ACTA PHYSICA
ACADEMIAE SCIENTIARUM HUNGARICAE

TOMUS XXI FASCICULUS 1

AKADÉMIAI KIADÓ, BUDAPEST
1966

ACTA PHYS. HUNG.

ACTA PHYSICA

A MAGYAR TUDOMÁNYOS AKADÉMIA FIZIKAI KÖZLEMÉNYEI

SZERKESZTŐSÉG ÉS KIADÓHIVATAL: BUDAPEST V., ALKOTMÁNY UTCA 21.

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Abonnementspreis pro Band: 110 Forint. Bestellbar bei dem Buch- und Zeitungs-Aussenhandels-Unternehmen »Kultúra« (Budapest I., Fő u. 32. Bankkonto Nr. 43-790-057-181) oder bei seinen Auslandsvertretungen und Kommissionären.

ACTA PHYSICA
ACADEMIAE SCIENTIARUM HUNGARICAE

ADIUVANTIBUS
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REDIGIT
P. GOMBÁS

TOMUS XXI

AKADÉMIAI KIADÓ, BUDAPEST
1966

ACTA PHYSICA

Tomus XXI

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (1), pp. 1—15, (1966)

THE LORENTZ PRINCIPLE AND THE GENERAL THEORY OF RELATIVITY

PART I

HOMOGENEOUS PROPAGATION OF LIGHT

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(Received 23. XI. 1965)

This paper is the first of a series in which the formulation of the general theory of relativity in terms of the Lorentz principle is attempted. In this first part the Lorentz transformation is generalized so as to be applicable to parts of space where light is propagated homogeneously but possibly unisotropically. It is shown that the Lorentz principle in its ordinary form remains valid for such regions.

Introduction

§ 1. In the present article we show that the Lorentz principle which we have formulated in a number of papers [1]—[4] can be generalized so as to apply to the problems of general relativity. Just as in the case of the special theory, in the generalized form the principle leads to a mathematical formalism equivalent to that of the general theory of relativity. The approach through the generalized Lorentz principle gives, however, new physical aspect to the problems. In particular although the mathematical formalism of Riemann geometry is made use of the concept of curved space is left out of the considerations. We hope to come back to the philosophical aspects of the problem elsewhere, here we try to restrict ourselves to such an extent as possible to physical considerations only.

§ 2. Our considerations start from the fact that the mode of propagation of light is affected by gravitational fields. In a gravitational field the propagation of light can thus not any more be regarded to be isotropic and the velocity of propagation may vary both in time and with location.

So as to be able to generalize the Lorentz principle to the case of inhomogeneous mode of propagation of light we shall, as a first step, generalize the Lorentz transformation to regions with homogeneous mode of propagation. In the present Part I of this work we shall give the generalization of the Lorentz transformation to the case of unisotropic but what we shall call homogeneous mode of propagation of light. In Part II we shall further generalize the Lorentz transformation to the case of inhomogeneous propagation of light.

It will be seen that the Lorentz principle when interpreted in terms of the Lorentz transformation thus generalized yields essential parts of the formalism of general theory of relativity.

In Part III we shall re-interpret the considerations of Einstein giving the connection between gravitational field and its sources. We shall thus give the connection between the mode of propagation of light and the sources of gravitation.

With the considerations of Part III we shall arrive from our approach at the whole of the mathematical formalism of the general theory of relativity.

§ 3. Let us consider part of space in which light is propagated unisotropically so that the velocity of light in different directions should be different. Let us suppose, however, that the directional distribution is the same in different points and that it does not vary in time. Thus suppose that the velocity of propagation of light can be written as

$$\mathbf{c}(\varkappa) = \varkappa a(\varkappa) \qquad \begin{array}{l}\text{independent of } \mathbf{r}, t\\ \text{for any direction } \varkappa\end{array} \tag{1}$$

where $\varkappa$ is a unit vector.

Furthermore we shall restrict the function $a(\varkappa)$. Supposing that light is propagated unisotropically in the manner as we know light to be propagated in a homogeneous but unisotropic medium, we may suppose the following connection between the vector $\mathbf{r}$ pointing from a point P to Q and the measure of time t in which a signal starting from P reaches Q,

$$\mathbf{rGr} - c_0^2 t^2 = 0, \tag{2}$$

where $\mathbf{G}$ is a symmetric positive definite tensor with components $G_{ik} = G_{ki}$, $i, k = 1, 2, 3$ and c_0 is a velocity. The particular case $\mathbf{G} = 1$, $c_0 = c$, i.e. $G_{ik} = \delta_{ik}$ corresponds to the isotropic propagation of light.

§ 4. So as to generalize (2) a little further, we may suppose that the carrier of light moves with the constant velocity $\mathbf{v}$ relative to our system. If we describe the propagation of light with respect to a system K' in which the carrier of light is at rest, then we find for the coordinates of the two points P and Q which are at rest with respect to the system K:

$$\left.\begin{aligned}\mathbf{r}'_P(t) &= \mathbf{a} - \mathbf{v}t,\\ \mathbf{r}'_Q(t) &= \mathbf{a} - \mathbf{v}t + \mathbf{r}\end{aligned}\right\}. \tag{3}$$

If a signal starts at $t = t_1$ from P and arrives at $t = t_2$ in Q we have to write

$$\left(\mathbf{r}'_P(t_1) - \mathbf{r}'_Q(t_2)\right) \mathbf{G} \left(\mathbf{r}'_P(t_1) - \mathbf{r}'_Q(t_2)\right) - c_0^2(t_1 - t_2)^2 = 0.$$

Rewriting the above relation and writing $t_2 - t_1 = t$ we find with the help of (3)

$$\mathbf{rGr} + 2\,\mathbf{rV}\,t - c^2 t^2 = 0,$$

where we wrote $\mathbf{Gv} = \mathbf{V}$ and $c^2 = c_0^2 - \mathbf{vV}$. The above relation can also be written

$$\mathbf{xgx} = 0, \tag{4}$$

where we suppose $\mathbf{x}$ to be a four-vector with components

$$\mathbf{x} = \mathbf{r}, t$$

and $\mathbf{g}$ is a symmetric tensor of the fourth order with components

$$\mathbf{g} = \begin{pmatrix} \mathbf{G} & \mathbf{V} \\ \mathbf{V} & -c^2 \end{pmatrix}. \tag{5}$$

In the following we shall say that light is propagated homogeneously in a region if the propagation inside all parts of this region can be described by relation (4) and the tensor $\mathbf{g}$ has the form (5).

We suppose the components of $\mathbf{g}$ to be independent of $\mathbf{x}$ furthermore we suppose $-g_{44} = c^2 > 0$.

A particular case of (4) and (5) is the case considered in previous works, (see for instance [1]), i.e.

$$\mathbf{x\Gamma x} = 0 \text{ with } \mathbf{\Gamma} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -c^2 \end{pmatrix}. \tag{6}$$

§ 5. Suppose relation (4) (with given elements of the tensor $\mathbf{g}$) is valid in the measures of a system of reference K. We can form transforms of the coordinates, e.g.*

$$\mathbf{x}' = \mathbf{S}^{-1}\,\mathbf{x}, \tag{7}$$

and inserting (7) into (4) we find

$$\left.\begin{aligned} \mathbf{x}'\,\mathbf{g}'\,\mathbf{x}' &= 0 \\ \mathbf{g}' &= \widetilde{\mathbf{S}}\,\mathbf{g}\,\mathbf{S} \end{aligned}\right\}. \tag{8}$$

Thus taking the transformed coordinates to refer to a system K' we see that the propagation of light appears homogeneous also in the measures of K' but the tensor $\mathfrak{g}$ giving the detailed mode of propagation has in general different elements in the representation relative to K' than $\mathbf{g}$ representing

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* The coordinate transformation itself may be an inhomogeneous transformation. $\mathbf{x}$ as used in relation (4) expresses a four-distance, thus it can be taken as the difference between two coordinate vectors e.g. $\mathbf{x} = \mathbf{x}_P - \mathbf{x}_Q$ and thus its transformation is homogeneous.

the propagation relative to K. (Here we denote by gothic symbols quantities irrespective of their representation).

§ 6. In particular if we prescribe the elements of the matrix $\mathbf{g}'$ we find a transformation $\mathbf{S}$ which leads from $\mathbf{g} \rightarrow \mathbf{g}'$ thus prescribed. Indeed, putting

$$\mathbf{S} = \mathbf{g}^{-1/2} \mathbf{g}'^{1/2} \tag{9}$$

(8) reduces to an identity. Thus the transformation with the matrix $\mathbf{S}$ as defined by (9) seems to give one suitable transformation, however, the transformation matrix $\mathbf{S}$ defined by (9) has in general complex elements. Writing $\mathbf{g}$ as a hypermatrix in the form (5) and using an analogous notation for the matrix $\mathbf{g}'$ we find that a matrix $\mathbf{S}$ giving the transformation (8) can be written

$$\mathbf{S} = \begin{pmatrix} \mathbf{G}^{-1/2}\,\mathbf{G}'^{1/2} & \mathbf{G}^{-1/2}\,\mathbf{G}'^{1/2}\,\mathbf{v}' - \mathbf{v}\,c'/c \\ 0 & c'/c \end{pmatrix}. \tag{9a}$$

Since $\mathbf{G}$ and $\mathbf{G}'$ are symmetric positive definite matrices, the matrix $\mathbf{S}$ as defined by (9a) has real elements only. For $\mathbf{v} = \mathbf{v}'$ or more generally if

$$\mathbf{G}'^{1/2}\,\mathbf{v}'/c' = \mathbf{G}^{1/2}\,\mathbf{v}/c$$

(9a) reduces to (9).*

Another transformation can be obtained as follows: denote by $\mathbf{O}$ and $\mathbf{O}'$ matrices with the help of which $\mathbf{g}$ respectively $\mathbf{g}'$ can be brought into diagonal form; thus suppose

$$\mathbf{O}^{-1}\,\mathbf{g}\,\mathbf{O} = \mathbf{D}, \qquad \mathbf{O}'^{-1}\,\mathbf{g}'\,\mathbf{O}' = \mathbf{D}'.$$

Thus remembering that $\mathbf{O}$ is an orthogonal matrix obeying $\widetilde{\mathbf{O}} = \mathbf{O}^{-1}$ we can also put

$$\mathbf{S} = \mathbf{O}'\,\mathbf{D}'^{1/2}\mathbf{D}^{-1/2}\,\widetilde{\mathbf{O}}, \tag{9b}$$

and we find that (9b) also satisfies (8).

Both transformations (9a) and (9b) have the following features:

1) If $\mathbf{g}' \rightarrow \mathbf{g}$ then $\mathbf{S} \rightarrow 1$.

2) The matrices thus defined are associative, i.e. if

$$\widetilde{\mathbf{S}}\mathbf{g}\mathbf{S} = \mathbf{g}' \quad \text{and} \quad \widetilde{\mathbf{S}}'\,\mathbf{g}'\,\mathbf{S}' = \mathbf{g}''$$

then we have also

$$\mathbf{g}'' = \widetilde{\mathbf{S}}''\,\mathbf{g}\,\mathbf{S}'',$$

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* I am indebted to P. Király for drawing my attention to the fact that the definition (9) leads to matrices $\mathbf{S}$ with complex elements and also for pointing out that the alternative definition (9a) leads to transformation matrices with real elements only.

where **S**, **S**$'$ and **S**$''$ are all three given either by expressions of the type (9a), or all three are given by the expressions of the type (9b).

In particular we may put

$$\mathbf{g}' = \mathbf{\Gamma}$$

and thus we find that in the measures of K' the propagation appears isotropic. Conversely even if the real propagation of light is isotropic we can construct systems of references in which the propagation of light is characterized by an arbitrarily given tensor **g**.

Thus from the fact that the propagation of light appears homogeneous in one representation, it follows that it appears so in all other representations which are obtained from the former by linear transformation. There exist always among the possible representations such in which the propagation appears isotropic.

§ 7. One infers from the above that it is impossible to determine the elements of **g** from the result of measurement of the times of travels of signals of light. That this is indeed impossible we show presently by a consideration which is a generalization of considerations given earlier [4].

§ 8. We show presently that one can easily generalize the considerations which we have given elsewhere [2] for the case of isotropic propagation of light. Consider for this purpose a number of clocks near points $P_0, P_1, P_2, \ldots, P_n$. We show that taking, say, the clock P_0 as standard, we can synchronize the remaining clocks using light signals between the clocks and we can at the same time express the components of the coordinate vectors $r_0, r_1, r_2, \ldots, r_n$ of the position of the clocks in terms of the observed times of travels of light signals.

§ 9. So as to carry out the above synchronization, suppose P_0 to be the standard clock, we may synchronize the rates of the clocks P_k $k = 1, 2, \ldots$ by emitting signals with a period T from P_0 and adjust the rates of the clocks P_k $k > 0$ to the rythm of the signals thus received.

The procedure of synchronizing the rates of the clocks can be repeated by emitting in turn periodic signals from the points $P_1, P_2, \ldots$, etc. and it is to be expected that the signals thus emitted and received by the remaining clocks appear to be periodic when timed with the receiving clocks.

The latter procedure can be taken as a test of the assumption that the velocity of propagation of light is indeed constant in time and also a test of the assumption that the clocks P_k, $k = 0, 1, 2$ are in positions at constant distances from each other. Furthermore the possibility of synchronizing the rates of the clocks in a consistent manner supports the assumption that the rates of the clocks are constant indeed. We shall come back elsewhere to the analysis of this problem in greater detail.

We suppose thus that the rates of the clocks P_k, $k = 0, 1, 2, \ldots$ have been successfully synchronized. We show how the coordinate vectors $\mathbf{r}_k$ of the positions of the clocks can be determined in terms of the times of travels of signals between the clocks so synchronized.

§ 10. So as to obtain definite values for the coordinates we define a system of reference with the help of the positions of four of the clocks. Let us suppose that P_0, P_1, P_2, P_3 lie on the corners of a non degenerated tetrahedron. We can take P_0 to fix the origin of K while the points P_1, P_2, P_3 fix the direction of the axis of the system of reference K. In the system thus defined the coordinate vectors of the positions of the four clocks can be written

$$\mathbf{r}_0 = 0; \qquad \mathbf{r}_1 = a_1, 0, 0; \qquad \mathbf{r}_2 = 0, a_2, 0; \qquad \mathbf{r}_3 = 0, 0, a_3 . \tag{10}$$

The numerical values of the components of the coordinate vector $\mathbf{r}_k$, $k = 1, 2, 3$ can be determined from the times of travels of light signals provided the components of $\mathbf{g}$ relative to K are known. This determination can be carried out in the following manner.

Denote the time of travel of a signal from P_n to P_m by $t_{n,m}$; denote the return time from P_n to P_m and back by

$$t_{n,m} + t_{m,n} = 2\, t_{nm} \tag{11}$$

further denote the difference

$$t_{n,m} - t_{m,n} = 2\, \Delta t_{nm} \tag{12}$$

(in the case of isotropic propagation of light we have of course $\Delta\, t_{n\,m} = 0$). Writing for the moment

$$\begin{gathered} t_{n,m} = t_1, \qquad t_{m,n} = t_2, \\ \mathbf{r}_m - \mathbf{r}_n = \mathbf{r}, \end{gathered} \tag{13}$$

then we have for the times of exchange of light signals between P_n and P_m

$$\left.\begin{aligned} \mathbf{rGr} + 2\,\mathbf{Vr}t_1 - c^2t_1^2 &= 0, \qquad (\mathrm{a}) \\ \mathbf{rGr} - 2\,\mathbf{Vr}t_2 - c^2t_2^2 &= 0. \qquad (\mathrm{b}) \end{aligned}\right\} \tag{14}$$

Solving the above equations into t_1 and t_2 we find using the notations (11), (12) and remembering (13)

$$\left.\begin{aligned} t_{nm}^2 &= (\mathbf{rGr})/c^2 + (\mathbf{Vr})^2/c^4, \qquad (\mathrm{a}) \\ \Delta t_{nm} &= \mathbf{Vr}/c^2, \qquad (\mathrm{b}) \\ \mathbf{r} &= \mathbf{r}_m - \mathbf{r}_n. \qquad (\mathrm{c}) \end{aligned}\right\} \tag{15}$$

In place of (15a) we may also write

$$c^2 t_{nm}^2 = (\mathbf{r}_m - \mathbf{r}_n)\,\overset{(3)}{\mathbf{g}}\,(\mathbf{r}_m - \mathbf{r}_n), \qquad \text{(a)}$$

where

$$\overset{(3)}{\mathbf{g}} = \mathbf{G} + (\mathbf{V} \circ \mathbf{V})/c^2. \qquad \text{(b)} \qquad\qquad (16)$$

Observing the times t_{nm}, $nm = 0, 1, 2, \ldots$ we are in a position to determine the components of the coordinate vectors $\mathbf{r}_n$, $n = 1, 2, 3, \ldots$. In particular for $n = 0$, $m = k = 1, 2, 3$ we find from (16) and (10)

$$\boldsymbol{a}_k = c t_{0k} \Big/ \sqrt{\overset{(3)}{g}_{kk}}\,, \quad k = 1, 2, 3. \qquad (17)$$

Further introducing a vector $\mathbf{D}^{(n)}$ with components

$$D_k^{(n)} = c^2 \frac{t_{kn}^2 - t_{0n}^2 - t_{0k}^2}{2\,\boldsymbol{a}_k} \qquad k = 1, 2, 3. \qquad (18)$$

We find from (16a)

$$\mathbf{r}_n = \overset{(3)}{\mathbf{g}}{}^{-1}\,\mathbf{D}^{(n)} \qquad n = 0, 1, 2, \ldots \qquad (18a)$$

However, (18a) gives only a necessary condition which the coordinates $\mathbf{r}_n$ have to satisfy. Whether the coordinates as given by (18a) in terms of the return times indeed satisfy the relations (16) has to be ascertained separately.

We consider the procedure in some more detail. Considering the four points P_k, $k = 0, 1, 2, 3$ and a fifth point P_l, $l > 3$, we may observe twenty return times between the various pairs of the five points. It follows from (16) that we must expect

$$t_{nm} = t_{mn}. \qquad n, m = 0, 1, 2, 3, l. \qquad (19)$$

Equ. (19) gives thus ten conditions which have to be fulfilled by the observed return times if our assumptions about the mode of propagation of light is to be correct.

Supposing (19) to be fulfilled by the observed values, equ. (16a) provides us with further ten conditions. However, inserting (18) into (16a) remembering (17) nine out of the ten relations reduce to identities and we are left with one non trivial relation, i.e.

$$c^2 t_{0l}^2 = \mathbf{r}_l\,\overset{(3)}{\mathbf{g}}\,\mathbf{r}_l\,. \qquad (20)$$

The above relation gives thus a further check of consistency of our assumptions.

One further check is obtained if we consider the time a signal takes to go round a triangle formed of three points. Writing thus

$$t_{klm} = t_{k,l} + t_{l,m} + t_{m,k}$$

we find with the help of (12)

$$t_{klm} - t_{kml} = 2(\Delta t_{kl} + \Delta t_{lm} + \Delta t_{mk})$$

and with the help of (15b) and (15c) we obtain

$$t_{klm} = t_{kml} \,. \tag{21}$$

The above relation can be checked directly by experiment.

If all the checks described above lead to satisfactory results then we may conclude: The fact that the rates of the clocks can be synchronized consistently, further the facts that (19), (20), and (21) are obeyed by the observed times of travels of signals support the hypothesis that in the region considered light is propagated homogeneously with a propagation tensor **g**.

However, the checks do not really prove that the propagation tensor has indeed the value **g** used for the determination of the coordinates $\mathbf{r}_n$. Indeed, had we supposed that the propagation was not given by **g** but by a tensor

$$\mathbf{g}' = \widetilde{\mathbf{S}}\mathbf{g}\mathbf{S} \,,$$

where **S** is a matrix with constant elements and det $\mathbf{S} \neq 0$, then the procedure described above would have led to coordinate vectors

$$\mathbf{r}'_n = \mathbf{S}^{-1}\, \mathbf{r}_n \,. \tag{22}$$

It is verified easily that provided the $\mathbf{r}_n$ obtained assuming the propagation to be given by **g** satisfy the checks described above, then automatically the coordinate vectors $\mathbf{r}'_n$ satisfy the corresponding relations involving the tensor $\mathbf{g}'$. We see therefore that *the analysis of times of travel of light signals can be used to ascertain whether or not light is propagated homogeneously, but no information can be obtained as to the components of the propagation tensor* **g** *from such measurements.*

It is interesting to note that it is usually strongly emphasized that observing the return times of light signals one cannot determine the velocity of the observer relative to the carrier of light.

We see from the above considerations that the latter statement contains only part of the real facts. The velocity of the observer relative to the carrier of light is contained in the components $V_k = g_{4k}$, $k = 1, 2, 3$ of **g**.

As, however, *none* of the components of **g** can be determined by the exchange of light signals, it follows that *the observation of times of travels of signals are also unsuitable to determine whether or not light is propagated isotropically relative to its carrier*. Thus the ambiguity of the interpretation of the results is considerably larger than it is usually supposed to be.

§ 11. We may define as the measure $\mathbf{r}_{nm}$ of the distance between the points P_n and P_m as

$$\mathbf{r}_{nm} = ct_{nm} = (\mathbf{r}_{nm} \overset{(3)}{\mathbf{g}} \mathbf{r}_{nm})^{1/2}. \tag{23}$$

The above relation in itself is a mere definition and has no physical contents. So as to obtain a physical statement we may take a solid rod AB, fix one of its ends A in the point P_n and turn it round into different directions. The end B of the rod thus will take up points upon a surface given by coordinate vectors

$$\mathbf{r}(\varkappa) = \mathbf{r}_n + \mathbf{l}(\varkappa)\,, \tag{24}$$

where $\varkappa$ is a two-component parameter defining the various orientations of the rod. Determining the $\mathbf{l}(\varkappa)$ by observing the behaviour of a real rod, we conclude from (23) and (24)

$$\mathrm{l}(\varkappa) = (\mathbf{l}(\varkappa) \overset{(3)}{\mathbf{g}} \mathbf{l}(\varkappa))^{1/2}$$

where $\mathrm{l}(\varkappa)$ is the measure of the length the rod takes up when is pointed into the direction defined by $\varkappa$.

From experiments of the Michelson—Morley type it follows that the return time of a light signal travelling between the ends of a solid rod is not affected if the rod is turned round. This experimental result may be expressed by stating that for a solid rod turned round adiabatically we have

$$\mathrm{l}(\varkappa) = \mathrm{l} = \text{independent of } \varkappa \tag{25}$$

The latter relation implies that when it is turned round physical processes take place which make the solid rod to adapt itself to the measures obtained from light signals and defined by (23).

The observed relation (25) can be taken as the first step in formulating the Lorentz principle in its generalized form.

The Lorentz principle in the case of homogeneous propagation of light

§ 12. Let us consider a system of reference in which the propagation of light can be described by

$$\mathbf{xgx} = 0\,, \tag{26}$$

with a given tensor **g**. We may change the system of reference and thus obtain new coordinates so that

$$\mathbf{x}' = \mathbf{M}\mathbf{x}\,. \tag{27}$$

(The transformation must be taken in the homogeneous form as $\mathbf{x}$ and $\mathbf{x}'$ represent four-distances.)

Introducing (27) into (26) we find

$$\mathbf{x}\widetilde{\mathbf{M}}\mathbf{g}\,\mathbf{M}\mathbf{x} = \mathbf{x}'\,\mathbf{g}\mathbf{x}'. \tag{28}$$

We see thus that if the matrix $\mathbf{M}$ is such as to obey relation

$$\widetilde{\mathbf{M}}\mathbf{g}\mathbf{M} = \Theta\mathbf{g} \qquad \Theta \neq 0, \tag{29}$$

then relation (26) written in terms of the coordinates $\mathbf{x}'$ reduces to

$$\mathbf{x}'\mathbf{g}\mathbf{x}' = 0\,. \tag{30}$$

We see therefore that there exists a set of systems of references K, K', . . . in all of which the propagation of light is expressed by the same algebraic expression of the form (26), i.e. by the same propagation tensor $\mathbf{g}$.

Relation (29) is the generalization of the definition of the Lorentz matrices [1], [4], i.e. of

$$\widetilde{\mathbf{\Lambda}}\mathbf{\Gamma}\mathbf{\Lambda} = \Theta\mathbf{\Gamma}\,. \tag{31}$$

In the following we shall restrict ourselves to consider transformations with $\Theta = +1$.

§ 13. The matrices $\mathbf{M}$ obeying (29) connect thus the systems of reference relative to which the propagation of light appears in the same form. The transformations $\mathbf{M}$ form (like the Lorentz transformations) a group. Indeed from

$$\widetilde{\mathbf{M}}\mathbf{g}\mathbf{M} = \mathbf{g} \tag{32}$$

follows, since $\det \mathbf{g} \neq 0$

$$\det \mathbf{M} = \pm 1\,. \tag{33}$$

Thus $\mathbf{M}$ possesses a reciprocal. We find thus from (32)

$$\mathbf{M}^{-1} = \mathbf{g}^{-1}\,\widetilde{\mathbf{M}}\mathbf{g}\,, \tag{34}$$

and therefore

$$\widetilde{\mathbf{M}}^{-1}\,\mathbf{g}\,\mathbf{M}^{-1} = \mathbf{g}\,. \tag{35}$$

Thus if $\mathbf{M}$ is a generalized Lorentz matrix, then $\mathbf{M}^{-1}$ is also such a matrix.

Furthermore we find that if two matrices **M** and **N** obey

$$\tilde{\mathbf{M}}\mathbf{g}\mathbf{M} = \mathbf{g} \quad \text{and} \quad \tilde{\mathbf{N}}\mathbf{g}\mathbf{N} = \mathbf{g}$$

then we have also

$$(\widetilde{\mathbf{M}\mathbf{N}})\,\mathbf{g}\,\mathbf{M}\mathbf{N} = \mathbf{g}\,.$$

Thus the matrices **M** obeying (32) form indeed a group.

§ 14. The generalized Lorentz transformation, which was introduced as giving transformation between the coordinates of different system of reference, can — just like the ordinary Lorentz transformation — be given a new meaning.

Considering the inhomogeneous transformation

$$\mathbf{X}^* = \mathbf{M}\mathbf{X} + \mathbf{m}\,, \tag{36}$$

where we write capital **X** for a coordinate four vector so as to distinguish it from the four-distances for which we wrote **x**.

We may consider **X** and $\mathbf{X}^*$ as four-coordinates of two events, say $\mathfrak{E}$ and $\mathfrak{E}^*$ both coordinates relative to one system of reference K. Thus the transformation (36) can be taken as to refer to coordinates relative to one system of reference only and thus the transformation orders to an event $\mathfrak{E}$ represented by **X** another event $\mathfrak{E}^*$ represented by the coordinate $\mathbf{X}^*$.

Considering instead of a single event $\mathfrak{E}$ some physical system $\mathfrak{Q}$ containing a number of points which may be also moving relative to each other, then transforming the coordinates of the points $\mathfrak{P}_1, \mathfrak{P}_2, \ldots, \mathfrak{P}_n$ of $\mathfrak{Q}$ we obtain new points $\mathfrak{P}_1^*, \mathfrak{P}_2^*, \ldots, \mathfrak{P}_n^*$ forming a new physical system $\mathfrak{Q}^*$. The system $\mathfrak{Q}^*$ is obtained from $\mathfrak{Q}$ by generalized Lorentz transformation. We may write symbolically

$$\mathscr{M}_{\mathfrak{p}}(\mathfrak{Q}) = \mathfrak{Q}^*\,, \tag{37}$$

where $\mathscr{M}_{\mathfrak{p}}$ is the operator describing the change from $\mathfrak{Q}$ into $\mathfrak{Q}^*$ and $\mathfrak{p}$ stands for the parameter characterizing the transformation. Relation (37) expressed in its representation relative to a system K of reference may be written

$$\mathscr{M}_{\mathfrak{p}}(\mathbf{Q}) = \mathbf{Q}^* \tag{38}$$

where

$$\mathbf{p} = K(\mathfrak{p})\,, \qquad \mathbf{Q} = K(\mathfrak{Q})\,, \qquad \mathbf{Q}^* = K(\mathfrak{Q}^*)$$

are the representations of the various quantities relative to K.

Written more explicitly, if we denote the representation of the four-coordinate vectors of a point $\mathfrak{P}_\nu$ of $\mathfrak{Q}$ by $\mathbf{x}_\nu$

$$\mathbf{x}_\nu^* = \mathbf{M}_{\mathbf{p}}\,\mathbf{x}_\nu + \mathbf{m} \qquad \nu = 1, 2, \ldots, n\,. \tag{39}$$

where $\mathbf{M}_\mathbf{p}$ is a matrix obeying the relation (32), the components of $\mathbf{p}$ are the parameters specifying the transformation and $\mathbf{m}$ is a four-vector with constant components.

§ 15. Considering the transition $\mathfrak{D} \rightarrow \mathfrak{D}^*$, i.e. the Lorentz deformation with parameter $\mathfrak{g}$ relative to a new system of reference, then we find

$$\mathbf{x}_\nu'^* = \mathbf{M}_{\mathbf{p}'} \mathbf{x}_\nu' + \mathbf{m}' \tag{40}$$

where we have

$$\mathbf{M}_{\mathbf{p}'} = \mathbf{M}^{(\mathbf{q})} \mathbf{M}_\mathbf{p} \mathbf{M}^{(\mathbf{q})^{-1}}; \tag{41}$$

here $\mathbf{M}^{(\mathbf{q})}$ is the matrix of the coordinate transformation leading from $K \rightarrow K'$ Thus the latter coordinate transformation written explicitly

$$\mathbf{x}_\nu' = \mathbf{M}^{(\mathbf{q})} \mathbf{x}_\nu + \mu \qquad \nu = 1, 2, \ldots, n \tag{42}$$

in place of the above relation we may also write

$$K' = \mathscr{M}^{(\mathbf{q})}(K),$$

where we have denoted by $\mathscr{M}^{(\mathbf{q})}$ the inhomogeneous operator containing the matrix $\mathbf{M}^{(\mathbf{q})}$ and the vector μ.

§ 16. From relation (41) we see how the deformation $\mathfrak{D} \rightarrow \mathfrak{D}^*$ is represented relative to various systems of references in which the propagation tensor $\mathfrak{g}$ has the same representation.

More precisely, we may state that the propagation of light in a certain region of space is given by a tensor $\mathfrak{g}$. The representation of $\mathfrak{g}$ relative to a number of systems of references $K, K', \ldots, K''$ is the same, e.g.

$$K(\mathfrak{g}) = K'(\mathfrak{g}) = K''(\mathfrak{g}) = \ldots = \mathbf{g}.$$

Considering a coordinate transformation of the type

$$\overline{\mathbf{X}} = \mathbf{S}\mathbf{X} + \mathbf{s},$$

where

$$\widetilde{\mathbf{S}}\mathbf{g}\mathbf{S} = \overline{\mathbf{g}} \neq \mathbf{g}.$$

We obtain from a system of reference K another system of reference $\overline{K}$ so that in the latter the propagation of light is described by a tensor $\overline{\mathbf{g}}$.

From the system of reference $\overline{K}$ we can form a group of systems of references $\overline{K}, \overline{K}', \overline{K}'', \ldots$ in each of which the tensor $\mathfrak{g}$ has the same representation $\overline{\mathbf{g}}$. The latter are connected by matrices $\overline{\mathbf{M}}$ obeying the relation

$$\widetilde{\overline{\mathbf{M}}}\mathbf{g}\overline{\mathbf{M}} = \overline{\mathbf{g}}.$$

A Lorentz deformation $\mathfrak{Q} \to \mathfrak{Q}^*$ can be expressed by an operator of the set $\overline{\mathbf{M}}$ if we consider it in one of the representations $\overline{K}, \overline{K}', \overline{K}'', \ldots$. We find easily that the connection between the operators $\mathbf{M}$ and $\overline{\mathbf{M}}$ is given by

$$\overline{\mathbf{M}}_{\mathbf{q}} = \mathbf{S}^{-1} \mathbf{M}_{\mathbf{q}} \mathbf{S} . \tag{43}$$

Thus a Lorentz deformation $\mathfrak{Q} \neq \mathfrak{Q}^*$ can be represented by a set of operators

$$\mathbf{M}_{\mathbf{q}}, \mathbf{M}_{\mathbf{q}'}, \mathbf{M}_{\mathbf{q}''}, \ldots$$

relative to systems of references K, K', K'', ... in all of which $\mathfrak{g}$ is represented by a tensor $\mathbf{g}$.

The same Lorentz deformation can also be represented by operators

$$\overline{\mathbf{M}}_{\mathbf{q}}, \overline{\mathbf{M}}_{\mathbf{q}'}, \overline{\mathbf{M}}_{\mathbf{q}''},$$

relative to systems of references $\overline{K}, \overline{K}', \overline{K}'', \ldots$ in which $\mathfrak{g}$ appears to be represented by a tensor $\overline{\mathbf{g}}$ different from $\mathbf{g}$.

Considering relations (41) and (43) we find an important common feature of all the representations of a deformation $\mathfrak{Q} \to \mathfrak{Q}^*$. Indeed, *the matrices*

$$\mathbf{M}_{\mathbf{q}}, \mathbf{M}_{\mathbf{q}'}, \ldots, \overline{\mathbf{M}}_{\mathbf{q}}, \overline{\mathbf{M}}_{\mathbf{q}'}, \ldots,$$

have all the same eigenvalues.

The eigenvalues of a Lorentz matrix can be chosen to be of the form (see [3])

$$e^{i\varphi}, \; e^{-i\varphi}, \; \sqrt{\frac{c+v}{c-v}}, \; \sqrt{\frac{c-v}{c+v}}$$

we see thus that *any representation of one Lorentz deformation has the same eigenvalues characterized by the parameters φ and v.* The latter result holds — as we see — also in the case of unisotropic propagation of light and it holds also if we consider systems of references in which the propagation tensor $\mathfrak{g}$ is represented by different matrices $\mathbf{g}, \overline{\mathbf{g}}, \ldots$, etc.

§ 17. We are now in a position to generalize the Lorentz principle to the case of homogeneous but possibly unisotropic propagation of light.

We state: *the laws of nature possess such symmetries that, provided $\mathfrak{Q}$ is a real physical system, then any Lorentz deformed form $\mathfrak{Q}^* = \mathscr{M}\mathfrak{p}\,(\mathfrak{Q})$ of $\mathfrak{Q}^*$ is also a possible system obeying the same laws of as $\mathfrak{Q}$.*

Furthermore, *if a system $\mathfrak{Q}$ is adiabatically accelerated then it changes its configuration into a Lorentz deformed form of its original configuration.*

The above formulation of the Lorentz principle regarding its form is identical with the former formulation (see [2]). We have extended its content by generalizing the Lorentz transformation to the case of unisotropic but homogeneous propagation of light.

§ 18. We make a concluding remark. The formulation of the Lorentz principle in its restricted form as was done in a previous work is based on the failure of a series of experiments to observe effects of translational motion. This failure is attributed to a peculiar symmetry of laws of nature which symmetry causes that to any effect which might arise from the translational motion relative to the aether, other effects appear which exactly compensate the former. This symmetry itself could be described adequately by the Lorentz principle.

The earlier considerations are based on the assumption that light is propagated isotropically relative to its carrier, the aether.

The generalized considerations show that supposing light was after all not carried isotropically in the aether but if the propagation be of the more general type which we denoted as homogeneous, even then, the symmetry discussed above might persist and this symmetry might prevent us not only to locate the distinguished system of reference K_0 which is at rest to the carrier of the light, but it equally prevents us to determine the propagation tensor $\mathbf{g}_0$ which describes the propagation of light relative to its carrier.

The extension of the symmetry properties of nature in this fashion is based on pure speculation. Experimentally the adequacy of this extension could be checked if we could carry out experiments, say with a Michelson interferometer in a region of space where we have good reason to believe the propagation of light to be unisotropic. If an experiment in such a region were to lead to a negative effect in spite of the unisotropy, then this result would directly justify the extension of the Lorentz principle.

At the moment such experiments do not exist. The generalization of the Lorentz principle we have given here can be in spite of the lack of direct evidence be justified.

Indeed, we shall show that the generalization of the Lorentz principle we have given here is a necessary intermediate step to its further generalization to the case of inhomogeneous propagation of light. In the case of the inhomogeneous propagation of light observable effects are found and the theory of these effects can be obtained by a straightforward further generalization which we discuss in the second part of this paper.

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ПРИНЦИП ЛОРЕНЦА И ОБЩАЯ ТЕОРИЯ ОТНОСИТЕЛЬНОСТИ

Часть I.

Л. ЯНОШИ

Резюме

Настоящая работа является первой из серии работ, в которых предлагается формулировка общей теории относительности на основе принципа Лоренца. В этой первой части преобразование Лоренца обобщается так, что оно становится применимым к областям пространства, где свет распространяется однородно, но быть может неизотропно. Показано, что для таких областей принцип Лоренца остается верным в своей обычной форме.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (1), pp. 17—32, (1966)

THE LORENTZ PRINCIPLE AND THE GENERAL THEORY OF RELATIVITY

PART II

INHOMOGENEOUS PROPAGATION OF LIGHT

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(Received 22. XII. 1965)

The generalization of the Lorentz transformation to regions where light is propagated inhomogeneously is given and it is shown that the Lorentz principle can be maintained in its ordinary form provided the Lorentz transformation is taken in its more general form formulated for such regions. The well-known equations for the geodetic lines in a gravitational field are obtained from the Lorentz principle thus generalized.

Generalized definition of the Lorentz transformation

§ 1. In this section we shall formulate the Lorentz principle for regions of space where light is propagated inhomogeneously. We shall assume, however, that even if the propagation at large is inhomogeneous still in sufficiently small regions the propagation remains homogeneous. Thus we suppose that a light signal starting from a point P with coordinates $\mathbf{r}$ at the time t arrives in a point Q with coordinate vector $\mathbf{r} + \boldsymbol{\rho}$ at the time $t + \tau$ so that

$$\boldsymbol{\xi}\mathbf{g}(\mathbf{x})\boldsymbol{\xi} = 0\,, \tag{1}$$

where

$$\mathbf{x} = \mathbf{r}, t \qquad \text{and} \qquad \boldsymbol{\xi} = \boldsymbol{\rho}, \tau$$

provided the components of $\boldsymbol{\xi}$ are sufficiently small so that the change of $\mathbf{g}(\mathbf{x})$ while $\mathbf{x}$ changes by $\boldsymbol{\xi}$ should be negligible.

As a first step we generalize the Lorentz transformation to the case of inhomogeneous propagation of light.

Let us consider to start with an arbitrary transformation of coordinates. Suppose the coordinates $\mathbf{x}$ and $\boldsymbol{\xi}$ refer to a system K. We introduce a system K' in which the four coordinate vectors are given by

$$\mathbf{x}' + \boldsymbol{\xi}' = \mathbf{f}(\mathbf{x} + \boldsymbol{\xi})\,, \tag{2}$$

where $\mathbf{f}$ has four components f_ν, $\nu = 1, 2, 3, 4$ and all four components are supposed to be slowly varying functions of their argument. More precisely we shall consider only such values of $\boldsymbol{\xi}$ for which we can write in a good approximation

$$\mathbf{f}(\mathbf{x}+\boldsymbol{\xi}) = \mathbf{f}(\mathbf{x}) + \boldsymbol{\xi}\,\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}}.$$

Writing more explicitly

$$\frac{\partial f_\nu(\mathbf{x})}{\partial x_\mu} = S_{\nu\mu} \qquad \nu, \mu = 1, 2, 3, 4\,.$$

The transformation (2) can also be written as

$$\boldsymbol{\xi}' = \mathbf{S}\boldsymbol{\xi} \qquad \text{and} \qquad \mathbf{x}' = \mathbf{x} + \boldsymbol{\mu}\,, \tag{3}$$

where

$$\boldsymbol{\mu} = \mathbf{f}(\mathbf{x}) - \mathbf{x}\,. \tag{3a}$$

The transformation (2) should possess a unique inverse and therefore we suppose

$$\det\ \mathbf{S} \neq 0. \tag{4}$$

§ 2. The propagation of light in the vicinity of the point P can thus be expressed relative to K' expressing (1) in terms of the transformed variables. Neglecting small terms we find thus

$$\boldsymbol{\xi}'\,\mathbf{g}'(\mathbf{x}')\,\boldsymbol{\xi}' = 0\,, \tag{5}$$

where

$$\mathbf{g}'(\mathbf{x}') = \widetilde{\mathbf{S}}^{-1}\,\mathbf{g}(\mathbf{x})\,\mathbf{S}^{-1}. \tag{6}$$

There exist coordinate transformations which leave the components of $\mathbf{g}(\mathbf{x})$ unchanged. We consider these transformations as the generalized Lorentz transformations. Thus a generalized Lorentz transformation $\mathscr{M}(\mathbf{x}, \boldsymbol{\mu})$ is expressed with the help of a shift $\boldsymbol{\mu}$ and a matrix $\mathbf{M}$ such that

$$\mathbf{x}' = \mathbf{x} + \boldsymbol{\mu} \tag{7a}$$

and

$$\widetilde{\mathbf{M}}\mathbf{g}(\mathbf{x}+\boldsymbol{\mu})\,\mathbf{M} = \mathbf{g}(\mathbf{x})\,. \tag{7b}$$

It must be emphasized that the transformation $\mathscr{M}$ does not change the components of $\mathbf{g}(\mathbf{x})$ in the fixed point $\mathbf{x}$ but it may change the values $\mathbf{g}\,(\mathbf{x}+\boldsymbol{\xi})$ in the vicinity of $\mathbf{x}$ and therefore it may change the derivatives of $\mathbf{g}(\mathbf{x})$ in $\mathbf{x}$ (see Parts IV and V)

The transformations defined by (7a) and (7b) form a structure with the following properties. Consider two transformations $\mathscr{M}(\mathbf{x}+\boldsymbol{\mu}_1)$ and $\mathscr{N}(\mathbf{x}+\boldsymbol{\mu}_1, \boldsymbol{\mu}_2)$, we have thus

$$\left.\begin{aligned} &\widetilde{\mathbf{M}}\mathbf{g}(\mathbf{x}+\boldsymbol{\mu}_1)\,\mathbf{M} = \mathbf{g}\,, && \text{(a)}\\ &\widetilde{\mathbf{N}}\mathbf{g}(\mathbf{x}+\boldsymbol{\mu}_1+\boldsymbol{\mu}_2)\,\mathbf{N} = \mathbf{g}(\mathbf{x}+\boldsymbol{\mu}_1)\,. && \text{(b)}\end{aligned}\right\} \tag{8}$$

Multiplying (8b) from the left by $\widetilde{\mathbf{M}}$ and from the right by $\mathbf{M}$ we find

$$(\widetilde{\mathbf{NM}})\, \mathbf{g}(\mathbf{x} + \mu_1 + \mu_2)\, \mathbf{NM} = \mathbf{g}(\mathbf{x}) \ .$$

Thus **NM** and $\mu_1 + \mu_2$ define a transformation $\mathscr{M}(\mathbf{x}, \mu_1 + \mu_2)$ and **NM** is thus itself a Lorentz matrix.

Thus Lorentz transformations consecutively applied give again Lorentz ransformations, however, a given Lorentz transformation refers to the fixed point, say $\mathbf{x}$ and produces a shift to another point, say $\mathbf{x}'$. Therefore applying a Lorentz transformation which produces a shift $\mathbf{x} \to \mathbf{x}'$ we can apply on the transformed quantities only such further transformations which produce shifts from $\mathbf{x}' \to \mathbf{x}''$. Therefore, if $\mathbf{x} \neq \mathbf{x}'$, then the two transformations are of different categories. These transformations fulfill the postulates of a partial algebraic structure and may be denoted a semi-group.* In the case of a homogeneous propagation of light the dependence of the transformation on the coordinates of the points upon which it is to be applied disappears and so the semi-group degenerates into an ordinary group — in this way the semi-groups of Lorentz transformations defined for the inhomogeneous case degenerate into the Lorentz group if the inhomogeneity disappears.

§ 3. The generalized Lorentz transformation can also be interpreted (like the more special transformation) to give not a coordinate transformation but to describe a deformation of some physical system $\mathfrak{Q}$. Suppose thus $\mathfrak{Q}$ to be a physical system in the vicinity of $\mathbf{x} = \mathbf{r}, t$; various points $\mathfrak{P}_1, \mathfrak{P}_2, \ldots$ of $\mathfrak{Q}$ can be described by four vectors

$$\mathbf{x} + \xi_\varkappa \quad \varkappa = 1, 2, \ldots .$$

Thus the point $\mathfrak{P}_\varkappa$ as represented in K moves along an orbit which at a time $t + \tau$ has a distance $\rho(\tau)$ from $\mathbf{r}$.

The deformed system $\mathfrak{Q}^*$ consists of points $\mathfrak{P}_1^*, \mathfrak{P}_2^*, \ldots$ with coordinate vectors

$$\mathbf{x}^* + \xi_\varkappa^* \quad \varkappa = 1, 2, \ldots ,$$

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* The expression semi-group is used somewhat loosely. In the usual sense the structure we use is that known as a BRANDT gruppoid with unit element, i.e. a special type of partial algebraic structure. If an algebraic structure is partial, then the product *ab* does not exist for an arbitrary pair *ab* of its elements. In our case of the semi-group, if *a*, *b*, *c* are any three elements of it and *ab* = *c* holds, then any of the elements *a*, *b*, *c* is uniquely determined by the other two. If *ab* and *bc* exist, the product *abc* may be written without parenthesis, thus the associativity law holds. Although in the case of BRANDT gruppoid every element has uniquely determined right and left unit elements, and conversely for two unit elements e_1, e_2 there is an element whose right and left unit elements are e_1 and e_2, in our case every element in the gruppoid has the same left and right unit elements. The existence of the inverse element is needed too. Gruppoid was introduced by BRANDT. (H. BRANDT: "Über die Axiome des Gruppoids". Vierteljahrsschrift der Naturforschenden Gesellschaft in Zürich, LXXXV [1940], 95—104.)

I am greatly indebted to Mr. J. DÉNES for having put at my disposal the above information.

where

$$\mathbf{x}^* = \mathbf{x} + \mu \,, \tag{9a}$$

and

$$\boldsymbol{\xi}^*_\varkappa = \mathbf{M}\boldsymbol{\xi}_\varkappa \quad \varkappa = 1, 2, 3, \dots \tag{9b}$$

and $\mathbf{M}$ and μ are the parameters of a transformation $\mathbf{M}\,(\mathbf{x}, \mu)$ which gives the deformation $\mathfrak{Q} \to \mathfrak{Q}^*$ in terms of representation in K.

The Lorentz principle can now be formulated for regions with inhomogeneous propagation of light as follows. *The laws of nature possess such forms that provided $\mathfrak{Q}$ is a real system obeying certain laws, then any Lorentz deformed system $\mathfrak{Q}^*$ obeys the same laws.*

Furthermore we may add: *if a system is accelerated adiabatically then it changes its configuration as a result of the acceleration into a Lorentz deformed configuration $\mathfrak{Q}^* = \mathbf{M}(\mathfrak{Q})$.*

The above formulation of the Lorentz principle is identic in form to former formulation, however, its contents are enlarged as it is supposed to be valid to the generalized family of Lorentz transformations $\mathbf{M}\,(\mathbf{x}, \mu)$. We show in the following that the latter form of the principle leads to results which are obtained usually from the general theory of relativity.

§ 4. It may appear as a deficiency of the Lorentz transformation as defined above, that it can be applied to small systems only, i.e. to systems which occupy such parts of space in which effects of the inhomogeneity of propagation of light can be neglected. However, this apparent deficiency is not a real one, it simply reflects upon material properties of physical systems.

Indeed, considering a system which is so large that the propagation of light inside the space occupied by the system is inhomogeneous to a noticeable extent, then gravitational stresses will appear in the system and its state of equilibrium will be determined partly by the gravitational field, but also by the material properties (compressibility, rigidity, etc.) of the system. If we shift such a system to different parts of space, then it will readjust itself to the field of the new surroundings and the change of configuration which thus arises depends very much on the actual physical properties of the system. If the Lorentz transformation depends only upon the distribution of the gravitational field, then it cannot possibly describe the material changes of a large system the changes of which depend — apart from the gravitational field — also upon the material properties of the system. We see thus, that it would be unreasonable to expect the existence of a general transformation which describes the changes of large physical systems when moved about in gravitational fields — since changes thus arising depend very much on the actual material properties of the system.

The fact that Lorentz transformations are suitable to express the changes small physical systems suffer when transported adiabatically into regions in which the gravitational field differs, shows that the reaction of micro-structures upon gravitational field obey general laws.

We have here an analogy of the circumstance that the Lorentz deformations described by the special theory of relativity are independent of the material properties of the systems provided the interferences causing the deformations are adiabatic.

§ 5. The Lorentz transformations $\mathbf{M}(\mathbf{x}, \mu)$ can be divided into two kinds: 1) transformations with $\mu = 0$, the latter may be denoted *local transformations*, as they produce no immediate shift of the system $\mathfrak{Q}$. 2) We may consider transformations $\mathbf{M}_0(\mathbf{x}, \mu)$ which produce a parallel shift, i.e. a shift, with as little changes apart from the parallel displacement, as it is possible.

Concerning the local transformations we find from (9a, b) that they contain matrices $\mathbf{M}$ obeying

$$\tilde{\mathbf{M}}\mathbf{g}(\mathbf{x})\,\mathbf{M} = \mathbf{g}(\mathbf{x})\,. \tag{10}$$

Thus the matrices of the local transformations are exactly those which are obtained for the case of homogeneous propagation of light, these matrices were considered in Part I — we explained there that the Lorentz principle can be supposed to be valid for such transformations.

The local transformations in distant points have, however, different forms. Consider a number of locations $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \ldots$. Let us denote

$$\mathbf{g}(\mathbf{x}_k) = \mathbf{g}_k\,. \tag{10a}$$

Further we write $\mathbf{M}_k$ for the transformation matrix relating to transformations in $\mathbf{x}_k$. Thus we suppose

$$\tilde{\mathbf{M}}_k\,\mathbf{g}_k\,\mathbf{M}_k = \mathbf{g}_k\,, \qquad k = 1, 2, 3. \tag{11}$$

The matrices $\mathbf{M}_1, \mathbf{M}_2, \ldots$ define local transformations near $\mathbf{x}_1, \mathbf{x}_2, \ldots$ A connection between the matrices $\mathbf{M}_k$ for different k can be found. Denote

$$\mathbf{g}_l^{-1/2}\,\mathbf{g}_k^{1/2} = \mathbf{S}_{lk}\,, \tag{12}$$

or *alternatively*, if S_{lk} thus defined possessed complex elements, then (12) can be replaced by matrices defined in equations (9a), or by those defined by (9b); the latter have real elements only and behave algebraically similar to the matrices (12).

We may put

$$\mathbf{M}_k = \mathbf{S}_{lk}^{-1}\,\mathbf{M}_l\,\mathbf{S}_{lk}\,. \tag{13}$$

Introducing (13) into (11) we find with the help of (12)

$$\tilde{\mathbf{M}}_l\,\mathbf{g}_l\,\mathbf{M}_l = \mathbf{g}_l\,.$$

Thus relation (13) can be taken as the transformation formula between matrices of local transformation in different locations.

§ 6. The matrices $\mathbf{S}_{lk}$ can be taken to define parallel shifts. The $\mathbf{S}_{lk}$ are matrices corresponding to Lorentz transformations producing shifts from $\mathbf{x}_k \rightarrow \mathbf{x}_l$. Indeed with the help of (12) we obtain

$$\widetilde{\mathbf{S}}_{lk}\, \mathbf{g}_l\, \mathbf{S}_{lk} = \mathbf{g}_k \,. \tag{14}$$

Remembering the definition (10a) and comparing (14) with (7b) we see that $\mathbf{S}_{lk}$ is indeed a matrix producing the shift $\mathbf{x}_k \rightarrow \mathbf{x}_l$.

We note that according to (12) the matrices $\mathbf{S}_{lk}$ obey the relation

$$\mathbf{S}_{lk}\, \mathbf{S}_{km} = \mathbf{S}_{lm} \tag{14a}$$

and also

$$\mathbf{S}_{lm}^{-1} = \mathbf{S}_{ml} \,. \tag{14b}$$

If we make three parallel shifts which compensate each other, i.e. $\mathbf{x}_k \rightarrow \mathbf{x}_l$, $\mathbf{x}_l \rightarrow \mathbf{x}_m$ and finally $\mathbf{x}_m \rightarrow \mathbf{x}_n$, then the corresponding matrix is found to be

$$\mathbf{S}_{kl}\, \mathbf{S}_{lm}\, \mathbf{S}_{mk} = \mathbf{1} \,. \tag{15}$$

If instead of (12) alternative definitions of S in accordance with (9a) or (9b) of Part I are taken, then relations (14a), (14b) and (15) remain valid. Thus if we carry out a number of adiabatic parallel shifts with a system $\mathfrak{Q}$ such that we return in the end to the original positions, then the configuration of the system $\mathfrak{Q}$ also returns to its original form.

The latter statement in this form has, however, no real physical content. Indeed, a shift $\mathbf{x}_k \rightarrow \mathbf{x}_l$ takes some time to carry out and therefore we have necessarily $x_{k4} < x_{l4}$. When carrying out a series of shifts we cannot arrive back to the first position $\mathbf{x}_k$ from which we started.

However, relation (14) expresses the real physical fact; it follows from (14) that shifting $\mathfrak{Q}$ first from $\mathbf{x}_k \rightarrow \mathbf{x}_l$ and then from $\mathbf{x}_l \rightarrow \mathbf{x}_m$ we obtain the same result as if we had carried out directly a parallel shift $\mathbf{x}_k \rightarrow \mathbf{x}_l$. I.e. the parallel shift here defined is a true parallel shift and *the result of such a shift does not depend on the path along which the shift is carried out as long as the end points are kept fixed.*

§ 7. The most general form of the Lorentz transformation is obtained by combining a local transformation and a parallel shift. We may put

$$\mathbf{M}_{lk} = \mathbf{S}_{lk}\, \mathbf{M}_k \tag{16a}$$

or inserting for $\mathbf{M}_k$ the expression (13), the identical relation

$$\mathbf{M}_{lk} = \mathbf{M}_l\, \mathbf{S}_{lk} \,. \tag{16b}$$

The transformations $\mathbf{M}\,(\mathbf{x}_k;\ \mathbf{x}_l - \mathbf{x}_k)$ possess matrices each of which can be written in the form (16a) respectively in the form (16b). We see thus that any transformation $\mathbf{M}\,(\mathbf{x}, \boldsymbol{\mu})$ can be taken as to consist of a local transformation $\mathbf{M}_k$ at $\mathbf{x}_k$ and a parallel shift μ — but it can also be represented by a parallel shift $\mathbf{M}_l$ in the final position $\mathbf{x}_l$. The connection between the local transformations $\mathbf{M}_k$ and $\mathbf{M}_l$ which lead to the same final result is given by relation (13).

Small displacements

§ 8. Let us consider that approximation of the Lorentz transformation which is valid in the case of small shifts. We consider as a small shift one which might be very much larger than the dimensions of the system subjected to the shift, but which is small on a cosmical scale, i.e. a shift μ such that we have in a good approximation

$$\mathbf{g}(\mathbf{x} + \mu) = \mathbf{g}(\mathbf{x}) + \mu \frac{\partial \mathbf{g}(\mathbf{x})}{\partial \mathbf{x}}. \tag{17}$$

A small shift in general can be expressed by a matrix

$$\mathbf{S} = \mathbf{1} + \sigma \mu, \tag{18}$$

where we suppose

$$\sigma \mu = \sum_{\varkappa} \sigma^{(\varkappa)} \mu_{\varkappa}. \tag{19}$$

Introducing (18) into (7b) and neglecting terms of higher order we find for the condition that S should be a Lorentz matrix

$$\tilde{\sigma}^{(\varkappa)} \mathbf{g} + \mathbf{g} \sigma^{(\varkappa)} = - \frac{\partial \mathbf{g}}{\partial \mathbf{x}_{\varkappa}}.$$

Thus we find

$$\sigma^{(\varkappa)} = - \frac{1}{2} \mathbf{g}^{-1} \left(\frac{\partial \mathbf{g}}{\partial \mathbf{x}_{\varkappa}} + \mathbf{A}^{(\varkappa)} \right), \tag{20}$$

where $\mathbf{A}^{(\varkappa)}$ (for any value of $\varkappa$) is an arbitrary antisymmetric matrix, i.e. a matrix obeying

$$\tilde{\mathbf{A}}^{(\varkappa)} = - \mathbf{A}^{(\varkappa)}. \tag{20a}$$

A small shift is thus produced by a transformation containing the matrix

$$\mathbf{S} = \mathbf{1} - \frac{1}{2} \mathbf{g}^{-1} \left(\frac{\partial \mathbf{g}}{\partial \mathbf{x}} \mu + \mathbf{A} \right). \tag{21}$$

The parallel shift is obtained for $\mathbf{A} = 0$. For $\mathbf{A} \neq 0$ we obtain a parallel shift superimposed on a local transformation which differs from unity only by terms of the order of μ.

Geodetic orbits

§ 9. In regions where the propagation of light is inhomogeneous there exists, apart from the parallel shift described above, another type of transformation.

Indeed, a physical system $\mathfrak{Q}$ even if no outside interference takes place may drift away if it has an initial velocity $\mathbf{v}$ and thus it moves into regions in which the tensor $\mathbf{g}$ differs from that in the original position. The question arises what changes occur due to the changing environment of the system?

It may be supposed that the changes which take place in the course of the free motion of a system can be described also by Lorentz transformations. We give presently an argument as the result of which the latter type of Lorentz transformation can be determined.

In the homogeneous case a closed system may move with some constant velocity and suffers no changes, therefore the transformation describing this motion corresponds to $\mathbf{M} = 1$ and a displacement $\mu = \mathbf{m}, t$ with $\mathbf{m} = \mathbf{v}t$.

If we transform the coordinates as described in § 1, we obtain in the new representation a tensor $\mathbf{g}'(\mathbf{x}')$ which depends on $\mathbf{x}'$ and thus the propagation of light appears relative to K' inhomogeneous.

Conversely, if in the representation K the propagation appears inhomogeneous the question arises whether it is possible by means of a suitable coordinate transformations to obtain a new representation in which the propagation appears to be homogeneous.

Considering thus the vicinity of a fixed four vector $\mathbf{x}$ we ask whether it is possible to find a transformation

$$\mathbf{x}' + \boldsymbol{\xi}' = \mathbf{f}(\mathbf{x} + \boldsymbol{\xi}) \tag{22}$$

such that

$$\widetilde{\mathbf{S}}(\mathbf{x} + \boldsymbol{\xi})\, \mathbf{g}'\, \mathbf{S}(\mathbf{x} + \boldsymbol{\xi}) = \mathbf{g}(\mathbf{x} + \boldsymbol{\xi}), \tag{23a}$$

where $\mathbf{g}'$ has constant components and describes the homogeneous propagation of light relative to K', further

$$S_{\nu\mu}(\mathbf{x} + \boldsymbol{\xi}) = \frac{\partial f_\nu(\mathbf{x} + \boldsymbol{\xi})}{\partial \xi_\mu}. \tag{23b}$$

In the above relations we have not neglected the terms of higher order in $\boldsymbol{\xi}$ as we wanted to define the transformation which leads from the representation of an apparently inhomogeneous region to a representation in which the region appears homogeneous.

Equations (23a) and (23b) give a system of ten partial differential equations to the four unknown functions f_ν and thus the system is as a rule overdetermined. We may therefore consider those cases where the equations (23a) and (23b) have solutions as exceptional cases and we may regard them as representing the cases where light is truly propagated homogeneously. Thus we may suppose that a propagation tensor $\mathbf{g}(\mathbf{x})$ if it possesses a representation $\mathbf{g}' =$ constant, then $\mathbf{g}(\mathbf{x})$ represents homogeneous propagation, only the representation is given in terms of curved coordinates. We note if in the above case we were to construct coordinates according to the methods described in Part I the latter method would automatically lead to a representation in which the propagation appeared to be homogeneous.

§ 10. In general it is impossible to "transform away" the inhomogeneity of propagation of light which appears in a given representation K. It is, however, possible to find by transformation of $\mathbf{g}(\mathbf{x})$ a representation $\mathbf{g}'(\mathbf{x}')$ the first derivatives of which are zero, thus a representation in which

$$\frac{\partial \mathbf{g}'(\mathbf{x}' + \boldsymbol{\xi}')}{\partial \boldsymbol{\xi}'} = 0 \quad \text{for} \quad \boldsymbol{\xi}' = 0\,. \tag{24}$$

In the latter representation the propagation of light appears as near as possible to homogeneous propagation.

We note that if there exists a transformation of the form (23) which leads to a transformed $\mathbf{g}'$ satisfying (24), then there exists also a transformation such that the transformed quantities satisfying apart from (24) also

$$\mathbf{x}' = \mathbf{x}\,, \qquad \mathbf{g}' = \mathbf{g}(\mathbf{x}). \tag{25}$$

Relations (25) are satisfied if the transformation functions obey

$$f_\nu(\mathbf{x}) = x_\nu \quad \text{and} \quad S_{\nu\mu}(\mathbf{x}) = \left(\frac{\partial f_\nu(\mathbf{x} + \boldsymbol{\xi})}{\partial \xi_\mu}\right)_{\xi = 0} = \delta_{\nu\mu}\,. \tag{26}$$

Differentiating (23c) into $\xi_\varkappa$ we find in the limit $\boldsymbol{\xi} = 0$ using (24) and (25)

$$\frac{\partial \mathbf{S}}{\partial \xi_\varkappa}\, \mathbf{g} + \mathbf{g}\, \frac{\partial \mathbf{S}}{\partial \xi_\varkappa} = \frac{\partial \mathbf{g}}{\partial \xi_\varkappa} \quad \text{for} \quad \boldsymbol{\xi} = 0. \tag{27}$$

The above equations admit solutions

$$\frac{\partial \mathbf{S}}{\partial \xi_\varkappa} = \frac{1}{2}\, \mathbf{g}^{-1} \left(\frac{\partial \mathbf{g}}{\partial \xi_\varkappa} + \mathbf{A}^{(\varkappa)}\right) \qquad \boldsymbol{\xi} = 0, \tag{28}$$

where $\mathbf{A}^{(\varkappa)}$ for $\varkappa = 1, 2, 3, 4$ are antisymmetric matrices obeying

$$\tilde{\mathbf{A}}^{(\varkappa)} = -\mathbf{A}^{(\varkappa)} . \tag{28a}$$

The latter transformation is of the form given in § 7, equs. (20) and (20a), however, in the present case the matrices $\mathbf{A}^{(\varkappa)}$ can be determined. Indeed, differentiating (23b) into $\xi_\varkappa$ we find

$$\frac{\partial S_{\nu\mu}}{\partial \xi_\varkappa} = \frac{\partial^2 f_\nu(\mathbf{x} + \boldsymbol{\xi})}{\partial \xi_\mu \partial \xi_\varkappa}$$

Thus we find interchanging μ and $\varkappa$ in the above relation

$$\frac{\partial S_{\nu\mu}}{\partial x_\varkappa} = \frac{\partial S_{\nu\varkappa}}{\partial x_\mu} . \tag{29}$$

Comparing (28a) and (29) we find

$$A_{\nu\mu}^{(\varkappa)} = \frac{\partial g_{\nu\varkappa}}{\partial x_\mu} - \frac{\partial g_{\mu\varkappa}}{\partial x_\nu} .$$

We may write in place of (22)

$$\frac{\partial \mathbf{S}}{\partial \xi_\varkappa} = -\frac{1}{2} \mathbf{g}^{-1} \mathbf{C}^{(\varkappa)} , \tag{30}$$

where

$$C_{\nu\mu}^{\varkappa} = -\frac{1}{2} \left(\frac{\partial g_{\nu\mu}}{\partial x_\varkappa} + \frac{\partial g_{\nu\varkappa}}{\partial x_\mu} - \frac{\partial g_{\mu\varkappa}}{\partial x_\varkappa} \right) , \tag{30a}$$

thus the $C_{\nu\mu}^{(\varkappa)}$ are equal to the well-known Christoffel brackets

$$C_{\nu\mu}^{(\varkappa)} = \begin{bmatrix} \nu\mu \\ \varkappa \end{bmatrix} \qquad \nu, \mu, \varkappa = 1, 2, 3, 4. \tag{30b}$$

Furthermore using the usual notation

$$\frac{\partial S_{\nu\mu}}{\partial \xi_\varkappa} = \begin{Bmatrix} \nu\,\mu \\ \varkappa \end{Bmatrix} \tag{30c}$$

we shall also use the following notation

$$\frac{\partial \mathbf{S}}{\partial \xi_\varkappa} = \mathcal{C}^{(\varkappa)} \qquad \varkappa = 1, 2, 3, 4. \tag{30d}$$

§ 11. So as to return to the transformation describing the free drift of a system we remark the following. Consider some four vector $\mathfrak{B}$ with a representation **B** relative to K which describes a feature of $\mathfrak{Q}$. The four-vector may be the four distance $\xi_k - \xi_\lambda$ between two points of $\mathfrak{Q}$ — but it might describe alternatively a velocity, an electromagnetic potential, etc.

If the propagation tensor $\mathfrak{g}$ as represented relative to K' is constant, i.e. if $\mathbf{g}' =$ constant, then in the representation K' the system $\mathfrak{Q}$ drifts freely and denoting the configuration of $\mathfrak{Q}$ after it has drifted some distance μ' by $\mathfrak{Q}^*$ we find

$$\mathbf{B}'^* = \mathbf{B}' \tag{31}$$

for the representations of the four-vector $\mathfrak{B}$ appearing in $\mathfrak{Q}$ respectively of $\mathfrak{B}^*$ appearing in $\mathfrak{Q}^*$ the shifted system. In the original representation K we have, however,

$$\mathbf{B} = \mathbf{S}^{-1}(\mathbf{x}')\,\mathbf{B}', \qquad \mathbf{B}^* = \mathbf{S}^{-1}(\mathbf{x}' + \mu')\,B'^*.$$

From (26) we find

$$\mathbf{S}(\mathbf{x}') = \mathbf{S}^{-1}(\mathbf{x}') = \mathbf{1} \quad \text{and} \quad \frac{\partial \mathbf{S}}{\partial \mathbf{x}} = -\frac{\partial \mathbf{S}^{-1}}{\partial \mathbf{x}} \quad \text{for} \quad \xi = 0$$

and therefore since neglecting higher order terms we may put $\mu' = \mu$, $\mathbf{B}' = \mathbf{B}$

$$\delta \mathbf{B} = \mathbf{B}^* - \mathbf{B} = \mu \frac{\partial \mathbf{S}^{-1}}{\partial \mathbf{x}} \mathbf{B}.$$

Thus with the help of (30d) we find

$$\delta \mathbf{B} = -\Sigma\, \mu_\varkappa\, \mathcal{C}^{(\varkappa)}\, \mathbf{B}\,, \tag{32a}$$

we may also write explicitly

$$\delta B_\nu = -\sum_{\mu\varkappa} \begin{Bmatrix} \mu\varkappa \\ \nu \end{Bmatrix} B_\mu\, \mu_\varkappa\,. \tag{32b}$$

§ 12. Relations (32a) or (32b) give the change of the measures of the components of a vector **B** in the course of the drift in the particular case where the system $\mathfrak{Q}$ is drifting in a homogeneous region and therefore in the proper representation K' (where $\mathbf{g}' =$ constant) the vector $\mathfrak{B}$ does not change at all because of the drift. The change $\delta\mathbf{B}$ reflects on changes of measures of the components of **B** which appear because the coordinates in K must be taken to be curved coordinates.

Thus relations (32a) or (32b) express only the result of a coordinate transformation if applied to a region in which the propagation is truly homogeneous in the sense of § 8. Following the idea of EINSTEIN, we may suppose that (32) remains valid whether or not the propagation of light is truly homogeneous. Thus it may be assumed that the free drift of a system $\mathfrak{Q}$ is characterized so that in a representation K' in which

$$\frac{\partial \mathbf{g}'(\mathbf{x}' + \boldsymbol{\xi}')}{\partial \boldsymbol{\xi}'} = 0 \qquad \text{for } \boldsymbol{\xi}' = 0,$$

i.e. in the representation K' where the propagation appears as near to homogeneous as possible — in that representation the change of a vector is characterized by

$$\delta \mathbf{B}' = 0$$

or more precisely

$$\delta \mathbf{B}' = \text{order of } \mu^2 .$$

If the latter assumption is made then we are led to relation (32) irrespective of the true mode of propagation of light.

As we suppose that the inhomogeneity of propagation of light is connected with the gravitational field, we may thus suppose that (32) describes the changes which occur in a system moving freely in a gravitational field, i.e. the changes occurring in a free falling system.

§ 13. It is very important that the change although spontaneous should take place adiabatically. If a system would be subjected to a sudden impact through some sudden change of gravitational field, then it might very well deform non-adiabatically. Thus relation (32) can be taken only to be valid for sufficiently slow changes. We have here a complete analogy with the limitations of the adiabatic principle attached to the Lorentz principle in the case of homogeneous propagation of light.

Relation (32) describes the deformations a free falling system suffers, while the parallel shifts discussed in § 5 and which are given (in the case of small shifts) by (18) arise if a system is shifted adiabatically in such a manner that the gravitational action is compensated by outside forces and thus the system is not allowed to fall but is made to move with some small velocity.

From the above remark it becomes clear that a system, which is not allowed to fall freely but is brought adiabatically with small velocity from one position into another, when thus treated will take up in its final position a configuration which is independent of the path along which it was brought there.

On the contrary if a system $\mathfrak{Q}$ falls freely from $\mathbf{x}_k \to \mathbf{x}_m$ then it will arrive in $\mathbf{x}_m$ with a velocity which it acquired in the course of its fall. However, if the system is made first to fall from $\mathbf{x}_k \to \mathbf{x}_l$ then to fall from $\mathbf{x}_l \to \mathbf{x}_m$ then it must receive in $\mathbf{x}_m$ the intermediate position $\mathbf{x}_l$ an impact which make it to change its direction so as to proceed towards $\mathbf{x}_m$. Because of this impact the system will arrive in $\mathbf{x}_m$ with a different velocity when it travelled via $\mathbf{x}_l$ than in the case of the direct journey. The difference of velocity of $\mathfrak{Q}$ when it arrives directly from $\mathbf{x}_k$ or when it arrives on a round about way $\mathbf{x}_m$ can be represented by a local Lorentz transformation, namely the one which corresponds to the change between the two velocities.

From the above consideration we see clearly that the analogy to the conventional parallel shift of a system is not the free fall but the parallel shift where gravitational effects are compensated by outside forces.

We note, that in the usual relativistic terminology the shift as a result of free falling is denoted "parallel shift" and therefore the parallel shift so defined depends on the path in a manner as explained further above. If we define alternatively the parallel shift as a shift which takes place while the gravitational action is compensated by outside forces, then we obtain a type of parallel shift independent of the orbit. Here we use this latter definition.

Adiabatic orbits

§ 14. With the help of relation (32) it is possible to determine the orbit of a free falling system. Consider thus a system the centre of which can be described by some vector $\mathbf{x}(p)$, i.e. we suppose that at the time

$$t = x_4(p) \tag{33}$$

its coordinates are given by

$$\mathbf{r}(t) = x_1(p),\ x_2(p),\ x_3(p). \tag{34}$$

The motion of the centre of the system is thus given in a parameter representation. The velocity of the system can be written

$$\mathbf{v}(p) = \dot{\mathbf{r}}(p)/\dot{x}_4(p), \tag{35}$$

where the dot denotes derivation into p. Further the acceleration is given by

$$\mathbf{a}(p) = \frac{d\mathbf{v}(p)}{dt} = \dot{\mathbf{v}}(p)/\dot{x}_4(p). \tag{36}$$

With the help of (35) and (36) we have also

$$\mathbf{a}(p) = \frac{\ddot{\mathbf{r}}(p) - \mathbf{v}(p)\,\ddot{x}_4(p)}{\dot{x}_4^2(p)}. \tag{37}$$

A system left on its own will thus move in first approximation with a constant velocity. In a time

$$\delta t = \dot{x}_4(p)\,\delta p\,,$$

it will shift by

$$\delta \mathbf{r} = \dot{\mathbf{r}}(p)\,\delta p\,,$$

and we may thus suppose that it will shift by

$$\mu = \delta \mathbf{r}, \delta t\,. \tag{38}$$

We may introduce (38) into (32) and introducing $\dot{\mathbf{x}}(p)$ in place of **B** we find

$$\delta \dot{x}_\nu(p) = -\sum_{\varkappa\lambda} \left\{ {\varkappa\lambda \atop \nu} \right\} \dot{x}_\varkappa(p)\,\dot{x}_\lambda(p)\,\delta p$$

or writing $\ddot{x}_\nu(p)$ for $\delta\,\dot{x}_\nu(p)/\delta p$ we have

$$\ddot{x}_\nu(p) + \sum_{\varkappa\lambda} \left\{ {\varkappa\lambda \atop \nu} \right\} \dot{x}_\varkappa(p)\,\dot{x}_\lambda(p) = 0\,. \tag{39}$$

The above relation is the well-known equation of the so-called four dimensionat geodetic line. We see that supposing a system if left on its own suffers Lorentzl deformations of the particular form (32) we are led to equation (39) for the orbit of a free particle or of a free closed system.

Since relation (39) contains no specific quantity of the moving system this leads to the conclusion that any small closed system left on its own, will move on the same orbit (determined only by initial conditions). Thus the fact that relation (39) contains only the coordinates of the moving system and their derivatives reflects the general law of the equivalence of inertial and gravitational masses.

§ 15. It is well known that the equation of motion (39) can also be derived from a variational principle. It can be shown that (39) are the Euler equations

$$\delta \int_{\mathbf{x}_1}^{\mathbf{x}_2} \left(\frac{ds}{dp} \right)^2 dp = 0, \tag{40}$$

where

$$\left(\frac{ds}{dp} \right)^2 = \dot{\mathbf{x}}\mathbf{g}\dot{\mathbf{x}}\,.$$

Multiplying (40) with the mass m_0 of the particle we may write if we choose the parameter p equal to x_4 with the help of notation used in Part I,

$$m_0\left(\frac{ds}{dp}\right)^2 = m_0(\mathbf{v}+\mathbf{V})\,\mathbf{G}(\mathbf{v}+\mathbf{V}) - m_0\,\Phi\,.$$

The first term can be regarded as a kind of kinetic energy (the velocity of the particle being taken to the aether drifting with a velocity $-\mathbf{V}$). The second term is a kind of negative potential energy, thus relation (40) is reminiscent of the Lagrange equation

$$\delta \int L\,\mathrm{d}t = 0\,,$$

with

$$L = K - U\,.$$

Furthermore it can be shown that (39) can also be derived from the following variational principle

$$\delta \int_{\mathbf{x}_1}^{\mathbf{x}_2} \mathrm{d}s = 0\,. \tag{41}$$

The latter principle requires that the orbit of the system should be a four dimensional geodetic line.

From the physical point of view, we prefer the derivation of the equation of motion (39) through the generalization of the Lorentz principle and thus to consider the tensor $\mathbf{g}(\mathbf{x})$ as characteristic for the propagation of light in the vicinity of $\mathbf{x}$. However, the fact that (39) gives mathematically the solution of a variational problem is very important from another point of view. In deriving (39) we have used approximations and have considered shifts μ small on a cosmical scale. A larger shift can be built up from the succession of a number of small shifts, but it is not immediately obvious that the small errors committed considering the small steps do not accumulate.

From the fact that (39) is the solution of a variational problem one concludes that the orbits obtained as a solution of (39) are independent of the particular choice of coordinates. Therefore one is inclined to take equation (39) to be exact — or at least to be strictly independent of the choice of coordinates.

In the case of homogeneous propagation of light we have $d\mathbf{g}/d\mathbf{x} = 0$ and therefore all the Christoffel brackets vanish. In the latter case we find $\ddot{\mathbf{x}}(p) = 0$ and thus

$$\mathbf{x} = \boldsymbol{\alpha} p + \boldsymbol{\beta}\,,$$

or eliminating p we have

$$\mathbf{r} = \mathbf{v}t + \mathbf{b}\,, \tag{42}$$

where $\mathbf{v}$ has components $v_k = \alpha_k/\alpha_4$, $k = 1, 2, 3$. Thus in a region with homogeneous propagation of light Newton's first law appears to be valid. If we consider the same region in terms of transformed coordinates $\mathbf{x}' = \mathbf{x}'(\mathbf{x})$, then in the latter the Christoffel brackets will not vanish, but we obtain the exact representation of the translational motion in terms of the transformed coordinates. This result, however, is only a check of consistency of one assumption as the concept of motion with constant velocity in the space free of gravitation was made use of in the derivation of the equations of motion.

For physical application it is of course necessary to establish the connection between the tensor $\mathbf{g}(\mathbf{x})$ and the gravitational field or more exactly it is necessary to obtain $\mathbf{g}(\mathbf{x})$ from the distribution of gravitating matter. The latter problem was solved by Einstein, we give certain aspects of the problem in Part III of this series.

ПРИНЦИП ЛОРЕНЦА И ОБЩАЯ ТЕОРИЯ ОТНОСИТЕЛЬНОСТИ

Часть II.

Л. ЯНОШИ

Резюме

Дано обобщение преобразования Лоренца для областей где свет распространяется неоднородно, и показано, что принцип Лоренца может быть сохранён в своей обычной форме если преобразование Лоренца взять в своем более общем виде, формулированном для таких областей. Известные уравнения геодезических линий в гравитационном поле выводятся из обобщенного таким образом принципа Лоренца.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (1), pp. 33—54, (1966)

COMPLETE CLASSIFICATION OF THE STATES OF NUCLEAR CONFIGURATIONS j^k FOR $j=\frac{9}{2}$

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The states of equivalent $j=\frac{9}{2}$ nucleon configurations are classified and enumerated. New formulae are given for the dimensionalities of the relevant partitions. Several general rules are deduced for the interpretation of non-standard partitions.

1. Introduction

This paper is a direct extension of an article published by Flowers, [1] in which the techniques of group theory were first applied to the problem of classifying the states of systems of equivalent nucleons in jj-coupling. Flowers completely classified the states of equivalent nucleon configurations for the cases $j=\frac{3}{2}$, $j=\frac{5}{2}$ and $j=\frac{7}{2}$. It is the purpose of this paper to extend these classifications to the case $j=\frac{9}{2}$.

In addition, new formulae are obtained for the dimensionalities $N[\lambda]$ and $N(\sigma)$ of the partitions $[\lambda]$ and (σ) associated with the irreducible representations of the unitary unimodular group SU $(2j+1)$ and the symplectic group Sp $(2j+1)$ respectively. These new formulae reduce considerably the computations required to obtain the values of the dimensionalities $N[\lambda]$ and $N(\sigma)$ for the various partitions $[\lambda]$ and (σ).

Furthermore, the formula for $N(\sigma)$ provides for the interpretation of non-standard partitions (σ) on the basis of dimensionality. This formula is used to deduce several general rules regarding these interpretations.

2. Results of the classification

Tables 1 to 6, particularly Table 6, give the results of the classification of the states of the nucleon configuration j^k for the case $j=\frac{9}{2}$. These Tables are completely analogous to those presented by FLOWERS [1] for the cases $j = \frac{3}{2}, \frac{5}{2}$, and $\frac{7}{2}$. The length of Table 6 is here minimized by not repeating the J-structure, which is already given in Table 5 for each partition (σ). The reader is referred to FLOWERS' article [1] or to ref. [2] for both the general theory and the detailed techniques of the calculations.

The state classification and the coefficients of fractional parentage for the case of *identical* $j = \frac{9}{2}$ particles have recently been given by SATO [4]. SATO's classification results correspond to those entries in Table 6 for which $T = \frac{k}{2}$ with $t = \frac{s}{2}$.

3. Non-standard (σ) partitions and dimensionality

3.1 *Interpretation of those non-standard (σ) partitions which occur in state classification calculations for selected j values*

In the performance of the reduction of the irreducible representations of SU (10) to the irreducible representations of Sp (10) given in Table 4, certain (σ) symbols occur which have more than the allowed $\nu = \frac{1}{2}(2j+1)$ integers.

Similar non-standard (σ) partitions occurred also in FLOWERS' calculations [1] with $j \leq \frac{7}{2}$, and for these cases he was able to interpret the occurring non-standard (σ) partitions by using the unimodular conditions to obtain sets of equivalent $[\lambda]$ partitions which upon reduction yielded sets of equivalent (σ) structures. His interpretations, based on this equivalent $[\lambda]$ partition technique [3], can be stated in a single sentence, which we shall refer to as FLOWERS' Rule; namely, that all non-standard (σ) partitions, occurring in the state classification calculations for $j \leq \frac{7}{2}$, are null except for those having either of the following forms

$$(\sigma_1 \ldots \sigma_\nu\ 11) = -(\sigma_1 \ldots \sigma_\nu), \tag{1}$$

$$(\sigma_1 \ldots \sigma_{\nu-1}\ 1111) = -(\sigma_1 \ldots \sigma_{\nu-1}\ 0). \tag{2}$$

In the present state classification calculation the following nine and ten row non-standard (σ) partitions occur: (111111111), (1111111111) and (211111111). Of these the first two may be interpreted by the equivalent $[\lambda]$

Table 1

The dimensions of the irreducible representations of SU (10)

k	$[\lambda]$	$N[\lambda]$
0	[0]	1
1	[1]	10
2	[2]	55
	[11]	45
3	[21]	330
	[111]	120
4	[22]	825
	[211]	990
	[1111]	210
5	[221]	3300
	[2111]	1848
	[11111]	252
6	[222]	4950
	[2211]	6930
	[21111]	2310
	[111111] = [1111]	210
7	[2221]	13860
	[22111]	9240
	[211111]	1980
	[1111111] = [111]	120
8	[2222]	13860
	[22211]	20790
	[221111]	8250
	[2111111]	1155
	[11111111] = [11]	45
9	[22221]	27720
	[222111]	19800
	[2211111]	4950
	[21111111]	440
	[111111111] = [1]	10
10	[22222]	19404
	[222211]	29700
	[2221111]	12375
	[22111111]	1925
	[211111111]	99
	[1111111111]	1

Table 2

The reduction of representations of SU (10) to representations of R (3)

k	$[\lambda]$	J-structure
0	[0]	0
1	[1]	$\frac{9}{2}$
2	[2]	$9\;\;7\;\;5\;\;3\;\;1$
	[11]	$8\;\;6\;\;4\;\;2\;\;0$
3	[21]	$\frac{25}{2}\;\frac{23}{2}\;\frac{21}{2}\;\left(\frac{19}{2}\right)^2\left(\frac{17}{2}\right)^2\left(\frac{15}{2}\right)^2\left(\frac{13}{2}\right)^3\left(\frac{11}{2}\right)^3\left(\frac{9}{2}\right)^3\left(\frac{7}{2}\right)^3\left(\frac{5}{2}\right)^2\;\frac{3}{2}\;\frac{1}{2}$
	[111]	$\frac{21}{2}\;\frac{17}{2}\;\frac{15}{2}\;\frac{13}{2}\;\frac{11}{2}\;\left(\frac{9}{2}\right)^2\;\frac{7}{2}\;\frac{5}{2}\;\frac{3}{2}$
4	[22]	$16\;\;14^2\;\;13\;\;12^3\;\;11^2\;\;10^5\;\;9^3\;\;8^7\;\;7^4\;\;6^7\;\;5^4\;\;4^7\;\;3^2\;\;2^6\;\;0^3$
	[211]	$15\;\;14\;\;13^2\;\;12^2\;\;11^4\;\;10^4\;\;9^6\;\;8^6\;\;7^8\;\;6^7\;\;5^8\;\;4^6\;\;3^7\;\;2^4\;\;1^4$
	[1111]	$12\;\;10\;\;9\;\;8^2\;\;7\;\;6^3\;\;5\;\;4^3\;\;3\;\;2^2\;\;0^2$
5	[221]	$\frac{37}{2}\;\frac{35}{2}\;\left(\frac{33}{2}\right)^2\left(\frac{31}{2}\right)^3\left(\frac{29}{2}\right)^5\left(\frac{27}{2}\right)^6\left(\frac{25}{2}\right)^9\left(\frac{23}{2}\right)^{11}\left(\frac{21}{2}\right)^{14}\left(\frac{19}{2}\right)^{16}\left(\frac{17}{2}\right)^{18}\left(\frac{15}{2}\right)^{19}\left(\frac{13}{2}\right)^{21}\left(\frac{11}{2}\right)^{20}\left(\frac{9}{2}\right)^{19}\left(\frac{7}{2}\right)^{17}\left(\frac{5}{2}\right)^{14}\left(\frac{3}{2}\right)^9\left(\frac{1}{2}\right)^5$
	[2111]	$\frac{33}{2}\;\frac{31}{2}\;\left(\frac{29}{2}\right)^2\left(\frac{27}{2}\right)^3\left(\frac{25}{2}\right)^4\left(\frac{23}{2}\right)^6\left(\frac{21}{2}\right)^8\left(\frac{19}{2}\right)^9\left(\frac{17}{2}\right)^{11}\left(\frac{15}{2}\right)^{12}\left(\frac{13}{2}\right)^{13}\left(\frac{11}{2}\right)^{13}\left(\frac{9}{2}\right)^{13}\left(\frac{7}{2}\right)^{11}\left(\frac{5}{2}\right)^9\left(\frac{3}{2}\right)^7\left(\frac{1}{2}\right)^3$
	[11111]	$\frac{25}{2}\;\frac{21}{2}\;\frac{19}{2}\;\left(\frac{17}{2}\right)^2\left(\frac{15}{2}\right)^2\left(\frac{13}{2}\right)^2\left(\frac{11}{2}\right)^2\left(\frac{9}{2}\right)^3\left(\frac{7}{2}\right)^2\left(\frac{5}{2}\right)^2\left(\frac{3}{2}\right)\left(\frac{1}{2}\right)$
6	[222]	$21\;\;19^2\;\;18^2\;\;17^4\;\;16^4\;\;15^9\;\;14^8\;\;13^{14}\;\;12^{14}\;\;11^{20}\;\;10^{19}\;\;9^{27}\;\;8^{22}\;\;7^{30}\;\;6^{24}\;\;5^{28}\;\;4^{19}\;\;3^{24}\;\;2^{10}\;\;1^{13}$
	[2211]	$20\;\;19\;\;18^3\;\;17^3\;\;16^7\;\;15^8\;\;14^{14}\;\;13^{15}\;\;12^{23}\;\;11^{24}\;\;10^{33}\;\;9^{32}\;\;8^{41}\;\;7^{37}\;\;6^{44}\;\;5^{35}\;\;4^{39}\;\;3^{26}\;\;2^{27}\;\;1^{10}\;\;0^9$
	[21111]	$17\;\;16\;\;15^2\;\;14^3\;\;13^5\;\;12^6\;\;11^9\;\;10^{10}\;\;9^{13}\;\;8^{14}\;\;7^{16}\;\;6^{15}\;\;5^{17}\;\;4^{14}\;\;3^{13}\;\;2^9\;\;1^7\;\;0$
	[111111] = [1111]	$12\;\;10\;\;9\;\;8^2\;\;7\;\;6^3\;\;5\;\;4^3\;\;3\;\;2^2\;\;0^2$

Table 2 (continued)

k	[λ]	*J*-structure
7	[2221]	$\frac{45}{2}\ \frac{43}{2}\ \left(\frac{41}{2}\right)^{2} \left(\frac{39}{2}\right)^{4} \left(\frac{37}{2}\right)^{6} \left(\frac{35}{2}\right)^{9} \left(\frac{33}{2}\right)^{14} \left(\frac{31}{2}\right)^{18} \left(\frac{29}{2}\right)^{25} \left(\frac{27}{2}\right)^{32} \left(\frac{25}{2}\right)^{39} \left(\frac{23}{2}\right)^{47} \left(\frac{21}{2}\right)^{56} \left(\frac{19}{2}\right)^{61} \left(\frac{17}{2}\right)^{67} \left(\frac{15}{2}\right)^{71} \left(\frac{13}{2}\right)^{71} \left(\frac{11}{2}\right)^{69} \left(\frac{9}{2}\right)^{65} \left(\frac{7}{2}\right)^{55} \left(\frac{5}{2}\right)^{45} \left(\frac{3}{2}\right)^{32} \left(\frac{1}{2}\right)^{15}$
	[22111]	$\frac{41}{2}\ \frac{39}{2}\ \left(\frac{37}{2}\right)^{3} \left(\frac{35}{2}\right)^{4} \left(\frac{33}{2}\right)^{7} \left(\frac{31}{2}\right)^{10} \left(\frac{29}{2}\right)^{15} \left(\frac{27}{2}\right)^{19} \left(\frac{25}{2}\right)^{26} \left(\frac{23}{2}\right)^{31} \left(\frac{21}{2}\right)^{38} \left(\frac{19}{2}\right)^{43} \left(\frac{17}{2}\right)^{49} \left(\frac{15}{2}\right)^{51} \left(\frac{13}{2}\right)^{54} \left(\frac{11}{2}\right)^{52} \left(\frac{9}{2}\right)^{49} \left(\frac{7}{2}\right)^{43} \left(\frac{5}{2}\right)^{35} \left(\frac{3}{2}\right)^{24} \left(\frac{1}{2}\right)^{13}$
	[211111]	$\frac{33}{2}\ \frac{31}{2}\ \left(\frac{29}{2}\right)^{2} \left(\frac{27}{2}\right)^{3} \left(\frac{25}{2}\right)^{5} \left(\frac{23}{2}\right)^{6} \left(\frac{21}{2}\right)^{8} \left(\frac{19}{2}\right)^{10} \left(\frac{17}{2}\right)^{12} \left(\frac{15}{2}\right)^{13} \left(\frac{13}{2}\right)^{14} \left(\frac{11}{2}\right)^{14} \left(\frac{9}{2}\right)^{14} \left(\frac{7}{2}\right)^{12} \left(\frac{5}{2}\right)^{10} \left(\frac{3}{2}\right)^{7} \left(\frac{1}{2}\right)^{4}$
	[1111111] = [111]	$\frac{21}{2}\ \frac{17}{2}\ \frac{15}{2}\ \frac{13}{2}\ \frac{11}{2}\ \left(\frac{9}{2}\right)^{2} \frac{7}{2}\ \frac{5}{2}\ \frac{3}{2}$
8	[2222]	$24\ 22^{2}\ 21^{2}\ 20^{5}\ 19^{5}\ 18^{11}\ 17^{11}\ 16^{20}\ 15^{21}\ 14^{32}\ 13^{33}\ 12^{48}\ 11^{45}\ 10^{61}\ 9^{57}\ 8^{70}\ 7^{60}\ 6^{72}\ 5^{54}\ 4^{62}\ 3^{39}\ 2^{41}\ 1^{14}\ 0^{16}$
	[22211]	$23\ 22\ 21^{3}\ 20^{4}\ 19^{8}\ 18^{11}\ 17^{18}\ 16^{23}\ 15^{34}\ 14^{41}\ 13^{55}\ 12^{63}\ 11^{79}\ 10^{85}\ 9^{99}\ 8^{100}\ 7^{109}\ 6^{102}\ 5^{103}\ 4^{86}\ 3^{79}\ 2^{53}\ 1^{39}\ 0^{8}$
	[221111]	$20\ 19\ 18^{3}\ 17^{4}\ 16^{8}\ 15^{9}\ 14^{16}\ 13^{18}\ 12^{27}\ 11^{29}\ 10^{39}\ 9^{39}\ 8^{49}\ 7^{45}\ 6^{52}\ 5^{44}\ 4^{47}\ 3^{32}\ 2^{32}\ 1^{13}\ 0^{10}$
	[2111111]	$15\ 14\ 13^{2}\ 12^{3}\ 11^{4}\ 10^{5}\ 9^{7}\ 8^{7}\ 7^{9}\ 6^{9}\ 5^{9}\ 4^{8}\ 3^{8}\ 2^{5}\ 1^{4}\ 0$
	[11111111] = [11]	8 6 4 2 0
9	[22221]	$\frac{49}{2}\ \frac{47}{2}\ \left(\frac{45}{2}\right)^{2} \left(\frac{43}{2}\right)^{4} \left(\frac{41}{2}\right)^{7} \left(\frac{39}{2}\right)^{10} \left(\frac{37}{2}\right)^{16} \left(\frac{35}{2}\right)^{22} \left(\frac{33}{2}\right)^{31} \left(\frac{31}{2}\right)^{41} \left(\frac{29}{2}\right)^{53} \left(\frac{27}{2}\right)^{65} \left(\frac{25}{2}\right)^{81} \left(\frac{23}{2}\right)^{93} \left(\frac{21}{2}\right)^{106} \left(\frac{19}{2}\right)^{118} \left(\frac{17}{2}\right)^{127} \left(\frac{15}{2}\right)^{130} \left(\frac{13}{2}\right)^{132} \left(\frac{11}{2}\right)^{126} \left(\frac{9}{2}\right)^{116} \left(\frac{7}{2}\right)^{101} \left(\frac{5}{2}\right)^{80} \left(\frac{3}{2}\right)^{55} \left(\frac{1}{2}\right)^{30}$

Table 2 (continued)

k	[λ]	*J*-structure
	[222111]	$\frac{45}{2}\ \frac{43}{2}\ \left(\frac{41}{2}\right)^{3} \left(\frac{39}{2}\right)^{5} \left(\frac{37}{2}\right)^{8} \left(\frac{35}{2}\right)^{12} \left(\frac{33}{2}\right)^{19} \left(\frac{31}{2}\right)^{25}$ $\left(\frac{29}{2}\right)^{35} \left(\frac{27}{2}\right)^{45} \left(\frac{25}{2}\right)^{56} \left(\frac{23}{2}\right)^{67} \left(\frac{21}{2}\right)^{80} \left(\frac{19}{2}\right)^{88} \left(\frac{17}{2}\right)^{98}$ $\left(\frac{15}{2}\right)^{103} \left(\frac{13}{2}\right)^{104} \left(\frac{11}{2}\right)^{101} \left(\frac{9}{2}\right)^{95} \left(\frac{7}{2}\right)^{81} \left(\frac{5}{2}\right)^{66} \left(\frac{3}{2}\right)^{47} \left(\frac{1}{2}\right)^{33}$
	[2211111]	$\frac{37}{2}\ \frac{35}{2}\ \left(\frac{33}{2}\right)^{3} \left(\frac{31}{2}\right)^{4} \left(\frac{29}{2}\right)^{7} \left(\frac{27}{2}\right)^{9} \left(\frac{25}{2}\right)^{13} \left(\frac{23}{2}\right)^{16}$ $\left(\frac{21}{2}\right)^{21} \left(\frac{19}{2}\right)^{24} \left(\frac{17}{2}\right)^{28} \left(\frac{15}{2}\right)^{30} \left(\frac{13}{2}\right)^{32} \left(\frac{11}{2}\right)^{31} \left(\frac{9}{2}\right)^{30}$ $\left(\frac{7}{2}\right)^{26} \left(\frac{5}{2}\right)^{22} \left(\frac{3}{2}\right)^{15} \left(\frac{1}{2}\right)^{8}$
	[21111111]	$\frac{25}{2}\ \frac{23}{2}\ \left(\frac{21}{2}\right)^{2} \left(\frac{19}{2}\right)^{2} \left(\frac{17}{2}\right)^{3} \left(\frac{15}{2}\right)^{3} \left(\frac{13}{2}\right)^{4} \left(\frac{11}{2}\right)^{4}$ $\left(\frac{9}{2}\right)^{4} \left(\frac{7}{2}\right)^{4} \left(\frac{5}{2}\right)^{3} \left(\frac{3}{2}\right)^{2} \left(\frac{1}{2}\right)$
	[11111111] = [1]	$\frac{9}{2}$
10	[22222]	$25\ \ 23^{2}\ \ 22^{2}\ \ 21^{5}\ \ 20^{6}\ \ 19^{11}\ \ 18^{12}\ \ 17^{22}\ \ 16^{24}\ \ 15^{36}\ \ 14^{39}$ $13^{55}\ \ 12^{56}\ \ 11^{74}\ \ 10^{73}\ \ 9^{88}\ \ 8^{83}\ \ 7^{95}\ \ 6^{80}\ \ 5^{90}\ \ 4^{66}\ \ 3^{67}\ \ 2^{39}$ $1^{36}\ \ 0^{2}$
	[222211]	$24\ \ 23\ \ 22^{3}\ \ 21^{4}\ \ 20^{9}\ \ 19^{11}\ \ 18^{20}\ \ 17^{25}\ \ 16^{39}\ \ 15^{46}\ \ 14^{65}$ $13^{74}\ \ 12^{97}\ \ 11^{104}\ \ 10^{127}\ \ 9^{129}\ \ 8^{148}\ \ 7^{139}\ \ 6^{150}\ \ 5^{129}\ \ 4^{129}$ $3^{94}\ \ 2^{84}\ \ 1^{40}\ \ 0^{24}$
	[2221111]	$21\ \ 20\ \ 19^{3}\ \ 18^{5}\ \ 17^{8}\ \ 16^{11}\ \ 15^{18}\ \ 14^{22}\ \ 13^{31}\ \ 12^{38}\ \ 11^{47}$ $10^{53}\ \ 9^{63}\ \ 8^{64}\ \ 7^{71}\ \ 6^{69}\ \ 5^{68}\ \ 4^{59}\ \ 3^{54}\ \ 2^{36}\ \ 1^{26}\ \ 0^{7}$
	[22111111]	$16\ \ 15\ \ 14^{3}\ \ 13^{3}\ \ 12^{6}\ \ 11^{6}\ \ 10^{10}\ \ 9^{9}\ \ 8^{14}\ \ 7^{12}\ \ 6^{16}\ \ 5^{12}$ $4^{15}\ \ 3^{9}\ \ 2^{11}\ \ 1^{3}\ \ 0^{4}$
	[211111111]	9 8 7 6 5 4 3 2 1
	[1111111111] = [0]	0

partition technique with the results

$$(111111111) = -(11100) \tag{3}$$

and

$$(1111111111) = -(11000). \tag{4}$$

An interpretation of the non-standard partition (211111111) by the same technique did not appear forthcoming, but it was found possible to

Table 3

The dimensions of the irreducible representations of Sp (10)

s	(σ)	$N(\sigma)$
0	(00000)	1
1	(10000)	10
2	(20000)	55
	(11000)	44
3	(21000)	320
	(11100)	110
4	(22000)	780
	(21100)	891
	(11110)	165
5	(22100)	2860
	(21110)	1408
	(11111)	132
6	(22200)	4004
	(22110)	5005
	(21111)	1155
7	(22210)	9152
	(22111)	4290
8	(22220)	7865
	(22211)	8580
9	(22221)	9438
10	(22222)	4719

infer the interpretation of this partition from the following argument based on dimensionality.

The (σ) structure of [211111111] is

$$\begin{aligned}[211111111] &= (211111111) + (2111111) + (1111111) \\ &+ (21111) + (111111) + (21100) + (11110) \\ &+ (20000) + (11000). \end{aligned} \tag{5}$$

If we temporarily assume (we shall argue this result later) that FLOWERS' Rule can be applied with $j = \frac{9}{2}$, i.e., $\nu = 5$, we obtain

$$\begin{aligned}(2111111) &= -(21111), \\ (11111111) &= -(11110),\end{aligned}$$

Table 4

The reduction of the representations of SU (10) to representations of Sp (10)

k	$[\lambda]$	(σ)-structure
0	[0]	(00000)
1	[1]	(10000)
2	[2]	(20000)
	[11]	(00000) (11000)
3	[21]	(10000) (21000)
	[111]	(10000) (111000)
4	[22]	(00000) (11000) (22000)
	[211]	(20000) (11000) (21100)
	[1111]	(00000) (11000) (11110)
5	[221]	(10000) (21000) (11100) (22100)
	[2111]	(10000) (21000) (11100) (21110)
	[11111]	(10000) (11100) (11111)
6	[222]	(20000) (21100) (22200)
	[2211]	(00000) (11000)^2 (22000) (21100) (11110) (22110)
	[21111]	(20000) (11000) (21100) (11110) (21111)
	[111111] = [1111]	(00000) (11000) (11110)
7	[2221]	(10000) (21000) (11100) (22100) (21110) (22210)
	[22111]	(10000) (21000) (11100)^2 (22100) (21110) (11111) (22111)
	[211111]	(10000) (21000) (11100) (21110) (11111)
	[1111111] = [111]	(10000) (11100)
8	[2222]	(00000) (11000) (22000) (11110) (22110) (22220)
	[22211]	(20000) (11000) (21100)^2 (11110) (22200) (22110) (21111) (22211)
	[221111]	(00000) (11000)^2 (22000) (21100) (11110)^2 (22110) (21111)
	[2111111]	(20000) (11000) (21100) (11110)
	[11111111] = [11]	(00000) (11000)
9	[22221]	(10000) (21000) (11100) (22100) (21110) (11111) (22210) (22111) (22221)
	[222111]	(10000) (21000) (11100)^2 (22100) (21110)^2 (11111) (22210) (22111)
	[2211111]	(10000) (21000) (11100)^2 (22100) (21110) (11111)
	[21111111]	(10000) (21000) (11100)
	[111111111] = [1]	(10000)
10	[22222]	(20000) (21100) (22200) (21111) (22211) (22222)
	[222211]	(00000) (11000)^2 (22000) (21100) (11110)^2 (22110)^2 (21111) (22220) (22211)
	[2221111]	(20000) (11000) (21100)^2 (11110)^2 (22000) (22110) (21111)
	[22111111]	(00000) (11000)^2 (22000) (21100) (11110)
	[211111111]	(20000) (11000)
	[1111111111[= [0]	(00000)

Table 5

The reduction of representations of Sp (10) to representations of *R* (3)

k	(σ)	J-structure
0	(00000)	0
1	(10000)	$\frac{9}{2}$
2	(20000)	$9\ 7\ 5\ 3\ 1$
	(11000)	$8\ 6\ 4\ 2$
3	(21000)	$\frac{25}{2}\ \frac{23}{2}\ \frac{21}{2}\ \left(\frac{19}{2}\right)^2 \left(\frac{17}{2}\right)^2 \left(\frac{15}{2}\right)^2 \left(\frac{13}{2}\right)^3 \left(\frac{11}{2}\right)^3 \left(\frac{9}{2}\right)^2 \left(\frac{7}{2}\right)^3 \left(\frac{5}{2}\right)^2 \frac{3}{2}\ \frac{1}{2}$
	(11100)	$\frac{21}{2}\ \frac{17}{2}\ \frac{15}{2}\ \frac{13}{2}\ \frac{11}{2}\ \frac{9}{2}\ \frac{7}{2}\ \frac{5}{2}\ \frac{3}{2}$
4	(22000)	$16\ 14^2\ 13\ 12^3\ 11^2\ 10^5\ 9^3\ 8^6\ 7^4\ 6^6\ 5^4\ 4^6\ 3^2\ 2^5\ 0^2$
	(21100)	$15\ 14\ 13^2\ 12^2\ 11^4\ 10^4\ 9^5\ 8^5\ 7^7\ 6^6\ 5^7\ 4^5\ 3^6\ 2^3\ 1^3$
	(11110)	$12\ 11\ 10\ 9\ 8\ 7\ 6^2\ 5\ 4^2\ 3\ 2\ 0$
5	(22100)	$\frac{37}{2}\ \frac{35}{2}\ \left(\frac{33}{2}\right)^2 \left(\frac{31}{2}\right)^3 \left(\frac{29}{2}\right)^5 \left(\frac{27}{2}\right)^6 \left(\frac{25}{2}\right)^8 \left(\frac{23}{2}\right)^{10} \left(\frac{21}{2}\right)^{12} \left(\frac{19}{2}\right)^{14} \left(\frac{17}{2}\right)^{15} \left(\frac{15}{2}\right)^{16} \left(\frac{13}{2}\right)^{17} \left(\frac{11}{2}\right)^{16} \left(\frac{9}{2}\right)^{15} \left(\frac{7}{2}\right)^{13} \left(\frac{5}{2}\right)^{11} \left(\frac{3}{2}\right)^7 \left(\frac{1}{2}\right)^4$
	(21110)	$\frac{33}{2}\ \frac{31}{2}\ \left(\frac{29}{2}\right)^2 \left(\frac{27}{2}\right)^3 \left(\frac{25}{2}\right)^3 \left(\frac{23}{2}\right)^5 \left(\frac{21}{2}\right)^6 \left(\frac{19}{2}\right)^7 \left(\frac{17}{2}\right)^8 \left(\frac{15}{2}\right)^9 \left(\frac{13}{2}\right)^9 \left(\frac{11}{2}\right)^9 \left(\frac{9}{2}\right)^9 \left(\frac{7}{2}\right)^7 \left(\frac{5}{2}\right)^6 \left(\frac{3}{2}\right)^5 \left(\frac{1}{2}\right)^2$
	(11111)	$\frac{25}{2}\ \frac{19}{2}\ \frac{17}{2}\ \frac{15}{2}\ \frac{13}{2}\ \frac{11}{2}\ \frac{9}{2}\ \frac{7}{2}\ \frac{5}{2}\ \frac{1}{2}$
6	(22200)	$21\ 19^2\ 18^2\ 17^4\ 16^4\ 15^8\ 14^7\ 13^{12}\ 12^{12}\ 11^{16}\ 10^{15}\ 9^{21}\ 8^{17}\ 7^{22}\ 6^{18}\ 5^{20}\ 4^{14}\ 3^{17}\ 2^7\ 1^9$
	(22110)	$20\ 19\ 18^3\ 17^3\ 16^6\ 15^7\ 14^{11}\ 13^{12}\ 12^{17}\ 11^{18}\ 10^{23}\ 9^{23}\ 8^{27}\ 7^{25}\ 6^{28}\ 5^{23}\ 4^{24}\ 3^{17}\ 2^{16}\ 1^7\ 0^5$
	(21111)	$17\ 16\ 15\ 14^2\ 13^3\ 12^3\ 11^5\ 10^5\ 9^6\ 8^7\ 7^7\ 6^6\ 5^8\ 4^6\ 3^5\ 2^4\ 1^3$
7	(22210)	$\frac{45}{2}\ \frac{43}{2}\ \left(\frac{41}{2}\right)^2 \left(\frac{39}{2}\right)^4 \left(\frac{37}{2}\right)^5 \left(\frac{35}{2}\right)^8 \left(\frac{33}{2}\right)^{11} \left(\frac{31}{2}\right)^{14} \left(\frac{29}{2}\right)^{18} \left(\frac{27}{2}\right)^{23} \left(\frac{25}{2}\right)^{27} \left(\frac{23}{2}\right)^{31} \left(\frac{21}{2}\right)^{26} \left(\frac{19}{2}\right)^{38} \left(\frac{17}{2}\right)^{41} \left(\frac{15}{2}\right)^{43} \left(\frac{13}{2}\right)^{41} \left(\frac{11}{2}\right)^{40} \left(\frac{9}{2}\right)^{37} \left(\frac{7}{2}\right)^{31} \left(\frac{5}{2}\right)^{25} \left(\frac{3}{2}\right)^{18} \left(\frac{1}{2}\right)^8$

Table 5 (continued)

k	(σ)	J-structure
	(22111)	$\frac{41}{2}\ \frac{39}{2}\ \left(\frac{37}{2}\right)^2 \left(\frac{35}{2}\right)^3 \left(\frac{33}{2}\right)^4 \left(\frac{31}{2}\right)^6 \left(\frac{29}{2}\right)^8 \left(\frac{27}{2}\right)^{10} \left(\frac{25}{2}\right)^{13} \left(\frac{23}{2}\right)^{15} \left(\frac{21}{2}\right)^{17} \left(\frac{19}{2}\right)^{19} \left(\frac{17}{2}\right)^{21} \left(\frac{15}{2}\right)^{21} \left(\frac{13}{2}\right)^{22} \left(\frac{11}{2}\right)^{21} \left(\frac{9}{2}\right)^{19} \left(\frac{7}{2}\right)^{17} \left(\frac{5}{2}\right)^{13} \left(\frac{3}{2}\right)^9 \left(\frac{1}{2}\right)^5$
8	(22220)	$24\ 22^2\ 21^2\ 20^4\ 19^4\ 18^8\ 17^8\ 16^{13}\ 15^{14}\ 14^{19}\ 13^{20}\ 12^{27}\ 11^{25}\ 10^{32}\ 9^{30}\ 8^{35}\ 7^{30}\ 6^{35}\ 5^{26}\ 4^{29}\ 3^{19}\ 2^{18}\ 1^7\ 0^7$
	(22211)	$23\ 22\ 21^2\ 20^3\ 19^5\ 18^6\ 17^{10}\ 16^{12}\ 15^{16}\ 14^{19}\ 13^{24}\ 12^{26}\ 11^{32}\ 10^{33}\ 9^{37}\ 8^{37}\ 7^{39}\ 6^{35}\ 5^{36}\ 4^{29}\ 3^{26}\ 2^{18}\ 1^{13}\ 0^2$
9	(22221)	$\frac{49}{2}\ \frac{47}{2}\ \frac{45}{2}\ \left(\frac{43}{2}\right)^3 \left(\frac{41}{2}\right)^4 \left(\frac{39}{2}\right)^5 \left(\frac{37}{2}\right)^8 \left(\frac{35}{2}\right)^{10} \left(\frac{33}{2}\right)^{13} \left(\frac{31}{2}\right)^{17} \left(\frac{29}{2}\right)^{20} \left(\frac{27}{2}\right)^{23} \left(\frac{25}{2}\right)^{28} \left(\frac{23}{2}\right)^{31} \left(\frac{21}{2}\right)^{33} \left(\frac{19}{2}\right)^{37} \left(\frac{17}{2}\right)^{38} \left(\frac{15}{2}\right)^{37} \left(\frac{13}{2}\right)^{38} \left(\frac{11}{2}\right)^{35} \left(\frac{9}{2}\right)^{31} \left(\frac{7}{2}\right)^{28} \left(\frac{5}{2}\right)^{21} \left(\frac{3}{2}\right)^{14} \left(\frac{1}{2}\right)^9$
10	(22222)	$25\ 23\ 22\ 21^2\ 20^3\ 19^4\ 18^4\ 17^7\ 16^7\ 15^{10}\ 14^{10}\ 13^{13}\ 12^{13}\ 11^{17}\ 10^{16}\ 9^{18}\ 8^{17}\ 7^{19}\ 6^{15}\ 5^{18}\ 4^{12}\ 3^{12}\ 2^7\ 1^7$

and

$$(111111) \quad = 0.$$

Upon substituting the above three results into eq. (5) there remains

$$[211111111] = (211111111) + (21100) + (20000) + (11000). \tag{6}$$

The dimension [see eq. (11)] of the partition [211111111] is 99, while the dimensions [see eq. (13)] of the standard partitions (σ) occurring in eq. (6), i.e., of the latter three partitions, are 891, 55, and 44, respectively.

From these values, it can be seen that the required dimension equality of the two sides of eq. (6) will be obtained only if the contribution of (211111111) cancels that of (21100), i.e., if

$$(211111111) = -(21100). \tag{7}$$

The above dimensionality considerations suggest the possibility of assigning negative dimensionality to certain non-standard partitions, e.g., it is inferred above that a dimension of -891 could be assigned to the non-standard partition (211111111). We support this consideration later.

Table 6

The classification of the states of the nucleon configuration j^k

k	$[\lambda]$	T	(σ)	(s, t)
0	[0]	0	(00000)	(0,0)
1	[1]	$\frac{1}{2}$	(10000)	$\left(1, \frac{1}{2}\right)$
2	[2]	0	(20000)	(2,0)
	[11]	1	(00000)	(0,0)
			(11000)	(2,1)
3	[21]	$\frac{1}{2}$	(21000)	$\left(3, \frac{1}{2}\right)$
			(10000)	$\left(1, \frac{1}{2}\right)$
	[111]	$\frac{3}{2}$	(11100)	$\left(3, \frac{3}{2}\right)$
			(10000)	$\left(1, \frac{1}{2}\right)$
4	[22]	0	(00000)	(0,0)
			(11000)	(2,1)
			(22000)	(4,0)
	[211]	1	(20000)	(2,0)
			(11000)	(2,1)
			(21100)	(4,1)
	[1111]	2	(00000)	(0,0)
			(11000)	(2,1)
			(11110)	(4,2)
5	[221]	$\frac{1}{2}$	(10000)	$\left(1, \frac{1}{2}\right)$
			(21000)	$\left(3, \frac{1}{2}\right)$
			(11100)	$\left(3, \frac{3}{2}\right)$
			(22100)	$\left(5, \frac{1}{2}\right)$
	[2111]	$\frac{3}{2}$	(10000)	$\left(1, \frac{1}{2}\right)$
			(21000)	$\left(3, \frac{1}{2}\right)$
			(11100)	$\left(3, \frac{3}{2}\right)$
			(21110)	$\left(5, \frac{3}{2}\right)$

Table 6 (continued)

k	$[\lambda]$	T	(σ)	(s, t)
	[11111]	$\frac{5}{2}$	(10000)	$\left(1, \frac{1}{2}\right)$
			(11100)	$\left(3, \frac{3}{2}\right)$
			(11111)	$\left(5, \frac{5}{2}\right)$
6	[222]	0	(20000)	(2,0)
			(21100)	(4,1)
			(22200)	(6,0)
	[2211]	1	(00000)	(0,0)
			$(11000)^2$	$(2,1)^2$
			(22000)	(4,0)
			(21100)	(4,1)
			(11110)	(4,2)
			(22110)	(6,1)
	[21111]	2	(20000)	(2,0)
			(11000)	(2,1)
			(21100)	(4,1)
			(11110)	(4,2)
			(21111)	(6,2)
	[111111] = [1111]	3	(00000)	(0,0)
			(11000)	(2,1)
			(11110)	(4,2)
7	[2221]	$\frac{1}{2}$	(10000)	$\left(1, \frac{1}{2}\right)$
			(21000)	$\left(3, \frac{1}{2}\right)$
			(11100)	$\left(3, \frac{3}{2}\right)$
			(22100)	$\left(5, \frac{1}{2}\right)$
			(21110)	$\left(5, \frac{3}{2}\right)$
			(22210)	$\left(7, \frac{1}{2}\right)$
	[22111]	$\frac{3}{2}$	(10000)	$\left(1, \frac{1}{2}\right)$
			(21000)	$\left(3, \frac{1}{2}\right)$
			$(11100)^2$	$\left(3, \frac{3}{2}\right)^2$

Table 6 (continued)

k	$[\lambda]$	T	(σ)	(s, t)
			(22100)	$\left(5, \frac{1}{2}\right)$
			(21110)	$\left(5, \frac{3}{2}\right)$
			(11111)	$\left(5, \frac{5}{2}\right)$
			(22111)	$\left(7, \frac{3}{2}\right)$
	[211111]	$\frac{5}{2}$	(10000)	$\left(1, \frac{1}{2}\right)$
			(21000)	$\left(3, \frac{1}{2}\right)$
			(11100)	$\left(3, \frac{3}{2}\right)$
			(21110)	$\left(5, \frac{3}{2}\right)$
			(11111)	$\left(5, \frac{5}{2}\right)$
	[1111111] = [111]	$\frac{7}{2}$	(10000)	$\left(1, \frac{1}{2}\right)$
			(11100)	$\left(3, \frac{3}{2}\right)$
8	[2222]	0	(00000)	(0,0)
			(11000)	(2,1)
			(22000)	(4,0)
			(11110)	(4,2)
			(22110)	(6,1)
			(22220)	(8,0)
	[22211]	1	(20000)	(2,0)
			(11000)	(2,1)
			$(21100)^2$	$(4,1)^2$
			(11110)	(4,2)
			(22200)	(6,0)
			(22110)	(6,1)
			(21111)	(6,2)
			(22211)	(8,1)
	[221111]	2	(00000)	(0,0)
			$(11000)^2$	$(2,1)^2$
			(22000)	(4,0)
			(21100)	(4,1)
			$(11110)^2$	$(4,2)^2$

Table 6 (continued)

k	$[\lambda]$	T	(σ)	(s, t)
			(22110)	(6,1)
			(21111)	(6,2)
	[2111111]	3	(20000)	(2,0)
			(11000)	(2,1)
			(21100)	(4,1)
			(11110)	(4,2)
	[11111111]	4	(00000)	(0,0)
			(11000)	(2,1)
9	[22221]	$\frac{1}{2}$	(10000)	$\left(1, \frac{1}{2}\right)$
			(21000)	$\left(3, \frac{1}{2}\right)$
			(11100)	$\left(3, \frac{3}{2}\right)$
			(22100)	$\left(5, \frac{1}{2}\right)$
			(21110)	$\left(5, \frac{3}{2}\right)$
			(11111)	$\left(5, \frac{5}{2}\right)$
			(22210)	$\left(7, \frac{1}{2}\right)$
			(22111)	$\left(7, \frac{3}{2}\right)$
			(22221)	$\left(9, \frac{1}{2}\right)$
	[222111]	$\frac{3}{2}$	(10000)	$\left(1, \frac{1}{2}\right)$
			(21000)	$\left(3, \frac{1}{2}\right)$
			$(11100)^2$	$\left(3, \frac{3}{2}\right)^2$
			(22100)	$\left(5, \frac{1}{2}\right)$
			$(21110)^2$	$\left(5, \frac{3}{2}\right)^2$
			(11111)	$\left(5, \frac{5}{2}\right)$
			(22210)	$\left(7, \frac{1}{2}\right)$

Table 6 (continued)

k	$[\lambda]$	T	(σ)	(s, t)
			(22111)	$\left(7, \frac{3}{2}\right)$
	[2211111]	$\frac{5}{2}$	(10000)	$\left(1, \frac{1}{2}\right)$
			(21000)	$\left(3, \frac{1}{2}\right)$
			$(11100)^2$	$\left(3, \frac{3}{2}\right)^2$
			(22100)	$\left(5, \frac{1}{2}\right)$
			(21110)	$\left(5, \frac{3}{2}\right)$
			(11111)	$\left(5, \frac{5}{2}\right)$
	[21111111]	$\frac{7}{2}$	(10000)	$\left(1, \frac{1}{2}\right)$
			(21000)	$\left(3, \frac{1}{2}\right)$
			(11100)	$\left(3, \frac{3}{2}\right)$
	[111111111]	$\frac{9}{2}$	(10000)	$\left(1, \frac{1}{2}\right)$
10	[22222]	0	(20000)	(2,0)
			(21100)	(4,1)
			(22200)	(6,0)
			(21111)	(6,2)
			(22211)	(8,1)
			(22222)	(10,0)
	[222211]	1	(00000)	(0,0)
			$(11000)^2$	$(2,1)^2$
			(22000)	(4,0)
			(21100)	(4,1)
			$(11110)^2$	$(4,2)^2$
			$(22110)^2$	$(6,1)^2$
			(21111)	(6,2)
			(22220)	(8,0)
			(22211)	(8,1)
	[2221111]	2	(20000)	(2,0)
			(11000)	(2,1)
			$(21100)^2$	$(4,1)^2$
			$(11110)^2$	$(4,2)^2$

Table 6 (continued)

k	$[\lambda]$	T	(σ)	(s, t)
			(22200)	(6,0)
			(22110)	(6,1)
			(21111)	(6,2)
	[22111111]	3	(00000)	(0,0)
			$(11000)^2$	$(2,1)^2$
			(22000)	(4,0)
			(21100)	(4,1)
			(11110)	(4,2)
	[211111111]	4	(20000)	(2,0)
			(11000)	(2,1)
	[1111111111]	5	(00000)	(0,0)

* The length of Table 6 is minimized by not repeating the *J*-structure, which is already given in Table 5 for each partition (σ).

3.2 *General expression for the interpretation of occurring non-standard* (σ) *for arbitrary j*

The non-standard (σ) partition interpretation eqs. (1), (2), (3), (4) and (7) can all be summarized by a single general expression. To see this, note that eqs. (3) and (7) are of the form

$$(\sigma_1 \ldots \sigma_{\nu-2} \quad 111111) = -(\sigma_1 \ldots \sigma_{\nu-2} \quad 00) \tag{8}$$

and eq. (4) is of the form

$$(\sigma_1 \ldots \sigma_{\nu-3}\, 11111111) = -(\sigma_1 \ldots \sigma_{\nu-3}\, 000). \tag{9}$$

Eqs. (1), (2), (8) and (9) suggest the following general expression for the interpretation of non-standard partitions (σ)

$$\begin{aligned}(\sigma_1 \ldots \sigma_{\nu-n+1}\ 111 \ldots 1_{\nu+n+1}) &= \\ = -(\sigma_1 \ldots \sigma_{\nu-n+1}\ 000 \ldots 0_\nu),\end{aligned} \tag{10}$$

for $n = 1, 2, 3, \ldots \nu - 1$. The upper limit on n results from the fact that the number of rows $\nu + n + 1$ in occurring (σ) partitions can not exceed the number of rows in the [λ] partition from which they were obtained. Since the maximum number of rows in occurring [λ] partitions is $2j + 1 = 2\nu$ we conclude that $n \leq \nu - 1$.

Verification of eq. (10) is given in section 3.4.

3.3 *Alternative formulae for the dimensionalities* $N[\lambda]$ *and* $N(\sigma)$

The dimensionality $N[\lambda]$ of a given partition $[\lambda]$ may be calculated from the formula [1]

$$N[\lambda] = \Pi^{2j+1}_{k>i=1}\left(\frac{\lambda_i - \lambda_k + k - i}{k - i}\right). \tag{11}$$

Alternatively, it can be shown that $N[\lambda]$ can be expressed in terms of k_1 and k_2, the lengths of the first and second columns, respectively, of the given $[\lambda]$ as

$$N[\lambda] = \frac{(k_1 - k_2 + 1)(2j + 1)!\,(2j + 2)!}{(k_2)!\,(k_1 + 1)!\,(2j - k_2 + 2)!\,(2j - k_1 + 1)!}\,. \tag{12}$$

For a given partition (σ), the dimensionality $N(\sigma)$ may be obtained from the expression [1]

$$N(\sigma) = \Pi^{\nu}_{i=1}\left(\frac{\sigma_i + \nu - i + 1}{\nu - i + 1}\right),$$

$$\Pi^{\nu}_{k>i=1}\frac{(\sigma_i - \sigma_k + k - i)(\sigma_i + \sigma_k + 2\nu + 2 - i - k)}{(k - i)(2\nu + 2 - i - k)} \tag{13}$$

Or, defining s_1 and s_2 respectively as the lengths of the first and second columns of the given partition (σ), it can be verified that the dimensionality $N(\sigma)$ can be written as

$$N(\sigma) = \frac{(2\nu + 1)!\,(2\nu + 3)!\,(s_1 - s_2 + 1)(2\nu - 2s_2 + 4)(2\nu - s_2 - s_1 + 3)(2\nu - 2s_1 + 2)}{(s_2)!\,(s_1 + 1)!\,(2\nu - s_2 + 4)!\,(2\nu - s_1 + 3)!} \tag{14}$$

Considerable effort is saved in obtaining the various dimensions by use of eqs. (12) and (14).

Substitution of the two equations

$$k_1 = \frac{1}{2}k + T \quad\text{and}\quad k_2 = \frac{1}{2}k - T$$

into eq. (12) would yield an expression for the dimensionality $N[\lambda]$ of a given partition $[\lambda]$ in terms of the number of nucleons k and the total isospin T of the corresponding nucleon configuration.

Similarly substitution of the two equations

$$s_1 = \frac{1}{2}s + t \quad\text{and}\quad s_2 = \frac{1}{2}s - t$$

into eq. (14) would yield an expression for the dimensionality in terms of the seniority s and the reduced isospin t.

It should be noted that eqs. (12) and (14) apply only to partitions $[\lambda]$ and (σ) having two or fewer columns. They are, however, completely general for systems of equivalent particles in jj-coupling.

3.4 *The interpretation of non-standard partitions (σ) on the basis of dimensionality*

Eq. (14) provides for the interpretation of the various non-standard partitions (σ) through the comparison of the dimensions obtained for non-standard (σ) with those for standard (σ). It is worth noting that such a comparison is not possible through the use of the more usual dimensionality expression, eq. (13), since it is limited in application to only standard partitions.

Consider, for example, the application of eq. (14) to the two partitions occurring in eq. (7). Using either of eqs. (13) or (14) the standard partition (21100) is found to have dimension 891. Application of eq. (14) to the non-standard partition (211111111), which has $s_1 = 9$ and $s_2 = 1$, yields dimension -891, and thereby verifies eq. (7).

Dimensionality verification of eq. (10), the general occurring non-standard (σ), may also be obtained by means of eq. (14). For the partition $(\sigma_1 \ldots \sigma_{\nu-n+1}\, 111 \ldots 1_{\nu+n+1})$, $s_1 = \nu + n + 1$ and $s_2 \leq \nu - n + 1$ whereas for the partition $(\sigma_1 \ldots \sigma_{\nu-n+1}\, 000 \ldots 0_\nu)$, $s_1' = \nu - n + 1$ and $s_2' = s_2$. Substitution of the sets of values, $s_1\, s_2$ and $s_1'\, s_2'$, into equation (14) reveals that the dimensionalities of the two partitions differ only in sign and thereby verifies eq. (10).

3.5 *General rules for the interpretation of non-standard partitions (σ)*

In this section two general expressions, deduced from eq. (14), are given for relating various partitions (σ). These general expressions are then specialized to non-standard (σ), resulting in a set of rules for the interpretation of non-standard partitions (σ).

The results are most conveniently stated in terms of the dual or adjoint $(\widetilde{\sigma})$, instead of the partition (σ) itself. We write the adjoint $(\widetilde{\sigma})$ in the form (s_1, s_2), where s_1 and s_2 represent the lengths of the first and second columns, respectively, of the partition (σ).

Using eq. (14), one may easily verify the following two general expressions

$$(s_1, s_2) = -(2\nu + 2 - s_1, s_2), \tag{E1}$$

$$(s_1, s_2) = (s_2 - 1, 2\nu + 3 - s_1). \tag{E2}$$

We can derive other useful expressions by successive applications of eqs. (E1) and (E2). Eq. (E2) followed by eq. (E1) yields

$$(s_1, s_2) = -(2\nu + 3 - s_2, 2\nu + 3 - s_1). \tag{E3}$$

Then eq. (E3) followed by eq. (E2) gives

$$(s_1, s_2) = -(s_1, 2\nu + 4 - s_2). \tag{E4}$$

These expressions are completely general, but it is our purpose to use these expressions to interpret non-standard (σ) partitions, i.e., (σ) partitions with more than ν rows, but first column at least as long as second, either as standard (σ) or as partitions of null dimensionality. We shall refer to the general expressions, when restricted to this application, as the general rules for the interpretation of non-standard (σ).

By way of illustration, consider expression (E1). It will relate a non-standard (σ) to a standard (σ) only if all of the following conditions are satisfied:

$$s_1 > \nu, \quad 2\nu + 2 - s_1 \leq \nu, \quad s_2 \leq s_1, \quad s_2 \leq 2\nu + 2 - s_1 .$$

Clearly these will be satisfied if $s_1 \geqslant \nu + 2$ with $s_2 \leq 2\nu + 2 - s_1$. Thus we have our first rule:

$$(s_1, s_2) = -(2\nu + 2 - s_1, s_2) \quad \text{with} \quad \left\{ \begin{array}{l} s_1 \geqslant \nu + 2, \\ s_2 \leq 2\nu + 2 - s_1 . \end{array} \right. \tag{R1}$$

Restricting expressions (E2) and (E3) in a similar manner we obtain, respectively,

$$(s_1, s_2) = (s_2 - 1, 2\nu + 3 - s_1) \quad \text{with} \quad \left\{ \begin{array}{l} s_1 \geqslant \nu + 3, \\ 2\nu + 4 - s_1 \leq s_2 \leq \nu + 1, \end{array} \right. \tag{R2}$$

$$(s_1, s_2) = -(2\nu + 3 - s_2,\ 2\nu + 3 - s_1) \quad \text{with} \quad s_1 \geq s_2 \geq \nu + 3. \tag{R3}$$

It should be pointed out that the interpretation expression, eq. (10), is eq. (R1), more precisely its adjoint, with $s_1 = \nu + n + 1$.

We can also deduce three cases in which non-standard (σ) are null. To see this consider the following three special cases:

If $s_1 = \nu + 1$ expression (E1) becomes $(\nu + 1,\ s_2) = -(\nu + 1,\ s_2)$.
If $s_2 = 2\nu + 3 - s_1$ expression (E3) becomes $(s_1,\ 2\nu + 3 - s_1) = -(s_1,\ 2\nu + 3 - s_1)$.
If $s_2 = \nu + 2$ expression (E4) becomes $(s_1,\ \nu + 2) = -(s_1,\ \nu + 2)$.

The fact that in each of these special cases a partition is equal to its own negative lets us formulate three additional rules

$$N(\sigma) = 0, \quad \text{when} \quad s_1 = \nu + 1; \tag{R1$'$}$$

$$N(\sigma) = 0, \quad \text{when} \quad s_1 + s_2 = 2\nu + 3; \tag{R3$'$}$$

$$N(\sigma) = 0, \quad \text{when} \quad s_2 = \nu + 2; \tag{R4$'$}$$

The rule numbers refer to the expressions from which the rules were obtained. The primes denote special cases of the corresponding expressions. Notice that the last three rules could, alternatively, have easily been deduced by considering, individually, the factors in the numerator of the $N(\sigma)$ expression, eq. (14).

The non-standard (σ) partitions, their standard partition interpretations, and the pertinent interpretation rules are summarized, for the present case ($j = \frac{9}{2}$ or $\nu = 5$) in Table 7.

Table 7

The non-standard partitions (σ) for the case $j = \frac{9}{2}$

s_1	s_2	(σ)	$N(\sigma)$	Interpretation	Rule
6	0	(111111)	0	X	1′
	1	(211111)	0	X	1′
	2	(221111)	0	X	1′
	3	(222111)	0	X	1′
	4	(222211)	0	X	1′
	5	(222221)	0	X	1′
	6	(222222)	0	X	1′
7	0	(1111111)	− 132	−(11111)	1
	1	(2111111)	−1155	−(21111)	1
	2	(2211111)	−4290	−(22111)	1
	3	(2221111)	−8580	−(22211)	1
	4	(2222111)	−9438	−(22221)	1
	5	(2222211)	−4719	−(22222)	1
	6	(2222221)	0	X	3′
	7	(2222222)	0	X	4′
8	0	(11111111)	− 165	−(11110)	1
	1	(21111111)	−1408	−(21110)	1
	2	(22111111)	−5005	−(22110)	1
	3	(22211111)	−9152	−(22210)	1

Table 7 (continued)

s_1	s_2	(σ)	$N(\sigma)$	Interpretation	Rule
	4	(22221111)	−7865	−(22220)	1
	5	(22222111)	0	X	3′
	6	(22222211)	4719	(22222)	2
	7	(22222221)	0	X	4′
	8	(22222222)	−4719	−(22222)	3
9	0	(111111111)	− 110	−(11100)	1
	1	(211111111)	− 891	−(21100)	1
	2	(221111111)	−2860	−(22100)	1
	3	(222111111)	−4004	−(22200)	1
	4	(222211111)	0	X	3′
	5	(222221111)	7865	(22220)	2
	6	(222222111)	9438	(22221)	2
	7	(222222211)	0	X	4′
	8	(222222221)	−9438	−(22221)	3
	9	(222222222)	−7865	−(22220)	3
10	0	(1111111111)	− 44	−(11000)	1
	1	(2111111111)	− 320	−(21000)	1
	2	(2211111111)	− 780	−(22000)	1
	3	(2221111111)	0	X	3′
	4	(2222111111)	4004	(22200)	2
	5	(2222211111)	9152	(22210)	2
	6	(2222221111)	8580	(22211)	2
	7	(2222222111)	0	X	4′
	8	(2222222211)	−8580	−(22211)	3
	9	(2222222221)	−9152	−(22210)	3
	10	(2222222222)	−4004	−(22200)	3

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ПОЛНАЯ КЛАССИФИКАЦИЯ ЯДЕРНЫХ СОСТОЯНИЙ КОНФИГУРАЦИИ j^k ДЛЯ $j = \frac{9}{2}$

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Резюме

Производятся классификация и перечень состояний эквивалентных $j = \frac{9}{2}$ ядерных конфигураций. Для размерности важнейших разделений даются новые формулы. Для объяснения нестандартных разделений выводится несколько общих правил.

Acta Physica Academiae Scientiarum Hungaricae, Tomus (1), p. 55—105, (1966)

VARIATIONSPRINZIPIEN ZUR BESCHREIBUNG VON SYSTEMEN VIELER TEILCHEN

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(Vorgelegt von A. Kónya. — Eingegangen 18. I. 1966)

Es wird ein Überblick über die Anwendung von Variationsprinzipien zur Lösung des Vielkörperproblems gegeben. Nach einer Diskussion allgemeiner Bedingungen für die Existenz von Variationsprinzipien wird ihre Anwendung in der klassischen Gleichgewichts- und Nichtgleichgewichtsstatistik untersucht. Anschliessend werden Verfahren zur Berechnung stationärer und nichtstationärer quantenmechanischer Systeme zusammengestellt. Irreversible Phänomene werden mit dem Prinzip der extremalen Entropieproduktion beschrieben. Speziell werden damit zusammenhängende Lösungsverfahren der Boltzmanngleichung behandelt.

Inhaltsverzeichnis

1. Einleitung

Die Grundaufgabe der Physik ist die Beobachtung und Beschreibung aller Vorgänge in der Natur. Die Aufgabe der Theoretischen Physik ist es, die beobachteten Erscheinungen in abstrakter Form darzustellen, um daraus wieder experimentell zu realisierende Ereignisse herauszulesen. Die Methoden der gedanklichen Abstraktion werden aus der Mathematik entnommen. Im allgemeinen wird das Naturgeschehen durch Differentialgleichungen beschrieben. Über die Integration dieser Gleichungen können zunächst keine weiteren Aussagen gemacht werden, ausser dass bei Gültigkeit bestimmter Erhaltungssätze Teilintegrationen möglich sind. Oft erweist es sich als sinnvoll, den Differentialgleichungen äquivalente mathematische Methoden zu benutzen, die in speziellen Fällen rascher zur Lösung des Problems führen. Eine solche Methode ist die Variationsrechnung.

Der erste wesentliche Anstoss zu ihrer Entwicklung entstammt dem berühmten Streit der Gebrüder BERNOUILLI (1696). In dieser Auseinandersetzung wurde unter anderem das Problem zur Diskussion gestellt, auf welcher Kurve sich ein Stein im Schwerefeld von einem Punkt P_1 zu einem Punkt P_2 bewegen müsste, um diese Strecke in kürzester Zeit zurückzulegen (Brachystochronenproblem). Die Fallzeit T ist offensichtlich vom Bahnverlauf $s(t)$ abhängig. T ist ein Funktional von $s(t)$. Die die Aufgabe lösende Kurve $\bar{s}(t)$ ergibt sich aus der Klasse aller möglichen Bahnen (aller Variationen von $s(t)$) dadurch, dass sie T zum Minimum macht, d. h. T darf sich bei kleinen Schwankungen $\delta s = s(t) - \bar{s}(t)$ der Bahn $s(t)$ um die optimale Kurve $\bar{s}(t)$ in erster Ordnung von δs nicht ändern, in zweiter Ordnung von δs muss die Änderung von T positiv sein. Man sagt: Die erste Variation von T ist Null, die zweite Variation ist positiv

$$\delta^1 T = 0, \qquad \delta^2 T > 0 .$$

Schon kurze Zeit nach dem Bekanntwerden der BERNOUILLIschen Aufgabe äusserte LEIBNIZ den Gedanken, dass alle Naturereignisse einem Prinzip der minimalen Wirkung unterliegen. Damit wurde eine Epoche der allgemeinen Anwendung des Variationskalküls zur Beschreibung physikalischer Erscheinungen eingeleitet, die bis zum heutigen Zeitpunkt andauert. Zunächst versuchte spekulative Interpretationen, die in der Existenz von Variationsprinzipien das Walten höherer Mächte erblickten (MAUPERTUIS u. a.), mussten der Erkenntnis Platz machen, dass das Variationsprinzip nur eine äquivalente Formulierung einer dasselbe Problem beschreibenden Differentialgleichung ist.

Obwohl also ein Variationsverfahren keine prinzipiell neuen Aussagen liefert, besitzt es bei bestimmten Fragestellungen gewisse Vorteile gegenüber anderen Darstellungsweisen. So wird es häufig wegen der Übersichtlichkeit und Eleganz der Rechnungen als mathematisches Hilfsmittel für die Deduktion physikalischer Gesetzmässigkeiten benutzt. Dabei werden bekannte Tatbestände auf verkürztem Weg verifiziert und zum Teil auch neue Aussagen abgeleitet. Weiterhin können die Untersuchung von Invarianzeigenschaften der Differentialgleichungen und das Auffinden von Erhaltungssätzen als Folge dieser Invarianzeigenschaften erheblich erleichtert werden (NOETHER-Theorem [1]).

Oft ist allein die Kenntnis der Existenz eines Variationsprinzips für bestimmte Teilaussagen hinreichend. Z. B. lassen sich damit in der Elastomechanik und Optik Reziprozitätsbeziehungen zwischen den in der LAGRANGE-funktion vorkommenden Variablen herleiten, die im wesentlichen auf der Gleichheit bestimmter gemischter Ableitungen des stationären Funktionals beruhen. In der Elastomechanik geben sie differentielle Beziehungen zwischen Randbedingungen und den interessierenden Grössen an einem beliebigen Ort im Innern an, während sie in der Optik Relationen zwischen Bild und Gegenstand beinhalten.

Ein weiteres Anwendungsgebiet sind bei Variationsproblemen häufig mögliche Analogiebetrachtungen, falls zwei zunächst grundsätzlich verschiedene physikalische Phänomene durch dasselbe stationäre Funktional beschrieben werden. Bekannt ist die sogenannte »KIRCHHOFFsche Analogie« zwischen den Bewegungsgleichungen für den schweren symmetrischen Kreisel und den Gleichungen eines durch Druck und Drill beanspruchten Stabes im dreidimensionalen Raum [2]. Das Erkennen der Analogie kann einen Ansatzpunkt für Näherungsverfahren bieten.

Ein rechentechnischer Vorzug eines Variationsverfahrens ist der, dass das zu variierende Funktional ein Skalar ist. Wegen der koordinatenunabhängigen Formulierung sind ohne Schwierigkeiten Übergänge von einem Koordinatensystem zu einem anderen möglich. Diese Übergänge bieten sich besonders deshalb an, weil in dem jeweils betrachteten Funktional stets Ableitungen vorkommen, die um eine Ordnung niedriger sind als in den entsprechenden Differentialgleichungen.

Ein wesentliches Kennzeichen eines Variationsprinzips ist die Tatsache, dass durch Ausführen von Teilvariationen Näherungsausdrücke für die Bewegungsgleichungen angebbar sind. Das ist besonders bei der im folgenden zu behandelnden Beschreibung von Vielteilchensystemen von Bedeutung. Durch die Auswahl einer bestimmten Klasse von Funktionen, die zur Konkurrenz stehen sollen, werden den Lösungen des jeweiligen Problems automatisch Beschränkungen auferlegt, so dass diese nur noch näherungsweise gelten können.

Die Möglichkeit, Variationsprinzipien anzugeben, besteht nicht nur in der klassischen Mechanik. Während dort das Zeitintegral über die Differenz der kinetischen und potentiellen Energie das gesuchte Funktional ist, dessen erste Variation verschwindet [3], können in der Quantenmechanik der Energieerwartungswert [4] bzw. eine Verallgemeinerung im zeitabhängigen Fall, im thermischen Gleichgewicht die thermodynamischen Potentiale [5] und in der Theorie irreversibler Prozesse, die stationär verlaufen, die Entropieproduktion an diese Stelle treten.

Die weiteren Ausführungen werden sich damit befassen, ob prinzipiell zu jeder Differentialgleichung ein Variationsprinzip angegeben werden kann, und die dabei auftretenden Schwierigkeiten bei irreversiblen Phänomenen in Teil 2 darlegen. Es soll ein Überblick über Variationsprinzipien in der klassischen Statistik in Teil 3 und der Quantentheorie stationärer und nichtstationärer Erscheinungen in Teil 4 bzw. Teil 5 gegeben werden. Teil 6 beschäftigt sich mit der Beschreibung irreversibler Prozesse in Vielteilchensystemen durch Variationsprinzipien.

2. Bedingungen für die Existenz von Variationsprinzipien

Die Tatsache, dass zu den meisten physikalischen Problemstellungen Variationsprinzipien angebbar sind, lässt die Frage entstehen, ob das prinzipiell möglich ist. Die Selbstadjungiertheit der das entsprechende Problem beschreibenden Differentialgleichung ist eine notwendige und hinreichende Bedingung dafür (Kap. 21). Ein in Kap. 22 behandeltes Beispiel zeigt, dass diese Forderung bei irreversiblen Differentialgleichungen erst durch geeignete Manipulationen erfüllt werden kann.

21. Das Umkehrproblem der Variationsrechnung

Bei der Beschreibung physikalischer Erscheinungen ist es in den meisten Fällen so, dass zunächst die Differentialgleichungen für die interessierenden physikalischen Grössen bekannt sind. Soll eine äquivalente Darstellung mit einem Variationsprinzip gegeben werden, so muss letzteres auf irgendeinem Weg gewonnen werden. Dieses Umkehrproblem der Variationsrechnung besteht darin, zur gegebenen Differentialgleichung ein Funktional F zu konstruieren, das stationär ist, d. h. für das die erste Variation verschwindet

$$\delta^1 F = 0 . \tag{1}$$

Für den Fall, dass die entsprechende physikalische Erscheinung durch lineare Differentialgleichungen beschrieben wird, existiert dazu eine ausführliche Theorie.

Hirsch [6] und andere konnten zeigen, dass für die Lösbarkeit des Umkehrproblems folgende Tatsache eine notwendige und hinreichende Bedingung zugleich darstellt:

Die Differentialgleichung (gewöhnliche oder partielle) muss selbstadjungiert sein, falls sie die EULERsche Gleichung eines dazugehörigen Variationsprin zips ist. Eine Differentialgleichung ist selbstadjungiert, wenn für den darin vorkommenden Operator (es handelt sich hierbei stets um lineare Operatoren) nach Definition eines bestimmten Skalarproduktes gilt

$$(\Psi, A\,\Phi) = (A\,\Psi, \Phi)\,. \tag{2}$$

In dem aus der Quantentheorie bekannten HILBERTraum entspricht das der Hermitizität. Ob ein Operator selbstadjungiert ist, hängt von der Art des betrachteten Skalarproduktes und den jeweiligen Randbedingungen ab.

Das Umkehrproblem der Variationsrechnung ist ohne grössere Schwierigkeiten lösbar, wenn selbstadjungierte Differentialgleichungen vorliegen. Ist das nicht der Fall, muss die Differentialgleichung geeignet umgeformt werden. Dabei gibt es verschiedene Möglichkeiten. Einmal kann man das Skalarprodukt geeignet umdefinieren, so dass Selbstadjungiertheit erreicht wird. Weiterhin ist es möglich, durch Umformung der Differentialgleichung (zusätzliche Multiplikation mit Operatoren) dasselbe zu erreichen. Schliesslich wird man häufig versuchen, der nichtselbstadjungierten Gleichung die adjungierte zuzuordnen. Beide Gleichungen zusammen lassen sich in einem Variationsprinzip formulieren.

22. *Einfache Spezialfälle*

Als Beispiel soll der harmonische Oszillator unter Reibung betrachtet werden.

$$m(\ddot{x}_1 + \gamma\dot{x}_1 + \omega_0^2 x_1) \equiv A x_1 = 0\,. \tag{1}$$

Der in dieser Differentialgleichung auftretende Operator ist nicht selbstadjungiert, wenn man als Skalarprodukt

$$(x_2, x_1) \equiv \int dt\, x_2(t)\, x_1(t) \quad \text{mit} \quad x(+\infty) = x(-\infty) = 0 \tag{2}$$

einführt. Es gilt

$$\begin{aligned}(x_2, A x_1) &= \int dt\, x_2\, m \left(\frac{d^2}{dt^2} + \gamma\frac{d}{dt} + \omega_0^2\right) x_1 \\ &= \int dt\, x_1\, m \left(\frac{d^2}{dt^2} - \gamma\frac{d}{dt} + \omega_0^2\right) x_2 \equiv (A^T x_2, x_1) \\ &\qquad A^T \neq A\,.\end{aligned} \tag{3}$$

Die Umformung von (1) erfolgt:

a) durch Multiplikation mit einem geeigneten Faktor.

$$e^{\gamma t}\, m(\ddot{x}_1 + \gamma\dot{x}_1 + \omega_0^2 x_1) = 0\,. \tag{4}$$

Bezüglich des in (2) definierten Skalarproduktes ist der in (4) vorkommende Operator selbstadjungiert. Es kann leicht eine LAGRANGEfunktion für (4) angegeben werden:

$$L = e^{\gamma t}\left(\frac{m}{2}\dot{x}_1^2 - \frac{m}{2}\omega_0^2 x_1^2\right) \qquad \delta^1 \int dt\, L = 0\,. \tag{5}$$

Dasselbe Ergebnis wie in (5) erhält man, wenn man von der Gleichung (1) ausgeht und ein neues Skalarprodukt einführt

$$< x, y > \equiv \int dt\, e^{\gamma t} x(t)\, y(t). \tag{6}$$

Methoden zur Bestimmung des multiplikativen Faktors bei beliebigen gewöhnlichen Differentialgleichungen werden zum Beispiel bei FUNK [7] angegeben.
b) durch Einführen einer zusätzlichen Differentialgleichung (adjungierte Dgl.).

Aus (3) entnimmt man sofort, dass die zu (1) adjungierte Differentialgleichung die Gestalt

$$m(\ddot{x}_2 - \gamma \dot{x}_2 + \omega_0^2 x_2) \equiv A^T x_2 = 0 \tag{7}$$

hat. Die Gleichungen (1) und (7) lassen sich aus einem einzigen Variationsprinzip von der Form

$$L = m\left[\dot{x}_1 \dot{x}_2 + \frac{1}{2}\gamma(x_1 \dot{x}_2^0 - \dot{x}_1^0 x_2) - \omega_0^2 x_1 x_2\right] \qquad \delta^1 \int dt\, L = 0 \tag{8}$$

gewinnen. Dabei werden x_1 und x_2 unabhängig voneinander variiert.

Der unter b) angegebene Weg erscheint verallgemeinerungsfähiger. Dem dissipativen System (1) wird ein adjungiertes (7) zugeordnet. Bei diesem Vorgehen existiert eine enge Verbindung mit der Lösung von Eigenwertproblemen nichthermitischer Matrizen

$$A e_1 = \lambda e_1 \qquad A^\dagger e_2^* = \lambda^* e_2^* \qquad A^\dagger \neq A\,. \tag{9}$$

Die Eigenwertgleichungen ergeben sich, wenn man fordert, dass der Ausdruck

$$\tilde{\lambda} = \frac{e_2 A e_1}{e_2 e_1} \tag{10}$$

stationär wird.

Das Beispiel des harmonischen Oszillators unter Reibung ist zunächst nicht typisch für die im folgenden zu behandelnde Problemstellung, da im Falle des Oszillators ein echtes Einteilchenproblem vorliegt. Es wird sich aber herausstellen, dass auch bei irreversiblen Prozessen in Vielteilchensystemen, die durch nichtselbstadjungierte Differentialgleichungen beschrieben werden, analoge Methoden Anwendung finden (siehe Teil 6). Offenstehende Fragen sind noch folgende: Lässt das Hinzufügen eines adjungierten Systems eine sinnvolle physikalische Interpretation zu? Für die in diesem Kapitel betrachteten linearen Operatoren gilt mit dem Skalarprodukt (2)

$$A^T(t) = A(-t), \tag{11}$$

falls die Zeit in A nur als Differentialoperator auftaucht. Eine Lösung von

$$A^T(t)\, x_2(t) = A(-t)\, x_2(t) = 0 \tag{12}$$

erhält man sofort mit

$$x_2(t) = x_1(-t). \tag{13}$$

In diesem Fall beschreibt die Lösung des adjungierten Problems also ein gegenüber dem ursprünglichen zeitlich umgekehrt ablaufendes Ereignis. Beim Beispiel des harmonischen Oszillators wäre das ein sich aufschaukelndes System.

Von Bedeutung ist auch die Frage, ob die Tatsache, dass in (8) zwei unabhängig zu variierende Funktionen auftreten, das Verfahren unbrauchbar macht. Zunächst existieren für diese Annahme keine Anhaltspunkte. Mathematisch formal ist die Aufgabe in dieser Weise lösbar. Die Rechnung wird natürlich wegen der zwei verschiedenen Funktionen komplizierter. Echte Schwierigkeiten dürften dann auftreten, wenn für die Funktionen plausible Näherungsansätze gemacht werden sollen, was für das adjungierte System nicht möglich sein wird, falls ihm keine anschauliche Bedeutung gegeben werden kann.

3. Variationsprinzipien zur Berechnung klassischer Verteilungsfunktionen

Es soll ein Überblick über Variationsprinzipien für klassische Verteilungsfunktionen gegeben werden. Im allgemeinsten Fall kann für die zeitabhängige Verteilungsfunktion, die der LIOUVILLEgleichung genügt, ein stationäres Funktional konstruiert werden, wie in Kap. 31 gezeigt wird. Näherungsansätze führen zu reversiblen kinetischen Gleichungen vom VLASOVtyp (Kap. 32). Variationsprinzipien für Verteilungsfunktionen im thermischen Gleichgewicht lassen sich mit Hilfe der Extremaleigenschaft der thermodynamischen Potentiale angeben (Kap. 33). Der Fall, dass die zu berechnende Verteilungsfunktion einer irreversiblen kinetischen Gleichung genügt, wird später in Teil 6 behandelt.

31. *Die* LIOUVILLE*gleichung*

Die Beschreibung des Vielkörperproblems in der klassischen Statistik erfolgt durch die LIOUVILLEgleichung

$$\frac{\partial}{\partial t} f_N + [H, f_N]_P = 0 . \tag{1}$$

$f_N (\mathfrak{p}_1, \mathfrak{r}_1; \ldots \mathfrak{p}_N, \mathfrak{r}_N; t) = f_N (1, \ldots, N; t)$ ist eine Dichteverteilung im 6 N-dimensionalen Phasenraum, dem Γ-Raum. $[H, \ldots]_P$ ist die bekannte POISSONklammer. Physikalisch interessierende Messwerte $\bar{A}$ werden durch Scharmittelwerte über die Verteilung f_N berechnet

$$\bar{A} = \int d1 \ldots dN f_N (1, \ldots N, t) A(1, \ldots N, t) . \tag{2}$$

f_N erfüllt die Normierungsbedingung

$$\int d1 \ldots dN f_N (1, .. N, t) = 1 . \tag{3}$$

Mit der Angabe von f_N wäre das Problem in allgemeinster Weise gelöst. Für die Berechnung physikalischer Grössen ist aber nur die Kenntnis der reduzierten Verteilungsfunktionen

$$f_n = f_n (1, \ldots n, t) \qquad n = 1, 2 \tag{4}$$

erforderlich.

Die Aufgabe der Theorie besteht nun darin, Näherungsverfahren für die exakt nicht lösbare LIOUVILLEgleichung zu entwickeln, was bereits auf verschiedene Weise mit Erfolg durchgeführt wurde [8]. Den Versuch, Variationsprinzipien dafür nutzbar zu machen, hat GARTENHAUS [9] unternommen.

Der Grundgedanke ist der, dass gewisse Analogien zwischen der LIOUVILLEgleichung und der quantenmechanischen SCHRÖDINGERgleichung bestehen. Beide sind lineare partielle Differentialgleichungen erster Ordnung in der Zeit. Es kann deshalb vermutet werden, dass das Variationsprinzip für die LIOUVILLEgleichung eine ähnliche Gestalt wie das für die zeitabhängige SCHRÖDINGERgleichung besitzt. Definiert man ein Skalarprodukt

$$< u_N, v_N > \equiv \int dt \, d1 \ldots dN \, u_N^*(1, \ldots N, t) v_N (1, \ldots N, t) , \tag{5}$$

so ist der Operator

$$\mathscr{L} = \left\{ \frac{\partial}{\partial t} + [H]_P, \right\} \tag{6}$$

antihermitisch. $\mathscr{L}$ besitzt ein System von komplexen Eigenfunktionen u_N, die der Gleichung

$$\mathscr{L}\, u_N = \lambda\, u_N \tag{7}$$

genügen. In Analogie zum Vorgehen bei Eigenwertproblemen antisymmetrischer Matrizen [10] lässt sich (7) äquivalent in einem Variationsprinzip formulieren:

$$F \equiv \langle u_N, \mathscr{L}\, u_N \rangle - \lambda \langle u_N, u_N \rangle \qquad \delta^1 F = 0\,. \tag{8}$$

Die Eigenwerte von (7) können nur rein imaginär bzw. Null sein. Multipliziert man (7) mit u_N^* und integriert über Orte, Impulse und Zeit, erhält man dieses Ergebnis unmittelbar, wenn man die Antihermitizität von $\mathscr{L}$ ausnutzt. Deshalb kann sofort eine Lösung $\bar{u}_N$ zum Eigenwert 0 angegeben werden, die sich von u_N um einen, wie es sich herausstellen wird, belanglosen Phasenfaktor unterscheidet

$$\bar{u}_N = u_N\, \mathrm{e}^{-\lambda t}\,. \tag{9}$$

Es ist das Ziel, Lösungen zu berechnen, die (7) für $\lambda = 0$ befriedigen und ausserdem reelle und stets positive Funktionen der Variablen $1, \ldots N$ und t sind. Wegen der speziellen Form von $\mathscr{L}$ (linearer Operator, der nur Differentiationen von erster Ordnung enthält), gilt

$$\mathscr{L}\, F(\bar{u}_N) = (dF/d\bar{u}_N)\, \mathscr{L}\, u_N\,. \tag{10}$$

Neben $\bar{u}_N$ ist auch eine beliebige Funktion von $\bar{u}_N$ Eigenfunktion zu $\lambda = 0$. Wählt man speziell

$$f_N = |\,\bar{u}_N\,|^2 = |\,u_N\,|^2\,, \tag{11}$$

so erhält man die Lösung von (1). Die aus der Forderung (8) bestimmte Funktion u_N liefert damit unmittelbar die Verteilungsfunktion f_N.

Zu bemerken ist noch, dass das Funktional in (8) lediglich stationär ist; es besitzt keine Extremaleigenschaften. Aussagen über die Art des Fehlers bei Näherungsverfahren sind deshalb nicht möglich.

Um einen Beweis für die innere Konsistenz des Variationsverfahrens (8) zu geben, sollen durch einen geeigneten Variationsansatz die kanonischen Bewegungsgleichungen abgeleitet werden. Als Versuchsfunktion wird

$$u_N = \prod_{i=1}^{N} \sqrt{\delta(i - \bar{i}(t))}\; \mathrm{e}^{j\psi(1,\ldots N,t)} \qquad \text{mit } \psi^* = \psi \tag{12}$$

in (8) eingesetzt. Mit i bzw. $\bar{i}(t)$ werden die Orte und Impulse $\mathfrak{r}_i$, $\mathfrak{p}_i$ bzw. $\mathfrak{s}_i(t)$, $\mathfrak{q}_i(t)$ zusammengefasst. $\bar{i}(t)$ und $\psi\,(1, \ldots N, t)$ sind zunächst völlig beliebige Funktionen, die unabhängig voneinander variiert werden können.

Dem Ansatz (12) entspricht die Verteilungsfunktion

$$f_N = \prod_{i=1}^{N} \delta(i - \bar{i}(t)) \,. \tag{13}$$

Dieser Ausdruck entspräche der exakten Verteilung von N Teilchen, wenn $\bar{i}(t)$ die durch die kanonischen Gleichungen beschriebene Bewegung des Teilchens i darstellen würde. Mit (12) erhält man nach einfachen Umformungen für das stationäre Funktional aus (8)

$$\begin{aligned} F &= j \int dt\, d1 \ldots dN \prod_{1=i}^{N} \delta(i - \bar{i}(t))\, \mathscr{L}(1, \ldots N, t)\, \psi(1, \ldots N, t) \\ &= j \int dt\, \mathscr{L}(\bar{1}(t), \ldots \bar{N}(t), t)\, \psi(\bar{1}(t), \ldots \bar{N}(t), t) \\ &= j \int dt \left\{ \frac{\partial \psi}{\partial t} + \sum_i \left(\frac{\partial H}{\partial \mathfrak{q}_i} \frac{\partial \psi}{\partial \mathfrak{s}_i} - \frac{\partial H}{\partial \mathfrak{s}_i} \frac{\partial \psi}{\partial \mathfrak{q}_i} \right) \right\}, \\ F &= j \int dt \left\{ \frac{d\psi}{dt} + \sum_i \left(\frac{\partial \psi}{\partial \mathfrak{s}_i} \left[\frac{\partial H}{\partial \mathfrak{q}_i} - \dot{\mathfrak{s}}_i \right] + \frac{\partial \psi}{\partial \mathfrak{q}_i} \left[- \frac{\partial H}{\partial \mathfrak{s}_i} - \dot{\mathfrak{q}}_i \right] \right) \right\}. \end{aligned} \tag{14}$$

Werden ψ und $\bar{i}(t)$ nun unabhängig voneinander variiert, entstehen sofort die kanonischen Bewegungsgleichungen

$$\dot{\mathfrak{s}}_i = \frac{\partial H}{\partial \mathfrak{q}_i} \qquad \dot{\mathfrak{q}}_i = - \frac{\partial H}{\partial \mathfrak{s}_i} . \tag{15}$$

Wie bereits oben fällt auch hier die Phase als unwesentlich aus der Rechnung heraus.

32. Kinetische Gleichungen

Das in (31.8) formulierte Variationsprinzip für die LIOUVILLEgleichung gestattet es, durch Teilvariation Näherungsgleichungen für die Verteilungsfunktion abzuleiten.

Zunächst soll der Ansatz

$$u_N = \prod_{i=1}^{N} v_i(i, t) \qquad \int di\, v_i^*(i, t)\, v_i(i, t) = 1 \tag{1}$$

für die zu variierende Funktion gewählt werden [9]. Im folgenden wird ein System ununterscheidbarer Teilchen betrachtet (z. B. Elektronen mit gleichmässig verschmiertem positiven Untergrund). Dann sind alle v_i gleich. Es gilt:

$$v_i(i, t) = v(i, t) \,. \tag{2}$$

Der Ansatz (1) beschreibt ein System statistisch unabhängiger Teilchen. Die Verteilungsfunktion f_N ergibt sich als Produkt von Einteilchenverteilungsfunktionen

$$f_N = \prod_{i=1}^{N} f(i,t) \qquad f(i,t) = |v(i,t)|^2 . \tag{3}$$

Setzt man (1) in

$$F = < u_N, \mathscr{L}\, u_N > - \lambda < u_N, u_N > \tag{4}$$

ein und fordert

$$\delta^1 F = 0, \tag{5}$$

so erhält man für v die Bestimmungsgleichung

$$\frac{\partial}{\partial t} v(1,t) + [H_1 + H_{1\bar{2}}, v(1,t)]_P = 0 . \tag{6}$$

$H_{1\bar{2}}$ ist der Teil der Hamiltonfunktion, der die über die Variable 2 gemittelte Wechselwirkung zwischen den Teilchen 1 und 2 berücksichtigt

$$H_{1\bar{2}} = \int d2\, v^*(2,t)\, H(1,2)\, v(2,t) . \tag{7}$$

Multiplikation von (6) mit $v^*(1,t)$ und Addition der konjugiert-komplexen Gleichung ergibt unmittelbar die Vlasovgleichung für die Einteilchenverteilungsfunktion

$$\frac{\partial}{\partial t} f(1,t) + [H_1 + H_{1\bar{2}}, f(1,t)]_P = 0 . \tag{8}$$

Die Gleichung (8) kann auch ohne Verwendung des Variationsprinzips aus der Liouvillegleichung hergeleitet werden. Dabei wird die durch Reduktion der Liouvillegleichung entstehende Gleichungshierarchie abgebrochen, indem

$$f_2(1,2,t) = f(1,t) f(2,t) \tag{9}$$

gesetzt wird. Die Tatsache, dass dann ebenfalls die Vlasovgleichung entsteht, zeigt deutlich, dass das Variationsprinzip nur eine äquivalente Formulierung der entsprechenden Differentialgleichung ist. Der Vorteil des Variationsprinzips wird sich erst bei allgemeineren Näherungsansätzen bemerkbar machen, da dann mit diesem Verfahren Näherungsgleichungen oft auf kürzerem Weg erhalten werden können, als es über die Hierarchie möglich ist.

Ein der Vlasovgleichung ähnlicher Ausdruck ergibt sich mit dem Ansatz [9]

$$u_N = \frac{1}{\sqrt{N!}} \prod_{i=1}^{N} v(i,t) \det w_j(\mathfrak{r}_k, t) . \tag{10}$$

Die im Unterschied zu (1) zusätzlich auftretende Determinante wird eingeführt, weil man hofft, damit in gewissen Grenzen den Einfluss kurzreichweitiger abstossender Wechselwirkungen zu beschreiben.

Zunächst ist zu erkennen, dass mit diesem Ansatz die Wahrscheinlichkeit Null sein muss, zwei Teilchen in einem Intervall $d\mathfrak{r}$ bei $\mathfrak{r} = \mathfrak{r}_0$ zu finden. Das wird durch den Ansatz (1) nicht garantiert; es entspricht der physikalischen Realität aber besser als die völlige statistische Unabhängigkeit. Mit (10) erhält man eine Gleichung vom Vlasovtyp. Die Antisymmetrie bzgl. der Orte erzeugt einen nur für kleine Abstände wesentlichen Zusatzterm. Kinetische Gleichungen dieser Struktur wurden auf anderem Weg bereits früher von Kadomtsev [11] bzw. von Rostoker und Rosenbluth [12] abgeleitet.

33. Variationsprinzipien für Systeme im thermischen Gleichgewicht

Im folgenden sollen Systeme im thermischen Gleichgewicht betrachtet werden. Geht man von einem System aus, das sich in einem gehemmten Gleichgewichtszustand befindet und überlässt das System nach Entfernen der äusseren Hemmung sich selbst, so wird es sich irreversibel auf das Gleichgewicht zubewegen. Über die dabei auftretende Entropieänderung dS macht der II. Hauptsatz der Thermodynamik die Aussage

$$T\,dS \geq dE + \sum_{i=1}^{f-1} k_i\,dX_i\,. \tag{1}$$

Die X_i bzw. k_i können als verallgemeinerte Koordinaten bzw. Kräfte eines thermodynamischen Systems mit f Freiheitsgraden aufgefasst werden (z. B. $X_1 = V$, $k_1 = p$) [5].

Es werden nun Prozesse betrachtet, bei denen während des Weges zum Gleichgewicht f voneinander unabhängige Variable konstant gehalten werden. Erfolgt solch ein Prozess mit konstanter Energie E und konstanten X_i $(i = 1, \ldots f-1)$, d. h. liegt ein abgeschlossenes System vor, dann nimmt die Entropie im Gleichgewicht ein Maximum an

$$dS \geq 0\,. \tag{2}$$

Es ist aber auch möglich, dass nicht diese, sondern andere Variable konstant gehalten werden. Wie in [5] gezeigt wurde, folgt mit (1), dass dann diejenige Grösse, die bezüglich der konstant zu haltenden Variablen thermodynamisches Potential ist, Extremalcharakter besitzt. Stellt sich der Gleichgewichtszustand eines Systems mit drei thermodynamischen Freiheitsgraden zum Beispiel bei konstanter Temperatur, konstantem Volumen und konstanter Teilchenzahl ein, so strebt die Freie Energie einem Minimum zu.

Bekanntlich lassen sich im Rahmen einer statistischen Theorie die thermodynamischen Potentiale durch die in Kap. 31 eingeführte Verteilungsfunktion f_N darstellen. Extremalprinzipien, denen die thermodynamischen Potentiale genügen, müssen deshalb auch Aussagen über die Gleichgewichtsverteilung liefern. Im weiteren werden Gleichgewichtszustände betrachtet, bei denen die Freie Energie zum Minimum wird. Für solche Systeme werden Näherungsgleichungen für die Verteilungsfunktion abgeleitet.

Setzt man f_N als Produkt von Korrelationsfunktionen an, die ab einer bestimmten Ordnung näherungsweise gleich Eins werden, erhält man Integralgleichungen für die Korrelationsfunktionen, die eine ähnliche Struktur wie die aus der Flüssigkeitstheorie bekannten besitzen. Bei einem anderen möglichen Ansatz führt man als f_N die Verteilungsfunktion eines mathematisch besser zu behandelnden Systems mit einer HAMILTONfunktion $\widetilde{H}$ ein. Weitere Näherungsverfahren ergeben sich mit der Verwendung von Clusterentwicklungen zur näherungsweisen Darstellung von f_N.

Es wird ein System konstanter Temperatur T, konstanten Volumens V und konstanter Teilchenzahl N betrachtet. Im Gleichgewicht nimmt bei solch einem System die Freie Energie F ein Minimum an

$$\delta^1 F = 0 \qquad \delta^2 F > 0\,. \tag{3}$$

Für ein reales Gas hat die Freie Energie die Gestalt

$$\begin{gathered} F = F_{\text{ideal}} + \beta^{-1} \int d\mathfrak{r}_1, \ldots\, d\mathfrak{r}_N f_{|N} (\ln f_{|N} + \beta u_N) \\ \text{mit} \qquad u_N \equiv \textstyle\sum_{i,j} u_{ij} \quad , \qquad \beta^{-1} \equiv kT\,. \end{gathered} \tag{4}$$

$f_{|N}$ stellt die nur noch von den Orten abhängige N-Teilchenverteilungsfunktion dar. Die Impulsabhängigkeit wird in den meisten Fällen trivial gleich einer MAXWELLverteilung sein. F_{ideal} ist die Freie Energie eines idealen Gases, für das die Wechselwirkungspotentiale u_{ij} verschwinden würden.

Die f_{IN} werden durch Minimalisierung der Freien Energie bestimmt. Bei unbeschränkter Variation folgt

$$\delta^1 F = 0 \qquad f_{|N} = \frac{e^{-\beta u_N}}{\int d\mathfrak{r}_1 \ldots d\mathfrak{r}_N \, e^{-\beta u_N}}\,. \tag{5}$$

Ein geeigneter Ansatz zur Ableitung von Näherungsgleichungen für f_{IN} ist ein Produkt von Korrelationsfunktionen [13] in der Form

$$f_{|N} = \frac{1}{V^N} \prod_{i<j} g_2(i,j) \prod_{i<j<k} g_3(i,j,k) \ldots \; g_N(1, 2 \ldots N)\,. \tag{6}$$

Der Ausdruck (6) für $f_{|N}$ scheint zunächst unnötig allgemein zu sein, da die exakte Lösung (5) mit u_N aus (4) ein Produkt von Zweiteilchenfunktionen ist. Er bekommt einen Sinn, wenn gefordert wird, dass beim Übergang von der N-Teilchenverteilungsfunktion zur reduzierten s-Teilchenverteilungsfunktion diese wieder aus denselben Korrelationsfunktionen $g_2 \ldots g_s$ in der Weise

$$f_{|s} = \frac{1}{V^s} \prod_{i<j} g_2(i,j) \prod_{i<j<k} g_3(i,j,k) \ldots g_s(1,2\ldots s) \qquad s = 2, \ldots N-1 \tag{7}$$

$$f_{|1} = \frac{1}{V}$$

zusammengesetzt werden kann. Damit müssen die Korrelationsfunktionen zusätzliche integrale Nebenbedingungen erfüllen. Aus (7) folgt, dass $g_2(1,2)$ mit der radialen Verteilungsfunktion identisch ist.

Mit dem Ansatz (6) wird die Freie Energie berechnet. Unter Berücksichtigung von (7) kann sie in der Form

$$F = F_{\text{ideal}} + \frac{1}{2!} \mathcal{N}^2 \int d\mathfrak{r}_1\, d\mathfrak{r}_2\, g_2(1,2)\,[\ln g_2(1,2) + \beta u(1,2)]$$

$$+ \frac{1}{3!} \mathcal{N}^3 \int d\mathfrak{r}_1\, d\mathfrak{r}_2\, d\mathfrak{r}_3\, g_2(1,2)\, g_2(2,3)\, g_2(3,1) \ln g_3(1,2,3) + \ldots \tag{8}$$

$$\text{mit } \mathcal{N} = \frac{N}{V}$$

dargestellt werden. Die Entwicklung ist exakt für grosse N. Dann gilt für die Entwicklungskoeffizienten

$$\binom{N}{2} \approx \frac{N^2}{2!} \qquad \binom{N}{3} \approx \frac{N^3}{3!}. \tag{9}$$

Der Vorteil dieser Entwicklung besteht darin, dass in den ersten k Gliedern nur Korrelationsfunktionen k-ter Ordnung auftreten.

Bis hierhin ist die Theorie exakt. Zur Ableitung von Näherungsgleichungen für die Verteilungsfunktion setzt man die g_n von einer bestimmten Ordnung ab gleich Eins. Fordert man, dass $g_3 = g_4 = \ldots = g_N = 1$ werden, so erhält man die in der Flüssigkeitstheorie bekannte KIRKWOODsche Superpositionsapproximation. Eine bessere Näherung ergibt sich mit

$$g_3(1,2,3) = 1 - \gamma = \text{const.} \qquad g_4 = g_5 = \ldots = 1, \tag{10}$$

wobei γ eine zunächst beliebige Konstante ist, die aus der Forderung

$$\int d\mathfrak{r}_1\, d\mathfrak{r}_2\, d\mathfrak{r}_3\, f_{|3} = 1 \tag{11}$$

in Abhängigkeit von g_2 bestimmt wird.

Wird mit dem Ansatz (10) die Freie Energie minimalisiert, entsteht eine Integrodifferentialgleichung für die radiale Verteilungsfunktion

$$\begin{gathered} -\beta^{-1} \frac{\partial}{\partial \mathfrak{r}_1} \ln g_2(1,2) = \frac{\partial}{\partial \mathfrak{r}_1} u(1,2) + \mathcal{N} \int d\mathfrak{r}_3\, g_2(1,2)\, g_2(2,3) \frac{\partial}{\partial \mathfrak{r}_1} w(1,3) \\ \text{mit} \quad w(1,3) \equiv -\beta^{-1} \ln g_2(1,3)\,. \end{gathered} \tag{12}$$

Die Gleichung hat eine ähnliche Struktur wie die aus der Flüssigkeitstheorie bekannten Gleichungen von KIRKWOOD, YVON, BORN und GREEN und MAYER. Die BORN-GREENsche Gleichung unterscheidet sich von (12) nur dadurch, dass das Potential der Durchschnittskräfte $w\,(1, 3)$ durch das zwischen 1 und 3 bei Abwesenheit aller anderen Teilchen bestehende Potential $u\,(1, 3)$ ersetzt wird. Im Falle langreichweitiger Kräfte können beide Potentiale beträchtlich voneinander abweichen. Die Gültigkeit der Gleichung (12) scheint überhaupt nur auf kurzreichweitige Wechselwirkungen beschränkt zu sein, da dann das Vernachlässigen höherer Korrelationen berechtigt ist.

Das Verfahren bietet die Möglichkeit, neben der Freien Energie auch die anderen thermodynamischen Grössen in Abhängigkeit von T, V und N zu berechnen, die sich aus der Freien Energie durch Differentiationen nach T, V und N ergeben.

Schwierigkeiten bereitet das Variationsverfahren bei unendlich ausgedehnten Systemen, da dann die Nebenbedingungen für die Korrelationsfunktionen nicht ohne weiteres eindeutig formuliert werden können. Dadurch treten beim Grenzübergang $V \to \infty$ in dem Ausdruck für die Freie Energie zunächst divergierende Integrale auf. Nach GURIKOV [14] lassen sich diese Terme in einem komplizierten Regularisierungsverfahren streichen (bei [13] nicht richtig gelöst). Anschliessend wird die Freie Energie minimalisiert.

Näherungsweise Ansätze für die Verteilungsfunktion lassen sich nicht nur durch die Methode gewinnen, die Korrelationsfunktionen bis zu einer bestimmten Ordnung zu berücksichtigen, sondern man kann sie auch noch auf eine andere Weise finden. Das oben behandelte Verfahren hat, vom Standpunkt der Anschaulichkeit aus betrachtet, noch gewisse Mängel. Es lässt sich nicht ohne weiteres sagen, für welch ein System der jeweilige Näherungsansatz die exakte Lösung darstellen würde. Das ist im folgenden besser möglich [15].

Für f_N wird der Ansatz

$$f_N = \frac{\exp(-\beta \widetilde{H})}{\int \exp(-\beta \widetilde{H})\, d1 \ldots dN} \qquad di \equiv d\mathfrak{p}_i\, d\mathfrak{r}_i \tag{13}$$

gemacht. $\widetilde{H}$ soll die HAMILTONfunktion eines geeignet zu wählenden Modellsystems sein. Für die Freie Energie erhält man mit (13)

$$F = -\beta^{-1}\ln[\int \exp(-\beta\widetilde{H})\,d1\ldots dN] + \frac{\int (H-\widetilde{H})\exp(-\beta\widetilde{H})\,d1\ldots dN}{\int \exp(-\beta\widetilde{H})\,d1\ldots dN}. \tag{14}$$

Den Näherungsausdruck (14) kann man als eine Störungsentwicklung von F bis zur ersten Ordnung nach $H - \widetilde{H}$ betrachten. Teilvariationen sind durchführbar, wenn man z. B. $\widetilde{H}$ in Abhängigkeit eines Satzes von Parametern darstellt. Der optimale Satz wird durch die Minimalforderung für F bestimmt. Eine Analogie zum temperaturabhängigen HARTREE—FOCK-Verfahren besteht, wenn man als $\widetilde{H}$ die HAMILTONfunktion eines Modells unabhängiger Teilchen wählt. In Fällen, wo $\widetilde{H}$ eine realistischere Form hat, die explizite Rechnungen nicht zulässt, kann man das Variationsprinzip verwenden, um Beziehungen zwischen verschiedenen Systemen zu begründen.

Die Extremaleigenschaften der thermodynamischen Potentiale bieten die Möglichkeit, zahlreiche andere Variationsverfahren anzugeben. Sie unterscheiden sich sowohl in der Auswahl des thermodynamischen Potentials (entsprechend dem betrachteten Gleichgewicht) als auch in dem Ansatz für f_N. Die für klassische Verteilungsfunktionen geltenden Variationsprinzipien müssen die gleiche Struktur haben wie die in der Quantenstatistik für die Dichtematrix bekannten [16]. Wegen der im Formalismus der Quantentheorie zunächst übersichtlicheren Darstellungsweise müsste es möglich sein, von letzterer ausgehend, diese auch in anderen als den bisher bekannten Fällen auf die klassische Statistik zu übertragen.

Eine weitere Anwendungsmöglichkeit besitzen Variationsprinzipien noch bei Clusterdarstellungen der Freien Energie. MORITA und HIROIKE [17] zeigen, dass durch Variation der Einteilchendichte bzw. einer modifizierten Zweiteilchendichte sich die exakten Integralgleichungen für die Ein- und Zweiteilchendichte ableiten lassen, die selbstverständlich wieder Clusterentwicklungen enthalten. Näherungsgleichungen (hypernetted chain approximation) ergeben sich, wenn man in dem Ausdruck für die Freie Energie bestimmte Clustersummen streicht.

4. Stationäre quantenmechanische Systeme

Der quantenmechanische Zustand eines Systems kann durch eine Wellenfunktion beschrieben werden, die je nach der Art des zu untersuchenden Problems der stationären bzw. instationären SCHRÖDINGERgleichung genügen muss [4]. Bei Vielteilchenproblemen sind die exakten Lösungen der SCHRÖDINGERgleichung mit Ausnahme weniger Spezialfälle nicht angebbar. Deshalb müssen entsprechende Näherungsverfahren entwickelt werden. Unter ihnen nehmen Variationsprinzipien eine wichtige Stellung ein.

Die stationäre SCHRÖDINGERgleichung kann wegen der Tatsache, dass der Energieerwartungswert im Grundzustand ein Minimum annimmt, leicht äquivalent in einem Variationsprinzip formuliert werden [4]. In Kap. 41 wird in allgemeiner Weise die Darstellbarkeit von Näherungslösungen durch unitäre Transformationen diskutiert. Diese Methode wird dann im Fall der HARTREE—FOCK-Näherung in Kap. 42 und der BOGOLJUBOVtransformation in Kap. 43 angewendet. In Kap. 44 werden Näherungsmethoden zur Behandlung von Atomkernen zusammengestellt. Indem man bei der näherungsweisen Auswertung des Energieminimums von vornherein nur bestimmte Zustände zur Variation zulässt, begeht man einen Fehler, der durch zusätzlichen Einbau von Nebenbedingungen teilweise korrigiert werden kann (Kap. 45). Ein kurzer Überblick über Schwierigkeiten, die bei der Berechnung der Dichtematrix mit Variationsmethoden entstehen, und über nichtintegrale Variationsverfahren wird in Kap. 46 gegeben.

41. Beschreibung von Näherungsverfahren durch unitäre Transformationen

Eine äquivalente Formulierung der stationären SCHRÖDINGERgleichung

$$H\Phi = E\Phi \qquad H = H^\dagger \tag{1}$$

kann wegen der Minimaleigenschaft des Erwartungswertes der Grundzustandsenergie [4] leicht durch das Variationsprinzip

$$\delta^1[(\Phi, H\Phi) + \lambda(\Phi, \Phi)] = 0 \tag{2}$$

angegeben werden.

Durch Teilvariation sind daraus Näherungsverfahren ableitbar. Man kann dabei zunächst ähnlich vorgehen wie in der Störungsrechnung. Ausgangspunkt ist ein möglichst einfacher Zustand Φ_0, z. B. der Grundzustand eines aus H durch Vereinfachung entstehenden Modellsystems H_0, der durch eine Transformation S mit dem tatsächlich interessierenden Zustand Φ verknüpft ist

$$\Phi = S\Phi_0 . \tag{3}$$

Fordert man, dass die Transformation unitär ist

$$S^{-1} = S^\dagger \qquad S = e^{i\eta} \qquad \eta^\dagger = \eta , \tag{4}$$

so hat man damit von vornherein die Erhaltung der Normierung sichergestellt.

Die Aufgabe besteht nun darin, einen sinnvollen Näherungsausdruck für η anzugeben. Während in der Störungsrechnung eine näherungsweise

Berechnung durch Partialsummation bestimmter Graphen einer Störungsentwicklung erfolgt, stellt man hier $\eta = \eta\,(\alpha, \beta, \ldots\, a_i^\dagger, \ldots\, a_j \ldots)$ in Abhängigkeit geeignet zu wählender Sätze von Parametern $\alpha, \beta, \ldots$ und Operatoren $a_i^\dagger, a_j \ldots$ dar, unter denen die optimale Kombination durch das Minimalprinzip (2) ausgewählt wird.

Beim Bestimmen der günstigsten Transformation S kann man auf verschiedene Weise vorgehen. Im allgemeinen wird man von einem vorgegebenen Satz von Operatoren ausgehen und nur die Parameter $\alpha, \beta, \ldots$ variieren. Eine andere Möglichkeit besteht darin, dass zu einem festen Parametersatz $\alpha, \beta, \ldots$ die optimalen Operatoren $a_i^\dagger, a_j \ldots$ durch Variation ermittelt werden. Der Charakter der Näherung wird bei beiden Methoden sowohl durch die Struktur von η als auch durch die Wahl des Ausgangszustandes bestimmt.

42. *Das* HARTREE—FOCK-*Verfahren*

Zunächst soll eine Darstellung des HARTREE—FOCK-Verfahrens in dem Formalismus von Kap. 41 gegeben werden (hierzu siehe auch [18]). Dabei wird der zweite der in Kap. 41 beschriebenen Wege benutzt.

Gegeben sei ein beliebiges System mit dem HAMILTONoperator

$$H = \Sigma_{i,j} < i\,|\,t\,|\,j > a_i^\dagger a_j^\dagger + \frac{1}{2} \Sigma_{i,j,k,l} < ij\,|\,v\,|\,kl > a_i^\dagger a_j^\dagger a_k a_l$$

$$\text{mit} \qquad < i\,|\,1\,|\,j > = \int d\mathfrak{r}\, \varphi_i^*(\mathfrak{r}) \cdot 1 \cdot \varphi_j(\mathfrak{r}) \,. \tag{1}$$

Als Modellsystem wird ein System unabhängiger Teilchen betrachtet. Ein möglicher Zustand solch eines Systems ist

$$\Phi_0 = \prod_{K=1}^{N} a_K^\dagger \Phi_{Vak} \tag{2}$$

$$\text{mit} \qquad a_i \Phi_{Vak} = 0 \,.$$

Beliebige andere Zustände Φ im Rahmen einer Näherung unabhängiger Teilchen können entsprechend Kap. 41 aus Φ_0 durch eine unitäre Transformation S erzeugt werden, wenn S folgende Gestalt hat:

$$\Phi = S\Phi_0 \,, \quad S = \mathrm{e}^{i\eta}, \quad \eta = \Sigma_m \Sigma_p \alpha_{mp} a_m^\dagger a_p \ \text{ mit } \ \alpha_{pm}^* = \alpha_{mp} \,. \tag{3}$$

Φ geht damit über in

$$\Phi = \prod_{K=1}^{N} c_K^\dagger \Phi_{Vak}$$

$$\text{mit} \quad c_K^\dagger = S a_K^\dagger S^\dagger = \mathrm{e}^{i[\eta,]_-} a_K^\dagger = a_K^\dagger + i\Sigma_j \alpha_{kj} a_j^\dagger + \frac{i^2}{2!} \Sigma_{j,l} \alpha_{kl} \alpha_{lj} a_j^\dagger \tag{4}$$

$$= \Sigma_j (\mathrm{e}^{i\alpha})_{kj} a_j^\dagger = \Sigma_j \beta_{kj} a_j^\dagger \,.$$

Wie Φ_0 stellt also auch Φ einen Zustand unabhängiger Teilchen dar. Die Aufgabe besteht nun darin, den optimalen Zustand zu bestimmen. Er folgt aus der Minimalisierung des Energieerwartungswertes $\bar{H}$:

$$\begin{aligned} \bar{H} &= (\Phi, H\Phi) = (\Phi_0, e^{-i\eta} H e^{+i\eta} \Phi_0) \\ &= (\Phi_0, e^{-i[\eta,]_-} H \Phi_0) = (\Phi_0, H\Phi_0) - i(\Phi_0, [\eta, H]_- \Phi_0) + \ldots . \end{aligned} \tag{5}$$

Frei wählbar sind zunächst die $c_K^\dagger$. Variationen der $c_K^\dagger$ entsprechen Änderungen der α_{ik} bzw. $\alpha_i^\dagger$. Im folgenden sollen nur die $a_i^\dagger$, die zunächst frei wählbar waren, verändert werden, während die α_{ik} festgehalten werden. Speziell wird gefordert, dass der optimale Zustand für $\alpha_{ik} = 0$ angenommen wird. Das ist nur möglich, wenn der in den α_{ik} lineare Term verschwindet

$$(\Phi_0, [\eta, H]_- \Phi_0) = 0 . \tag{6}$$

(6) stellt eine Bestimmungsgleichung für die $a_i^\dagger$, a_k und damit für die φ_i aus (1) dar. Aus (6) folgt

$$\begin{gathered} < p \,|\, t \,|\, m > + \Sigma_{l=1}^N (< pl \,|\, v \,|\, lm > - < pl \,|\, v \,|\, ml >) = 0 \\ < m \,|\, t \,|\, p > + \Sigma_{l=1}^N (< ml \,|\, v \,|\, lp > - < ml \,|\, v \,|\, pl >) = 0 \\ m = N + 1 \ldots \infty \\ p = 1 \ldots N. \end{gathered} \tag{7}$$

Da p und m beliebig Werte innerhalb der in (7) angegebenen Grenzen annehmen können, folgt sofort

$$\begin{gathered} | t \,|\, m > + \Sigma_{l=1}^N l \,|\, v \,|\, lm > - l \,|\, v \,|\, ml > = \Sigma_{n=N+1}^\infty \lambda_n \varphi_n \\ | t \,|\, p > + \Sigma_{l=1}^N l \,|\, v \,|\, lp > - l \,|\, v \,|\, pl > = \Sigma_{q=1}^N \lambda_q \varphi_q . \end{gathered} \tag{8}$$

Durch orthogonale Transformationen der φ_m und φ_p

$$\bar{\varphi}_n = \Sigma_m a_{nm} \varphi_m \qquad \bar{\varphi}_q = \Sigma_p a_{qp} \varphi_p \tag{9}$$

wird (8) diagonalisiert, und man erhält sofort die bekannten HARTREE—FOCK-Gleichungen

$$\begin{gathered} | t \,|\, \bar{m} > + \Sigma_{l=1}^N \bar{l} \,|\, v \,|\, \bar{l}\bar{m} > - \bar{l} \,|\, v \,|\, \bar{m}\bar{l} > = \varepsilon_m \bar{\varphi}_m , \\ | t \,|\, \bar{p} > + \Sigma_{l=1}^N \bar{l} \,|\, v \,|\, \bar{l}\bar{p} > - \bar{l} \,|\, v \,|\, \bar{p}\bar{l} > = \varepsilon_p \bar{\varphi}_p . \end{gathered} \tag{10}$$

Der interessierende Zustand Φ ändert sich bei der orthogonalen Transformation nicht. In Ortsdarstellung

$$\Phi = \begin{vmatrix} \varphi_1(\mathfrak{r}_1) \ldots \varphi_1(\mathfrak{r}_N) \\ \vdots \\ \varphi_N(\mathfrak{r}_1) \quad \varphi_N(\mathfrak{r}_N) \end{vmatrix} = \begin{vmatrix} \bar{\varphi}_1(\mathfrak{r}_1) \ldots \bar{\varphi}_1(\mathfrak{r}_N) \\ \vdots \\ \bar{\varphi}_N(\mathfrak{r}_1) \quad \bar{\varphi}_N(\mathfrak{r}_N) \end{vmatrix} \tag{11}$$

geht die Determinante der $\overline{p}_1$ nur durch Addition und Subtraktion entsprechender Zeilen aus der ersten hervor.

43. *Die* Bogoljubov*transformation*

Das Verfahren wurde entwickelt, um für supraleitende Systeme eine geeignete Näherungsmethode abzuleiten. Zunächst wird der Hamiltonoperator eines beliebigen Vielteilchensystems mit Zweierwechselwirkung betrachtet. Er kann in der Form

$$H = \Sigma_k \, \varepsilon_k \, a_k^\dagger \, a_k + \frac{1}{2} \Sigma_{k,k',q} \, v_{kk'q} \, a_k^\dagger \, a_{k'}^\dagger \, a_{k'+q} \, a_{k-q}. \tag{1}$$

eargestellt werden. $a_k^\dagger$ bzw. a_k sind Erzeugungs- bzw. Vernichtungsoperatoren von Fermionen mit dem Impuls $\hbar \, \mathfrak{k}$ und dem Spin $s_z = \hbar/2$. Operatoren zu dntgegengesetztem Impuls und Spin werden folgendermassen unterschieden:

$$a_k^\dagger = a_{\mathfrak{k}\uparrow}^\dagger \qquad a_{-k}^\dagger = a_{\dagger -\mathfrak{k}\downarrow}\,. \tag{2}$$

Schwierigkeiten bei der Berechnung dieses Systems bereiten stets die im zweiten Term enthaltenen Zweierwechselwirkungen. Im allgemeinen Fall ist eine exakte Auswertung der Schrödingergleichung deshalb nicht möglich.

Zur Lösung des Problems kann man nach Bogoljubov folgendes Näherungsverfahren anwenden [19]:

Ausgehend von einem möglichst einfachen Zustand Φ_0, wird der zu berechnende Grundzustand Φ durch eine unitäre Transformation S erzeugt

$$\Phi = S \Phi_0. \tag{3}$$

Durch geeignete Wahl von S kann aus einem in bestimmter Weise vorgegebenen Zustand Φ_0 jeder beliebige Zustand Φ entstehen. Setzt man für Φ_0 speziell ein Produkt von Einteilchenzuständen

$$\Phi_0 = \prod_{k=1}^{n} a_k^\dagger \Phi_{Vak}\,, \quad a_k \Phi_{Vak} = 0\,, \quad n \text{ beliebig} \tag{4}$$

an, dann erhält man für Φ die Darstellung

$$\Phi = \prod_{k=1}^{n} c_k^\dagger \tilde{\Phi}_{Vak} \qquad \text{mit} \qquad \begin{aligned} c_k^\dagger &= S\, a_k^\dagger S^\dagger \\ \tilde{\Phi}_{Vak} &= S\, \Phi_{Vak} . \end{aligned} \tag{5}$$

Im folgenden wird versucht, als Grundzustand des supraleitenden Systems einen solchen Zustand $\Phi = \Phi_{BCS}$ auszuwählen, der Vakuumzustand für die durch $c_k^\dagger$ erzeugten Quasiteilchen ist.

$$c_k \Phi_{BCS} = 0. \tag{6}$$

Das wird erfüllt, wenn für Φ_0 der Vakuumzustand Φ_{Vak} der durch die $a_k^\dagger$ erzeugten Teilchen mit dem Impuls $\hbar\mathfrak{k}$ und dem Spin $s_z = \hbar/2$ eingesetzt wird (also $n = 0$ in (4)). Dann gilt

$$c_k \Phi_{BCS} = c_k S \Phi_{Vak} = S a_k \Phi_{Vak} = 0 . \tag{7}$$

Die Transformation S muss nun dem realen System so angepasst werden, dass die neu eingeführten Quasiteilchen zumindest für kleine Anregungsenergien als wechselwirkungsfrei behandelt werden können.

Bogoljubov schlägt deshalb für supraleitende Fermionensysteme die Transformation

$$S = e^{i\eta}$$

$$\eta = - i\Sigma_k \alpha_k (a_k^\dagger a_{-k}^\dagger - a_{-k} a_k) \qquad \text{mit} \qquad \alpha_k = \alpha_k^* = -\alpha_{-k} \tag{8}$$

vor. Damit erhält man für den Vakuumzustand der Quasiteilchen aus (5)

$$\Phi_{BCS} = S \Phi_{Vak} = \prod_k (\cos \alpha_k + \sin \alpha_k \, a_k^\dagger a_{-k}^\dagger) \Phi_{Vak} . \tag{9}$$

Der Grundzustand ist entsprechend (9) ein Zustand unabhängiger Fermionenpaare (Cooperpaare). Das hier erhaltene Ergebnis ist identisch mit einem von Bardeen, Cooper und Schrieffer [20] auf Grund anderer Überlegungen erhaltenen Ansatz für den Grundzustand Φ_{BCS}.

Die α_k sind durch Energieminimalisierung geeignet zu bestimmen. Dabei ist zu beachten, dass mit der angegebenen Transformation Zustände erzeugt werden, für die die Teilchenzahl $N = \Sigma_k a_k^\dagger a_k$ keine Erhaltungsgrösse mehr ist. Deshalb muss als Nebenbedingung die Konstanz des Teilchenzahlerwartungswertes gefordert werden. Das Variationsprinzip hat die Gestalt

$$\delta^1 [(\Phi_{BCS} , H \Phi_{BCS}) + \lambda_1 (\Phi_{BCS} , N \Phi_{BCS})] = 0 . \tag{10}$$

Die Variation liefert eine Integralgleichung für die α_k, die noch zu gewissen Vereinfachungen des HAMILTONoperators führt. Stellt man ihn durch die Quasiteilchenoperatoren $c_k^\dagger$, $c_{k'}$ dar, so hat er ursprünglich die Form

$$H(a_k^\dagger, a_{k'}) = H(S^\dagger c_k^\dagger S,\ S^\dagger c_{k'} S) = H_0 + H_1 + H_2 + H_3$$

mit

$$H_0 = \Sigma_k E_{0k}(\alpha_k) \qquad H_1 = \Sigma_k E_k(\alpha_k)\, c_k^\dagger c_k \tag{11}$$

$$H_2 = \Sigma_k E_{2k}(\alpha_k)\,(c_k^\dagger c_{-k}^\dagger + c_{-k} c_k).$$

H_3 ist eine Summe aller möglichen Kombinationen von insgesamt vier Erzeugungs- oder Vernichtungsoperatoren $c_k^\dagger$ und c_k, wobei die Erzeugungsoperatoren links von den Vernichtungsoperatoren stehen.

Für die aus (10) bestimmten optimalen α_k verschwindet H_2. Wegen der speziellen Form (8) der Transformation S kann für niedrige Anregungsenergien H_3 als kleine Störung näherungsweise vernachlässigt werden. Der dann aus (11) durch Streichen von H_3 entstehende genäherte HAMILTONoperator $\widetilde{H}$ beschreibt ein System freier Quasiteilchen

$$\widetilde{H} = H_0 + \Sigma_k E_k c_k^\dagger c_k\,. \tag{12}$$

Angeregte Zustände von $\widetilde{H}$ sind sofort angebbar. Der n-te angeregte Zustand besitzt die Gestalt

$$\Phi_{BCS}^{(n)} = \prod_{k=1}^{n} c_k^\dagger \Phi_{BCS}\,. \tag{13}$$

Das Verfahren, optimale Quasiteilchen zur Beschreibung einer bestimmten physikalischen Situation einzuführen, lässt sich in zwei Näherungsschritte zusammenfassen. Einmal werden durch die Wahl einer bestimmten Klasse von Transformationen S — genauso wie bei jedem anderen Variationsprinzip — nur noch Teilvariationen zugelassen, was zu Näherungsgleichungen führen muss. Zum anderen wählt man eine solche Transformation aus, die es erlaubt, bei Rechnungen in Bereichen niedriger Anregungsenergien die Wechselwirkungsterme zu vernachlässigen.

Die Forderung, Wechselwirkungsterme zu streichen, wie es oben gemacht wird, muss natürlich nicht immer erhoben werden. Damit entstehen zwar neue Schwierigkeiten bei der Auswertung, das Verfahren wird jedoch allgemeiner anwendbar.

Ansätze zu einer solchen Erweiterung sind in Arbeiten von KELLY, SESSLER [21] und PROVIDENCIA [22, 23] zu finden. Sie führen Mehrfachanregungen ein, indem sie für S den Ausdruck

$$S = \exp i\,(\Sigma_{i,k}\, \alpha_{ik}\, a_i^\dagger a_k + \Sigma_{j,l,p,r}\, \alpha_{jl,pr}\, a_j^\dagger a_l^\dagger a_p a_r \tag{14}$$

verwenden. PROVIDENCIA [23] zeigt, dass man gute Näherungsansätze für Systeme mit singulären Potentialen kurzer Reichweite durch Berücksichtigung von Zweifachanregung erhält. Er bricht deshalb die Entwicklung im Exponenten von S nach dem zweiten Glied ab. Bei der Berechnung des Energieerwartungswertes treten schon bei dem einfachen Ansatz

$$\Phi = S\Phi_0 \qquad \Phi_0 = \prod_{k=1}^{N} a_k^{\dagger}\Phi_{Vak} \tag{15}$$

für den Grundzustand komplizierte Integrale auf, die mit Clusterentwicklungen in Analogie zur klassischen Statistik berechnet werden. Die so gewonnene Darstellung für den Energieerwartungswert erlaubt nun die Verwendung von Variationsmethoden zum Bestimmen der optimalen Transformation S. Bisher wurden diese Rechnungen aber noch nicht explizit ausgeführt.

44. *Variationsmethoden beim Atomkern*

Der Grundzustand eines Systems vieler Teilchen mit kurzreichweitiger singulärer Wechselwirkung (hard core-Potential) kann mit dem JASTROWschen Variationsverfahren [24] berechnet werden. Als Ansatzfunktion werden Produkte von Zweiteilchenfunktionen benutzt. Die komplizierte Auswertung des Energieerwartungswertes erfolgt mit Mitteln der klassischen Statistik. Falls man hard core-Potentiale durch geeignete Umformungen umgeht, können einfachere Näherungsansätze verwendet werden. Eine rechentechnisch gut zu bewältigende Methode ist ein auf wellenmechanischer Grundlage verbessertes statistisches Verfahren von MACKE [25].

Die Anwendung von Variationsprinzipien bei Potentialen mit singulärer Wechselwirkung wurde bereits von JASTROW [24] und anderen mit Erfolg erprobt. Verfahren dieser Art werden bei der Beschreibung von Atomkernen wegen der dort auftretenden hard core-Potentiale notwendig. Methoden vom HARTREE—FOCK-Typ müssen versagen, da dabei wegen der Existenz singulärer Potentiale divergente Ausdrücke entstehen. Das Modell der unabhängigen Teilchen kann aber durch das der unabhängigen Paare ersetzt werden, da Korrelationen zwischen mehr als zwei Teilchen vernachlässigt werden dürfen. Das ist deshalb der Fall, weil im Atomkern die effektive Reichweite der Wechselwirkungskräfte zwischen den Teilchen klein gegen ihren mittleren Abstand ist.

JASTROW führt dementsprechend als Versuchsfunktion ein Produkt von Zweiteilchenfunktionen ein. Dieses Produkt wird bei FERMIonensystemen zusätzlich mit einer HARTREE—FOCK-Determinante multipliziert, um das PAULIprinzip zu berücksichtigen. Im folgenden sollen zur Vereinfachung der Rechnung nur Teilchen betrachtet werden, die der BOSEstatistik genügen, da für Fermionen keine qualitativ neuen Ergebnisse erhalten werden. Der verbesserte Ansatz für den Grundzustand nach JASTROW verursacht natürlich Schwierigkeiten beim Durchführen der Variation. Aus Zweckmässigkeitsgründen wird Φ in der Form

$$\Phi(\mathfrak{r}_1, \ldots \mathfrak{r}_N) = \prod_{i<j} \exp \frac{1}{2} w(i,j) \tag{1}$$

dargestellt. Für den Energieerwartungswert ergibt sich dann:

$$\begin{aligned} E &= (\Phi, H\Phi) = (\Phi, [\Sigma_i h_i + \Sigma_{i<j} v(i,j)]\,\Phi) = \\ &= \frac{\hbar^2}{8m} \int d\mathfrak{r}_1\, d\mathfrak{r}_2 \left[\frac{\partial w(1,2)}{\partial \mathfrak{r}_1} \cdot \frac{\partial \varrho_2(1,2)}{\partial \mathfrak{r}_1} + \frac{1}{2} v(1,2)\, \varrho_2(1,2)\right]. \end{aligned} \tag{2}$$

Dabei soll ϱ_2 die Zweiteilchendichte sein. Allgemein gilt für die s-Teilchendichte

$$\varrho_s = \frac{N!}{(N-s)!} \cdot \frac{\int d\mathfrak{r}_{s+1} \ldots d\mathfrak{r}_N\, \Phi^* \Phi}{\int d\mathfrak{r}_1 \ldots d\mathfrak{r}_N\, \Phi^* \Phi}. \tag{3}$$

Die weitere Aufgabe besteht nun darin, E zu minimalisieren, indem man für Φ alle möglichen Werte zulässt. In (2) werden also $w\,(1,2)$ und $\varrho_2\,(1,2)$ variiert. Diese Variationen dürfen jedoch wegen (3) nicht unabhängig voneinander erfolgen. Zwischen ϱ_2 und $w\,(1,2)$ existiert entsprechend der Definition (3) der Zusammenhang

$$\frac{\partial}{\partial \mathfrak{r}_1} \varrho_2(1,2) = \varrho_2(1,2) \frac{\partial}{\partial \mathfrak{r}_1} w(1,2) + \int d\mathfrak{r}_3\, \varrho_3(1,2,3) \frac{\partial}{\partial \mathfrak{r}_1} w(1,3). \tag{4}$$

Gleichung (4) ist nicht abgeschlossen, da sie als neue unbekannte Grösse die Dreiteilchendichte ϱ_3 enthält. Um die Variation durchführen zu können, sind deshalb von mehreren Autoren Näherungsverfahren entwickelt worden [26], [27], [28].

ABE [27] benutzt zur Elimination von ϱ_3 aus (4) die KIRKWOODsche Näherung

$$\mathcal{N}^3 \varrho_3(1,2,3) = \varrho_2(1,2)\, \varrho_2(2,3)\, \varrho_2(3,1) \quad \text{mit} \quad \mathcal{N} = \frac{N}{V}. \tag{5}$$

Diese Approximation ist gut bei Systemen mit kurzer Reichweite und nicht zu grossen Teilchendichten, da dann im allgemeinen nur zwei Teilchen gleichzeitig miteinander wechselwirken werden. Mit (4) und (5) kann man für $\partial w\,(1,2)/\partial \mathfrak{r}_1$ eine Entwicklung nach der Teilchendichte $\mathcal{N}$ angeben, in der nur noch ϱ_2 auftaucht. Bricht man die Entwicklung in einer bestimmten Ordnung ab und minimalisiert

$$E = E\,[\varrho_2(1,2)], \tag{6}$$

so erhält man eine Bestimmungsgleichung für die Zweiteilchendichte $\varrho_2(1,2)$.

HIROIKE [28] baut die in der Reihenentwicklung bzgl. $\mathcal{N}$ bestehende Analogie zur klassischen Statistik weiter aus. Setzt man für $w(1,2) = -\beta\,u(1,2)$, so kann man die zur Berechnung der Zweiteilchendichte in der klassischen Statistik geltenden Integralgleichungen übernehmen, falls $u(1,2)$ formal mit dem Wechselwirkungspotential zwischen zwei Teilchen identifiziert wird. Die Integralgleichungen gestatten es, $w(1,2)$ in E durch $\varrho_2(1,2)$ auszudrücken. Näherungsverfahren, die von klassischen Clusterentwicklungen her bekannt sind, ermöglichen eine Auswertung des Variationsprinzips. Es wird z. B. die hyper-netted chain approximation (HNC) verwendet, bei der nur Cluster einer bestimmten topologischen Struktur aufsummiert werden [17]. Wird anschliessend die Energie zum Minimum gemacht, erhält man im Rahmen der HNC-Approximation gültige Integralgleichungen für $\varrho_2(1,2)$. Das JASTROWsche Verfahren enthält also neben der Näherung durch den speziellen Ansatz für den Grundzustand stets weitere Näherungen bei der Auswertung des Energieerwartungswertes.

Wie gezeigt wurde, bereitet das JASTROWsche Variationsverfahren für Systeme mit singulären Wechselwirkungen bei der Auswertung erhebliche Schwierigkeiten. Da aber in der Theorie der Atomkerne durch den hard core-Anteil des Nukleonenpotentials solche Fragestellungen entstehen, wurden Wege gesucht, um dieses Hindernis zu umgehen. Stets ist es das Ziel, zur näherungsweisen Bestimmung des Grundzustandes mathematisch einfacher durchführbare Variationsmethoden wie das HARTREE—FOCK-Verfahren oder statistische Verfahren anwenden zu können.

Eine Möglichkeit ergibt sich dadurch, dass man das singuläre Potential durch ein geglättetes Effektivpotential ersetzt, wie es in der BRUECKNERtheorie gemacht wird. Für eine Behandlung von Atomkernen mit Variationsprinzipien wird das zum Beispiel von KUMAR [29] und BRUNNER [30] ausgenutzt.

Ein zweiter Weg besteht darin, hard core-Potentiale durch geschwindigkeitsabhängige zu ersetzen. Es lässt sich zeigen, dass beide Potentialtypen durch eine Variablentransformation ineinander überführt werden können [31]. Wegen des jetzt nicht mehr singulären HAMILTONoperators ist es erlaubt, HARTREE—FOCK-Ansätze zu machen. Bei Systemen mit grosser Teilchenzahl N wird das Berechnen der HARTREE—FOCK-Einteilchenwellenfunktionen nach der Methode des »self consistent field« sehr mühevoll sein. Deshalb benutzt man statistische Beschreibungen, bei denen zumindest das PAULIprinzip gewahrt bleibt [32].

Eine Verfeinerung des statistischen Modells auf wellenmechanischer Grundlage wurde von Macke [25] angegeben. Er verwendet für den Grundzustand einen Näherungsansatz vom Hartree—Fock-Typ in der Form

$$\Phi(\mathfrak{r}_1, \ldots \mathfrak{r}_N) = \frac{1}{\sqrt{N!}} \left| \varphi_n(\mathfrak{r}_k) \right|$$

mit (7)

$$\varphi_n(\mathfrak{r}) = \sqrt{\frac{\sigma(\mathfrak{r})}{N}}\, \tilde{\varphi}_n(\mathfrak{y}(\mathfrak{r})) \,.$$

Die $\tilde{\varphi}_n$ stellen einen in bestimmter Weise vorgegebenen Satz von Einteilchenfunktionen dar. Sie sollen nach Konstruktion in einem durch die Variable $\mathfrak{y}(\mathfrak{r})$ beschriebenen Bereich orthogonal sein, d. h. es gilt

$$\int d\mathfrak{y}\, \tilde{\varphi}_n^*(\mathfrak{y})\, \tilde{\varphi}_m(\mathfrak{y}) = \delta_{mn} \,. \tag{8}$$

Es wird angenommen, dass zwischen den Raumpunkten $\mathfrak{r}$ und dem Bereich $\mathfrak{y}$ eine eindeutige, aber sonst zunächst beliebige Transformation $\mathfrak{y} = \mathfrak{y}(\mathfrak{r})$ vorgegeben werden kann. σ/N soll gleich der Funktionaldeterminante der Transformation sein

$$\frac{\sigma(\mathfrak{r})}{N} = \left| \frac{\partial y_i}{\partial x_k} \right| . \tag{9}$$

Aus (8) und (9) kann man folgern, dass auch die $\varphi_n(\mathfrak{r})$ zueinander orthogonal sein müssen. Es gilt

$$\begin{aligned} \int d\mathfrak{r}\, \varphi_n^*(\mathfrak{r})\, \varphi_m(\mathfrak{r}) &= \int d\mathfrak{r} \left| \frac{\partial y_i}{\partial x_k} \right| \tilde{\varphi}_n^*(\mathfrak{y}(\mathfrak{r}))\, \varphi_m(\mathfrak{y}(\mathfrak{r})) = \\ &= \int d\mathfrak{y}\, \tilde{\varphi}_n^*(\mathfrak{y})\, \tilde{\varphi}_m(\mathfrak{y}) = \delta_{nm} \,. \end{aligned} \tag{10}$$

Durch die Forderung, dass mit dem Ansatz (7) die Energie zum Minimum wird, kann die Transformation $\mathfrak{y} = \mathfrak{y}(\mathfrak{r})$ bestimmt werden.

Will man die Energie nur in statistischer Näherung $N \to \infty$ berechnen, so ist die spezielle Form der $\tilde{\varphi}_n$ nicht sehr wichtig, z. B. können sie die Eigenfunktionen eines Einheitswürfels sein.

Mit diesem Ansatz liefert das Variationsverfahren eine Verfeinerung der Thomas—Fermi—Dirac-Methode [33]. Als Verbesserung tritt in der kinetischen Energie zusätzlich der Weizsäckerterm auf

$$E_{kin,w} = \frac{\hbar^2}{2m} \int d\mathfrak{r} \left(\frac{\partial \sqrt{\varrho}}{\partial \mathfrak{r}} \right)^2 \quad \text{mit} \quad \varrho = \frac{\sigma}{N} \sum_{n=1}^{N} |\tilde{\varphi}_n|^2 , \tag{11}$$

der die Ortsabhängigkeit der Teilchendichte berücksichtigt.

45. Einbau von Nebenbedingungen—cranking-Modell

In den bisher behandelten Verfahren werden Näherungslösungen der stationären SCHRÖDINGERgleichung ermittelt, indem der Energieerwartungswert unter der Nebenbedingung konstanter Normierung zum Minimum gemacht wird.

$$\delta\,[(\Phi, H\,\Phi) - \lambda\,(\Phi, \Phi)] = 0. \tag{1}$$

Dabei werden den zu variierenden Zuständen Φ durch spezielle Ansätze von vornherein Beschränkungen auferlegt, die zwangsläufig zu Näherungslösungen führen müssen. Von guten Näherungslösungen wird man sprechen, wenn der Energieerwartungswert möglichst gut approximiert wird. Um darüber hinaus auch vernünftige Ergebnisse in bezug auf andere Fragestellungen zu erhalten, werden oft mit grossem Erfolg zusätzliche Nebenbedingungen in die Variationsaufgabe eingebaut.

Es soll z. B. einmal eine HARTREE—FOCK-Näherung betrachtet werden. Während die exakte Lösung Φ des Problems Eigenzustand zum wahren HAMILTONoperator H ist, kann die Näherungslösung Φ_0 als Eigenzustand eines Modelloperators H_0 interpretiert werden. Der exakte HAMILTONoperator H ist invariant gegen beliebige Translationen und Drehungen, es gilt also

$$[H, \mathfrak{P}]_- = 0\,, \qquad [H, \mathfrak{J}]_- = 0\,. \tag{2}$$

Die Eigenlösungen Φ sind damit auch Eigenzustände des Gesamtimpulses $\mathfrak{p}$ sowie von Quadrat und z-Komponente des Gesamtdrehimpulses $\mathfrak{h}$. Beim Übergang zum Modelloperator H_0 geht die Symmetrie von H zumindest teilweise verloren. Durch Einführung eines raumfesten mittleren Einteilchenpotentials, das in H_0 enthalten ist, wird

$$[H_0, \mathfrak{P}]_- \neq 0\,. \tag{3}$$

Die Modellzustände sind nicht mehr Eigenzustände von $\mathfrak{P}$, ausserdem verschwindet dessen Erwartungswert. Eine freie Translation des Schwerpunktes und eine zugehörige Schwerpunktsenergie sind also nicht mehr im Modell enthalten.

Bei deformierten Kernen verliert H_0 die Kugelsymmetrie, die H besitzt. Bleibt der Kern axialsymmetrisch, dann enthält H_0 eine ausgezeichnete Richtung $\mathfrak{e}$, die Figurenachse des Kernes. Es gilt dann

$$\begin{aligned} &[H_0, \mathfrak{e}\mathfrak{J}]_- = 0\,, \qquad [H_0, Q\,\mathfrak{J}] \neq 0 \\ \text{mit}\quad &Q \equiv \mathrm{I} - \mathfrak{e} \circ \mathfrak{e} \qquad \mathrm{I} = \text{Einheitstensor.} \end{aligned} \tag{4}$$

H_0 besitzt also nur Eigenzustände, die keine Drehimpulskomponente senkrecht zu $\mathfrak{e}$ enthalten, im Gegesatz zum exakten Problem. Durch den speziellen Ansatz Φ_0 werden damit auch Kernrotationen nicht mitgeliefert, denn diese können ja nur um Achsen senkrecht zur Figurenachse erfolgen.

Um diesen Fehler zu beseitigen, kann man durch Einbau von Nebenbedingungen in (1) an Φ_0 zusätzliche Forderungen stellen. So kann man z. B. verlangen, dass der Kern einen Drehimpuls

$$(\Phi, \mathfrak{J}\,\Phi) \equiv \mathfrak{J} = \mathfrak{a} \tag{5}$$

besitzen soll. (1) geht dann in

$$\delta\,[(\Phi, H\,\Phi) - \vec{\omega}\,(\Phi, \mathfrak{J}\,\Phi) - \lambda\,(\Phi, \Phi)] = 0 \tag{6}$$

über [37].

Bei vollständiger Variation der Φ sind (1) und (6) gleichwertig, da die Lösungen von (1) stets Eigenzustände einer Komponente von $\mathfrak{J}$, etwa der Komponente in Richtung $\mathfrak{a}$ aus (5), sind. Bei teilweiser Variation dagegen ist die Nebenbedingung entscheidend, sie führt bei deformierten Kernen zu neuen Lösungen, die durch H_0 nicht erfasst werden. (6) geht aus (1) hervor, indem man entsprechend

$$H \to H - \vec{\omega}\,\mathfrak{J} \tag{7}$$

zum HAMILTONoperator den Term-$\vec{\omega}\,\mathfrak{J}$ hinzufügt. Das entspricht einem Übergang von einem ruhenden zu einem mit $\vec{\omega}$ rotierenden Koordinatensystem. Die Variation in (6) mit einem HARTREE—FOCK-Ansatz beschreibt demnach ein System mit $\vec{\omega}$ rotierender Teilchen, die sich im rotierenden Bezugssystem unabhängig voneinander in einem Einteilchenpotential bewegen.

Führt man die Rechnung in (6) durch, so erhält man einen Energieerwartungswert, der für $\mathfrak{a} \neq 0$ grösser als der bei einem HARTREE—FOCK-Verfahren ohne die zusätzliche Nebenbedingung ist. Der Zusatzterm hängt in erster Näherung quadratisch von der Winkelgeschwindigkeit $\vec{\omega}$ ab. Der Proportionalitätsfaktor wird als Trägheitsmoment interpretiert. Mit diesem Verfahren erhält man damit verbesserte Ergebnisse des cranking-Modells [35].

Dieselben Überlegungen sind für den Impuls $\mathfrak{P}$ möglich. Der Variationsforderung

$$\delta\,[(\Phi, H\,\Phi) - \mathfrak{v}\,(\Phi, \mathfrak{P}\,\Phi) - \lambda\,(\Phi, \Phi)] = 0 \tag{8}$$

entspricht hierbei ein Übergang zu einem mit der Geschwindigkeit $\mathfrak{v}$ bewegten System.

4.6. *Weitere Variationsverfahren*

Der Zustand eines quantenmechanischen Systems kann durch eine Wellenfunktion beschrieben werden. Eine allgemeinere Darstellung ist mit der Dichtematrix möglich. Diese muss auf jeden Fall dann eingeführt werden, wenn nur unvollständige Information über das System vorliegt [36]. Zur Berechnung der Dichtematrix eines Systems vieler Teilchen müssen ebenso wie zur Bestimmung der Wellenfunktion Näherungsverfahren entwickelt werden, da das Problem nicht exakt lösbar ist. Ein möglicher Weg besteht in der Verwendung des Variationskalküls. Die Dichtematrix für den Grundzustand eines Systems kann im Formalismus der Variationsrechnung durch Energieminimalisierung berechnet werden. Man kann zeigen, dass der Energieerwartungswert nur von der durch Reduktion aus der N-Teilchendichtematrix ϱ_N entstehenden Zweiteilchendichtematrix ϱ_2 in der Form

$$E = \mathrm{Sp}_2\, H\, \varrho_2 \tag{1}$$

abhängt. ϱ_2 darf als Ansatzfunktion nicht beliebig gewählt werden, sondern muss einem Satz von Nebenbedingungen genügen. Diese Nebenbedingungen entstehen aus Forderungen an ϱ_N (z. B. Normierung, Hermitizität, Ununterscheidbarkeit der Teilchen und — für Fermionen — Pauliprinzip). Durch Reduktion tauchen die Bedingungen in komplizierter Form wieder in ϱ_2 auf. Bei einem beliebigen Näherungsansatz für ϱ_2 ist stets zu untersuchen, ob sie erfüllt sind. (N-Darstellbarkeit von ϱ_2). Ausführlichere Untersuchungen darüber wurden u. a. von Ando [37] und von Coleman [38] angestellt. Bisher ist es aber nur gelungen, eine Vielzahl von entweder nur notwendigen oder nur hinreichenden Bedingungen für ϱ_2 anzugeben; es konnte nicht gezeigt werden, dass sie beides zugleich sind. In jüngster Zeit ist es scheinbar gelungen, notwendige und hinreichende Bedingungen zugleich für die N-Darstellbarkeit von ϱ_2 anzugeben [39]. Diese Bedingungen sind jedoch so kompliziert, dass sie für Anwendungen ungeeignet zu sein scheinen.

Alle bisher angeführten Variationsprinzipien zur Bestimmung des quantenmechanischen Grundzustandes haben ein gemeinsames Merkmal. Sie stellen integrale Variationsprobleme dar. Wie man z. B. beim Jastrowschen Verfahren feststellen konnte, bereiten die Integrationen über die Variablen aller Teilchen oft erhebliche Schwierigkeiten. Deshalb ist ein Extremalprinzip, bei dem die Integrationen umgegangen werden, teilweise aus rechentechnischen Gründen vorzuziehen.

Die local energy-Methode [40] besitzt diesen Vorzug. Das Verfahren soll der Einfachheit halber an einem Einteilchenmodell erläutert werden. Es ist aber genauso auf Vielkörperprobleme anwendbar. Ausgangspunkt ist die stationäre Schrödingergleichung in Ortsdarstellung

$$H\, \varphi(\mathfrak{r}) = E\, \varphi(\mathfrak{r}). \tag{2}$$

Für eine genäherte Funktion $\tilde{\varphi}(\mathfrak{r})$ geht sie in

$$H\,\tilde{\varphi}(\mathfrak{r}) = \varepsilon(\mathfrak{r})\,\tilde{\varphi}(\mathfrak{r}) \tag{3}$$

über. Die Wellenfunktion ist optimal, wenn $\varepsilon(\mathfrak{r})$ unabhängig vom Ort einen konstanten Wert annimmt, d. h. wenn die mittlere quadratische Schwankung

$$(\Delta\varepsilon)^2 = \overline{\varepsilon^2} - \bar{\varepsilon}^2 \tag{4}$$

ein Minimum annimmt.

Um Integrationen zu vermeiden, werden die Mittelungen über die Umgebungen $\Delta\tau_p$ eines Systems von endlich vielen Punkten vorgenommen. Dann gilt

$$\bar{\varepsilon} = \frac{\Sigma_p\,\varepsilon_p\,g_p}{\Sigma_p g_p} \qquad \overline{\varepsilon^2} = \frac{\Sigma_p\,\varepsilon_p^2\,g_p}{\Sigma_p\,g_p}\,,$$

mit

$$g_p(\mathfrak{r}_p) = \Delta\tau_p\,\tilde{\varphi}(\mathfrak{r}_p)^2\,. \tag{5}$$

Für $\tilde{\varphi}$ werden Näherungsausdrücke eingeführt. Wählt man speziell

$$\tilde{\varphi} = \Sigma_i\,c_i\,\varphi_i\,, \tag{6}$$

so erhält man aus der Minimalforderung für (4) ein System von Bestimmungsgleichungen für die c_i, das mit einem Iterationsverfahren gelöst werden kann. Denkbare Ansätze für die φ_i wären z. B. bei einem FERMIonensystem HARTREE—FOCK-Determinanten.

5. Nichtstationäre quantenmechanische Systeme

Für die zeitabhängige SCHRÖDINGERgleichung können sowohl ein nur stationäres Funktional als auch solch ein Funktional angegeben werden, das einen Minimalwert annimmt (Kap. 51). Das letztere hat die anschauliche Bedeutung, dass das Quadrat vom Abstand des wahren Zustandes und des näherungsweise gültigen im Zeitablauf ein Minimum annimmt. Mit diesen Variationsverfahren können zeitabhängige HARTREE—FOCK-Gleichungen abgeleitet werden. Das Minimalprinzip ist ausserdem bei Stabilitätsuntersuchungen von Nutzen. In Kap. 52 werden Streuprobleme behandelt. Diese instationären Vorgänge können speziell bei elastischer Streuung durch stationäre Gleichungen beschrieben werden, die mit Variationsprinzipien von KOHN [41], HULTHEN [42] und SCHWINGER [43] näherungsweise gelöst werden.

51. Die zeitabhängige SCHRÖDINGER*gleichung*

Der Ausgangspunkt aller Variationsverfahren für die stationäre SCHRÖDINGERgleichung ist die Minimaleigenschaft des Energieerwartungswertes. Für die zeitabhängige SCHRÖDINGERgleichung

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\Psi = H\Psi \qquad H = H^{\dagger} \tag{1}$$

lässt sich auf diesem Weg jedoch kein Variationsprinzip ableiten. Es bieten sich dafür aber verschiedene andere Möglichkeiten an.

Entsprechend den in Kap. 21 gemachten Aussagen kann man versuchen, in dem durch (1) beschriebenen Raum aller Zustandsvektoren Ψ ein Skalarprodukt zu definieren, bei dem der Operator $\hbar\partial/i\,\partial t + H$ selbstadjungiert ist. H soll nach Voraussetzung hermitisch sein. Dann erhält man sofort ein Variationsprinzip, wenn man das in der Quantentheorie übliche Skalarprodukt um eine Zeitintegration erweitert. Fordert man, dass das Funktional

$$F = \int dt\left(\Psi, \left\{\frac{\hbar}{i}\frac{\partial}{\partial t} + H\right\}\Psi\right) \tag{2}$$

stationär wird

$$\begin{aligned}\delta^1 F &= \int dt\left(\delta\Psi, \left\{\frac{\hbar}{i}\frac{\partial}{\partial t} + H\right\}\Psi\right) + \int dt\left(\Psi, \left\{\frac{\hbar}{i}\frac{\partial}{\partial t} + H\right\}\delta\Psi\right) \\ &= \int dt\left(\delta\Psi, \left\{\frac{\hbar}{i}\frac{\partial}{\partial t} + H\right\}\Psi\right) + \int dt\left(\delta\Psi, \left\{\frac{\hbar}{i}\frac{\partial}{\partial t} + H\right\}\Psi\right)^{*} = 0\,,\end{aligned} \tag{3}$$

so erhält man bei beliebiger Variation der Ψ die Gleichung (1).

Das Verfahren hat aber einen Nachteil. Betrachtet man die zweite Variation

$$\delta^2 F = \int dt\left(\delta\Psi, \frac{\hbar}{i}\frac{\partial}{\partial t}\delta\Psi\right) + \int dt\,(\delta\Psi, H\,\delta\Psi) \gtrless 0\,, \tag{4}$$

dann kann man zwar mit Sicherheit sagen, dass der zweite Term immer positiv sein wird [4], dagegen sind für den ersten Ausdruck beide Vorzeichen möglich. Das Funktional F ist also nur stationär. Es nimmt keinen Extremwert an.

Ein Minimalprinzip für die zeitabhängige SCHRÖDINGERgleichung wird von MCLACHLAN [44] angegeben. Es kann auf anschauliche Weise hergeleitet werden.

Nach Vorgabe eines Zustandes zur festen Zeit t $\Psi(t) = \Psi_0$ ist mit (1) die weitere Entwicklung des Systems im Zeitablauf eindeutig bestimmt. Für den Zustand zur Zeit $t + \delta t$ gilt

$$\Psi(t+\delta t) = \Psi(t) - \frac{i}{\hbar} H\Psi(t)\cdot dt\,. \tag{5}$$

Falls $\Psi(t)$ in einem Unterraum a liegt, wird $\Psi\,(t+\delta\,t)$ im Zeitablauf im allgemeinen aus a herauslaufen.

In Abb. 1 wird der HILBERTraum durch die Papierebene charakterisiert. Die Zustandsvektoren $\Psi(t)$ sollen wie Ortsvektoren, von einem Ursprung O ausgehend, aufgetragen werden. Die im Rahmen eines Näherungsverfahrens zu berechnenden Zustände $\widetilde{\Psi}$ bleiben durch einen speziellen Ansatz auf den Unterraum a beschränkt. Zu dem festen Zeitpunkt t soll der näherungsweise gültige Zustand $\widetilde{\Psi}(t)$ gleich dem von dem realen System exakt angenommenen Zustand $\Psi(t)$ sein

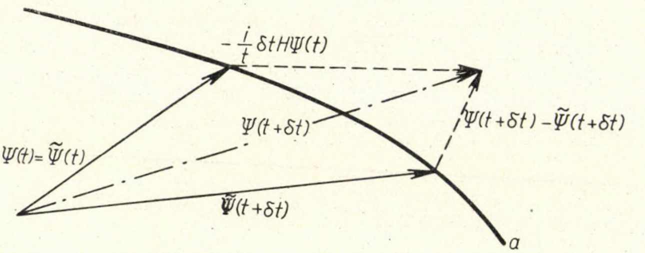

Abb. 1. Beispiel für die Beschränkung der Zustandsvektoren durch eine Nebenbedingung a

$$\widetilde{\Psi}(t)=\Psi(t)=\Psi_0\,. \tag{6}$$

Es wird nun nicht $\Psi\,(t+\delta\,t)$, sondern derjenige im Unterraum a liegende Zustand $\widetilde{\Psi}\,(t+\delta\,t)$ bestimmt, der das tatsächlich zu beschreibende System optimal approximiert. Eine sinnvolle Forderung für eine möglichst gute Näherung ist die, dass das Quadrat des Abstandes von $\widetilde{\Psi}\,(t+\delta\,t)$ und $\Psi\,(t+\delta\,t)$

$$\Delta\,(t+\delta\,t)=([\widetilde{\Psi}\,(t+\delta\,t)-\Psi\,(t+\delta\,t)],\;[\widetilde{\Psi}\,(t+\delta\,t)-\Psi\,(t+\delta\,t)]) \tag{7}$$

ein Minimum annimmt. Dann muss also gelten:

$$\delta^1\,\Delta\,(t+\delta t)=0. \tag{8}$$

Es bleibt nun noch zu untersuchen, welche Grösse in $\Delta\,(t+\delta\,t)$ variiert werden darf. $\Psi\,(t+\delta\,t)$ wird sich nicht ändern, da bei Vorgabe des Anfangszustandes $\Psi(t)$ die SCHRÖDINGERgleichung $\Psi\,(t+\delta\,t)$ eindeutig bestimmt. Variationen sind nur für $\widetilde{\Psi}\,(t+\delta\,t)$ möglich, aber auch nicht in unbeschränktem Umfange. Entwickelt man $\widetilde{\Psi}\,(t+\delta\,t)$ um die Stelle t

$$\widetilde{\Psi}\,(t+\delta t)=\widetilde{\Psi}\,(t)+\delta t\frac{\partial}{\partial t}\,\widetilde{\Psi}\,(t)=\Psi(t)+\delta t\frac{\partial}{\partial t}\widetilde{\Psi}\,(t)\,, \tag{9}$$

so sieht man, dass nur

$$\frac{\partial}{\partial t}\tilde{\Psi}(t) = -\frac{i}{\hbar}\chi(t) \tag{10}$$

variiert werden kann. Die möglichen Werte von $\chi(t)$ müssen dabei den mit *a* gegebenen Nebenbedingungen genügen.

Es gilt

$$\Psi(t+\delta t) - \tilde{\Psi}(t+\delta t) = -\frac{i}{\hbar}\,\delta t\big(H\tilde{\Psi}(t) - \chi(t)\big)\,. \tag{11}$$

Damit erhält man für (7)

$$\Delta(t+\delta t) = \frac{\delta t^2}{\hbar^2}\big(\chi(t) - H\tilde{\Psi}(t),\, \chi(t) - H\tilde{\Psi}(t)\big)\,. \tag{12}$$

Das Minimalprinzip hat die Gestalt (der konstante Faktor $\frac{\delta t^2}{\hbar^2}$ kann unberücksichtigt bleiben):

$$\delta^1\bar{\Delta}(t) = 0\,, \qquad \bar{\Delta}(t) = \frac{\hbar^2}{\delta t^2}\Delta(t+\delta t) \tag{13}$$

mit der Nebenbedingung

$$\chi(t) = -\frac{\hbar}{i}\frac{\partial}{\partial t}\tilde{\Psi}(t)\,.$$

(13) ergibt bei unbeschränkter Variation

$$\delta^1\bar{\Delta}(t) = (\delta\chi, \chi - H\Psi) + (\chi - H\Psi, \delta\chi) \tag{14}$$

die Gleichung (1), wenn man noch die Nebenbedingung (10) berücksichtigt. Die zweite Variation

$$\delta^2\bar{\Delta}(t) = (\delta\chi, \delta\chi) > 0 \tag{15}$$

ist stets positiv.

Die oben angegebenen Variationsmethoden ermöglichen es, prinzipiell dieselben Näherungsverfahren anzuwenden wie im zeitunabhängigen Fall. So kann z. B. ein zeitabhängiges HARTREE—FOCK-Verfahren abgeleitet werden. Mit dem Ansatz

$$\Psi(\mathfrak{r}_1,\ldots\mathfrak{r}_N, t) = \frac{1}{\sqrt{N!}}\det\psi_i(\mathfrak{r}_j, t) \tag{16}$$

erhält man aus beiden Variationsprinzipien HARTREE—FOCK-Gleichungen, die sich von den zeitunabhängigen nur durch

$$\varphi_i(\mathfrak{r}) \rightarrow \psi_i(\mathfrak{r}, t) \quad \text{und} \quad \varepsilon_i \rightarrow -\frac{\hbar}{i}\frac{\partial}{\partial t} \tag{17}$$

unterscheiden. Sie haben die Form

$$-\frac{\hbar}{i}\,\frac{\partial}{\partial t}\,\psi_i(\mathfrak{r},t) = h\,\psi_i(\mathfrak{r},t)$$

mit
$$h = -\frac{\hbar^2}{2m}\,\frac{\partial^2}{\partial \mathfrak{r}^2} + \Sigma_j \int d\mathfrak{r}'\,\psi_j^*(\mathfrak{r}',t)\,v(\mathfrak{r},\mathfrak{r}')\,[1-P]\,\psi_j(\mathfrak{r}',t) \tag{18}$$

und
$$P\psi_j(\mathfrak{r}',t)\,\psi_i(\mathfrak{r},t) = \psi_j(\mathfrak{r},t)\,\psi_i(\mathfrak{r}',t)\,, \qquad P^2 = 1\,.$$

Für stationäre Lösungen $\psi_i(\mathfrak{r}, t) = \varphi_i(\mathfrak{r}) \exp(-i\,\varepsilon_i\,t/\hbar)$ gehen sie in die zeitunabhängigen HARTREE—FOCK-Gleichungen über. Im allgemeinen werden kompliziertere Näherungsansätze durchaus zu verschiedenen Resultaten führen, je nachdem welches Variationsprinzip verwendet wird. Wegen seiner echten Minimaleigenschaft ist dann das letztere vorzuziehen.

Mit dem Minimalprinzip (13) können Stabilitätsuntersuchungen für Näherungslösungen vorgenommen werden. Sie lassen sich auf ein »Verfahren der kleinen Schwingungen« zurückführen. Die dabei auftretenden Eigenschwingungen entsprechen kollektiven Anregungen des Grundzustandes [45].

52. *Streuprozesse*

In ihrer allgemeinsten Fragestellung sind Streuprozesse instationäre Vielkörperprobleme. Ein einzelnes Teilchen wird auf ein Target geschossen. Seine physikalischen Eigenschaften nach dem Verlassen des Targets geben Auskunft über die Wechselwirkung des Teilchens mit dem Target und damit, weil dieses aus vielen Teilchen besteht, auch über die Wechselwirkung der das Target aufbauenden Teilchen selbst.

Prinzipiell interessiert nur das asymptotische Verhalten der ein- und auslaufenden Teilchen. Da das wegen der Vielkörperstruktur in seiner Komplexität nicht vollständig erfassbar ist, begnügt man sich mit Näherungen. Die einfachste besteht darin, dass man annimmt: Ein Teilchen wird an einem lokalen (oder nichtlokalen) Potential elastisch gestreut. Damit werden Prozesse, bei denen das Teilchen eingefangen wird oder ein oder mehrere Teilchen aus dem Target herausschlägt, von vornherein ausgeschlossen. Setzt man elastische Streuung voraus, so ist eine FOURIERzerlegung der Gesamtwellenfunktion in einzelne Komponenten mit voneinander verschiedenen Impulsen $\hbar\mathfrak{k}$ möglich, die der stationären SCHRÖDINGERgleichung (1) genügen. Zur Vereinfachung soll ein reines Zentralkraftpotential betrachtet werden.

$$\left[\frac{\partial^2}{\partial \mathfrak{r}^2} + k^2 + w(r)\right]\varphi(\mathfrak{r}) = 0 \qquad w(r) = -\frac{2m\,V(r)}{\hbar^2}\,. \tag{1}$$

In grossem Abstand vom Target setzt sich φ aus einer bezüglich des Targets einlaufenden ebenen Welle und einer auslaufenden Kugelwelle zusammen.

$$\varphi(\mathfrak{r}) \to e^{i\mathfrak{k}\mathfrak{r}} + f(\vartheta)\frac{e^{ikr}}{r} \quad \text{mit} \quad r \to \infty\,. \tag{2}$$

Eine einfache Darstellung erhält man, wenn (2) nach Eigenfunktionen des Drehimpulsquadrates $P_l(\vartheta)$ entwickelt wird.

$$\varphi(\mathfrak{r}) = \Sigma_l\, C_l \frac{u_l(r)}{r} P_l(\vartheta)\,. \tag{3}$$

Die $u_l(r)$ genügen der Differentialgleichung

$$[L - k^2]\, u_l(r) \equiv \left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 + w(r)\right] u_l(r) = 0 \tag{4}$$

mit dem asymptotischen Verlauf

$$\begin{aligned} u_l(0) &= 0 \qquad \text{für } r = 0 \\ u_l &\to A \sin\left(kr - \frac{l\pi}{2} + \eta_l\right) \quad \text{für } r \to \infty\,. \end{aligned} \tag{5}$$

Es kann gezeigt werden, dass mit Kenntnis der Streuphasen η_l der gesamte Streuprozess eindeutig beschrieben wird [46].

Zur Berechnung von Streuphasen haben sich Variationsverfahren als geeignet erwiesen. Die möglichen Variationsmethoden lassen sich grundsätzlich in zwei Gruppen unterteilen. Bei der ersten geht man von der Differentialgleichung für $u_l(r)$ aus (Hulthen [42], Kohn [41]), während die zweite auf einer Integralgleichung für $u_l(r)$ beruht (Schwinger [43]). Hulthen benutzt als Ausgangspunkt ein Funktional I_l, das eine ähnliche Gestalt hat wie das zur Berechnung gebundener Zustände (Teil 4) verwendete

$$I_l = \int_0^\infty dr\, u_l(r)\,(L - k^2)\, u_l(r). \tag{6}$$

Die Variationen der $u_l(r)$ unterliegen den Nebenbedingungen

$$\begin{aligned} \delta u_l(r) &= 0 \qquad \text{für} \quad r = 0 \\ \delta u_l(r) &\to (A + \delta A)\cdot \cos\left(kr - \frac{l\pi}{2} + \eta_l\right)\delta\eta_l \qquad \text{für} \quad r \to \infty\,. \end{aligned} \tag{7}$$

Unter Berücksichtigung von (7) erhält man für δI_l

$$\begin{aligned} \delta I_l &= 2\int dr\, \delta u_l\, (L - k^2)\, u_l + \left(u_l \frac{d}{dr} \delta u_l - \delta u_l \frac{d}{dr} u_l \right) \Bigg|_0^\infty \\ \delta I_l &= 2\int dr\, \delta u_l\, (L - k^2)\, u_l - k A^2\, \delta\eta_l\,. \end{aligned} \tag{8}$$

Genügt $u_l(r)$ der Gleichung (4), dann folgt aus (8)

$$\delta I_l = -k A^2 \delta \eta_l\,. \tag{9}$$

Die Amplitude A kann möglicherweise noch von η_l abhängen. Mit

$$A = \sqrt{f'(\eta_l)} \tag{10}$$

geht (8) in

$$\delta I_l = -k\, \delta f(\eta_l) \tag{11}$$

über. Hulthen stellt an die Variation von u_l eine weitere Bedingung. Es soll stets gelten

$$I_l = 0\,. \tag{12}$$

Während aus (11) folgt, dass damit η_l nicht variiert werden darf, kann $u_l(r)$ für endliche r durchaus allen möglichen Variationen unterliegen. Stellt man $u_l(r)$ in der Form

$$u_l(r) = u_l\,(r;\, c_1, \ldots c_n,\, \eta_l) \tag{13}$$

dar, ergibt sich aus (11) und (12) ein Satz von $n + 1$ Bestimmungsgleichungen für $c_1, \ldots c_n$ und η_l

$$\frac{\partial I_l}{\partial c_i} = 0 \qquad i = 1 \ldots n \qquad I_l = 0\,. \tag{14}$$

Im Gegensatz zu Hulthen lässt Kohn Variationen der η_l zu. Mit (11) lässt sich in diesem Fall ein stationäres Funktional der Gestalt

$$F_l \equiv k f(\eta_l) + I_l \quad \text{mit} \quad \delta F_l = 0 \tag{15}$$

konstruieren. Bei beliebigen Variationen (bis auf die Randbedingungen aus (7)) der u_l folgt (4). Hat $u_l(r)$ die Form (13), so erhält man ebenfalls $n + 1$ Gleichungen für die Variationsparameter

$$\frac{\partial F_l}{\partial c_i} = \frac{\partial I_l}{\partial c_i} = 0 \qquad i = 1 \ldots n \qquad \frac{\partial I_l}{\partial \eta_l} = -k f'(\eta_l)\,. \tag{16}$$

Mit speziellen Ansätzen für A in (10) können verschiedene Formen für F_l angegeben werden:

$$A_l = 1 \qquad F_l = k\eta_l; \qquad A_l = \cos^{-1}\eta_l \qquad F_l = k\tan\eta_l \tag{17}$$

$$A_l = \sin^{-1}\eta_l \qquad F_l = -k\cot\eta_l\,.$$

Während die Variationsverfahren von HULTHEN—KOHN von der Differentialgleichung ausgehen, benutzt SCHWINGER die aus der Differentialgleichung und den Randbedingungen für $u_l(r)$ folgende Integralgleichung

$$u_l(r) = \sin\left(kr - \frac{l\pi}{2} + \eta_l\right) + \int dr'\, G(r, r')\, w(r')\, u_l(r')\,. \tag{18}$$

Die GREENsche Funktion $G(r, r')$ lässt sich aus der Differentialgleichung bestimmen [46]. Die Gleichung (18) wird als EULERsche Gleichung des stationären Funktionals

$$k^{-1}\cot\eta_l = \frac{\int dr\, u_l\, w\, u_l - \int\int dr\, dr'\, u_l\, w\, G(r, r')\, w'\, u_l'}{\left[\int dr\, \sin\left(kr - \frac{l\pi}{2} + \eta_l\right) w\, u_l\right]^2} \tag{19}$$

erhalten.

Das SCHWINGERsche Variationsverfahren stellt eine sehr elegante Formulierung für Streuprobleme dar. Wegen der etwas komplizierten GREENschen Funktion $G(r, r')$ entstehen bei detaillierteren Variationsansätzen aber Schwierigkeiten beim Auswerten der Integrale. Deshalb wird die Methode nach HULTHEN—KOHN der von SCHWINGER häufig vorgezogen. Beiden Verfahren ist gemeinsam, dass sie keine Extremalprinzipien sind. Deshalb ist bei Näherungen eine Aussage über den Fehler nicht möglich.

Sowohl das HULTHEN—KOHNsche als auch das SCHWINGERsche Variationsverfahren besitzen noch einen Mangel. Bei der Wahl beliebiger Versuchsfunktionen kann es vorkommen, dass die zur Ableitung der EULERschen Gleichung zu erfüllenden Nebenbedingungen (asymptotisches Verhalten) nicht gewahrt bleiben. Dadurch entstehen Inkonsistenzen in der Rechnung, die z. B. das Auftreten von Singularitäten der Variationsparameter c_i bei bestimmten Wellenzahlen k nach sich ziehen können [47]. Die Schwierigkeiten lassen sich bei genauerer Betrachtung der auszuwählenden Nebenbedingungen beheben, wie von MALIK [48] gezeigt werden konnte. Eine zusammenfassende Darstellung von Variationsprinzipien bei Streuprozessen, die nicht nur auf elastische Streuung im Zentralkraftfeld beschränkt bleiben, wird von DEMKOW [49] gegeben.

6. Irreversible Phänomene

Bei stationären irreversiblen Prozessen hat die Entropieproduktion $N_S = dS/dt$ Extremaleigenschaften. Diese Tatsache wird zur Konstruktion von Variationsprinzipien ausgenutzt. In Kap. 61 und Kap. 62 werden zunächst die verschiedenen Extremalprinzipien zusammengestellt. Dabei wird eine makroskopische Beschreibungsweise gewählt, die keine unmittelbaren Aussagen über Vielkörperstrukturen zulässt. Es kann aber gezeigt werden (Kap. 63), dass auch bei einer mikroskopischen Theorie die Variationsprinzipien für stationäre irreversible Prozesse den Gedanken der extremalen Entropieproduktion als Grundlage enthalten. Anwendungen der so abgeleiteten Variationsverfahren werden in Kap. 64 behandelt.

61. Das Prigogine*sche Minimalprinzip*

Im folgenden soll der zeitliche Ablauf eines Systems betrachtet werden, dass sich anfangs in einem Nichtgleichgewichtszustand befindet. Ohne irgendwelchen Eingriff von aussen würde sich das System nach genügend grosser Zeit einem Gleichgewichtszustand nähern. Hier werden dagegen Systeme untersucht, deren Endzustand auch noch ein Nichtgleichgewichtszustand ist, bei dem aber eine stationäre Stromverteilung vorliegen soll. Damit solch ein Endzustand möglich ist, muss ein Eingriff von aussen erfolgen (z. B. Anlegen einer konstanten äusseren Kraft).

Prigogine [50] konnte zeigen, dass für diesen stationären Endzustand die Entropieproduktion ein Minimum annimmt. Das wird hier vereinfachend für ein System mit nur einem inneren Parameter a, der sich im Zeitablauf ändert, abgeleitet.

Betrachtet wird die zeitliche Änderung der Entropie $S(a(t))$, die bei dem zu untersuchenden irreversiblen Übergang nach dem II. Hauptsatz der Thermodynamik stets die Bedingung

$$N_s = \frac{dS}{dt} = \dot{a}\,\frac{dS}{da} \geq 0 \tag{1}$$

erfüllt. $\dot{a}$ bzw. dS/da können als verallgemeinerter thermodynamischer Strom bzw. als thermodynamische Kraft aufgefasst werden. Entsprechend (1) muss zwischen beiden im Rahmen einer linearen Näherung (nur kleine Ströme $\dot{a}$)

$$\dot{a} = \lambda \frac{dS}{da} \qquad \text{mit} \quad \lambda > 0 \tag{2}$$

gelten. Für die Änderung der Entropieproduktion im Zeitablauf erhält man dagegen mit (2) und $d\lambda/dt = 0$

$$\delta N_S = \delta t \left(\ddot{a}\,\frac{dS}{da} + \dot{a}\,\frac{d}{dt}\,\frac{dS}{da} \right) = 2\,\delta t\,\dot{a}\,\frac{d}{dt}\,\frac{dS}{da}\,. \tag{3}$$

Entwickelt man die Kraft dS/da um die Gleichgewichtslage

$$\frac{dS}{da} = \left(\frac{dS}{da}\right)_0 + (a - a_0)\left(\frac{d^2 S}{da^2}\right)_0 \tag{4}$$

und berücksichtigt man, dass die Entropie im Gleichgewicht ein Maximum annimmt, dann folgt mit (3) sofort

$$\delta N_s = 2\,\delta t\,\dot{a}^2 \left(\frac{d^2 S}{da^2}\right)_0 \leq 0. \tag{5}$$

Das Ergebnis ist plausibel, wenn man (3) betrachtet. Es besagt, dass die zeitliche Änderung der verallgemeinerten Kräfte den zu einem bestimmten Zeitpunkt fliessenden Strömen stets entgegengerichtet ist. Aus (1) und (5) ergibt sich nun unmittelbar, dass die Entropieproduktion im stationären Endzustand ein Minimum annimmt. Diese Minimaleigenschaft der Entropieproduktion ist nicht nur auf einparametrige Systeme beschränkt. Sie existiert ebenso, wenn sich mehrere Parameter gleichzeitig ändern. Voraussetzung ist nur, dass zwischen den verallgemeinerten Strömen I_i und Kräften K_i die Beziehungen

$$I_i = \Sigma_k L_{ik} K_k \tag{6}$$

mit $L_{ik} = L_{ki}$ als den bekannten ONSAGERrelationen (zu deren Ableitung siehe [51]) gelten. Gleichzeitig kann das hier erhaltene Resultat auf ortsabhängige Phänomene ausgedehnt werden. Die Parameter a_i werden durch »lokale« Parameter $\xi_i(\mathfrak{r}, t)$ mit den dazugehörigen Stromdichten $\mathfrak{j}_i(\mathfrak{r}, t)$ ersetzt. Es gilt dann

$$\begin{aligned} \frac{dS}{dt} = \int d\mathfrak{r}\,\frac{d\sigma}{dt} &= -\oiint d\mathfrak{f}\,\Sigma_i\,\mathfrak{j}_i\,\frac{\partial\sigma}{\partial\xi_i} + \int d\mathfrak{r}\,\Sigma_i\,\mathfrak{j}_i\,\frac{\partial}{\partial\mathfrak{r}}\,\frac{\partial\sigma}{\partial\xi_i} \\ &\equiv -\oiint d\mathfrak{f}\,\mathfrak{J}_s + N_s. \end{aligned} \tag{7}$$

Während $\mathfrak{J}_s$ als Entropiestromdichte interpretiert werden kann, stellt N_s die im betrachteten Integrationsbereich erzeugte Entropie, die Entropieproduktion, dar. Aus (7) folgt, dass sich die Entropieproduktionsdichte als Produkt verallgemeinerter Ströme I_i und Kräfte K_i (die den $\mathfrak{j}_i$ und $\partial^2\sigma/\partial\mathfrak{r}\,\partial\xi_i$ aus (7) entsprechen) darstellen lässt. Im stationären Endzustand nimmt die Entropieproduktion ein Minimum an. Das folgende Beispiel soll die hier angestellten Überlegungen etwas illustrieren.

Zwischen zwei Äquipotentialflächen U_1, U_2 befindet sich ein den elektrischen Strom leitendes Medium. Die Potentiale U_1 und U_2 werden während der ganzen Zeit konstant gehalten. Im Innern der Substanz wird zu Beginn des Prozesses als Störung eine ungleichmässig verteilte Ladungsverteilung angebracht. In der Nähe der linken Platte sollen vor allem positive, in der Nähe der rechten vor allem negative Ladungen angehäuft sein. Der Stromfluss wird diese Störung ausgleichen, d. h. er wird eine ihm entgegengerichtete zeitliche Änderung des elektrischen Feldes verursachen. Während die Entropieproduktion bis auf einen Faktor T^{-1} gleich der JOULEschen Wärme ist und deshalb stets grösser als Null sein muss, ist ihre Änderung beim Einstellen des stationären Endzustandes negativ:

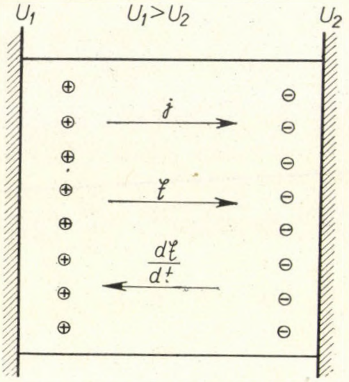

Abb. 2. Zur Veranschaulichung des PRIGOGINEschen Minimalprinzips

$$N_s = \frac{1}{T}\int d\mathfrak{r}\,\mathfrak{j}\mathfrak{E} > 0\,, \qquad \delta N_s = \frac{2\delta t}{T}\int d\mathfrak{r}\,\mathfrak{j}\,\frac{d\mathfrak{E}}{dt} \leq 0. \tag{8}$$

Im stationären Endzustand nimmt die Entropieproduktion ein Minimum an.

Mit
$$\mathfrak{E} = -\frac{\partial U}{\partial \mathfrak{r}}\,, \quad \mathfrak{j} = \sigma\mathfrak{E} \quad \text{und} \quad \sigma = \text{konst} \tag{9}$$

gilt im stationären Endzustand:

$$N_s = \int d\mathfrak{r}\,\sigma\left(\frac{\partial U}{\partial \mathfrak{r}}\right)^2$$

$$\delta^1 N_s = 2\int d\mathfrak{r}\,\frac{\partial \delta U}{\partial \mathfrak{r}}\cdot\frac{\partial U}{\partial \mathfrak{r}} = 2\oiint d\mathfrak{f}\,\sigma\,\delta U\,\frac{\partial U}{\partial \mathfrak{r}} - 2\int d\mathfrak{r}\,\sigma\,\delta U\,\frac{\partial^2 U}{\partial \mathfrak{r}^2} \tag{10}$$

$$= 0 - 2\int d\mathfrak{r}\,\sigma\,\delta U\,\frac{\partial^2 U}{\partial \mathfrak{r}^2} = 0\,,$$

d. h.

$$\frac{\partial^2}{\partial \mathfrak{r}^2}\,U = 0\,.$$

Das Oberflächenintegral verschwindet, da am Rand U konstant ist bzw. $\partial U / \partial \mathfrak{r}$ senkrecht zur Flächennormale gerichtet ist. Im stationären Endzustand befinden sich zwischen den Äquipotentialflächen keine Ladungen mehr, denn aus (10) folgt

$$-\frac{\partial^2 U}{\partial \mathfrak{r}^2} = \frac{\partial \mathfrak{E}}{\partial \mathfrak{r}} = \varrho(\mathfrak{r}) = 0 . \tag{11}$$

Bei der Ableitung des PRIGOGINEschen Minimalprinzips werden über den Zusammenhang zwischen den verallgemeinerten Kräften und Strömen

$$I_i = \Sigma_k L_{ik} K_k \tag{12}$$

folgende Voraussetzungen gemacht:

1. Gültigkeit des ONSAGERrelationen $L_{ik} = L_{ki}$
2. Konstanz der L_{ik} .

Während die erste Forderung beim Fehlen von Magnetfeldern im allgemeinen erfüllt ist (der Fall $\mathfrak{B} \neq 0$ wird in Kap. 63 behandelt), kann die Konstanz der L_{ik} gegebenenfalls verletzt werden. Wie GLANSDORFF u. a. [52] zeigten, gilt dann das Minimalprinzip der Entropieproduktion nicht mehr. Als Beispiel behandeln sie die Bewegung einer zähen inkompressiblen Flüssigkeit mit ungleichmässiger Temperaturverteilung.

Sie führen ein »lokales Potential« N_s^* ein, indem sie für die L_{ik} in den Ausdruck für die Entropieproduktion die nullte Ordnung einer Entwicklung um den stationären Endzustand einsetzen:

$$N_s^* = \int d\mathfrak{r}\, \Sigma_{i,k} L_{ik}^0 K_i K_k . \tag{13}$$

Die K_i stellen die verallgemeinerten Kräfte des jeweiligen Zustandes dar, dagegen sind die L_{ik}^0 die ONSAGERkoeffizienten für den stationären Endzustand. N_s^* nimmt im stationären Endzustand ein Minimum bezüglich aller Zustände in seiner engeren Nachbarschaft an. Diese einschränkende Bedingung besteht bei konstanten L_{ik} nicht. Eine Schwierigkeit besteht darin, dass die L_{ik}^0 zunächst unbekannt sind. Der stationäre Endzustand soll ja erst berechnet werden. Ein möglicher Weg zur Bestimmung der L_{ik}^0 bietet sich in einem Iterationsverfahren an. Ausgehend von einem Anfangssatz der L_{ik}^0 können diese mit den sich jeweils daraus ergebenden K_i und I_i für den stationären Endzustand beliebig verbessert werden. Die Methode des »lokalen Potentials« wird teilweise schon benutzt, um nicht nur rein dissipative Erscheinungen zu beschreiben, sondern mit ihr können auch Prozesse erfasst werden, die reversible und irreversible Anteile (z. B. Wärmekonvektion und Wärmeleitung) enthalten [53].

62. Minimal- und Maximalprinzip der Entropieproduktion

Das PRIGOGINEsche Minimalprinzip macht Aussagen über die Annäherung eines Systems an einen stationären Zustand von einem von diesem makroskopisch verschiedenen Ausgangszustand aus. Der stationäre Endzustand besitzt gegenüber allen von ihm verschiedenen Zuständen

$$\text{mit} \qquad \begin{gathered} I_i = I_i^0 + \delta I_i^{Ma} \qquad K_i = K_i^0 + \delta K_i^{Ma} \\ \delta I_i^{Ma} = \Sigma_k L_{ik} \, \delta K_k^{Ma} \end{gathered} \tag{1}$$

minimale Entropieproduktion. δI_i^{Ma} und δK_i^{Ma} sind makroskopische Änderungen der verallgemeinerten Ströme und Kräfte, die miteinander eindeutig verbunden sind. Anstelle makroskopischer Variationen der Ströme und Kräfte können auch nur mikroskopische zugelassen werden, für die die dritte Beziehung aus (1) nicht mehr gelten muss. Betrachtet man beliebige mikroskopische Schwankungen der Ströme und hält dabei die Kräfte konstant, so kann ein dissipatives System im stationären Endzustand durch folgendes Variationsprinzip [54] beschrieben werden:

$$\begin{gathered} \int d\mathfrak{r} \, (2\,\nu_s - \bar{\nu}_s) = \text{Max.} \\ \text{mit} \quad \nu_s = \Sigma_i \, I_i \, K_i \quad \text{und} \quad \bar{\nu}_s = \Sigma_{i,k} \, I_i \, R_{ik} \, I_k \, . \end{gathered} \tag{2}$$

Die Variation erfolgt unter der Nebenbedingung konstanter Kräfte. Die EULERschen Gleichungen von (2) haben die Gestalt

$$K_i = \Sigma_k R_{ik} I_k \quad \text{bzw.} \quad I_i = \Sigma_k L_{ik} K_k \quad \text{mit} \quad (R_{ik}) \equiv (L_{ik})^{-1} \, . \tag{3}$$

Betrachtet man die zweite Variation

$$\delta^2 \int d\mathfrak{r} \, (2\nu_s - \bar{\nu}_s) = - \int d\mathfrak{r} \, \Sigma_{i,k} \, R_{ik} \, \delta I_i \, \delta I_k \, , \tag{4}$$

so erkennt man, da sie gleich dem negativen der zweiten Variation beim PRIGOGINEschen Minimalprinzip ist, dass hier im stationären Endzustand ein Maximum angenommen wird.

Da das Prinzip auf den stationären Endzustand angewandt wird, muss die Entropiebilanz für diesen Zustand

$$\frac{dS}{dt} = - \oint\!\!\oint d\mathfrak{f} \, \mathfrak{J}_s + \int d\mathfrak{r} \Sigma_i \, I_i \, K_i = 0 \tag{5}$$

zur Betrachtung mit hinzugezogen werden. (5) stellt eine Bedingung für die möglichen Schwankungen der I_i dar, denn nach Voraussetzung soll bei diesen mikroskopischen Änderungen der makroskopische Zustand nicht geändert werden. (5) muss also stets erfüllt sein.

Es werden jetzt zwei Fälle unterschieden. Einmal kann man Schwankungen betrachten, die am Rande verschwinden. Mit (5) folgt dann

$$\delta \int d\mathfrak{f}\, \mathfrak{J}_s = \delta \int d\mathfrak{r}\, \nu_s = 0\,. \tag{6}$$

Das Variationsprinzip (2) geht in ein Minimalprinzip

$$\int d\mathfrak{r}\, \bar{\nu}_s = \text{Min.} \tag{7}$$

über. Erlaubt man dagegen, dass die Randströme auch den Schwankungen unterliegen, so kann man ν_s beliebig variieren. Der Einfachheit halber werden Variationen betrachtet, bei denen stets

$$\nu_s = \bar{\nu}_s \tag{8}$$

sein soll. Aus (2) folgt dann ein Prinzip der maximalen Entropieproduktion

$$\int d\mathfrak{r}\, \bar{\nu}_s = \text{Max.} \tag{9}$$

Zusammenfassend kann man sagen: Der stationäre Zustand eines dissipativen Systems ist ein Sattelpunkt auf einer hypothetisch einführbaren Entropieproduktionsfläche. Dieser Sattelpunkt ist ein Minimum bezüglich makroskopischer Variationen, bei denen alle möglichen instabilen Zustände vom Anfangszustand aus durchlaufen werden. Für mikroskopische Variationen wird die Entropieproduktion minimal bei Schwankungen der Ströme und festen Kräften, wenn die Randströme konstant sind. Gegenüber Variationen mit veränderlichen Randströmen nimmt sie einen Maximalwert an.

63. Lösung der BOLTZMANN*gleichung mit Variationsprinzipien*

Wie gezeigt wurde, bietet das Prinzip der extremalen Entropieproduktion eine Möglichkeit, stationäre irreversible Prozesse zu behandeln. Es ist deshalb zu erwarten, dass sich ein Variationsprinzip zur Lösung der BOLTZMANNgleichung bei kleinen Abweichungen vom lokalen Gleichgewicht darauf zurückführen lassen muss. Zunächst wird die BOLTZMANNgleichung durch Linearisierung in eine Form gebracht, die eine Auswertung durch Variationsverfahren zulässt. Gleichzeitig wird die Verbindung zwischen der BOLTZMANNgleichung und der Entropieerzeugung klargestellt. Für die linearisierte BOLTZMANNgleichung werden für den Fall $\mathfrak{B} = 0$ bzw. $\mathfrak{B} \neq 0$ Variationsprinzipien angegeben, die sich im wesentlichen mit dem Prinzip der maximalen Entropieproduktion identifizieren lassen.

Die BOLTZMANNgleichung

$$D_1 f(1,t) = \int dl'\, d2\, d2'\, \{f(1',t) f(2',t) - f(1,t) f(2,t)\}\ \Gamma(1',2' \rightarrow 1,2)$$

$$f(i,t) \equiv f(\mathfrak{r}_1, \mathfrak{p}_i, t) \qquad \int di \equiv \int d\mathfrak{p}_i \tag{1}$$

$$D_1 \equiv \frac{\partial}{\partial t} + \frac{\mathfrak{p}_1}{m} \frac{\partial}{\partial \mathfrak{r}_1} + \mathfrak{K}_1 \frac{\partial}{\partial \mathfrak{p}_1}$$

beschreibt irreversible Prozesse in der kinetischen Gastheorie. Im folgenden soll wie in Gleichung (1) entgegen den sonstigen Gepflogenheiten $d1$ nur eine Integration über $\mathfrak{p}_1$ darstellen.

Da (1) eine nichtlineare Bestimmungsgleichung für die Einteilchenverteilungsfunktion ist, bereitet ihre Auswertung im allgemeinen Schwierigkeiten. Für den Fall, dass nur Lösungen gesucht werden, die sich in der Nähe eines lokalen Gleichgewichts $f^0(1,t)$ befinden, kann die Gleichung (1) mit dem Ansatz

$$f(1,t) = f^0(1,t)\,(1 + \Phi(1,t)) \qquad \Phi \ll 1 \tag{2}$$

linearisiert werden. Man erhält damit für (1)

$$\begin{aligned} -D_1 f^0(1,t) = \int d1'\, d2\, d2' f^0(1,t) f^0(2,t)\, [\Phi(1,t) + \Phi(2,t) - \Phi(1',t) - \\ - \Phi(2',t)]\ \Gamma(1',2' \rightarrow 1,2)\,, \end{aligned} \tag{3}$$

was künftig in der verkürzten Form

$$K(1,t) = R\, \Phi(1,t) \tag{4}$$

geschrieben werden soll. Dabei hängt die linke Seite von (4) nur noch von $f^0(1,t)$ ab.

Um die Irreversibilität der durch (1) bzw. (4) beschriebenen Prozesse zu zeigen, wird für diese Gleichung die Entropiebilanz aufgestellt. Mit dem in der kinetischen Theorie definierten Ausdruck

$$\mu\, s = -k \int d1\, f(1)\, (\ln f(1) - 1) \tag{5}$$

für die Entropie pro Volumeneinheit ergibt sich aus (1) die Bilanzgleichung

$$\frac{\partial \mu s}{\partial t} + \frac{\partial}{\partial \mathfrak{r}} (\mu s \bar{\mathfrak{v}} + \mathfrak{J}_s) = \nu_s\,, \tag{6}$$

wobei $\bar{\mathfrak{v}}$ die mittlere Geschwindigkeit, $\mathfrak{S}_s$ die Entropiestromdichte und ν_s die Entropieproduktionsdichte sind. ν_s hat die Gestalt

$$\nu_s = -k \int d1\, d2\, d1'\, d2' \ln f(1)\, [f(1')f(2') - f(1)f(2)]\, \Gamma(1',2' \rightarrow 1,2). \quad (7)$$

Für die linearisierte Boltzmanngleichung gilt dieselbe Entropiebilanz mit

$$\nu_s = k \int d1\, \Phi(1,t)\, R\, \Phi(1,t) \equiv k \langle \Phi, R\, \Phi \rangle. \quad (8)$$

(8) folgt aus (7), wenn man für $f(1,t)$ den Ansatz (2) benutzt und Glieder bis zur zweiten Ordnung in Φ berücksichtigt.

Um für die linearisierte Boltzmanngleichung

$$K(1,t) = R\, \Phi(1,t) \quad (9)$$

ein Variationsprinzip zu konstruieren, kann man den in Kap. 62 abgeleiteten Formalismus benutzen. Die Gleichung (9) lässt sich in diesem Rahmen als verallgemeinerte Strom-Kraft-Relation interpretieren [55]. Die verallgemeinerte Kraft K ist durch den hier als Integraloperator auftretenden reziproken »Onsagerkoeffizienten« R mit dem verallgemeinerten Strom Φ verknüpft. Wie man aus der Definition von $K(1,t)$ (4) sieht, bleibt $K(1,t)$ bei beliebigen Änderungen von $\Phi(1,t)$ konstant. Die Änderungen des verallgemeinerten Stromes Φ können als Schwankungen im Sinne der von Onsager abgeleiteten Theorie gedeutet werden. Da sie im allgemeinen keinen speziellen Randbedingungen unterworfen sein werden, wird das Variationsprinzip für (9) die Struktur von (62.9) haben.

Mit dem in (8) definierten Skalarprodukt

$$\langle \Phi, \Psi \rangle = \int \Phi(1)\, \Psi(1)\, d1 \quad (10)$$

wird das Funktional

$$F = \langle \Phi, R\, \Phi \rangle \quad (11)$$

unter der Nebenbedingung

$$\langle \Phi, R\, \Phi \rangle = \langle \Phi, K \rangle \quad (12)$$

zum Extremum gemacht. F nimmt ein Maximum an. Vergleicht man (11) mit (8), so sieht man, dass das Funktional F bis auf einen konstanten Faktor k gleich der Entropieproduktion ist. Führt man die Variation in (11) aus

$$\delta\, (\langle \Phi, R\, \Phi \rangle + \lambda\, \{\langle \Phi, R\, \Phi \rangle - \langle \Phi, K \rangle\}) = 0 \quad (13)$$

und benutzt zur Bestimmung von λ die Nebenbedingung (12), so erhält man schliesslich

$$\frac{1}{2}(R + R^T)\, \Phi = K\,, \quad (14)$$

was mit (9) identisch ist, falls der Operator R gleich seinem adjungierten Operator R^T ist. Diese den ONSAGERrelationen entsprechende Forderung an R ist erfüllt, wenn die mikroskopische Reversibilität $\Gamma(1', 2' \rightarrow 1, 2) = \Gamma(1, 2 \rightarrow 1', 2')$ garantiert ist. Rückblickend kann man feststellen, dass das in (13) angegebene Variationsprinzip mit dem aus (62.9) identisch ist. Die Nebenbedingung (12) entspricht der Forderung (62.8).

Bei Anwesenheit von Magnetfeldern muss in der linearisierten BOLTZMANNgleichung der Zusatzterm der magnetischen Kraft berücksichtigt werden, der linear vom Magnetfeld $\mathfrak{B}$ abhängt. Die linearisierte Gleichung hat nun die Form (15), wobei der Operator M bezüglich des in (10) eingeführten Skalarproduktes nicht mehr selbstadjungiert ist (16).

$$K = M\,\Phi \tag{15}$$

$$M^T(\mathfrak{B}) = M(-\mathfrak{B}). \tag{16}$$

Wegen (16) leistet das Magnetfeld keinen expliziten Beitrag zur Entropieproduktion

$$\nu_S = k \langle \Phi, M\,\Phi \rangle. \tag{17}$$

Der in $\mathfrak{B}$ lineare Term fällt aus ν_S heraus. Diese Tatsache ist verständlich, da Entropiezuwachs nur durch Streuprozesse, nicht aber durch die reversible Bewegung im Magnetfeld erfolgt. Implizit hängt ν_S natürlich doch von $\mathfrak{B}$ ab, da durch (15) Φ mit $\mathfrak{B}$ zusammenhängt.

In dem in (11) abgeleiteten Variationsprinzip würde der Term proportional zu $\mathfrak{B}$ auch verschwinden. Das darf aber nicht eintreten, da dann die Φ bestimmende Integralgleichung unabhängig von $\mathfrak{B}$ wäre. Deshalb muss nach ZIMAN [56], GARCIA-MOLINER [57] u. a. zur Formulierung eines Variationsverfahrens für (15) ein neues Skalarprodukt der Art

$$\ll \Phi, \Psi \gg\; = \langle \Phi(-\mathfrak{B}), \Psi(\mathfrak{B}) \rangle \tag{18}$$

eingeführt werden, für das M dann selbstadjungiert ist. Damit kann das Variationsprinzip aus (13) übernommen werden:

$$\delta \{\ll \Phi, M\,\Phi \gg + \lambda (\ll \Phi, M\,\Phi \gg - \ll \Phi, K \gg)\} = 0. \tag{19}$$

Beim Einführen der neuen Metrik (18) bleibt M nicht mehr positiv definit. Das hat zur Folge, dass (19) kein Extremalprinzip ist. Für nichtselbstadjungierte Operatoren ist entsprechend Kap. 21 auch ein anderes Vorgehen möglich. Man fügt zu (15) die (bzgl. des Skalarproduktes (10)) adjungierte Gleichung

$$K = M^T\,\Psi \tag{20}$$

hinzu. Beide Gleichungen folgen aus

$$\delta\,\{\langle \Psi, K\rangle + \langle K, \Phi\rangle - \langle \Psi, M\,\Phi\rangle\} = 0, \tag{21}$$

falls Ψ und Φ bei konstantem K unabhängig voneinander variiert werden.

64. *Anwendungen*

Die angegebenen Variationsverfahren wurden vor allem mit Erfolg bei der Beschreibung von Transportphänomenen in elektrischen Leitern angewendet. Ausgangspunkt ist nicht die Boltzmanngleichung aus Kap. 63, sondern eine modifizierte Form (Blochgleichung), die im Stossterm den quantenmechanischen Charakter der Prozesse berücksichtigt. Für stationäre Vorgänge hat sie die Gestalt

$$\mathfrak{v}_\mathfrak{k}\frac{\partial f_\mathfrak{k}}{\partial \mathfrak{r}} + \frac{e\mathfrak{E}}{\hbar}\frac{\partial f_\mathfrak{k}}{\partial \mathfrak{k}} = \int d\mathfrak{k}'\,Q(\mathfrak{k}'\,\mathfrak{k})\left[f_{\mathfrak{k}'}(1-f_\mathfrak{k}) - f_\mathfrak{k}(1-f_{\mathfrak{k}'})\right]. \tag{1}$$

$f_\mathfrak{k}(\mathfrak{r})\,d\mathfrak{k}\,d\mathfrak{r}$ ist die Wahrscheinlichkeit dafür, dass ein Teilchen in einem Intervall $d\mathfrak{r}$ am Ort $\mathfrak{r}$ und innerhalb des Intervalls $\hbar\,d\mathfrak{k}$ mit dem Impuls $\hbar\mathfrak{k}$ angetroffen wird. Im Stossterm wird berücksichtigt, dass die mit der Wahrscheinlichkeit $Q(\mathfrak{k},\mathfrak{k}')$ stattfindenden Übergänge nur von besetzten zu unbesetzten Zuständen möglich sind. Für die Verteilung $f_\mathfrak{k}$ wird in (1) der Ansatz

$$f_\mathfrak{k} = f^0_\mathfrak{k} - \Phi_\mathfrak{k}\frac{\partial f^0_\mathfrak{k}}{\partial E_\mathfrak{k}} \tag{2}$$

eingeführt, um (1) zu linearisieren. $f^0_\mathfrak{k}$ ist die Verteilung für ein lokales Gleichgewicht (lokale Fermiverteilung). $E_\mathfrak{k}$ soll die Energie eines Teilchens mit dem Impuls $\hbar\mathfrak{k}$ sein.

Die linearisierte Gleichung hat die Gestalt

$$\begin{gathered}-\mathfrak{v}_\mathfrak{k}\left[\frac{\partial f^0_\mathfrak{k}}{\partial T}\frac{\partial T}{\partial \mathfrak{r}} + e\,\mathfrak{E}\,\frac{\partial f^0_\mathfrak{k}}{\partial E_\mathfrak{k}}\right] = \frac{1}{k\,T}\int d\mathfrak{k}'\,Q\,(\mathfrak{k},\mathfrak{k}')\,(\Phi_\mathfrak{k}-\Phi_{\mathfrak{k}'})\,f^0_\mathfrak{k}(1-f^0_{\mathfrak{k}'})\\ K' = R'\,\Phi\,.\end{gathered} \tag{3}$$

Gleichung (3) hat dieselbe Struktur wie (63.9). Der hier nicht betrachtete Fall $\mathfrak{B} \neq 0$ würde auf (63.19) führen. Lösungen von (3) sind wie in (63.11) alle die Funktionen, die der Extremalforderung

$$\langle \Phi, R'\Phi\rangle = \text{Max.} \tag{4}$$

unter der Nebenbedingung

$$\langle \Phi, R'\Phi \rangle = \langle \Phi, K' \rangle \tag{5}$$

genügen. Das Maximalprinzip mit Nebenbedingung lässt sich auch in das Minimalprinzip ohne Nebenbedingung

$$\frac{\langle \Phi, R'\,\Phi \rangle}{\{\langle \Phi, K' \rangle\}^2} = \mathrm{Min.} \tag{6}$$

umschreiben. Während (6) für Anwendungen geeigneter ist, besitzt (5) grössere physikalische Anschaulichkeit.

Mit (6) erhält man sehr leicht Ausdrücke zur Berechnung von Transportkoeffizienten. Als Beispiel wird ein Variationsprinzip für den spezifischen elektrischen Widerstand ϱ abgeleitet. Es wird ein System konstanter Temperatur betrachtet, bei dem ausserdem der Widerstand noch richtungsunabhängig sein soll (z. B. kubisches Kristallgitter). Für die Entropieproduktion gilt:

$$\nu_s = \varrho\, \mathfrak{j}^2/T. \tag{7}$$

$\mathfrak{j}$ ist die über $f_{\mathfrak{k}}$ gemittelte Stromdichte

$$\mathfrak{j} = \int d\mathfrak{k}\, e\, \mathfrak{v}_{\mathfrak{k}} f_{\mathfrak{k}} = -\int d\mathfrak{k}\, e\, \mathfrak{v}_{\mathfrak{k}}\, \Phi_{\mathfrak{k}} \frac{\partial f_{\mathfrak{k}}^0}{\partial E_{\mathfrak{k}}}. \tag{8}$$

Das letzte Gleichheitszeichen gilt, da für ϱ Isotropie vorausgesetzt wurde. Aus der linearisierten BLOCHgleichung ergibt sich in Analogie zu Kap. 63 für die durch die Streuung verursachte Entropieproduktion

$$\nu_s = \langle \Phi, R'\Phi \rangle / T. \tag{9}$$

Mit (7), (8) und (9) erhält man für ϱ den Ausdruck

$$\varrho = \frac{\langle \varphi, R'\,\varphi \rangle}{\{\langle \Phi, K'\,(|\mathfrak{E}| = 1) \rangle\}^2}, \tag{10}$$

der im stationären Endzustand ein Minimum annimmt. Ausgehend von Formel (10) wird ϱ mit geeigneten Ansätzen für Φ in entsprechender Näherung berechnet.

KOHLER [58] gelang es, auf diesem Weg die Temperaturabhängigkeit von ϱ in qualitativ guter Übereinstimmung mit der zunächst nur experimentell bekannten GRÜNEISENschen Widerstandsformel zu berechnen. Er erhielt für tiefe Temperaturen eine Abhängigkeit $\varrho \sim T^5$, die bei hohen Werten von T in $\varrho \sim T$ übergeht. Weiterhin konnte er die näherungsweise Gültigkeit der MATHIESSENschen Regel bestätigen, nach der sich der Gesamtwiderstand aus der Summe des idealen Widerstandes und des Restwiderstandes zusammensetzt. Thermoelektrische Effekte berechnet er, indem er in (3) auch den Term proportional $\partial T/\partial \mathfrak{r}$ berücksichtigte. Die Abhängigkeit des Widerstandes von einem Magnetfeld erhält man, falls (3) um das Glied mit der magnetischen Kraft erweitert und ein zu (63.19) analoges Variationsverfahren verwendet wird [57]. Die gesamte Theorie ist zur Berechnung anderer Transportkoeffizienten (z. B. Wärmeleitfähigkeit) ebenso anwendbar.

In neueren Arbeiten wird nicht mehr von der BOLTZMANNgleichung bzw. ihren quantenmechanischen Modifikationen ausgegangen, sondern man benutzt dazu eine linearisierte Form der NEUMANNgleichung für die Dichtematrix im Fall einer vorübergehend eingeschalteten Störung. Das der Gleichung äquivalente Variationsprinzip lässt sich bis auf unwesentliche Faktoren mit der Entropieproduktion identifizieren. Die Formulierungen besitzen teilsweise einen allgemeineren Charakter als die aus der BOLTZMANNgleichung abgeleiteten. Es lässt sich zeigen, dass das Variationsprinzip für die BOLTZMANNgleichung als erstes Glied aus einer Störungsentwicklung des von NAKANO [59] angegebenen Variationsprinzips für die linearisierte NEUMANNgleichung folgt.

7. Zusammenfassung

In der vorliegenden Arbeit wurde gezeigt, welche wichtige Stellung die Variationsrechnung im methodischen Apparat der Theoretischen Physik einnimmt. Es stellte sich heraus, dass Variationsprinzipien zur Beschreibung fast aller physikalischen Erscheinungen anwendbar sind. Die noch vorhandenen Schwierigkeiten (z. B. Thermodynamik irreversibler Prozesse, Teil 6; N-Darstellbarkeit der Dichtematrix, Kap. 46) sind nicht von grundsätzlicher Natur, so dass auch dort ein erfolgreicher Einsatz von Variationsmethoden zu erwarten ist.

Der wesentliche Vorteil, den ein Variationsverfahren zur Behandlung von Vielteilchenstrukturen bietet, besteht darin, dass das Vielkörperproblem durch Teilvariation entsprechend den ausgewählten Ansätzen näherungsweise gelöst werden kann.

Bei der Auswertung der Variationsprinzipien entstehen wegen der Vielzahl der auszuführenden Integrationen oft erhebliche Schwierigkeiten. Durch geeignet gewählte Entwicklungen lassen sich diese Integrationen auf sehr viele in sich gleichartige Rechenvorschriften überführen. Bei deren Auswertung scheint das konsequente Anwenden der Graphenrechnung die weitere Entwicklung zu bestimmen. Im Zusammenhang damit wird die Verwendung von Funktionalableitungen in der Variationsrechnung an Bedeutung gewinnen.

Im Augenblick besteht eine gewisse Konzentration der Bemühungen darauf, eine umfassende Beschreibung irreversibler Phänomene mit Variationsmethoden zu ermöglichen. Erfolge wurden bisher nur bei stationären irreversiblen Prozessen erzielt. Von Interesse ist auch die Frage, wie man mit Variationsprinzipien den Übergang von reversiblen zu irreversiblen Gleichungen vollziehen kann. Untersuchungen an einfachen Modellsystemen sollten dazu weitere Hinweise geben.

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ПРИМЕНЕНИЕ ВАРИАЦИОННЫХ ПРИНЦИПОВ ДЛЯ РЕШЕНИЯ ПРОБЛЕМ МНОГИХ ТЕЛ

В. ПОМПЕ, К. ЭЛК и В. МАККЕ

Резюме

В этой работе дан обзор о применении вариационных принципов для решения проблем многих тел. После обсуждения общих условий существования вариационных принципов исследуется их применение в классической статистике равновесных и неравновесных состояний. Следует составление методов для трактовки стационарных и нестационарных квантовых систем. Необратимые процессы описываются принципом экстремального возникновения энтропии. В частности рассматриваются связанные с этим принципом методы, служащие для решения уравнения Больцмана.

Printed in Hungary

A kiadásért felel az Akadémiai Kiadó igazgatója Műszaki szerkesztő: Farkas Sándor
A kézirat nyomdába érkezett: 1966. III. 12. — Terjedelem: 9,25 (A/5) ív, 2 ábra

66.62111 Akadémiai Nyomda, Budapest — Felelős vezető: Bernát György

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Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (2), pp. 107—120 (1966)

ON THE KINETICS OF SURFACE RECOMBINATION IN GERMANIUM*

By

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(Presented by G. Szigeti — Received 31. VIII. 1965)

In this paper the kinetics of surface recombination is examined both experimentally and theoretically. The photoconductivity decay was measured over the temperature range 77° K—340° K. At low temperatures, the decay curves could be composed of two exponents (τ_r, τ_t). It is shown that the temperature dependence of both relaxation times, apart from the saturation of τ_r can be well described assuming one kind of recombination centres and also traps for holes. The system of differential equations of recombination is given, taking into consideration the space charge region (Appendix). For the simplest case it is shown how to obtain the formulae for the surface model from those for the bulk model.

Introduction

Recently, the kinetics of surface recombination has become a widespread method in the investigation of surface phenomena in semiconductors. This can mainly be explained by the fact that, especially below room temperature, some relaxation effects arise which cannot be observed under steady-state conditions. The measurements of these relaxation effects give new information on the parameters of the centres. The following more important and characteristic effects are observable: a) the quasistationary lifetime (τ_r) increases with decreasing temperature; b) in the photoconductivity decay a short relaxation effect (τ_t) appears; c) both relaxation processes are sensitive to steady illumination.

The effects a) and c) have been investigated by several authors for both Ge and Si, e.g. by **Lindley** and **Banbury** [1, 5], **Rupprecht** [2], **Harnick** et al. [3] and **Litovchenko** and **Lyashenko** [4]. The effect b) has been observed by **Lyashenko** et al. [6] and also in papers [3, 5]. Detailed experimental results were published for Si by **Primachenko** et al. [8].

In the present work, the behaviours a) and b) are studied for Ge both theoretically and experimentally. The experimental techniques are described

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* Part of this work was presented at the Conference on the "Electronic Processes on Semiconductor Surface" held in Kiev, 1965.

in Sec. 1 and the experimental results are given in Sec. 3. Sec. 3a deals with the kinetics of bulk recombination in the presence of hole-traps. In 3b the transference of the above model to surface recombination and surface trapping is discussed, based on the equations given in the Appendix. It is explained how, in a very simple case, the formulae for the surface model can be derived from those for the bulk model. In Sec. 4 the interpretation of experimental results, with special respect to the possible origin of the saturation of τ_r at low temperature, is given.

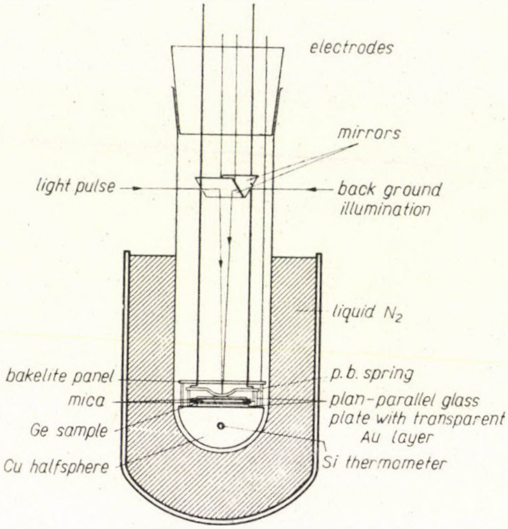

Fig. 1. Evacuable glass vessel with sample holder, immersed in liquid nitrogen

1. Experimental techniques

Photoconductivity decay was used to investigate the kinetics of surface recombination. The condition of a small signal case was always fulfilled with $\frac{\Delta\sigma}{\sigma_0} \leq 0{,}1\%$. The samples used were cut from n-type germanium of 20—25 Ωcm. The sample sizes were 1,3 × 0,4 × (0,05 or 0,03) cm. After polishing, the samples were etched in etchant "A" (100 ccm HNO_3 of 65% + 300 ccm H_2F_2 of 38% + 50 cg J_2). Contacts from Sn containing 0,5% Sb were prepared, having ohmic characteristics down to liquid nitrogen temperature. Before measurements, the samples were freshed in the etchant "A".

The measurements were carried out over the temperature range 77°K—340°K. Figure 1 shows the cryostat evacuated to less than 10^{-3} mm Hg. The terminals held the copper hemisphere with the sample and also provided the electrical contacts.

The lower part of the glass vessel was immersed in liquid nitrogen to cool the copper hemisphere and the sample to the required temperature. The sample holder was used to measure both the field effect and photoconductivity decay (the transparent electrodes had a capacity of 200 pF). For temperature measurement a Si resistance thermometer was used.

The cooling procedure described above has some advantages over others.* The liquid nitrogen temperature can in fact be reached; the cooling and, thus, the condensation of water vapour begins on the wall of the vessel instead of on the sample and, finally the system can be evacuated easily owing to the absence of metal-glass junctions.

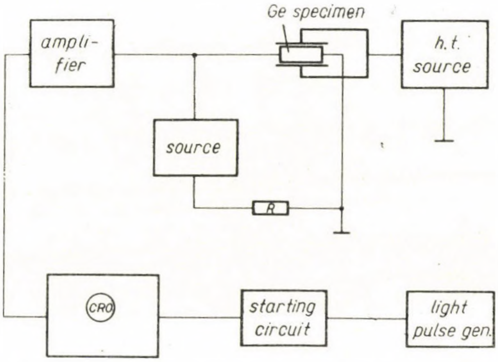

Fig. 2. Schematic diagram for photoconductivity decay measurements

The light pulses were produced by a hydrogen lamp. The duration of pulse was sufficiently short ($\sim 1{,}5$ μsec) to measure the shortest relaxation times in question (~ 20 μsec). The measurements were carried out using an equipment with the block scheme shown in Fig. 2. The current through the sample was varied between 100 μA$-$1 mA depending on the temperature, i.e. on the resistivity of the sample.

After adequate wide-band amplification the signal was photographed with an oscilloscope, type OGl$-$10.

2. Experimental results

The photoconductivity-decay below room temperature could be decomposed into two exponential curves with relaxation times τ_r and τ_l. A typical curve, obtained from analyzing the corresponding decay is shown in Fig. 3. The two relaxation times or life-times are well determinable from this curve. Our aim was to investigate the effects a) and b) to obtain experimental data

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* This method of cooling was proposed by Mr. J. Tihanyi.

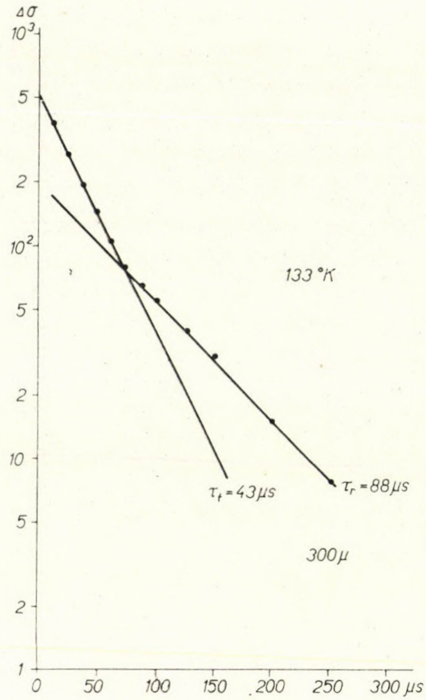

Fig. 3. Photoconductivity decay. The points are obtained by analyzing the photographs of the oscilloscope traces

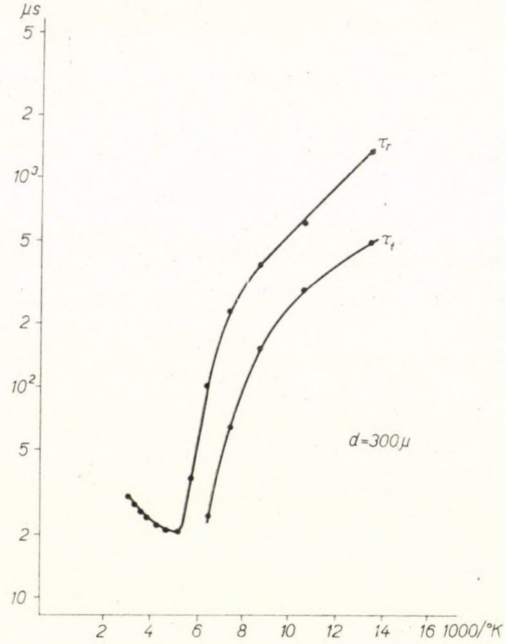

Fig. 4. Lifetimes τ_r and τ_t as functions of reciprocal absolute temperature for sample thickness $d = 300\ \mu$

concerning the temperature dependence of τ_r and τ_t. The measurements were carried out on numerous samples with two different thicknesses ($d = 300\ \mu$, $d = 500\ \mu$).

Figures 4 and 5 show the temperature dependence of both lifetimes. The longer relaxation time τ_r after a short decrease, begins to increase exponentially with decreasing temperature. Below 100°K, τ_r shows a tendency to become saturated. It is interesting to remark that near the liquid nitrogen temperature, in some cases, the value of τ_r decreases again. With our apparatus the shorter relaxation time becomes measurable only at relatively low temperatures. In the range measured, the τ_t is a monotonic function of temperature: it increases with decreasing temperature and shows saturation characteristics. The curves, as can be seen in Figures 4 and 5, are nowhere exponential.

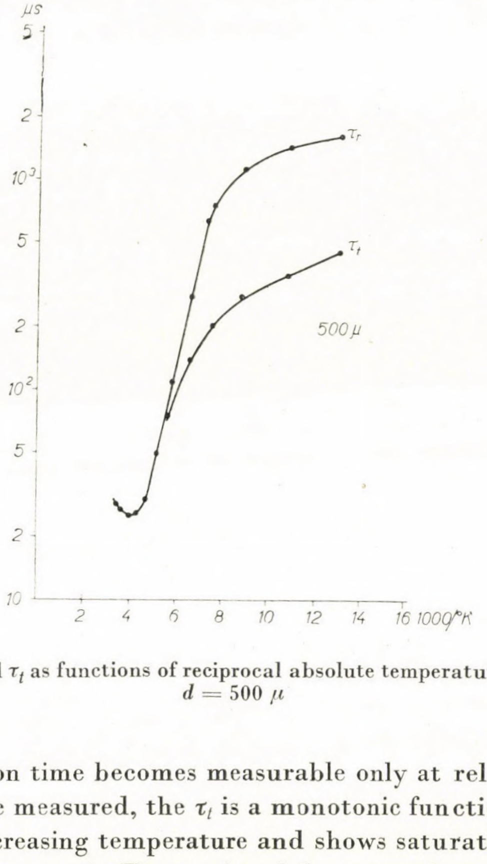

Fig. 5. Lifetimes τ_r and τ_t as functions of reciprocal absolute temperature for sample thickness $d = 500\ \mu$

The apparatus used (see Fig. 1) is capable of measuring the field effect and also of applying a steady illumination. Some preliminary measurements have been carried out in both respects, but the results are insufficient to allow any valuable conclusion to be drawn. It is worth remarking however, that with the given geometry of the field effect experiments (200 pF), the applied voltage (±100 V) does not markedly alter the slope of the $\tau_r \left(\frac{1}{T}\right)$ curves.

The background illumination causes a strong diminution of τ_r, which accords with the observations of other authors. The effect of illumination on the shorter relaxation time τ_t, on the other hand, could not be analyzed because the amplitude of signal was greatly decreased.

3. The kinetics of recombination in the presence of traps

a) Bulk model

To interpret the experimental results given in the previous section, we shall discuss in detail the model proposed first by WERTHEIM [9], and also accepted by LINDLEY and BANBURY in their later paper [5]. According to this model, there are recombination centres of one kind and also traps for holes. The parameters of these centres, with the usual notation, are:

$$N_r, E_r, C_{rp}, C_{rn}, n_{r1}, p_{r1}, \text{ and } N_t, E_t, C_{tp}\; C_{tn} = 0\; n_{t1}, p_{t1}, \text{ respectively}.$$

Here n_{r1}, n_{t1} denote the electron concentrations in the conduction band if the Fermi level F_0 is equal to E_r resp. E_t. The quantitites p_{r1}, p_{t1} referring to holes have similar meanings. If n_r and p_r denote the full and empty recombination centres, respectively (a similar notation is used for traps) then the system of differential equations governing the recombination is:

$$\begin{aligned} \frac{dn}{dt} &= -C_{rn}\,(np_r - n_{r1}\,n_r)\,, \\ \frac{dp}{dt} &= -\,C_{rp}\,(pn_r - p_{r1}\,p_r) - C_{tp}\,(pn_t - p_{t1}\,p_t)\,, \qquad (1) \\ \frac{dn_t}{dt} &= -\,C_{tp}\,(pn_t - p_{t1}\,p_t)\,. \end{aligned}$$

To solve Eq. (1) further relations are needed. It is possible without restriction of generality, to assume neutrality for both the recombination centres and traps in the lower charge condition. Hence, we obtain the following subsidiary conditions:

$$\begin{aligned} \delta n_r + \delta p_r &= 0\,, \\ \delta n_t + \delta p_t &= 0\,, \qquad (2) \\ \delta n + \delta n_t + \delta n_r &= \delta p\,, \end{aligned}$$

where the first two equations are the conditions of normalization and the third is the conditions of electrical neutrality. If the variables δn_r, δp_r, δp_t are eliminated by the aid of Eq. (2), then for the column vector α of elements δn, δp and δn_t, the following equation is obtained in matrix form:

$$\dot{\alpha} = -A\alpha \, , \tag{3}$$

where the lifetime matrix A has the form

$$A = \begin{pmatrix} A_n + C_{rn} p_{r0}; & -A_n; & -A_n \\ -A_p; & +(A_p + C_{rp} n_{r0} + C_{tp} n_{t0}); & -A_n + A_t \\ 0; & C_{tp} n_{t0}; & +A_t \end{pmatrix}; \tag{4}$$

here $A_n = C_{rn}(n_0 + n_{r1})$; $A_p = C_{rp}(p_0 + p_{r1})$; $A_t = C_{tp}(p_0 + p_{t1})$. The lifetimes τ_i can be determined from the characteristic equation of matrix A; $| A - \lambda \mathrm{I} | = 0$, using $\tau_i = \dfrac{1}{\lambda_i}$.

A simple calculation gives the coefficients b_i of the equation of third order:

$$b_0 \lambda^3 + b_1 \lambda^2 + b_2 \lambda + b_3 = 0 \, , \tag{5}$$

$$\begin{aligned} b_0 &= -1 \, , \\ b_1 &= +[A_t + T(A_r) + C_{tp} n_{t0}] \, , \\ b_2 &= -[A_t \, T(A_r) + A_p C_{tp} n_{t0} + D(A_r) + C_{rn} p_{r0} C_{tp} n_{t0} + A_n C_{tp} n_{t0}] \, , \\ b_3 &= +[C_{tp} n_{t0} C_{rn} p_{r0} A_p + A_t D(A_r)] \, . \end{aligned} \tag{6}$$

Here $T(A_r)$ and $D(A_r)$ are the trace and determinant of the lifetime matrix A_r of the simple $S-R$ model ($N_t = 0$):

$$T(A_r) = A_n + A_p + C_{rn} p_{r0} + C_{rp} n_{r0} \, ,$$

$$D(A_r) = A_n C_{rp} n_{r0} + A_p C_{rn} p_{r0} + C_{rn} C_{rp} n_{r0} p_{r0} \, .$$

The lifetimes of the $S-R$ model are determined by the roots of the equation

$$\lambda^2 - T(A_r)\lambda + D(A_r) = 0 \, . \tag{7}$$

We shall give the approximate roots of Eq. (5). If the roots are well separated i.e. $\lambda_1 \gg \lambda_2 \gg \lambda_3$ then the following approximation is valid:

$$\frac{1}{\tau_i} = \lambda_i \approx - \frac{b_i}{b_{i-1}} \, .$$

Using the notation $\tau_3 \equiv \tau_r$ and $\tau_2 \equiv \tau_t$, we obtain:

$$\tau_r = -\frac{b_2}{b_3}; \qquad \tau_t = -\frac{b_1}{b_2}.$$

Let us now examine the temperature dependence of coefficients b_i. We shall assume the material to be n-type and $N_r \ll n_0$, i.e. the recombination centres do not play any part in the determination of the Fermi-level F_0 (the Fermi level, with decreasing temperature, passes through the recombination level E_r). A simple estimate shows that in the whole temperature range the following approximation is valid:

$$b_3 \approx +A_t D(A_r).$$

For coefficient b_2, on the other hand:
$b_2 \approx -A_t T(A_r)$ (high temperature); $b_2 \approx -A_n C_{tp} n_{t0}$ (low temperature).
Using the above approximations, one obtains for τ_r

$$\tau_r \approx \frac{T(A_r)}{D(A_r)} \quad \text{(high temperature)}, \tag{8a}$$

$$\tau_r \approx \frac{A_n n_{t0} C_{tp}}{A_t D(A_r)} \quad \text{(low temperature)}. \tag{8b}$$

From Eqs. (8) it is seen that at higher temperature the simple $S-R$ model works, while if the temperature is sufficiently low the lifetime τ_r is determined mainly by the trap parameters. In fact, taking into consideration that $n_{t0} \approx N_t$ and $n_{r0} \approx N_r$ we get:

$$\tau_r \approx \frac{N_t}{N_r C_{rp} (p_0 + p_{t1})} \approx \frac{N_t}{N_r C_{rp} N_v} \cdot e^{+\frac{E_t - E_v}{kT}} \tag{9}$$

if the relation $p_{t1} \gg p_0$ is valid.

A quite similar approximation may be used also for τ_t. At higher temperatures the recombination centre works, being

$$\tau_t = \frac{1}{T(A_r)} \tag{10a}$$

while at lower temperatures one obtains if $C_{rn} n_0 \gg C_{rp} N_r$; $C_{tp} N_t$ and $n_{r0} \approx \approx N_r$; $n_{t0} \approx N_t$

$$\tau_t \approx \frac{1}{C_{tp} N_t}\left(1 + \frac{C_{rp} N_r}{C_{rn} n_0}\right) + \frac{1}{C_{rn} n_0} \approx \frac{1}{C_{tp} N_t}. \tag{10b}$$

b) Surface recombination

The kinetics of surface recombination involving space charge effects has not yet been solved to the best knowledge of the authors. In paper [5] some attempts were made to transfer the bulk recombination model to the surface case, but the calculations were mainly heuristic in character. In the Appendix of the present paper the equations to be solved are given for the model treated in 3a. Equations (A1)—(A4), however, cannot be solved for the general case, and therefore, it will be of interest to show that formula (9) is also valid for the case of surface centres and to give a rule for transferring the formulae relating to bulk recombination to surface recombination, assuming a simple space charge region. Let the value of surface potential Y be small and let us also assume the small signal case. In this case the quantities Γ_n and Γ_p, introduced by GARRETT and BRATTAIN [10], take the following approximate values:

$$\Gamma_n \approx L'(n_Y - n^*)\,; \qquad \Gamma_p \approx L'(p_Y - p^*)\,.$$

Thus, in this approximation, the space-charge region can be described using an effective Debye length L' and concentrations on the surface. The quantities n^* and p^* denote the concentrations just below the space-charge layer, effectively in the bulk (see Appendix). For the simplest model the L' does not depend either on the surface potential or on the non-equilibrium concentrations.* Based on this expression, the approximations

$$\frac{d\,\delta\bar{u}}{dt} \approx L'\,\frac{d\,\delta n_Y}{dt} \quad \text{and} \quad \frac{d\,\delta\bar{p}}{dt} \approx L'\,\frac{d\,\delta p_Y}{dt}$$

can be used in the linearized form of Eq. (A1). The rule for transferring bulk expressions to surface ones can readily be obtained. In fact, the proper formulae can be derived using the following correspondences:

$$n \rightarrow n_Y\,;\; p \rightarrow p_Y\,;\; N_r\,(\mathrm{cm}^{-3}) \rightarrow \frac{N_r\,(\mathrm{cm}^{-2})}{L'}\,.$$

(Similarly for concentrations n_r, p_r);

$$N_t\,(\mathrm{cm}^{-3}) \rightarrow \frac{N_t\,(\mathrm{cm}^{-2})}{L'} \qquad \text{(similarly for } n_t,\ p_t).$$

The parameters n_{r1}, p_{r1} and n_{t1}, p_{t1}, occurring in the equations in question do not contain the surface potential. Thus, finally we obtain:

$$\tau_r\,(Y) \approx \frac{N_t}{N_r\,C_{rp}\,(p_{Y0} + p_{t1})} \approx \frac{N_t}{N_r\,C_{rp}\,N_v}\,e^{+\frac{E_t - E_v}{kT}} \tag{11}$$

---

* The effective Debye length L' introduced here, for the simple model assumed, can be expressed as $L' = \sqrt{2}/2(\lambda + \lambda^{-1})^{1/2}\,L_{Di} = \frac{\sqrt{2}}{2}\,L_{De}$, where L_{De} is the extrinsic Debye length introduced by C. GOLDBERG [11]; L_{De} is not sensitive to the variation of temperature.

and the inconvenient quantity L' is eliminated. The formula, related to higher temperatures contains the quantity L', but from the expression $\frac{\tau}{\tau_{r\,\mathrm{min}}}$, examined in the function of the surface potential Y, it is also eliminated, assuming a small concentration of recombination centres.

It is worth remarking, finally, that expression (11) differs from that given in paper [5] in two respects: expression (11) contains the factor $\frac{N_t}{N_r}$ and also the quantity p_{Y0} depending on the surface potential. Owing to the first difference, the value of C_{rp} cannot be obtained directly from (11) while the second one may be significant if $p_{Y0} \gg p_0$.

4. Interpretation and discussion of the results

To interpret effects a) and b) several models must be taken into consideration. LINDLEY and BANBURY in their previous papers [1] tried to discuss the effect a) in terms of a simple $S-R$ model. They argued that because of the opposite temperature dependence of the two lifetimes of $S-R$-model, τ_t may become larger than τ_r and thus the explanation for a) is found. This, however, is not correct. Though from the approximate roots (8a) and (10a) it is not evident, the relation $\tau_t \ll \tau_r$ is always valid. This can be seen simply starting from the exact lifetime of $S-R$ model. In fact, in order for the roots of eq. (7) to be positive, the relation $\sqrt{T(A_r)^2 - 4D(A_r)} \geqslant 0$ should occur, whence the relation $\tau_r \geqslant \tau_t$ obviously follows.

From what has been said above it is clear that to interpret effects a) and b) it is necessary to employ more complicated models or assumptions. In fact, in their later work LINDLEY and BANBURY assumed the presence of one kind of recombination centres and also traps for holes [5].

In paper [3], on the contrary, HARNICK et al. assumed a temperature dependent capture constant and also that the position of recombination centre is temperature dependent.

In the present work, the model with traps is accepted and studied in detail. From calculations of Sec. 3. (formula (11)) it is clear that the low temperature behaviour of τ_r is determined by p_{t1}. This has the physical meaning that under the conditions assumed, the thermal emission of holes into the valence band by traps is the slowest process in the recombination. Thus, from the slopes of the experimental curves, the energy level of traps can be calculated. Experimentally, we obtained (see Figures 4 and 5) $E_t - E_v = 0{,}10-0{,}14$ eV. Below 120°K, as Figures 4 and 5 show, the lifetime τ_r has a tendency to saturate, what has been observed by some other authors, too [4, 6]. Starting from the model accepted, the saturation cannot be explained in a natural way.

This is clear from Fig. 6 where the quantity $\frac{\tau_r}{\tau_0}$ is plotted as a function of reciprocal temperature, assuming $C_{rn} = C_{rp} = C_{tp} = C$. According to expectation, at higher temperatures the traps have no effect on the lifetime (see formulae (8)), while at lower temperatures, depending on their concentration, the traps begin to play an important role in the recombination and τ_r increases exponentially showing no saturation.

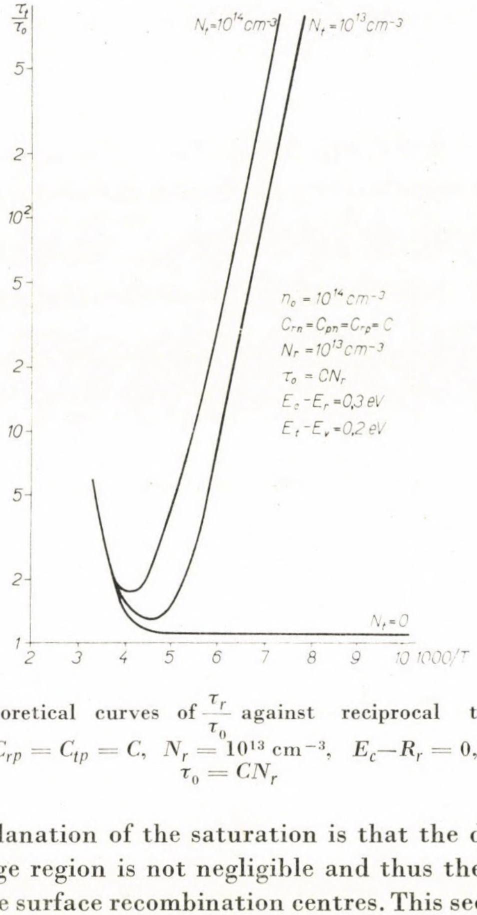

Fig. 6. Normalized theoretical curves of $\frac{\tau_r}{\tau_0}$ against reciprocal temperature, assuming $n_0 = 10^{14}\,\mathrm{cm}^{-5}$, $C_{rn} = C_{rp} = C_{tp} = C$, $N_r = 10^{13}\,\mathrm{cm}^{-3}$, $E_c—R_r = 0{,}3\mathrm{eV}$, $T_t—E_v = 0{,}2\mathrm{eV}$. $\tau_0 = CN_r$

A possible explanation of the saturation is that the diffusion of carriers from the space charge region is not negligible and thus the bulk centres may shunt the effect of the surface recombination centres. This seems to be supported by the observation that the thicker the sample the sooner saturation begins. It is possible also that at lower temperatures the communication between the traps and conduction band improves, and so the saturation becomes evident. Just becuase of the saturation effect, the model of multi-electron centres proposed by KALASHNIKOV et al. [12] for bulk recombination seems to be well applicable for this case too. Here it is noted only, that, assuming all capture constants to be equal, the desired temperature dependence of τ_r was obtained with a relatively high concentration of centres. In our case, on the contrary, the exponential temperature dependence of τ_r can be explained also for N_r, $N_t \ll n_0$ (see Fig. 6). It is important, however, to emphasize that based on the experimental results available, and without any knowledge of the origin of the centres, it seems to be impossible to make an unambiguous choice between these models.

The shorter relaxation time τ_t increases with decreasing temperature and also shows saturation. From the model studied in Sec. 3 such temperature dependence can be fully explained, as seen in Fig. 7. It is interesting to note that the short relaxation time found by **Primachenko** et al. for Si, has a temperature dependence opposite to that of τ_t in Figures 4 and 5. Therefore, our model is not applicable to this case. From the saturation value of τ_t the quantity $C_{tp}N_t$ can be calculated if the relaxation time is assumed to be determined by the traps alone.

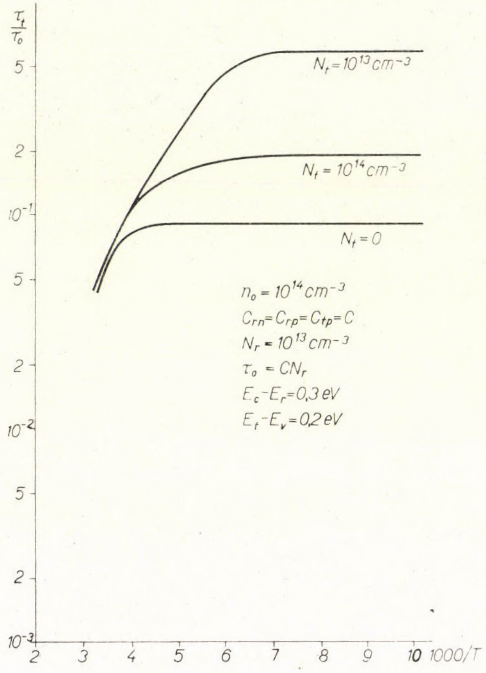

Fig. 7. Normalized theoretical curves of $\frac{\tau_t}{\tau_0}$ against reciprocal temperature for the same values of parameters as in Fig. 6

Further experiments are in progress to separate the effect of recombination centres from that of traps. For this purpose it is intended to combine the method of stationary field effect [13] with surface kinetics measurements and also to systematically study the behaviour c). By using different chemical treatments, it is hoped to obtain information concerning the origin of the traps.

Acknowledgements

The authors thank Professor Z. Bodó for valuable discussions, Mrs. M. Németh for the elaboration of chemical treatments and Mrs. J. Turcsányi for assistance in the experimental work.

Appendix

Integrating Eq. (1) over the space charge layer and assuming a δ-like distribution of centres, we obtain:

$$\frac{d\bar{n}}{dt} = -C_{rn}(n_Y p_{rY} - n_{r1} n_{rY}),$$

$$\frac{d\bar{p}}{dt} = -C_{rp}(p_Y n_{rY} - p_{r1} p_{rY}) - C_{tp}(p_Y n_{tY} - p_{t1} p_{tY}), \tag{A1}$$

$$\frac{dn_{tY}}{dt} = -C_{tp}(p_Y n_{tY} - p_{t1} p_{tY}),$$

where the relations $n_{r1Y} = n_{r1}$ etc. were taken into account and n_r, p_r, n_t, p_t are concentrations per unit area. Based on classical work of Garrett and Brattain [10] we have

$$\bar{n} = \Gamma_n + \bar{n}^* = -\frac{1}{2} n_i \lambda^{-1} e^{-N} L_{Di} \int_0^Y \frac{e^y\, dy}{F(y, \lambda, N, P)},$$

$$\bar{p} = \Gamma_p + \bar{p}^* = -\frac{1}{2} n_i \lambda e^P L_{Di} \int_0^Y \frac{e^{-y}\, dy}{F(y, \lambda, N, P,)}, \tag{A2}$$

where the concentrations are given by the expressions:

$$n = n^* e^y = n_i \lambda^{-1} a^{-N+y},$$

$$p = p^* e^{-y} = n_i \lambda e^{P-y}, \tag{A3}$$

The following notations were used: $\lambda = P_0/n_i = n_i/n_0$; $P = \beta(F_p - F_0)$; $N = \beta(F_n - F_0)$ and the quasi Fermi-levels F_n, F_p are taken independent of position (the condition for this was examined by Frankl [14]).
$y = \beta(\psi - \psi_0)$ is the dimensionless potential and Y is its value at the surface.
$L_{Di} = \left(\frac{\varepsilon\varepsilon_0}{2\pi e n_i \beta}\right)^{1/2}$ is the so called intrinsic Debye length,

$$F(y, \lambda, P, N) = \mp [\lambda e^{P}(e^{-y} - 1) + \lambda^{-1} e^{-N}(e^{y} - 1) + (\lambda - \lambda^{-1}) y]^{1/2}$$

where, by definition, $F < 0$ if $y > 0$. It is easy to see that Eq. (2) should be replaced by the following expressions:

$$\begin{aligned} \delta n_{rY} + \delta p_{rY} &= 0\,, \\ \delta n_{tY} + \delta p_{tY} &= 0\,, \\ \delta \bar{n} + \delta n_{tY} + \delta n_{rY} &= \delta \bar{p}\,. \end{aligned} \qquad \text{(A4)}$$

In the above equations the diffusion and the bulk centres have been neglected.

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О КИНЕТИКЕ ПОВЕРХНОСТНОЙ РЕКОМБИНАЦИИ В ГЕРМАНИИ

А. ЛЕРИНЦИ, Г. ПАТАКИ и Г. ПАСТОР

Резюме

В настоящей работе экспериментально и теоретически исследована кинетика поверхностной рекомбинации в Ge. Измеряется релаксация фотопроводимости между 77°—340°K. При пониженных температурах кривые релаксации фотопроводимости можно составить из двух экспонентов (τ_r, τ_t). В работе показано, что температурную зависимость τ_r и τ_t, с исключением насыщения τ_r, можно хорошо объяснить, предполагая существование центров рекомбинации одного типа и также центров прилипания для дырок. Получается систем дифференциальных уравнений рекомбинации, принимая во внимание влияние слоя объемного заряда (Приложение). Для самого простого случая дается правило получения формул, относящихся к поверхностной рекомбинации, если известны соответствующие формулы для объемных центров.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (2), pp. 121—127 (1966)

DENDRITIC GROWTH OF ZnS CRYSTALS

By

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(Presented by G. Szigeti — Received 31. VII. 1965)

The dendritic growth of ZnS crystals in the form of long ribbons, plates and needles was observed when ZnS crystallized from liquid Ga. The cubic ribbons and plates propagated in the ⟨211⟩ directions, the needles were hexagonal and their main propagation was parallel to the c-axis. It has been found that for a cubic lattice (ribbons and plates) the growth mechanism of ZnS show the same features as the growth of Ge, Si, In, Sb, etc. dendrites.

1. Introduction

Dendritic growth of crystals can be observed from melts, liquid and solid solutions, vapour-phase and during electrocrystallization.

Recently, the formation of dendrites aroused widespread interest but the origin of this phenomenon has not yet been clarified. (C. F. Bolling and W. A. Tiller 1961, [1, 2])

Dendrites usually possess a definite crystallographic orientation, and in this respect they belong to the monocrystals.

Generally, crystals of low symmetry show dendritic growth. In lattices of higher symmetry, chiefly when crystallizing metal-melts, dendritic growth frequently occurs.

Dendritic growth occurs very rarely in case of ZnS and CdS, whether they originate from the vapour, or melt phase.

Owing to the great importance of these crystals and because of some special properties of dendritic crystals it seems reasonable to use every effort to produce dendrites and to examine their characteristics.

This paper deals with the description of some features of ZnS dendrites produced in our laboratory. It has been stated by Kaluzhnaia (1964) that the ZnS can be dissolved and crystallized from Ga [3].

Concerning the dendritic growth of ZnS crystals, we only wish to remark that they have been produced from ZnS dissolved in metallic Ga by means of suitable apparatus. This paper does not deal with the method and technique of dendritic growth, which will be discussed elsewhere.

2. ZnS dendrites

When crystallyzing ZnS from the liquid phase of Ga, we succeeded in observing two different types of dendritic crystals. The one was the so called platelike dendrite, very similar to the crystals appearing in supersaturated solution and during the formation of ice.

The other type is needle-like, with numerous secondary dendrite branches growing perpendicular to the main growth direction.

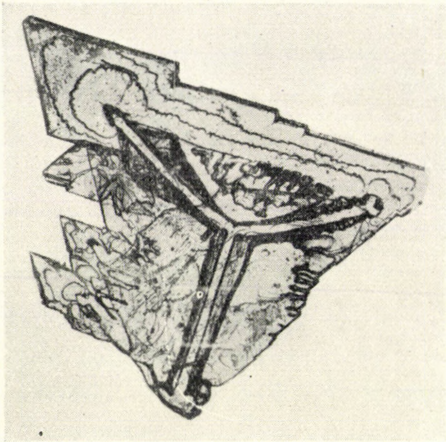

Fig. 1. Triangle-like ZnS dendrite plate. The propagation layers well observable on the surface of the plane are conform to the main propagation direction ⟨211⟩ of the dendrite

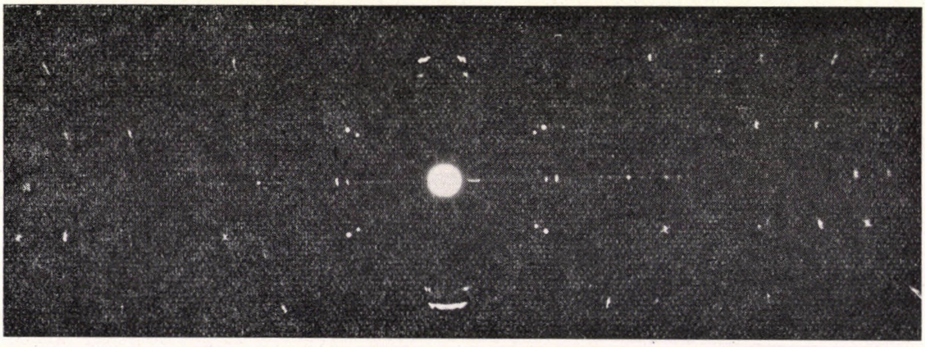

Fig. 2. X-ray pattern of the dendrite shown in Fig. 1. The pattern has been made by the rotating crystal method; the axis of rotation is parallel to the normal of the planes

The maximum length of the first crystal type very frequently exceeds 10 mm, its thickness is generally about 0,1 mm. Figure 1 shows a characteristic, triangular dendritic ZnS plate. The main propagation directions of the dendrite and its surface pattern are distinctly visible.

X-ray examination of the crystal proved that it has a cubic structure (sphalerite). The X-ray patterns were made in Weissenberg or oscillation type cameras of 57,3 mm diameter by irradiation with FeK_α and CuK_α radiation, respectively. According to the rotating crystal patterns the normal to the surface is parallel to the hexagonal *c* i.e. the cubic ⟨111⟩ axis .If we choose the rotation axis parallel to the direction of the bisectors, i..e. to the normals of the sides of the triangle-like crystal plates, the value *d* calculated from the distance of the layer-lines in the pattern is 6,6 Å (see Fig. 2); this is equal to the distance of two identical points lying in the direction of the normal of the (1000) plane, according to hexagonal indexing $2d_{1000} = a \cdot \sqrt{3} = 6{,}6166$ Å.

If we choose the axis of rotation parallel to one of the sides of the triangle-like crystal, the value *d*, calculated from the distance of the layer-lines comes to 3,84 Å. Thus, it is equal to the lattice-constant of the elementary cell ($a =$ 3,82 Å), within the measuring errors. All these results prove that the side planes of the triangle conform to the (1000), (0100) and $(\bar{1}\bar{1}10)$ lattice planes. The plate itself lies in the (0001) crystal plane, parallel to the closest packed lattice planes. Figure 1 shows that the dendritic growth occurs as the result of the repeated protrusion on the tips of the crystal. This phenomenon can be observed still better when examining ribbon-like dendrites. Figure 3 shows the tip of such a dendrite. The symmetry conditions and orientation of the dendrite are perfectly similar to that of the crystal shown in Fig. 1. It must be pointed out that the X-ray pattern of the above plate-like dendrites does not show any stacking faults and the crystals are very probably of pure, cubic structure. This fact has a great importance for further physical investigations.

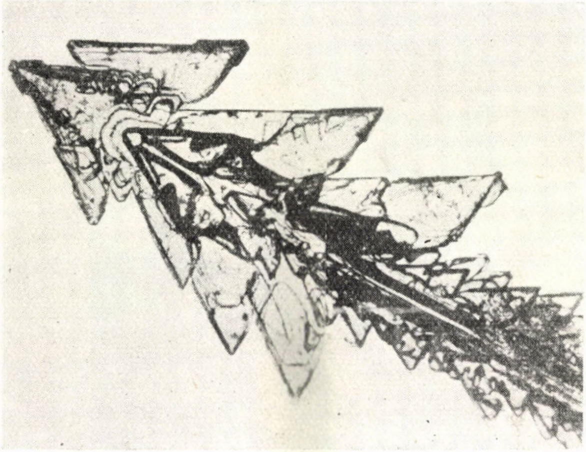

Fig. 3. Microphotography of the ZnS dendrite-ribbon. The morphological and structural features of the crystal are similar to those of the dendrite shown in Fig. 1. The only difference is that one of the three (211) directions is a preferred one

In some cases we succeeded in observing polytypes on plate-like dendrites with hexagonal morphology. The X-ray pattern of such plate-like dendrites proves that the structure of the plate is polytype with six layers without stacking faults, similar to the structure described by FRONDEL and PALACHE [4] (1948). We could also observe this type of structure on ZnS crystals grown from the vapour-phase. The only difference was that with needles grown from the vapour phase, the polytype-like lattice occurred only in a small, definite range of the crystal, whereas the dendritic plates are as a whole structurally pure polytype modifications.

A considerable difference in structure occurs with dendritic needles. These needles have a length of almost 10 mm and their width is 0,5—1,0 mm. Secondary dendrite branches, consisting of needles and plates branch off perpendicular to their main propagation direction. In many cases the characteristic dendritic form is followed by a hexagonal, hollow crystal along the needle axis. The faces of this are approximately perfect and only the hollow within the crystal proves its dendritic origin (see Fig. 4). The X-ray examination of such dendrites shows that the lattice of the hollow range is hexagonal. Stacking faults can be observed on it, as well. Considering the fact that the cubic plates and the hexagonal needles are occurring at the same time, the structure difference accompanying this morphology seems to be of great interest.

Fig. 4. Rod- and needle-like ZnS dendrites. On crystal *B* it is well observable that the continuation of the dendrite is a hexagonal, hollow crystal

3. Discussion

Up to now the investigation of dendritic growth has shown that it chiefly depends upon temperature gradients, due to heat-conduction effects, impurity gradients, or to the solvent, accumulated on the surface of the growing crystal. (See e.g. SARATOVKIN 1959, BOLLING and TILLER 1961 [5, 2]).

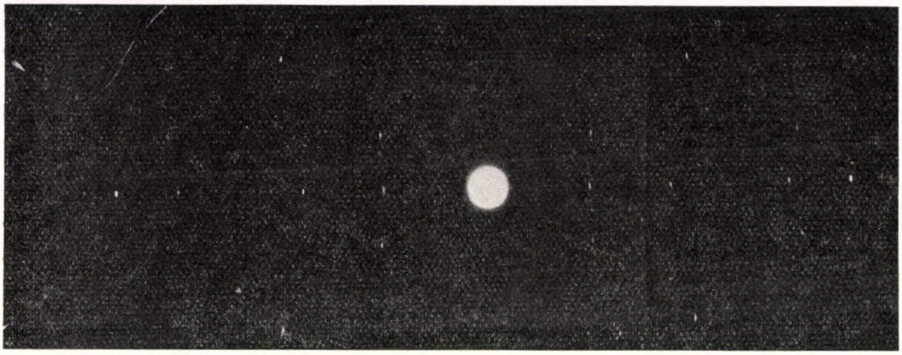

Fig. 5. X-ray pattern of the hollow section of crystal *B* shown in Fig. 4 made by rotating crystal method

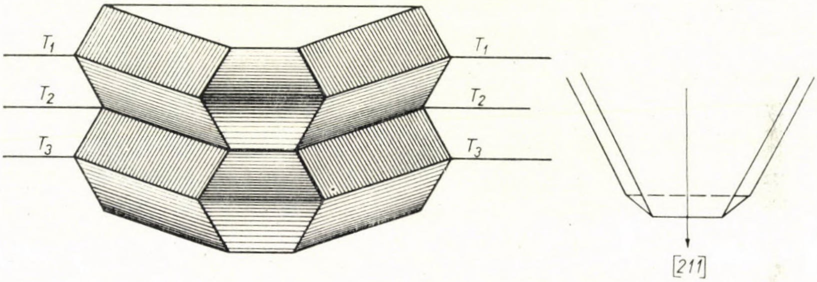

Fig. 6. Morphology of the tip of a dendritic crystal containing 3 twin-planes. The tip shows two reentrant grooves and one ridge. The neighbouring sides contain two ridges and one reentrant grove

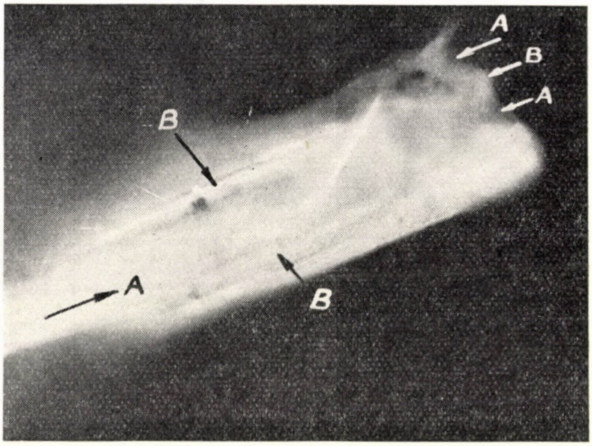

Fig. 7. Microphotography of the tip of a ZnS dendrite. The planes and edges of Fig. b are well observable on the tip and one of the side-planes. (A = reentrant groove, B = ridge)

Since, in the course of our experiments we used sufficiently pure Ga and ZnS, the mechanism caused by contaminants is excluded. It seems to be most probable that when growing ZnS from Ga the first or third mechanism is occurring. The fact that the dendritic plates differ considerably from the needles in structure and main propagation direction, proves that their atomic mechanism of growth is different.

The main propagation directions of the dendritic plates conform with $\langle \bar{1}2\bar{1} \rangle$, $\langle \bar{1}\bar{1}2 \rangle$ and $\langle 2\bar{1}\bar{1} \rangle$ (cubic indexing). This agrees perfectly with the observations made on other materials of diamond structure as InSb, Ge, Si, etc.

It is known that when using the above substances the twin planes parallel to the crystal face or ribbon-planes accelerate the quick growth of dendrites (see e.g. ALBON and OWEN 1962, BILLIG 1957, BILLIG and HOLMES 1957, LINDBERG and FAUST 1962) [6—10]. These twin planes produce ridges and reentrant grooves which are covered by faces (111) on the tip of the dendrite. A more detailed examination of dendritic plates and ribbons showed that these dendrites contain 3 twin planes.

In the case of Ge f.i. dendrites with 3 twin planes are of great importance. The theory of three-twinned dendrites has been described (BOLLING and TILLER 1961 [1]) in more detail. Such dendrites were supposed to have two re-entrant grooves and one ridge on their tips. The growth rate of the tip is about twice that of the neighbouring side planes, showing one re-entrant groove and two ridges (Fig. 6). This causes a continuous propagation in three $\langle 2\bar{1}\bar{1} \rangle$ directions. When examining the tips of the platelike ZnS dendrites, we succeeded in observing the characteristic morphology as shown in Fig. 6. Figure 7 shows such a dendrite tip with the faces and edges.

The growth of the rod-like dendrites does not show such unique features. The growth mechanism could not be determined by X-ray examination. Morphological examination shows that the dendrite-branches perpendicular to the *c*-axis have most probably a $\langle 11\bar{2}0 \rangle$ orientation. We did not succeed in observing tertiary branching on the secondary dendrite arms.

In any case, the fact that the main propagation directions of the two different types of dendrites (needles and plates) form a right angle and that there is a sharp difference in their structures, indicates that there must be an essential difference in their growth mechanism.

The explanation of the growth mechanism of the needlelike dendrites and their continuation, the hexagonal hollow crystals, needs further investigation.

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ДЕНДРИТОВЫЙ РОСТ КРИСТАЛЛОВ ZnS

И. БЕРТОТИ, Е. ЛЕНДВАИ, М. ФАРКАШ-ЯНКЕ, М. ХАРШИ и П. КОВАЧ

Резюме

Исследовался дендритовый рост кристаллов в длинной ленточной, плоской и игольчатой формах в случае кристаллизации ZnS из жидкого Ga. Выращивание кубических лент и плоских форм происходит в направлении ⟨211⟩, игольчатые имели гексагональную форму и рост их в основном характеризуется направлением, параллельным оси — *c*. Оказывается, что в случае кубических решеток (ленточных и плоских кристаллов) механизм роста кристаллов ZnS показывает такую же картину, как это наблюдалось при росте дендритов Ge, Si, In, Sb и т. д.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (2), pp. 129—136 (1966)

AN ELECTRON DIFFRACTION STUDY OF THE PHASE TRANSFORMATION OF CESIUM CHLORIDE

By

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(Presented by Z. Gyulai — Received 7. X. 1965)

The phase transformation of cesium chloride has been investigated by an electron diffraction method. Hybridization and recrystallization were observed in a temperature range below the transition temperature. The thermal expansion of the alpha phase showed an anomalous increase. The possibility of a defect mechanism to account for these effects is discussed.

It is well known that cesium chloride undergoes a crystallographic transition above 720°K from a bcc form (CsCl—α) to a fcc form (CsCl—β). Although much work has been done to explain the structural changes on an atomic scale during the transformation the conclusions drawn from the experimental results are still contradictory. According to **Wagner** and **Lippert** [1], **Buerger** [2], and **Hoodless** and **Morrison** [3] the transformation of cesium chloride might be accounted for by a simple differential dilatation of the lattice. On the other hand **Menary**, **Ubbelohde** and **Woodward** [4], who carried out X-ray measurements in the region of the crystallographic transition suggested that the transformation is accompanied by a gradual increase in the concentration of imperfections. Thus the transition is foreshadowed by considerable changes in the original phase. **Lantelme** and **Pauly** [5] have shown that neutron irradiated cesium-chloride crystals which were heated subsequent to the irradiation show an enhanced release of ^{35}S at about 753°K. This observation might be interpreted as indicating the presence of a high concentration of vacancies in the region of the transition.

In this paper electron diffraction studies are discussed the aim of which was to follow more closely the structural changes taking place in the region below and at the transformation temperature. The advantage of this method is the short exposure time (1—2 seconds) which enables a considerable number of diffraction pictures to be obtained during the whole process of transformation. This type of experiment can be carried out only with evaporated thin layers. However **Witt**, who had made absolute lattice constant measurements with the electron diffraction method, found that his results on TlCl were in agreement with X-ray measurements up to four decimals [6]. As will be shown later our own lattice spacing measurements corresponded reasonably with the X-ray results of **Wagner** and **Lippert** [1]. Thus, it appears to be feasible to draw more general conclusions from electron diffraction investigations.

Results

1. The experimental procedure and some results have been briefly described in a preliminary report [7]. The specimens were prepared from Merck pro analysi CsCl in a Balzers 350—G vacuum device at $2 \cdot 10^{-5}$ torr by evaporation from a molybdenum boat, and then investigated in a hot-stage electron diffraction specimen holder of a Hitachi HU—10A electron microscope operated at 75 kV. In order to prevent sublimation during the heating the cesium-chloride crystal-layers were coated in the vacuum evaporator with a thin carbon film. The contrast of the diffraction patterns was only slightly affected by this procedure. A typical picture of the bcc α-phase at room temperature is shown in Fig. 1. The layer thicknesses expected [8] were 20, 100 and

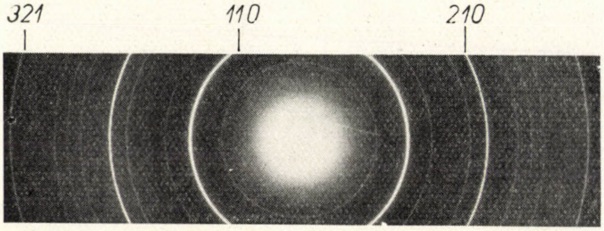

Fig. 1. Diffraction pattern of the α-phase (electron beam focussed on the object)

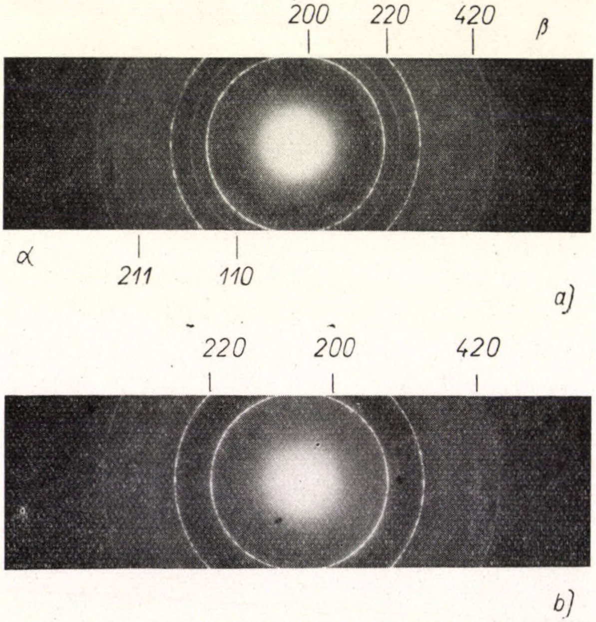

Fig. 2. Diffraction pattern of the mixed phase (a) and of the β-phase (electron beam focussed on the object)

300 Å. The $L\lambda$ values (L is the tube length and λ is the electron wave length) were determined with a thallium chloride standard [9]. The diffractograms were evaluated with a Zeiss Abbe comparator and a Zeiss autoregistering photometer with diffraction attachment. More than 50 experiments were carried out, the mean square error in the determination of the lattice constant was 0.2%. The accuracy of the temperature measurement was ±10°C as allowance had to be made for the heating effect of the electron beam.

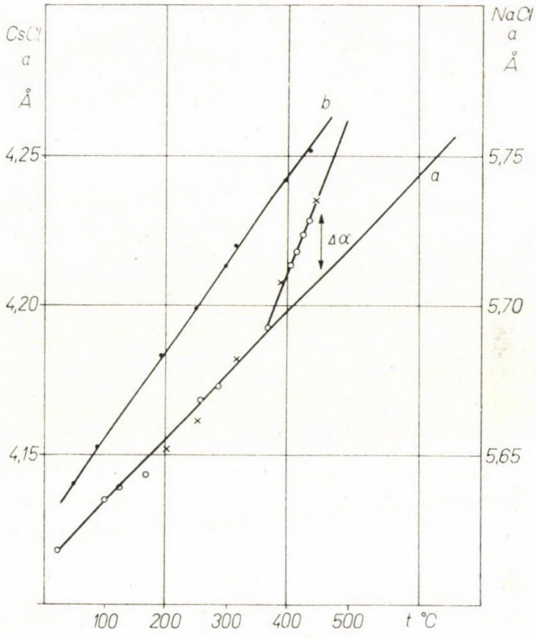

Fig. 3. Temperature dependence of the lattice spacing: a.) CsCl-α b.) NaCl (for comparison) mean square approximation. O: own measurements, x: results of WAGNER and LIPPERT

2. According to the experimental results the (200), (220) and (420) rings of the β phase appeared at about 673°K. However, the structure remained mixed at this temperature since a major part of the rings of the α-phase was also observed. Above 733°K only the β-phase remained (200), (220), (311) and (420) rings.

Fig. 2 shows typical pictures of the mixed phase and the β-phase.

Once the β-phase had developed it remained very stable and could be brought down to room temperature. The first rings of the α-phase (211), (221), (310) and (400) only appeared after several hours at room temperature.

The lattice spacing as determined from the (110) and (211) rings of the α-phase at room temperature was 4,118 ± 0,008 Å and for the β-phase as determined by the intensive (200) ring 7,020 ± 0,008 Å at 755°K. The lattice spacing of CsCl at 293°K obtained by other authors is given in Table 1. Utilizing the short exposition time of the electron diffraction method values of the lattice constant of CsCl—α were measured from 293°K to 733°K. In Fig. 3 the lattice spacing versus temperature is plotted, together with the X-ray results of Wagner and Lippert [1]. An exact transition temperature cannot be given because of the hybridization of the α- and β-phases already beginning at 673°K, an approximate temperature however as found by the disappearance of the strongest (211) bcc line is given in Table 1, together with the data of other authors.

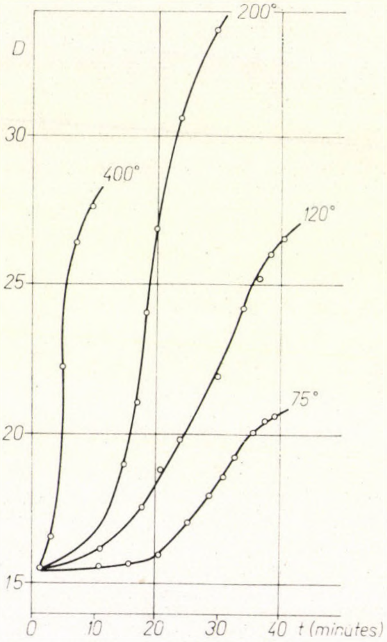

Fig. 4. Rate of recrystallization
Abscissa: time in minutes; ordinate: average grain size in Å

Our results — as can be seen from Fig. 3 — substantiated the results of Wagner and Lippert: the thermal expansion of the crystal lattice showed an anomalous increase in the neighbourhood of the transition CsCl— $\alpha \rightarrow \beta$. Fig. 3 contains for comparison also the thermal expansion of the lattice spacing of sodium-chloride samples prepared and measured in the same way as cesium-chloride. No anomalous expansion can be observed in the measured temperature range.

3. The growth of the mixed phase was investigated more closely by evaporating cesium-chloride in the diffraction-attachment of the HU—10A electron microscope from an evaporator, constructed specially for these

experiments in our laboratory, on carbon substrates at elevated temperatures. Depending upon the temperature of the substrate, mixed and pure β-phase was obtained below the $\alpha \rightarrow \beta$ transition temperature. These results are summarized in Table 2. If the experiments were repeated with substrate temperatures in the region of the transition no layer was obtained because of the sublimation which made it necessary to coat the layers with a thin carbon film as described in Section 1.

4. In order to obtain more information on the mechanism of transformation, electron diffraction photographs were taken by focussing the electron beam on the object. In this way the rings could be resolved into spots suggesting recrystallization, by raising the temperature. This recrystallization process was examined more closely by measuring the line broadening applying the theory of the scattering of the X-rays by small crystals developed by von Laue [10] to the diffraction of electrons. The average crystal size of the samples was determined in this way, according to Pinsker [11] with fair accuracy. As can be seen from Fig. 4, the results show curves approximately of the type $x = 1 - \exp(-Bt^K)$ (x = recrystallized fraction, t = time, B = temperature dependent constant, K = constant) well known from the theory of recrystallization [12, 13]. According to these measurements the samples undergo a remarkable recrystallization during heat treatment.

Discussion

To explain our results it is assumed that the phase transformation of cesium chloride can be related to the increasing concentration of thermally generated Schottky defects formed before and during recrystallization. This assumption seems to be substantiated by the observed recrystallization process (Figures 4 and 5), which must necessarily be connected with ionic movements. It is well known that in the case of alkali halides the diffusion of ions takes place via Schottky defects i.e. positive and negative ion-vacancies.

A further argument in favour of the above assumption appears to be the observed anomalous temperature dependence of the thermal expansion of the α-phase in the temperature range preceding the $\alpha \rightarrow \beta$ transition. Merriam, Smoluchowski and Wiegand [13] showed that for sodium chloride a similar deviation from the linearity of the thermal expansion was observed about 200°C below the melting point. The magnitude of this deviation ($\Delta\alpha$) increases exponentially with the temperature according to $\Delta\alpha = A \cdot \exp(-B/kT)$, where T is the temperature in °K, k = Boltzmann's constant, A is a constant and B should represent the energy of the formation of a cation or anion vacancy. This activation energy was consistent with that deduced from ionic conductivity measurements [14]. The authors concluded that the anomalous thermal expansion of sodium chloride can be related to the concentration of thermally generated Schottky defects.

We suggest that the same mechanism applies to cesium chloride still in the α-phase in the temperature range preceding the $\alpha \rightarrow \beta$-transition. This might be verified by plotting semilogarithmically the temperature dependence of the deviation from linearity ($\Delta\alpha$) in the thermal expansion of cesium chloride, (log $\Delta\alpha$ versus $1/T$). This plot gives a straight line, i.e. $\log \Delta\alpha = \log A - B. 1/kT$, as can be seen from Fig. 5. From the slope of the graph the B activation energy of a thermally generated positive or negative ion vacancy (Schottky defect) can be determined. For this the value 0,6 eV was obtained, which gives 1,2 eV for the formation of a Schottky defect pair.

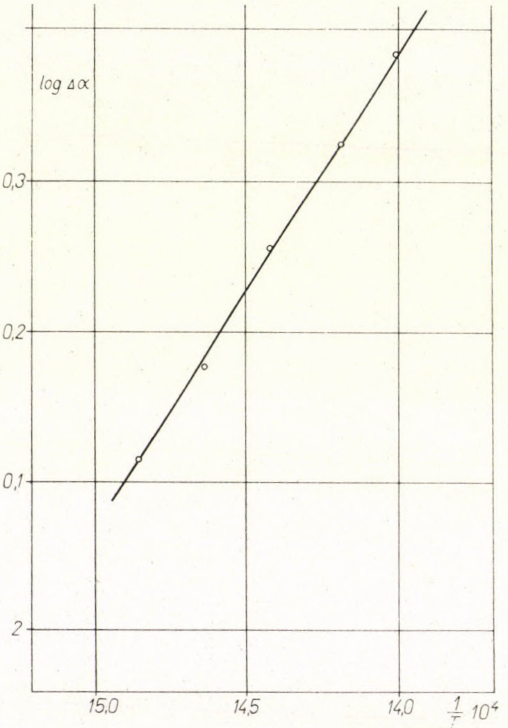

Fig. 5. Temperature dependence of $\Delta\alpha$ in semilogarithmic representation

Similar values were obtained by measuring the electrical conductivity of cesium chloride single crystals and polycrystalline samples. The results are presented and discussed in a following paper to be published.

Our results are apparently in accordance with those of MERRIAM, UBBELOHDE and WOODWARD [4] who explained the anomalous decrease of the intensities of their X-ray lines with the temperature by a gradual increase of the concentration of crystal defects.

Table 1

Lattice spacing at 293^{0}sK and transition temperature of CCl

Lattice spacing in A	Authors	Transition temperature in °K	Authors
4,12	W. P. Davy, F. G. Wick [1]	716	H. Keitel [6] cooling curve
4,121	E. Brock, J. Oftende, A. Probst [2]	718 ± 5	G. Wagner, R. Lippert [4] X-rays
4,118 ± 0,002	R. J. Havighurst E. Mack, F. C. Blake [3]	724	S. Zenczuzny, J. Ronbach [7], C. Sandonini, G. Scarpa [8] cooling curves
4,118 (298°K)	G. Wagner, L. Lippert [4]	752	E. Korrang [9] heating curves
4,1180 ± 0,0005	J. W. Menary, A. R. Ubbelohde, J. Woodward [5]	742	J. W. Menary, A. R. Ubbelohde, J. Woodward [5]
4,118 ± 0,008	present work	753 ± 10	present work

1. Phys. Rev., **17,** 403, 1921.
2. Z. Phys. Chem., **3B,** 209, 1929.
3. J. Amer. Chem. Soc., **46,** 2368, 1924.
4. Z. Phy . Chem., **31,** 263, 1936.
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It seems the conclusion might be drawn that the transition is foreshadowed by a considerable gradual increase in number and size of β nuclei. This, of course, does not exclude the possibility of a dilatational transformation in very small regions of some ten or hundred ions. This transformation of the β nuclei may take place below the transformation temperature. Once, however, they have been formed they start growing by some recrystallization mechanism at the expense of the original phase. The observed hybridization as well as the formation of the β-phase on substrates at elevated temperatures below the transition range might be accounted for in this way.

Table 2

The growth of the β-nuclei below the transition on substrates at elevated temperatures

Temperature of the substrate in ^{0}K	293	503	613	643
Presence of the α and β-component	$\alpha+\beta^*$	$\underline{\alpha}+\beta$	$\alpha+\underline{\beta}$	β

Note: *β-phase only in traces; the underlined letter refers to the predominant phase

We wish to thank Prof. S. **Lengyel** for his continuous interest, Mrs. **Fülöp**, Miss **Bartha** and Miss **Machovits** for helping us to carry out the experiments, and Mr. J. **Hernády** for the construction of the evaporating device attached to the HU—10A instrument.

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ЭЛЕКТРОННО-ДИФФРАКЦИОННОЕ ИССЛЕДОВАНИЕ ФАЗОВОГО ПЕРЕХОДА ХЛОРИСТОГО ЦЕЗИЯ

З. МОРЛИН и Й. ТРЕММЕЛ

Резюме

Электронно-диффракционным методом исследуется фазовый переход хлористого цезия. В температурном интервале, предшествующем температуру перехода, наблюдались гибридизация и рекристаллизация. Термическое расширение альфа-фазы показывает аномальное повышение. Истолкуется возможность добавочного дефектного механизма для этих эффектов.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (2), pp. 137—147 (1966)

THE ELECTRICAL CONDUCTIVITY AND THE PHASE TRANSFORMATION OF CESIUM CHLORIDE

By

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(Presented by Z. Gyulai — Received 14. X. 1965)

From the electrical conductivity of pure cesium chloride crystals and crystals doped with divalent impurities the energy of the formation of a Schottky defect pair can be calculated. The results obtained in this way and the comparison of the activation energy values as obtained from the measurements of the α- and β-phase indicate that the phase transformation is foreshadowed by the formation of termal vacancies. The phase transformation appears to be structure-sensitive.

In a previous paper the bcc (α) → fcc (β) phase transformation of cesium chloride was investigated with an electron diffraction method [1]. The observed hybridization (simultaneous presence of the α- and β-phase below the transformation temperature) and the measured anomalous thermal expansion could be explained by assuming a gradual increase in the concentration of thermally generated Schottky defects. Similar results were obtained by MENARY, UBBELOHDE and WOODWARD [2] who observed an anomalous decrease of the intensities of the X-ray lines with the temperature, and LANTELME and PAULY who showed that neutron irradiated cesium chloride crystals which, subsequent to the irradiation, were heat treated gave an enhanced release of ^{35}S at about 753°K [3]. Both observations might be interpreted by the presence of a high concentration of vacancies in the region of the transition.

In a series of experiments the ionic motion before, after, and in the transition region has been investigated directly by measuring the temperature dependent conductivity of cesium chloride single crystals and polycrystalline pressed samples. Similar measurements had already been carried out [4—6] but with varying results, which may be attributed to the relative small number of samples measured and to the fact that the experiments were carried out over a small temperature range (543°—754°K) only till the end of the transformation.

§ 1. Experimental method

Merck pro analysi and high grade spectral pure material (Johnson, Matley and Co) was used. From the pro analysi material single crystals were grown in a chlorine atmosphere according to the method of AVAKIAN and SMAKULA [7], and polycrystalline disks prepared at room temperature with a pressure of 10 000 kg · cm^{-2}. This method of preparation has already been described

[8, 9]. The conductivity of the samples was measured from 423°K up to 873°K (close to the melting point).

The measurements were carried out in the usual way with a direct current method at a stabilized voltage of 3 V. The current was measured with a Hartmann and Braun light spot galvanometer with a maximum sensitivity of $4{,}49 \cdot 10^{-9}$ amp./scale. The samples covered with a thin graphite layer were clamped between silver electrodes, and heated in an electric oven of stabilized current, which could be regulated with a thoroid transformer. The temperature of the specimens was measured with a Fe—Ko thermocouple and a Hartmann and Braun millivoltmeter.

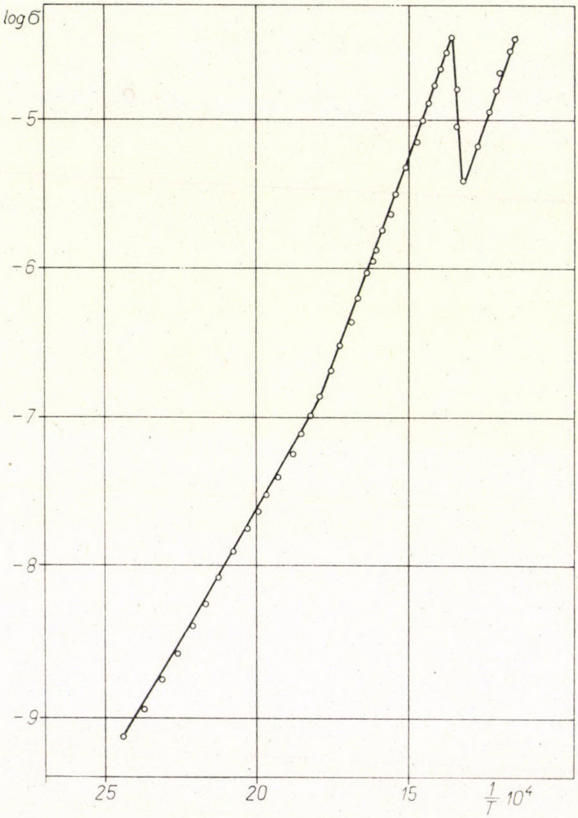

Fig. 1. log σ versus $1/T$ plot of the conductivity of a CsCl single crystal

The specimens were in air or maintained in a dry nitrogen atmosphere. No atmospheric dependent difference could be observed. About 25 samples were measured, and the results could be represented by the well known function $\sigma = \exp(-B/kT)$ (σ = conductivity in $\text{ohm}^{-1}\text{cm}^{-1}$, T = temperature in °K, k* Boltzmann's constant).

§ 2. Results

1. Fig. 1 shows a typical example of the conductivity measurements in semilogarithmical (log σ versus l/T) representation. The graph consists of two straight lines in the α-phase range with a knee at about 550°K. Similar results were obtained with all samples, single crystals and polycrystalline disks, except that the specimens made from spectral pure material had their knee at a lower temperature (about 500°K) as can be seen from Fig. 2.

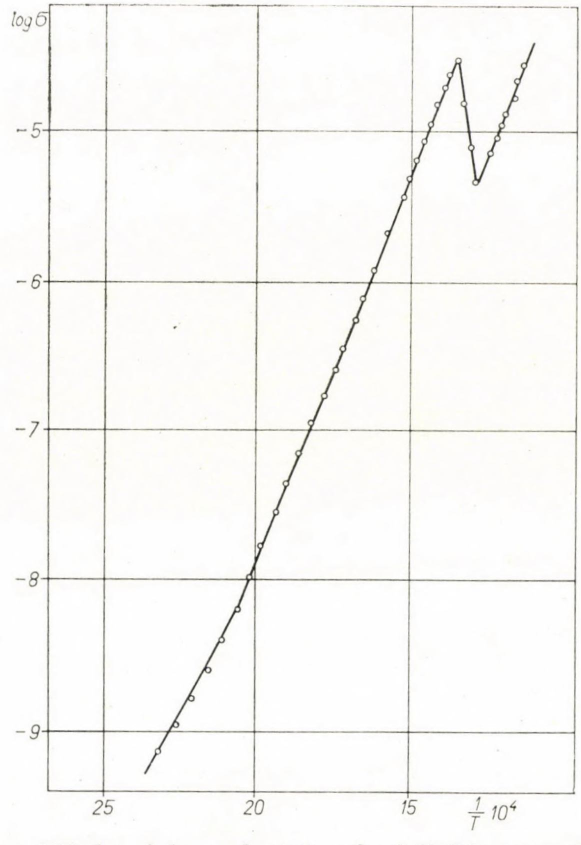

Fig. 2. log σ versus $1/T$ plot of the conductivity of a CsCl disk prepared from spectral-pure material

The phase transformation is indicated by a considerable decrease of conductivity in the transformation region. It may be noted that the conductivity of the β-phase is represented by only one straight line with a slope nearly the same as that of the α-phase line above the knee.

The activation energies as determined from the conductivity measurements in the usual way were 0,6 $\pm$ 0,2 eV for the first region below, and 1,05 $\pm$ 0,05 eV for the second above the knee. The same value was obtained for the single line of the β-phase. With one and the same specimen the difference between the second activation energy of the α-phase and the sole energy value of the β-phase was not more than 0,02 eV.

2. The break in the log σ versus $1/T$ curves is now generally interpreted as resulting from divalent impurities incorporated in the crystal. As the material becomes purer the break in the conductivity graph shifts to lower temperatures in agreement with this interpretation. In our experiments, a similar shift could be observed for the spectral pure specimens (Fig. 2).

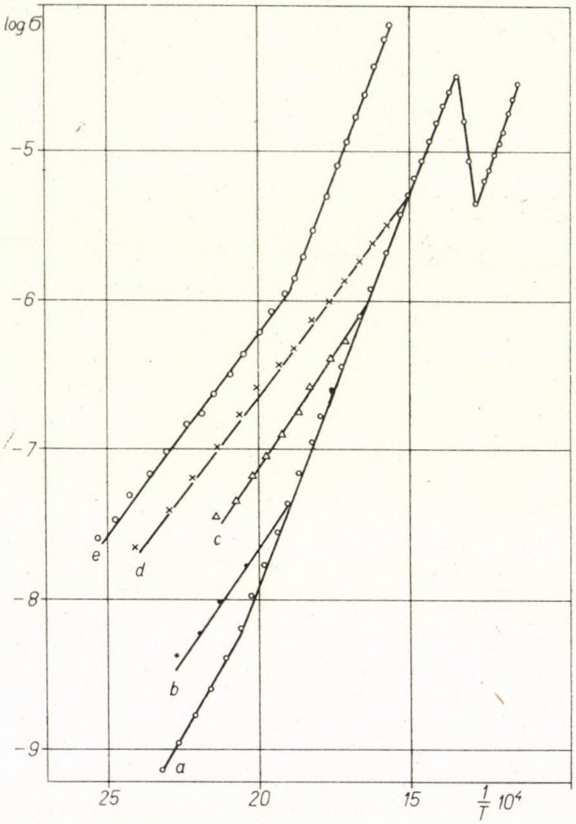

Fig. 3. log σ versus $1/T$ plot of spectral-pure disks doped with $SrCl_2$

a) undoped
b) $12{,}64 \cdot 10^{-7}$ mol ratio Sr/Cs
c) 25,28 mol ratio Sr/Cs
d) 37,92 mol ratio Sr/Cs
e) 94,84 mol ratio Sr/Cs

The influence of the divalent ions was investigated in the usual way developed for KCl and NaCl (KELTING and WITT [10], and ETZEL and MAURER

[11]). The spectral pure cesium chloride was doped with various amounts of $SrCl_2$ by a recrystallization technique already described, and used to incorporate TlCl in sodium chloride [12, 13]. The results of the conductivity measurements on such specimens are presented in Fig. 3. As can be seen, the curves come together to straight lines with the same slope. It should be noted that at a given temperature below the knee the conductivity induced by the divalent metal ion depends upon the concentration of the impurity.

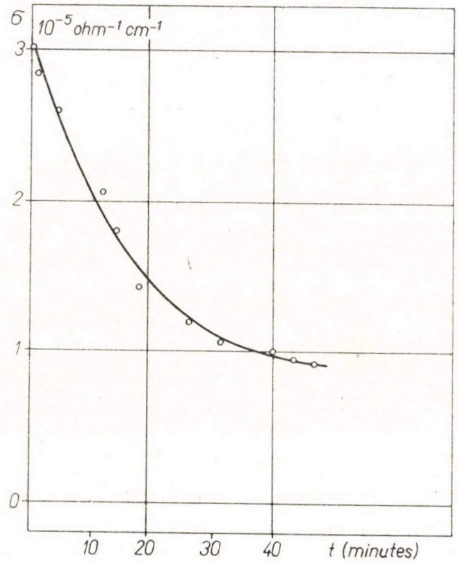

Fig. 4. Time dependence of the $\alpha \to \beta$ transition as indicated by the decrease of the conductivity at constant temperature

3. As can be seen from graphs 1 and 2 the $\alpha \to \beta$-phase transition is indicated by a considerable decrease of the conductivity in the temperature region of the transformation. If the temperature at which the transition was observed to begin was kept constant a relatively small decrease of the conductivity was initiated, which, however, did not indicate a full transformation (Fig. 4). This could be achieved only if the heat treatment at this temperature lasted for more than 10 hours or when the whole temperature range of the transition had been passed through.

The decrease of the conductivity during the transformation can be influenced by a heat treatment at the starting temperature (743° ± 5°K) of the transition. For such experiments the crystals were heat treated for various time intervals, brought down to room temperature and measured. Depending upon the time of the heat treatment, the decrease of the conductivity characteristic for the transition was gradually reduced (Fig. 5). Together with this

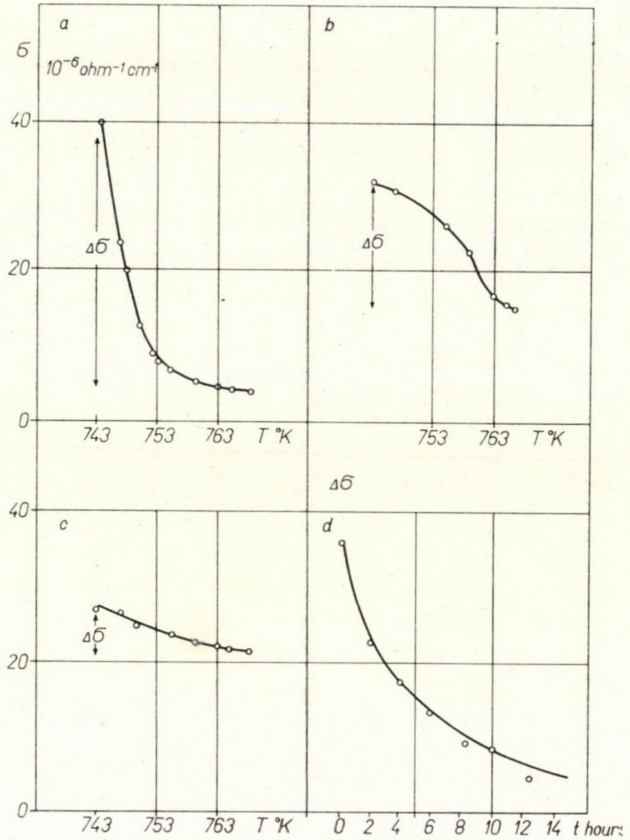

Fig. 5. The time-dependent reduction of the $\Delta\sigma$ values ($\Delta\sigma$ = decrease of the conductivity indicating the phase transformation) as a function of the heat treatment; (temperature of heat treatment: 743°K):

a) before the heat treatment
b) after a heat treatment of 4 hours
c) after a heat treatment of 12 hours
d) the time dependence of $\Delta\sigma$, heat treatment at 743°K

reduction ($\Delta\sigma$) a second knee and a third slope was formed in the α-phase at about 645°K with a very low apparent energy value (B), which varied together with the $\Delta\sigma$ values (Table 1).

§ 3. Discussion

1. The β-phase slope represents a temperature range approaching the melting point of cesium chloride (913°K). Consequently it is a high temperature range, where the conductivity is essentially intrinsic, and should be accounted for by thermally generated Schottky defects. From the fact that the activation energy as calculated from the second slope of the α-phase corresponds in a

Table 1

The variation of the apparent B-values of the third slope of the α-phase conductivity developed during the heat treatment

Time of heat treatment (hours)	$\Delta\sigma$ in 10^{-6} (ohm^{-1} cm^{-1})	B (absolute value)
0	36	no third slope
4	16	1400
6	12	1200
8	9	1000
12	4	850

easonable way with the values of the β-phase it might be assumed that the econd slope of the α-phase represents an intrinsic region, too. In this region, the termally generated defects become larger in number, and the activation energy represents the sum of the energy of formation and the jump energy of a vacancy. Our assumption is substantiated by the results of measurements carried out with $SrCl_2$ doped specimens. From these experiments according to Etzel and Maurer the mobility of the vacancies and the energy of formation of a Schottky defect pair was calculated [11]. Applying the mass action law one obtains

$$y = L\sigma^2 + F\sigma^{*}, \tag{1}$$

where y is the mole fraction of the impurity ion added to the crystal, σ is the conductivity of the crystal containing divalent impurities, and

$$L = x_0 \, H/\sigma_0^2 \tag{2}$$

and

$$F = M/\varrho \, N_0 \, e\mu \, . \tag{3}$$

In Eq. (2) x_0 represents the mole fraction of the positive ion vacancies present in the undoped crystal and σ_0 the conductivity of the undoped crystal. H is defined by the equilibrium constants of the mass action law. By introducing the experimental data as obtained from diagram 3 at constant temperature to Eq. (1) the constant F was evaluated. The mobility (μ) of the vacancies was obtained directly by substituting in Eq. (3) the known values of M (molecular weight), ϱ (density), e (electric charge) and N_0 (Avogadro's number) (Table 2). Plotting log μT versus l/T according to the well known equation

$$\mu = (\mu_0/T) \cdot \exp\,(-U/kT) \tag{4}$$

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* For the derivation of this equation see Etzel and Maurer [11].

Table 2

Evaluation of the F constant and determination of the mobility of the vacancies from measurements on $SrCl_2$-doped samples

Temperature °K	$F = M/\varrho N_0 e\mu$	Mobility cm² sec⁻¹ Volt⁻¹
425	$4{,}15 \cdot 10^4$	$1{,}05 \cdot 10^{-8}$
454	$2{,}45 \cdot 10^4$	$1{,}78 \cdot 10^{-8}$
477	$1{,}72 \cdot 10^4$	$2{,}54 \cdot 10^{-8}$
500	$0{,}90 \cdot 10^4$	$4{,}85 \cdot 10^{-8}$

the U activation energy for a jump of a vacancy was calculated (Fig. 6). For cesium chloride $U = 0{,}5 \pm 0{,}05$ eV was obtained. For the pure crystals an activation energy for the assumed intrinsic region of the α-phase $B = 1{,}05 \pm \pm 0{,}05$ eV was measured. As according to theory

$$B = W/2 + U \tag{5}$$

the W energy to form a pair of isolated positive and negative ion vacancies within the crystal is 1,1 eV.

Assuming that the experimentally measured temperature-dependence of the thermal expansion of cesium chloride in the anomalous region near the $\alpha \rightarrow \beta$ transition as discussed in the previous paper [1] can be related to the concentration of thermally generated Schottky defects, following MERRIAM, SMOLUCHOWSKI and WIEGAND [14] W was also calculated from diffraction measurements [1]. The activation energy for a Schottky defect pair obtained in this way ($W = 1{,}2$ eV) seems to be reasonably consistent with that deduced from the conductivity measurements.

From these results, the conclusion might be drawn that the phase transformation of cesium chloride is preceded by an enhanced release of vacancies as the transition range is approached just as the transition from the solid to the liquid state is accompanied by a rapid increase of vacancies in the crystal near the melting point.

2. The phenomenon described in section 3 of paragraph 2 can be explained by assuming that as a result of the heat treatment at the starting temperature of the $\alpha \rightarrow \beta$ transition β-nuclei start growing. The conductivity of the β-phase is less than that of the α-phase, the reason for which is readily explained by the lower co-ordination number of the fcc β-phase [15]. The slow time dependent transition shown in Fig. 4 may represent a slow growth of β-nuclei. As a result of these experiments it is suggested that the heat treatment produces a certain number of β-nuclei which seem to be very stable. When, after the heat treatment, the temperature dependent conductivity was mea-

sured the β-nuclei formed during the previous heat treatment are supposed to start growing even below the transition temperature. The α-phase is still in excess, and the conductivity increases with the temperature. This increase, however, is suppressed by the growing β-nuclei. As a result of these two opposed processes the slope of the conductivity graph, and with it the apparent activation energy, decreases. The starting temperature of the phase transformation is in the heat-treated cases lowered, it starts with the second knee, and is indicated by the lowering of the B-values, too. In these cases not only the decrease of the conductivity, but the formation of the second knee, and the B-values above it ought to be considered together as indicating the phase transformation.

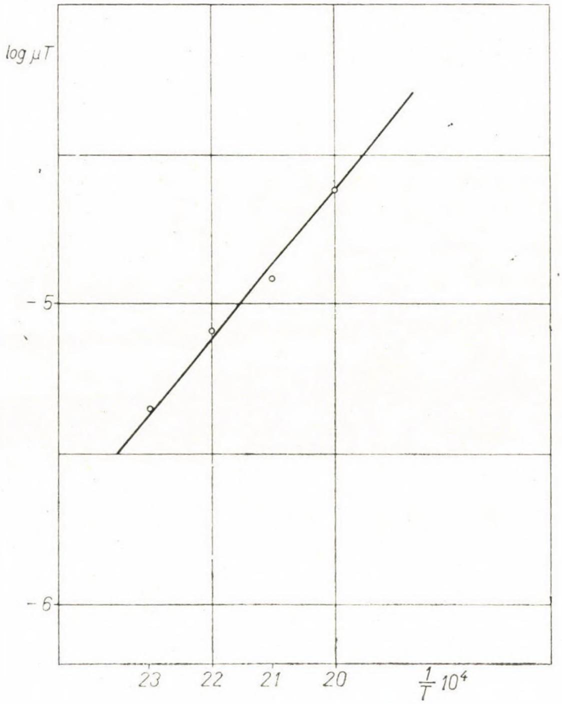

Fig. 6. Semilogarithmic representation of the temperature-dependent vacancy mobility as determined by the $SrCl_2$-doped specimens

The conclusion can be drawn that the phase transformation of cesium chloride is structure-sensitive. This structure sensitivity is also indicated by a hysteresis shown in the $\alpha \rightarrow \beta$ and $\beta \rightarrow \alpha$ transformation as can be seen from Fig. 7. Similar observations have already been reported [4].

Summary

1. The temperature dependence of the electrical conductivity of the α-phase of cesium chloride consists of two slopes The activation energy as determined from the second slope corresponds in a reasonable way with the values determined from the single slope of the β-phase.

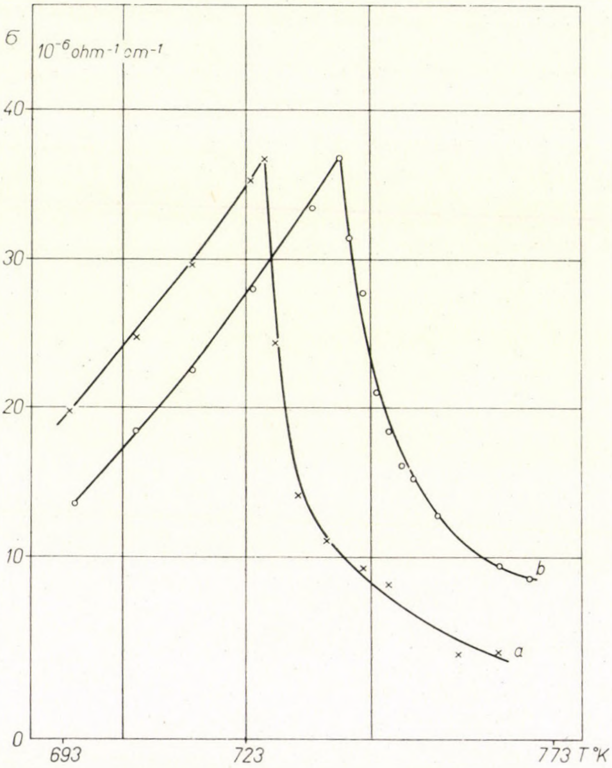

Fig. 7. Hysteresis of the $\alpha \rightarrow \beta$ and $\beta \rightarrow \alpha$ transition:

a) as measured at increasing temperature
b) measured at decreasing temperature

2. By doping the cesium chloride samples with $SrCl_2$ the activation energy for one ion jump can be calculated. From this and from the second slope of the conductivity graph of the α-phase the activation energy of the formation of a vacancy pair can be calculated. The values obtained in this way correspond in a good approximation with the values obtained from the anomalous increase of the thermal expansion.

3. The experimental results can be explained by assuming that the phase transformation is foreshadowed by the formation of thermal vacancies.

4. The process of the phase transformation as indicated by the electrical conductivity can be influenced with a proper heat treatment: the transformation appears to be structure sensitive.

Acknowledgement

I wish to thank Dr. G. Turchányi and Dr. S. Ujhelyi (Research Group for Crystal Physics of the Hungarian Academy of Sciences) for growing the single crystals, Dr. J. Teltow and Dr. P. Müller (Institute of Crystal Physics, Berlin-Adlershof), and Dr. R. Voszka (Research Group of Crystal Physics of the Hungarian Academy of Sciences) for valuable discussions. Further, I thank Mr. J. Hernády and Mr. P. Hölczl for constructing the measuring device, Miss M. Albekker for carrying out a great number of the measurements, and Miss J. Machovits for her help in evaluating the results.

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ЭЛЕКТРИЧЕСКАЯ ПРОВОДИМОСТЬ И ФАЗОВЫЙ ПЕРЕХОД ХЛОРИСТОГО ЦЕЗИЯ

З. МОРЛИН

Резюме

На основе электрической проводимости чистых кристаллов хлористого цезия и кристаллов, содержащих двухвалентные примеси, определяется энергия образования дефектных пар Шоттки. Полученные данным методом результаты и сравнение энергий активации, полученных на основе измерений α- и β-фаз, показывают, что фазовый переход предсказывается образованием термических вакансий. Фазовый переход оказывается чувствительным относительно структуре.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (2), pp. 149—167 (1966)

DIE LEBENSDAUER DER HELIUMZUSTÄNDE

Von

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(Vorgelegt von L. Jánossy. — Eingegangen 16. XI. 1965)

Die Lebensdauer der 4^3S-, 4^1D-, 3^3P-, 5^1D-, 4^3D- und 4^1S-Zustände von Helium werden durch Messungen der Zerfallskurven mit Hilfe eines Zeitanalysators bestimmt. Es ergeben sich der Reihe nach folgende Werte: $67 \pm 1{,}4$; $41 \pm 1{,}3$; 112 ± 6; 57 ± 2; 93 ± 6 und 90 ± 7 nsec.

Einleitung

Zur Bestimmung der Lebensdauer angeregter atomarer Zustände sind aus der Literatur mehrere indirekte [1, 2] bzw. direkte Messmethoden [1, 3—8] bekannt. Da bei Anwendung der früheren Messmethoden zahlreiche Störeffekte auftreten, die in den Messergebnissen beträchtliche Abweichungen hervorrufen [9—13], ist es von Interesse, eine neue Messmethode zu entwickeln. Vor einigen Jahren schlug HERON, McWHRITER und RHODERICK [14, 15] ein neues Verfahren zur unmittelbaren Messung der Lebensdauer angeregter Zustände vor. Bei dieser Methode werden die Atome durch Impulse von Elektronen angeregt und die durch die angeregten Atome ausgesandten Lichtquanten mit einem Elektronenvervielfacher detektiert. Der zeitliche Unterschied $t - T = \tau$ zwischen dem Ende der Anregung und dem Impuls aus dem Elektronenvervielfacher kann gemessen werden, wobei T die Zeitdauer der Anregung, d. h. die Länge des Erregerstromimpulses ist. Anhand der beobachteten Häufigkeit $n(\tau)$ der Zeitabstände τ lässt sich die Zerfallskurve auftragen. Durch Logarithmieren der Zerfallskurve erhält man die Zerfallsgerade. Die Richtungstangente der Zerfallsgeraden stellt die mittlere Lebensdauer τ_0 dar.

Der zeitliche Ablauf des Erregerstromes, die Wahrscheinlichkeit (W) des Erscheinens des Lichtquants als Funktionen der Zeit und die zeitliche Lage der beiden Kurven im Verhältnis zueinander sind aus Abb. 1 ersichtlich. Die Zerfallskurve kann entweder nach der verzögerten Koinzidenzmethode [16] oder mit Hilfe eines Zeitanalysators [17] gemessen werden.

Die Methode von HERON wurde für die Messung der angeregten Zustände von Helium und Neon bereits mehrmals benutzt [18, 19].

Die Versuchsanordnung, die für die Messung der Lebensdauer entwickelt wurde, beruht auf dem Zeitanalyseprinzip [20]. Abb. 2 zeigt das Termschema des Heliums. Bei den einzelnen Niveaus sind die berechneten [21] und gemessenen Lebensdauerwerte angegeben. Die letzteren sind mit einem * bezeichnet. Als Zeiteinheit gilt die Nanosekunde. Die unterhalb der Termen stehendnen Zahlen stellen die Kehrwerte der theoretischen Lebensdauer dar. Mit Ausnahme der Niveaus 5^1D und 4^3D stimmen unsere Messergebnisse mit den in der Literatur veröffentlichten experimentell bzw. rechnerisch ermittelten Werten gut überein. Die Abweichungen, die sich bei der Lebensdauer des Niveaus 5^1D zeigen, lassen sich durch Störeffekte erklären, bei der Lebensdauer des Zustandes 4^3D hingegen konnte die Abweichung vom theoretischen Wert nicht gedeutet werden.

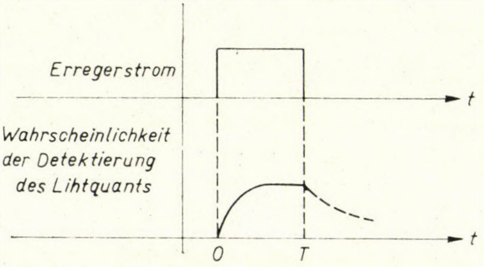

Abb. 1

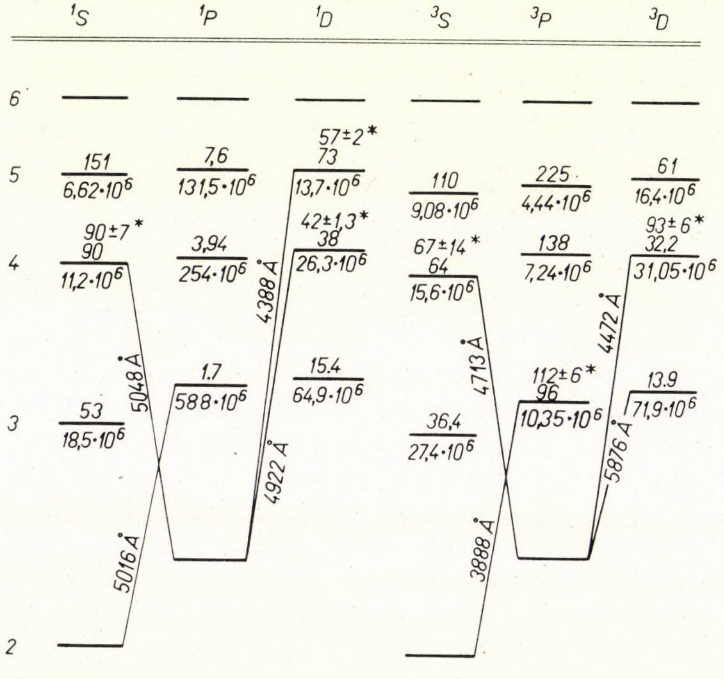

Abb. 2. Die Lebensdauer der Terme sind in nsec (obere Werte), ihre reziproken Werte in $\sec^{-1}$ (untere Werte) angegeben. Die mit einem Stern bezeichneten Werte sind die von uns gemessenen Werte

I. Die experimentelle Anordnung

Die Messungen wurden in einem mit einem Vakuumsystem verbundenen Versuchsrohr durchgeführt (Abb. 3).

Das Rohr wurde ausgeheizt, und bis zu einem Druck von 10^{-7} Torr ausgepumpt. Das System erwies sich auch zur Füllung des Rohres mit spektralreinem Gas des Druckes 10^{-3}—10^{-2} Torr als geeignet.

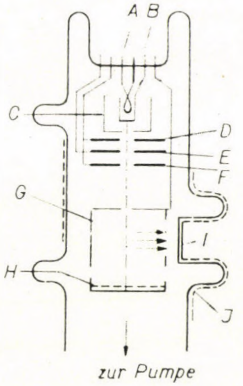

Abb. 3. A Heizfaden, B Kathode, C Wehnelt-Zylinder, D Beschleunigungselektrode, E Fokussierungselektrode, F letzte Elektrode der Elektronenlinse, G Beobachtungsraum, H Kollektor, I Fenster für das austretende Licht. Die gestrichelte Linie zeigt den schwarzen Anstrich des Rohres, mit dem störendes zerstreutes Licht eliminiert werden kann

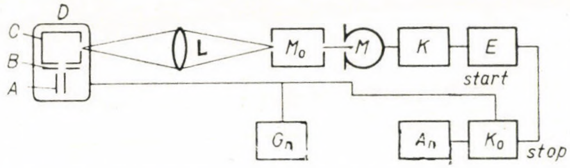

Abb. 4. A Elektronenquelle, B Steuerungselektrode, C Beobachtungsraum, D Versuchsrohr, L Kollimatorobjektiv, M_0 Monochromator, M Sekundärelektronenvervielfacher, K Kathodenverstärker, K_0 Zeit-Amplituden-Umformer, A_n 128-Kanal-Amplitudenanalysator, G_n Impulsgenerator, E Verstärker

Die He-Atome wurden durch Elektronenpakete aus einer Elektronenkanone erregt. Der Strom der Elektronenkanone wurde durch einen Generator gesteuert, der Impulse mit einer Amplitude von 40 V, einer Anstieg- und Abfallzeit von 3 nsec, einer Impulslänge von 100 nsec ($0-T$ Erregungszeit) und einer Frequenz von 10 kHz erzeugte. Die von der für gewöhnlich abgesperrten Kathode ausgesandten Stromimpulse von 100—200 μA, mit der Impulslänge von 100 nsec treten nach geeigneter Beschleunigung und Fokussierung in den Beobachtungsraum ein.

Das entstehende Licht wird durch ein optisches Abbildungssystem bzw. einen Monochromator — der die zu beobachtende Spektrallinie auswählt —, einem Photoelektronenvervielfacher Typ 1P21 (siehe Abb. 4) zugeführt.

Die Versuchsbedingungen (Gasdruck, Elektronenstrom, Abbildung) wurden so gewählt, dass allen 100 bzw. 500 erregenden Elektronenimpulsen ein einziger Spannungsimpuls aus dem Photoelektronenvervielfacher folgte. Zwischen dem Ende des erregenden Impulses und dem Auftreten des Spannungsimpulses kommt es zu einer Zeitverzögerung. Die Aufgabe bestand in der Messung der Verzögerungszeiten. Die aus dem Photoelektronenvervielfacher austretenden und entsprechend verstärkten Spannungsimpulse erreichen den Eingang des Zeit-Amplituden-Umformers System »Start-Stop«; die Amplitude der aus dem Umformer ausgesandten Impulse ist der Zeit proportional, die zwischen dem Ende des erregenden Impulses und dem Entstehen des photoelektrischen Impulses verstreicht.

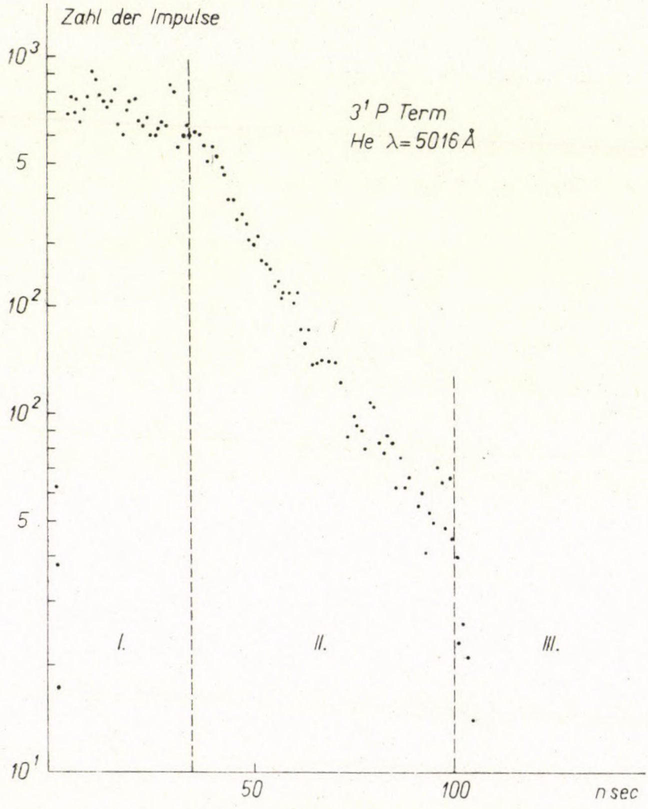

Abb. 5

Die Impulse werden mit Hilfe eines 128-Kanal-Amplitudenanalysators analysiert. Ein Kanal entspricht einer Zeit von 1 nsec.

Der für die Auswertung brauchbare Analysierbereich des Zeitanalysators liegt bei $(t - T)_{\max} \sim 60$ nsec. Abb. 5 zeigt eine im semilogarithmischen

Koordinatensystem dargestellte Zerfallskurve, deren erster Abschnitt der Zeit $t < T$ entspricht, bei der noch Erregerstrom fliesst. Der zweite Abschnitt der Kurve gibt den eigentlichen Zerfallsverlauf wieder: dies ist eine Gerade, die dem exponentiellen Zerfallgesetz folgt. Der letzte Abschnitt der Kurve fällt steil ab, woraus man auf die Grenze des Analysierbereiches schliessen kann.

II. Auswertung der Messergebnisse

Aus dem Logarithmus der im i-ten Messprozess erhaltenen Messwerte $\ln [n_i^{(l)}(k\Delta\tau)]$ wurde die Zerfallsgerade des betrachteten Zustandes (l) nach der Methode der kleinsten Quadrate [22] bestimmt, wo $\Delta\tau = 1$ nsec die Breite eines Kanals im Analysator und $k = 1, 2, 3 \ldots 60$ die laufende Nummer des Kanals ist. Die Richtungstangente der gewonnenen Zerfallsgerade stellt die mittlere Lebensdauer des Zustandes $\tau_0^{(l)}$ dar. Die Anwendung dieser Methode [23] zur Auswertung der Messergebnisse ist zulässig, da die kürzeste Lebensdauer, die sich bei dieser Versuchsanordnung überhaupt messen liess, bei $\tau_{0\min} \leqq 5$ nsec, also wesentlich unter der in der gegenwärtigen Arbeit gemessenen Lebensdauer lag (einige zehn nsec).

Für die Terme 4^3S, 4^1D wurden mehrere Messkurven des Zerfallprozesses aufgenommen. Aus den von diesen Kurven einzeln berechneten Lebensdauergrössen wurde danach der Mittelwert $\bar{\tau}_0$ errechnet. Der Messfehler wurde auf Grund der Messwerte zu $\sigma = \sqrt{\frac{(\tau_{i0} - \bar{\tau}_0)^2}{n(n-1)}}$ geschätzt, wobei n die Zahl der Zerfallskurven bezeichnet.

Für die weiteren Zustände 3^3P, 5^1D, 4^1S wurde nur je eine Zerfallsgerade gemessen. Die mittleren Lebensdauerwerte wurden für diese Terme auf Grund der Formel

$$1/\tau_{0i} = \frac{\ln[n(k_i \Delta \tau)] - \ln[n(k_j \Delta \tau)]}{(k_i - k_j)\Delta\tau}$$

berechnet, wobei $k_i - k_j = 55$ ist. Für $k_i = 1, 2, 3, 4, 5$ ergaben sich also fünf τ_i Werte, aus denen sich der Mittelwert, weiterhin unter Anwendung der angegebenen Formel der Fehler (σ) ermitteln liessen.

III. Physikalische Vorgänge in der Strahlungsquelle

Ausser dem Abklingen der erregten Zustände treten im Gas auch andere physikalische Vorgänge auf, zu deren gefolge die aus den Messergebnissen bestimmten Lebensdauerwerte mit den theoretischen Werten manchmal nicht übereinstimmen. Um die Messergebnisse mit den theoretischen Werten vergleichen zu können, müssen auch diese Störeffekte berücksichtigt werden. Es zeigen sich folgende Störeffekte [20]:

1. Resonanzabsorption [24—28]
2. Mit dem Anregungsaustausch verbundene Zusammenstösse zwischen Atomen im angeregten bzw. im Grundzustand (Stösse zweiter Art) [31—34, 21].
3. Kaskadenvorgänge zwischen den verschiedenen angeregten Zuständen [21, 29, 30].

Das hier folgende Gleichungssystem gibt die Zeitabhängigkeit der Population:

$$\frac{dn_i}{dt} = \frac{n_i}{\tau_0^{(i)}} - n_i N\bar{v} \sum_k Q_{ik} + \sum_{l>i} A_{li} n_l + N\bar{v} \sum_m Q_{im} n_m + N q_i (V) j; \qquad (1)$$

n_i ist die Besetzung des Niveaus i. Infolge der spontanen Übergänge nimmt die Population im Zustand i ab; dies kommt im ersten Glied der rechten Seite der Gl. (1) zum Ausdruck; $\tau_0^{(i)}$ ist die mittlere Lebensdauer des Zustandes i. Zwischen diesem Wert und den Einsteinschen spontanen Übergangswahrscheinlichkeiten A_{ik}, $(k < i)$ gilt die Beziehung

$$\tau_0^{(i)} = \frac{1}{\sum\limits_k A_{ik}} .$$

Handelt es sich um einen Resonanzzustand, dann ist

$$\tau_0^{(i)} = \frac{1}{g A_{i0} + \sum\limits_{i<k} A_{ik}} ,$$

worin g den Einkerkerungsfaktor (eine Folge der Resonanzabsorption) [24—26] bezeichnet, während das Niveau 0 dem Grundzustand des Atoms gleich ist.

Die Population im Zustand i kann sich auch dann vermindern, wenn ein Atom im angeregten Zustand i mit einem Atom im Grundzustand zusammenstösst (Stösse zweiter Art). Beim Zusammenstoss geht das Atom, das sich im Anregungszustand i befindet, in den Grundzustand über, während das im Grundzustand befindliche Atom in den angeregten Zustand k übergeht. Der Wirkungsquerschnitt eines derartigen Stosses ist Q_{ik}. Das zweite Glied der rechten Seite der Gl. (1) stellt eine auf diese Weise sich abspielende Besetzungsabnahme dar, wobei N die Zahl der im Grundzustand befindlichen Atome je cm^3 und $\bar{v}$ die mittlere Geschwindigkeit der beiden zusammenstossenden Atome gemäss

$$\bar{v} = \sqrt{\frac{16\,k\,T}{\pi\,\mu}}$$

ist. Hier ist k die Boltzmannsche Konstante, T die Gastemperatur und μ die Masse der Gasatome.

Als Folge des Strahlungsprozesses fallen die Atome von dem höheren Zustand l auf das Niveaus i und bewirken dort eine Besetzungszunahme. Das dritte Glied der rechten Seite der Gl. (1) stellt den mit dem Abfallen der Atome verbundenen Anstieg der Atomzahl dar.

Die Folgen der Stösse zweiter Art zeigen sich nicht nur in der Abnahme des Besetzungswertes, sondern auch darin, dass die Atome vom Zustand m in den Zustand i gelangen. Dies kommt im vierten Glied der Gl. (1) zum Ausdruck.

Durchfliesst ein Strom der Dichte j das Heliumgas, werden die im Grundzustand befindlichen und von den Elektronen angestossenen Gasatome in einen höheren Zustand gehoben. Man hat also mit einem Anstieg der Population zu rechnen, was im fünften Glied der rechten Seite der Gl. (1) seinen Ausdruck findet, wobei $q_i(V)$ den Wirkungsquerschnitt bedeutet, mit dem zu rechnen ist, wenn ein Atom als Folge eines Zusammenstosses vom Grundzustand in den angeregten Zustand i gehoben wird, während V das auf die Elektronen auswirkende Potential des Beschleunigungsfeldes bezeichnet.

Im Ausgangzustand ist $t = 0$, $n_i = 0$, $i \neq 0$ und $n_0 = N$, d. h. sämtliche Atome können mit guter Näherung als im Grundzustand befindlich angesehen werden (Boltzmann-Verteilung). Im Zeitabstand $t = 0 - T$ (siehe Abb. 1) fliesst ein Strom der Dichte j durch das Gas, im Zeitpunkt T beträgt also die Atomverteilung $n_0, n_1, \ldots n_i \neq 0$. Der weitere Besetzungsverlauf ist durch die Gleichung

$$\frac{dn_i}{dt} = -\frac{n_i}{\tau_0^{(i)}} - n_i N \bar{v} \sum_k Q_{ik} + \sum_{l>i} A_{li}\, n_l + N\bar{v} \sum_m Q_{im}\, n_m \tag{2}$$

gegeben.

Die Zerfallskurve $n_i(\tau) = n_i(t - T)$ ist im allgemeinen eine Funktion der Parameter $\tau_0^{(i)}$, Q_{ik}, A_i. Da unsere Messungen die Bestimmung der Zeit $\tau_0^{(i)}$ bezweckten, müssten die experimentellen Bedingungen so gewählt werden, dass der Einfluss der übrigen Parameter vernachlässigbar klein bleibt. Dies ist jedoch nicht immer leicht zu erreichen. Beim Helium war die Aufgabe leichter, da über die Wirkungsquerschnitte Q_{ik} und q_i bereits Untersuchungen vorlagen [21, 32—34], die bei der Auswertung unserer Messergebnisse benützt werden konnten. Zwischen den experimentell und den rechnerisch ermittelten Werten liess sich eine gute Übereinstimmung feststellen.

IV. Diskussion der Messergebnisse

Die erhaltenen Messergebnisse sind aus Tabelle 1 ersichtlich. In der ersten Kolonne sind die betrachteten Übergänge, in der zweiten die Wellen-

Tabelle 1

Messergebnisse

Übergang	λ (Å)	Druck (μ)	V_H (Volt)	τ_{nsec}	$\bar{\tau} \pm \sigma_{\bar{\tau}}$ (nsec)	τ Literatur (nsec)
2^3S-3^3P	3889	40	31	112,5	112±6	100±8* [19]
				120,0		96,5 [21]
				112,5		118 [36]
				91,5		115±5* [14]
				125,6		
2^1P-5^1D	4388	40	50	57,9	57±2	72,0 [21]
				56,7		
				52,4		
				54,4		
				63,9		
2^3P-4^3D	4472	40	50	78,6	93±6	32,2 [21]
				92,0		
				84,8		
				112,0		
				98,3		
2^3P-4^3S	4713	18		70,3	67,0±1,4	102,0 [36]
		16	50	66,4		63,8 [21]
		40	30	61,8		67,5±1* [14]
		13	30	64,8		64,0 [35]
		4	30	70,6		
		4	30	67,4		
2^1P-4^1D	4922	7,5		42,0	41,6±1,3	37,8 [21]
		18	100	42,1		
		7	30	43,2		
		7	50	45,7		
		16	50	37,6		
		40	50	45,7		
		13	50	37,4		
2^1P-4^1S	5048	40		83,4	90±7	90,0 [21]
				112,2		
				94,8		
				74,3		
				84,6		

Tabelle 2

Energiedifferenzen in eV in bezug auf die ^1P-Terme im Falle der He-Atome [34]

	^1S	^1D	^3S	^3P	^3D
2^1P	0,598	—	0,9975	0,2521	—
3^1P	0,165	0,013	0,366	0,079	0,013
4^1P	0,068	0,006	0,147	0,034	0,006
5^1P	0,035	0,003	0,074	0,018	0,003
6^1P	0,020	0,002	0,042	0,010	0,002
7^1P	0,012	0,001	0,026	0,006	0,001

längen (λ) des Überganges angeführt. Die dritte Kolonne enthält die Werte der bei den einzelnen Messungen verwendeten Gasdrücke ($P \sim N$) in Mikron, während die vierte das Potential des Beschleunigungsfelds angibt. Die experimentell bestimmten Lebensdauerwerte finden sich in Kolonne 5 und die daraus gebildeten Mittelwerte (mit statistischem Fehler) in Kolonne 6. Zu Vergleichszwecken sind die aus der Literatur bekannten berechneten und die experimen-

Tabelle 3

Wirkungsquerschnitte für Stösse zweiter Art der He-Atome (Einheit 10^{-16} cm^2)

	^1S	^1D	^3S	^3P	^3D
3^1P				134 [21] 82 [38] 25,9 [39] 21,0 [34]	73 [21] 423 [38] 120 [34]
4^1P	92,1 [21] $<$17,8 [38] $<$30,0 [34]	121,7 [21] 29,7 [38] 86,1 [39] 120,0 [32] 67,0 [34]	74,3 [21] $<$ 5,9 [38] $<$15,0 [34]		123,2 [21] 56,4 [38] 66,8 [39] 26,0 [32] 150,0 [34]
5^1P	92,6 [21] $<$ 9,3 [38] 28,6 [39] $<$15,0 [34]	166 [21] 232 [38] 175 [39] 760 [32] 510 [34]	50,0 [21] $<$ 5,8 [38] $<$ 9,0 [34]		240 [21] 111 [38] 120 [32] 270 [34]

Die bei der Diskussion der Messergebnisse betrachteten Wirkungsquerschnittwerte sind unterstrichen.

tell ermittelten Lebensdauerwerte (letztere mit * bezeichnet) in Kolonne 7 angeführt.

Zustand 3^3P. Dieser Zustand ist kein Resonanzniveau, deshalb gibt es hier keinen Einkerkerungseffekt. Tabelle 2 gibt die zwischen den benachbarten Zuständen (von den gleichen Hauptquantenzahlen) vorhandenen Abstände [34] an. Die Termunterschiede gegenüber den ^1P-Termen sind in eV angegeben. Die Wirkungsquerschnitte der Stösse zweiter Art hängen weitgehend von den Energiedifferenzen ab. Ein Stoss zweiter Art mit einem 1,4-fachen gaskinetischen Wirkungsquerschnitt konnte experimentell nur zwischen 3^1P und 3^3P nachgewiesen werden (siehe Tabelle 3). Der Abklingprozess wird durch die Kleinheit des Wirkungsquerschnittes und die Kürze der Lebensdauer des Zustandes 3^1P nicht wesentlich gestört.

Da die Wirkungsquerschnitte der Anregung der Niveaus n^3S, n^3D ($n > 3$) durch Elektronenstoss kleiner sind als die Wirkungsquerschnitte der Anregung des Niveaus 3^3P (siehe Tabelle 4 und 5), beträgt die Besetzungszunahme durch Kaskadenübergänge nicht mehr als 15 Prozent. Die grösste prozentuale Populationszunahme ergab sich am Niveau 4^3S (siehe Tabelle 5):

Tabelle 4

Wirkungsquerschnitte der Erregung der He-Atome durch Elektronstösse von 30 eV Energie. (Einheit 10^{-20} cm^2) Nach GABRIEL und HEDDLE [21]

Hauptquantenzahl	^1S	^1P	^1D	^3S	^3P	^3D
6	14	10	4,5			
5	17	22	11	22	42	18
4	38	53	18	55	76	27
3	70	110	38	162	181	166

$$\alpha\left(\frac{0\to 4^3S\to 3^3P}{0\to 3^3P}\right) = 100\,\frac{q_{4^3S}(30V)\,A_{4^3S\to 3^3P}}{q_{3^3P}(30V)\sum_x A_{4^3S\to x}} \sim 12\%\,.$$

Wie aus Tabelle 1 ersichtlich, stimmt der experimentell ermittelte Wert der Lebensdauer mit dem aus der Literatur bekannten Wert gut überein.

Der *Zustand 5^1D* ist kein Resonanzzustand. Der Zustand 5^1D ist mit dem Zustand 5^1P in »thermischer« Kopplung. Tabelle 3 zeigt die Wirkungsquerschnitte der Zusammenstösse zweiter Art.

Obwohl der Wirkungsquerschnitt der Erregung des Zustandes 6^1P durch Elektronenstoss von derselben Grössenordnung ist wie der Wirkungsquerschnitt des Zustandes 5^1D (siehe Tabelle 6), ist die Übergangswahrscheinlichkeit

Tabelle 5

Übergangswahrscheinlichkeiten bei He-Atomen (Einheit 10^6 sec^{-1}
Nach GABRIEL und HEDDLE [21]

	2^1P	3^1P	4^1P	5^1P	6^1P	7^1P	8^1P
1^1S	1870	571	246	127	74,0	46,6	31,0
2^1S	1,97	13,4	6,81	3,85	2,56	1,60	1,07
3^1S	18,8	0,25	1,47	0,94	0,57	0,43	0,26
4^1S	6,60	4,54	0,06	0,30	0,25	0,19	0,14
5^1S	3,12	2,01	1,49	0,02	0,08	0,07	0,07
6^1S	1,76	1,07	0,72	0,61	0,01	0,03	0,05
7^1S	1,21	0,62	0,42	0,30	0,26	0	0,04
8^1S	0,74	0,41	0,27	0,21	0,15	0,14	0
3^1D	65,1	0	0,29	0,13	0,09	0,08	0,07
4^1D	19,3	7,14	0	0,16	0,08	0,05	0,03
5^1D	8,89	3,28	1,52	0	0,08	0,04	0,03
6^1D	4,94	1,80	0,84	0,47	0	0,04	0,02
7^1D	2,63	1,17	0,52	0,29	0,18	0	0,02
8^1D	1,82	0,66	0,38	0,22	0,15	0,14	0

	2^3P	3^3P	4^3P	5^3P	6^3P	7^3P	8^3P
2^3S	10,2	9,28	5,67	3,08	1,87	1,15	0,79
3^3S	27,5	1,07	0,71	0,60	0,41	0,29	0,21
4^3S	9,26	6,42	0,22	0,12	0,14	0,17	0,18
5^3S	4,33	2,68	2,05	0,06	0,03	0,05	0,07
6^3S	2,40	1,40	0,90	0,76	0,03	0,01	0,02
7^3S	1,75	0,86	0,51	0,37	0,36	0,01	0,01
8^3S	1,18	0,60	0,34	0,25	0,17	0,15	0,01
3^3D	71,7	0	0,65	0,27	0,06	0,01	0
4^3D	24,4	6,65	0	0,32	0,16	0,03	0,01
5^3D	11,9	3,38	1,26	0	0,16	0,09	0,02
6^3D	5,87	1,99	1,05	0,35	0	0,09	0,05
7^3D	4,53	1,33	0,60	0,26	0,13	0	0,03
8^3D	3,03	0,98	0,43	0,22	0,10	0,06	0

zwischen den Zuständen $6^1P \to 5^1D \sim 10^{-3}$-mal geringer, als die Summe der Übergangswahrscheinlichkeiten vom Niveau 6^1P (siehe Tabelle 5), so dass der Störeffekt des Kaskadenprozesses vernachlässigt werden kann.

Nach Gl. 2 der Anhang *A* lautet die Populationsformel für das Niveau 5^1D im Zeitpunkt $t > T$ wie folgt:*

$$\dot{n}_{5^1D} = -\left(\frac{1}{\tau_0^{(5^1D)}} + 16{,}8 \cdot 10^6\right) n_{5^1D} + 16{,}8 \cdot 10^6\, n_{5^1P}\,, \tag{3}$$

wobei der Druck $40\,\mu$, d. h. $N = \dfrac{P}{kT} = 1{,}25 \cdot 10^{15} \dfrac{1}{\text{cm}^3}$ ist. Bei einer Temperatur von $T = 300°$ K sind die mittlere Geschwindigkeit und der Wirkungsquerschnitt

$$\bar{v} = \sqrt{\frac{16k\,T}{\pi\,\mu}} = 1{,}77 \cdot 10^5\,,$$

$$Q_{5^1P - 5^1D} = 7{,}6 \cdot 10^{-14}\,.$$

Der für den $\dfrac{1}{\tau_0^{(5^1D)}}$ erwartete Wert beträgt somit $13{,}7 \cdot 10^6\ \text{sec}^{-1}$ (siehe Abb. 2). Die Population ist für den Term 5^1P in Gl. (2) gegeben:

$$\dot{n}_{5^1P} = -\left(\frac{1}{\tau_0^{(5^1D)}} + 16{,}8 \cdot 10^6\right) n_{5^1P} + 16{,}8 \cdot 10^6\, n_{5^1D}\,. \tag{4}$$

Mit Berücksichtigung der thermischen Stösse, die zum Übergang 5^3D führen ($Q_{5^1P-5^3D} = 1{,}2 \cdot 10^{-14}\ \text{cm}^2$; siehe Tabelle 3), und des Einkerkerungseffektes für diesen Term (für die Errechnung des Einkerkerungseffekts siehe [14]; der Radius des Beobachtungsrohres $\varrho = 0{,}5$ cm), ist für $1/\tau_0^{(5^1P)} = 20{,}5 \cdot 10^6\ \text{sec}^{-1}$ zu erwarten. Die Lösung der Gl. (3) und (4) nach n_{5^1D} lautet also nach Formel A4 (siehe Anhang A) wie folgt:

$$\begin{aligned} n_{5^1D}(\tau) = {} & \left[0{,}49 n_{5^1P}(T) + 0{,}60 n_{5^1D}(T)\right] e^{-\frac{\tau}{60}} - \\ & - \left[0{,}49 n_{5^1P}(T) - 0{,}40 n_{5^1D}(T)\right] e^{-\frac{\tau}{19{,}5}}\,. \end{aligned} \tag{5}$$

Hierin bedeutet $n_{5^1D}(T)$ und $n_{5^1P}(T)$ die Besetzung der betreffenden Niveaus im Zeitpunkt $t = T$. Als Zeiteinheit gilt in der Formel die Nanosekunde. $n_{5^1D}(T)$ und $n_{5^1P}(T)$ lassen sich aus den Lösungen des Gleichungssystems (1) ableiten, indem man berücksichtigt, dass die Stromdichte $j = 8 \cdot 10^{16} \dfrac{\text{Elektron}}{\text{cm}^2}$ und $q_{5^1P}(50) = 5{,}6 \cdot 10^{-19}\ \text{cm}^2$, $q_{5^1D}(50) = 1{,}3 \cdot 10^{-19}\ \text{cm}^2$ ist (siehe Tabelle 6). Bei der betrachteten Messung betragen die entsprechenden

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* Die Verschiedenheit der statistischen Gewichte von ^1D und ^1P wurde bei der Berechnung ausser acht gelassen.

Werte laut Formel B4 $n_{5^1P}(T) = 2 \cdot 10^6$ cm^{-3} und $n_{5^1D}(T) = 1{,}3 \cdot 10^6$ cm^{-3} (siehe Anhang B). Mit diesen Werten hat man aus Gleichung (5)

$$n_{5^1D}(\tau) = 1{,}8 \cdot 10^6 \cdot e^{-\frac{\tau}{60}} - 4{,}7 \cdot 10^5 \cdot e^{-\frac{\tau}{19{,}5}} . \qquad (6)$$

Es ist ohne weiteres klar, dass das erste Glied der Gleichung (6) ($\tau_0 = 60$ nsec) das zweite übertrifft. Die Messungen ergaben für die Lebensdauer $\tau_0 = 57$ nsec (siehe Tabelle 1), es besteht also eine gute Übereinstimmung mit den errechneten Werten.

Term 3^3D. Bei dem Term 3^3D spielen die Störeffekte eine besonders ausgeprägte Rolle. Bereits HERON hat bemerkt, dass die Zerfallskurve des Terms 3^3D als eine Überlagerung zweier Exponentialkurven anzusehen ist (Abb. 6). Wir haben die Zerfallskurve des Zustandes 3^3D gleichfalls gemessen, aus der Konfiguration die wir erhielten, konnten jedoch über die Lebensdauer keine Folgerungen gezogen werden, da es in der Kurve keinen geraden Abschnitt gab (Abb. 7).

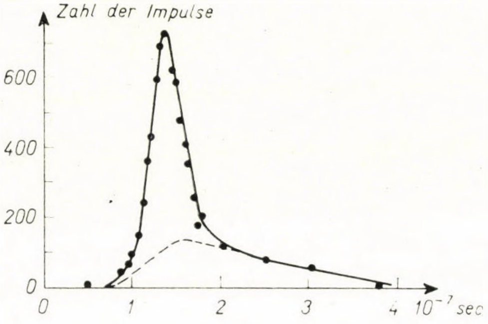

Abb. 6

Term 4^3D. Für diesen Term ergab die semilogarithmische Darstellung eine Gerade. Die daraus berechnete Lebensdauer beträgt das Dreifache des theoretischen Wertes. Anhand der bekannten Prozesse lässt sich die Abweichung kaum erklären, da einerseits die Übergangswahrscheinlichkeiten vom Niveau n^3P $n > 4$ zu klein sind (siehe Tabelle 5), als dass sie die Lebensdauer wesentlich beeinflussen könnten, andererseits ist die Lebensdauer des mit dem Zustand 4^3D in »thermischer« Kopplung befindlichen Niveaus 4^1P zu kurz (sie beträgt bei einem Gasdruck von 40 μ 41,5 nsec), als dass sie die Lebensdauer des Termes 4^3D auf das Dreifache verlängern könnte.

Term 4^3S. Für den grössten Wirkungsquerschnitt der Stösse zweiter Art, der von GABRIEL und HEDDLE bestimmt wurde, beträgt die prozentuale Besetzung des Zustandes 4^3S, d. h. die Besetzung über den Weg $0-4^1P-4^3S$ relativ zur Besetzung über den direkten Weg $0-4^3S$ ungefähr 6% (siehe

Tabelle 3, 4, 5), und der Einkerkerungsfaktor $g(p = 40\,\mu;\ \varrho = 0{,}5\ \text{cm}) = 4{,}3 \cdot 10^{-2}$.

$$\alpha\left(\frac{0\rightarrow 4^1P - 4^3S}{0 - 4^3S}\right) = 100\, \frac{q_{4^1P}(30V)\, N(40\mu)\, Q_{4^1P\rightarrow 4^3S}\, \bar{v}(300^\circ K)}{q_{4^3S}(30V)\left[gA_{4P^1\rightarrow 0} + \sum\limits_x A_{4^1P\rightarrow x} + N\bar{v}\sum\limits_x Q_{4^1P\rightarrow x}\right]} \sim 6\%.$$

Die prozentuale Besetzung durch Kaskadenübergänge vom Term 4^3P beträgt ungefähr 4,5% und vom Term 5^3P ungefähr 2,5% (siehe Tabelle 4 und 5). Die gemessene Lebensdauer muss mit dem wahren Wert zusammenfallen. Wie aus Tabelle 1 ersichtlich, ist hieı dies der Fall.

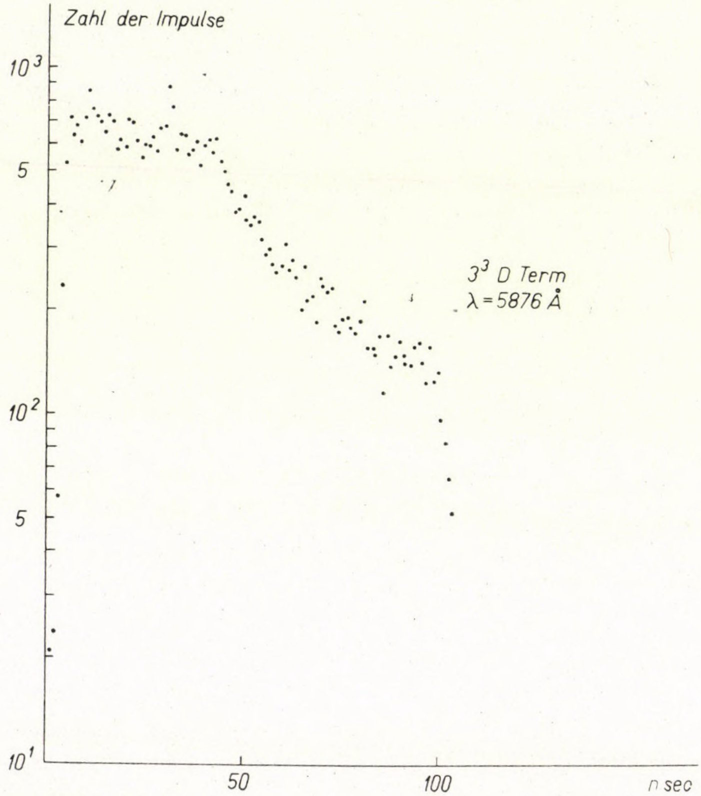

Abb. 7

Term 4^1D. Die prozentuale Besetzung durch Stösse zweiter Art ist bei einem Druck von 7 μ und einer Energie von 50 eV

$$\alpha\left(\frac{0\rightarrow 4^1P\rightarrow 4^1D}{0\rightarrow 4^1D}\right) = \frac{q_{4^1P}(50V)\, N(7\mu)\, Q_{4^1P\rightarrow 4^1D}\, \bar{v}(300^\circ K)\cdot 100}{q_{4^1D}(50V)\left[gA_{4^1P\rightarrow 0} + \sum\limits_x A_{4^1P\rightarrow x} + N\bar{v}\sum\limits_x Q_{4^1P\rightarrow x}\right]} \sim 2{,}2\%,$$

während bei 18 μ Druck $\alpha \sim 21\%$ und bei 40 μ Druck $\alpha \sim 67\%$ ist. Diese

Variation der prozentuale Besetzung ist aus den Zerfallsgeraden nicht ersichtlich, weil die Lebensdauer des 4^1P-Terms infolge des Imprisonments parallel mit dem Anstieg des Druckes zunimmt und ihr Wert z. B. bei $40\,\mu$ Druck 41,5 nsec wird, d. h. selbst wenn der Effekt der prozentualen Besetzung wegen strenger Kopplung sichtbar wäre, könnte dies infolge der gleichen Lebensdauer der Niveaus nicht wahrgenommen werden.

Die höchste prozentuale Besetzungszunahme durch Kaskaden vom Niveau 5^1P ist bei $40\,\mu$ geringer als 2,4%, demnach kann ihre Wirkung vernachlässigt werden (siehe Tabelle 5 und 6). Die experimentell ermittelten Lebensdauerwerte stimmen mit den theoretischen Werten — wie sich dies aus Tabelle 1 feststellen lässt — gut überein.

Zustand 4^1S. Bei einem Druck von $40\,\mu$ beträgt die für den Wirkungsquerschnitt der Stösse zweiter Art auf Grund der experimentell bestimmten Werte von GABRIEL und HEDDLE berechnete prozentuale Besetzungszunahme ungefähr 39%, während die von WOLF und MAURER gemessenen Werte einen niedrigeren Wert (2,1%) ergeben (siehe Tabelle 3, 6).

Die durch Kaskadenübergänge vom Niveau 5^1P entstehende Besetzungszunahme beträgt ungefähr 3% (siehe Tabelle 5, 6). Der experimentell ermittelte Wert stimmt mit der theoretischen Lebensdauer gut überein, der WOLF—MAURER Wert scheint also der richtigere zu sein.

V. Zusammenfassung

Es wurde die Lebensdauer der Zustände 4^3S, 4^1D, 3^3P, 5^1D, 4^3D und 4^1S gemessen, wobei sich der Reihe nach folgenden Werte ergaben: $67 \pm 1{,}4$; $41 \pm 1{,}3$; 112 ± 6; 57 ± 2; 93 ± 6 und 90 ± 7 nsec. Die Diskussion der Messergebnisse beruht auf den aus der Literatur bekannten Werten der Übergangswahrscheinlichkeiten und Wirkungsquerschnitte der Stösse zweiter Art sowie auf jenen der Elektronenstösse. Bei der Berechnung der theoretischen Lebensdauerwerte und Wirkungsquerschnitte der Erregung durch Elektronenstösse wurden die Werte von GABRIEL und HEDDLE benutzt. Anhand der Wirkungsquerschnittwerte der Stösse zweiter Art von STEWART und GABATHULER bzw. jener von WOLF und MAURER konnten die Messergebnisse gedeutet werden. Nach unseren Daten erweisen sich die Wirkungsquerschnittwerte der Stösse zweiter Art von GABRIEL und HEDDLE manchmal als zu hoch (siehe z. B. den Term 4^1S); dieser Wert zeigt sich bei einer Messung als höchster möglicher Wert (siehe z. B. den Term 4^3S). Die Lebensdauerwerte der Zustände 3^3P, 4^3S, 4^1D, 4^1S stimmen mit den theoretischen Werten ziemlich gut überein. Die Abweichung des Lebensdauerwertes des Zustandes 5^1D lässt sich auf Grund der aus der Literatur bekannten Angaben erklären, im Falle des Termes 4^3D jedoch konnte die Abweichung nicht gedeutet werden. Die Zerfallskurve des Niveaus 3^3D erwies sich ebenfalls als unauswertbar.

Aus den Gleichungen (1) und (2) geht hervor, dass die Ergebnisse der Lebensdauermessungen auch durch andere Vorgänge beeinflusst werden, die sich im Gas abspielen. Dies gilt auch für die Messung von Wirkungsquerschnitten der Stösse zweiter Art bzw. von Wirkungsquerschnitten der Erregung durch Elektronenstösse. Die Resultate solcher Messungen hängen von den gemessenen Lebensdauerwerten ab.

Da in den gemessenen Zerfallskurven sämtliche Wirkungsquerschnitt- sowie Lebensdauerwerte enthalten sind, ermöglicht die Anwendung einer modifizierten Auswertungsmethode die Bestimmung dieser Werte.

Anhang

A) Der Zustand 5^1D ist mit dem Term 5^1P in thermischer Kopplung. Nach Gleichung (2) ist die zeitabhängige Variation der Population der Zustände

$$\begin{aligned} \dot{n}_1 &= -(A_1 + B)n_1 + Bn_2 , \\ \dot{n}_2 &= -(A_2 + B)n_2 + Bn_1 . \end{aligned} \qquad \text{A. 1.}$$

n_1 bzw. n_2 sind n_{5^1P} bzw. n_{5^1D}; $B = N\bar{v}Q_{5^1P-5^1D}$;

$$A_1 = gA_{5^1P\to 0} + \sum_x A_{5^1P\to x} + N\bar{v}\sum_y Q_{5^1P\to y}\,; \qquad y \neq 5^1D$$

$$A_2 = \sum_x A_{5^1D\to x} = \frac{1}{\tau_0^{(5^1D)}} .$$

Nach der Laplaceschen Transformation [37] gilt

$$\begin{aligned} p\bar{n}_1 - n_1(T) &= -(A_1 + B)\bar{n}_1 + B\bar{n}_2 , \\ p\bar{n}_2 - n_2(T) &= -(A_2 + B)\bar{n}_2 + B\bar{n}_1 . \end{aligned} \qquad \text{A. 2.}$$

Hier ist $n_1(T)$ bzw. $n_2(T)$ die Population des Niveaus 5^1P bzw. 5^1D am Ende der Erregung. Die Lösung dieser Gleichungen schreibt sich zu

$$\begin{aligned} \bar{n}_1 &= \frac{n_2(T)\,B + n_1(T)\,(p + A_2 + B)}{p^2 + p(A_1 + A_2 + 2B) + A_1A_2 + B(A_1 + A_2)} , \\ \bar{n}_2 &= \frac{n_1(T)\,B + n_2(T)\,(p + A_1 + B)}{p^2 + p\,(A_1 + A_2 + 2B) + A_1A_2 + B(A_1 + A_2)} . \end{aligned} \qquad \text{A. 3.}$$

Bei inverser Transformation hat man

$$\begin{aligned} n_1(\tau) &= \frac{n_2(T)\,B + n_1(T)(p_1 + A_2 + B)}{2p_1 + A_1 + A_2 + 2B}\, e^{p_1\tau} + \\ &+ \frac{n_2(T)\,B + n_1(T)(p_2 + A_2 + B)}{2p_2 + A_1 + A_2 + 2B}\, e^{p_2\tau}, \\ n_2(\tau) &= \frac{n_1(T)\,B + n_2(T)(p_1 + A_1 + B)}{2p_1 + A_1 + A_2 + 2B}\, e^{p_1\tau} + \\ &+ \frac{n_1(T)\,B + n_2(T)(p_2 + A_1 + B)}{2p_2 + A_1 + A_2 + 2B}\, e^{p_2\tau}, \end{aligned} \tag{A. 4.}$$

worin

$$p_{1-2} = \frac{-(A_1 + A_2 + 2B) \pm \sqrt{(A_1 - A_2)^2 + 4B^2}}{2}\,. \tag{A. 5.}$$

B) Die Werte $n_1(T)$ und $n_2(T)$ sind durch die Gleichung (1) definiert:

$$\begin{aligned} \dot{n}_1 &= -(A_1 + B)n_1 + Bn_2 + D_1\,, \\ \dot{n}_2 &= -(A_2 + B)n_2 + Bn_1 + D_2\,, \end{aligned} \tag{B. 1.}$$

wobei $D_1 = Njq_{5^1P}(V)$ und $D_2 = Njq_{5^1D}(V)$. Nach der Laplaceschen Transformation wird

$$\begin{aligned} p\bar{n}_1 &= -(A_1 + B)\,\bar{n} + B\bar{n}_2 + \frac{D_1}{p}\,, \\ p\bar{n}_2 &= -(A_2 + B)\,\bar{n}_2 + B\bar{n}_1 - \frac{D_2}{p}\,. \end{aligned} \tag{B. 2.}$$

Die Lösung dieser Gleichungen lautet

$$\begin{aligned} \bar{n}_2 &= \frac{D_2(p + A_1 + B) + D_1 B}{p[(p + A_1 + B)(p + A_2 + B) - B^2]}\,, \\ \bar{n}_1 &= \frac{D_2 B + D_1(p + A_2 + B)}{p[(p + A_1 + B)(p + A_2 + B) - B^2]}\,. \end{aligned} \tag{B. 3.}$$

Durch inverse Transformation erhält man

$$\begin{aligned} n_1(t) &= \frac{D_2 B + D_1(A_2 + B)}{A_1 A_2 + B(A_1 + A_2)} + \frac{D_2 B + D_1(p_1 + A_2 + B)}{p_1(2p_1 + A_1 + A_2 + 2B)}\, e^{p_1 t} + \\ &+ \frac{D_2 B + D_1(p_1 + A_2 + B)}{p_2(2p_2 + A_1 + A_2 + 2B)}\, e^{p_2 t}, \end{aligned}$$

B. 4

$$n_2 (t) \frac{D_2 (A_1 + B) + D_1 B}{A_1 A_2 + B(A_1 + A_2)} + \frac{D_1 B + D_2 (p_1 + A_1 + B)}{p_1(2p_1 + A_1 + A_2 + 2B)} e^{p_1 t} + + \frac{D_1 B + D_2 (p_2 + A_1 + B)}{p_2 (2p_2 + A_1 + A_2 + 2B)} e^{p_2 t} .$$

P_{1-2} ergibt sich aus Gleichung A 5.

Tabelle 6

Wirkungsquerschnitte der Erregung der He-Atome durch Elektronenstösse von 50 eV Energie. (Einheit 10^{-20} cm^2) Nach GABRIEL und HEDDLE [21]

Haupt-quanten-zahl	^1S	^1P	^1D	^3S	^3P	^3D
6	10	26	5,4	—	—	—
5	12	56	13,0	7	19	10
4	27,5	144	21,5	19	34	15
3	49	310	45	57	80	93

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СРЕДНЕЕ ВРЕМЯ ЖИЗНИ ВОЗБУЖДЕННЫХ УРОВНЕЙ ГЕЛИЯ

И. БАКОШ и Я. СИГЕТИ

Резюме

При помощи временного анализатора посредством измерения кривых распада определяются средние времени жизни состояний 4^3S, 4^1D, 3^3P, 5^1D, 4^3D и 4^1S гелия. Для этих состояний получены значения 67 ± 1,4; 41 ± 1,3; 112 ± 6; 57 ± 2; 93 ± 6 и 90 ± 7 нсек. соответственно.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (2), pp. 169—184 (1966)

AN ALGEBRAIC APPROACH TO QUANTUM MECHANICS II.

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(Presented by K. Novobátzky — Received 21. XII. 1965)

The mathematical definitions and theorems for the algebraic formulation of quantum mechanics are given. This formulation is based on a certain kind of group algebras (δ-group algebras) instead of the direct use of operator algebras on Hilbert space. The properties of the δ-group algebras in general and the δ-group algebra of quantum mechanics are investigated in detail.

I. Introduction

The purpose of this paper is to summarize certain results — elementary and in part very well known for mathematicians but probably much less familiar for physicists. The results here concern the "δ-group algebras", used in the algebraic quantum mechanics. The most important features of this theory were dealt with in a preceding paper [1] but there the theorems were announced generally without rigorous proof. Our main task is now to remedy this deficiency.

The (ordinary) group algebras are extensively used in the mathematical theory of groups as well as in the physical applications of group theory. A group algebra can be defined [2] on a *locally compact topological group* G: a group which is at the same time a Hausdorff (topological) space is called *topological group* if the "function of two variables" $f(g, h) = gh^{-1}$, $g, h \in G$ is continuous in the topology of G. G is *locally compact* if its topology is locally compact. Let μ be the *left invariant measure* on G, i.e. the measure with the property $\mu(V) = \mu(gV)$ if $V \subseteq G$ and $g \in G$. [It is possible to show that this requirement determines μ up to a constant factor on G [2]. The *right invariant measure* μ_r has the property $\mu_r(V) = \mu_r(Vg)$ for every $V \subseteq G$, $g \in G$. The set of μ-summable (complex valued) functions on G is $L^1_\mu(G) = L^1$. Defining the algebraic operations on L^1 as

$$(\alpha a + \beta b)(g) = \alpha a(g) + \beta b(g)\,, \quad a, b \in L^1\,, \ \alpha, \beta \text{ complex numbers;}$$

$$(a \cdot b)(g) = \int_G a(h) b(h^{-1}g) d\mu(h)\,; \tag{GA}$$

$$(a^*)(g) = \lambda^{-1}(g)\, \bar{a}(g^{-1})\,, \qquad \lambda(g) = \frac{d\mu(g)}{d\mu_r(g)}\,;$$

and the norm as

$$|a|_1 = \int_G |a(g)|\, d\mu(g)\,, \tag{N}$$

L^1 becomes a ***Banach*-algebra***. (See A.8. in the Appendix where the most important algebraic definitions are collected.) An adjunction of the unit (A.11) to L^1 (if it has no unit) gives the ***Banach*-algebra with unit element*** $\mathbf{L}(G) = \mathbf{L}$ which is the ***group algebra of G***.

A certain generalization of the group algebras leads to the concept of the δ-group algebra. Let us suppose the existence of a continuous function $\delta(g \mid h)$ of the two variables g, h on G, which has the properties

$$\begin{gathered} |\,\delta(g \mid h)\,| = 1\,; \quad \delta(g \mid g) = 1\,; \\ \delta(g \mid g_1 g_2) = \delta(g \mid g_1)\,\delta(g \mid g_2)\,; \\ \delta(g \mid h) = \delta(h^{-1} \mid g)\,. \end{gathered} \tag{δ}$$

We define on L^1 the addition, the multiplication with a complex number and the involution in the same way as in (GA), but the multiplication of two elements is now

$$(a \cdot b)(g) = \int_G \delta(g \mid h) a(h) b(h^{-1} g) d\mu(h)\,. \tag{δM}$$

It is easy to show that the set L^1 supplied with these algebraic operations and with the norm (N) is a ***Banach*-algebra***. An adjunction of the unit (A.11,) gives $\mathbf{L}_\delta(G) = \mathbf{L}_\delta$ which is the ***δ-group algebra of G***.

Two remarks: 1. $\mathbf{L}_\delta$ is indeed the generalization of $\mathbf{L}$, because the function $\delta(g \mid h) \equiv 1$ satisfies trivially the conditions (δ). 2. If $\delta(g \mid h) \not\equiv 1$ then the commutativity of G generally does not imply the commutativity of the multiplication (δM) in $\mathbf{L}_\delta$.

It was shown in [1] that the local observables in quantum mechanics form a δ-group algebra. There the relevant group is the abelian group of $2n$ dimensional vectors (in the case of n degrees of freedom): $G_{qm}^{(n)} = \{(x_1, x_2, \ldots, x_n, p_1, \ldots, p_n)\}$. The function $\delta(g \mid h)$ is determined here by the Heisenberg commutation relations and is equal to

$$\delta(g, h) = \exp\left\{\frac{i}{2} \sum_{k=1}^{n} (y_k p_k - x_k r_k)\right\},$$

$$\text{if } g = (x_1, \ldots, x_n, p_1, \ldots, p_n) \text{ and } h = (y_1, \ldots, y_n, r_1, \ldots, r_n). \tag{δQ}$$

Thus the multiplication of the local observables $a(x_k, p_k)$ and $b(x_k, p_k)$ is given by

$$\begin{aligned} &(a \cdot b)(x_k, p_k) = \\ &= \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} \exp\left\{\frac{i}{2} \sum_{k=1}^{n} (y_k p_k - x_k r_k)\right\} a(y_k, r_k)\, b(x_k - y_k, p_k - r_k)\, dy_1 \ldots \\ &\ldots dy_n\, dr_1 \ldots dr_n\,. \end{aligned} \tag{QM}$$

This algebra was used already by J. v. NEUMANN in his famous paper about the unitary equivalence of different representations of the commutation relations [3].

In the present paper we shall be concerned with the general properties of δ-group algebras (Sec. II.). In Section III we deal with δ-group algebras of a certain more special character to prepare Sec. IV, where the problems of algebraic quantum mechanics are investigated.

II. δ — group algebras (general)

In the whole Section G is a locally compact topological group, μ is the left invariant measure on it, $L^1_\mu(G) = L^1$ is the set of μ-summable functions and $\mathbf{L}_\delta(G) = \mathbf{L}_\delta'$ is the δ-group algebra of G determined by the function $\delta(g \mid h)$ satisfying Eq. (δ).

First of all we mention some properties of $\delta(g \mid h)$ which immediately follow from Eq. (δ):

$$\delta(g_1 g_2 \mid g) = \delta(g_1 \mid g)\delta(g_2 \mid g) , \tag{1}$$

$$\delta(e \mid g) = \delta(g \mid e) = 1 \text{ where } e \text{ is the unit of } G, \tag{2}$$

$$\delta(h \mid g) = \delta(g \mid h)^{-1} = \delta(g \mid h^{-1}) = \delta(g^{-1} \mid h) = \bar{\delta}(g \mid h) . \tag{3}$$

Using Eqs. (δ), (1), (2) and (3) it is easy to show that the algebraic operations defined in Eqs. (GA) and (δM) satisfy in fact the requirements of A.1, and A.6, respectively and $\mathbf{L}_\delta$ is indeed a Banach *-algebra in the norm (N) (see A.3, A.7, A. 8).

The well known theorems on group algebras [2] (the case $\delta(g \mid h) \equiv 1$) can be translated almost word for word into the case of δ-group algebras. Generally also the proofs can be carried over with trivial alterations to δ-group algebras. Therefore we give here the most important theorems of NN Chap. VI. translated in the δ-algebraic language without proof.

Definition 1. Let $x(g)$ be an element of $L^1_\mu(G)$, then the mapping $L^1_\mu(G) \to L^1_\mu(G)$ defined by

$$x \to x_h^\delta ; \quad x_h^\delta(g) = \delta(g \mid h) x(h^{-1}g) \tag{4}$$

is the *δ-left-shift with h.* Similarly

$$x \to x_\delta^h ; \quad x_\delta^h(g) = \delta(g \mid h) x(gh) \tag{5}$$

defines the *δ-right-shift with h* in $L^1_\mu(G)$ [4].

Theorem 2. (The corresponding result in group algebras can be found in NN

§28.2.I.) If $x(g) \in L^1_\mu(G)$ then x_h^δ and x_δ^h depends continuously on h in the norm of L^1, i.e. to every $\varepsilon > 0$ and $h_0 \in L^1$ there is a neighbourhood $U_{h_0}^{(\varepsilon)}$ of h_0 such that

$$|x_{h_0}^\delta - x_h^\delta| < \varepsilon \qquad \text{if} \qquad h \in U_{h_0}^{(\varepsilon)} .$$

Theorem 3. (See in NN § 28.2.IV.) The closed subspace $J \subseteq L^1_\mu(G)$ is a (left/right) ideal if and only if J is invariant under every δ-left-(right-) shift.

Definition 4. (NN §18.2.) **R** is a *reduced *-algebra* if it is a *-algebra with unit element and if from $x \in \mathbf{R}$ and $\{f \mid x^* \cdot x\} = 0$ follows $x = 0$ for every positive functional f.

Theorem 5. (See in NN § 28.2.V.) Every δ-group algebra of a locally compact topological group is a reduced *-algebra.

Theorem 6. (See in NN § 28.2.VII.) $\mathbf{L}_\delta(G)$ is semisimple.

Theorem 7. In $\mathbf{L}_\delta$ there exists minimal regular norm $|\, x \,|$ which is completely regular, and we have $|\, x \,| \leq |\, x \,|_1$ for every $x \in \mathbf{L}_\delta$.

Proof: this is a direct consequence of *Theorem 5* and NN § 18.3, Theorem 1 and Corollary.

Definition 8. Because $|\, x \,| \leq |\, x \,|_1$, $\mathbf{L}_\delta$ is generally not complete in the minimal regular norm $|\, x \,|$. Let us denote the completion of $\mathbf{L}_\delta$ with respect to this norm by $\mathbf{D}_\Delta(G) = \mathbf{D}_\Delta$. $\mathbf{D}_\Delta$ is a C^*-algebra (A.10.) and we call it the *Δ-group algebra of G* for the sake of brevity. Generally there is a very close connection between $\mathbf{L}_\delta$ and $\mathbf{D}_\delta$, and in the literature sometimes $\mathbf{D}(G)$ ($\delta \equiv 1$!) is called the group algebra of G. This close connection will appear also in the next Section.

Definition 9. Let us denote the set of unitary operators on the Hilbert space H by $\mathbf{U}(H)$. The mapping $g \rightarrow U_g$, $g \in G$, $U_g \in \mathbf{U}(H)$ is a *unitary δ-representation* of G on H if

$$U_e = I \ \text{(the unit operator)}\,, \tag{6}$$

$$U_{gh} = \delta(g \mid h) U_g U_h \,.$$

The unitary δ-representation $g \rightarrow U_g$ is *measurable* if the function $(\xi, U_g \eta)$ is measurable on G for every $\xi, \eta \in H$. The unitary δ-representation $g \rightarrow U_g$ is *continuous* if for every $\xi \in H$ we have $|\, U_g\xi - U_h\xi \,| \rightarrow 0$ if $g \rightarrow h$.

Definition 10. (NN §29.2.) The *-representation $x \rightarrow T(x)$ of $\mathbf{L}_\delta$ on H is *degenerate* if $T(a)\xi = 0$ for every $\xi \in H$ and $a \in L^1$.

The *-representation $x \rightarrow T(x)$ *does not contain the degenerate representation* if there is no $0 \neq \xi \in H$ with the property $T(a)\xi = 0$ for every $a \in L^1_\mu(G)$.

Theorem 11. (See in NN §29.2. Theorem 1.) To every *-representation $x \rightarrow T(x)$ of $\mathbf{L}_\delta$ which does not contain the degenerate representation belongs a continuous unitary δ-representation $g \rightarrow U_g$ of G. Conversely: every measurable δ-representation $g \rightarrow U_g$ of G determines a *-representation $x \rightarrow T(x)$ of $\mathbf{L}_\delta$

which does not contain the degenerate representation. The connection between $g \to U_g$ and $x \to T(x)$ is given by

$$T(\lambda e + a) = \lambda I + \int a(g) U_g \, d\mu(g) \; ; \; [a \in L^1] \, .$$

Corollary 12. (See in NN § 29.3.) It is evident from *Theorem 11* that the measurable unitary δ-representation $g \to U_g$ is irreducible if and only if the corresponding *-representation $x \to T(x)$ is irreducible. Moreover, two measurable unitary δ-representations are unitarily equivalent if and only if the corresponding *-representations of $\mathbf{L}_\delta$ are equivalent.

Definition 13. The function $\varphi(g)$ on G is ***δ-positive definite*** if for every system $g_1, g_2, \ldots, g_n$ of elements of G and for arbitrary complex numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$ we have

$$\sum_{k,l=1}^{n} \varphi(g_e^{-1} g_k) \, \lambda_k \, \bar{\lambda}_l \, \delta(g_l | g_k) \geq 0 \, .$$

Theorem 14. (See in NN § 30.1. Theorem 1.) The function $\varphi(g) = (\xi_0, U_g \xi_0)$ is a continuous δ-positive definite function for every continuous unitary δ-representation $g \to U_g$ of G on H and for every $\xi_0 \in H$. Conversely: every continuous δ-positive definite function $\varphi(g) \not\equiv 0$ determines a cyclic continuous unitary δ-representation $g \to U_g$ with the cyclic vector ξ_0 and $\varphi(g) = (\xi_0, U_g \xi_0)$.

Definition 15. The positive functional $\{f_0 \mid x\}$ on $\mathbf{L}_\delta$ is *degenerate* if $\{f_0 \mid \lambda e + a\} = c\lambda$, $a \in L^1$. The positive functional $\{f \mid x\}$ on $\mathbf{L}_\delta$ is *regular* if the functional $(\lambda f - f_0)$ is not positive at any value of the complex number λ (here f_0 is a degenerate functional).

Theorem 16. (See in NN § 30.2. Theorem 2.) There is an one-to-one correspondence between the regular positive functionals f on $\mathbf{L}_\delta$ and the continuous δ-positive definite functions φ on G. This correspondence is given by

$$\{f \mid \lambda e + a\} = \lambda \varphi(e) + \int a(g) \varphi(g) d\mu(g) \, , \quad a \in L^1 \, .$$

Definition 17. The function $\varphi(g) \in L_\mu^\infty(G)$ ($L_\mu^\infty(G)$ = the set of μ-essentially bounded functions on G) is ***integrally δ-positive definite*** if it satisfies

$$\int (a^* \cdot a)(g) \varphi(g) d\mu(g) = \int\int \delta(h \mid g) \bar{a}(h) a(hg) \varphi(g) d\mu(h) d\mu(g) \geq 0$$

for every $a \in L^1$.

Theorem 18. (See in NN §30.2.III. and IV.) Every integrally δ-positive definite function on G is locally almost everywhere equal to a continuous δ-positive definite function and every continuous δ-positive definite function is at the same time integrally δ-positive definite.

III. δ-group algebras (special)

In this Section we specialize the group G and the functions δ in order to come nearer to the δ-group algebra of quantum mechanical "local observables". In all this Section we suppose that G_c is a commutative locally compact topological group, μ is the invariant measure on it, $L(G_c)$ is the set of continuous functions with compact support on G_c, $L^1_\mu(G_c) = L^1$ is the set of μ-summable functions on G_c, $L^\infty_\mu(G_c) = L^\infty$ is the set of μ-essentially bounded functions on G_c and $\mathbf{L}_\delta(G_c) = \mathbf{L}_\delta$ is the δ-group algebra of G_c. We suppose further that δ and $\mathbf{L}_\delta$ have the properties [Pl]: every character $\chi(g)$ of the group G_c can be written with some $h \in G_c$ in the form $\chi(g) = \chi_h(g) = \delta(hh \mid g)$, [5] [P2]: there is an element $h \in L^1$ such that $h = h^*$ and in every *-representation $x \to T(x)$ of $\mathbf{L}_\delta$ which does not contain the degenerate representation we have

$$T(h)U_gT(h) = \gamma(g)T(h) \, ,$$

where $\gamma(g)$ is a function on G_c and $\gamma(e) \neq 0$ [6].

The properties [P1] and [P2] restrict very much the possible *-representations of $\mathbf{L}_\Delta$ as it can be seen from the *Theorems* P_1 and P_2:

Theorem P_1. Every non-degenerate *-representation of $\mathbf{L}_\delta$ is faithful.

Proof: Every non-degenerate *-representation $x \to T(x)$ of $\mathbf{L}_\delta$ which contains the degenerate representation can be written as $T = T' \oplus D$, where D is a degenerate representation and T' does not contain already the degenerate representation. Therefore it is enough to consider only such *-representations which do not contain the degenerate representation. Let $x \to T(x)$ be such a *-representation. It is easy to see [*Theorem 11.* and Eq. (6)] that if $a \in L^1$ and $g \in G$ then

$$U_{g^{-1}} \, T(a)U_g = \int \delta(gg \mid k)a(k)U_k d\mu(k) \, .$$

Thus if $T(a) = 0$ then taking into account [P1] we have

$$\int \chi(k)a(k)U_k d\mu(k) = 0 \quad \text{for every character } \chi \in \bar{G}_c.$$

This can be true only if $a(k) = 0$ almost everywhere (that is if $a = 0$ in L^1) To prove this we must use two lemmas:

Lemma 19. Every element of $L(G_c)$ can be approximated in the weak topology of L^∞ by linear combinations of characters on G_c.

Proof: a theorem of I. M. GELFAND and D. A. RAIKOV (NN §30.3, Theorem 3) assures that every positive definite function on G_c can be approximated in the weak topology of L^∞ by trigonometrical polynomials. But NN, §31.1, Corollary 2 and NN §30.4 together say that a trigonometrical polynomial is a linear combination of characters. Now $\varphi = f \cdot f^*$ is positive definite for every $f \in L(G_c)$ and

$$f_1 \cdot f_2^* = \frac{1}{4} [(f_1 + f_2)(f_1 + f_2)^* - (f_1 - f_2)(f_1 - f_2)^* + i(f_1 + if_2)(f_1 + if_2)^* -$$
$$- i(f_1 - if_2)(f_1 - if_2)^*].$$

Thus every element of the form $f_1 \cdot f_2^*$ can be approximated by linear combinations of characters. But NN §28.2, Remark 2 assures that every $x \in L(G_c)$ can be uniformly (i.e. in the norm of L^∞ *!*) approximated by elements of the form $f_1 \cdot x$, thus the proof of the lemma is complete because the norm topology in L^∞ is more strong than the weak topology.

Lemma 20. If $a_0(g) \in L^1$ and for every $f(g) \in L(G_c)$ we have $\int f(g) a_0(g) d\mu(g) = 0$ then $a_0(g) = 0$ almost everywhere.

The proof is elementary and is left to the reader. Combining *Lemmas 19* and *20* the proof of *Theorem* P_1 can be easily completed.

Theorem P_2. Every *-representation $x \to T(x)$ of $\mathbf{L}_\delta$ can be written as $T = T_k \oplus D$, $k = 0, 1, 2, \ldots, \infty$ where D is the degenerate representation and $T_k = \sum_{i=1}^{k} \oplus T_0^{(i)}$, where $T_0^{(i)}$ is equivalent to a *certain* irreducible *-representation T_0 of $\mathbf{L}_\delta$.

The proof of this theorem is essentially given in a paper of J. v. NEUMANN [3] We reconstruct it briefly for the sake of convenience: Let N be the set of elements $\xi \in H$ (H is the Hilbert space of the *-representation T) with the property: $T(a)\xi = 0$ for every $a \in L^1$. N is clearly an invariant closed subspace, and in N the *-representation T is equal to the degenerate representation D. Later on we shall consider the *-representation T only in $H' = H \ominus N$ which already does not contain the degenerate representation. Therefore *Theorem 11.* and [P2] gives $T(h)U_gT(h) = \gamma(g)T(h)$ and thus $T(h)^2 = \gamma(e)T(h)$. Hence the set $M = T(h)H'$ is not void (*Theorem* P_1) and it is a closed subspace in H', because $M = \{\psi : \psi \in H', T(h)\psi = \gamma(e)\psi\}$. Using [P2], Eqs. (3) and (6) we obviously have for $\varphi, \varphi' \in M$

$$(U_g \varphi,\ U_k \varphi') = Ug\, T(h)\, \varphi_0\,,\ U_k\, T(h)\, \varphi_0') =$$
$$= \frac{\gamma(kg^{-1})}{\gamma(e)}\, \delta(g, k)\ (\varphi, \varphi)'. \tag{7}$$

Therefore if $\{\varphi_k\}$ is a complete orthonormed system in M and if M_k is the closed subspace in H' spanned by the elements of the form $U_g\varphi_k$, $g \in G_c$ then M_i is orthogonal to M_k if $i \neq k$. Further the subspaces M_k are clearly invariant under U_g and thus also under $T(x)$ (*Theorem 11.*). $\sum_k \oplus M_k$ is the whole H' because in $H' \ominus \left(\sum_k \oplus M_k\right) = U$ we have $T(h) = 0$ and in virtue of *Theorem* P_1

this is possible only if $U = \{0\}$. From Eq. (7) it is clear that the *-representations $T_0^{(k)}$ in M_k are unitarily equivalent. The irreducibility of $T_0 = T_0^{(k)}$ follows from the definition of M_k and from *Corollary 12.*

We mention a simple consequence of *Theorem P_2*: *Corollary 21.* The non-degenerate irreducible *-representations of $\mathbf{L}_\delta$ are unitarily equivalent to each other.

Up to now we dealt with the δ-group algebra $\mathbf{L}_\delta$ but earlier we remarked that there is a close connection between $\mathbf{L}_\delta$ and $\mathbf{D}_\Delta$ (*Definition 8.*). In the remaining part of this Section we shall be concerned with this connection. *Lemma 22.* If G is a locally compact topological group then the positive functionals on $\mathbf{L}_\delta(G)$ and $\mathbf{D}_\Delta(G)$ are the same: every positive functional of $\mathbf{L}_\delta$ can be (uniquely) extended to $\mathbf{D}_\Delta$. Therefore every *-representation of $\mathbf{L}_\delta$ can be "extended" to a *-representation of $\mathbf{D}_\Delta$. In this (one-to-one) correspondence the pure functionals go over into pure functionals and irreducible *-representations go over into irredubible *-representations.
Proof: the first statement is a simple consequence of *Theorem 7* and A.27. The second one follows from the GNS construction of *-representations: A.(29). The other statements are trivial.
Theorem 23. On $\mathbf{L}_\delta(G_c)$ there is only one completely regular norm and this is even the minimal regular norm. Let $x \to T(x)$ be an irreducible *-representation of $\mathbf{L}_\delta$ then the closure of $T(\mathbf{L}_\delta)$ in the operator norm is an irreducible *-representation of $\mathbf{D}_\Delta(G_c)$.
Proof: let us suppose that there are two different completely regular norms, and let $\mathbf{D}_\Delta$ resp. $\mathbf{D}'_\Delta$ be the completion of $\mathbf{L}_\delta$ with respect to these norms. Let us consider a faithful irreducible *-representation of $\mathbf{D}_\Delta(T')$ and $\mathbf{D}'_\Delta(T')$ respectively. T and T' are both norm preserving (NN. §24.1, Theorem 3). The restrictions of T and T' to $\mathbf{L}_\delta$ are faithful irreducible *-representations of $\mathbf{L}_\delta$ according to *Lemma 22* and they are equivalent because of *Corollary 21.* Thus the two norms must coincide. Therefore there is only one completely regular norm. But the minimal regular norm exists on $\mathbf{L}_\delta$ (*Theorem 7.*), thus the minimal regular norm is the unique completely regular norm on $\mathbf{L}_\delta$. The last statement of the theorem directly follows from this and *Lemma 22*, because the operator norm is completely regular on Hilbert spaces.
Corollary 24. Theorem P_2 and *Corollary 21* are valid for $\mathbf{D}_\Delta$ too instead of $\mathbf{L}_\delta$.
Theorem 25. Let us consider an irreducible *-representation T of $\mathbf{D}_\Delta$ on H. The necessary and sufficient condition for a positive functional f on $\mathbf{D}_\Delta$ to be pure and faithful is that there exists an element $\psi \in H$ for which $\{f \mid x\} = (\psi, T(x)\psi)$.
Proof: if $\{f \mid x\} = (\psi, T(x)\psi)$ then f is a faithful positive functional (*Corollary 24*) and also pure according to A.(31) and A.(29) or NN §17.3.I.
If f is pure and faithful then the corresponding *-representation T_f of $\mathbf{D}_\Delta$ [see A.(29)] is irreducible according to A.(31) and faithful because of A.32.

But every irreducible *-representation is equivalent (*Corollary 24*) therefore also T_f and T are equivalent and this completes the proof.

Theorem 26. Every positive functional f on $\mathbf{D}_\Delta$ can be written in the form

$$\{f|x\} = c\{f_0|x\} + \sum_{i=1}^{k}\{f_i|x\}, \quad k=0, 1, 2, \ldots, \infty$$

where c is a number, f_0 is a degenerate functional and f_i $(i = 1, 2, \ldots)$ is a pure positive functional.

Proof: Considering the *-representation T_f on H belonging to f [see A.(29)] we can apply *Theorem* P_2: $T_f = D \oplus \sum_{i=1}^{k} \oplus T_0^{(i)}$. Let us denote the subspace of D by H_D, and the subspace of $T_0^{(i)}$ by H_i. A.(29) says that $\{f \mid x\} = (\xi_0, T_f(x)\xi_0)$. Because $H = H_D \oplus \sum_{i=1}^{k} \oplus T_0^{(i)}$ we can decompose the vector ξ_0 into the components $\xi_0 = \xi_e + \sum_{i=1}^{k} \xi_i$ with $\xi_e \in H_D$, $\xi_i \in H_i$. H_D and H_i are invariant subspaces, therefore we get $\{f \mid x\} = (\xi_e, T_f(x)\xi_e) + \sum_{i=1}^{k} (\xi_i, T_f(x)\xi_i)$. Here $(\xi_e, T_f(x)\xi_e)$ is clearly a degenerate functional (if H_D is void then $c = 0$ in the theorem) and $(\xi_i, T_f(x)\xi_i)$ is pure according to *Theorem* P_2 and A.(31).

IV. The algebra of quasilocal observables in quantum mechanics

The mathematical results obtained make possible the rigorous discussion of algebraic quantum mechanics treated in I. Also, we can now incorporate quantum mechanics in the general frame of algebraic quantum theory in an easier way [7, 8]. Algebraic quantum theory is based on the algebra of observables and states of quantum systems are characterized by positive functionals on this algebra.

The algebra of local observables in quantum mechanics was defined in I. In the case of *one degree of freedom* the physical quantity described in classical mechanics by the function $f(p, x)$ is represented in the algebra of local observables by the element

$$a(x, p) = (2\pi)^{-2} \int e^{-i(rx+yp)} f(r, y)drdy\,. \tag{8}$$

The elements $a(x, p)$ form an algebra which is in fact the δ-group algebra $\mathbf{L}^\delta$ of the group $G_{qm}^{(1)}$ (= the abelian group of two dimensional vectors; see I and also the Introduction). It is easy to show that $\mathbf{L}_\delta(G_{qm}^{(1)}) = \mathbf{A}'$ has the properties [P1] and [P2]: If $h = (y, r)$ and $g(x, p)$ then from (δQ) we have

$$\delta(hh|g) = e^{-i(yp-xr)} . \tag{9}$$

It is possible to write every character of $G_{qm}^{(1)}$ in this form, thus [P1] is valid. Furthermore an easy computation shows that if

$$h(x, p) = e^{-\frac{1}{4}(x^2+p^2)} \tag{10a}$$

then from *Theorem 11* follows

$$T(h)\, U_{(x,y)}\, T(h) = 2\pi\, e^{-\frac{1}{4}(x^2+p^2)}\, T(h) ,$$

and thus [P2] is fulfilled with

$$\gamma(x, p) = 2\pi e^{-\frac{1}{4}(x^2+p^2)} . \tag{10b}$$

The algebra **A**′ of local observables in quantum mechanics is a Banach *-algebra (as every δ-group algebra). In general algebraic quantum theory, however, one considers the *algebra of quasilocal observables* **A** which is a C^*-algebra and can be obtained from **A**′ by completing it in the minimal regular norm (see in [8]). Thus now **A** is just the Δ-group algebra of $G_{qm}^{(1)}$: $\mathbf{D}_\Delta(G_{qm}^{(1)}) = \mathbf{A}$. It is worthy to note that on **A**′ there is only one completely regular norm (*Theorem 23*) and thus there is only one possibility to construct a C^*-algebra from **A**′. According to *Theorem 23* a possibility for this construction is the following: We consider an arbitrary (nondegenerate) irreducible *-representation T of **A**′ and then completing $T(\mathbf{A}')$ in the operator norm we get even **A**. The uniqueness of this procedure is assured also by *Corollary 21* which tells that the irreducible *-representations of **A**′ are all equivalent.

The close connection between **A**′ and **A** (expressed also by *Lemma 22*) shows that it does not make very much difference whether we built algebraic quantum mechanics on **A**′ or on **A**. But the mathematical properties of a C*-algebra are more simple and beautiful and we shall see below that the set of possible states can be given with the help of **A** as follows: *We shall use the algebra* **A** *of quasilocal observables as a starting point of our investigations in quantum mechanics.*

First we give the definition of the possible states (in I this was omitted because of the lack of sufficient mathematical preparations):

Postulate: the set of possible states of the system is the "surface" of the closed unit sphere in $\mathbf{A}^{*(+)}$ i.e. the positive functionals f with $\{f \mid e\} = 1$ [9]. The expectation value of the quasilocal observable $a = a^*$ in the state f is equal to $\{f \mid a\}$.

Taking into account *Theorem 25* we see that the pure states f_p are given by the elements ψ in the Hilbert space of an (arbitrary!) irreducible *-representation T of $\mathbf{A}$ in the form

$$\{f_p \mid x\} = (\psi, T(x)\psi) . \tag{11}$$

This relation shows the content of the above postulate in the "old" language: $(\psi, \psi) = \| \psi \|^2$ must be equal to 1 and the expectation value is given by $(\psi, T(x)\psi)$. Naturally there are other possible states of the pure ones too and as it can be seen from *Theorem 26* the most general state has the form

$$\sum_{i=1}^{k} \{f_i | x\} = \sum_{i=1}^{k} (\psi_i , T(x)\, \psi_i) , \tag{12}$$

where f_i's are pure and $k = 1, 2, \ldots, \infty$. Here the case $k \neq 1$ clearly corresponds to the *mixed states* of conventional quantum mechanics.

A very important feature of quantum mechanics is that every (non-degenerate) irreducible *-representation of $\mathbf{A}$ is unitarily equivalent (Corollary 24). Therefore quantum mechanics (even algebraic quantum mechanics!) can be formulated in the Hilbert space of a given irreducible *-representation. This is guaranteed by the properties [P1] and [P2]. But one cannot expect a similar situation generally in quantum theory and this has essential consequences:

1. There is not necessarily such a close connection between $\mathbf{A}$ and $\mathbf{A}'$ (lack of *Theorem 23*),

2. the possible (and the possible pure) states are more general (lack of *Theorems 25* and *26*),

3. the algebraic- and the Hilbert space-formulations are not equivalent because the different *-representations are not (unitarily) equivalent (lack of *Theorems* P_1 and P_2).

From the study of algebraic quantum mechanics one can draw another conclusion too. In I and now we defined the algebra of quasilocal observables by means of the *concrete* δ-group algebra $\mathbf{A}'$. This can be looked upon as a certain kind of representation of the *abstract* Banach *-algebra relevant in quantum mechanics as the algebra of local observables. The advantage of this "*representation*" is that the elements of $\mathbf{A}'$ are common functions of two variables, which seem to be more "palpable" than the corresponding operators in Hilbert space.

Appendix (algebraic syllabus)

Here we give a short review of definitions and fundamental facts following the book of M. A. Neumark [2]. We suppose that the reader is familiar with topology, integration, linear space and Hilbert space (these topics are dealt with also in NN Chap. I., thus we refer for uniformity in this paper always to NN. Further details on these subjects can be found for example in the books quoted in [10].

A.1. *Algebra.* The set $\mathbf{R} = \{x, y, \ldots\}$ is an algebra if it is a *linear space* (in the present paper always a complex one) and if in $\mathbf{R}$ the *multiplication* of two elements $x \cdot y$ is defined and the multiplication has the properties:

$$\alpha(x \cdot y) = (\alpha x) \cdot y = x \cdot (\alpha y) ;$$

$$(x \cdot y) \cdot z = x \cdot (y \cdot z) ; (x + y) \cdot z = x \cdot z + y \cdot z ; \; x \cdot (y + z) = x \cdot y + xz.$$

Here (and henceforth) α is a complex number and $x, y, z \in \mathbf{R}$.

A.2. *Algebra with unit element* ($\mathbf{R}$). $\mathbf{R}$ is an *algebra* having an element e (the *unity*) for which $e \cdot x = x \cdot e = x$ for every $x \in \mathbf{R}$.

A.3. *Normed algebra* ($\mathbf{R}$). $\mathbf{R}$ is an *algebra* with a *norm* defined on it, i.e. a nonnegative number $| x |$ (the norm of x) is given for every $x \in \mathbf{R}$ which has the properties

$$| x | = 0 \text{ if and only if } x = 0 ;$$

$$| \alpha x | = | \alpha | \cdot | x | ; \quad | x + y | \leq | x | + | y | ; \quad | x \cdot y | \leq | x | \cdot | y | .$$

A.4. *Normed algebra with unit element* ($\mathbf{R}$). $\mathbf{R}$ is a *normed algebra* and an *algebra with unit element* and $| e | = 1$.

A.5. *Banach algebra* ($\mathbf{R}$). $\mathbf{R}$ is a *normed algebra* and if $\lim\limits_{n,m \to \infty} | x_n - x_m | = 0$ then there exists an $x_0 \in \mathbf{R}$ for which $\lim\limits_{n \to \infty} | x_n - x_0 | = 0$. (Or in other terms: $\mathbf{R}$ is *complete* in its norm, that is $\mathbf{R}$ is a normed algebra and a *Banach space* in its norm.)

A.6. **-algebra* ($\mathbf{R}$). $\mathbf{R}$ is an *algebra* and an *involution* $x \to x^*$ is defined on it, that is every $x \in \mathbf{R}$ has an *adjoint* $x^* \in \mathbf{R}$. The involution must have the properties

$$(x \cdot y)^* = y^* \cdot x^* ; \quad (x^*)^* = x ; \quad (\alpha_1 x_1 + \alpha_2 x_2)^* = \overline{\alpha}_1 x_1^* + \overline{\alpha}_2 x_2^* ,$$

where $\overline{\alpha}$ is the complex conjugate of α and $x_1, x_2 \in \mathbf{R}$.

A.7. *Normed *-algebra* ($\mathbf{R}$). $\mathbf{R}$ is a **-algebra*, $\mathbf{R}$ is a *normed algebra* and $| x^* | = | x |$ for every $x \in \mathbf{R}$.

A.8. *Banach *-algebra* ($\mathbf{R}$). $\mathbf{R}$ is a *Banach algebra* and with the same norm a *normed *-algebra*.

A.9. *Completely regular norm.* The norm in the *normed *-algebra* $\mathbf{R}$ is called completely regular if $| x^* \cdot x | = | x |^2$ for every $x \in \mathbf{R}$.

A.10. *C*-algebra* (**R**). **R** is a *Banach *-algebra* and its norm is *completely regular.*

A.11. *Adjunction of a unit.* If **R** is an algebra without unit then it is possible to enlarge **R** into an algebra with unit element $\mathbf{R}_e$. Namely: Let $\mathbf{R}_e$ be the set of pairs $[\alpha, x]$ where α is a complex number and $x \in \mathbf{R}$, that is

$$\mathbf{R}_e = \{[\alpha, x]: \alpha \text{ is a complex number, } x \in \mathbf{R}\} .$$

We define the algebraic operations in $\mathbf{R}_e$ in the following way:

$$[\alpha_1, x_1] + [\alpha_2, x_2] = [\alpha_1 + \alpha_2, x_1 + x_2] , \qquad \alpha[\alpha_1, x_1] = [\alpha\alpha_1, \alpha x_1] ,$$
$$[\alpha_1, x_1] \cdot [\alpha_2, x_2] = [a_1 \alpha_2, \alpha_1 x_2 + \alpha_2 x_1 + x_1 \cdot x_2] .$$

Then clearly $[1, 0] = e$ is the unit element of $\mathbf{R}_e$ and $[0, x]$ correspond to the elements of **R**, hence every element of $\mathbf{R}_e$ can be written as $[\alpha, x] = \alpha e + x$, where $x = [0, x] \in \mathbf{R}$.

If **R** is a *-algebra then we define the *involution* in $\mathbf{R}_e$ as

$$[\alpha, x]^* = [\bar{\alpha}, x^*] , \text{ that is } (\alpha e + x)^* = \bar{\alpha} e + x^* .$$

Thus $\mathbf{R}_e$ becomes a *-algebra with unit element. If **R** is a normed algebra then the *norm* in $\mathbf{R}_e$ can be defined as $| \alpha e + x | = | \alpha | + | x |$.

A.12. *Ideal.* A *subset* of the algebra is a left (right) ideal if it is a *linear subspace* (J) of **R** and if from $x \in \mathbf{R}$, $n \in \mathrm{J}$ follows that $x \cdot n \in \mathrm{J}$ $(n \cdot x \in \mathrm{J}$, respectively).
A left ideal which is at the same time also a right ideal is called *two-sided ideal.* A (left, right, two-sided) ideal is a *proper* or *nontrivial* (left, right, two-sided) ideal if it does not coincide neither with **R** nor with $\{0\}$. **R** and $\{0\}$ are always two-sided ideals, they are the *trivial ideals.*

A.13. *Simple algebra.* An algebra **R** is *simple* if it does not contain a proper two-sided ideal.

A.14. *Maximal ideal.* A (left, right, two-sided) ideal $\mathrm{J} \neq \mathbf{R}$ is *maximal* if there is not other proper (left, right, two-sided) ideal which contains J.

A.15. *Radical.* The *intersection* of the maximal left ideals is the *radical.*

A.16. *Semisimple algebra.* An algebra **R** is called *semisimple* if its radical is equal to $\{0\}$.

A.(17). The radical coincides with the intersection of the maximal right ideals, therefore it is a two-sided ideal. Hence a simple algebra is always semisimple (NN §7.5.III).

A.18. **-ideal* (J). J is an ideal in a *-algebra and from $x \in \mathrm{J}$ follows that $x^* \in \mathrm{J}$.

A.19. *Homomorphism.* If $\mathbf{R}_1$ and $\mathbf{R}_2$ are two algebras then the *mapping* h: $\mathbf{R}_1 \rightarrow \mathbf{R}_2$ is a *homomorphism* if it keeps the algebraic relations, that is if

$$h(\alpha_1 x_1 + \alpha_2 x_2) = \alpha_1 h(x_1) + \alpha_2 h(x_2) , \qquad h(x_1 \cdot x_2) = h(x_1) \cdot h(x_2)$$

for every $x_1, x_2 \in \mathbf{R}_1$ and α_1, α_2 complex numbers. A homomorphism which is one-to-one is an *isomorphism.*

A.20. **-homomorphism.* A *homomorphism* between two *-algebras $\mathbf{R}_1$ and $\mathbf{R}_2$ is a **-homomorphism* if $h(x^*) = h(x)^*$ for every $\mathbf{R}_1$.
An one-to-one *-homomorphism is a **-isomorphism.*

A.(21) There is a one-to-one correspondence between the (*-) homomorphisms and the two-sided (*-) ideals of a (*-) algebra **R**. A given (*-) homomorphism h determines a two-sided (*-) ideal **K**, the *kernel* of the (*-) homomorphism, in the following way:

$$\mathbf{K} = \{x : x \in \mathbf{R} , \ h(x) = 0\} .$$

Conversely: if **K** is a (*-) ideal and $\mathbf{R}/\mathbf{K}$ is the *factor-algebra* determined by **K** then the mapping $h_K : \mathbf{R} \rightarrow \mathbf{R}/\mathbf{K}$, $h_K(x) = \{x + \mathbf{K}\}$ is a (*-) homomorphism. (The elements of the *factor algebra* $\mathbf{R}/\mathbf{K}$ are the cosets $\{x + \mathbf{K}\}$ in **R** determined by **K**. The algebraic operations are defined in $\mathbf{R}/\mathbf{K}$ as

$$\alpha_1\{x_1 + \mathbf{K}\} + \alpha_2\{x_2 + \mathbf{K}\} = \{\alpha_1 x_1 + \alpha_2 x_2 + \mathbf{K}\} ;$$
$$\{x_1 + \mathbf{K}\} \cdot \{x_2 + \mathbf{K}\} = \{x_1 \cdot x_2 + \mathbf{K}\} ; \quad \{x_1 + \mathbf{K}\}^* = \{x_1^* + \mathbf{K}\} .$$

A.22. **-representation.* The set $\mathbf{B}(H)$ of bounded linear operators on the Hilbert space H with usual definitions of algebraic operations is clearly a *-algebra. A **-representation* of a *-algebra **R** on the Hilbert space H is a **-homomorphism*: $\mathbf{R} \rightarrow \mathbf{B}(H)$. If a *-representation is in addition one-to-one (i.e. it is a *-isomorphism) then it is a *faithful* *-representation.
The *-representations T_1 on H_1 and T_2 on H_2 are (unitarily) *equivalent* if there is a unitary operator $U : H_1 \rightarrow H_2$ such that $UT_1(x)U^{-1} = T_2(x)$ for every $x \in \mathbf{R}$.

A.23. *Irreducible *-representation.* Let $x \rightarrow T(x)$ be a *-representation (T) of the *-algebra **R** on the Hilbert space H. If there is an *invariant subspace* in H, that is a (closed) subspace $M \neq H$, $\{0\}$ for which $T(x)M \subseteq M$ for every $x \in \mathbf{R}$, then the *-representation T is *reducible.*
If T is not reducible then it is *irreducible.*

A.24. *Cyclic *-representation.* A *-representation T of **R** on H is *cyclic* if there is an element $\xi_0 \in H$ for which the set $\{T(x)\xi_0, x \in \mathbf{R}\}$ is dense in H. The vector ξ_0 is a *cyclic vector* of the cyclic *-representation T.

A.25. *Linear functional.* A mapping f which orders a complex number $\{f \mid x\}$ to every element x of an algebra $\mathbf{R}$ is a *linear functional* if $\{f \mid \alpha_1 x_1 + + \alpha_2 x_2\} = \alpha_1\{f \mid x_1\} + \alpha_2\{f \mid x_2\}$.
A linear functional f on a normed algebra $\mathbf{R}$ is *continuous* if from $| x_n - x_0 | \to 0$ follows $\{f \mid x_n\} \to \{f \mid x_0\}$. The set of continuous linear functionals is the *dual space* $\mathbf{R}^*$ of $\mathbf{R}$.

A.26. *Positive functional.* A linear functional f on the *-algebra $\mathbf{R}$ is a *positive functional* if it is not identically zero and if $\{f \mid x^* \cdot x\} \geq 0$ for every $x \in \mathbf{R}$.
The set of positive (continuous positive) functionals can be denoted by $\mathbf{R}^{(+)}$ ($\mathbf{R}^{*(+)}$, respectively).
A positive functional f_p is *pure* if from $f_p = \lambda f_1 + (1 - \lambda) f_2$, $1 > \lambda > 0$; $f_1, f_2 \in \mathbf{R}^{(+)}$ follows that f_1 and f_2 are equal to f_p.

A.27. *Regular norm.* The norm $| x |$ in the *-algebra $\mathbf{R}$ with unit element is called *regular* if every positive functional of $\mathbf{R}$ can be extended as a positive functional onto the completion of $\mathbf{R}$ with respect to the norm $| x |$.
The *minimal regular norm* on $\mathbf{R}$ is a regular norm $| x |_0$ with the property $| x |_0 \leq | x |$ for every regular norm $| x |$ and for arbitrary $x \in \mathbf{R}$.

A.(28). If we have a positive functional f on the *-algebra $\mathbf{R}$ then for every $x, y \in \mathbf{R}$

$$| \{f \mid x^* \cdot y\} |^2 \leq \{f \mid y^* \cdot y\} \{f \mid x^* \cdot x\}$$

(NN §10.2.III.).

A.(29). To every cyclic *-representation $x \to T(x)$ of the *-algebra $\mathbf{R}$ with the cyclic vector ξ_0 corresponds a positive functional $\{f \mid x\} = (\xi_0, T(x)\xi_0)$. This functional determines the *-representation up to unitary equivalence. Conversely, every positive functional f on a Banach *-algebra with unit element determines a cyclic *-representation T_f of $\mathbf{R}$ with the cyclic vector ξ_0 for which $\{f \mid x\} = (\xi_0, T_f(x)\xi_0)$ (NN § 17.3, Theorem 2).
The *-representation T_f is determined by the GELFAND—NEUMARK—SEGAL (GNS) construction: We define a scalar product on $\mathbf{R}/\mathrm{N}_f$ by $(\{x_1 + \mathrm{N}_f\}, \{x_2 + \mathrm{N}_f\}) = \{f \mid x_1^* \cdot x_2\}$. Here $\mathrm{N}_f = \{n : n \in \mathbf{R},\ \{f \mid n^* \cdot n\} = 0\}$ is a left ideal according to A.(28). Thus $T(x)\{y + \mathrm{N}_f\} = \{x \cdot y + \mathrm{N}_f\}$ determines a *-representation on the completion of $\mathbf{R}/\mathrm{N}_f$ with respect to the scalar product defined above.

A.(30). Every positive functional f in a Banach *-algebra with unit element is continuous and $|\{f \mid x\}| \leq \{f \mid e\} \, | x |$. Moreover, the norm of f is *equal* to $\{f \mid e\}$ (NN § 10.4.I. and II.).

A.(31). A cyclic *-representation is irreducible if and only if the corresponding positive functional is pure (NN § 19.3, Theorem 2).

A.32. *Faithful positive functional.* A positive functional is called *faithful* if the corresponding *-representation is faithful.

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5. From Eq. (1) the mapping $h \rightarrow x_h$ is clearly a homomorphism: $G_c \rightarrow \overline{G}_c$ (where $\overline{G}_c$ denotes the character group of G_c). We suppose here that the image of G_c in this homomorphism is the whole $\overline{G}_c$.
6. Here U_g is the δ-representation of G_c belonging to $x \rightarrow T(x)$ in virtue of *Theorem* 11.
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АЛГЕБРАИЧЕСКОЕ ПРИБЛИЖЕНИЕ В КВАНТОВОЙ МЕХАНИКЕ II.

И. МОНТВАИ

Резюме

Даются математические определения и теоремы для алгебраического формулирования квантовой механики. Данное формулирование основывается на определенном виде групповых алгебр (δ-групповые алгебры) вместо непосредственного использования операторной алгебры в Гильбертовом пространстве. Подробно исследуются свойства δ-групповых алгебр в общем и δ-групповая алгебра квантовой механики.

COMMUNICATIONES BREVES

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (2), pp. 185—189 (1966)

BEMERKUNGEN ZUR FRAGE DER WECHSELSEITIGEN BEZIEHUNG DER KONSTANTEN EINIGER THEORIEN ÜBER DIE KONZENTRATIONSDEPOLARISATION DER PHOTOLUMINESZENZ VON LÖSUNGEN

Von

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(Eingegangen 3. XI. 1964)

Die Frage der Bestimmung der Konstante R_0, die in der von FÖRSTER [1,2] aufgestellten Theorie der Übertragung von Elektronenanregungsenergie auftritt, sowie die Frage der Beziehung dieser Konstante zu den in den Theorien anderer Autoren [3—5] über den Einfluss der Konzentration auf die Lumineszenz von Lösungen auftretenden Konstanten, ist in einer Anzahl von Abhandlungen diskutiert worden [6—11]. Die genannte Konstante R_0, der die Bedeutung jener wechselseitigen Entfernung zwischen zwei aufeinander einwirkenden Molekülen zukommt, bei der die Wahrscheinlichkeiten der Emission und der Übertragung von Energie einander gleich sind, kann aus folgender Formel bestimmt werden [2]:

$$R_0 = \left[\frac{9\varkappa^2 (\ln 10)^2 \, c\tau \, I\tilde{\nu}}{16\, \pi^4 \, n^2 \, N'^2 \, \tilde{\nu}_0^2} \right]^{1/6} . \qquad (1)$$

Hierbei ist $\varkappa$ ein von der wechselseitigen Orientierung beider Moleküle abhängiger Zahlenfaktor, n der Brechungsindex der Lösung,c die Lichtgeschwindigkeit im Vakuum, τ die natürliche Lebensdauer des angeregten Sensibilisators, N' die Molekülzahl in Millimol, $\tilde{\nu}_0$ die Wellenzahl des Elektronenübergangs im Spektrum in cm^{-1} (mittlerer Wert zwischen Absorptions- und Fluoreszenzmaximum) und $I\tilde{\nu}$ der Wert, der den Grad der Überdeckung der Spektren von Absorption und Fluoreszenz bedeutet. Zwischen der Konstante R_0 und dem Radius der Wirkungssphäre R_J, die in der Theorie von JABŁOŃSKI über die Konzentrationsdepolarisation auftritt, besteht eine bestimmte zahlenmässige Beziehung, wobei die von verschiedenen Autoren gefundenen Werte des Verhältnisses $\frac{R_J}{R_0}$ recht beträchtlich variieren. In vorliegender Notiz werden wir die Gründe dieser Unstimmigkeiten und die falschen Voraussetzungen aufzeigen, die in einigen Fällen bei der Bestimmung des Verhältnisses zwischen R_J und R_0 angenommen wurden.

In einer unlängst veröffentlichten Abhandlung beschäftigt sich **Kawski** [12] unter anderem mit der experimentellen Bestimmung der Konstante R_0 sowie mit der kritischen Konzentration C_0, die miteinander durch folgende Beziehung verbunden sind [2]:

$$n' = C_0 N' = \frac{3}{4\pi R_0^3}, \tag{2}$$

wobei C_0 in $\frac{\text{Mol}}{l}$, n' die entsprechende Molekülzahl in 1 cm^3 bedeutet. Hierbei benützt er die von ihm gefundene Beziehung [13]

$$R_J = 3^{1/3} R_0 . \tag{3}$$

Den Wert R_J bestimmt er durch Vergleich der Erfahrungsergebnisse, die sich auf die Konzentrationsdepolarisation der Photolumineszenz von Fluorescein-, Rhodamin B-, Rhodamin 6G- und Trypaflavin-Glycerinlösungen beziehen, mit dem aus der Theorie von **Jabłoński** [5] sich ergebenden Ausdruck, der vom Autor [14] vorliegender Notiz in der Form

$$\frac{1}{p} - \frac{1}{3} = \left(\frac{1}{p_0} - \frac{1}{3}\right) \frac{\nu^2}{2[\nu - 1 + e^{-\nu}]} \tag{4}$$

aufgeführt wird. P_0 bedeutet hier den Grundpolarisationsgrad $\nu = v_J n$, wobei v_J das Volumen der Wirkungssphäre und n die Zahl der lumineszierenden Moleküle in 1 cm^3 ist. Alsdann berechnet **Kawski** aus den Gleichungen (3) und (2) die Werte R_0 und C_0. Für die auf diese Weise gefundenen Werte C_0 stellt er eine gute Übereinstimmung der Erfahrungsergebnisse mit der Theorie von **Förster—Ore** [1, 15] fest. Im weiteren werden wir beweisen, dass die Beziehung (3), auf der die Berechnung von R_0 und C_0 basiert, nicht einwandfrei begründet ist.

Es sei kurz daran erinnert, dass sich **Kawski** bei der Entwicklung der Beziehung (3) auf folgende Ergebnisse stützte:

1. auf die Methode [7] zur Bestimmung von R_0, die auf die Bestimmung der Molekülzahl n' hinausläuft, was dem Polarisationsgrad entspricht:

$$\frac{1}{p} = \frac{1}{p_0} + \left(\frac{1}{p_0} - \frac{1}{3}\right), \tag{5}$$

2. auf die vom Autor [8] angegebene Abhängigkeit[1]

---

[1] Erstaunlich erscheint die Tatsache, dass sich **Kawski**, während er die Beziehung (6) benützt, die von mir in einer allgemein zugänglichen Zeitschrift [8] veröffentlicht wurde, auf seine Arbeit [13] beruft, die in einer schwer erhältlichen Zeitschrift ein Jahr nach Erscheinen der Abhandlung [8] veröffentlicht wurde. Bei Benützung der Beziehung (6) stützt er sich übrigens auf dieselben Voraussetzungen, auf denen die Abhandlung [8] basiert.

$$\frac{1}{n'} = \frac{\tau_0}{k_2} = \frac{4}{3} \pi R_0^3 , \tag{6}$$

in der $\frac{\tau_0}{k_2}$ eine Konstante ist, die in der von WAWILOW aufgestellten Theorie über den Einfluss der Konzentration auf die Fluoreszenz der Lösungen auftritt. Durch Vergleich des Ausdruckes

$$\frac{1}{p} = \frac{1}{p_0} + \left(\frac{1}{p_0} - \frac{1}{3} \right) \frac{1}{3} v_J n , \tag{7}$$

der sich aus der Gleichung (4) für $\nu = v_J n \ll 1$ ergibt, mit der Formel von WAWILOW

$$\frac{1}{p} = \frac{1}{p_0} + \left(\frac{1}{p_0} - \frac{1}{3} \right) \frac{\tau_0}{k_2} n , \tag{8}$$

die gleichfalls die Konzentrationsdepolarisation bei Vernachlässigung der Auslöschung beschreibt, erhielt er

$$v_J = \frac{4}{3} \pi R_J^3 = 3 \frac{\tau_0}{k_2} , \tag{9}$$

was bei Berücksichtigung der Abhängigkeit (6) schliesslich die Beziehung (3) ergibt.

Wir stellen fest, dass KAWSKI beim Vergleich der Gleichungen (7) und (8) die Gültigkeit beider Formeln bis zur Konzentration n' voraussetzt, bei welcher der Polarisationsgrad den Wert (5) annimmt. Dieser Wert der kritischen Konzentration n' bestimmt nämlich die Konstanten $\frac{\tau_0}{k_2}$ und R_0. (Vergleiche die Gleichungen (6) und (8)). Indessen darf man sich des Ausdrucks (7) im Gegensatz zu (8) nicht in diesem weiten Bereich der Konzentrationen bedienen. Insofern nämlich die lineare Abhängigkeit (8) unmittelbar aus WAWILOWS allgemeinem Ausdruck für die Konzentrationsdepolarisation auf Grund der Vernachlässigung des Auslöschens ohne sonstige Vereinfachungen hervorgeht, führt JABŁONSKIS Theorie bei Vernachlässigung des Auslöschens zu einer nicht linearen Beziehung (4), aus der man erst für $\nu \ll 1$ die Abhängigkeit (7) erhält. Somit steht die Voraussetzung der Gültigkeit des Ausdrucks (7) bis zur Konzentration n', der $\nu = 3$ entspricht, in ausdrücklichem Widerspruch zu der Bedingung $\nu \ll 1$. Wie wir bewiesen haben [14], ist der Ausdruck (7) nur für $\nu < 0{,}3$ eine gute Näherung der Gleichung (4). Zu bemerken ist, dass sich KAWSKI ganz unnötigerweise auf die Theorie von WAWILOW (Ausdruck (8)), desgleichen auf die Beziehung (6) beruft, da sich die Relation

$R_J = 3^{1/3} R_0$ sofort ergibt, wenn man die Unrichtigkeit der Voraussetzung von der Gültigkeit des Ausdrucks (7) für die Konzentration n' in Betracht zieht. Da der Polarisationsgrad für die Konzentration n' den Wert (5) annimmt, geht aus der Gleichung (7) hervor, dass $\frac{4}{3} \pi R_J^3 n' = 3$, was wegen der Gleichheit $n' = 3/4\pi R_0^3$ sofort $R_J = 3^{1/3} R_0$ ergibt.

Ein weiterer Fehler **Kawskis** bei der Entwicklung der Beziehung (3) besteht darin, dass er Ausdrücke (z. B. (7) und (8) sowie (7) und (5)) vergleicht, die auf verschiedenen Voraussetzungen basieren. So berücksichtigt z. B. die Theorie von **Jabłonski** die Fluktuation der Konzentration lumineszierender Moleküle und die Rückwanderung der Anregungsenergie und lässt keine Möglichkeit der Übertragung von Anregungsenergie an die Moleküle zu, die sich in einer Entfernung von $R > R_J$ befinden, während die Ausdrücke (8) und (5) von der Voraussetzung aus entwickelt wurden, dass die lumineszierenden Moleküle in der Lösung der gleichmässigen Verteilung unterliegen. Die von **Kawski** festgestellte zufriedenstellende Übereinstimmung jener Werte einerseits, die sich nach Formel (1) auf Grund von Messungen der Absorptions- und Fluoreszenzspektren sowie der mittleren Lebensdauer des Moleküls im angeregten Zustand errechnen, und der aus der Kurve der Konzentrationsdepolarisation anhand der Gleichungen (4) und (3) errechneten Werte andererseits, ist eine teilweise wechselseitige Kompensation der Fehler, die bei Aufstellung der Beziehung (3) begangen worden sind.

Die Frage der wechselseitigen Beziehung zwischen R_J und R_0 im Falle der Konzentrationsauslöschung der Photolumineszenz durch fremde Stoffe ist in der Arbeit von **Jabłoński** [6] und im Falle der Konzentrationsdepolarisation in den Abhandlungen [10, 11] behandelt worden.

Bei Bestimmung der Beziehung zwischen R_J und R_0 wurde dort unter anderen das von **Förster** angegebene Gesetz der Wechselwirkung der Moleküle berücksichtigt, da sich die Wahrscheinlichkeit der Energieübertragung mit der Entfernung wie R^{-6} verringert. Der gefundene Wert für das Verhältnis $\frac{R_J}{R_0}$ beim Modell mit Wirkungssphäre [6, 10] betrug 1,327. Im Falle des Schichtmodells [16] erhielten wir für das gleiche Verhältnis den Wert 1,279, der mit den Versuchsergebnissen von **Szalay** und **Sárkány** [9] sehr gut übereinstimmt.[2]

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[2] Diese Autoren bestimmten gleichfalls die Beziehung zwischen R_J und R_0 in der Gestalt $R_J = 1{,}367\ R_0$. Die Diskussion hierüber ist in Abhandlung [11] angegeben.

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Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (2), pp. 191—194 (1966)

ÜBER DIE ERSCHEINUNGEN DER ELEKTRODENZERSTÄUBUNG BEI Hg—A GLEICHSTROMENTLADUNG

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(Eingegangen: 28. IX. 1965)

Während dieses Experiments wurden vom Verfasser die Zerstäubungserscheinungen in Entladungsröhren mit Oxydkathoden untersucht. Die 1200 mm langen gläsernen Entladungsröhren ∅ 38 mm, hatten eine A-Gasfüllung unter einem Druck von 3 Torr. Die Messungen wurden bei einer Umgebungstemperatur von 25 ± 2° C bei Gleichstromentladung nach der Methode von KÜHL [1] durchgeführt. Der Entladungsstrom (i_L) diente als Parameter; in Abhängigkeit von diesem wurden die Zerstäubungsgeschwindigkeit (V_z) weiterhin die Temperaturänderungen an den auf den Elektroden entstehenden Anoden- (T_{F_a}) bzw. Kathodenflecken (T_{Fk}) geprüft. Der Gleichstrom wurde mit einer spannungsstabilisierten Gleichstromquelle erzeugt. Zur Messung der Geschwindigkeit der Zerstäubung der einzelnen Oxydüberzügekomponenten diente eine aus Monochromator-Multiplier-Verstärker-Oszilloskop-Einheiten [2] zusammengestellte Messeinrichtung. Die Temperatur wurde unter Berücksichtigung der in solchen Fällen erforderlichen Korrektion mit Hilfe eines optischen Pyrometers bestimmt.

Obwohl während der Messungen die Bestimmung der Veränderungen in den Oberflächen der Anoden- und Kathodenflecke nicht die wichtigste Rolle spielte, wurde mit Hilfe eines Kathetometers festgestellt, dass sich die Grösse der Flecken in dem hier untersuchten Strombereich nicht wesentlich änderte. Die Messung der Zerstäubung erstreckte sich auf alle drei Komponenten des die Oxyde von Ba, Sr und Ca enthaltenden Drei-Oxyds. Die Untersuchungen wurden bei Ba mit $\lambda = 451$ nm, bei Sr mit $\lambda = 460$ nm bei Ca mit $\lambda = 412$ nm durchgeführt. Die Zerstäubung von Sr und Ca verläuft ähnlich wie die von Ba, und erwartungsgemäss zeigte der Ablauf des Sr und besonders des Ca in dem untersuchten Fall einen niedrigeren Wert. Deshalb sollen die Änderungen dieser beiden Komponenten (Sr und Ca) hier nicht diskutiert werden.

Die Kennlinien der Brennspannung (V_L) und der Leistung (W) sind sowohl bei der Anode (Abb. 2) als auch bei der Kathode (Abb. 1) gleich, weil die Zerstäubungsgeschwindigkeit in beiden Fällen unter Anwendung der gleichen Röhren bestimmt wurde. Die Beachtung der Fehlergrenzen bei den angewandten Messungen führte zu der Feststellung, dass die bei verschiedenen

Entladungsströmen (i_L) aufgenommenen Werte der einzelnen Parameter graphisch durch die auf den Abbildungen 1 und 2 gegebenen Geraden dargestellt werden können. Die Messungen bestätigen die Literaturangaben [3], dass der Anodenfleck bei gegebenem Entladungstrom eine höhere Temperatur hat als der Kathodenfleck, wenn es sich um eine Gleichstromentladung handelt. Darüber hinaus wurde die ***bisher in der Literatur nicht erwähnte Tatsache*** bewiesen, dass die Geschwindigkeit der Zerstäubungen der Kathode trotzdem einen höheren Wert aufweist als bei der Anode.

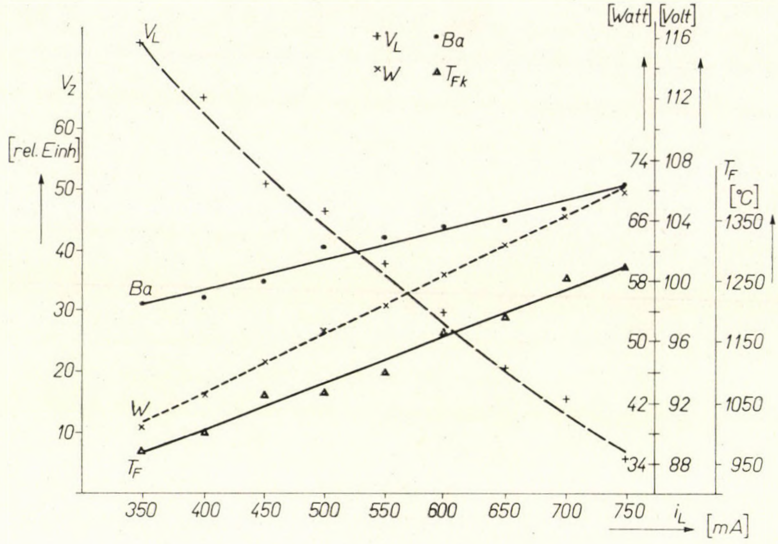

Abb. 1

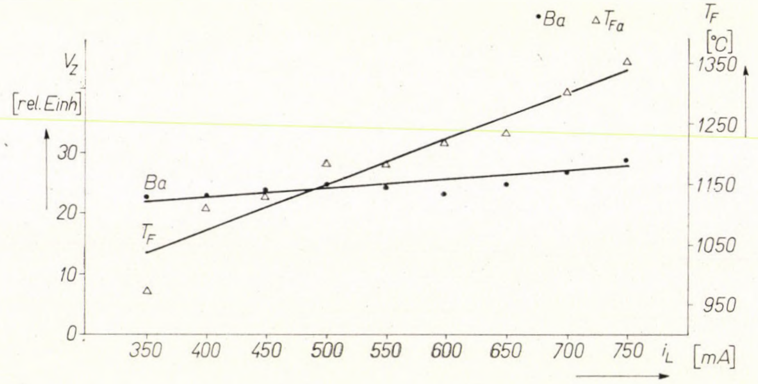

Abb. 2

Entsprechend den Abbildungen 1 und 2 kann die Zerstäubungsgeschwindigkeit (V_z) in dem untersuchten Bereich sowohl bei der Anode- als auch bei der Kathode mit guter Annäherung als lineare Funktion des Entladungsstromes (i_L) aufgefasst werden; dies bezieht sich auf die beiden Fleckentemperaturen T_{Fk} und T_{Fa}, auf die Brennspannung (U_L) und auf die elektrische Leistung (W). Daraus folgt, dass auch das Verhältnis zwischen der Zerstäubungsgeschwindigkeit und der Flecktemperatur linear ist (Abb. 3).

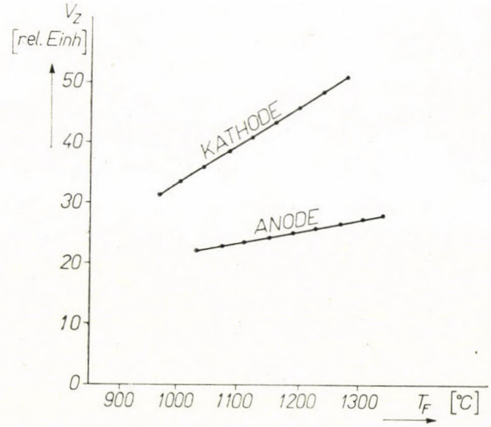

Abb. 3

Diesen Zusammenhang beschreiben innerhalb des untersuchten Bereiches folgende Beziehungen:
an der Kathodenseite

$$V_{zk} = A_k \cdot T_{Fk} + B_k = f(T_{Fk}), \tag{1a}$$

an der Anodenseite

$$V_{za} + A_a \cdot T_{Fa} + B_a = f(T_{Fa}), \tag{1b}$$

wobei A_k und B_k die Kennwertkonstanten an der Kathodenseite, A_a und B_a hingegen die an der Anodenseite bezeichnen.

Die Abbildung 3 zeigt die den Gleichungen (1a) und (1b) entsprechend aufgetragene Kathodenkurve $V_{zk} = f(T_{Fk})$ und die Anodenkurve $V_{za} = f(T_{Fa})$.

Aus der Abbildung kann geschlossen werden, dass

$$A_k > A_a, \tag{2}$$

$$V_{zk} > V_{za} \text{ (bei gleichen Temperaturen } T). \tag{3}$$

Der Quotient A_a/A_k, gebildet aus der Steilheit der Kennlinien

$$A_a/A_k = 0{,}04 \tag{4}$$

weist darauf hin, dass es eine weitere Wirkung gibt, die von der Polarität der Elektroden abhängig ist, und neben der die auf den Elektrodenoberflächen auftretende Flecktemperatur die Zerstäubungsgeschwindigkeit (V_z) gleichfalls deutlich beeinflusst.

Wie bereits erwähnt, ändert sich die Grösse der Anoden- und Kathodenflecke nur unmerklich, die Fleckoberfläche kann also nicht als Ursache für die Abweichung der Kurven $V_{zk} = A_k \cdot T_{Fk} + B_k$ bzw. $V_{za} = A_a \cdot T_{Fa} + B_a$ betrachtet werden.

Die Eigenschaften der Kennlinien V_{zk} und V_{za} werden ausser durch die Temperatur auch durch die im Anoden- und Kathodenraum wirkenden Mechanismen wesentlich beeinflusst. Diese sind:

bei der Kathode — Elektronenemission, Ioneneinschlag, der die Kathoden auch mechanisch beschädigt, ausserdem der Verlust durch Wärmestrahlung, Wärmekonvektion, Wärmeübertragung sowie der durch die Elektronenemission entstehende, weiterhin der durch die Verdampfung und die mechanische Zerstäubung des Kathodenüberzuges verursachte Wärmeverlust;

bei der Anode — Elektroneneinschalg, die Wärmeverluste durch Strahlung, Konvektion und Übertragung.

Die Abweichungen der hier angeführten Kennlinien von anodischen und kathodischen Erscheinungen können auf die Abweichungen infolge dieser Mechanismen zurückgeführt werden.

Die hier gemessene Zerstäubungsgeschwindigkeit vereinigt in sich die Verdampfung wie auch den mechanischen Zerfall: die Zerstörung. Welchen unter diesen Entladungsparametern im gegebenen Elektrodenfall die grössere Bedeutung zukommt, wird die Weiterführung der hier mitgeteilten Untersuchung zu entscheiden haben.

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Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (2), pp. 195—198 (1966)

THE EFFECT OF IMPURITY CONTENT AND HEAT TREATMENT ON THE R_{273}/R_{78} RESISTIVITY RATIO OF ALUMINIUM AND COPPER

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(Received 16. XI. 1965)

Introduction

The resistivity ratio as measured in ice, or in liquid He, H_2 or N_2 is often used to characterize the purity of different metals. It is generally accepted in the literature that this resistivity ratio varies according to the purity of the sample, after a suitable heat treatment has been employed to remove the various physical lattice defects (point defects, dislocations). However, the question arises as to what is to be regarded as "suitable" heat treatment, and how for this ratio is characteristic of the chemical purity of the given metal, because it has been shown [1—3] that the resistivity ratio of a given sample may change by further heat treatment even after the removal of physical lattice defects.

The resistivity ratio of 99,999% copper varies with the residual pressure of the vacuum heat treatment: Dolecek and Schultz [1] studied the effect in liquid He, Lange and Haeussler [2] in liquid H_2. The results of the two investigations differed considerably. The resistivity ratio of aluminium of different purity, has also shown some anomaly during measurement in liquid H_2, after heat treatment in air [3].

In this paper we wish to submit some results, related to the effect of heat treatment and of the impurity content of various aluminium and copper samples, with measuring the resistivity ratio in liquid N_2 and ice temperatures.

Aluminium

Results for several aluminium wires of different purities are shown in Figure 1. The samples were drawn to a diameter of 1 mm and were held for a long period at room temperature before further treatment. The heat treatment was effected in vacuo, at 5.10^{-5} Torr, holding the samples for a period of 30 minutes at a given temperature. As can be seen in Figure 1, the value of the R_{273}/R_{78} resistivity ratio of aluminium samples of different purity depends considerably on the temperature of the previous heat treatment.

The zone refined sample "1" of 99,999% purity softens considerably at room temperature within a few hours after deformation, i.e. lattice defects, responsible for the work hardening, are removed during this annealing. The further decrease of low temperature resistivity after a heat treatment at 200 to 300° C can be related to the removal of those lattice defects, which remained for a longer period in the samples held at room temperature. The increase of the resistivity ratio of the less pure samples "2" and "3" up to a temperature of 200° C resp. 300° C can be explained again by the removal of lattice defects, mainly dislocations, as was shown by parallel mechanical tests. For anneals at still higher temperatures the resistivity ratio increases with the annealing temperature, but later it decreases. The decrease is more pronounced in the case of samples of lower purity. This fact can be related to some inter-

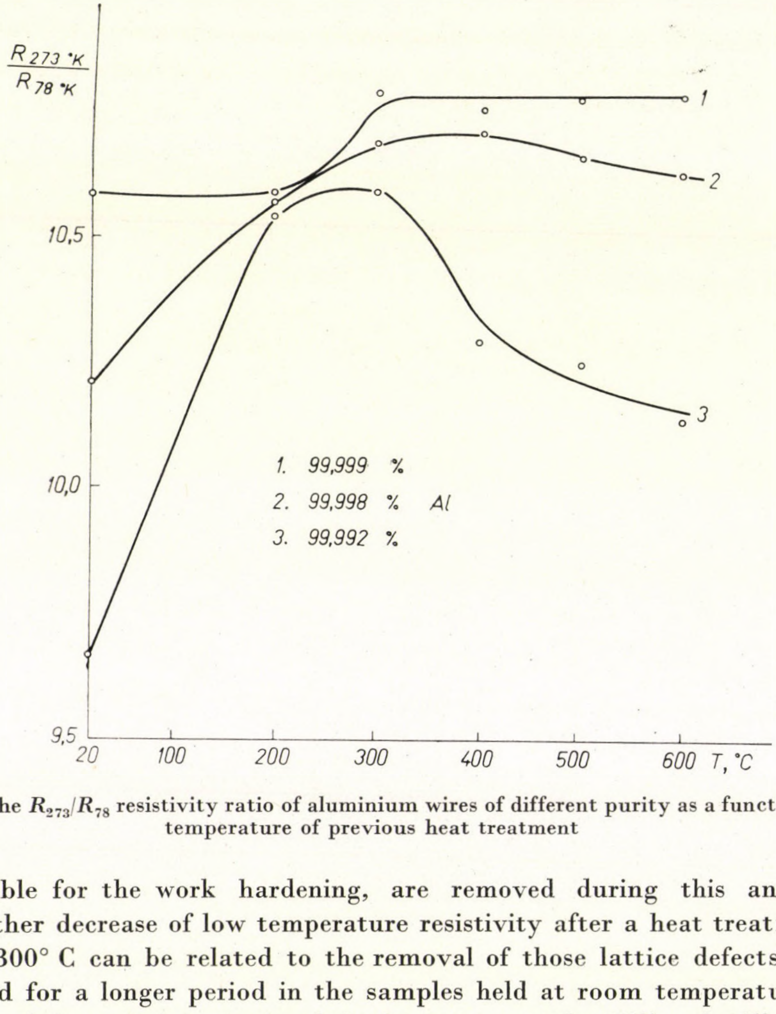

Fig. 1. The R_{273}/R_{78} resistivity ratio of aluminium wires of different purity as a function of the temperature of previous heat treatment

action between the different impurities, or between impurities and lattice defects.

According to these considerations it is highly debatable what heat treatment must be applied, when the purity of a given sample is to be characterized by the resistivity ratio. The different R_{273}/R_{78} ratios show *nearly the same value after a heat treatment at 200 to 250° C, regardless of great differences in their purities.* It is therefore uncertain what heat treatment leads to resistivity ratios characteristic of the impurity content of the different samples.

Our further investigations have shown that the resistivity ratio maxima, produced by anneals of roughly between 200 and 400° C, can hardly be related to the solution, precipitation or evaporation of any impurities present in smell concentrations. It seems to be necessary therefore to investigate *in conjunction with the change of the resistivity ratio as a function of the previous heat treatment, the response of the samples to deformation and recovery, and to characterize* the physical state of the given samples *by these joint properties.*

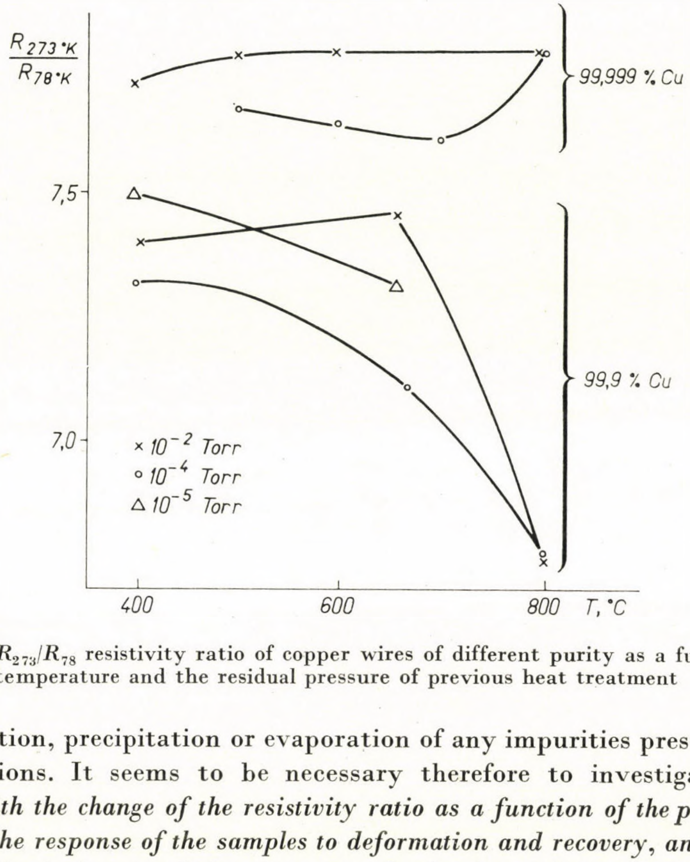

Fig. 2. The R_{273}/R_{78} resistivity ratio of copper wires of different purity as a function of the temperature and the residual pressure of previous heat treatment

Copper

Results of the measurement of the resistivity ratio of different copper wires are shown in Figure 2, as a function of the temperature of previous heat treatment. This was effected for a period of 4 hours at different degrees of vacuum, on zone-refined copper (99,999%) and electrolytic-grade copper (99,9%). It can be seen that the value of the R_{273}/R_{78} ratio depends considerably on the annealing atmosphere. For the purer samples the effect is smaller. In a poor vacuum (10^{-2} Torr) the ratio becomes generally higher, and for less pure samples decreases only above 600° C. This effect can be explained in various ways. It may be possible that the oxygen in the residual atmosphere combines with the iron impurity content of the given copper sample, showing a great R_{273}/R_{78} ratio. The decrease of this ratio in the case of the less pure copper samples can also be related to the resolution of the iron content [2]. It is possible, however, that the interaction of other impurities with oxygen gives rise to this anomalous behaviour.

If we compare the results of Figure 2 with the data of DOLECEK and SCHULTZ [1], resp. LANGE and HAEUSSLER [2], we come to the conclusion, that besides the factors already listed, the cooling liquid used during the measurement of the resistivity may also influence the value of the low temperature resistivity, leading to the large discrepancies between the data of various experimenters. The measurements, made on different copper samples show, in conformity with the considerations related to the aluminium samples, that the absolute value of the resistivity ratio in itself alone is not an equivocal characteristic of the purity of the metal, and should be coupled with the investigation of other physical processes.

Our thanks are due to Mrs. J. P. KUKONYA for her help during the measurements.

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Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (2), pp. 199—206 (1966)

LOW ENERGY SCATTERING OF ELECTRONS BY HARTREE-FOCK NEUTRAL ATOMS

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(Received 5. X. 1965)

It is known that the elastic scattering of electrons by neutral atoms is of great interest in connection with upper atmosphere physics and astrophysics. The range of the energy of the scattered electrons is of the order of 0 to 50 eV. The accuracy of the calculated phase shifts depends very much on the approximation method as well as on the atomic potential. The purpose of this paper is to calculate the phase shifts using HULTHÉN's method and the approximation for the HARTREE—FOCK potential of neutral atoms. According to STRAND an BONHAM [1] the radial electron density of neutral HARTREE—FOCK atoms can be accurately represented by the expression corresponding to the following form of the screening factor $Z_p(r)/Z$

$$Z_p(r)/Z = \sum_{i=1}^{2} {}^a\gamma_i \exp(-{}^a\lambda_i r) + r \sum_{j=1}^{m} {}^b\gamma_j \exp(-{}^b\lambda_j r), \tag{1}$$

where r is the radial distance, $Z_p(r)$ the effective nuclear charge for the potential, Z is the atomic number, $m = 2$ for $Z = 2$ to $Z = 18$ and $m = 3$ for $Z = 19$ to $Z = 36$ and ${}^a\gamma_i$, ${}^a\lambda_i$, ${}^b\gamma_j$ and ${}^b\lambda_j$ are parameters to be obtained for each atom. For the point $r = 0$ the condition $\sum_{i=1}^{2} {}^a\gamma_i = 1$ is obtained for the ${}^a\gamma_i$. The electrostatic potential $V(r)$ in atomic units is related to $Z_p(r)$ as $V(r) = -Z_p(r)/r$. In order to find the phase shift for low energy scattering of electrons by HARTREE—FOCK neutral atoms we apply the HULTHÉN [2] variational method for the quantum number $l = 0$ using eq. (1). In this case we write

$$L = \int_0^\infty R_0(r)\left[\frac{d^2}{dr^2} + k^2\right] R_0(r)\, dr + 2Z \sum_{i=1}^{2} {}^a\gamma_i \int_0^\infty \frac{e^{-{}^a\lambda_i r}}{r} R_0^2(r)\, dr \tag{2}$$

$$+ 2Z \sum_{j=1}^{m} {}^{b}\gamma_j \int_0^\infty e^{-b\lambda_j r} R_0^2(r)\, dr ,$$

where $R_0(r)$ is the approximate solution for the SCHRÖDINGER eq. for $l = 0$ satisfying the following boundary condition

$$R_0(0) = 0 \text{ and } \lim_{r\to\infty} R_0(r) \to \sin kr + a \cos kr. \tag{3}$$

In eq. (2) $k^2 = 2E$, where E is the incident energy of the scattered electron and a in eq. (3) is related to the phase shift η_0 as follows $a = \tan \eta_0$. If a suitable trial function for $R_0(r)$ containing $n + 1$ independent parameters $c_1, \ldots c_2, \ldots$ is chosen then according to HULTHÉN's variational method these parameters are determined by the conditions $L = 0$ and $\partial L/\partial c_i = 0$, $i = 1, \ldots, n$, where $a = \tan \eta_0$ determines the phase shift. In this paper we calculated the phase shifts η_0 using for $R_0(r)$ following expression [3]

$$R_0(r) = \sin kr + (a + be^{-cr})\,(1 - e^{-cr}) \cos kr\, . \tag{4}$$

This approximate solution of the SCHRÖDINGER equation for the case $l = 0$ fulfills the required boundary conditions given by eq. (3) and contains the independent parameters a, b and c where $a = \tan \eta_0$. At first we have calculated $R_0^2(r)$ and $R_0(r) \left[\dfrac{d^2}{dr^2} + k^2\right] R_0(r)$ namely:

$$\begin{aligned} R_0^2(r) = {} & a^2(1 - 2e^{-cr} + e^{-2cr}) \cos^2 kr + b^2(e^{-2cr} - 2e^{-3cr} + e^{-4cr}) \cos^2 kr + \\ & + 2ab(e^{-cr} - 2e^{-2cr} + e^{-3cr}) \cos^2 kr \\ & + 2a(1 - e^{-cr}) \sin kr \cos kr + 2b(e^{-cr} - e^{-2cr}) \sin kr \cos kr + \sin^2 kr \end{aligned} \tag{5}$$

and

$$\begin{aligned} R_0 \frac{d^2 R_0}{dr} + k^2 R_0^2 = {} & a^2[2ck(e^{-2cr} - e^{-cr}) \sin kr \cos kr + \\ & + c^2(e^{-2cr} - e^{-cr}) \cos^2 kr] + b^2 [2ck(e^{-2cr} - 3e^{-3cr} + \\ & + 2e^{-4cr}) \sin kr \cos kr + c^2(e^{-2cr} - 5e^{-3cr} + 4e^{-4cr}) \cos^2 kr] + \\ & + ab[2ck(e^{-cr} - 4e^{-2cr} + 3e^{-3cr}) \sin kr \cos kr + c^2(e^{-cr} - \\ & - 6e^{-2cr} + 5e^{-3cr}) \cos^2 kr] + a[-2cke^{-cr} \sin^2 kr - \\ & - c^2 e^{-cr} \sin kr \cos kr] + b[2ck(e^{-cr} - 2e^{-2cr}) \sin^2 kr + \\ & + c^2 (e^{-cr} - 4e^{-2cr}) \sin kr \cos kr]\, . \end{aligned} \tag{6}$$

Substituting $R_0^2(r)$ and $R_0 \dfrac{d^2 R_0}{dr} + k^2 R_0^2$ into the expression for L given by eq. (2) we obtain

$$L = A_1 a^2 + B_1 b^2 + C_1 ab + D_1 a + E_1 b + A_2 a^2 + B_2 b^2 + C_2 ab + D_2 a + \\ + E_2 b + F_2 + A_3 a^2 + B_3 b^2 + C_3 ab + D_3 a + E_3 b + F_3\,, \qquad (7)$$

where the symbols A_1, B_1, C_1, D_1, E_1, ... A_2, B_2, C_2, D_2, E_2, F_2 and A_3, B_3, C_3, D_3, E_3, F_3 are given by

$$A_1 = -\frac{c(2c^2 + k^2)}{4(c^2 + k^2)}\,,$$

$$B_1 = \frac{c(2c^2 + 3k^2)}{4(c^2 + k^2)} - \frac{c(45c^2 + 28k^2)}{3(9c^2 + 4k^2)} + \frac{c(8c^2 + 3k^2)}{2(4c^2 + k^2)}\,,$$

$$C_1 = -\frac{c(4c^2 + 5k^2)}{2(c^2 + k^2)} + \frac{c(45c^2 + 28k^2)}{3(9c^2 + 4k^2)}\,,$$

$$D_1 = -k\,, \quad E_1 = 0\,,$$

$$A_2 = Z \sum_{i=1}^{2} {}^{a}\gamma_i \left\{ \ln \frac{({}^{a}\lambda_i + c)^2}{{}^{a}\lambda_i ({}^{a}\lambda_i + 2c)} + \frac{1}{2} \ln \frac{[({}^{a}\lambda_i + c)^2 + 4k^2]^2}{[{}^{a}\lambda_i^2 + 4k^2][({}^{a}\lambda_i + 2c)^2 + 4k^2]} \right\},$$

$$B_2 = Z \sum_{i=1}^{2} {}^{a}\gamma_i \left\{ \ln \frac{({}^{a}\lambda_i + 3c)^2}{{}^{a}\lambda_i + 2c)({}^{a}\lambda_i + 4c)} + \right. \\ \left. + \frac{1}{2} \ln \frac{[({}^{a}\lambda_i + 3c^2)^2 + 4k^2]^2}{[({}^{a}\lambda_i + 2c)^2 + 4k^2]^2 [({}^{a}\lambda_i + 4c)^2 + 4k^2]} \right\},$$

$$C_2 = 2Z \sum_{i=2}^{2} {}^{a}\gamma_i \left\{ \ln \frac{({}^{a}\lambda_i + 2c)^2}{({}^{a}\lambda_i + c)\,({}^{a}\lambda_i + 3c)} + \right. \\ \left. + \frac{1}{2} \ln \frac{[({}^{a}\lambda_i + 2c)^2 + 4k^2]^2}{[({}^{a}\lambda_i + c)^2 + 4k^2]\,[({}^{a}\lambda_i + 3c)^2 + 4k^2]} \right\},$$

$$D_2 = 2Z \sum_{i=1}^{2} {}^{a}\gamma_i \left\{ \tan^{-1} \frac{2k}{{}^{a}\lambda_i} - \tan^{-1} \frac{2k}{{}^{a}\lambda_i + c} \right\} = \\ = 2Z \sum_{i=1}^{2} {}^{a}\gamma_i \tan^{-1} \frac{2ck}{4k^2 + {}^{a}\lambda_i ({}^{a}\lambda_i + c)}\,,$$

$$E_2 = 2Z \sum_{i=1}^{2} {}^{a}\gamma_i \left\{ \tan^{-1} \frac{2k}{{}^{a}\lambda_i + c} - \tan^{-1} \frac{2k}{{}^{a}\lambda_i + 2c} \right\} = \\ = 2Z \sum_{i=1}^{2} {}^{a}\gamma_i \tan^{-1} \frac{2ck}{4k^2 + ({}^{a}\lambda_i + c)\,({}^{a}\lambda_i + 2c)}\,,$$

$$F_2 = \frac{Z}{2} \sum_{i=1}^{2} {}^a\gamma_i \ln\left[1 + \left(\frac{2k}{{}^a\lambda_i}\right)^2\right] \tag{8}$$

and

$$A_3 = 2Z \sum_{j=1}^{m} {}^b\gamma_j \left\{ \frac{{}^b\lambda_j^2 + 2k^2}{{}^b\lambda_j ({}^b\lambda_j^2 + 4k^2)} - \frac{2({}^b\lambda_j + c)^2 + 4k^2}{({}^b\lambda_j + c)\left[({}^b\lambda_j + c)^2 + 4k^2\right]} + \right.$$
$$\left. + \frac{({}^b\lambda_j + 2c)^2 + 2k^2}{({}^b\lambda_j + 2c)\left[({}^b\lambda_j + 2c)^2 + 4k^2\right]} \right\},$$

$$B_3 = 2Z \sum_{j=1}^{m} {}^b\gamma_j \left\{ \frac{({}^b\lambda_j + 2c)^2 + 2k^2}{({}^b\lambda_j + 2c)\left[({}^b\lambda_j + 2c)^2 + 4k^2\right]} - \right.$$
$$\left. - \frac{2({}^b\lambda_j + 3c)^2 + 4k^2}{({}^b\lambda_j + 3c)\left[({}^b\lambda_j + 3c)^2 + 4k^2\right]} + \frac{({}^b\lambda_j + 4c)^2 + 2k^2}{({}^b\lambda_j + 4c)\left[({}^b\lambda_j + 4c)^2 + 4k^2\right]} \right\},$$

$$C_3 = 4Z \sum_{j=1}^{m} {}^b\gamma_j \left\{ \frac{({}^b\lambda_j + c)^2 + 2k^2}{({}^b\lambda_j + c)\left[({}^b\lambda_j + c)^2 + 4k^2\right]} - \frac{2({}^b\lambda_j + 2c)^2 + 4k^2}{({}^b\lambda_j + 2c)\left[({}^b\lambda_j + 2c)^2 + 4k^2\right]} + \right.$$
$$\left. + \frac{({}^b\lambda_j + 3c)^2 + 2k^2}{({}^b\lambda_j + 3c)\left[({}^b\lambda_j + 3c)^2 + 4k^2\right]} \right\},$$

$$D_3 = 4Zk \sum_{j=1}^{m} {}^b\gamma_j \left\{ \frac{1}{{}^b\lambda_j^2 + 4k^2} - \frac{1}{({}^b\lambda_j + c)^2 + 4k^2} \right\},$$

$$E_3 = 4Zk \sum_{j=1}^{m} {}^b\gamma_j \left\{ \frac{1}{({}^b\lambda_j + c)^2 + 4k^2} - \frac{1}{({}^b\lambda_j + 2c)^2 + 4k^2} \right\},$$

$$F_3 = 4Zk^2 \sum_{j=1}^{m} \frac{{}^b\gamma_j}{{}^b\lambda_j ({}^b\lambda_j^2 + 4k^2)} \,.$$

The numerical values of the parameters ${}^a\lambda_1$, ${}^a\gamma_2$, ${}^a\lambda_2$, ${}^b\gamma_1$, . . . ${}^b\lambda_3$ and ${}^b\gamma_3$ from $Z = 2$ to $Z = 36$ are tabulated in Table I. The parameters a, b and c for several k-values and atomic numbers $Z = 2$, $Z = 6$, $Z = 7$, $Z = 8$ and $Z = 10$ have been collected in Tables II, III, IV, V and VI. The numerical values of these parameters are determined using Hulthén's method by the help of an IBM709 digital computer.

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a) D. R. Hartree and W. Hartree, Proc. Roy. Soc. (London) A, **193**, 299, 1948.

b) d) For references see [1].

c) 3s wavefunction is from L. Biermann and E. Trefftz, Z. Astrophys., **26**, 213, 1949, wavefunction for Mg** from W. J. Vost, Phys. Rev., **58**, 557, 1940.

Table I

Values of the parameters ${}^{a}\lambda_1, {}^{a}\gamma_2, {}^{a}\lambda_2, {}^{b}\gamma_1 \ldots, {}^{b}\gamma_3, {}^{b}\lambda_3$ and ${}^{a}\gamma_1 = 1 - {}^{a}\gamma_2$

Z	${}^{a}\lambda_1$	${}^{a}\gamma_2$	${}^{a}\lambda_2$	${}^{b}\gamma_1$	${}^{b}\lambda_1$	${}^{b}\gamma_2$	${}^{b}\lambda_2$	${}^{b}\gamma_3$	${}^{b}\lambda_3$
1	2.000			1.000	2.000				
2	2.4907			0.5489	3.219	0.2546	5.244		
3	0.8776	—0.2197	7.951	— 1.2520	1.795	— 1.3296	3.192		
4	1.1824	—0.3171	9.624	— 2.0940	2.877	— 1.5037	5.186		
5	1.4333	—0.3002	11.848	— 2.3256	3.796	— 1.6440	6.667		
6	1.7315	—0.3391	13.713	— 2.7379	4.718	— 2.0444	8.333		
7	2.0249	—0.3521	15.700	— 3.0744	5.671	— 2.3369	9.960		
8	2.2376	—0.2806	18.263	— 3.0715	6.803	— 1.9710	11.548		
9	2.4796	—0.2538	20.644	— 3.2697	7.971	— 1.8073	13.392		
10	2.7385	—0.2464	22.850	— 3.5467	9.129	— 1.7746	15.381		
11[a)]	1.2009	—0.1353	25.776	— 1.7781	2.013	— 3.576	11.463		
11[b)]	1.1968	—0.1317	25.996	— 1.7673	2.006	— 3.531	11.469		
12[c)]	1.2709	—0.1630	26.644	— 2.0702	2.334	— 4.138	12.784		
12[d)]	1.2724	—0.1670	26.519	— 2.0859	2.340	— 4.198	12.780		
13	1.3532	—0.1951	27.522	— 2.3888	2.674	— 4.804	14.036		
14	1.4722	—0.2293	28.407	— 2.7089	3.061	— 5.531	15.233		
15	1.6115	—0.2655	29.329	— 3.0555	3.483	— 6.323	16.392		
16	1.7525	—0.2979	30.417	— 3.4114	3.915	— 7.095	17.546		
17	1.9037	—0.3336	31.476	— 3.8189	4.373	— 7.952	18.675		
18	2.0636	—0.3740	32.485	— 4.2960	4.853	— 8.916	19.772		
19	2.320	—0.4523	32.78	— 5.045	5.439	—10.448	20.656	0.0470	0.6328
20	2.625	—0.5426	33.24	— 5.945	6.058	—12.224	21.541	0.1212	0.8498
21	2.742	—0.5290	35.50	— 6.075	6.450	—12.47	22.83	0.1353	0.936
22	2.883	—0.5397	36.70	— 6.508	6.885	—13.191	23.986	0.1487	1.0169
23	2.032	—0.5507	38.11	— 6.885	7.324	—13.823	25.095	0.1597	1.0919
24	3.177	—0.5574	39.56	— 7.225	7.760	—14.381	26.212	0.1683	1.1610
25	3.318	—0.5604	41.04	— 7.533	8.195	—14.876	27.339	0.1733	1.2204
26	3.458	—0.5587	42.59	— 7.792	8.629	—15.285	28.493	0.1828	1.2952
27	3.594	—0.5551	44.17	— 8.028	9.064	—15.653	29.656	0.1890	1.3613
28	3.726	—0.5498	45.78	— 8.242	9.499	—15.981	30.831	0.1938	1.4240
29[a)]	3.856	—0.5436	47.41	— 8.439	9.935	—16.284	32.013	0.1973	1.4838
30	3.985	—0.5379	49.03	— 8.637	10.374	—16.587	33.195	0.1989	1.5376
31	4.293	—0.5978	49.65	— 9.658	11.000	—18.278	34.056	0.2718	1.5819
32	4.581	—0.6485	50.42	—10.601	11.584	—19.792	34.943	0.3455	1.6531
33	4.911	—0.7128	51.05	—11.765	12.189	—21.619	35.768	0.4386	1.769
34	5.256	—0.7818	51.70	—13.044	12.795	—23.579	36.589	0.5406	1.8922
35	5.629	—0.8621	52.29	—14.530	13.410	—25.805	37.376	0.6557	2.0288
36	6.029	—0.9534	52.84	—16.230	14.032	—28.297	38.138	0.7832	2.1740

Table II
The numerical values of the parameters a, b, c for $Z = 2$ and for small values of k

k	a	b	c
0.0707	—0.0016	0.0055	1.971
0.2236	—0.0356	0.1124	1.964
0.3162	—0.0903	0.2644	1.943
0.7071	0.5392	—1.1064	1.565
0.8944	0.4851	—1.2021	1.662
1.0	0.4603	—1.210	1.703
1.0954	0.4420	—1.202	1.734
1.2247	0.4221	—1.181	1.767
1.4142	0.4004	—1.140	1.802

Table III
The numerical values of the parameters a, b, c for $Z = 6$ and for small values of k

k	a	b	c
0.0707	—0.0026	0.0046	1.971
0.2236	—0.0599	0.0937	1.959
0.3162	—0.1659	0.2238	1.917
0.7071	0.6509	—0.6329	1.505
0.8944	0.6032	—0.7454	1.598
1.00	0.5844	—0.7760	1.639
1.0954	0.5716	—0.7900	1.670
1.2247	0.5592	—0.7956	1.703
1.4142	0.5475	—0.7889	1.741

Table IV
The numerical values of the parameters a, b, c for $Z = 7$ and for small values of k

k	a	b	c
0.0707	—0.0027	0.6045	1.971
0.2236	—0.0630	0.0914	1.958
0.3162	—0.1763	0.2184	1.913
0.7071	0.6672	—0.5960	1.499
0.8944	0.6001	—0.7393	1.633
1.0954	0.5876	—0.7541	1.663
1.2247	0.5158	—0.9611	1.697
1.4142	0.5652	—0.7560	1.735

Table V

The numerical values of the parameters a, b, c for $Z = 8$ and for small values of k

k	a	b	c
0.0707	−0.0028	0.0044	1.971
0.2236	−0.0655	0.0895	1.958
0.3162	−0.1851	0.2139	1.918
0.7071	0.6808	−0.5675	1.494
0.8944	0.6314	−0.6789	1.587
1.00	0.6129	−0.7108	1.628
1.0954	0.6007	−0.7263	1.659
1.2247	0.5894	−0.7341	1.692
1.4142	0.5797	−0.7301	1.739

Table VI

The numerical values of the parameters a, b, c for $Z = 10$ and for small values of k

k	a	b	c
0.0707	−0.0029	0.0043	1.971
0.2236	−0.0694	0.0865	1.957
0.3162	−0.1990	0.2069	1.905
0.7071	0.7022	−0.5264	1.487
0.8944	0.6512	−0.6369	1.580
1.0	0.6328	−0.6694	1.621
1.0954	0.6209	−0.6857	1.651
1.225	0.6103	−0.6945	1.685
1.414	0.6019	−0.6921	1.722

In case when a is known then according to the relation $a = \tan \eta_0$ the phase shift η_0 for low energy scattering of electrons by HARTREE—FOCK neutral atoms can be calculated.

Since the screening factor [4] $Z_p(r)/Z$ given by eq. (1) with the numerical values of the parameters ${}^a\lambda_1$, ${}^a\gamma_2$, ${}^a\lambda_2$, ${}^b\gamma_1$, . . ., ${}^b\gamma_3$ and ${}^b\lambda_3$ collected in Table I fit to a great accuracy the true HARTREE field from $Z = 2$ to $Z = 36$ and the HULTHÉN method as well as $R_0(r)$ given by eq. (4) is sufficiently accurate for low energy scattering of electrons by neutral atoms, so we can expect that the considerations of this paper are sufficiently accurate to this problem.

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3. H. S. W. Massey—Moiseiwitch, Proc. Roy. Soc. Lond. A, **205**, 483, 1951.
4. For reference see [1].

RECENSIONES

Problems of Low Temperature Physics and Thermodynamics

edited by Prof. A. VAN ITTERBEEK (Belgium) published by Pergamon Press, 1962

Volume 3

The volume contains the discussions of Commission No. 1 of the International Institute of Refrigeration. In the working sessions between September 20th and 22nd 1961 140 delegates coming from 14 countries discussed 24 papers. The first day of the session was devoted to discussing methods for the large scale production, transport and storage of liquid gases, the second and third days were assigned to the physics of very low temperatures, particularly to the attainment and measurement of temperatures below 1° K.

Various branches of industry demand large quantities of liquid gases, particularly oxygen and hydrogen, which are consumed in big steel works and chemical plants at the rate of thousands of tons a day. One report discussed the use of aluminium alloys as heat exchangers, pointing out the low specific gravity, outstanding heat conductivity and the high strength of aluminium. Cooler surfaces of various designs were shown.

Messrs. COULON, SIMONET and STOULS reported on the work of low-temperature distillation columns used in the production of deuterium.

J. W. L. KÖHLER and J. R. VAN GEUNS from the Netherland Philips Laboratories described a small liquid oxygen plant developed by them; the plant weighing three tons produces 15 kg liquid oxygen of 99,5% purity per hour after a running-in period of three hours.

Insulation techniques introduced by two American experts M. A. DUBS and L. I. DANA have brought about a small revolution in the transport of large quantities of liquid gases. The process is also suitable for the handling of liquid hydrogen and helium.

J. W. T. DABBS of the Oak Ridge National Laboratory (USA) reported on a reliable helium liquefaction plant. This plant producing 250—400 litres per month was in operation for six month attended by a single technician.

In the Clarendon Laboratory a pulsating core magnetic resonance meter was used in an investigation into the electronic structure of transition metals below 1° K temperatures.

Two papers discussed the use of H^3 in temperature measurement below 1° K and in specific heat determination.

One of the delegates suggested the use of a H^3 cooling cycle to produce temperatures below 0,2° K. To obtain a higher osmotic pressure a weak solution of H^3 in H^4 was used.

R. D. PARKS and W. A. LITTLE of the Stanford University (California) discussed cooling methods by the adiabatic demagnetization of metal alloys.

A. VAN ITTERBEEK, W. VAN DAEL and G. FORREZ (Belgium) described the measurement of sound velocities in gases and liquids at 1 Mc/s frequency at various temperatures. The results were used to investigate the pressure dependence of the quotient C_p/C_v and the equation of state. A. VAN ITTERBEEK and O. VERBEKE discussed the dependence on pressure of the density of liquified gases up to pressures of 850 kg/cm^2 (H_2, O_2, N_2 and A).

The extremely interesting papers of the symposium dealt with practical problems and important results concerning the liquefaction of gases.

Z. GYULAI

V. F. NOZDREV: **The Use of Ultrasonics in Molecular Physics.** (Pergamon Press. Oxford—London—Edinburgh—New York—Paris—Frankfurt. 1965, 424 pages, £ 5 net.)

Of the wide-ranging experimental techniques of investigation into the structure of materials, acoustic methods have gained considerable ground. Significant results have been obtained in the last 15 years by subjecting matter to ultrasonic high-frequencies (10^9 c/s) and the great number of publications on this topic demands the development of a new special field: molecular acoustics.

The increasing use of molecular acoustics involving molecular physics in the interpretation of events occurring in sound space and its major stages has been marked by the following works: И. Михайлов: Распространение ультразвуковых волн в жидкостях (Гостехиздат, Москва 1949), Б. Кудрявцев: Применение ультраакустических методов в практике физико-химических исследований (Гостехиздат, Москва 1952) L. **Bergmann**: Der Ultraschall (Hirzel, Zürich, 1954) (in some of its parts); the first Russian edition of **Nozdrev**'s book (1958); K. F. **Herzfeld**, Th. A. **Litowitz**: Absorption and Dispersion of Ultrasonic Waves (Academic Press, New York—London, 1959); D. **Sette**: Dispersion and Absorption of Sound by Molecular Processes (Academic Press, New York—London, 1964). The interest of the scientific world in this special field is reflected by this list of books. The English translation of **Nozdrev**'s books is significant for making the connection between various research trends, which are often independent of each other both in the East and West. The results published in the first edition have been confirmed by recent investigations which qualify them as "classical" results in this young branch of science. One of the important advantages of the English edition is a well-compiled summary of the results obtained by Soviet scientists since the publication of the first edition. The publication of this summary as an Appendix brings the book up-to-date. It is regrettable that the restricted space (four pages) reserved for it has prevented any detailed discussion.

V. F. **Nozdrev**'s book deals with the research work carried out in the Molecular Acoustical Laboratory of the Krupski Moscow Provincial Pedagogical Institute and in the Laboratory for Molecular Physics of the University of Moscow. From among 278 publications reviewed 21 are from the Soviet literature and works of Soviet authors. From the achievements obtained in Western countries, **Nozdrev** lists only the fundamental ones, whereas **Herzfeld** and **Litowitz**'s book, published at nearly the same time almost entirely neglects any results from Eastern countries. As a result, the two books together give a comprehensive description of, and reference list to the literature of this special branch. To draw a parallel between the two books is the more interesting as **Nozdrev**'s book is devoted to experimental work and, in addition to results, also gives full details of experimental techniques. The **Herzfeld—Litowitz** book is more theoretical in character, although the lack of a comprehensive theory is also felt here, as well as in **Nozdrev**'s interpretation.

The monograph examines the mechanism of propagation of ultrasonic waves in saturated, overheated vapours of organic matters, in multi-component solutions and mixtures, in the frequency range from 2 to 150 Mc/s, temperature interval from —50° C to +600° C, under pressure varying from 0 to 400 kg/cm^2. The matter is discussed in six chapters.

1. Measurement of the velocity and absorption of ultrasonic waves in liquids and gases by optical methods;
2. Determination of the velocity and absorption of ultrasonic waves in liquids and gases by pulse techniques;
3. Propagation of ultrasonic waves in liquids;
4. Propagation of ultrasonic waves in some compounds and in their binary mixtures in the critical region;
5. Propagation of ultrasonic waves in saturated and overheated vapours of organic liquids;
6. Absorption of ultrasonic waves in organic liquids and their mixtures over a wide range of temperature, concentration and frequency.

The titles of the chapters give a good idea of the material discussed in the book. Two remarks should be added. Chapters 3 and 4 are completed with the discussion of relaxation processes and with the representation of a relationship between the phenomena of sound space and the kinetic theory of molecules. The absence of a comprehensive theory is again noticeable. Recent investigations discussed in the Appendix attempt to make up for this drawback. **Adkhamov**, in his works published in 1960—1961, gives an original direction based on **Bogoliubov**'s statistics, and a number of theoretical publications in the Soviet literature of these past years have approached the problem. Their results give an explanation of the anomaly of sound absorption in monoatomic and polyatomic gases in the critical zone.

Another remark relates to the experimental techniques discussed in Chapters 1 and 2. Owing to the detailed descriptions of experimental methods and apparatus close to the level of documentation these chapters gain a particular significance for the experimental physicist. The multiple difficulties inherent in investigations conducted through wide temperature and pressure ranges are too well-known. Useful, well-proved guidance is given in these chapters for many practical problems. Measurements in the vicinity of the critical point, the examination of the dynamic equilibrium of phases, a systematic check of the results demand a well-reasoned, purposeful experimental technique. To supply this was one of the aims of the book which it has done with unquestionable success.

The lucid discussion is completed by two Appendices, an Authors' Index and a Subject Index. The first Appendix lists the latest results, the second the characteristics of the materials examined. 22 tables give the main molecular-acoustical characteristics of aliphatic and aromatic hydrocarbons, esters, alcohols and of their aqueous and nonaqueous solutions. Including these, the book gives measurement results for more than fifty organic compounds and 17 binary mixtures, in 59 tables. 125 figures illustrate the text.

Careful presentation, the annotations of a careful Editor, the listing of the Western equivalents of Soviet tubes, testify to the high standards of the Pergamon Press.

A. Illényi

Collected Papers

of P. L. Kapitza (Vol. 1. Pergamon Press, 1964)

Professor P. L. Kapitza, Member of the Academy of Sciences of the USSR, and Fellow of the Royal Society celebrated his 70th birthday not long ago. On this occasion the 1st volume of the collected works of this great scientist was published.

The volume includes the papers and studies of Prof. Kapitza published between 1916 and 1934, written partly in Leningrad and partly in Cambridge. Originally the papers were published in Soviet, British and German periodicals. For the convenience of English speaking readers, publications first printed in an other language have been translated into English. The book includes all the figures, tables and photographs of the original publications. The papers are preceded by a short preface by D. ter Haar, and by a six-page introductory survey of Kapitza's activities.

33 papers make a volume of 503 pages. Kapitza's scientific activity covers a fairly wide range including nuclear physics, the generation of strong magnetic fields, the behaviour of matter in magnetic fields, techniques for the production of low temperatures, liquid helium, and high-energy electronics.

The first six studies of this volume deal with the Leningrad period. They cover the subjects of electron inertia, the magnetic moment of atoms, X-ray reflection on crystals, and microphotometry. The Leningrad papers are followed by other publications giving an account of investigations carried out in the Cavendish Laboratory at Cambridge University under Rutherford's guidance. The most important point here is the loss of energy of α and β rays on passing through gases. The measurement results led to another subject — strong magnetic fields. The examination of the trajectories of patricles in strong magnetic fields raised the technical problems of the generation of such fields. The generation of strong magnetic fields rendered the approach to a number of other investigations possible. The Zeeman effect could be measured and the electric properties of a number of materials in magnetic fields examined. The problems of magnetostriction, magnetic susceptibility, superconduction have been brought forward. Investigation into superconduction has led to the physics of low temperatures which are discussed in several studies dealing with the problems of the liquefaction of hydrogen and helium.

This is contained in the first volume. Physicists of today are sure to have an interest in this book which contains the collected works of a Soviet scientist of international reputation. Kapitza's scientific career reflects the development of the physical sciences witnessed by the generation of physicists who grew up after World War I.

J. Boros

J. Friedel: Dislocations

(International Series of Monographs on Solid State Physics Vol. 3. Pergamon Press, 1964. pp. XXI—491, 120s.)

Dies Buch von Friedel, der bekanntlich eine der kompetentesten Autoritäten auf diesem Gebiet ist, kann sowohl dem Studenten als auch dem auf diesem Gebiet arbeitenden Physiker wärmstens empfohlen werden. Es umfasst das Gebiet der Versetzungen in 3 Teilen. Der erste Teil gibt eine allgemeine Übersicht der Eigenschaften der Versetzungen, der zweite bringt die Versetzungs-Netzwerke, die sich in Kristallen ausbilden können und behandelt plastische Eigenschaften, der dritte Teil befasst sich mit der Wechselwirkung der Versetzungen mit anderen Kristalldefekten. Es ist leicht verständlich geschrieben und mit zahlreichen Figuren illustriert. Den Schluss bildet ein sehr ausführliches Literaturverzeichnis. Das Buch kann man geradeso wie das in 1956 erschienene französische Original Les Dislocations (Gauthier—Villars, Paris), als Standardwerk auf diesem Gebiet betrachten.

P. Gombás

INDEX

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A kézirat nyomdába érkezett: 1966. IV. 14. — Terjedelem: 9,25 (A/5) ív, 38 ábra

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TOMUS XXI FASCICULI 3–4

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Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3—4), pp. 211—217 (1966)

PRODUCTION OF ELECTRON AND POLARIZED BARYON IN THE HIGH ENERGY INTERACTION OF NEUTRINO WITH POLARIZED NUCLEON

By

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(Presented by A. Kónya — Received 20. XII. 1965)

The purpose of the paper is to calculate the cross section for the production of an electron or positron and a polarized baryon which may be a nucleon, or a hyperon, when a very high energy neutrino or antineutrino interacts with a polarized nucleon target. The general result is discussed in laboratory system of coordinates for some special cases which may facilitate the determination of the form factors associated with the various terms of weak interaction.

Introduction

In the collision of $\nu(\bar{\nu})$ with nucleons, baryons (nucleons and hyperons) and leptons are produced. The general weak interaction is of current-current type. The baryon current in general contains vector, axial vector, induced scalar and induced pseudoscalar terms with form factors associated with each of them. The structures of the form factors are dependent upon the strong interaction properties of the baryons. They are dependent upon the square of the momentum transfer between the incident neutrino and the outgoing lepton and in order to effectively study this dependence we require high energy $\nu(\bar{\nu})$ beam for the experiment. Apart from the study of angular correlation, the polarization measurements of the particles involved in the reaction provide us with additional means of determining the structure of various from factors. Lee and Yang [1] have considered the longitudinal polarisation of outgoing nucleons in the reaction $\nu + n \rightarrow l^- + p$ and $\bar{\nu} + p \rightarrow l^+ + n$ where l stands for lepton. Azimov and Shekhter [2] have discussed the case of μ^--polarization effect in the reaction $\mu^- + p \rightarrow \Lambda + \nu$. Egardt [3] has calculated the cross section for the production of polarized baryons both in a covariant form and in the laboratory system of coordinates. In a recent paper Adler [4] has evaluated the cross section for the production of polarized leptons and baryons both in a covariant form and in the centre of mass system. He has further expressed his result directly in terms of lepton (here μ meson) and baryon decay asymmetries. In the work of Egardt [3] and Adler [4] beside the scattering experiment another experiment is to be carried out involving the measurement of decay asymmetries of stopped μ mesons and baryons to analyse the polarization states of the particles produced. Now, as Adler [4] has observed, an attempt to stop a μ meson produced in a reaction in order to observe its decay may be very difficult from the experimental standpoint. In our case when we polarise the target and then observe the dependence of the reaction cross section on the polarisation of the target nucleon only no such second experiment like measurement of decay asymmetry is required. The purpose of the paper is to give a general expression for the reaction cross section, containing terms related to the polarization of nucleon and that of the baryon and the correlation effects involving both polarisations. Some examples of ν and $\bar{\nu}$ induced reactions are given below

$$\nu + n \rightarrow l^- + p\,,$$
$$\bar{\nu} + n \rightarrow l^+ + \Sigma^-\,,$$
$$\bar{\nu} + p \rightarrow l^+ + n,\quad l^+ + \Lambda,\quad l^+ + \Sigma^0\,.$$

In our investigation we consider electrons and positrons, rather than μ-mesons, because the calculation can be simplified in the former case for the very high energy production process, where the mass of the electron can be neglected in comparison with its energy.

Calculations

In the following we use the notation of Adler [4]. Let us take k_1, k_2, p_1 and p_2 to be the momentum four vectors of $\nu(\bar{\nu})$, $e^-(e^+)$, N (nucleon of mass M_1) and b (baryon of mass M_2) respectively in the reaction

$$\nu(\bar{\nu}) + N \rightarrow b + e^-(e^+)\,. \tag{1}$$

Let E, E^ν and E^e be the energies of baryon, neutrino and electron, respectively, in the laboratory system. We take s and t to be the polarization four-vectors of the proton and the baryon, respectively.

The matrix element of ν induced reaction is given by

$$M = 2^{-1/2}\bar{u}_e(k_2)\,\gamma_\lambda(1+\gamma_5)\,u_\nu(k_1)\,\bar{u}_b(p_2)\,O_\lambda\,u_N(p_1)\,, \tag{2}$$
$$O_\lambda = \gamma_\lambda(g_V + g_A\gamma_5) + i(p_1+p_2)_\lambda(f_V + f_A\gamma_5) + i(p_1-p_2)_\lambda(h_V + h_A\gamma_5)\,.$$

It may be remarked that the weak magnetism term $\dfrac{i\mu F_1}{2M}\sigma_{\mu\nu}(p_1-p_2)_\nu$ and the weak electricity term $(icF_2/M)\,\sigma_{\mu\nu}(p_1-p_2)_\nu\,\gamma_5$ are implicitly present in the general form of O_λ, since these terms containing $\sigma_{\mu\nu}$, a product of two γ matrices can be reduced to terms containing single γ matrices by using the commutation relation between γ matrices and Dirac equation. The form factors g_V, g_A, f_V and f_A are functions of the square of the momentum transfer $(p_1 - p_2)^2$ and can be determined experimentally. For a very high energy encounter we can neglect the mass of the electron in comparison with its energy and can then rewrite O_λ as

$$O_\lambda = \gamma_\lambda (g_V + g_A \gamma_5) + 2ip_{1\lambda} (f_V + f_A \gamma_5).$$

The matrix element for $\bar{\nu}$ induced reaction is similarly given by

$$M = 2^{-1/2} \bar{u}_{\bar{e}} (k_2) \gamma_\lambda (1 - \gamma_5) u_{\bar{\nu}} (k_1) \bar{u}_b (p_2) O'_\lambda u_N (p_1), \tag{3}$$

where

$$O'_\lambda = \gamma_\lambda (g_V - g_A \gamma_5) + 2ip_{1\lambda} (f_V - f_A \gamma_5).$$

Here we have taken g_A and f_A with a minus sign for convenience in writing the results of our investigation.

The expressions for the cross section of ν and $\bar{\nu}$ induced reaction involving the polarizations of the nucleon and the baryon are given by

$$d\sigma = \frac{1}{16\pi^2} \delta (p_2 + k_2 - p_1 - k_1) \frac{d_3 \bar{p}_2 \, d^3 \bar{k}_2}{E E^e E^\nu M_1} K, \tag{4}$$

where

$$K = A_1 + B(t) + C(s) + D(s,t),$$

where K is split into terms which are independent of polarizations, dependent upon polarisation s, t separately and another term involving both s and t simultaneously.

$B(t)$ is given by

$$\begin{aligned}
B(t) = {} & \pm 2M_2 (|g_V|^2 + |g_A|^2) (k_2 \cdot p_1 \, k_1 \cdot t - k_2 \cdot t k_1 \cdot p_1) \mp \\
& \mp 2M_1 (|g_V|^2 - |g_A|^2) (k_2 \cdot p_2 \, k_1 \cdot t - k_2 \cdot t p_2 \cdot k_1) \mp \\
& \mp 4M_2 \operatorname{Re} (g_V g_A^*) (p_1 \cdot k_1 \, t \cdot k_2 + p_1 \cdot k_2 \, t \cdot k_1) \pm \\
& \pm 4 \operatorname{Re} (g_A f_V^* + g_V f_A^*) \{ t \cdot p_1 (p_1 \cdot k_2 \, p_2 \cdot k_1 + p_1 \cdot k_1 \, p_2 \cdot k_2) - \\
& - p_1 \cdot p_2 (p_1 \cdot k_1 \, t \cdot k_2 + p_1 \cdot k_2 \, t \cdot k_1) \} \pm \\
& \pm 4M_1 M_2 \operatorname{Re} (g_A f_V^* - g_V f_A^*) (p_1 \cdot k_1 \, t \cdot k_2 + p_1 \cdot k_2 \, t \cdot k_1 - \\
& - t \cdot p_1 \, k_1 \cdot k_2) \mp 8M_2 \operatorname{Re} (f_V \cdot f_A^*) \, p_1 \cdot t \, (2p_1 \cdot k_1 \, p_1 \cdot k_2 + M_1^2 k_1 \cdot k_2) \\
& \mp 4 \operatorname{Re} (g_V f_V^* + g_A f_A^*) \{ t \cdot k_1 (k_2 \cdot p_2 \, p_1 \cdot p_2 + M_2 k_2 \cdot p_1) - \\
& - t \cdot k_2 (k_1 \cdot p_2 \, p_1 \cdot p_2 + M_2^2 k_1 \cdot p_1) \} + \\
& + 4_i \, \varepsilon_{\mu\nu p\sigma} t_\mu p_{1\mu} k_{1p} k_{2\sigma} \{ M_1 \operatorname{Im} (g_V g_A^*) - \operatorname{Im} (g_V f_V^* + \\
& + g_A f_A^*) \, p_1 \cdot (k_1 + k_2) - \operatorname{Im} (g_A f_V^*) (p_1 \cdot p_2 - M_1 M_2) - \\
& - \operatorname{Im} (g_V f_A^*) (p_1 \cdot p_2 + M_1 M_2) \} .
\end{aligned}$$

$C(s)$ is obtained from $B(t)$ by making the following replacements:

$$g_A \to -g_A, \quad p_1 \to p_2, \quad p_2 \to p_1, \quad M_1 \to M_2, \quad M_2 \to M_1 \quad \text{and} \quad t \to -S$$

$$\begin{aligned}
D(s,t) = {} & 4M_2 \operatorname{Re}(g_V f_V^* - g_A f_A^*) \{t \cdot p_1 (p_1 \cdot k_1\, s \cdot k_2 + p_1 \cdot k_2\, s \cdot k_1) - \\
& - s \cdot t (2p_1 \cdot k_1\, p_1 \cdot k_2 + M_1^2 k_1 \cdot k_2)\} + 4M_1 \operatorname{Re}(g_V f_V^* + \\
& + g_A f_A^*) \{s \cdot p_2 (p_2 \cdot k_1\, t \cdot k_2 + p_2 \cdot k_2\, t \cdot k_1) - \\
& - s \cdot t (2p_1 \cdot k_1\, p_1 \cdot k_2 + M_1^2 k_1 \cdot k_2)\} - \\
& - 4M_1 M_2 \operatorname{Re}(g_V g_A^*) (k_2 \cdot s\, k_1 \cdot t - k_2 \cdot t\, k_1 \cdot s) + \\
& + 4M_2 \operatorname{Re}(f_A g_V^* - f_V g_A^*) \{p_1 \cdot t (k_2 \cdot p_1\, k_1 \cdot s - k_2 \cdot s\, k_1 \cdot p_1) + \\
& + M_1^2 (k_2 \cdot t\, k_1 \cdot s - k_2 \cdot s\, k_1 \cdot t)\} - 4M_1 \operatorname{Re}(f_A g_V^* + \\
& + f_V g_A^*) \{p_1 \cdot t (k_2 \cdot p_2\, k_1 \cdot s - k_2 \cdot s\, k_1 \cdot p_2) - p_1 \cdot p_2 (k_2 \cdot t\, k_1 \cdot s - \\
& - k_2 \cdot s k_1 \cdot t)\} - 2 (|g_V|^2 - |g_A|^2) \{t \cdot p_1 (s \cdot k_1\, p_2 \cdot k_2 + \\
& + s \cdot k_2\, p_2 \cdot k_1) + s \cdot p_2 (t \cdot k_2\, p_1 \cdot k_1 + t \cdot k_1\, p_1 \cdot k_2 - t \cdot p_1\, k_1 \cdot k_2) - \\
& - p_1 \cdot p_2 (s \cdot k_1\, t \cdot k_2 + s \cdot k_2\, t \cdot k_1) - s \cdot t (2p_1 \cdot k_2\, p_1 \cdot k_1 + \\
& + M_1^2 k_1 \cdot k_2)\} - 2M_1 M_2 (|g_V|^2 + |g_A|^2) (s \cdot k_2\, t \cdot k_1 + \\
& + s \cdot k_1\, t \cdot k_2) + 4 \{(|f_V|^2 - |f_A|^2) (p_1 \cdot t\, s \cdot p_2 - p_1 \cdot p_2\, s \cdot t) + \\
& + M_1 M_2 (|f_V|^2 + |f_A|^2) s \cdot t\} (2k_2 \cdot p_1\, k_1 \cdot p_1 + M_1^2 k_1 \cdot k_2) \mp \\
& \mp 4i\varepsilon_{\mu\nu\varrho\sigma} \{M_2 \operatorname{Im}(g_V f_V^* - g_A f_A^*)\, t \cdot p_1\, s_\mu p_{1\nu} k_{2\varrho} k_{1\sigma} + \\
& + M_1 \operatorname{Im}(g_V f_V^* + g_A f_A^*)\, s \cdot p_2\, t_\mu p_{1\nu} k_{2\varrho} k_{1\sigma} + \\
& + 2\operatorname{Im}(f_V f_A^*) (2k_1 \cdot p_1\, k_2 \cdot p_1 + M_1^2 k_1 \cdot k_2)\, p_{1\mu} s_\nu p_{2\varrho} t_\sigma - \\
& - \operatorname{Im}(g_V g_A^*)(2t \cdot k_1\, s_\mu k_{2\nu} k_{i\varrho} p_{1\sigma} - 2p_1 \cdot k_2\, s_\mu p_{1\nu} k_{1\varrho} t_\sigma - \\
& - M_1^2 s_\mu k_{2\nu} k_{1\varrho} t_\sigma) - M_2 \operatorname{Im}(f_A g_V^* - f_V g_A^*)(p_1 \cdot k_2\, k_{1\mu} p_{1\nu} s_\varrho t_\sigma + \\
& + p_1 \cdot k_1\, k_{2\mu} p_{1\nu} s_\varrho t_\sigma) + M_1 \operatorname{Im}(f_A g_V^* + \\
& + f_V g_A^*) (p_2 \cdot k_2\, k_{1\mu} p_{2\nu} s_\varrho t_\sigma + p_2 \cdot k_1\, k_{2\mu} p_{2\nu} s_\varrho t_\sigma)\}.
\end{aligned}$$

Expression for A_1 is obtained from that of ADLER's [4] paper after putting lepton mass $m_1 = 0$. Upper and lower signs correspond to reactions induced by neutrino and antineutrino, respectively. $\varepsilon_{\mu\nu\varrho\sigma}$ is completely antisymmetric in its indices and $\varepsilon_{1234} = 1$. The terms involving $\varepsilon_{\mu\nu\varrho\sigma}$ all vanish if time reversal invariance holds.

We may investigate some special cases of the general expression for $d\sigma$ which may facilitate the determination of coupling constants associated with various terms of the weak interaction. First we discuss properties of $B(t)$ for some special cases (in the laboratory system) which are mostly given by

Egardt [3] also. We see that some of the properties of $B(t)$ discussed here are shared by $C(s)$ also. Next we investigate the behaviour of $B(t)$ for some hypothetical cases of pure $V - A$ and $V + A$ interactions in the laboratory system, then the same things in the centre of mass system as given by **Adler** are also stated. We discuss here the corresponding behaviour of $C(s)$ also. Lastly we consider $D(s, t)$ for the case when both s and t are perpendicular to the scattering plane. Then $B(t)$ and $C(s)$ vanish and for purely $V \pm A$ interaction (i.e. $g_V = \pm g_A$) $D(s, t)$ is non vanishing only when the weak interaction contains induced scalar and pseudoscalar terms.

For the case of forward scattering **Egardt** [3] has observed that in the expression for $B(t)$ the coefficients of $|g_V|^2$ and $|g_A|^2$ vanish in general but the coefficient of $\mathrm{Re}(g_V g_A^*)$ vanishes only when $M_1 = M_2$ and further the $\mathrm{Re}(g_V g_A^*)$ occurring in the expression for A_1 also has vanishing coefficient. In addition to these findings of **Egardt** [3] we see that the coefficient of $\mathrm{Re}(g_V f_V^* + g_A f_A^*)$ in $B(t)$ is zero for forward scattering. Actually the term proportional to $\mathrm{Re}(g_V f_V^* + g_A f_A^*)$ is absent in the result given by **Egardt** [3], which is not correct. In the case of backward scattering **Egardt** [3] has observed that all the coefficients associated with induced form factors in both A_1 and $B(t)$ vanish. He has made all these observations regarding $B(t)$ for longitudinal polarisation of baryon but it is easy to see from the expression of $B(t)$ that all the findings of **Egardt** [3] are true for any arbitrary direction of polarization of the baryon. We next find that all the above mentioned properties of $B(t)$ except the following one are true for $C(s)$ also, in forward scattering the coefficient of $\mathrm{Re}(g_V g_A^*)$ occurring in the expression for $C(s)$ is not zero even for $M_1 = M_2$. In the limiting case of backward scattering we can determine g_V and g_A without knowing the values of f_V and f_A.

Adler [4] has investigated the behaviour of $B(t)$ in the centre of mass system for the hypothetical case when $f_V = f_A = 0$, the mass of the lepton is zero and g_V, g_A are real. Let us study the properties of $B(t)$ under the same sort of assumptions but in the laboratory system of coordinates. In this case we have

$$\begin{aligned} B(t) = &\mp 2M_2 (g_V + g_A)^2 k_2 \cdot t\, k_1 \cdot p_1 \pm 2M_2 (g_V - g_A)^2 k_2 \cdot p_1\, t \cdot k_1 \\ &\mp 2M_1 (g_V^2 - g_A^2)(k_2 \cdot p_2 \cdot k_1 \cdot t - k_2 \cdot t\, p_2 \cdot k_1). \end{aligned} \tag{5}$$

For $g_V = g_A$ we find that the effect of $B(t)$ in the case of forward and backward scattering is maximum when the baryon is longitudinally polarized, whereas in the centre of mass system the effect of $B(t)$ for all scattering angles is maximum when the baryon is longitudinally polarized. For $g_V = -g_A$ we find that the effect of $B(t)$ in the case of forward and backward scattering is maximum when the baryon is longitudinally polarised. This result holds good for both centre of mass and laboratory system of coordinates.

For $g_V = -g_A$, $M_1 = M_2$ and in laboratory system of coordinates

$$B(t) = \pm 2M_2 (g_V - g_A)^2 k_2 \cdot p_1 \, t \cdot k_1 =$$

$$= \mp 2M_1^2 E^e (g_V - g_A)^2 \left\{ \frac{\bar{\zeta} \cdot \bar{p}_2}{E + M_1} M_1 \left(1 - \frac{E^\nu}{M_1 + 2E^\nu \sin^2 \theta/2} \right) + \bar{\zeta}_\perp \cdot \bar{k}_1, \right\} \tag{6}$$

where we have put

$$t = \bar{\zeta} + \frac{\bar{\zeta} \cdot \bar{p}_2 \, \bar{p}_2}{M_2 (E + M_2)}, \qquad \frac{i \bar{\zeta} \cdot \bar{p}_2}{M_2}$$

and $\bar{\zeta}_\perp$ is the component of $\bar{\zeta}$ orthogonal to $\bar{p}_2$. We see from equ. (6) that, for the scattering angle between the incident neutrino and outgoing electron in the laboratory system given by $\theta = \cos^{-1} \dfrac{M_1}{E^\nu}$, the effect of $B(t)$ is maximum when the baryon is transversely polarized. In the center of mass system ADLER [4] has noted that for $g_V = -g_A$ the baryon is 100% transversely polarized at $\theta_\perp = 2 \operatorname{tg}^{-1} W/M_2$, where W is the centre of mass energy and $\theta_\perp$ is the centre of mass scattering angle between the incident neutrino and outgoing lepton.

Similarly for the hypothetical case $f_V = f_A = 0$, $C(s)$ is given by

$$C(s) = \pm 2M_1 (g_V - g_A)^2 k_2 \cdot s \, k_1 \cdot p_2 \mp 2M_1 (g_V + g_A)^2 k_2 \cdot p_2 \, s \cdot k_1$$
$$\pm 2M_2 (g_V^2 - g_A^2)(k_2 \cdot p_1 \, k_1 \cdot s - k_2 \cdot s \, p_1 \cdot k_1). \tag{7}$$

We see that for pure $V - A$ interaction i.e. $g_V = +g_A$ the effect of $C(s)$ is maximum when the polarization of the nucleon is parallel to the neutrino momentum and for pure $V + A$ interaction i.e. $g_V = -g_A$ the effect of $C(s)$ is maximum when polarisation of the nucleon is parallel to the electron momentum.

Finally we consider under assumption of time reversal invariance, the expression for $D(s, t)$ which gives the correlation effects involving polarizations of both the nucleon and the baryon. In $D(s, t)$ the coefficients of $Re(g_V f_V^*)$, $\mathrm{Re}(g_A f_A^*)$, $|f_V|^2$ and $|f_A|^2$ vanish in the case of backward scattering. The coefficient of $\mathrm{Re}(g_V g_A^*)$ reduces to zero in the case of forward scattering. The coefficients of $\mathrm{Re}(f_A g_V^*)$ and $\mathrm{Re}(f_V g_A^*)$ are zero for both forward and backward scattering. When s and t are both normal to the scattering plane, we have in the laboratory system

$$d\sigma = A_1 - 4s \cdot t \, (2p_1 \cdot k_1 \, p_1 \cdot k_2 + M_1^2 \, k_1 \cdot k_2) \mathrm{Re} \left\{ g_V f_V^* (M_1 + M_2) + \right.$$
$$\left. + g_A f_A^* (M_1 - M_2) + \frac{g_A^2 - g_V^2}{2} - M_1 (E_1 + E_2) f_V^2 + M_1 (E - M_2) \, f_A^2 \right\} =$$
$$= A_1 - 8 \, s \cdot t \, M_1^2 E^\nu \left(E^\nu - \frac{M_2^2 - M_1^2}{2M_1} \right)$$

$$\left\{1-\left(1+\frac{M_1}{2E^{\nu}}\right)\frac{2E^{\nu}\sin^2\theta/2}{M_1+2E^{\nu}\sin^2\theta/2}\right\}\times \operatorname{Re}\Big\{g_V f_V^*(M_1+M_2)+$$

$$+\ g_A f_A^*(M_1-M_2)+\frac{g_A^2-g_V^2}{2}-M_1(E+M_2)f_V^2+M_1(E-M_2)f_A^2\Big\}. \qquad (8)$$

We see that when $g_V = \mp g_A$ (pure $V \pm A$ interaction) the polarization-dependent term exists only when induced scalar and pseudoscalar terms are present, i.e., when both s and t are directed normal to the scattering plane we get the polarisation effect if at least any one of the conditions $|g_V| \neq |g_A|$, $f_V \neq 0$ and $f_A \neq 0$ is satisfied. The effect of the polarization-dependent term in equ. (8) is maximum when $\theta = 0$ and minimum when $\theta = \pi$.

Acknowledgement

The author wishes to thank Prof. D. Basu and Dr. N. C. Sil for stimulating discussion during the progress of the work.

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ОБРАЗОВАНИЕ ЭЛЕКТРОНА И ПОЛЯРИЗОВАННОГО БАРИОНА ВО ВЫСОКОЭНЕРГЕТИЧЕСКОМ ВЗАИМОДЕЙСТВИИ НЕЙТРИНО С ПОЛЯРИЗОВАННЫМ НУКЛОНОМ

Ш. ШАРКАР

Резюме

Целью настоящей работы является определение сечения образования электрона или позитрона и поляризованного бариона, являющегося или нуклоном, или гипероном, в случае, когда нейтрино или антинейтрино очень высокой энергии взаимодействует с поляризованной нуклонной мишенью. Общий результат дискутируется в лабораторной системе координат для нескольких специальных случаев, облегчающих определение формфакторов, связанных с различными условиями слабых взаимодействий.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3—4), pp. 219—227 (1966)

FORMALE ENTKOPPLUNG DES *S*-OPERATORS DER QUANTEN-ELEKTRODYNAMIK

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(Vorgelegt von A. Kónya — Eingegangen: 21. XII. 1965)

Die bekannte geschlossene Darstellung für das erzeugende Funktional der Ausbreitungsfunktionen als formale Lösung der Schwingerschen Funktional-Differentialgleichungen wird ohne Verwendung der Störungstheorie einfach durch eine formale Entkopplung des *S*-Operators gewonnen.

Einleitung

Wegen der bekannten Mängel der Störungsrechnung besteht allgemein der Wunsch, für relativistische und nichtrelativistische Vielteilchenprobleme Lösungen und Formulierungen zu finden, die nicht auf der Entwickelbarkeit nach der Kopplungskonstanten beruhen. Einen Weg in dieser Richtung bietet die Anwendung funktionaler Methoden. So hat Schwinger [1] die Ausbreitungsfunktionen, in denen praktisch alle Informationen eines Vielteilchensystems enthalten sind, zu einem erzeugenden Funktional vorgegebener Quellen zusammengefasst und dessen Bestimmungsgleichungen untersucht. Diese Funktional-Differentialgleichungen können ohne jede Störungstheorie durch geeignete Ansätze formal gelöst werden [2]. Das Ergebnis ist eine geschlossene Darstellung des erzeugenden Funktionals. Die entsprechende geschlossene Darstellung für den *S*-Operator selbst, aus dem das erzeugende Funktional durch Bildung des Vakuum-Erwartungswertes hervorgeht, wurde bereits von Nambu, Yamazaki und Katayama [3, 4] durch Anwendung des Wickschen Theorems, das später von Hori, Anderson und Matsubara [4, 5] kompakt formuliert wurde, und durch formale Aufsummierung von Graphen gewonnen. Im folgenden wird gezeigt, wie sich durch eine formale Entkopplung des *S*-Operators, die, sinngemäss angewendet, auch für nichtrelativistische Vielteilchensysteme nützlich ist [6], die formale Lösung der erwähnten Funktional-Differentialgleichungen etwas vereinfachen lässt.

1. Einführung der Informationsgrösse

Da die in dem erzeugenden Funktional

$$G(\bar{\eta},\eta,j) = \ll T e^{-\frac{i}{\hbar}\left(\bar{\eta}\psi+\bar{\psi}\eta+\frac{j}{c}A\right)} \gg \tag{1}$$

enthaltenen Feldoperatoren $\varphi = \overline{\psi}, \psi, A$ die üblichen Vertauschungseigenschaften besitzen und auch den Bewegungsgleichungen der Quantenelektrodynamik [7]

$$(p - mc - eA^c - eA)\,\psi = 0\,, \quad \Box A_\nu - \mu_0\, c\overline{\psi}\, e\gamma_\nu\, \psi = 0 \tag{2}$$

genügen, erfüllt G bekanntlich die äusserlich ähnlichen Funktional-Differentialgleichungen [1]

$$(p - mc - eA^c - e\tilde{A})\,\widetilde{\psi}\, G = \eta G \qquad (\Box \tilde{A}_\nu - \mu_0\, c\widetilde{\overline{\psi}}\, e\gamma_\nu\, \widetilde{\psi})\, G = \mu_0\, j_\nu\, G \tag{3}$$

mit

$$\widetilde{\psi} \equiv -\frac{\hbar}{i}\,\frac{\delta}{\delta\overline{\eta}}\,, \quad \widetilde{\overline{\psi}} \equiv \frac{\hbar}{i}\,\frac{\delta}{\delta\eta}\,, \quad \tilde{A}_\nu \equiv -\frac{\hbar}{i}\,\frac{\delta}{\delta j^\nu/c} \tag{4}$$

als Funktional-Differentialoperatoren. Dabei wird in (1) und im folgenden in Analogie zur Einsteinschen Summenregel die abkürzende Schreibung

$$\begin{aligned}
\overline{\eta}\,\psi &\equiv \int dx \sum_a \overline{\eta}_a(x)\, \psi_a(x)\,,\\
jA &\equiv \int dx \sum_\nu j^\nu(x)\, A_\nu(x),\\
\overline{\psi} A\psi &\equiv \int dx \sum_{a,b} \sum_\nu \overline{\psi}_a(x)\, \gamma^\nu_{ab}\, A_\nu(x)\, \psi_b(x),\\
A\psi &= \sum_b \sum_\nu \gamma^\nu_{ab}\, A_\nu(x)\, \psi_b(x)
\end{aligned} \tag{5}$$

mit $dx = cdtd\mathfrak{r}$ benutzt; bei Verknüpfung von Spinor- und Vierergrössen, wie in $A\,\psi$ und $\overline{\psi}\, A\, \psi$, sollen die auftretenden Diracschen Matrizen $\gamma^\nu_{\alpha b}$ in den Summationsvorschriften enthalten sein. Weiter bedeutet », « in (1) das polarisierbare Vakuum des Gesamtsystems (2). A^c bedeutet ein klassisches äusseres Feld. T ist der Wicksche Zeitordnungsoperator [4]. Aus (1) geht hervor, dass G die Vakuum-Erwartung «S» des S-Operators eines durch die Quellen $\overline{\eta}, \eta, j$ »gestörten« Systems darstellt. Übrigens ist dieses um die Quellen erweiterte System nur dann in sich widerspruchsfrei, wenn von den Spinorquellen $\overline{\eta}, \eta$ Plus-Vertauschbarkeit mit sich, miteinander und mit $\overline{\psi}, \psi$ und weiter die Ladungserhaltung für die Photonenquellen j verlangt wird, wobei auch die Differentialoperatoren (4) die entsprechenden Vertauschungseigenschaften übernehmen. Schliesslich werden die Differentialgleichungen (3) noch durch die Randbedingungen $G\,(0, 0, 0,) = 1$ und $\widetilde{\varphi} G =$ «φ S» bzw. «S φ» für t + bzw. $-\infty$ ergänzt.

Mit dem von Gell-Mann und Low [7] angegebenen Theorem über die quasistatische Einschaltung der Wechselwirkung kann die Erzeugende (1) in die Form

$$G(\overline{\eta}, \eta, j) = \frac{< Te^{-\frac{i}{\hbar}\left(\overline{\eta}\psi + \overline{\psi}\eta + \frac{j}{c}A + \overline{\psi}e(A+A^c)\psi\right)} >}{< Te^{-\frac{i}{\hbar}\overline{\psi}e(A+A^c)\psi} >} \equiv \frac{U(\overline{\eta}, \eta, j)}{U(0, 0, 0)} \tag{6}$$

gebracht werden. Da hier in (6) und im folgenden die Feldoperatoren $\varphi = \overline{\psi}, \psi, A$ nicht mehr (2), sondern nur noch den »ungestörten« Bewegungsgleichungen

$$(p - mc)\,\psi = 0, \qquad \Box A_\nu = 0 \tag{7}$$

genügen, erfüllt (6) auch (3), so dass man (6) auch ohne Rücksicht auf das erwähnte Theorem als Ansatz für (3) auffassen kann. In (6) bedeutet $>, <$ das »nackte« Vakuum des ungestörten Systems (7). In (6) ist eine Grösse U eingeführt, die hier Informationsgrösse genannt werden soll, weil sie alle möglichen Informationen über das System (2) kompakt zusammenfasst. U stellt die Vakuum-Erwartung eines S-Operators dar, bei dem nicht nur die Quellen, sondern auch das äussere Feld A^c sowie die eigentliche Kopplung der Felder als »Störung« betrachtet wird.

2. Formale Entkopplung des S-Operators

Mit der Volterra-Entwicklung

$$f(\varphi + u) = e^{u\frac{\delta}{\delta\varphi}} f(\varphi) \tag{1}$$

lässt sich nun der in (1.6) enthaltene S-Operator formal entkoppeln [13]

$$\boxed{Te^{-\frac{1}{\hbar}\overline{\psi}e(A+A^c)\psi} = Te^{A\frac{\delta}{\delta A^c}}\; Te^{-\frac{i}{\hbar}\overline{\psi}eA^c\psi}} \tag{2}$$

Hierbei wird die Anwendung von (1) unter dem T-Operator dadurch ermöglicht, dass das Photonenfeld A mit dem Elektron/Positron-Feld $\overline{\psi}, \psi$ vertauschbar ist, und daher T lediglich voneinander unabhängig die Zeitordnung der Photonenoperatoren A und der Elektron/Positron-Operatoren $\overline{\psi}$, ψ untereinander verlangt. Damit wird auch die Informationsgrösse U formal entkoppelt

$$\boxed{\begin{aligned} U(\overline{\eta}, \eta, j) &\equiv < Te^{-\frac{i}{\hbar}\left(\overline{\eta}\psi + \overline{\psi}\eta + \frac{j}{c}A + \overline{\psi}e(A+A^c)\psi\right)} > \\ &= < Te^{\left(-\frac{i}{\hbar}\frac{j}{c} + \frac{\delta}{\delta A^c}\right)A} > < Te^{-\frac{i}{\hbar}(\overline{\eta}\psi + \overline{\psi}eA\psi)} > \\ &\equiv U_{ph}\left(j, \frac{\delta}{\delta A^c}\right) U_{ep}(\overline{\psi}, \psi, A^c)\,. \end{aligned}} \tag{3}$$

Die nach dem zweiten Gleichheitszeichen vorgenommene Zerlegung der Vakuum-Erwartung in ein Produkt von Erwartungswerten stützt sich auf die Separierbarkeit des ungestörten Systems (1.7). Während der erste Faktor U die Photonen-Erzeugung durch äussere Ströme beschreibt, gibt der zweite Faktor U die Elektron/Positron-Bewegung im äusseren Feld an. Nachdem diese beiden jeweils rückwirkungsfreien, halbklassischen Grenzfälle gelöst sind, wird die vollständige Kopplung zwischen beiden Feldern durch den Differentialoperator

$$\frac{j^c}{c} = -\frac{\hbar}{i}\frac{\delta}{\delta A^c} \tag{4}$$

schliesslich wieder hergestellt.

Dass die Quellen j, j^c einerseits und $\overline{\eta}, \eta, A^c$ andererseits im Photonen- bzw. Elektron/Positron-Anteil so verschieden auftreten, hängt mit dem Verschwinden der Photonen-Ruhemasse zusammen. So gibt es zwar für Elektronen und Positronen neben der Möglichkeit, Teilchen zur erzeugen und zu vernichten (dies wird durch die Spinorquellen $\overline{\eta}, \eta$ als »Kathode und Anode« besorgt), auch noch die Möglichkeit, den Bewegungszustand der Teilchen zu ändern (dies wird durch das äussere Feld A^c sozusagen als Quelle der kinetischen Energie bewirkt), während sich für die Photonen mit ihren primitiveren Eigenschaften die gesamte Dynamik im Erzeugen und Vernichten erschöpft. Aus diesem Grunde unterscheiden sich zwar die Quellen $\overline{\eta}, \eta$ von A^c, wogegen es keinen Unterschied zwischen j und j^c gibt, weswegen sie in der Form $j + j^c$ auftreten.

Im folgenden werden U_{ph} und U_{ep} durch Lösung der sie bestimmenden Differentialgleichungen gewonnen.

3. Photonen-Erzeugung durch äussere Ströme

Da der in

$$\boxed{U_{ph}(j) = < T e^{-\frac{i}{\hbar}\frac{j}{c}A} >} \tag{1}$$

enthaltene Operator A gemäss (1.7) die MAXWELLschen Gleichungen $\Box A = 0$ befriedigt, genügt U_{ph}, wie in (1.2), der entsprechenden Funktional-Differentialgleichung

$$\Box \tilde{A}\, U_{ph} = \mu_0 j U_{ph} \qquad U_{ph}(0) = 1\,, \tag{2}$$

die mit der Photonen-Ausbreitungsfunktion

$$D_{12} = ((\Box + \varkappa^2)^{-1})_{12} = -\frac{i}{\hbar}\frac{1}{\mu_0 c} < T A_1 A_2 > \qquad \begin{matrix} \operatorname{Re} \varkappa \to 0 \\ \operatorname{Im} \varkappa \underset{\to}{\leq} 0 \end{matrix} \tag{3}$$

in Übereinstimmung mit [3, 4, 9], sofort durch

$$\boxed{U_{ph}(j) = e^{-\frac{i}{\hbar}\frac{\mu_0}{2c} jDj}} \tag{4}$$

gelöst wird.

4. Elektron/Positron-Bewegung im äusseren Feld A^c

Da die in

$$U_{ep}(\overline{\eta}, \eta) = <Te^{-\frac{i}{\hbar}(\eta\psi + \overline{\psi}\eta + \overline{\psi} e A^c \psi)}> \tag{1}$$

enthaltenen Operatoren $\overline{\psi}$, ψ gemäss (1.7) die Diracsche Gleichung $(p - mc)\psi = 0$ erfüllen, genügt U_{ep} wie in (1.2) der entsprechenden Funktional-Differentialgleichung

$$\begin{gathered}(p - mc - eA^c)\,\widetilde{\psi}\,U_{ep} = \eta U_{ep},\\ (U_{ep})_0 = U_{ep}(0,0) = <Te^{-\frac{i}{\hbar}\overline{\psi} e A^c \psi}>,\end{gathered} \tag{2}$$

die mit der Elektron/Positron-Ausbreitungsfunktion

$$\begin{aligned}&S_{12}(A^c) = ((p - mc - eA^c)^{-1})_{12} =\\ &= -\frac{i}{\hbar} <T\psi_1\,\overline{\psi}_2\,e^{-\frac{i}{\hbar}\overline{\psi} e A^c \psi}> <Te^{-\frac{i}{\hbar}\overline{\psi} e A^c \psi}>^{-1}\end{aligned} \tag{3}$$

durch

$$U_{ep} = (U_{ep})_0\, e^{-\frac{i}{\hbar}\overline{\eta} S(A^c)\eta} \tag{4}$$

gelöst wird. Der nur noch vom äusseren Feld A^c abhängige Faktor $(U_{ep})_0$ genügt einer einfachen Differentialgleichung bezüglich der Kopplungskonstanten e

$$\begin{aligned}&e\frac{\partial}{\partial e}(U_{ep})_0 = -\frac{i}{\hbar} <T\overline{\psi}\,eA^c\,\psi e^{-\frac{i}{\hbar}\overline{\psi} e A^c \psi}> =\\ &= -eA^c\left(-\frac{i}{\hbar}\right) <T\psi\,\overline{\psi}\,e^{-\frac{i}{\hbar}\overline{\psi} e A^c \psi}> = -eA^c S(A^c)(U_{ep}),\end{aligned} \tag{5}$$

die durch

$$(U_{ep})_0 = e^{-F(A^c)}\quad F(A^c) = \int_0^e de\, A^c\, S(A^c) \tag{6}$$

gelöst wird. Zusammenfassend lautet (4) und (6) in Übereinstimmung mit [3, 4, 10]

$$\boxed{U_{ep}(\bar{\eta}, \eta) = e^{-\int_0^e de A^c S(A^c) + \left(-\frac{i}{\hbar}\right) \bar{\eta} S(A^c) \eta} .} \tag{7}$$

Übrigens kann der Vakuumanteil $F(A^c)$ bei Gültigkeit der Reihenentwicklung

$$S(A^c) = S^0 + S^0 e A^c S^0 + S^0 e A^c S^0 e A^c S^0 + \dots \tag{8}$$

mit $S^0 = S(0)$ auch in die bekannte Form der zu (3) gehörigen **Fredholm**-Determinante

$$\begin{aligned} F(A^c) = S^0 e A^c + \frac{1}{2} S^0 e A^c S^0 e A^c + \dots = - Sp\, ln\, (1 - S^0 e A^c) \\ = - ln \, \| 1 - S^0 e A^c \| \end{aligned} \tag{9}$$

gebracht werden.

5. Kopplung der Felder

Mit (2.3), (3.4), (4.7) entsteht schliesslich für U der bekannte Ausdruck

$$\boxed{U(\bar{\eta}, \eta, j) = e^{-\frac{i}{\hbar} \frac{\mu_0}{2c} (j + j^c) D (j + j^c)} \; e^{-\frac{i}{\hbar} \bar{\eta} S(A^c) \eta - \int_0^e de A^c S(A^c)}} \tag{1}$$

der mit (2.4) sowie mit der Produktregel der Differentialrechnung auch in der Form

$$U(\bar{\eta}, \eta, j) = e^{-\frac{i}{\hbar} \frac{\mu_0}{2c} j D j} \; e^{-\frac{i}{\hbar} \frac{\mu_0}{2c} j^c D j^c} \; e^{-\frac{i}{\hbar} \bar{\eta} S(A^c) \eta - \int_0^e de A^c S(A^c)} \Big|_{A^c \to A^c + \mu_0 j D} \tag{2}$$

geschrieben werden kann. Statt (2.2) hätte natürlich auch die Entkopplung

$$T e^{-\frac{i}{\hbar} \left(\frac{j}{c} - e \psi \bar{\psi} \right) A} = \left(T e^{-e \psi \bar{\psi} \frac{\delta}{\delta j^c / c}} \right) \left(T e^{-\frac{i}{\hbar} \frac{j^c}{c} A} \right) \tag{3}$$

in (1.6) praktisch dasselbe Ergebnis (1) oder (2) geliefert, doch hätten dann j^c und A^c ihre Rollen als Differentialoperator (2.4) und Funktion vertauscht.

Setzt man die Gültigkeit der Störungsrechnung voraus, lassen sich die in (1) verlangten Differentiationen sukzessive ausführen, und in Verbindung mit kombinatorischen Betrachtungen entsteht für U wie in [10] die Exponentialform $U = \exp \Gamma$ mit Γ als der Summe aller Verbundgraphen. In diesem bislang nur auf störungstheoretischem Wege zu gewinnenden, aber sicher grundsätzlichere Bedeutung besitzenden Funktional $\Gamma(\bar{\eta}, \eta, j)$ sind nun alle

Informationen über (1.2) enthalten. So stellen die Koeffizienten-Funktionen der Volterra-Entwicklung von Γ nach Potenzen der Quellen $\bar{\eta}, \eta, j$ die nichtfaktorisierbaren und daher die Korrelationen beschreibenden Anteile der Ausbreitungsfunktionen dar. Weiterhin gibt $\Gamma_0 = \Gamma(0, 0, 0)$ nach dem GELL-MANN/LOW-Theorem [7] gemäss $\Delta E = (-\hbar/i)\,\Gamma_0 \tau$ die Energieverschiebung ΔE gebundener Zustände an, sofern man in (1.6) statt der Vakuum-Erwartung die entsprechenden Erwartungswerte betrachtet.

Übrigens stellt sich heraus, dass die Begriffe Informationsgrösse U und Energie/Korrelationsfunktional Γ auch in nichtrelativistische sowie in thermodynamische Vielteilchensysteme zwanglos eingeführt werden können, womit sich eventuell ein einheitliches Begriffssystem für beliebige Vielteilchensysteme andeutet.

Herrn Prof. Dr. W. MACKE danke ich für die Unterstützung der Arbeit und wertvolle Anregungen zum Thema.

Anhang

I. Zum Aufstellen der Bewegungsgleichungen (1.3)

Zum Aufschreiben der funktionalen Bewegungsgleichungen (1.3) für $G = «S»$ wird die Beziehung

$$\frac{d}{dt} S\varphi_t = \frac{d}{dt}\, T e^{-\frac{i}{\hbar}\int_t dt'W'} \varphi_t\, e^{-\frac{i}{\hbar}\int^t dt'W'} =$$

$$= T e^{-\frac{i}{\hbar}\int_t dt'W'} ([W, \varphi] + \dot{\varphi})_t\, e^{-\frac{i}{\hbar}\int^t dt'W'} = S([W, \varphi] + \dot{\varphi})_t$$

benötigt. Dabei soll der in S enthaltene Zeitordnungsoperator auch auf die rechts neben S stehenden Feldoperatoren $\varphi = \bar{\psi}, \psi, A$ wirken.

II. Direkte Lösung der Bewegungsgleichungen (1.3)

Die formale Lösung (5.1) entsteht auch aus den funktionalen Bewegungsgleichungen (1.3) für G bzw. U durch den Ansatz

$$U(\bar{\eta}, \eta, j) = e^{-\frac{i}{\hbar}\frac{\mu_0}{2c}(j+j^c)D(j+j^c)} H(\bar{\eta}, \eta, A^c). \tag{1}$$

Mit

$$e^{\frac{i}{\hbar}\frac{\mu_0}{2c}(j+j^c)D(j+j^c)} (\tilde{A} + A^c)\, e^{-\frac{i}{\hbar}\frac{\mu_0}{2c}(j+j^c)D(j+j^c)} = A^c \tag{2}$$

wird aus der DIRACschen Gleichung (1.3)

$$(p - mc - eA^c)\, \widetilde{\psi}\, H = \eta\, H, \tag{3}$$

während die MAXWELLsche Gleichung (13) in

$$A^c \frac{\delta}{\delta A^c} H = \frac{\hbar}{i} \frac{\delta}{\delta \eta}\, e A^c \frac{\delta}{\delta \overline{\eta}} H \tag{4}$$

übergeht. Da e und A^c in den Bestimmungsgleichungen (2) und (4) nur in der Kombination eA^c vorkommen, gilt bei Anwendung auf H die Beziehung $e\partial/\partial e = A\,\delta/\delta\, A$, so dass (4) auch durch

$$e \frac{\partial}{\partial e} H = \frac{\hbar}{i} \frac{\delta}{\delta \eta}\, e A^c \frac{\delta}{\delta \overline{\eta}} H \tag{5}$$

ersetzt werden kann. Der Ansatz

$$H = e^{-F(A^c) - \frac{i}{\hbar} \overline{\eta} S(A^c) \eta} \tag{6}$$

löst (3) und überführt (5) in

$$e \frac{\partial}{\partial e} F(A^c) = eA^c S(A^c), \qquad e \frac{\partial}{\partial e} S(A^c) = S(A^c) eA^c S(A^c). \tag{7}$$

Die erste Gleichung liefert die den Virial-Theoremen nichtrelativistischer Theorien [12] entsprechende Beziehung (4.6), während die zweite Gleichung lediglich eine aus (4.3) folgende Identität darstellt. Mit (1) und (6) entsteht dann wieder (5.1).

III. Beweis der formalen Entkopplung über die Bewegungsgleichung für S

Die Richtigkeit der Entkopplung (2.2) folgt auch aus den Bewegungsgleichungen. Einerseits genügt

$$S(t, t') = T e^{-\frac{i}{\hbar} \int_{t'}^{t} dt_1 (\overline{\psi} e (A + A^c) \psi)_{t_1}} \tag{1}$$

der Differentialgleichung

$$-\frac{\hbar}{i} \frac{\partial}{\partial t} S = (\overline{\psi} e (A + A^c)\, \psi)_t\, S\,, \tag{2}$$

andererseits erfüllt

$$S(t,t') = (T e^{\int_{t'}^{t} dt_1 \left(A \frac{\delta}{\delta A^c}\right)_{t_1}})(T e^{-\frac{i}{\hbar} \int_{t'-\delta}^{t+\delta} ct_1 (\overline{\psi} e A^c \psi)_{t_1}}) \tag{3}$$

dieselbe Differentialgleichung

$$-\frac{\hbar}{i}\frac{\partial}{\partial t} S = -\frac{\hbar}{i}\left(A \frac{\delta}{\delta A^c}\right)_t S + (T e^{\int_{t'}^{t} dt_1 \left(A \frac{\delta}{\delta A^c}\right)_{t_1}})(\overline{\psi} e \; A^c \psi)_{t+\delta} \cdot$$

$$\cdot (T e^{-\frac{i}{\hbar} \int_{t'-\delta}^{t+\delta} dt_1 \; (\overline{\psi} e A^c \psi)_{t_1}}) = (\overline{\psi}\, e\, (A + A^c)\, \psi)_t\, S.$$

Da die Ausdrücke (1) und (3) dieselben Differentialgleichungen und Anfangsbedingungen befriedigen, müssen sie identisch sein, q. e. d. In (1) bis (4) erstreckt sich die Schreibung (1.5) ausnahmsweise nur auf die Orte sowie auf die Spinor- und Viererindices, nicht dagegen auf die Zeiten.

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ФОРМАЛЬНОЕ РАЗЪЕДИНЕНИЕ S-ОПЕРАТОРА КВАНТОВОЙ ЭЛЕКТРОДИНАМИКИ

П. ЦИШЕ

Резюме

Выводится известное закрытое представление для функционала функции распространения как формальное решение функционально-дифференциального уравнения Швингера без применения теории возмущений путем формального разъединения S-оператора.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3—4), pp. 229—233 (1966)

INVESTIGATION OF $Rh^{103}(n, He^3)\,Tc^{101}$ REACTION

By

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(Presented by A. Szalay. — Received 20. I. 1966)

The cross-section of the $Rh^{103}(n, He^3)\,Tc^{101}$ reaction was determined at 14.7 MeV neutron energy by the activation method. $\sigma(n, He^3) = (1{,}2 \pm {}^{1,0}_{0,6})\,\mu$b value was observed. The cross-section ratio of the (n, He^3) and (n, α) reactions for nucleus Rh^{103} was calculated on the basis of the statistical model. The comparison of the values of the measured ratio and that calculated shows that the relatively high yield of the n, He^3 reaction cannot be explained on the basis of the statistical model.

Introduction

In our earlier investigations the existence of the (n, He^3) reaction was verified at Cs^{133} nucleus by activation method. For the cross-section of the reaction $(5 \pm 3)\,\mu$b value was found at 14,7 MeV neutron energy [1]. The present work was undertaken with the aim of obtaining additional information on the (n, He^3) reaction. For this investigation Rh^{103} nucleus has rather favourable properties [2]. In the case of Rh^{103} there is no need for radiochemical separation because of the suitable half lives of the reaction products. The half life of the required Tc^{101} isotope is 14 min., 91,5% of the decays is followed by the emission of 307 keV energy gamma quanta rendering the use of a gamma-spectrometer possible. To determine the cross-section the $Rh^{103}(n, \gamma)\,Rh^{104m}$ reaction can be used as internal monitor.

Experimental method and results

5g rhodium metal in polyethylene holder was irradiated with 14,7 MeV neutrons produced by the $H^3(d, n)\,He^4$ reaction using the 300 kV neutron generator of ATOMKI [3]. The sample was irradiated with an average flux of $\sim 5.10^9$ neutron $\cdot$ cm^{-2} $\cdot$ sec^{-1} for 25 min. During the irradiation the flux was continuously monitored by a $B^{10}F_3$ "long-counter". The activity of the irradiated sample was measured with a scintillation gamma-spectrometer [4], consisting of 5×5 cm NaI(Tl) crystal and 400-channel TMC pulse height analyzer. The 0—1 MeV energy interval of the gamma spectrum as a function of time was measured. Analysing the decay curve obtained in 270—340 keV interval (Fig. 1) the half lives of 210 d, 15,5 min. and 4,5 min. were found. The activity of 15,5 min. half life could not be distinguished from the background in other regions of the gamma spectrum. The gamma activity of 15,5 ± 1,5 min. half life observed at ~300 KeV verifies the existence of $Rh^{103}(n, He^3)\,Tc^{101}$ reaction. The activities of 210 d and 4,5 min half lives belong to $Rh^{103}(n, 2n)\,Rh^{102}$ and $Rh^{103}(n, \gamma)\,Rh^{104m}$ reactions, respectively. For the determination of the cross-section $Rh^{103}(n, \gamma)\,Rh^{104m}$ reaction was used as internal monitor. Rh^{104m} with 4,5 min half life decays into the ground state of Rh^{104}. In 1,8% of Rh^{104} decays a 556 keV gamma particle is emitted that can be used as internal monitor. The gamma spectrometer was calibrated by Na^{22}, Mn^{54}, Co^{60}, Co^{57}, Y^{88}, Cs^{137}, Hg^{203}, Am^{241} (IAEA Vienna) absolute standard sources.

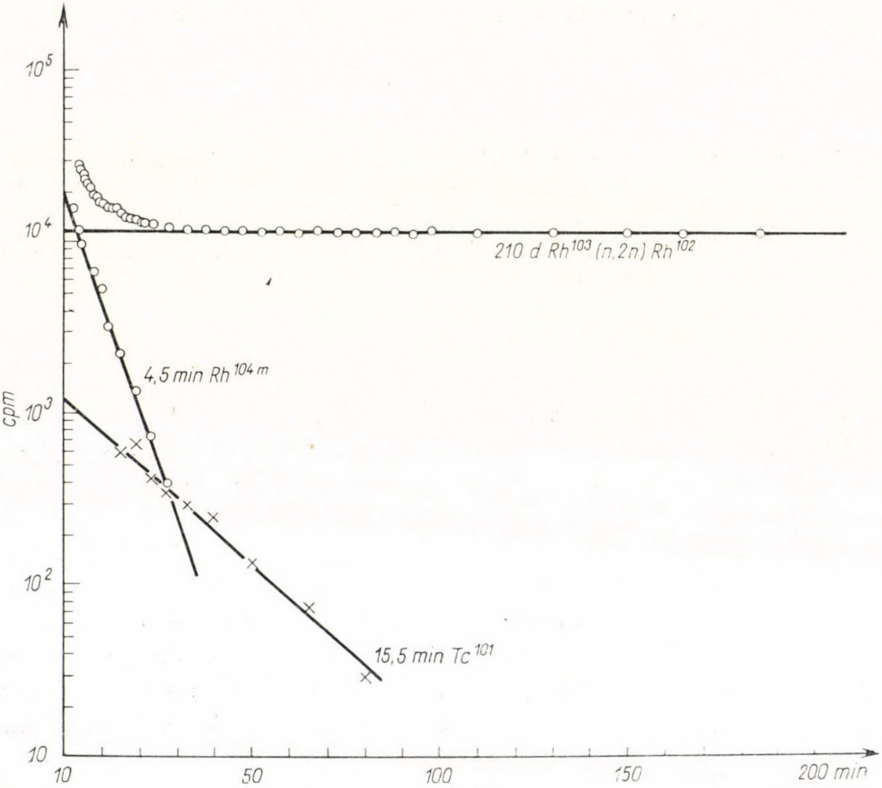

Fig. 1. The analysed complex decay curve

If we take into consideration the necessary corrections to be made for the irradiation and the activity measurements for the cross-section ratio we obtain:

$$\frac{\sigma[Rh^{103}/n,\ He^3/Tc^{101}]}{\sigma[Rh^{103}/n,\ \gamma/Rh^{104m}]} = 3{,}8 \cdot 10^{-4} .$$

Accepting the earlier results [5] for the absolute cross-section of $Rh^{103}(n, \gamma)\,Rh^{104m}$ and $Rh^{103}(n, \alpha)\,Tc^{100}$ reactions (i.e. $\sigma(n, \gamma) = 3{,}23$ mb, $\sigma(n, \alpha) = 11$ mb) our measurement gives the following values

$$\sigma(n, He^3) = \left(1{,}2 \pm \begin{matrix} 1{,}0 \\ 0{,}6 \end{matrix}\right) \mu b ,$$

$$\frac{\sigma(n, He^3)}{\sigma(n, \alpha)} = \left(1{,}1 \pm \begin{matrix} 1{,}0 \\ 0{,}6 \end{matrix}\right) 10^{-4} .$$

Calculation of cross-section ratio from statistical model

The investigation of the reaction mechanism for (n, He^3) with heavy nuclei is possible only by comparing the measured and calculated cross-sections, because of the low value of $\sigma(n, He^3)$. For this reason, in the case of Rh^{103} nucleus the cross-section ratio of (n, α) and (n, He^3) reactions was calculated on the basis of the statistical model at 14,7 MeV neutron energy.

The calculation of cross-section ratio in the case of a compound mechanism is reduced to the determination of the $\Gamma_{He}/\Gamma_\alpha$ ratio.

The emission probability for particle b generally is:

$$\Gamma_b = M_b\,(2s_b + 1) \int\limits_{\varepsilon_{b\min}}^{\varepsilon_{b\max}} \varepsilon_b\, \sigma_b\,(\varepsilon_b)\, \omega(u)\, d\varepsilon_b ,$$

where M_b, s_b and ε_b are the mass, spin and kinetic energy of the emitted particle, $\sigma_b(\varepsilon_b)$ is the cross-section for compound nucleus formation by the inverse reaction, $\omega(u)$ is the level density of residual nucleus at u excitation energy.

The even-odd effect was taken into consideration in the excitation energy $u = \varepsilon_{b\max} - \varepsilon_b + n\delta$ by adding $n\delta$, where n is 0, 1 and 2 in the case of even, odd-mass and odd end-nuclei, respectively;

$$\delta = 10 \cdot A^{-1/2}\ \text{MeV} ,$$

where A is the mass number [6]. The $\sigma_b(\varepsilon_b)$ values were taken by interpolating the data of the SHAPIRO tables [7]. These data are given for rectangular potential. The data of the same table were applied to the rounded-off potential taking into account the KIKUCHI relation [8] between the B maximum of the

rectangular potential and the B_{eff} maximum of the rounded-off potential

$$B_{\mathrm{eff}} = B\left(1 - \frac{1{,}7}{R}\right).$$

$R = 1{,}5\ A^{1/3}$ fm was taken as a nuclear radius. In calculating the inverse cross-section no distinction was made between the He^3 and α particles. For the energy dependence of the level density a simplified form derived from the Fermi gas model was adopted:

$$\omega(u) = c \cdot \exp\left[2(au)^{1/2}\right].$$

The value of the level density parameter was taken from the relation $a = 0{,}115 \cdot A$ [9]. The multiplication constant C was disregarded for the cross-section ratio because of its weak mass number dependence [10]. Since the $\sigma(n, \mathrm{He}^3)/\sigma(n, \alpha)$ ratio was determined experimentally containing neither $(n, n'\,\alpha)$ nor $(n, n'\,\mathrm{He}^3)$ processes, therefore — in order to compare with the experimental data — the calculated spectra were integrated over the energy region of emitted particles in which the emission of a second particle is energetically forbidden. The Q values were calculated using the data of KUNZ et al. tables [11], $Q(n, \alpha) = 3{,}94$ MeV and $Q(n, \mathrm{He}^3) = -7{,}85$ MeV.

The value for the cross-section ratio obtained by calculation:

$$\frac{\sigma(n, \mathrm{He}^3)}{\sigma(n, \alpha)} = \frac{\Gamma_{\mathrm{He}^3}}{\Gamma_\alpha} = 1{,}5 \cdot 10^{-9},$$

is 5 orders of magnitude less than the measured one. The calculated low value is due to the large negative Q value of the (n, He^3) reaction. At $A \sim 100$ nuclei the cross-section values for (n, α) reactions calculated on the basis of the statistical model are in the same order of magnitude as the measured ones [12]. Therefore, the great difference between the measured and calculated cross-section ratios may arise mostly from (n, He^3) reaction. This means that the cross-section of (n, He^3) reaction is more orders of magnitude higher than the one we should expect on the basis of the statistical model.

With $N > 82$ nuclei the measured value of $\sigma(n, \alpha)$ is, in several cases, 2—3 orders of magnitude higher than those calculated on the basis of the statistical model [12]. The measurements of the energy spectra and angular distributions show a strong, direct effect in the α emission with $N > 82$ nuclei. This supports the observation that the value of the cross-section is high in the case of direct reactions. Considering the above mentioned facts one can suppose that the high cross-section value observed at (n, He^3) reaction is caused by direct effects. Unfortunately, the proof of this by the measurement of He^3

energy spectrum and angular distribution cannot be carried out with present techniques since $\sigma(n, He^3)$ is too low.

The author is grateful to Professor A. SZALAY for his kind interest in this work.

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ИССЛЕДОВАНИЕ РЕАКЦИИ $Rh^{103}(n, He^3)\,Tc^{101}$

Й. ЧИКАИ

Резюме

Методом активации определяется поперечное сечение реакции $Rh^{103}(n, He^3)\,Tc^{101}$ при энергии нейтронов в 14,7 MeV для чего получено значение $\sigma(n, He^3) = (1,2 \pm {}^{1,0}_{0,6}\ \mu b$. Отношение поперечных сечений реакций (n, He^3) и (n, α) для ядра Rh^{103} определяется на основе статистической модели. Сравнение значений измеренного и вычисленного отношений поперечных сечений показывает, что относительно большой выход реакции (n, He^3) не может быть объяснен на основе статистической модели.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3–4), pp. 235–241 (1966)

CALCULATION OF ATOMIC FORM FACTORS FROM THE STATISTICAL ELECTRON DENSITY DISTRIBUTIONS

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The atomic form factors and the cross-sections for electron scattering are calculated for rare gases using a statistical atom model, which contains both the Dirac exchange energy and the improved kinetic energy correction of Gombás. Results are compared with the empirical data.

1. Introduction

The Thomas—Fermi [1] model of atoms is based on the assumption that the electrons of a heavy atom can be considered as a free-electron gas and accordingly, the kinetic energy of the atom can be identified with the Fermi energy of the electron gas. In calculating the potential energy of the atom one makes the assumption, that the negative electric charge is distributed continuously and that the electrons are present in this gas in a "smeared-out" state. Consequently, only the electrostatic Coulomb interaction between electrons has been taken into account.

Many improvements have been made on this original Thomas—Fermi model, which take into account more exactly both the potential energy and the kinetic energy of the atom. The most important correction to the potential energy, introduced by Dirac [2], is the exchange interaction energy of the electrons. The corrections to the kinetic energy arise from the fact that the density of the electron gas in an atom, especially in the neighbourhood of the nucleus, cannot be regarded as constant. The Weizsäcker [3] kinetic-energy correction has the effect that some defects of the statistical atom model disappear. In particular, as a result of this correction, the electron density at the nucleus is finite and falls off exponentially at infinity. These are in agreement with the corresponding results of wave mechanics, while in the Thomas—Fermi—Dirac model the electron density at the nucleus is infinite and the radius of the atom has a finite value, at which the electron density drops discontinuously from a finite value to zero. However, the Weizsäcker correction has the defect that the agreement of energies with empirical data is not so good. The energies of the model, including the Weizsäcker correction are 20—25% higher than the empirical ones. The origin of this discrepancy has been pointed out by Gombás [4]. The addition of the Fermi energy of the electrons and the Weizsäcker correction results in an error, because the two expressions partly overlap and, consequently, a part of the kinetic energy is taken into account twice. This discrepancy can be eliminated by decomposing the kinetic energy to an azymuthal and a radial part and then subtracting the radial self energy of electrons from the radial kinetic energy of the atom.

If we add both the Dirac exchange energy and the Gombás kinetic energy correction to the Thomas—Fermi model, we arrive at an atom model which besides its simplicity, describes many features of atoms in a very good approximation. The electron density of this model approximates better the wavemechanical Hartree—Fock distribution than the original Weizsäcker distribution, and it behaves exactly like the wave-mechanical distribution at the nucleus and at large distances from the nucleus [6]. The atomic energies of this model show, from the lightest to the heaviest atoms, a deviation smaller than 2% from the empirical values [5]. Considering that these energies are distributed in a range of 5 orders of magnitude the agreement is excellent.

The aim of this paper is to calculate the atomic form factors and the cross-sections for collisions of electrons with atoms using the electron distribution of the above mentioned statistical atom model [6]. The comparison of the computed and measured differential cross-sections is the best way to compare the calculated electron distribution with empirical data. Our aim is to control, by this comparison, the reliability of the Gombás statistical atom model.

2. Calculation of atomic form factors and cross-sections

The collision of high energy electrons ($E_{\text{kin}} \sim 1$ keV) with atoms can be treated in first Born approximation. The differential cross-section for elastic scattering is given by

$$\sigma(\vartheta) = \sigma_R(\vartheta) \left(\frac{Z - F(q)}{Z} \right)^2 , \tag{1}$$

where $\sigma_R(\vartheta)$ is the Rutherford cross-section of a point charge Ze, Z is the atomic number and F is the atomic form factor which characterizes the screening of the nucleus due to the electrons.

$$\sigma_R(\vartheta) = \left(\frac{Ze^2}{2m_0 c^2} \right)^2 \frac{1 - \beta^2}{\beta^4} \quad \frac{1 - \beta^2 \sin^2(\vartheta/2)}{\sin^4(\vartheta/2)} , \tag{2}$$

$$F(q) = 4\pi \int_0^\infty \varrho(r) \frac{\sin qr}{qr} r^2 \, dr , \tag{3}$$

$$q = \frac{2m_0\,c}{\hbar}\;\frac{\beta}{\sqrt{1-\beta^2}}\sin(\vartheta/2)\,. \tag{4}$$

Here e is the electronic charge, c the velocity of light, $\hbar$ the Planck constant divided by 2π, m_0 the rest mass of electron, ϑ the angle of scattering and

$$\beta = \frac{v}{c} = \frac{\sqrt{E_{\text{kin}}(E_{\text{kin}} + 2m_0\,c^2)}}{E_{\text{kin}} + m_0\,c^2}\,, \tag{5}$$

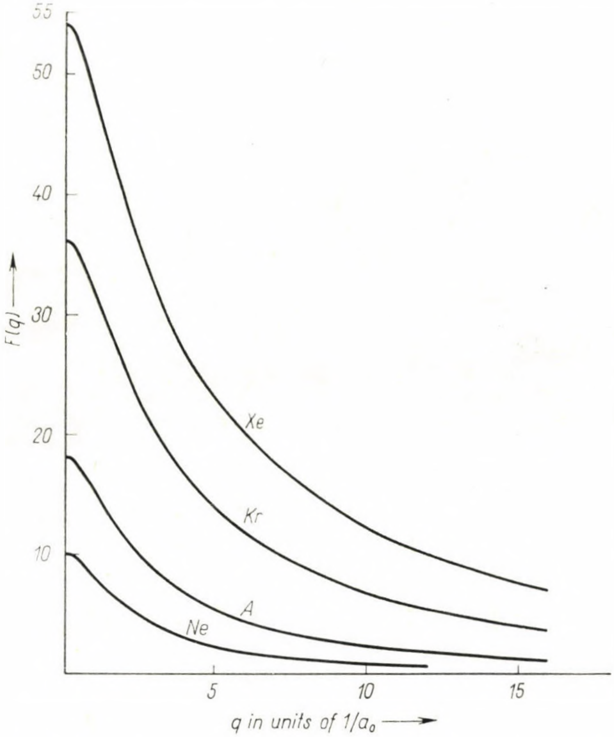

Fig. 1. Atomic form factors for rare gases as functions of q

where v is the velocity and E_{kin} the kinetic energy of incident electrons. In (3) $\varrho(r)$ is the density distribution of atomic electrons and the form factor $F(q)$ is essentially the Fourier-transform of the electron density distribution.

$\varrho(r)$ has been calculated by Gombás for rare gas atoms and the radial density $D(r) = 4\pi\, r^2\, \varrho(r)$ is given for Ne, A, Kr and Xe in his paper [6]. Using these $D(r)$-s we have calculated the atomic form factors

$$F(q) = \int_0^\infty D(r)\,\frac{\sin qr}{qr}\,dr \tag{6}$$

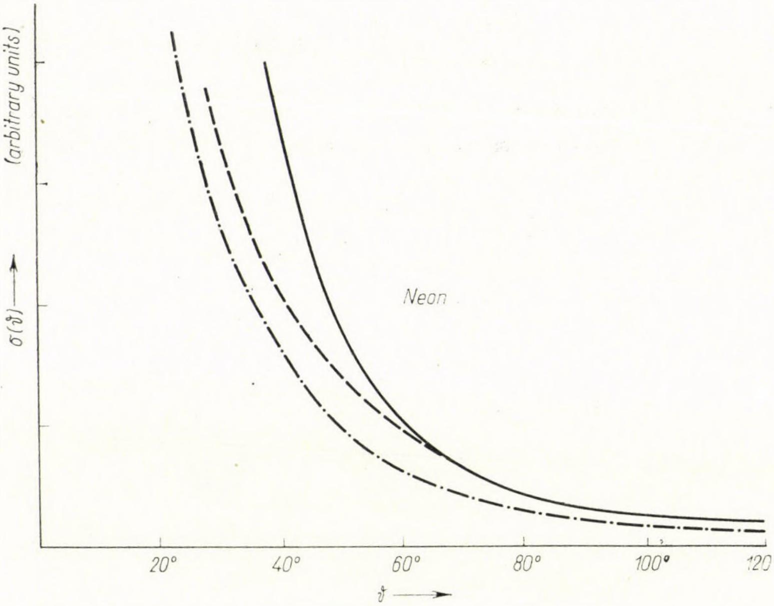

Fig. 2. **Differential cross-section for scattering of 412 eV electrons by Ne atoms**

——————— present calculation
—.—.—.— THOMAS—FERMI model
— — — — measured by ARNOT [7]

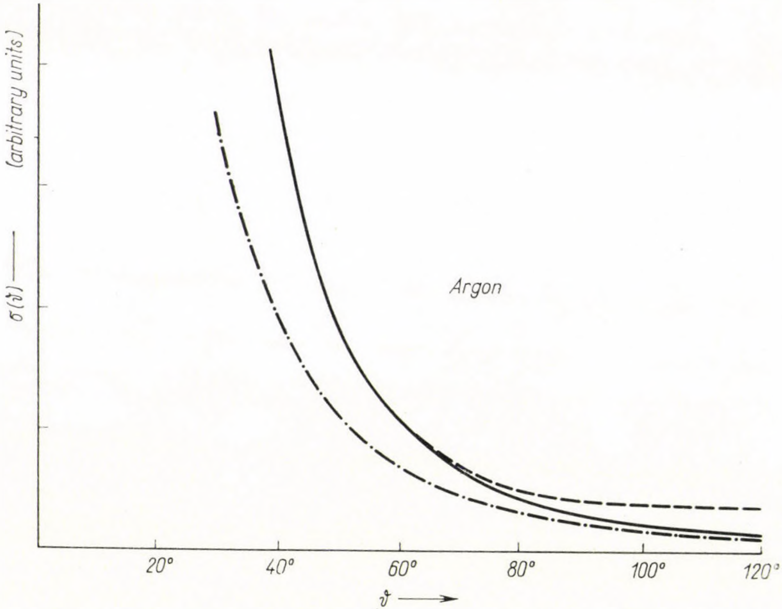

Fig. 3. **Differential cctin for soross-escattering of 708 eV electrons by A atoms**

——————— present calculations
—.—.—.— THOMAS—FERMI model
— — — — measured by ARNOT [7]

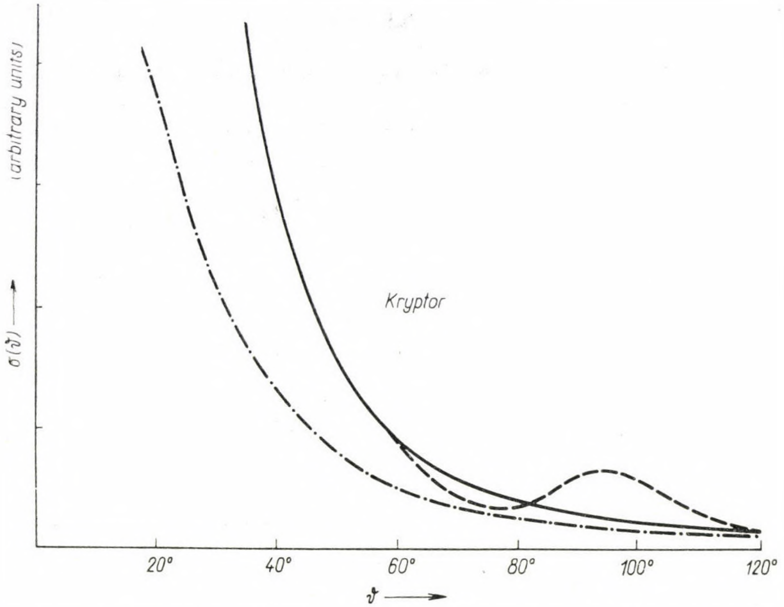

Fig. 4. Differential cross-section for scattering of 820 eV electrons by Kr atoms

———— present calculation
—.—.—.— THOMAS—FERMI model
— — — — measured by ARNOT [7]

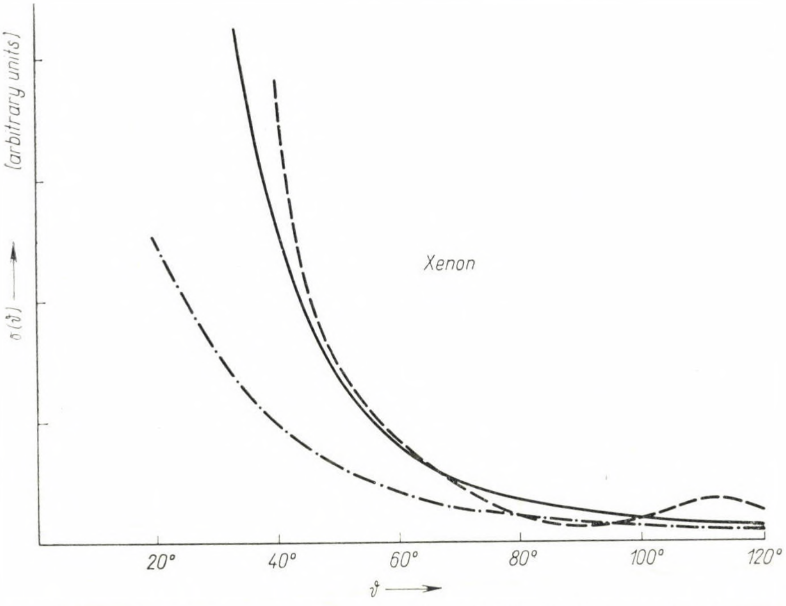

Fig. 5. Differential cross-section for scattering of 800 eV electrons by Xe atoms

———— present calculation
—.—.—.— THOMAS—FERMI model
— — — — measured by ARNOT [7]

Table I

Atomic form factors for rare gases. q in units of $1/a_0$

Gas	Neon	Argon	Krypton	Xenon
q	F	F	F	F
0.	10.	18.	36.	54.
0.25	9.887	17.725	35.682	53.544
0.50	9.436	17.080	34.688	52.237
0.75	8.803	16.250	33.222	50.350
1.00	8.099	15.126	31.549	48.148
1.25	7.399	14.073	29.763	45.852
1.50	6.744	13.068	28.232	43.581
2.00	5.623	11.287	25.425	39.368
2.50	4.729	9.811	22.394	35.648
3.00	4.020	8.598	20.200	32.413
3.50	3.447	7.582	18.176	29.585
4.00	2.982	6.734	16.499	27.118
4.50	2.600	6.020	15.048	25.008
5.00	2.279	5.409	13.784	23.051
6.00	1.792	4.431	11.698	19.862
7.00	1.436	3.691	10.061	17.316
8.00	1.165	3.109	8.737	15.230
9.00	0.956	2.645	7.637	13.661
10.00	0.792	2.268	6.751	12.051
11.00	0.668	1.967	6.010	10.842
12.00	0.584	1.774	5.359	9.815
13.00	0.487	1.530	4.856	8.933
14.00	0.429	1.448	4.389	8.153
15.00	0.372	1.174	3.988	7.477
16.00	0.328	1.101	3.640	6.886

for several values of q. We have performed the integration in (6) numerically, the mesh of r used was 0 (0,001) 0,01 (0,002) 0,02 (0,004) 0,06 (0,008) 0,108 (0,016) 0,284 (0,032) 0,508 (0,064) 1,212 (0,128) 3,132 (0,256) 10,044 in units of Bohr radius a_0. The results for Ne, A, Kr and Xe are given in Table I and are shown in Fig. 1. For $q = 0$ the form factor F equals to Z; F decreases monotonically with increasing q and vanishes for $q = \infty$.

The scattering cross-sections have been calculated from the form factors according to (1)—(4). The results for the rare gas atoms and for scattering energy of about 800 eV are shown in Figs. 2—5, where the cross-sections measured by ARNOT [7] are also plotted. Both the calculated and measured curves fall off rapidly with increasing ϑ. Except for the case of Ne, the agreement between the two curves for small and intermediate ϑ-s is quite good. For large angles of scattering the measured cross-section of heavier elements Kr and Xe exhibits a weak oscillation. The theoretical curve cannot reproduce this oscillation but averages it. These results emphasized the reliability of the electron distribution of the statistical atom model which contains both the Dirac and the Gombás corrections.

The author wishes to express her thanks to Prof. Dr. P. Gombás for helpful advices and discussions.

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ВЫЧИСЛЕНИЕ АТОМНЫХ ФОРМФАКТОРОВ ИЗ СТАТИСТИЧЕСКОГО РАСПРЕДЕЛЕНИЯ ПЛОТНОСТИ ЭЛЕКТРОНОВ

А. ДОБАИ-СЕГЛЕТ

Резюме

В работе определяются атомные формфакторы и поперечные сечения для рассеяния электронов в случае благородных газов на основе статистической атомной модели, содержащей обменную энергию Дирака и исправленную Гомбашом коррекцию к кинетической энергии. Результаты сравниваются с эмпирическими данными.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3—4), pp. 243—253 (1966)

ALGEBRAIC METHODS IN THE THEORY OF SPECIAL UNITARY GROUPS

I. CALCULATION OF GENERATOR MATRIX ELEMENTS

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(Presented by L. Jánossy. — Received 2. II. 1966)

In this paper and a few following ones the efficiency of simple algebraic methods is demonstrated in the theory of the special unitary groups. The present work deals with the calculation of the generator matrix elements. The procedure is considered in detail in the framework of $SU(3)$.

In the last few years the role of the Lie groups in theoretical physics, especially in the domain of elementary particles has become dominant. A large amount of work has been done in this field, mainly in connection with special unitary groups. Most of the results have been obtained by using the general and very aesthetic theory of semisimple compact Lie groups. However, almost every calculation can be carried out by much more simple methods very similar to the tricks of $SU(2)$ which can be found in every textbook.

On the other hand, the theory of n-dimensional special unitary groups has developed so rapidly, that some subsidiary questions, such as the general reduction of product spaces and their new quantum numbers, and the determination of isoscalar factors in closed form, have not received the attention deserved.

In the present paper and in those following we should like to demonstrate the effectiveness of fairly simple algebraic methods in the theory of $SU(n)$ both in the treatment of older results obtained by more complicated reasoning, and in attacking some problems, as yet unsolved.

In our work we make an attempt to formulate the results for any $SU(n)$ though some of the calculations will be carried out only for $SU(3)$. In some cases we shall emphasize the connections with the general theory of semisimple compact Lie groups.

In this paper we show the method of determination of generator matrix elements of $SU(n)$.

In Part 1 we outline an inductive way of these calculations in $SU(n)$ on the basis of the knowledge of matrix elements in $SU(n-1)$. In Part 2 we develop the whole procedure in detail for $SU(3)$. The results of this section agree with those of Biedenharn obtained on the basis of Weyl's branching laws [1] and Mukunda and Pandit [2], who obtained the same expressions by means of tensor methods.

1.

In the WEYL basis of generators of $SU(n)$ the commutation rules are as follows:*

$$[A'_{ik}, A'_{lm}] = \delta_{kl} A'_{im} - \delta_{im} A'_{lk}, \qquad 1 \leqslant i, k \leqslant n. \tag{1}$$

A'_{ik} satisfies the conditions $\Sigma A'_{rr} = 0$ and $A'^{+}_{ik} = A'_{ki}$.**

The fundamental representation (F. R.) of the generators is:

$$(A'_{ik})_{rs} = \delta_{ir}\,\delta_{ks} - \frac{\delta_{ik}}{n}\,\delta_{rs}, \qquad 1 \leqslant i,\ k,\ r,\ s \leqslant n. \tag{2}$$

Let us introduce a linear combination of the generators:

$$A_{ik} = \left(A'_{ik} + \frac{\delta_{ik}}{n-1} A'_{nn}\right)\left(1 + \frac{1-2n}{n}\,\delta_{in}\,\delta_{kn}\right), \tag{3}$$

which in detail gives the equations:

$$A_{ik} = A'_{ik}, \quad i \neq k,$$
$$A_{ii} = A'_{ii} + \frac{1}{n-1} A'_{nn}, \quad i < n,$$
$$A_{nn} = -A'_{nn}.$$

This new set of generators might be arranged in three classes:

a) A_{ik} $\quad i, k < n \quad \sum_{i=1}^{n-1} A_{ii} = 0$

b) A_{in} $\quad i < n;$ $\quad A_{nk}$ $\quad k < n$

c) A_{nn}.

It is instructive to look into the structure of the generators of these classes separately in the F. R.

a) $i, k < n.$

We have, from formulae (2) and (3)

$$(A_{ik})_{rs} = \delta_{ir}\,\delta_{ks} - \frac{\delta_{ik}}{n-1}\,\delta_{rs} + \frac{\delta_{ik}}{n-1}\,\delta_{nr}\,\delta_{ns}.$$

---

* No upper indices are used either in this note or in the following ones, as we do not intend to work with tensor notation.

** An arbitrary element of $SU(n)$ can be written in the form:

$$U = \exp i \sum_{jk} \frac{1}{2}\left(\alpha_{jk} A'_{jk} + \alpha^{*}_{jk} A'_{kj}\right).$$

This formula shows that if $r=n$ or $s=n$, then

$$(A_{ik})_{rs}=0 \quad \text{and} \quad \sum_{i=1}^{n-1} A_{ii}=0.$$

It is easily seen that the matrices of this class in the F. R. are simply the matrices of $SU(n-1)$ with one column and one row of zeros attached to them:

$$\left(\begin{array}{ccc|c} \multicolumn{3}{c|}{\text{Generators}} & 0 \\ \multicolumn{3}{c|}{\text{of } SU\,(n-1)} & \vdots \\ & & & 0 \\ \hline 0 & \cdots\cdots & 0 & 0 \end{array}\right);$$

b) If $i<n$ $(k<n)$, then in the F. R. $A_{in}(A_{nk})$ contain 1 in the i-th (k-th) position of the last column (row)

$$\text{e.g.} \qquad A_{in}=\left(\begin{array}{ccc|c} & & & 0 \\ & & & \vdots \\ & & & 0 \\ & 0 & & \vdots \\ & & & 1 \\ & & & \vdots \\ & & & 0 \\ \hline 0 & \cdots\cdots & 0 & 0 \end{array}\right) \qquad (1 \text{ in the } i\text{—th row})$$

c) This class consists of one matrix

$$(A_{nn})_{rs}=-\,\delta_{nr}\,\delta_{ns}+\frac{1}{n}\,\delta_{rs}$$

with $\frac{1}{n}$ in the diagonal except its last element which is equal to $\frac{1-n}{n}$.

$$\left(\begin{array}{cccc|c} \frac{1}{n} & & & & \\ & \frac{1}{n} & & & \\ & & \ddots & & \\ & & & \frac{1}{n} & \\ \hline & & & & \frac{1-n}{n} \end{array}\right)$$

Using formulae (1) and (2) we can write down the commutators of our generators. If we examine the commutators of the generators in class a), we see, that

$$[A_{ik}, A_{lm}]=\delta_{kl}\,A_{im}-\delta_{im}\,A_{lk}, \qquad i,k,l,m\leqslant n-1. \tag{4}$$

These commutation rules are exactly the rules of $SU(n-1)$. The commutators of generators belonging to class a) and b), respectively, are

$$[A_{ik}, A_{ln}] = [(A'_{ik} + \frac{\delta_{ik}}{n-1} A'_{nn}), A'_{ln}] =$$

$$= \delta_{kl} A'_{in} - \frac{\delta_{ik}}{n-1} A'_{ln} = \sum_r \left(\delta_{kl}\, \delta_{ir} - \frac{\delta_{ik}}{n-1}\, \delta_{rl}\right) A'_{rn}. \qquad i,\ k,\ l < n \tag{5}$$

In the last formula the bracket contains the matrix of the generator A_{ik} of $SU(n-1)$ in its F. R. which can be seen by replacing n by $n-1$ in (2). This shows that A_{ln} is an irreducible tensor operator of $SU(n-1)$ transforming according to its F. R.

A_{nn} and the generators of class a) commute:

$$[A_{ik},\ A_{nn}] = 0 \qquad i, k < n\,. \tag{6}$$

A_{nn} and the generators of class b) have the following commutator:

$$\begin{aligned} [A_{nn},\ A_{ln}] &= -[A'_{nn},\ A'_{ln}] = A'_{ln} = A_{ln} \\ [A_{nn},\ A_{nk}] &= -A_{nk} \qquad\qquad k, l < n \end{aligned}\,. \tag{7}$$

Two further types of commutation rules involving generators of class b) exist, i.e.

$$[A_{in},\ A_{kn}] = 0 \tag{8}$$

and

$$[A_{in},\ A_{nk}] = A_{ik} + \frac{n}{n-1}\, \delta_{ik}\, A_{nn}\,. \tag{9}$$

With this method we have separated the generators of an $SU(n-1)$ subgroup of $SU(n)$.

Let us turn our attention to the calculation of generator matrix elements of $SU(n)$ in an irreducible representation. First we have to make one remark. BIEDENHARN shows [3] that the states of a given irreducible representation of $SU(n)$ may be completely characterized by quantum numbers of $SU(n-1)$ — that is, numbers specifying an irreducible representation of this subgroup, and numbers, specifying a state in this irreducible representation — plus one new additive quantum number, which in our scheme is the eigenvalue of A_{nn}. The generators of the $SU(n-1)$ subgroup are exactly A_{ik} $i, k < n$ in our picture.

Thus, since we know the generator matrix elements of $SU(n-1)$, only the matrix elements of the type A_{in} $(i < n)$ must be calculated as $A_{nk} =$

$= A^{+}_{kn}$ and A_{nn} is diagonal in this representation. Equation (5) gives further information, showing that A_{in} is an irreducible tensor operator of $SU(n-1)$ transforming according to its F. R.; consequently in the determination of A_{in} the WIGNER—ECKART theorem of $SU(n-1)$ can be used.

In the next section we apply these general results to the calculation of the generator matrix elements of $SU(3)$.

2.

In $SU(3)$ it is more convenient to introduce the following notation:

$$\begin{array}{lll} I_z = A_{11}\,, & Y = A_{33}\,, & \\ I_+ = A_{12}\,, & F_+ = A_{13}\,, & G_+ = -A_{32}\,, \\ I_- = A_{21}\,, & F_- = A_{23}\,, & G_- = A_{31} \end{array}$$

and

$$I_+^+ = I_-\,, \qquad F_+^+ = G_-\,, \qquad F_-^+ = -G_+\,.$$

The generators $I_\pm$, I_z; $F_\pm$, $G_\pm$; and Y constitute classes a), b) and c) of the previous section respectively.

Since $A_{11} + A_{22} = 0$, we have $A_{22} = -I_z$.

The commutators corresponding to equations (4)—(9) are the following:

$$[I_z\,, I_\pm] = \pm I_\pm\,, \qquad [I_+\,, I_-] = 2I_z\,, \tag{4'}$$

$$\left.\begin{array}{l} [I_+\,, F_-] = F_+\,, \quad [I_-\,, F_+] = F_-\,, \quad [I_z\,, F_\pm] = \pm\dfrac{1}{2}F_\pm\,, \\ [I_+\,, G_-] = G_+\,, \quad [I_-\,, G_+] = G_-\,, \quad [I_z\,, G_\pm] = \pm\dfrac{1}{2}G_\pm\,, \\ [I_+\,, F_+] =]I_-\,, F_-] = [I_+\,, G_+] = [I_-\,, G_-] = 0\,, \end{array}\right\} \tag{5'}$$

$$[I_+\,, Y] = [I_-\,, Y] = [I_z\,, Y] = 0\,, \tag{6'}$$

$$[Y, F_\pm] = F_\pm\,, \qquad [Y, G_\pm] = -G_\pm\,, \tag{7'}$$

$$[F_+\,, F_-] = [G_+\,, G_-] = 0\,, \tag{8'}$$

$$\left.\begin{array}{ll} [F_+\,, G_+] = -I_+\,, & [F_-\,, G_-] = I_-\,, \\ [F_+\,, G_-] = I_z + \dfrac{3}{2}Y\,, & [F_-\,, G_+] = I_z - \dfrac{3}{2}Y\,. \end{array}\right\} \tag{9'}$$

As for an irreducible representation of $SU(3)$ the theorem of **Biedenharn** states that an eigenvector has the following labelling:

$$|TMY\rangle\,.^{*}$$

T and M specify an irreducible representation of the $SU(2)$ subgroup of the generators $I_{\pm}$, I_z, and its magnetic quantum number, respectively. Y is the new additive quantum number of $SU(3)$. This labelling system might be constructed in an inductive manner, too. We have two mutually commuting operators I_z and Y. Let us denote a simultaneous eigenvector of them by $|MY\rangle$;

$$I_z|MY\rangle = M|MY\rangle\,,$$
$$Y|\,MY\rangle = Y\,|\,MY\rangle\,.$$

Following the tricks of $SU(2)$ with generators I_+, I_- and I_z, and taking into account that they commute with Y, we see that for a fixed eigenvalue of Y we must characterize the eigenvector by a number T, i.e. we must write $|\,TMY\rangle$, and we get the possible values of M:

$$-T \leqslant M \leqslant T\,.$$

T is the eigenvalue of

$$I^2 = \frac{1}{2}(I_+ I_- + I_- I_+) + I_z^2:$$

$$I^2\,|\,TMY\rangle = T(T+1)\,|\,TMY\rangle\,.$$

For I_+, I_- we get the well-known relation:

$$I_{\pm}|\,TMY\rangle = \sqrt{(T \mp M)\,(T \pm M + 1)}\,|T\,M \pm 1Y\rangle\,.$$

Concerning F_+, F_- we remark that according to equations (5′) they are irreducible spinor operators. This fact together with (7′) gives the equations:

$$\sqrt{\frac{T-M+1}{2T+1}}\,F_-\,|\,TMY\rangle + \sqrt{\frac{T+M}{2T+1}}\,F_+\,|\,TM-1Y\rangle =$$
$$= \alpha(TY)\Big|\;T + \frac{1}{2}M - \frac{1}{2}Y + 1\Big\rangle,$$

$$\sqrt{\frac{T+M}{2T+1}}\,F_-\,|TMY\rangle - \sqrt{\frac{T-M+1}{2T+1}}\,F_+\,|TM-1Y\rangle =$$
$$= \beta(TY)\Big|T - \frac{1}{2}\,M - \frac{1}{2}Y + 1\Big\rangle,$$

---

[*] As can be seen, we have adopted **Dirac**'s notation. The scalar product of two kets is defined: $\langle TMY\,|\,T'M'Y'\rangle = \delta_{TT'}\delta_{MM'}\delta_{YY'}$.

where $\alpha(TY)$ and $\beta(TY)$ are independent of the quantum number M. (WIGNER—ECKART theorem.)

From these equations we get:

$$F_{\pm}\,|TMY\rangle=\sqrt{\frac{T\pm M+1}{2T+1}}\,\alpha(TY)\left|T+\frac{1}{2}\,M\pm\frac{1}{2}\,Y+1\right\rangle\mp \mp\sqrt{\frac{T\mp M}{2T+1}}\,\beta(TY)\left|T-\frac{1}{2}\,M\pm\frac{1}{2}\,Y+1\right\rangle \tag{10}$$

and

$$G_{\pm}\,|TMY\rangle=\mp F_{\pm}^{+}\,|TMY\rangle= =\mp\sqrt{\frac{T\mp M}{2T}}\,\alpha^{*}\left(T-\frac{1}{2}\,Y-1\right)\left|T-\frac{1}{2}\,M\pm\frac{1}{2}\,Y-1\right\rangle- -\sqrt{\frac{T\pm M+1}{2T+2}}\,\beta^{*}\left(T+\frac{1}{2}\,Y-1\right)\left|T+\frac{1}{2}\,M\pm\frac{1}{2}\,Y-1\right\rangle. \tag{11}$$

To compute $\alpha(TY)$ and $\beta(TY)$ we use the two relations:

$$[F_{+}\,,\,F_{-}]=0\,, \tag{12}$$

$$[F_{+}\,,\,G_{-}]=I_{z}+\frac{3}{2}\,Y. \tag{13}$$

We remark that all the remaining commutators of F and G can be obtained from these either by taking hermitian adjoints, or by commuting the second relation with $I_{\pm}$ and using the JACOBI-identity:

$$[A,[B,C]]+[B,[C,A]]+[C,[A,B]]=0$$

Commutator (12) gives the following equation:

$$\frac{\alpha(TY)}{\alpha\left(T-\frac{1}{2}\,Y+1\right)}=\sqrt{\frac{T}{T+1}}\;\frac{\beta(TY)}{\beta\left(T+\frac{1}{2}\,Y+1\right)}\,. \tag{14}$$

Commutator (13) gives two equations with respect to diagonal and non-diagonal elements

$$\frac{T+M}{2T}\left|\alpha\,(T-\frac{1}{2}\,Y-1)\right|^{2}-\frac{T+M+1}{2T+1}\left|\alpha\,(TY)\right|^{2}+ +\frac{T-M+1}{2T+2}\left|\beta\left(T+\frac{1}{2}\,Y-1\right)\right|^{2}- -\frac{T-M}{2T+1}\,|\beta\,(TY)|^{2}-M-\frac{3}{2}\,Y=0 \tag{15}$$

and

$$\frac{\alpha(TY)}{\alpha\left(T-\frac{1}{2}Y+1\right)}=\frac{2T+1}{\sqrt{2T(2T+2)}}\,\frac{\beta\left(T+\frac{1}{2}Y+1\right)}{\beta(TY)}. \tag{16}$$

From equations (14) and (16) we can derive the following relations equivalent to them:

$$\left|\alpha\left(T+\frac{1}{2}Y-1\right)\right|^2=\frac{2T+2}{2T+3}\,|\alpha(TY)|^2, \tag{17}$$

$$\left|\beta\left(T-\frac{1}{2}Y-1\right)\right|^2=\frac{2T}{2T-1}\,|\beta(TY)|^2. \tag{18}$$

Making use of the fact that $\alpha(TY)$ and $\beta(TY)$ are independent of M and replacing M by T and $-T$, respectively, (15) gives two further equations:

$$\left|\alpha\left(T-\frac{1}{2}Y-1\right)\right|^2+\frac{1}{2T+2}\left|\beta\left(T+\frac{1}{2}Y-1\right)\right|^2= \\ =|\alpha(TY)|^2+T+\frac{3}{2}Y, \tag{19}$$

$$\frac{2T+1}{2T+2}\left|\beta\left(T+\frac{1}{2}Y-1\right)\right|^2=\frac{1}{2T+1}\,|\alpha(TY)|^2+ \\ +\frac{2T}{2T+1}\,|\beta(TY)|^2-T+\frac{3}{2}Y. \tag{20}$$

Equations (17)—(20) constitute a system of difference equations for $\alpha(TY)$ and $\beta(TY)$. To solve this system, it is necessary to impose initial conditions. As we are considering finite dimensional representations, the eigenvalues of Y must terminate at some Y_0. Let us denote the corresponding T value by T_0, that means that there exists a state $|T_0MY_0\rangle$ for which:

$$F_+|T_0MY_0\rangle=F_-|T_0MY_0\rangle=0$$

as F increase the eigenvalue of Y by 1 [see(7′)]. It is easily seen by considering $I_+|T_0MY_0\rangle$, that this property is valid for any value of M ($-T_0\leqslant M\leqslant T_0$) for the state $|T_0MY_0\rangle$, i.e.

$$F_+|T_0T_0Y_0\rangle=F_-|T_0T_0Y_0\rangle=0.$$

From these and (10) it becomes clear that

$$\alpha(T_0Y_0)=\beta(T_0Y_0)=0\,.$$

On the other hand (16) and (17) give:

$$\left|\alpha\left(T+\frac{k}{2},\ Y-k\right)\right|^2=\frac{2T+2}{2T+k+2}\,|\alpha(TY)|^2\,, \tag{21}$$

$$\left|\beta\left(T-\frac{l}{2},\ Y-l\right)\right|^2=\frac{2T}{2T-l}\,|\beta(TY)|^2\,, \tag{22}$$

(k and l are integers).

For any value of T and $Y\,(Y<Y_0)$ we may introduce two integer variables, m and n by the equations:

$$T=T_0+\frac{m-n}{2}\,,\qquad Y=Y_0-(m+n),\qquad m+n>0\,.$$

This is justified, as when examining the difference equations we find that T and Y values involved differ from each other by half-integer and integer numbers, respectively. In the following we present the calculations of $\beta(TY)$.

$$\begin{aligned}|\beta(TY)|^2&=\left|\beta\left(T_0+\frac{m}{2}-\frac{n}{2},\ Y_0-m-n\right)\right|^2=\\&=\frac{2T}{2T-n}\left|\beta\left(T_0+\frac{m}{2}Y_0-m\right)\right|^2,\end{aligned} \tag{23}$$

where we have used (22).

Replacing T by $T_0+\frac{m-1}{2}$ and Y by $Y_0-(m-1)$ equation (20) gives the following relation

$$\begin{aligned}&\frac{2T_0+m}{2T_0+m+1}\left|\beta\left(T_0+\frac{m}{2}Y_0-m\right)\right|^2-\\&\qquad-\frac{2T_0+m-1}{2T_0+m}\left|\beta\left(T_0+\frac{m-1}{2}Y_0-(m-1)\right)\right|^2=\\&\qquad=\frac{1}{2T_0+m}\left|\alpha\left(T_0+\frac{m-1}{2}Y_0-(m-1)\right)\right|^2-\\&\qquad-T_0-\frac{m-1}{2}+\frac{3}{2}Y_0-\frac{3}{2}(m-1).\end{aligned}$$

According to equation (21) the first term on the right-hand side is proportional to $\left| \alpha(T_0 Y_0) \right|^2$, and that is equal to zero. The remaining equation is a difference equation, which may be summed up, and leads to the result:

$$\left|\beta\left(T_0 + \frac{m}{2} Y_0 - m\right)\right|^2 = \frac{2T_0 + m + 1}{2T_0 + m}\left(\frac{3}{2} Y_0 - T_0 + 1 - m\right) m\,.$$

This and (23) give:

$$|\beta(TY)|^2 = \left|\beta\left(T_0 + \frac{m-n}{2} Y_0 - (m-n)\right)\right|^2 =$$

$$= \frac{2T_0 + m + 1}{2T_0 + m + n}\left(\frac{3}{2} Y_0 - T_0 + 1 - m\right) m.$$

Using now the value T and Y instead of m and n, and considering that we have a freedom in the choice of phases as all the equations involve only squares of absolute values of $\alpha(TY)$ and $\beta(TY)$, we get

$$\beta(TY) =$$

$$= \left[\frac{\left(T_0 + \frac{Y_0}{2} + T - \frac{Y}{2} + 1\right)\left(\frac{Y_0}{2} - T_0 + T - \frac{Y}{2}\right)\left(Y_0 - T + \frac{Y}{2} + 1\right)}{2T}\right]^{1/2}. \tag{24}$$

Equally, $\alpha(TY)$ can be determined in a similar way, and then we obtain

$$\alpha(TY) =$$

$$= \left[\frac{\left(T_0 - \frac{Y_0}{2} + T + \frac{Y}{2} + 1\right)\left(T_0 + \frac{Y_0}{2} - T - \frac{Y}{2}\right)\left(Y_0 + T + \frac{Y}{2} + 2\right)}{2T + 2}\right]^{1/2}$$

(25

From $SU(2)$ considerations it is obvious that any T value, and so T_0, is a non-negative integer or half-integer, i.e.

$$T_0 = \frac{\lambda}{2} \qquad (\lambda \geqslant 0, \quad \text{integer}).$$

From the finite dimensionality of the representation it is also obvious that

$$(G_+)^\mu |T_0 T_0 Y_0> \neq 0$$

but

$$(G_+)^{\mu+1} |T_0 T_0 Y_0> = 0$$

as G_+ decreases the eigenvalue of Y by 1.

The structure of G_+ [see (11)] shows, that the last two equations lead to the condition:

$$\beta\left(T_0 + \frac{\mu+1}{2} Y_0 - \frac{\mu+1}{2}\right) = 0,$$

which together with $T_0 = \frac{\lambda}{2}$ and taking into account (24) gives $Y_0 = \frac{\lambda + 2\mu}{3}$.

So, finally, we may state that the two non-negative integer values λ and μ specify the irreducible representation in question, and the expressions for $\alpha(TY)$ and $\beta(TY)$ in terms of λ and μ are the following:

$$\alpha(TY) = \\ = \left[\frac{\left(\frac{\lambda-\mu}{3} + T + \frac{Y}{2} + 1\right)\left(\frac{2\lambda+\mu}{3} - T - \frac{Y}{2}\right)\left(\frac{\lambda+2\mu}{3} + T + \frac{Y}{2} + 2\right)}{2T+2}\right]^{1/2}, \tag{26}$$

$$\beta(TY) = \\ = \left[\frac{\left(\frac{2\lambda+\mu}{3} + T - \frac{Y}{2} + 1\right)\left(-\frac{\lambda-\mu}{3} + T - \frac{Y}{2}\right)\left(\frac{\lambda+2\mu}{3} - T + \frac{Y}{2} + 1\right)}{2T}\right]^{1/2}. \tag{27}$$

Thus, the problem of determination of generator matrix elements in the irreducible representation characterized by λ and μ is completely solved.

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АЛГЕБРАИЧЕСКИЕ МЕТОДЫ В ТЕОРИИ СПЕЦИАЛЬНЫХ УНИТАРНЫХ ГРУПП I

Ю. НИРИ и А. ШЕБЕШТЕН

Резюме

В данной работе и в последующих использованы простые алгебраические методы в теории специальных унитарных групп. В настоящей статье определяются матричные элементы генераторов. Подробные расчеты приведены для SU(3).

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3—4), pp. 255—276 (1966)

A FEW USES OF ELEMENTARY PARTICLES IN NUCLEAR STRUCTURE STUDIES*

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A selective review is given of some of the ways in which "elementary particles "and the techniques of high energy physics in general may be used for the investigations of nuclear structure. It is pointed out that our ability to extract new nuclear structure information from such experiments is often limited by our present ignorance on other aspects of nuclear structure.

Introduction

We are very familiar with the use of the great accelerating machines for the study of elementary particles in their own right. Beams of nucleons, pions, muons, K-mesons, anti-protons, neutrinos and so on are generated and used to provoke collisions or reactions that brings us information about the elementary particles themselves. These same beams will, of course, interact also with complex nuclei, and sometimes such interactions have been used either because targets of complex nuclei were demanded in order to get nucleons in sufficiently concentrated form or, more rarely, because complex nuclei, by virtue of the spin or some other quantum number, enabled us to place restrictions on the character of the elementary particle interactions. However, the availability of such beams of elementary particles naturally leads us to ask the question whether, by their interaction with complex nuclei, we may not be able to gain information about the complex nuclei themselves of a character that cannot be obtained by the normal methods of nuclear structure experimentation or that may perhaps confirm the results of such conventional methods of experimentation from this novel point of view.

So far work has been confined to elementary particle beams that "naturally" found themselves available from having been prepared for elementary particles research purposes. We are now beginning, however, to think seriously about developing such beams and indeed special accelerators, largely or even solely for the purposes of nuclear structure research. It is therefore appropriate to examine the sort of information one can hope to gain about the nucleus

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* A lecture delivered in Budapest on 25th October 1965 to the Hungarian Physical Society.

through the medium of elementary particles and to assess whether it is sufficiently important and sufficiently novel to justify the very considerable expenditure that this form of experimentation will entail. I shall not attempt, in this lecture, to shoulder the responsibility of recommending for or against such expenditure. I am in no way attempting a synoptic account of the subject — great areas will be left untouched: I shall, for example, omit nucleons and electrons completely. Still less am I writing a proposal for a meson factory — that document would look very different from this lecture. But I shall try to show by a few eclectic examples: (a) that we have already benefitted in our knowledge of nuclear structure from the use of elementary particles; (b) that there is a wealth of important nuclear structure information to which elementary particles might lead us in the future; (c) that care is going to be needed in interpreting the results. I shall have to strike some sort of balance of emphasis between (a), (b) and (c); I shall hope to do this fairly but I should also say that (c) would have had to loom large in some of the topics I have omitted had time allowed their inclusion.

The composition of the nuclear surface

Before examining, particle by particle, the type of nuclear structure information that we might obtain, it may be interesting to illustrate the knowledge about the nucleus that has already been gained through elementary particle probes by reference to a single problem. This will, I hope, convince you that use can be, and already has been, made of elementary particles for giving us information that it would be very difficult to get by conventional means. The problem is the composition of the nuclear surface: is the nuclear surface composed chiefly of neutrons or chiefly of protons or is it composed of neutrons and protons in more or less the same $N:Z$ proportion as for the nucleus as a whole?

This is obviously a very important question for nuclear structure; that it is an open question may be shown by two simple contradictory arguments. The first of these is that the protons in the nucleus are positively charged while the neutrons are neutral; the protons therefore repel each other which the neutrons do not and so tend to get as far apart as possible making the edge of the nucleus proton-rich. The second argument is a little more complicated and is illustrated in Figure 1. This Figure shows the potential felt by a neutron as it enters the nucleus and also the potential felt by a proton. Owing to the charge independence of the specifically-nuclear force, the proton potential differs from the neutron potential essentially by the addition of the repulsive Coulomb force which lifts up the proton potential and makes it, as shown, not so deep as the neutron potential inside the nucleus. The nucleus may then be thought of, crudely, as built up by siting neutrons and protons in their respective potentials up to a certain level that represents the binding energies. This level must be more-or-less the same for neutrons and for protons, otherwise beta-decay will convert one into the other until equilibrium is reached. As may be seen from the Figure, owing to the sloping sides of the nuclear potential this means that the protons are confined by an effectively narrower potential than the neutrons and so the edge of the nucleus must be neutron-rich.

These two contrary arguments are both false but are also both superficially plausible. They at least suffice to show that the question about the composition of the nuclear surface does not have a simple common-sense answer. Nor is an answer given by the most sophisticated analysis that we are yet able to make; an experimental answer is clearly demanded to provide a boundary condition for further speculation about nuclear structure.

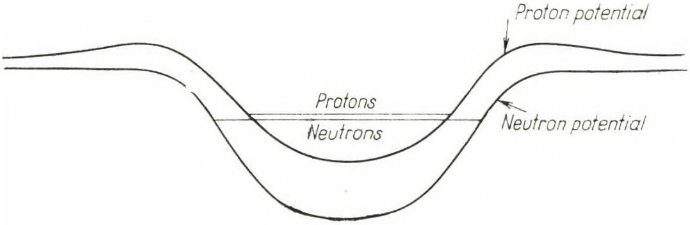

Fig. 1

To some degree, the conventional methods of nuclear structure experimentation are sensitive to the neutron-versus-proton ratio in the nuclear surface, for example relative nucleon reduced widths are clearly dependent on the relative nucleon distribution. However, the extraction of such widths from experimental data is a delicate and by no means unambiguous procedure and demands full faith in the Distorted Wave Born Approximation on which one knows one cannot rely for really quantitative answers. One is therefore led to seek a completely new approach. The use of elementary particle probes has provided three such approaches which will now be briefly summarized.

(i) π^+ *versus* π^- *cross-sections*

Generally speaking the nucleon cross-section for the collision of a particular charge of pion will be different for neutrons and for protons. Charge independence then provides:

$$\sigma_{\pi+p} = \sigma_{\pi-n} \neq \sigma_{\pi+n} = \sigma_{\pi-p} \, .$$

Imagine now, for the sake of argument, that we could find a pion energy at which the above inequality sign reads "very much smaller than". Imagine also that the nucleus has, in fact, a neutron-rich surface so that the "neutron nucleus" is bigger than the "proton nucleus". In this case bombardment of the nucleus with positive pions will see chiefly the neutron nucleus while bombardment with negative pions will see chiefly the proton nucleus. Since the neutron nucleus is bigger than the proton nucleus the cross-section for positive pions will be bigger than that for negative pions. In fact, at a pion energy of about 700 MeV $\sigma_{\pi-p}$ is more than twice as big as $\sigma_{\pi+p}$. Under these circumstances calculation shows a 6 to 8% difference in $(\sigma_{\pi-} - \sigma_{\pi+})/\sigma_{\pi+}$ for a heavy nucleus depending on whether the neutrons and protons occupy the same region of space or whether there is a neutron-rich surface such as would correspond to the central density being the same for neutrons and protons. It is now 10 years since the theory was worked out [1] and the experiments performed [2] showing that, within experimental accuracy, the neutron and proton distributions have the same radius and there is no significant skin of either type of nucleon on the surface.

(ii) *Elastic neutral pion photoproduction*

We know quite well the distribution of protons in the nucleus from the elastic scattering of high-energy electrons, particularly the work of HOFSTADTER at Stanford. We have, however, rather little information on the distribution of matter in the nucleus, that is to say, neutrons and protons without regard to their charge. A nuclear reaction that does not basically distinguish between neutrons and protons is the photoproduction of neutral pions. If this is carried out elastically from a complex nucleus, that is to say, leaving the target nucleus in its ground state, then the process is a coherent one and the angular distribution of the resultant neutral pions represents the coherent superposition of the production amplitudes from all the individual nucleons; the angular distribution therefore depends, in the usual way of a diffraction pattern, on the spatial distribution of the nucleons. Careful measurement of this angular distribution then gives information about the matter distribution. These experiments have been done [3] and show an essentially-identical distribution for the matter as for the protons revealed through elastic electron scattering: there is no marked preponderance of either type of nucleon on the surface.

(iii) *Absorption of K^--mesons*

When a negatively-charged particle is slowed down in matter it eventually falls under the influence of a particular atom and spirals in towards the nucleuss passing through a very large number of quantum orbits and proceeding inwarde by a combination of Auger and radiative transitions. At first the Auger process will be the stronger but later radiative transitions will take over. At this stag, we should expect the orbits, semi-classically speaking, to become more and more circular because at each stage of the radiative process there will be a tendency to make the transition to the state of highest statistical weight, namely that of highest allowed l-value. It is anticipated that the orbits will become circular before the nucleus is closely approached and so the final capture will take place from states of $l = n - 1$. In the case of K$^-$-mesons, the absorption is so very strong that one may easily calculate that the absorption will, in fact, take place at the edge of the nucleus where the nucleon density is low [4]. This region we might term the "nuclear stratosphere". The absorption products therefore bring us information about the composition of this stratosphere. The absorption of K-mesons on single nucleons goes by the following processes:

$$\begin{aligned} K^- + p \to\ & \Sigma^- + \pi^+ \\ & \Sigma^0 + \pi^0 \\ & \Sigma^+ + \pi^- \\ & \Lambda^0 + \pi^0 \\ K^- + n \to\ & \Sigma^- + \pi^0 \\ & \Sigma^0 + \pi^- \\ & \Lambda^0 + \pi^- \end{aligned}$$

We see that, although absorption on protons can lead either to Σ^+ or to Σ^- absorption on neutrons cannot make Σ^+ but of the charged Σ-hyperons only Σ^-. The production of Σ^+ in K$^-$-meson absorption therefore signals the presence of protons in the nuclear stratosphere. Interpretation of the experiments is still somewhat complicated by our lack of complete knowledge of the elementary particle constants involved, but, so far as we can see at the moment, the results are completely consistent with there being the same $N : Z$ mixture of neutrons and protons in the stratosphere as there is in the depths of the nucleus.

These three elementary-particle approaches to this question are totally different the one from the other but all agree on the answer, namely that the nuclear surface is not noticeably richer in one sort of nucleon than the other and is most probably of about the same composition as average nuclear matter. This is already something of considerable nuclear structure interest that we know about essentially only from the elementary-particle experiments.

We will now look systematically but far from exhaustively at some kinds of information that some of the various elementary particles can bring us about nuclear structure.

Muons

The muon is a magnificent probe for the nucleus because it is so weakly coupled to the nucleon field. Interpretation of the $g - 2$ experiments on the muon show that $G^2/4\pi < 10^{-3}$. We can therefore neglect the nuclear interaction of the muon completely by comparison with its electric interaction. In this respect the muon is just like an electron but its greater mass brings it certain advantages.

Muonic atoms: nuclear charge distribution

The distribution of charge within the nucleus is a matter of intense interest. At the moment our chief knowledge about this comes from the elastic scattering of energetic electrons but the energies of muonic X-rays are also, in principle, capable of telling us a lot about the charge distribution. Because the muon is 200 times heavier than the electron its orbit is proportionally smaller and may be comparable with the size of the nucleus. The electric field within which it moves cannot then be taken as that of a point charge; the finite size of the nucleus is significant and there is a level shift from the value calculated for a point nucleus.

In the first approximation one treats the entire nuclear size as a perturbation, finding a level shift for the muonic atom of:

$$\Delta E = \frac{2\pi}{3} Z\alpha^2 \, |\Phi(0)|^2 \, \langle r^2 \rangle .$$

Here $\Phi(0)$ is the Schrödinger point-nucleus solution for the muon's wavefunction. In this approximation the experiments tell us only $\langle r^2 \rangle$ which does not put them into competition with electron scattering which is already sensitive to two parameters that measure the radius and the surface thickness.

To investigate the potentiality of the muonic X-ray method in more detail we must make an exact solution of the muon wavefunction in whatever charge distribution we care to investigate. The classical charge distribution for such purposes is the FERMI or SAXON—WOODS form:

$$\varrho(r) \sim [e^{(r-R)/a} + 1]^{-1} .$$

For this form of distribution for Pb using the values of R and a deriving from electron scattering a 10% change in the radial parameter R changes the energy of the $2p_{3/2}$ to $1s_{1/2}$ transition by 8,2%. Similarly a 10% change in the surface thickness parameter a changes the same transition energy by 1,1%.

We must now pause and ask ourselves how accurately can we hope to measure these muonic X-ray energies. Given sufficiently-intense beams of stopping muons we can apply either crystal spectrometer methods or Ge(Li) counter methods. These methods offer us an ultimate accuracy of perhaps 0,1 keV for the X-ray energies involved provided that the problem of calibration can be solved. It superficially appears, then, that the distribution parameters can be determined with enormous accuracy since the transition energies in question in the heavier elements are of the order of 6 MeV. This, however, is wholly illusory because we must determine both parameters at the same time and not assume that one of them is known a priori. In fact we are immediately led to ask whether we should not introduce a third parameter into our description of the charge distribution. The electron-scattering experiments are just beginning to become sensitive to a possible third parameter and so if the muonic X-ray work is to be competitive with the electron scattering it too must demonstrate a sensitivity to a third parameter. Consider the form:

$$\varrho(r) \sim [1 + \alpha r^2]/[e^{(r-R)/a} + 1] .$$

We will investigate the following reasonable ranges for the three parameters: a : (0,5 to 1,5) F; R : (1,0 to 1,2) $A^{1/3}$ F; α : (0 to 1,25) $(A^{1/3}\ F)^{-2}$. This form of charge distribution is taken to represent the tendency in a heavy nucleus for the mutual Coulomb repulsion of the protons to have some effect. Within these parameter ranges the energy for the $2p_{3/2}$ to $1s_{1/2}$ transition in Pb may change by as much as 1 MeV. Consider first the $2p_{3/2}$ to $1s_{1/2}$ transition. If this transition energy were known precisely then the whole range of variation of the parameters in the above expression would correspond to variations in the energy of other transitions by a few tens of keV. If, in addition, we knew the $3d_{5/2}$ to $2p_{3/2}$ transition energy precisely, then the above parameter range corresponds to a variation in energy of the $2s_{1/2}$ to $2p_{3/2}$ transition by about 2 keV [5]. Since we are hypothesizing an accuracy of 0.1 keV we see that, in principle, it may be possible to make a three-parameter determination to an accuracy of several percent on each of the three parameters. This would, of course, be extremely valuable although we must not forget the arbitrariness in the choice of the aspects of the charge distribution that we choose to parameterize. This corresponds to some doubt as to the relationship between our inferred distribution and physical reality and emphasizes the desirability of having available complementary approaches of comparable sensitivity — muonic X-rays and electron scattering in the present example.

Even before we doubt the relevance of the analysis to the real world we must examine critically various factors that might disturb the analysis. We have assumed that the problem is exactly described by the solution of the Dirac equation in the field of a structured but inert and unresponding nucleus. Both these assumptions must be questioned. As to the first one, our present level of understanding suggests that all we need to do is to allow for vacuum polarization; although this correction considerably exceeds the 0,1 keV of our assumed accuracy of measurement, it is well understood and we will take it that the correction can be made sufficiently exactly not to disturb the analysis as we have presented it so far.

A more serious difficulty is represented by the assumption that the nucleus is inert, is unaffected by finding itself in the electric field of the muon. This is obviously not correct and we must estimate, using second order perturbation theory, the shift in the muonic energy levels to be associated with excitation of the nucleus into and out of all possible virtual states. In other words, we must evaluate the shift:

$$\Delta E_k = \sum_{n,\mu} \frac{\langle \Psi_0 \Phi_k | H | \Psi_n \Phi_\mu \rangle \langle \Psi_n \Phi_\mu | H | \Psi_0 \Phi_k \rangle}{(E_0 + E_k - E_n - E_\mu)}$$

n, μ are the intermediate nuclear and mesonic states; Ψ and Φ are the nuclear and muonic wavefunctions; H is the muon-nucleus interaction Hamiltonian. Present calculations of this polarization shift for the $1s_{1/2}$ level in Pb range from 58 keV to 8,2 keV [6]. While the reason for this large range of theoretical result is understood in terms of the different sorts of approximation involved in the different calculations the fact that the correction is so enormously greater than the accuracy with which we have imagined the measurements can be made and interpreted is very worrying. It is not at the moment clear what can be done about this problem. Of course, it may be possible to tackle it to some degree semi-empirically by comparison of neighbouring elements, neighbouring transitions, and so on, but it is clear that it introduces a considerable complication into our attempts to extract a third parameter of the charge distribution by these methods. We may even be tempted to invert the process: say that we know sufficient about the charge distribution from the electron scattering measurements to use the muonic X-ray data for telling us something about nuclear polarization. It would indeed be interesting to know if there is any systematic dependence of nuclear polarizability on various parameters such as nearness to closed shells, deformation and so on.

Quadrupole effects

Other effects disturb the simple analysis but also bring us information of importance in their own right.

Consider quadrupole effects. In ordinary atoms the quadrupole splitting is seen as a perturbation of the magnetic hyperfine structure. In the case of muonic atoms the quadrupole effect dominates. This is because the ratio of the quadrupole effect to the hyperfine splitting is approximately: $[e^2 Q_n / r^3] / [\mu \mu_n / r^3]$ which has the value of about 200 for muons as against approximately unity for electrons because the muon's magnetic moment is about 200 times less than the electron's. In the case of muonic X-rays we have, therefore, the opportunity to gain information about the nuclear quadrupole moment with a directness that is denied us for electrons. If we consider the $2p$ to $1s$ transitions we should, in general, if the nuclear spin allows it, find not the two transitions $2p_{3/2}$ to $1s_{1/2}$ and $2p_{1/2}$ to $1s_{1/2}$ that arise if we neglect the quadrupole moment but rather five, from which the quadrupole moment may be extracted.

An interesting effect comes about owing to the coupling between the muon and the nucleus. This coupling implies that it is possible, in the course of the X-ray cascade, for the muon actually to excite the nucleus into a real excited state. This will be particularly likely in the heavy elements which have low-lying rotation states with large $E2$ transition moments and excitations comparable with the $2p_{3/2} - 2p_{1/2}$ splitting. This means that the five lines expected if this effect is neglected will become ten, five of which are associated with the real excitation of the nucleus. It turns out that the nuclear transition strengths and spacings are such that in certain heavy nuclei these two groups of five transitions may be of comparable intensity. Since this excitation can come about in a nucleus which has $J = 0$ in its ground state, we are able to measure quadrupole moments in nuclei that do not normally permit of such a measurement.

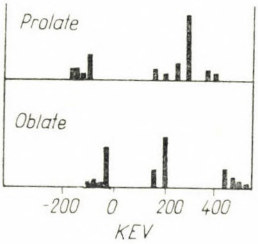

Fig. 2

An important and exciting point is that the distribution of the quadrupole splitting is sensitive to the *sign* of the quadrupole moment and not just to its magnitude. This is illustrated in Figure 2 which shows approximately the distribution and relative strength of the quadrupole-split transitions calculated for Th^{232} on the two assumptions: that the nucleus is prolate and that it is oblate. As may be seen the patterns for the two signs are very different and so comparison with experiment reveals the sign of the quadrupole moment which it is extremely difficult to determine by any other type of experiment. This in itself may be a matter of considerable importance and justify considerable effort in the measuring of muonic X-rays.

Magnetic splitting

The magnetic splitting is usually much smaller than the quadrupole splitting for muonic atoms but in the $1s_{1/2}$ state of heavy atoms the magnetic splitting may be as big as 1 to 5 keV with no complications from quadrupole splitting. This magnetic splitting should be measurable. If all that it told us were the magnetic moment of the nucleus there would be nothing to be excited about. However, in the heavy elements the $1s_{1/2}$ state lies to a large degree inside the nucleus so the magnetic splitting is determined not by the overall magnetic moment but involves the *distribution* of magnetic moment within the nucleus. This again is something that is extremely difficult to get at by conventional means and so there may be here also a considerable field for exploiting muons.

We may note in passing that it is in principle possible to make these magnetic measurements on the particle-bound excited states of nuclei by resonant scattering of muons [7]. There is an elastic scattering process in which the incident muon is captured into its $1s_{1/2}$ orbit with accompanying excitation of the nucleus into a definite state followed by ejection from the orbit and simultaneous de-excitation of the nucleus. This will be a resonant process of large cross section ($\approx \pi \lambda^2$) but very small width; it will show the magnetic hyperfine splitting due to the magnetic moment of the excited nuclear state: there will not be one resonance for each excited state but rather two, corresponding to the two orientations of the muon spin relative to that of the nucleus. This hyperfine splitting is then a measure of the distribution of magnetic moment in the excited state of the nucleus. It is not clear whether such measurements will ever be feasible in practice but in principle they open up another great and important field.

Nuclear diamagnetism

We may finally note the possibility of measuring nuclear diamagnetism using muons [7]. It will obviously be most interesting for nuclear structure work to know quantitatively the degree to which the nucleus is diamagnetic. Dimensionally we may expect an induced magnetic moment of about 10^{-17} H nuclear magnetons in a field of H gauss. For $Z = 20$ one nuclear magneton in the nucleus corresponds to a field of about 10^{13} gauss at the muon orbit. Therefore at the muon orbit, owing to the nuclear diamagnetism, we may expect a field of about 10^{-4} H gauss. This may be a just-measurable effect on the muon's precession frequency. This effect increases rapidly with Z. Again we may note that in principle we are sensitive to the spatial distribution of the induced diamagnetic moment.

Muon capture

The capture of negative muons by the nucleus is a weak interaction and is sensitive to the details of the nuclear wavefunction. At the moment, this process is too much bedevilled by our uncertainties about the basic muon capture process itself to begin to use it seriously as a tool for probing nuclear structure. We are still in the stage of using nuclei whose properties we believe we understand fairly well to learn about the muon and its interactions. When these are sufficiently well understood the process can be reversed and can in principle yield important information. In certain limited cases useful information could be had already if sufficiently intense muon sources were available. For example, the reaction $d + \mu^- \rightarrow 2n + \nu$ with simultaneous energy and angle measurement on both neutrons would bring valuable information about the nn interaction.

Inelastic scattering

Muons may also be useful for more conventional types of experiment. For example, muon inelastic scattering will be very much like electron inelastic scattering and will be valuable in bringing us information about nuclear wavefunctions and matrix elements. In this muons have the advantage over electrons that their bremsstrahlung is very much less; this will make possible certain types of investigation closed to electrons. Another technical advantage is that muons have more momentum for a given energy than electrons and so better energy resolution is available for a given momentum transfer. Muons are complementary to electrons in inelastic scattering experiments in that they explore different regions of energy-loss-momentum-transfer space.

Pions

The pion is the quantum of the nuclear force field, or at least of its tail, and so might be expected to be of direct relevance to the problem of nuclear structure. This, however, is not so, at least for this decade, but it is still very valuable as spinless, strongly-interacting $T = 1$ energy.

Elastic scattering

Little seems likely to come in the immediate future from elastic scattering optical model studies in the way of nuclear structure information. Confrontation with calculation based on the empirical pion-nucleon interaction is obviously interesting in its own right and is in principle an approach to correlation effects. There are, however, many complications; the way is only now becoming clear for a programme with the specific objective of telling us about nuclear structure.

Pionic atoms: nucleon-nucleon correlations

A matter closely related to elastic scattering that does hold more immediate promise of yielding important data is the study of pionic atoms. By studying the pionic X-rays we can measure directly the width and infer the shift of the 1*s*-level and can infer the shift of the 2*p*-level. Indirectly (from the X-ray intensities) we can determine the 2*p*- and 3*d*-widths. These shifts are due to the attraction or repulsion exerted on the pion by the nucleus and the widths are due to the absorption of the pion by the nucleus. We can compare the inferred magnitude of the force and the absorption with what we expect on the basis of various empirical pion-nucleon interactions and so infer something about the condition of the nucleons inside the nucleus, particularly their correlations.

To do this we must obviously have a theory that predicts the pion-nucleus optical model potential in terms of πN and πNN free space interactions. This theory is very difficult to make and it has not yet been done unambiguously. We may illustrate the way in which the calculation might go from the work of ERICSON and ERICSON [8]. The potential importance of pionic X-ray studies for giving us information about nuclear structure does not depend on the detailed correctness of this particular calculation; here we just use it as an illustration of the degree of sensitivity that the experiments might have to certain details of the nuclear wavefunction. ERICSON and ERICSON first of all derive that part of the optical model potential that is due to the multiple scattering of the pion on single nucleons; i.e. coming from the πN interaction. They write down the multiple scattering equations, truncate at the pair correlations and find in the nonrelativistic limit:

$$V(r) = \frac{-4\pi\hbar^2}{2\mu}\left[b\varrho(r) - \vec{\nabla}\cdot \frac{c\varrho(r)}{1+\dfrac{4\pi}{3}\,c\varrho(r)}\,\vec{\nabla} \right].$$

(This derivation assumes very short range correlations and negligible nuclear excitation energies.) The first term in this expression is a local potential that arises from the *s*-wave πN interaction. The second term is non-local or velocity dependent and comes from the *p*-wave πN interaction which for low energy pions is strong and attractive (the (3,3) resonance at a bombarding pion energy of about 200 MeV) as against the weak and repulsive *s*-wave πN interaction. The nonlinearity of the second term depends on the correlations and is the analogue of the LORENTZ—LORENTZ effect (the nonlinear dependence of refractive index on density for light passing through a dense homogeneous medium of polarizable atoms); as **Ericson** and **Ericson** have picturesquely pointed out, a low energy pion behaves somewhat like a strongly interacting photon. We must also consider the explicitly-two-nucleon scattering amplitude, coming from the πNN interaction, which contains terms such as $\{B + C\,\vec{k}_i \cdot \vec{k}_f + \ldots\}$ (the ks are the initial and final pion momenta). Here again the first term is local, coming from s-waves, and the second is non-local, coming from p-waves. The overall local interaction (which includes both the πN and the πNN terms) is determined to be, as expected, repulsive, from the 1s-shift. The 2p-shift shows an attractive force and with the local interaction already determined by the 1s-shift, enables us to get a measure of the non-local interaction. The widths are due to absorption and so determine the imaginary parts of the two-nucleon amplitudes (the contribution to absorption from the one-nucleon terms is negligible). The 1s-width determines ImB. The 2p- and 3d-widths then give ImC. These quantities may now be compared with expectation based on the free πN scattering cross sections and information about the πNN interaction deriving from reactions such as:

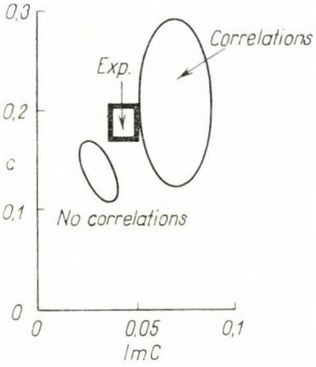

Fig. 3

$$p + p \to \pi^+ + d\,; \qquad p + p \to \pi^0 + p + p\,.$$

The calculated values of the shifts and widths obviously depend on the assumptions made about the nucleon-nucleon correlation inside the nucleus. Fig. 3 shows the comparison between the expectation based on the πN and πNN interactions both with and without a degree of nucleon-nucleon correlation inside the nucleus such as would correspond to the effect of the conventional hard core of the nucleon-nucleon interaction. It is seen that better agreement is obtained on the assumption of the reasonable short-range anti-correlation than for an uncorrelated nuclear wavefunction.

As was remarked earlier, we cannot interpret these experiments at the moment as proving the existence, inside the nucleus, of the expected nucleon-nucleon correlation because the theory is not yet free of ambiguities; the experiments are also rather crude. The purpose of the present comparison is to illustrate the sensitivity of the measurements to the nuclear-structure parameter of interest. It is clear that important information can be got from a more detailed experimental and theoretical study of pionic atoms.

Nuclear absorption

Another use that has already been made of pions and that can be considerably extended is the study of the details of their absorption by nuclei. Consider absorption of negative pions at rest. The pion brings a considerable amount of energy (about 140 MeV) into the nucleus on absorption but negligible momentum. The energy is ultimately transmitted to nucleons which must therefore leave the nucleus with considerable energy and momentum. Since the pion provides no momentum the momentum must come from the interaction of the nucleons with each other, either in the initial or the final state. Since the momentum involved is considerably higher than the Fermi momentum inside the nucleus, we should expect single nucleon absorption, in which the recoil is essentially taken up by the optical model potential of the rest of the nucleus, to be rather unlikely and the commonest event to be one of absorption on a closely-correlated nucleon-nucleon pair; the final state momentum then derives from the nucleon-nucleon rather than from the nucleon-nucleus interaction. In this case nucleons should emerge from such absorption events in pairs correlated very roughly at 180° to each other. If the nucleus is light it is quite likely that both members of the nucleon pair will emerge and will carry with them a fairly good memory of the momentum state associated with the primary absorption process. In heavier nuclei final state interactions of the nucleons with the rest of the nucleus on the way out will become important and it will be more difficult to derive information about the primary absorption process from the final products. Such nucleon pairs, with the expected strong anticorrelation, have been known for some considerable time [9] but have more recently been studied in greater detail. Their angular correlation, if the final state interaction can be understood, will give information about the momentum distribution of the absorbing pair itself inside the nucleus and this in turn is an important parameter, related, for example, to the degree of three-particle clustering.

What do we learn from the nature of the emergent nucleon pairs? The negative pion may be absorbed either by a pair of protons or by a neutron-proton pair. In the first case what we see emerge is a fast anticorrelated neutron-proton pair and in the second case a similar neutron-neutron pair. Off-hand we should expect there to be something like four times as many neutron-neutron final-state pairs as neutron-proton final-state pairs. This is because the capturing neutron-proton pair may be in either a triplet or a singlet state whereas the capturing proton-proton pair must be in a singlet state. This assumes that the chief NN states operative in the nucleus are s-states following the observed feebleness of the p-state interaction in free NN collisions. If, however, the p-state interaction were strong inside the nucleus, then the neutron-proton final-state pairs would be relatively boosted because the statistically-weighty triplet p-state would then be admitted for the initial proton-proton interaction. The possibility that the effective residual nucleon-nucleon interaction inside the nucleus is significantly different from the free nucleon-nucleon interaction is an extremely important and open nuclear structure question. We should therefore be very eager to pursue any investigation, such as the one now being discussed, which promises to bring us news about the nucleon-nucleon interaction *inside* nuclear matter.

In fact experiments show an excess of neutron-neutron final-state pairs over the number expected by mere counting. This may superficially appear to suggest that the triplet s-state interaction, operative only for neutron-proton absorbing pairs, is stronger at the distances of about 0,5 F relevant for this absorption process than the singlet s-state interaction. This would be an important conclusion. However, we have here an example of the caution that must be exercised in interpreting the results of elementary-particle-nucleus interaction experiments. The point is that the simple expectation that we have just described is based on the assumption that the pion is absorbed by that nucleon of the correlated pair with which it first interacts. We must, however, recognize the possibility that rescattering may be important: the pion scatters off the first nucleon of the correlated pair and is absorbed by the second. There are many diagrams that contribute to this type of high order process, This process may come about most simply, however, through a $\Phi\pi$ or $\Phi\Phi$ term in the Hamiltonian (where Φ represents the meson field and π is the conjugate field operator). That is to say, the initial interaction may be scattering without or with charge exchange. This rescattering mechanism would boost the triplet s-state absorption relative to the singlet s-state absorption because charge exchange contributes to the former but not to the latter. We therefore here have an alternative reason why the final-state neutron-neutron pairs are more abundant relative to the final-state neutron-proton pairs than we find by mere counting, and in this case we are learning nothing about the relative strengths at short distances of the NN interactions. In fact the rough magnitude of the rescattering phenomenon may be estimated using information from the $p + p \rightarrow \pi^+ + d$ and $p + p \rightarrow p + p + \pi^0$ reactions near threshold and appears to be of about the right size to explain the experimental π^--capture data.

We must obviously be careful about making a too-naive interpretation of experiments of this kind.

Other correlations

We have mentioned the use of negative-pion absorption to look for np and pp correlations. It will be also interesting to use finite but low-energy positive pions in reactions such as (π^+, np) and (π^+, pp) to supplement the information coming from the negative-pion absorption at rest.

We may finally note the possibility of using pion absorption to look for three-nucleon correlations with clusters such as:

$$\pi^+ + npp \rightarrow 3p\,,$$
$$\pi^- + ppp \rightarrow n + 2p\,.$$

Pion production

Other possible uses of pions are legion: for example the reaction $p + \begin{pmatrix} N \\ Z \end{pmatrix} \rightarrow \begin{pmatrix} N+1 \\ Z \end{pmatrix} + \pi^+$ for large momentum transfer is sensitive to the nucleon-nucleon correlation inside the nucleus and important information will be forthcoming particularly when the residual nucleus $\begin{pmatrix} N+1 \\ Z \end{pmatrix}$ is left in an identified state. Pion production from a complex nucleus below its threshold for free NN collisions will also tend to show up high momentum states in the target nucleus wavefunction (this is true of any production process).

Inelastic scattering

Pions possess certain advantages for straightforward inelastic scattering work in that they are spinless and are distinguishable from nucleons. Since pions are of $T = 1$ they can excite transitions of $\Delta T = 2$ and so may show up new forms of collective motion and can reach states difficult of access by other methods. $(\pi, \pi\gamma)$ reactions may have certain advantages for wavefunction studies over the corresponding nucleon-induced reactions since there is no spinflip possible for the bombarding pion.

Double charge exchange

The charge-exchange possibilities with pions also open up interesting fields. Of particular interest may be the double charge exchange reactions: $(\pi^\pm, \pi^\mp)$. With low energy pions we will tend to excite low-lying analogue states. It is not at the moment clear what nuclear structure information may be obtained from this although it will be interesting to look for the $T \cdot \tau$ term in the pion-nucleus potential. It will be interesting to discover whether the double charge exchange is to be associated with an isotopic tensor term in a two-nucleon effect or with the repeated application of the isotopic vector term. Such reactions should give information about nucleon-nucleon correlations if they can be interpreted unambiguously.

A further possibly-interesting use for pion double charge exchange is to reach systems that are otherwise very difficult to study. Some examples are:

$$\begin{aligned} &\mathrm{He}^3\,(\pi^-, \pi^+)\,3n\,, \\ &\mathrm{He}^4\,(\pi^-, \pi^+)\,4n\,, \\ &\mathrm{H}^3\,(\pi^+, \pi^-)\,3p\,, \\ &\mathrm{Li}^7\,(\pi^-, \pi^+)\,\mathrm{H}^7\,. \end{aligned}$$

Intrinsic nucleon magnetic moments

We have already discussed the elastic photoproduction of neutral pions as an approach to the problem of the matter distribution within the nucleus. Other sorts of photoproduction may also, in principle, yield valuable information. Much information of importance for nuclear structure is locked up in the many very accurate values of nuclear magnetic moments that we now possess. Unfortunately interpretation of these accurate data is bedevilled by our ignorance of the degree to which the mesonic exchange currents within the nucleus that are responsible for the nucleon binding concomitantly modify the nucleon intrinsic magnetic moments. It is clear that some such modification must take place, but it is unclear how important this effect may be. It is very difficult to disentangle this modification of the intrinsic magnetic moments from the detailed effects of the nuclear wavefunction that we want to use the overall magnetic moment to probe, particularly when one must recognize the likely importance of considerable amounts of two-particle-two-hole excitation and other forms of configuration interaction. An experiment that bore directly on the question of the nucleon intrinsic magnetic moments *inside* the nucleus would be extremely valuable. In principle, one can approach this problem through pion photoproduction since the reaction $\gamma + N \rightarrow \pi + N$ involves directly the intrinsic nucleon magnetic moments [11]. If we may treat pion photoproduction from a complex nucleus in the impulse approximation, if it is from single nucleons and if we may neglect the importance of final state interactions, then a comparison of that photproduction, particularly the nucleon polarization with the corresponding reaction on free nucleons gives us a measure of the desired nucleon intrinsic magnetic moment inside the nucleus. This determination is independent of the coupling scheme operative within the nucleus and of configuration mixing and so on. The difficulty here is the detailed assumptions that we have to make and on which it is very difficult to make a check. It is particularly doubtful whether the final state interactions will be sufficiently weak to enable the outgoing nucleon to carry away memory of its initial polarization without significant modification. However, systematic studies involving many nuclei may possibly enable the various disturbing effects to be unravelled.

Prospecting

We know very little about nuclear disintegrations provoked by pions. There may be unsuspected and revealing systematic phenomena to be found. It is worth looking to see.

The use of strange particles

Hypernuclei

When K^--mesons are absorbed by nuclei the initial act of absorption, which may be for example: $K^- + N \rightarrow \Lambda^\circ + \pi$, is often followed by a further process of Λ°-hyperon-capture to form a hypernucleus in which the Λ°-hyperon substitutes for a neutron. An example of such a reaction is: $K^- + \mathrm{He}^4 \rightarrow \rightarrow \mathrm{He}^4_\Lambda + \pi^-$. The absorption of Σ-hyperons may similarly produce hypernuclei following the basic interaction: $\Sigma + N \rightarrow \Lambda^\circ + N$. Hypernuclei are objects of intense interest in their own right; their study falls outside the scope of this present examination although we may note in passing that it may bring us information about the wavefunctions of ordinary nuclei, the cores to which the Λ°-hyperons are bound, as well as information about hypernuclei.

A possibly-important use of hypernuclei may be to study the stability of systems that are just unstable in the free state. The addition of a Λ°-hyperon may, by its binding to nucleons, stabilize an unstable nucleon system; our understanding of the Λ° N, $\Lambda^\circ NN$ force may then enable us to make deductions about the properties of the unbound nucleon core of the particle-stable hypernucleus. For example, the unstable nucleon systems n^3, n^4, H^4, H^5, He^7 may serve as the cores of the possibly-particle-stable hypernuclei n^4_Λ, n^5_Λ, H^5_Λ, H^6_Λ, He^8_Λ. These hypernuclei could be identifiably formed in, for example, the following reactions:

$$\begin{gathered}
\Sigma^- + \mathrm{He}^4 \rightarrow n^4_\Lambda + p\,, \\
K^- + \mathrm{He}^4 \rightarrow n^4_\Lambda + \pi^+\,, \\
\Sigma^- + \mathrm{Li}^6 \rightarrow n^5_\Lambda + 2p\,, \\
K^- + \mathrm{Li}^6 \rightarrow n^5_\Lambda + \pi^+ + p\,, \\
K^- + \mathrm{Li}^6 \rightarrow \mathrm{H}^5_\Lambda + p\,, \\
K^- + \mathrm{Li}^7 \rightarrow \mathrm{H}^6_\Lambda + p\,, \\
K^- + \mathrm{Li}^6 \rightarrow \mathrm{H}^6_\Lambda + \pi^+\,, \\
K^- + \mathrm{Li}^7 \rightarrow \mathrm{H}^6_\Lambda + p\,, \\
K^- + \mathrm{Be}^9 \rightarrow \mathrm{He}^8_\Lambda + p\,.
\end{gathered}$$

Another important property of hypernuclei is that they can, in their decay, populate high isotopic spin states that are difficult of access by other means. For example, the decay $\mathrm{He}_{\Lambda}^{4} \rightarrow \mathrm{Li}^{4*} + \pi^-$ can populate $T = 2$ states of Li^4 which may show up as sharp states revealed by a monokinetic π^--group [12]. Such states may be sharp because their decay is inhibited either by isotopic spin or by kinematic factors.

It is possible that a study of excited states of hypernuclei may bring us information about radiative transition probabilities of the hypernucleus cores that it is very difficult to obtain by other means. Consider, for example, the first excited $J^\pi = 2^+$ state of He^6 at 1,71 MeV. It is very important to determine the lifetime of this state for its electric quadrupole transition to the ground state of He^6 since, according to the simple shell model configuration, $(1s_{1/2})^4\,(1p)^2$, the radiation is due to two neutrons only and so the lifetime should be extremely long (infinite if one uses harmonic oscillator wavefunctions which must be quite a good approximation to the truth here). However, we know from experience in light nuclei that $E2$ transitions take place much more readily than the simple shell model suggests and, by analogy with the notorious case in O^{17}, we might guess that this $E2$ lifetime now under consideration will not be as long as we should predict from the simple model. Since this He^6 system is so extremely simple we have a good chance of carrying out the kind of explicit configuration-interaction calculation that is necessary if we are to understand the detailed mechanism of these $E2$ enhancements. Unfortunately, the state in question is unstable against disintegration $\mathrm{He}^6 \rightarrow \rightarrow \mathrm{He}^4 + 2n$ and so there is no chance of measuring the lifetime directly. However, when a Λ° hyperon is attached to He^6 it forms the particle-stable hypernucleus $\mathrm{He}_{\Lambda}^{7}$, the first excited state of which is probably also particle-stable and may be thought of as the first excited state of He^6 to which a Λ°-hyperon has been attached. If, as is likely, this excited He^7 state has $J^\pi = 5/2^+$ its radiative de-excitation to the $J^\pi = 1/2^+$ ground state will be closely related to the $E2$ transition in He^6 that we are discussing. An interesting and amusing aspect of the situation is that He^7 contains its own built-in clock in the form of the decay of the Λ°-hyperon $\Lambda^\circ \rightarrow N + \pi$ which will be competitive with the radiative de-excitation. A measurement of the branching ratio of the excited $\mathrm{He}_{\Lambda}^{7}$ state as between gamma-emission and hyperon decay therefore gives us a measure of the lifetime for the radiative process. We must, of course, be able to take into account the effect on the hyperon decay lifetime of its binding into the hypernucleus but this can be rather accurately estimated from lifetime studies on hypernuclear ground states.

The texture of the nuclear surface

We have already discussed one aspect of the capture of stopped K^--mesons by complex nuclei. We explained that the capture may well be peripheral, in the nuclear stratosphere, and that this capture can therefore bring us information about the state of the nucleus in its tenuous outer reaches. An experimentally-interesting aspect of this capture is that it occurs very frequently (about 20% of the time) not mesonically on single nucleons through reactions such as $K^- + N \rightarrow \Lambda$ or $\Sigma + \pi$ but by non-mesonic absorption on correlated nucleon pairs by the reactions: $K^- + NN \rightarrow \Lambda$ or $\Sigma + N$. The probability of such non-mesonic capture is very closely the same in complex nuclei as it is in He^4. If the capture is indeed peripheral this can only mean that in the tenuous outer reaches of the nucleus nucleons are as closely correlated as they are in the alpha-particle. The nuclear stratosphere is therefore not composed of a more-and-more-tenuous gas of single nucleons getting further and further apart but rather of sub-nuclear entities that we might tentatively label "alpha-particles"; these are presumably constantly dissolving and falling back into the body of the nucleus and reforming elsewhere in the stratosphere [13]. If this is true it is obviously nuclear structure information of the very first importance: the surface of the nucleus is not "smooth" but "knobbly".

It must be said at once that there is some evidence that K^--meson capture at rest is not in fact peripheral but takes place in the body of the nucleus in which case the present considerations are not relevant. Whether or not the capture is peripheral may be determined by studying the K-mesonic X-rays in just the same way as the muonic and pionic X-rays have been studied as already discussed: if the K-mesonic X-rays seen correspond to transitions between circular orbits and terminate as expected for peripheral capture then the case is proved. It is worth noting that if the normal capture process is found to be not overwhelmingly peripheral then we can still select out cases of surface capture by gating our detector for the absorption products on the appropriate K-mesonic X-ray, i.e. one corresponding to a transition to a circular orbit from which capture is overwhelmingly more probable than a further radiative transition. In this way it will be possible to filter from the bulk of the absorption process just those that are peripheral; this complicates the experiments but adds no difficulty of principle.

High momentum states

It is possible to look for high momentum states in strange particle absorption processes, for example the reaction: $C^{12} + K^- \rightarrow C^{11} + \Sigma^-$ in which the C^{11} is left intact in an identified state signals high momentum in the absorbing neutron. Similarly the reaction: $C^{12} + \Sigma^- \rightarrow B^{12} + \Lambda^\circ$ may be used for looking for a high momentum proton. These two types of reaction are complementary in that they are sensitive to different high momentum states.

Three-body forces

A section of nuclear structure physics about which we are quite astonishingly ignorant is the importance of three-body forces. We attempt to discuss the properties of complex nuclei as though only two-body forces operated between nucleons. We know very well that three-body forces must exist but have effectively no idea at all at the moment about their importance relative to two-body forces. The closest studies of the three-body systems, H^3 and He^3 are not yet good enough to approach this problem. If three-body forces exist they will tend to favour triangular nucleon configurations in which the momentum is shared more or less equally among the three nucleons. If we consider for example the reaction: $He^3 + K^- \rightarrow \Sigma^- + 2p$ using stopped K^--mesons then if two-body forces are dominant we shall expect to find final states consisting of a Σ-p pair in a high momentum state with the further proton as a low-momentum spectator. If three-body forces are important they will show up in events in which all three particles in the final state have high momentum. The analysis will be complicated as usual by the possibility of initial two-nucleon absorption followed by high momentum being transferred to the originally spectator particle by a final state collision with one of the original pair. However, in so simple a system as He^3, we have a chance to sort this out and still to pinpoint the three-body forces if they are at all reasonably strong. (We may note that pion absorption is also a possible way of looking for these correlations but K^--meson absorption will be easier to analyze since all final-state particles are then charged. The reaction: $\pi^+ + He^3 \rightarrow 3p$ also produces all charged particles in the final state but is not so satisfactory because the incident pion must now bring in significant momentum and so increases the probability of a more-or-less-equal sharing of the momentum in the final state among the three product particles.)

Conclusion

This has only been a light and selective passage over some of the ways in which elementary particles may be used as nuclear probes. Significant information may be had in other ways, for example by the use of antiprotons and, when sufficient fluxes are available, of neutrinos. There is no doubt that here is a field of considerable richness whose exploitation only awaits the making available of adequate resources.

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О НЕКОТОРЫХ ИСПОЛЬЗОВАНИЯХ ЭЛЕМЕНТАРНЫХ ЧАСТИЦ В ИЗУЧЕНИИ СТРУКТУРЫ ЯДЕР

Д. Г. УИЛКИНСОН

Резюме

Дается специальный обзор нескольких приемов, в рамках которых «элементарные частицы» и методы физики высоких энергий могут использоваться для исследования ядерной структуры. Подчеркивается, что наша способность получить новую информацию о структуре ядра из некоторых экспериментов часто ограничивается нашим незнанием на данном этапе других сторон ядерной структуры.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3—4), pp. 277—292 (1966)

ON THE DERIVATION OF GENERALIZED GINZBURG—LANDAU EQUATIONS

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(Presented by L. Pál. — Received 1. III. 1966)

The consequences of using more realistic effective electron-electron interactions than the BCS one in the derivation of the GINZBURG—LANDAU equations and their generalizations are examined. GORKOV's equations for the thermodynamic GREEN's functions are used as a starting point. The gap parameter is given in terms of a general non-local two-particle interaction and the anisotropy of the one particle spectrum is also taken into account. Generalized WERTHAMER's equations are obtained and shown to reduce to modified GINZBURG's equations for $T \lesssim T_c$. Within the same limit neglecting anisotropy effects the GINZBURG—LANDAU equations result.

1. Introduction

The GINZBURG—LANDAU [1] phenomenological equations for the description of the behaviour of a superconductor in a static magnetic field have been derived by GORKOV [2] from microscopic theory. GORKOV assumed that the temperature T is near to the critical temperature T_c therefore the gap Δ is a small quantity and the magnetic potential as well as Δ are slowly varying functions of positions.

Generalizations of the GINZBURG—LANDAU equations have been derived recently by WERTHAMER [3], TEWORDT [4], ZUMINO and UHLENBROCK [5] and EILENBERGER [6]. These authors relaxed the assumption that Δ is small but retained the others. Thus, their equations should also be valid at lower temperatures for local superconductors. In all the microscopic theories mentioned the BCS [7] interaction has been used in the calculation of the energy gap function which, as a consequence, depends only on the centre-of-mass coordinate of the pair, $\Delta = \Delta(R)$.

To describe the behaviour of anisotropic superconductors in a magnetic field GINZBURG [8] has given the analogues of the GINZBURG—LANDAU equations which differ from the GINZBURG—LANDAU equations in having a mass tensor instead of the isotropic mass. GINZBURG's equations have been derived by GORKOV and MELIK—BARKHUDAROV [9] on the basis of the microscopic theory taking into account the anisotropy of both the one-particle spectrum and the gap function, restricting themselves to $T \lesssim T_c$.

For strong coupling superconductors other generalizations of the BCS theory have also been necessitated by certain experimental facts. For example, the structure in the superconducting density of states showed that the non-instantaneous nature of the effective electron-electron interaction via phonon exchange leading to the dependence of the gap function on the energy is of great importance [10].

It would be of interest to see what effect taking into account the more realistic effective electron-electron interactions has on the GINZBURG—LANDAU equations and their generalizations. As a first step in this direction we have investigated the case of a general non-local two-particle interaction. A preliminary account of these investigations has been given previously [11].

The interaction Hamiltonian is given in a gauge-invariant form in Section 2. To get equations determining the gap function and current density for local superconductors we start from GORKOV's equations [12], [9] for the thermodynamic GREEN's functions (Section 3) and perform a gauge-invariant expansion [5] of these equations (Section 4). In this way generalizations of WERTHAMER's equations are obtained in which the gap function depends on the relative momentum of the pair, too, $\Delta = \Delta\,(p, R)$ and the anisotropy of the one particle spectrum is also taken into account. These equations represent the extension of GORKOV and MELIK—BARKHUDAROV's result [9] to lower temperatures (Section 5). In Section 6 the equations are given for $T < T_c$ and are shown to reduce to modified GINZBURG's equations in which the mass tensors occurring in the current density and gap equation are different from each other while they are the same in the original GINZBURG theory [8]. It is found that neglecting all the anisotropy effects the GINZBURG—LANDAU equations result but with parameters differing in general from those given by GORKOV [2].

2. The Hamiltonian

We consider the Hamiltonian

$$H = H_0 + H_{\text{int}} = \int \psi_\alpha^+(\mathbf{r})\; \xi \left(\frac{\partial}{\partial \mathbf{r}} - \frac{ie}{c}\, \mathbf{A}(\mathbf{r}) \right) \psi_\alpha(\mathbf{r})\, d\mathbf{r} +$$

$$+ \int V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4)\; \psi_\alpha^+(\mathbf{r}_1)\, \psi_\beta^+(\mathbf{r}_2)\, \psi_\beta(\mathbf{r}_3)\, \psi_\alpha(\mathbf{r}_4)\, d\mathbf{r}_1 \ldots d\mathbf{r}_4\,,$$

where α and β stand for definite spin directions (summation is to be performed over repeated indices), $\mathbf{A}$ is the vector potential, ξ is the energy of a Bloch electron and V is the interaction between Bloch electrons representing the effective interaction coming from the phonon exhange + the screened Coulomb interaction between the electrons. It is well known that retardation effects can be simulated to some extent by non-local interactions. Owing to the non-locality, however, the difficulty arises that H_{int} is not gauge-invariant. To avoid this problem we shall use the gauge-invariant interaction Hamiltonian [11]

$$H_{\rm int}^{\rm g.i.} = \int V_{\rm eff}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4;\ \mathbf{A})\, \psi_\alpha^+(\mathbf{r}_1)\, \psi_\beta^+(\mathbf{r}_2)\, \psi_\beta(r_3)\, \psi_\alpha(r_4)\, d\mathbf{r}_1 \ldots d\mathbf{r}_4\,,$$

where

$$V_{\rm eff} = V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) \exp\left[\frac{ie}{c}\left(\int\limits_{\mathbf{r}_1}^{\mathbf{R}} \mathbf{A} d\mathbf{r} + \int\limits_{\mathbf{r}_2}^{\mathbf{R}} \mathbf{A} d\mathbf{r} - \int\limits_{\mathbf{r}_3}^{\mathbf{R}'} \mathbf{A} d\mathbf{r} - \int\limits_{\mathbf{r}_4}^{\mathbf{R}'} \mathbf{A} dr + 2\int\limits_{\mathbf{R}}^{\mathbf{R}'} \mathbf{A} d\mathbf{r}\right)\right], \tag{1}$$

with $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$, $\mathbf{R}' = \frac{1}{2}(\mathbf{r}_3 + \mathbf{r}_4)$. Straight lines joining the two end points are chosen as integration paths.

It is worth noting that the gauge invariant interaction Hamiltonian proposed by ZAWADOWSKI [13]

$$\tilde{H}_{\rm int}^{\rm g.i.} = \int V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) \exp\left\{(\mathbf{r}_1 - \mathbf{r}_0)\left(\frac{\partial}{\partial \mathbf{r}_0} + \frac{ie}{c}\mathbf{A}(\mathbf{r}_0)\right)\right\} \psi_\alpha^+(\mathbf{r}_0)$$

$$\exp\left\{(\mathbf{r}_2 - \mathbf{r}_0)\left(\frac{\partial}{\partial \mathbf{r}_0} + \frac{ie}{c}\mathbf{A}(\mathbf{r}_0)\right)\right\} \psi_\beta^+(\mathbf{r}_0) \exp\left\{(\mathbf{r}_3 - \mathbf{r}_0)\right.$$

$$\left.\left(\frac{\partial}{\partial \mathbf{r}_0} - \frac{ie}{c}\mathbf{A}(\mathbf{r}_0)\right)\right\} \psi_\beta(\mathbf{r}_0)$$

$$\exp\left\{(\mathbf{r}_4 - \mathbf{r}_0)\left(\frac{\partial}{\partial r_0} - \frac{ie}{c}\mathbf{A}(\mathbf{r}_0)\right)\right\} \psi_\alpha(\mathbf{r}_0)\, d\mathbf{r}_1 \ldots d\mathbf{r}_4\,,$$

where $\mathbf{r}_0 = \frac{1}{2}(\mathbf{R} + \mathbf{R}')$, can be transformed to a form similar to that of $H_{\rm int}^{\rm g.i.}$ but $V_{\rm eff}$ is replaced by [14]

$$\tilde{V}_{\rm eff} = V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) \exp\left[\frac{ie}{c}\left(\int\limits_{\mathbf{r}_1}^{\mathbf{r}_0} \mathbf{A} d\mathbf{r} + \int\limits_{\mathbf{r}_2}^{\mathbf{r}_0} \mathbf{A} d\mathbf{r} - \int\limits_{\mathbf{r}_3}^{\mathbf{r}_0} \mathbf{A} d\mathbf{r} - \int\limits_{\mathbf{r}_4}^{\mathbf{r}_0} \mathbf{A} d\mathbf{r}\right)\right].$$

3. Basic equations

We start from GORKOV's equations [12], [9] in the coordinate representation

$$\left[i\omega - \xi\left(\frac{\partial}{\partial \mathbf{r}_1} - \frac{ie}{c}\mathbf{A}(\mathbf{r}_1)\right) + \mu\right] G_\omega(\mathbf{r}_1\, \mathbf{r}_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2) - \int \Delta(\mathbf{r}_1, \mathbf{r}_3)\, F_\omega^+(\mathbf{r}_3, \mathbf{r}_2)\, d\mathbf{r}_3\,, \tag{2}$$

$$\left[-i\omega - \xi\left(\frac{\partial}{\partial \mathbf{r}_1} + \frac{ie}{c}\mathbf{A}(\mathbf{r}_1)\right) + \mu\right] F_\omega^+(\mathbf{r}_1, \mathbf{r}_2) = \int \Delta^*(\mathbf{r}_1, \mathbf{r}_3)\, G_\omega(\mathbf{r}_3, \mathbf{r}_2)\, d\mathbf{r}_3\,, \tag{3}$$

where G_ω and F_ω^+ are the Fourier transforms with respect to $\tau_1 - \tau_2 \equiv \tau$ of the thermodynamic Green's functions defined as

$$G(\mathbf{r}_1, \mathbf{r}_2; \tau) = - < T_\tau (\psi_\uparrow (\mathbf{r}_1, \tau_1) \psi_\uparrow^+ (\mathbf{r}_2, \tau_2)) > ,$$

$$F^+ (\mathbf{r}_1, \mathbf{r}_2; \tau) = < T_\tau (\psi_\uparrow^+ (\mathbf{r}_1, \tau_1) \psi_\downarrow^+ (\mathbf{r}_2, \tau_2)) > .$$

Moreover $\omega = (2n + 1)\pi T$ $(n = 0, \pm 1, \pm 2, \ldots)$, μ is the chemical potential and $\Delta(\mathbf{r}_1, \mathbf{r}_2)$ is the gap function defined as

$$\Delta^* (\mathbf{r}_1, \mathbf{r}_2) = - T \sum_\omega \int V_{\text{eff}} (\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4; \mathbf{A}) F_\omega^+ (\mathbf{r}_3, \mathbf{r}_4) \, d\mathbf{r}_3 \, d\mathbf{r}_4 . \tag{4}$$

Let us introduce sum and difference coordinates and perform Fourier transformation of all the quantities appearing in eqs. (2) and (3) with respect to the difference coordinate (mixed representation), e.g.

$$G_\omega (\mathbf{p}, \mathbf{R}) = \int d(\mathbf{r}_1 - \mathbf{r}_2) \, e^{-i\mathbf{p}(\mathbf{r}_1 - \mathbf{r}_2)} G_\omega (\mathbf{r}_1, \mathbf{r}_2) ,$$

where $\mathbf{R} = \frac{1}{2} (\mathbf{r}_1 + \mathbf{r}_2)$. Thus eqs. (2) and (3) transform to

$$\begin{aligned} i\omega G_\omega (\mathbf{p}, \mathbf{R}) - \Theta\left[\varepsilon \left(\mathbf{p} - \frac{e}{c} \mathbf{A} (\mathbf{R}) \right) G_\omega (\mathbf{p}, \mathbf{R}) \right] = \\ = 1 - \Theta[\Delta (\mathbf{p}, \mathbf{R}) F_\omega^+ (\mathbf{p}, \mathbf{R})], \end{aligned} \tag{5}$$

$$\begin{aligned} - i\omega F_\omega^+ (\mathbf{p}, \mathbf{R}) - \Theta\left[\varepsilon \left(\mathbf{p} + \frac{e}{c} \mathbf{A} (\mathbf{R}) \right) F_\omega^+ (\mathbf{p}, \mathbf{R}) \right] = \\ = \Theta \left[\Delta^* (\mathbf{p}, \mathbf{R}) G_\omega (\mathbf{p}, \mathbf{R}) \right], \end{aligned} \tag{6}$$

where

$$\varepsilon \left(\mathbf{p} \pm \frac{e}{c} \mathbf{A} (\mathbf{R}) \right) \equiv \xi \left(\mathbf{p} \pm \frac{e}{c} \mathbf{A} (\mathbf{R}) \right) - \mu ,$$

$$\Delta^* (\mathbf{p}, \mathbf{R}) = - T \sum_\omega \int \frac{d\mathbf{p}'}{(2\pi)^3} \, d\mathbf{R}' \, V_{\text{eff}} (\mathbf{p}, \mathbf{p}' . \mathbf{R}, \mathbf{R}'; \mathbf{A}) F_\omega^+ (\mathbf{p}', \mathbf{R}')$$

and Θ is a differential operator of infinite order [15]

$$\Theta [f \; g] = \lim_{\substack{\mathbf{R}' \to \mathbf{R} \\ \mathbf{p}' \to \mathbf{p}}} \exp \left[\frac{i}{2} \sum_{xyz} \left(\frac{\partial}{\partial R_x} \frac{\partial}{\partial p_x'} - \frac{\partial}{\partial p_x} \frac{\partial}{\partial R_x'} \right) \right] f (\mathbf{p}, \mathbf{R}) \, g (\mathbf{p}', \mathbf{R}') .$$

The sum over x, y, z means that $x, y,$ and z are to replace each other cyclically.

4. Expansion procedure

To derive equations for local superconductors one assumes that the magnetic potential as well as other quantities entering the problem vary slowly over distances of the order of the coherence length. These assumptions allow one to apply the quasi-classical approximation which we use in a form developed by several authors for normal [15] and superfluid [3], [5], [16] systems. Moreover we assume that Δ is small and use as expansion parameter the small quantity σ introduced by ZUMINO and UHLENBROCK [5] by setting

$$\mathbf{A}(\mathbf{R}) = \sigma\widetilde{\mathbf{A}}(\sigma\mathbf{R}),$$

where $\widetilde{\mathbf{A}}$ is a fixed function. In this way simultaneous expansion can be performed in powers of $\nabla_{\mathbf{R}}$ and $\mathbf{A}$ which is necessary to get a gauge-invariant approximate expression for a gauge invariant quantity. To obtain manifestly gauge-invariant results we introduce, following ZUMINO and UHLENBROCK [5], the so-called gauge-invariant propagators, too, with the definition

$$\bar{G}_\omega(\mathbf{r}_1,\mathbf{r}_2) = G_\omega(\mathbf{r}_1,\mathbf{r}_2)\exp\left[\frac{ie}{c}\int\limits_{\mathbf{r}_1}^{\mathbf{r}_2}\mathbf{A}d\mathbf{r}\right], \tag{7}$$

$$\bar{F}^+_\omega(\mathbf{r}_1,\mathbf{r}_2) = F^+_\omega(\mathbf{r}_1,\mathbf{r}_2)\exp\left[-\frac{ie}{c}\left(\int\limits_{\mathbf{r}_1}^{\mathbf{R}}\mathbf{A}d\mathbf{r}+\int\limits_{\mathbf{r}_2}^{\mathbf{R}}\mathbf{A}d\mathbf{r}\right)\right] \tag{8}$$

and the new gap function

$$\bar{\Delta}^*(\mathbf{r}_1,\mathbf{r}_2) = \Delta^*(\mathbf{r}_1,\mathbf{r}_2)\exp\left[-\frac{ie}{c}\left(\int\limits_{\mathbf{r}_1}^{\mathbf{R}}\mathbf{A}d\mathbf{r}+\int\limits_{\mathbf{r}_2}^{\mathbf{R}}\mathbf{A}d\mathbf{r}\right)\right]. \tag{9}$$

$\bar{G}_\omega$ is gauge invariant while $\bar{F}^+_\omega$ and $\bar{\Delta}^*$ transform according to

$$\bar{F}^+_\omega(\mathbf{r}_1,\mathbf{r}_2) \to \bar{F}^+_\omega(\mathbf{r}_1,\mathbf{r}_2)\exp\left[-\frac{2ie}{c}\varphi(\mathbf{R})\right],$$

if

$$\mathbf{A}(\mathbf{r}) \to \mathbf{A}(\mathbf{r}) + \operatorname{grad}\varphi(\mathbf{r}).$$

The equation determining the gap function $\bar{\Delta}$ can be obtained from eq. (4), using eqs. (1), (8) and (9). In the mixed representation we get

$$\begin{aligned}\bar{\Delta}^*(\mathbf{p},\mathbf{R}) = -T\sum_\omega\int\frac{dp'}{(2\pi)^3}\,d\mathbf{R}'\,V(\mathbf{p},\mathbf{p}',\mathbf{R}-\mathbf{R}')\\ \exp\left[\frac{2ie}{c}\int\limits_{\mathbf{R}}^{\mathbf{R}'}\mathbf{A}d\mathbf{r}\right]\bar{F}^+_\omega(\mathbf{p}',\mathbf{R}'),\end{aligned} \tag{10}$$

where V is taken to be independent from $\mathbf{R} + \mathbf{R}'$ because of translational invariance of the interaction. Moreover, the expression for the current in terms of the gauge-invariant Green's function $\bar{G}_\omega$ is

$$j_i(\mathbf{R}) = 2eT \sum_\omega \int \frac{dp}{(2\pi)^3} v_{p_i} \bar{G}_\omega(\mathbf{p}, \mathbf{R}), \qquad v_{p_i} = \frac{\partial \varepsilon(p)}{\partial p_i} . \tag{11}$$

We want to obtain approximate expressions for $\bar{F}^+_\omega$ and $\bar{G}_\omega$ up to second order in σ. With this in mind, let us expand all the quantities appearing in eqs. (5) and (6) to this order

$$G_\omega = G^{(0)}_\omega + G^{(1)}_\omega + G^{(2)}_\omega , \qquad F^+_\omega = F^{+(0)}_\omega + F^{+(1)}_\omega + F^{+(2)}_\omega ,$$

$$\Theta = \Theta^{(0)} + \Theta^{(1)} + \Theta^{(2)} ,$$

$$\varepsilon\left(\mathbf{p} \pm \frac{e}{c}\mathbf{A}\right) = \varepsilon(\mathbf{p}) \pm \frac{e}{c} v_{p_i} A_i(\mathbf{R}) + \frac{e^2}{2c^2} w_{ij} A_i A_j ,$$

where

$$w_{ij} = \frac{\partial^2 \varepsilon(\mathbf{p})}{\partial p_i \partial p_j} .$$

Δ is considered as a zero-th order quantity. Equating terms of similar degree separately to zero

$$i\omega G^{(0)}_\omega(\mathbf{p}, \mathbf{R}) - \Theta^{(0)}\left[\varepsilon(\mathbf{p}) G^{(0)}_\omega(\mathbf{p}, \mathbf{R})\right] = 1 - \Theta^{(0)}\left[\Delta(\mathbf{p}, \mathbf{R}) F^{+(0)}_\omega(\mathbf{p}, \mathbf{R})\right] ,$$

$$- i\omega F^{+(0)}_\omega(\mathbf{p}, \mathbf{R}) - \Theta^{(0)}\left[\varepsilon(\mathbf{p}) F^{+(0)}_\omega(\mathbf{p}, \mathbf{R})\right] = \Theta^{(0)}\left[\Delta^*(\mathbf{p}, \mathbf{R}) G^{(0)}_\omega(\mathbf{p}, \mathbf{R})\right] ,$$

etc. straightforward but tedious calculation leads to the expressions of F^+_ω and G_ω up to second order in σ. $\bar{F}^+_\omega$ and $\bar{G}_\omega$ are obtained using eqs. (7) and (8) transformed into the mixed representation and expanded up to second order in σ (eqs. (33) and (32) of ref. [5])

$$\bar{G}_\omega(\mathbf{p}, \mathbf{R}) = \left(1 + \frac{e}{c}\mathbf{A}(\mathbf{R}) \triangle_\mathbf{p} + \frac{1}{2}\frac{e^2}{c^2}(\mathbf{A}\triangle_\mathbf{p})^2\right) G_\omega(\mathbf{p},\mathbf{R}),$$

$$\bar{F}^+_\omega(\mathbf{p}, \mathbf{R}) = \left(1 - \frac{ie}{4c}\frac{\partial A_i}{\partial R_j}\frac{\partial}{\partial p_i}\frac{\partial}{\partial p_j}\right) F^+_\omega(\mathbf{p}, \mathbf{R}) .$$

The results are given in the Appendix.

5. Generalized Werthamer's equations

In order to get equations determining the gap function and current density the expressions obtained for $\bar{F}^+_\omega$ and $\bar{G}_\omega$ have to be inserted into eqs. (10) and (11), respectively. Taking into account the consequences of the invariance under time reversal and space reflection i.e. that

$$\varepsilon(\mathbf{p}) = \varepsilon(-\mathbf{p}),$$

$$V(\mathbf{p},\mathbf{p}',\mathbf{R}-\mathbf{R}') = V(-\mathbf{p}',-\mathbf{p},-\mathbf{R}+\mathbf{R}') = V(\mathbf{p}',\mathbf{p},-\mathbf{R}+\mathbf{R}'), \quad (12)$$

it is easy to see that only $\bar{G}^{(1)}_{\omega}$ gives a non-zero contribution to the current density. As to the gap equation, in the general case only those terms of $\bar{F}^{+}_{\omega}$ will give vanishing contributions to it which are odd in ω. Moreover the gap equation is nonlocal in both variables. Its non-locality in the variable R can, however, be eliminated by making some restrictions on physical grounds concerning the form of the interaction $V(p, p', R - R')$. As the four-electron vertex part when calculated, using the electron-phonon interaction, in the lowest order approximation (one phonon exhange) contains the factor $\delta(R - R)'$, it is reasonable to assume that the dependence of $V(p, p', R - R')$ on $R - R'$ is δ-function-like. More precisely, we suppose that $V(p, p', R - R')$ differs from zero only in a region in the neighbourhood of $R' = R$ which is so small that the other two factors in eq. (10) can be expanded in powers of $R - R'$ in the vicinity of R and it is sufficient to retain terms up to second order in these series

$$\bar{F}^{+}_{\omega}(\mathbf{p}',\mathbf{R}') = \bar{F}^{+}_{\omega}(\mathbf{p}',\mathbf{R}) - \frac{\partial \bar{F}^{+}_{\omega}(\mathbf{p}',\mathbf{R})}{\partial R_i}(\mathbf{R}-\mathbf{R}')_i + \\ + \frac{1}{2}\frac{\partial^2 \bar{F}^{+}_{\omega}(\mathbf{p}',\mathbf{R})}{\partial R_i \partial R_j}(\mathbf{R}-\mathbf{R}')_i(\mathbf{R}-\mathbf{R}')_j, \quad (13)$$

$$\exp\left[-\frac{2ie}{c}\int\limits_{\mathbf{R}'}^{\mathbf{R}}\mathbf{A}d\mathbf{r}\right] = 1 - \frac{2ie}{c}A_i(\mathbf{R}-\mathbf{R}')_i - \\ - \frac{ie}{c}\frac{\partial A_i}{\partial R_j}(\mathbf{R}-\mathbf{R}')_i(\mathbf{R}-\mathbf{R}')_j - \quad (14) \\ - \frac{2e^2}{c^2}A_i A_j(\mathbf{R}-\mathbf{R}')_i(\mathbf{R}-\mathbf{R}')_j .$$

Thus we get from eq. (10)

$$\bar{\Delta}^*(\mathbf{p},\mathbf{R}) = -T\sum_{\omega}\int\frac{d\mathbf{p}'}{(2\pi)^3}\Big[V_0(\mathbf{p},\mathbf{p}')\bar{F}^{+}_{\omega}(\mathbf{p}',\mathbf{R}) + \quad (15) \\ + \frac{1}{2}V_{ij}(\mathbf{p},\mathbf{p}')\left(\nabla_{\mathbf{R}} + \frac{2ie}{c}\mathbf{A}(\mathbf{R})\right)_i\left(\nabla_{\mathbf{R}} + \frac{2ie}{c}\mathbf{A}(\mathbf{R})\right)_j\bar{F}^{+}_{\omega}(\mathbf{p}',\mathbf{R})\Big]$$

with

$$V_0(\mathbf{p},\mathbf{p}') \equiv \int V(\mathbf{p},\mathbf{p}',\mathbf{R}-\mathbf{R}')\,d\mathbf{R}',$$

$$V_{ij}(\mathbf{p},\mathbf{p}') = \int V(\mathbf{p},\mathbf{p}',\mathbf{R}-\mathbf{R}')(\mathbf{R}-\mathbf{R}')_i(\mathbf{R}-\mathbf{R}')_j\,d\mathbf{R}' .$$

The terms of first order in eqs. (13) and (14) do not contribute to the gap equation because $\int V(\mathbf{p}, \mathbf{p}', \mathbf{R} - \mathbf{R}')(\mathbf{R} - \mathbf{R}')_i \, d\mathbf{R}' \equiv 0$ as a consequence of eq. (12).

Let us assume, moreover, that

$$V(\mathbf{p}, \mathbf{p}', \mathbf{R} - \mathbf{R}') = \bar{V}(\varepsilon(\mathbf{p}), \varepsilon(\mathbf{p}'), \hat{\mathbf{p}}, \hat{\mathbf{p}}', \mathbf{R} - \mathbf{R}') \, (\hat{\mathbf{p}} = \mathbf{p}/|\mathbf{p}|, \ \hat{\mathbf{p}}' = \mathbf{p}'/|\mathbf{p}'|)$$

is an even function of $\varepsilon(\mathbf{p})$ and $\varepsilon(\mathbf{p}')$, which holds for all the interactions used in the theory of superconductivity. As a consequence $\Delta(\varepsilon, \hat{p}, \mathbf{R})$ can also be taken as being an even function of ε.

Changing the integration variables from $\mathbf{p}$ to ε and $\hat{p}$ $\left(d\mathbf{p} = d\varepsilon \dfrac{d\sigma}{v_F}\right.$, where $d\sigma$ is a surface element on the Fermi surface and v_F is the velocity on the Fermi surface) the contributions of all the terms odd in ε vanish when integrated over ε both in eqs. (11) and (12). Thus we get*

$$\begin{aligned} j_i(\mathbf{R}) = 2eT \sum_{\omega} \int \frac{dp}{(2\pi)^3} v_{p_i} v_{p_j} \Bigl[&- \frac{i}{2a^2} \bigl(\Delta^*(\mathbf{p}, \mathbf{R}) \, O_j \, \Delta(\mathbf{p}, \mathbf{R}) - \Delta(\mathbf{p}, \mathbf{R}) \cdot \\ &\cdot O_j^* \, \Delta^*(\mathbf{p}, \mathbf{R})\bigr) + \frac{i}{2a^2} \varepsilon(\mathbf{p}) \biggl(\frac{\partial \Delta^*(\mathbf{p}, \mathbf{R})}{\partial \varepsilon} O_j \, \Delta(\mathbf{p}, \mathbf{R}) - \\ &- \frac{\partial \Delta(\mathbf{p}, \mathbf{R})}{\partial \varepsilon} O_j^* \, \Delta^*(\mathbf{p}, \mathbf{R}) \biggr) \Bigr], \end{aligned} \tag{16}$$

$$\begin{aligned} \Delta^*(\mathbf{p}, \mathbf{R}) = - T \sum_{\omega} \int \frac{d\mathbf{p}'}{(2\pi)^3} V_0(\mathbf{p}, \mathbf{p}') \biggl[&\frac{\Delta^*(\mathbf{p}', \mathbf{R})}{a'} + \\ &+ \frac{O_i^* O_j^* \Delta^*(\mathbf{p}', \mathbf{R})}{4a'^2} \biggl(v_{p'_i} v_{p'_j} \biggl(3 - \frac{4\varepsilon^2(\mathbf{p}')}{a'} - \frac{4\varepsilon(\mathbf{p}')}{a'} \frac{\partial |\Delta|^2}{\partial \varepsilon'} \biggr) + \\ &+ \frac{2a' V_{ij}(\mathbf{p}, \mathbf{p}')}{V_0(\mathbf{p}, \mathbf{p}')} - \frac{1}{a'} \nabla_{p'_i} |\Delta|^2 \nabla_{p'_j} |\Delta|^2 - \Delta \nabla_{p'_i} \nabla_{p'_j} \Delta^* + \\ &+ \nabla_{p'_i} \nabla_{p'_j} |\Delta|^2 \biggr) + \frac{O_i^* \Delta^* O_j^* \Delta^*}{a'^2} \biggl(v_{p'_i} v_{p'_j} \biggl(- \frac{\Delta}{a'} + \frac{\varepsilon'}{a'} \frac{\partial \Delta}{\partial \varepsilon'} \biggr) + \\ &+ \frac{\Delta^*}{4a'} \nabla_{p'_i} \Delta \nabla_{p'_j} \Delta - \frac{1}{4} \nabla_{p'_i} \nabla_{p'_j} \Delta \biggr) + \\ &+ \frac{\nabla_{R_i} \nabla_{R_j} |\Delta|^2}{a'^2} \biggl(v_{p'_i} v_{p'_j} \biggl(- \frac{\Delta^*}{3a'} + \frac{\Delta^* \varepsilon'}{a'^2} \frac{\partial |\Delta|^2}{\partial \varepsilon'} \biggr) + \\ &+ \frac{1}{4} \triangle_{p'_i} \nabla_{p'_j} \Delta^* - \frac{\Delta^*}{4a'} \nabla_{p'_i} \nabla_{p'_j} |\Delta|^2 + \end{aligned}$$

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* From now on we shall write Δ instead of as Δ the original Δ will not reoccur.

$$\begin{aligned}
&+\frac{\varDelta^*}{4a'^2}\nabla_{p'_i}|\varDelta|^2\,\nabla_{p'_j}|\varDelta|^2\Bigg)+\frac{\nabla_{R_i}|\varDelta|^2\,\nabla_{R_j}|\varDelta|^2}{a'^3}\left(\frac{\varDelta^*}{2a'}v_{p'_i}v_{p'_j}+\right.\\
&\left.+\frac{\varDelta^*}{4a'}\nabla_{p'_i}\nabla_{p'_j}|\varDelta|^2-\frac{1}{4}\nabla_{p'_i}\nabla_{p'_j}\varDelta^*\right)+\\
&+\frac{1}{4a'^2}\left(\frac{\varDelta^*}{a'}O_i\varDelta O_j\varDelta-O_iO_j\varDelta\right)\nabla_{p'_i}\varDelta^*\,\nabla_{p'_j}\varDelta^*+\qquad\qquad (17)\\
&+\frac{\varDelta}{4a'^2}\nabla_{p'_i}O_j^*\varDelta^*\,\nabla_{p'_j}O_i^*\varDelta^*-\\
&\frac{1}{a'^3}O_i^*\varDelta^*O_j\varDelta\left(\frac{\varDelta^*}{2}\nabla_{p'_i}\varDelta\,\nabla_{p'_j}\varDelta^*+v_{p'_i}v_{p'_j}\,\varepsilon'\frac{\partial\varDelta^*}{\partial\varepsilon'}\right)+\\
&+\frac{1}{2a'^2}\nabla_{p'_i}O_j\varDelta\,\nabla_{p'_j}O_i^*\varDelta^*+\\
&+\frac{1}{2a'^2}\nabla_{p'_i}O_j^*\varDelta^*\left(\frac{1}{a'}\triangle_{p'_j}a'\,\nabla\boldsymbol{R}_i|\varDelta|^2-\nabla_{p'_j}\nabla_{R_i}|\varDelta|^2\right)+\\
&+\frac{\varDelta^*}{4a'^3}\nabla_{p'_i}\nabla_{R_j}|\varDelta|^2\,\nabla_{p'_j}\nabla_{R_i}|\varDelta|^2-\\
&-\frac{\varDelta^*}{2a'^4}\triangle_{R_i}|\varDelta|^2\,\nabla_{p'_i}\nabla_{R_j}|\varDelta|^2\,\nabla_{p'_j}a'\,,
\end{aligned}$$

where

$$O_i=\left(\nabla_{\mathbf{R}}-\frac{2ie}{c}\mathbf{A}(\mathbf{R})\right)_i,\qquad a=\omega^2+\varepsilon^2(\mathbf{p})+|\varDelta(\mathbf{p},\mathbf{R})|^2,$$

$$a'=\omega^2+\varepsilon^2(\mathbf{p}')+|\varDelta(\mathbf{p}',\mathbf{R})|^2.$$

Eqs. (16) and (17) are coupled equations determining $\varDelta(\mathbf{p},\mathbf{R})$ and $\mathbf{A}(\mathbf{R})$. They contain the analogues of the terms appearing in WERTHAMER's equations [3] as well as numerous additional terms containing the first and second derivatives of the gap function with respect to **p**. Moreover, they are generalizations of WERTHAMER's equations owing to the inclusion of the anisotropy of the one-particle spectrum too. Such equations may be expected to hold for a comparatively wide range of temperatures below T_c for pure local superconductors such as Nb which shows anisotropy effects [17] and is a strong coupling superconductor [18] at the same time.

6. Equations for $\mathbf{T} \lesssim \mathbf{T}_c$

Near the critical temperature T_c the gap function can be considered to be small and the Green's functions can also be expanded in powers of $|\varDelta|^2$. Thus we get from eqs. (16) and (17)

$$j_i(\mathbf{R}) = 2e\,T \sum_{\omega} \int \frac{d\mathbf{p}}{(2\pi)^3} \frac{v_{p_i} v_{p_j}}{(\omega^2+\varepsilon^2)^2} \left[\frac{e}{c} A_j \left(-2|\Delta|^2 + \frac{\partial |\Delta|^2}{\partial \varepsilon} \varepsilon \right) + \right.$$

$$\left. + \frac{i}{2} \frac{\partial \Delta}{\partial R_j} \left(\varepsilon \frac{\partial \Delta^*}{\partial \varepsilon} - \Delta^* \right) - \frac{i}{2} \frac{\partial \Delta^*}{\partial R_j} \left(\varepsilon \frac{\partial \Delta}{\partial \varepsilon} - \Delta \right) \right], \tag{18}$$

$$\Delta^*(\mathbf{p},\mathbf{R}) = -T \sum_{\omega} \int \frac{d\mathbf{p}'}{(2\pi)^3} V_0(\mathbf{p},\mathbf{p}') \left\{ \frac{\Delta^*(\mathbf{p}',\mathbf{R})}{\omega^2+\varepsilon'^2} - \frac{|\Delta(\mathbf{p}',\mathbf{R})|^2 \Delta^*(\mathbf{p}',\mathbf{R})}{(\omega^2+\varepsilon'^2)^2} \right.$$

$$+ \frac{1}{2} \left(\nabla_{\mathbf{R}} + \frac{2ie}{c} \mathbf{A}(\mathbf{R}) \right)_i \left(\Delta_{\mathbf{R}} + \frac{2ie}{c} \mathbf{A}(\mathbf{R}) \right)_j \Delta^*(\mathbf{p}',\mathbf{R}) \cdot \tag{19}$$

$$\left. \cdot \left[\left(1 + \frac{1}{2} \frac{\partial}{\partial \varepsilon'} \varepsilon' \right) \frac{v_{p'_i} v_{p'_j}}{(\omega^2+\varepsilon'^2)^2} + \frac{V_{ij}(\mathbf{p},\mathbf{p}')}{V_0(\mathbf{p},\mathbf{p}')} \frac{1}{\omega^2+\varepsilon'^2} \right] \right\}.$$

Our equations can further be simplified by generalizing the procedure given by ZUBARIEV et al. [19] to obtain approximate results for the gap near the critical temperature in the field-free case. Similar considerations have been made by GORKOV and MELIK—BARKHUDAROV [9]. Let us expand $\Delta(\mathbf{p}, \mathbf{R}, T)$ in powers of $[(T_c - T)/T_c]^{1/2} \equiv \vartheta^{1/2}$

$$\Delta(\mathbf{p},\mathbf{R},T) = \Delta_1(\mathbf{p},\mathbf{R},T) + \Delta_2(\mathbf{p},\mathbf{R},T) + \Delta_3(\mathbf{p},\mathbf{R},T) + \cdots$$

where $\Delta_1(\mathbf{p}, \mathbf{R}, T)$, $\Delta_2(\mathbf{p}, \mathbf{R}, T)$ and $\Delta_3(\mathbf{p}, \mathbf{R}, T)$ are of first, second and third order in $\vartheta^{1/2}$, respectively. Inserting this expansion into eq. (19), performing the summation over ω in the first term on the right hand side and expanding the resulting factor $\tan \frac{\varepsilon'}{2T}$ in powers of ϑ, too, we get to the lowest order

$$\Delta_1^*(\mathbf{p},\mathbf{R},T) = \varphi(\mathbf{p})\, \Delta_1^*(\mathbf{R},T), \tag{20}$$

where $\varphi(\mathbf{p})$ (and T_c) are determined by the eigenvalue equation

$$\varphi(\mathbf{p}) = -T_c \sum_{\omega_c} \int \frac{d\mathbf{p}'}{(2\pi)^3} V_0(\mathbf{p},\mathbf{p}') \frac{\varphi(\mathbf{p}')}{\omega_c^2+\varepsilon'^2} = \tag{21}$$

$$= \frac{-1}{2} \int \frac{dp'}{(2\pi)^3} V_0(\mathbf{p},\mathbf{p}') \tan \frac{\varepsilon'}{2T_c} \frac{\varphi(\mathbf{p}')}{\varepsilon'}\,;$$

$$\omega_c \equiv (2n+1)\,\pi\, T_c.$$

To get the equation determining $\Delta_1(\mathbf{R})$ we have to examine the equation obtainable from eq. (19) for the terms of third order

$$\Delta_3^*(\mathbf{p},\mathbf{R},T) = \frac{-1}{2}\int \frac{d\mathbf{p}'}{(2\pi)^3} V_0(\mathbf{p},\mathbf{p}')\tan\frac{\varepsilon'}{2T_c}\,\frac{\Delta_3^*(\mathbf{p}',\mathbf{R},T)}{\varepsilon'} -$$

$$- \frac{\vartheta}{4T_c}\int \frac{d\mathbf{p}'}{(2\pi)^3} V_0(\mathbf{p},\mathbf{p}')\,\frac{\Delta_1^*(\mathbf{p}',\mathbf{R},T)}{\mathrm{ch}^2(\varepsilon'/2T_c)} +$$

$$+ T_c\sum_{\omega_e}\int \frac{dp'}{(2\pi)^3}\,\frac{|\Delta_1|^2\Delta_1^*}{\omega_c^2+\varepsilon'^2} - \frac{1}{2}T_c\sum_{\omega_c}\int\frac{d\mathbf{p}'}{(2\pi)^3}\cdot$$

$$\cdot \left(\nabla_{\mathrm{R}} + \frac{2ie}{c}\mathbf{A}\right)_i \cdot \left(\nabla_{\mathrm{R}} + \frac{2ie}{c}\mathbf{A}\right)_j \Delta_1^*\Big[V_0(\mathbf{p},\mathbf{p}')\cdot$$

$$\cdot \left(1 + \frac{1}{2}\,\frac{\partial}{\partial\varepsilon'}\varepsilon'\right)\frac{v_{p'_i}v_{p'_j}}{(\omega_c^2+\varepsilon'^2)^2} + v_{ij}(\mathbf{p},\mathbf{p}')\frac{1}{\omega_c^2+\varepsilon'^2}\Big|.$$

The condition for the solvability of this equation, making use of eq. (20) is

$$\frac{C}{2m_{ij}}\left(\nabla_{\mathbf{R}} + \frac{2ie}{c}\mathbf{A}(\mathbf{R})\right)_i\left(\nabla_{\mathbf{R}} + \frac{2ie}{c}\mathbf{A}(\mathbf{R})\right)_j \Delta_1^*(\mathbf{R}) +$$

$$+ \left[f\frac{T_c-T}{T_c} - g|\Delta_1(\mathbf{R})|^2\right]\Delta_1^*(\mathbf{R}) = 0\,, \tag{22}$$

where

$$\frac{C}{\widetilde{m}_{ij}} \equiv \frac{C}{m_{ij}} + C\,\delta\frac{1}{m_{ij}}\,,$$

$$\frac{C}{m_{ij}} = T_c\sum_{\omega c}\int\frac{d\mathbf{p}}{(2\pi)^3}\,\frac{v_{pi}\,v_{pj}}{(\omega_c^2+\varepsilon^2)^2}\left[\varphi^2(\mathbf{p}) - \frac{1}{2}\varepsilon\,\frac{\partial\varphi^2(\mathbf{p})}{\partial\varepsilon}\right],$$

$$C\,\delta\frac{1}{m_{ij}} = T_c\sum_{\omega_e}\int\frac{d\mathbf{p}}{(2\pi)^3}\tan\frac{\varepsilon}{2T_c}\cdot\frac{\varphi(\mathbf{p})}{2\varepsilon}\int V_{ij}(\mathbf{p},\mathbf{p}')\,\frac{\varphi(\mathbf{p}')}{\omega_c^2+\varepsilon'^2}\,\frac{d\mathbf{p}'}{(2\pi)^3}\,,$$

$$g = T_c\sum_{\omega_e}\int\frac{d\mathbf{p}}{(2\pi)^3}\,\frac{\varphi^4(\mathbf{p})}{(\omega_c^2+\varepsilon^2)^2}\,, f = \frac{1}{4\,T_c}\int\frac{d\mathbf{p}}{(2\pi)^3}\,\frac{\varphi^2(\mathbf{p})}{Ch^2(\varepsilon/2T_c)}\,.$$

Using eq. (20), eq. (18) takes the form

$$j_i(\mathbf{R}) = C\left[-\frac{ie}{m_{ij}}\left(\Delta_1^*\frac{\partial\Delta_1}{\partial R_j} - \Delta_1\frac{\partial\Delta_1^*}{\partial R_j}\right) - \frac{4e^2}{m_{ij}C}A_j(\mathbf{R})\,|\Delta_1|^2\right|. \tag{23}$$

Let us normalize $\varphi(\mathbf{p})$ in such a way that

$$\int\varphi^2(|\mathbf{p}_F|,\hat{p})\,\frac{d\sigma}{v_F} = 1$$

and choose

$$C=\frac{7\zeta(3)\,\varepsilon_F}{(2\pi)^3\,12\,(\pi T_c)^2}\int\frac{d\sigma}{v_F}\,,$$

where ζ is the Riemann zeta function and ε_F is the Fermi energy. With this choice of C the expressions for $\tilde{m}_{ij}$ and m_{ij} reduce to $m\delta_{ij}$ (m is the electron mass) in the isotropic, weak coupling case [2].

Let us introduce the order parameter by

$$\Psi(\mathbf{R})=\sqrt{C}\Delta_1(\mathbf{R})\,.$$

Eqs. (22) and (23) go over to

$$\frac{1}{2\tilde{m}_{ij}}\left(\nabla_{\mathrm{R}}+\frac{2ie}{c}\mathbf{A}(\mathbf{R})\right)_i\left(\nabla_{\mathrm{R}}+\frac{2ie}{c}\mathbf{A}(\mathbf{R})\right)_j\psi^*(\mathbf{R})+$$

$$+\left[a\,\frac{T_c-T}{T_c}-b\,|\psi|^2\right]\psi^*(\mathbf{R})=0 \qquad (24)$$

with

$$a\equiv f/C\,,\qquad b\equiv g/C^2\,,$$

$$j_i(\mathbf{R})=-\frac{ie}{m_{ij}}\left(\psi^*\frac{\partial\psi}{\partial R_j}-\psi\frac{\partial\psi^*}{\partial R_j}\right)-\frac{4e^2}{m_{ij}\,c}A_j\,|\psi|^2\,. \qquad (25)$$

The equations obtained represent modified Ginzburg's equations because the mass tensors $\tilde{m}_{ij}$ and m_{ij} occurring in eqs. (24) and (25) differ from each other while they are the same in the original Ginzburg theory [8]. Neglecting $\delta\frac{1}{m_{ij}}$ the parameters in the Ginzburg's equations obtained are still different from those derived by Gorkov and Melik—Barkhudarov [9] because the gap function also depends on the absolute value of $\mathbf{p}$. Neglecting, on the other hand, all the anisotropy effects caused by the dependences on the directions in $V(\mathbf{p},\mathbf{p}',\mathbf{R}-\mathbf{R}')$ and $\varepsilon(\mathbf{p})$ but retaining dependences on the absolute values, we arrive at the Ginzburg—Landau equations with parameters in general differing from those derived by Gorkov [2].

7. Discussion

We have investigated the consequences of using a general non-local two-particle interaction in the derivation of the Ginzburg—Landau equations and their generalizations having strong coupling and anisotropic superconductors in mind. Restricting ourselves to local superconductors we have arrived at generalized WERTHAMER's equations containing even much more terms than the original ones. These equations are too complicated to find their solution. They simplify considerably for temperatures near the critical temperature T_c: modified GINZBURG's equations have been obtained for anisotropic superconductors and the GINZBURG—LANDAU equations for the isotropic ones. The parameters of these equations comprise the characteristic features of the interaction and differ, in general, from the expressions given by GORKOV in the isotropic, weak coupling case.

It is worth mentioning that similar results can be obtained if one starts from the equations of the coupled electron phonon system which are more adequate for the description of strong coupling superconductors [20].

The author wishes to thank P. SZÉPFALUSY and A. ZAWADOWSKI for many helpful discussions and to CS. HARGITAI for valuable remarks.

Appendix

The approximate expressions for the gauge-invariant Green's functions up to second order in σ are the following

$$\bar{G}_\omega^{(0)} = -\frac{i\omega + \varepsilon}{a}, \qquad a \equiv \omega^2 + \varepsilon^2 + |\Delta(\mathbf{p}, \mathbf{R})|^2 ,$$

$$\begin{aligned} \bar{G}_\omega^{(1)} = & -\frac{i}{2a^2} v_{p_i} [\Delta^* O_i \Delta - \Delta O_i^* \Delta^*] + \\ & + \frac{i(i\omega + \varepsilon)}{2a^2} [\nabla_{p_i} \Delta^* O_i \Delta - \nabla_{p_i} \Delta O_i^* \Delta^*] , \end{aligned}$$

$$O_i \equiv \left(\nabla \mathbf{R} - \frac{2ie}{c} \mathbf{A}(\mathbf{R}) \right|_i ,$$

$$\begin{aligned} \bar{G}_\omega^{(2)} = & -\frac{w_{ij}}{8a^2} \nabla_{R_i} \nabla_{R_j} |\Delta|^2 \left(1 - \frac{4\varepsilon(i\omega + \varepsilon)}{a} \right) + \\ & + \frac{w_{ij}}{4a^3} \nabla_{R_i} |\Delta|^2 \nabla_{R_j} |\Delta|^2 \left(1 - \frac{2\varepsilon(i\omega + \varepsilon)}{a} \right) - \\ & - \frac{w_{ij}}{2a^2} O_i^* \Delta^* O_j \Delta + \frac{1}{4} \frac{v_{p_i} v_{p_j}}{a^3 (i\omega + \varepsilon)} (\Delta^* O_i \Delta - \\ & - \Delta O_i^* \Delta^*)(\Delta^* O_j \Delta - \Delta O_j^* \Delta^*) + \\ & + \frac{i\omega + \varepsilon}{2a^3} \left(1 - \frac{2\varepsilon^2}{a} \right) v_{p_i} v_{p_j} \nabla_{R_i} \nabla_{R_j} |\Delta|^2 + \end{aligned}$$

$$\begin{aligned}
&+ \frac{v_{p_i} v_{p_j}}{a^2 (i\omega + \varepsilon)} O_i \Delta O_j^* \Delta^* - \frac{1}{4} \frac{v_{p_i} v_{p_j}}{a^3 (i\omega + \varepsilon)} \cdot \\
&\cdot \left(1 + \frac{2(i\omega + \varepsilon)^2}{a}\right) \nabla_{R_i} |\Delta|^2 \nabla_{R_j} |\Delta|^2 - \\
&- \frac{v_{p_i}}{2a^3} (\Delta^* O_i \Delta - \Delta O_i^* \Delta^*) (\nabla_{p_j} \Delta^* O_j \Delta - \nabla_{p_j} \Delta O_j^* \Delta^*) + \\
&+ \frac{1}{4} \frac{v_{p_i}}{a^2} \Big(\nabla_{p_i} \Delta^* O_i O_j \Delta + \nabla_{p_j} \Delta O_i^* O_j^* \Delta^*) - \\
&- \frac{v_{p_i}}{4a^2} (\nabla_{p_i} O_i \Delta O_j^* \Delta^* + \nabla_{p_j} O_i^* \Delta^* O_j \Delta) + \\
&+ \frac{1}{2} \frac{v_{p_i}}{a^4} \nabla_{R_i} |\Delta|^2 \nabla_{p_i} |\Delta|^2 \nabla_{R_j} |\Delta|^2 - \\
&- \frac{\varepsilon(i\omega + \varepsilon)}{a^4} v_{p_i} \nabla_{p_j} |\Delta|^2 \nabla_{R_i} \nabla_{R_j} |\Delta|^2 + \\
&+ \frac{i\omega + \varepsilon}{8a^2} [O_i^* O_j^* \Delta^* \nabla_{p_i} \nabla_{p_j} \Delta + O_i O_j \Delta \nabla_{p_i} \nabla_{p_j} \Delta^* - \\
&- 2 \nabla_{p_i} O_j \Delta \nabla_{p_j} O_i^* \Delta^*] + \\
&+ \frac{i\omega + \varepsilon}{4a^2} [2 \nabla_{R_i} \nabla_{p_j} |\Delta|^2 \nabla_{R_j} |\Delta|^2 \nabla_{p_i} |\Delta|^2 - \\
&- \nabla_{R_i} \nabla_{R_j} |\Delta|^2 \nabla_{p_i} |\Delta|^2 \nabla_{p_j} |\Delta|^2 - \\
&- \nabla_{R_i} |\Delta|^2 \nabla_{R_j} |\Delta|^2 \nabla_{p_i} \nabla_{p_j} |\Delta|^2] + \\
&+ \frac{i\omega + \varepsilon}{8a^3} [3 \nabla_{R_i} \nabla_{R_j} |\Delta|^2 \nabla_{p_i} \nabla_{p_j} |\Delta|^2 - \\
&- 2 \nabla_{R_i} \nabla_{p_j} |\Delta|^2 \nabla_{p_j} \nabla_{R_i} |\Delta|^2] \\
&+ \frac{i\omega + \varepsilon}{4a^3} [(O_i \Delta \nabla_{p_i} \Delta^* - O_i^* \Delta^* \nabla_{p_i} \Delta) \cdot \\
&\cdot (O_j \Delta \nabla_{p_j} \Delta^* - O_j^* \Delta^* \nabla_{p_j} \Delta)] ,
\end{aligned}$$

$$\bar{F}_\omega^{+(0)} = \frac{\Delta^*}{a} ,$$

$$\bar{F}_\omega^{+(1)} = \frac{\omega}{a^2} v_{p_i} O_i^* \Delta^* .$$

$$\begin{aligned}
\bar{F}_{\omega}^{+(2)} = {} & \frac{w_{ij}\,\varepsilon}{4a^2}\,{}^{*}_{i}\,O^*_j O\,\Delta^* - \frac{\varepsilon w_{ij}}{2a^3}\,\Delta^*\,\nabla_{R_i}\nabla_{R_j}|\Delta|^2 + \\
& + \frac{\varepsilon w_{ij}}{2a^4}\,\Delta^*\,\nabla_{R_i}|\Delta|^2\,\nabla_{R_j}|\Delta|^2 + \frac{v_{p_i} v_{p_j}}{4a^2}\,O^*_i O^*_j \Delta^*\left[3 - \frac{4\varepsilon^2}{a}\right] - \\
& - \frac{v_{p_i} v_{p_j}}{a^3}\,\Delta O^*_i \Delta^* O^*_j \Delta^* + \frac{v_{p_i} v_{p_j}}{2a^4}\,\Delta^*\,\nabla_{R_i}|\Delta|^2\,\nabla_{R_j}|\Delta|^2 - \\
& - \frac{v_{p_i} v_{p_j}}{2a^3}\,\Delta^*\,\nabla_{R_i}\nabla_{R_j}\,|\Delta|^2\left(1 - \frac{2\varepsilon^2}{a}\right) - \\
& - \frac{2ie}{c}\,\frac{\varepsilon}{4a^2}\,v_{p_i}\nabla_{p_j}\Delta^*\,(\nabla_{R_j}A_i - \nabla_{R_i}A_j) + \\
& + \frac{\varepsilon}{a^3}\,v_{p_i}\,[-\nabla_{p_j}|\Delta|^2\,O^*_i O^*_j\,\Delta^* + \nabla_{R_j}|\Delta|^2\,O^*_i\,\nabla_{p}\,\Delta^* - \\
& - \nabla_{p_j}\Delta^*\,O^*_i\,\Delta^*\,O_j\,\Delta + \nabla_{p_j}\Delta O^*_i\,\Delta^*\,O^*_j\,\Delta^*] + \\
& + \frac{\varepsilon}{a^4}\,v_{p_i}\Delta^*\,[\nabla_{p_j}|\Delta|^2\,\nabla_{R_i}\nabla_{R_j}|\Delta|^2 - \nabla_{R_j}|\Delta|^2\,\nabla_{R_i}\nabla_{p_j}|\Delta|^2] + \\
& + \frac{2ie}{c}\,\frac{\Delta^*}{8a^2}\,\nabla_{p_i}\Delta^*\,\nabla_{p_i}\Delta\,(\nabla_{R_j}A_i - \nabla_{R_i}A_j) + \\
& + \frac{1}{4a^2}\,[\nabla_{p_i}\nabla_{p_j}\Delta^*\,\triangle_{R_i}\nabla_{R_j}|\Delta|^2 - 2O^*_i\,\nabla_{p_j}\Delta^*\,\nabla_{p_i}\nabla \boldsymbol{R}_j\,|\Delta|^2 + \\
& 2O^*_i\,\nabla_{p_j}\Delta^*\,\nabla_{p_i}O_j\,\Delta + O^*_i O^*_j\,\Delta^*\,\nabla_{p_i}\nabla_{p_j}|\Delta|^2 - \\
& - O^*_i\,\Delta^*\,O^*_j\,\Delta^*\,\nabla_{p_i}\nabla_{p_i}\Delta - \nabla_{p_i}\Delta^*\,\nabla_{p_j}\Delta^*\,O_i\,O_j\,\Delta + \\
& + \Delta O^*_i\,\nabla_{p_j}\Delta^*\,\nabla_{p_i}O^*_j\,\Delta^* - \Delta O^*_i\,O^*_j\,\Delta^*\,\nabla_{p_i}\nabla_{p_j}\Delta^*] + \\
& + \frac{1}{4a^3}\,[2\nabla_{p_i}|\Delta|^2\,\nabla_{R_j}|\Delta|^2\,O^*_i\,\nabla_{p_j}\Delta^* - \\
& - \nabla_{p_i}|\Delta|^2\,\nabla_{p_j}|\Delta|^2\,O^*_i O^*_j\,\Delta^* + \Delta^*(\nabla_{p_i}\Delta O^*_i\,\Delta^* - \\
& - \nabla_{p_i}\Delta^*\,O_i\,\Delta)\,(\nabla_{p_i}\Delta O^*_j\,\Delta^* - \nabla_{p_j}\Delta^*\,O_j\,\Delta) + \\
& + \Delta^*\,\nabla_{R_i}\nabla_{p_j}|\Delta|^2\,\nabla_{p_i}\nabla_{R_j}|\Delta|^2 - \\
& - \Delta^*\,\nabla_{p_i}\nabla_{p_j}|\Delta|^2\,\nabla_{R_i}\nabla_{R_j}|\Delta|^2 - \\
& - \nabla_{R_i}|\Delta|^2\,\nabla_{R_j}|\Delta|^2\,\nabla_{p_i}\nabla_{p_j}\Delta^*] + \\
& + \frac{\Delta^*}{4a^4}\,[-2\nabla_{p_i}|\Delta|^2\,\nabla_{R_j}|\Delta|^2\,\nabla_{R_i}\nabla_{p_j}|\Delta|^2 + \\
& + \nabla_{p_i}|\Delta|^2\,\nabla_{R_j}|\Delta|^2\,\nabla_{p_i}\nabla_{p_j}|\Delta|^2 + \\
& + \nabla_{p_i}|\Delta|^2\,\nabla_{p_j}|\Delta|^2\,\nabla_{R_i}\nabla_{R_j}|\Delta|^2] \,.
\end{aligned}$$

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О ВЫВОДЕ ОБОБЩЕННЫХ УРАВНЕНИЙ ГИНЗБУРГА-ЛАНДАУ

Н. МЕНЬГАРД

Резюме

В работе исследуются следствия применения модели более реального, чем BCS эффективного электрон-электронного взаимодействия в выводе уравнений Гинсбурга—Ландау и их обобщений. Исходным пунктом взяты уравнения Горькова для термодинамических функций Грина, в которых параметр щели выратем через общий нелокальный двухчастичный потенциал. Принимается во внимание и анизотропия одночастичного спектра. Выводятся обобщенные уравнения Вертгамера и показывается приведение их к модифицированным уравнениям Гинсбурга для $T \lesssim T_c$. В той же области пренебрежение анизотропии приводит к результатам уравнений Гинсбурга—Ландау.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3–4), pp. 293–302 (1966)

CALCULATION OF THE DIFFUSION COEFFICIENT TO MOBILITY RATIO OF ELECTRONS FOR NOBLE GASES

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(Presented by I. Kovács. — Received 31. III. 1966)

Taking elastic scattering into consideration, but neglecting inelastic collision, with the application of the Boltzmann transport equation the equilibrium distribution function of electrons has been calculated with a view to determine the energy dependence of the diffusion cross section. In the knowledge of the equilibrium distribution function the ratio $\frac{D}{\mu}$ of diffusion coefficient to mobility was determined. In the case of very low electric field strength the calculated equilibrium distribution function gives the Maxwell—Boltzmann distribution and $\frac{D}{\mu} = \frac{kT}{e}$. With increasing electric field strength the equilibrium distribution function passes through an intermediate distribution and finally gives the distribution calculated by MORSE, ALLIS and LAMAR. The ratio $\frac{D}{\mu}$ increases with the electric field strength. With the assumption of a diffusion cross section independent from energy in the case of higher electric field strengths the ratio increases linearly with the field strength. The results have been applied to the calculation of the dependence of the ratio $\frac{D}{\mu}$ on electric field strength for helium and neon gases. The results have been compared with measured data.

Introduction

The first method for the measurement of the ratio of diffusion coefficient to mobility of electrons is due to TOWNSEND [1]. His method has been improved. The experimental results were summed up by HEALEY and REED [2], MASSEY and BURHOP [3], LOEB [4] and BROWN [5].

For the theoretical interpretation of the measurements it was first assumed that the electrons follow a MAXWELL or a DRUYVESTEIN [4] distribution and that the elastic collision cross section as well as the rotation and vibration cross sections are independent of energy [6], or only slightly change with energy [7]. These assumptions produced a fairly good agreement with measurements. A more precise solution of the problem may be obtained through the Boltzmann transport equation. For this a better knowledge of the processes that produce energy drops is needed. In many cases this is not available and inverse methods were preferred [8] [9]. By using measured data related to the ratio $\frac{D}{\mu}$ with the application of the Boltzmann transport equation the energy dependence of elastic and inelastic collision cross sections could be determined.

The ratio $\frac{D}{\mu}$, characteristic of the average energy of electrons in a gas, is sometimes called the characteristic energy of electrons. Recent measurements [10] have proved the ratio $\frac{D}{\mu}$ in case of very low electric field strengths to be equal to the quantity $\frac{kT}{e}$ (k = Boltzmann constant, T = absolute temperature of the gas and e = charge of the electron). In this case the electrons are in equilibrium with the gas and their energy distributions are identical. With an increase of the electric field strength characteristic energy increases, the increase being strongly dependent on the energy dependence of the cross sections related to the electrons.

By using the Boltzmann transport equation and taking only elastic scattering into consideration the equilibrium distribution function of the electrons have been determined and from this also the ratio $\frac{D}{\mu}$. The results have been applied to helium and neon gases.

Solution of the Boltzmann transport equation

Margenau [11] and Holstein [12] applied the Boltzmann transport equation to electrons moving in a gas of absolute temperature T for the cases of constant and of periodically changing electric field strengths. In a constant electric field the following differential equation has resulted for the equilibrium distribution function:

$$\begin{aligned} \frac{E^2}{3}\left[\frac{d}{du}\, u\lambda_D(u)\frac{df(u)}{du}\right] + \frac{2m}{M}\frac{d}{du}\left[\frac{u^2}{\lambda_D(u)}f(u)\right] + \\ + \frac{2mkT}{Me}\frac{d}{du}\left[\frac{u^2}{\lambda_D(u)}\frac{df(u)}{du}\right] + \qquad (1) \\ + \sum_n (u+u_n) f(u+u_n)\,\lambda_n^{-1}(u+u_n) = 0\,, \end{aligned}$$

where u is the energy of the electron in eV, E electric field strength in units of $\frac{\text{Volt}}{\text{cm}}$, $\frac{m}{M}$ the ratio of the mass of the electron to the mass of the molecule, $\lambda_D(u)$ the diffusion (momentum transfer) mean free path, $\lambda_n(u)$ the diffusion mean free path for the nth excitation and $f(u)$ the equilibrium distribution function.

The density of the electrons in the energy interval between u and $u + du$ is proportional to $u^{1/2} f(u)$. The probability that an electron will be found in this interval can be calculated as

$$n(u)\,du = \frac{u^{\frac{1}{2}} f(u)\,du}{\int\limits_0^\infty u^{\frac{1}{2}} f(u)\,du}\,. \tag{2}$$

The application of the equilibrium distribution function gives for the ratio $\frac{D}{\mu}$ the relationship [13]

$$\frac{D}{\mu} = -\frac{\int\limits_0^\infty u\lambda_D(u) f(u)\,du}{\int\limits_0^\infty u\lambda_D(u)\frac{df(u)}{du}\,du}\,. \tag{3}$$

The ratio $\frac{D}{\mu}$ is obtained in electronvolts.

As long as the electric field strength is not too high, the last term which takes excitation into consideration in differential equation (1) may be neglected, as in this case only the energy of a negligibly small number of electrons falls into the excitation range. Then equation (1) holds

$$\frac{E^2}{3}\frac{d}{du}\left[u\lambda_D(u)\frac{df(u)}{du}\right] + \frac{2m}{M}\frac{d}{du}\left[\frac{u^2}{\lambda_D(u)}f(u)\right] + \\ + \frac{2\,mkT}{Me}\frac{d}{du}\left[\frac{u^2}{\lambda_D(u)}\frac{df(u)}{du}\right] = 0\,.$$

We integrate with respect to u and obtain

$$\frac{E^2}{6}u\lambda_D(u)\frac{df(u)}{du} + \frac{m}{M}\frac{u^2}{\lambda_D(u)}f(u) + \frac{mkT}{Me}\frac{u^2}{\lambda_D(u)}\frac{df(u)}{du} = K,$$

where K is a constant. Integrate again to obtain

$$f(u) = \mathrm{C}e^{-\int\limits_0^u \frac{du}{\frac{E^2}{6}\frac{M}{m}\frac{\lambda_D^2(u)}{u} + \frac{kT}{e}}}\,, \tag{4}$$

where C is a constant. The equilibrium distribution function has been obtained in a not normalised form. Let us put into equation (4) the diffusion cross section instead of λ_D by using the relationship $\lambda_D = \frac{1}{pQ_D}$ (Pressure p is expressed in terms of Torr, Q_D in terms of $\frac{1}{\text{cm Torr}}$, both of them for the case of 300° K temperature).

$$f(u) = Ce^{-\int\limits_0^u \frac{du}{\frac{M}{6m}\left(\frac{E}{p}\right)^2 \frac{1}{Q_D^2 u} + \frac{kT}{e}}} . \tag{5}$$

For very low electric field strength to pressure ratio, when $\frac{E}{p} \to 0$, the equilibrium distribution function takes the form

$$f(u) = Ce^{-\frac{eu}{kT}} .$$

This is the Boltzmann equilibrium distribution function. In this case the electrons, like the gas molecules, have an energy distribution corresponding to thermal agitation.

When the electric field strength to pressure ratio is sufficiently high, expression (5) is replaced with a fairly good approximation by the relationship

$$f(u) = Ce^{-\frac{6m}{M\left(\frac{E}{p}\right)^2}\int\limits_0^u Q_D^2\, u\, du} . \tag{6}$$

As long as $\frac{D}{\mu} > 10\,\frac{kT}{e}$, relationship (6) holds. This distribution is identical with the result obtained by MORSE, ALLIS and LAMAR [14] calculated by taking into account the elastic collision of the electrons.

To calculate $\frac{D}{\mu}$ put distribution function (5) into equation (3):

$$\frac{D}{\mu} = \frac{\int\limits_0^\infty \frac{u}{Q_D} f(u)\, du}{\int\limits_0^\infty \frac{u}{Q_D}\left(\frac{f(u)}{\frac{M}{6m}\left(\frac{E}{p}\right)^2 \frac{1}{Q_D^2 u} + \frac{kT}{e}}\right) du} . \tag{7}$$

When the electric field strength to pressure ratio is very low, then

$$\frac{D}{\mu} = \frac{kT}{e} . \tag{8}$$

With the electric field strength to pressure ratio increasing in accordance with relationship (7), the ratio $\frac{D}{\mu}$ is increasing monotonously.

In the case of a constant diffusion cross section, when Q_D is independent of the electric field strength to pressure ratio, after the substitutions

$$A = \frac{kT}{e} \quad \text{and} \quad B = \frac{M}{6m}\left(\frac{E}{p}\right)^2 \frac{1}{Q_D^2}$$

equation (7) may be written as

$$\frac{D}{\mu} = \frac{\int\limits_0^\infty u e^{-\frac{u}{A}} (Au + B)^{\frac{B}{A}} du}{\int\limits_0^\infty u^2 e^{-\frac{u}{A}} (Au + B)^{\frac{B}{A} - 1} du} ,$$

The ratio of the two integrals may be transformed into an expression consisting of incomplete factorial functions:

$$\frac{D}{\mu} = A \frac{\int\limits_{\frac{B}{A^2}}^\infty t^{\frac{B}{A} + 1} e^{-t} dt - \frac{B}{A^2} \int\limits_{\frac{B}{A^2}}^\infty t^{\frac{B}{A}} e^{-t} dt}{\int\limits_{\frac{B}{A^2}}^\infty t^{\frac{B}{A} + 1} e^{-t} dt - \frac{2B}{A^2} \int\limits_{\frac{B}{A^2}}^\infty t^{\frac{B}{A}} e^{-t} dt + \frac{B^2}{A^4} \int\limits_{\frac{B}{A^2}}^\infty t^{\frac{B}{A} - 1} e^{-t} dt} . \tag{9}$$

The integrals can be calculated by making use of a Table [15]. If the electric field strength to pressure ratio is high enough $\left(\frac{D}{\mu} > 10 \frac{kT}{e}\right)$ by using distribution function (6) we may write

$$\frac{D}{\mu} = \frac{\left(\frac{E}{p}\right)^2 M}{3m Q_D^2} \frac{\int\limits_0^u u e^{-\frac{3m}{M} \frac{Q_D^2}{\left(\frac{E}{p}\right)^2} u^2} du}{\int\limits_0^u u^2 e^{-\frac{3m}{M} \frac{Q_D^2}{\left(\frac{E}{p}\right)^2} u^2} du} = \frac{E}{p} \frac{1}{Q_D} \left(\frac{M}{3\pi m}\right)^{\frac{1}{2}} \tag{10}$$

It is seen that in this case the ratio $\frac{D}{\mu}$ increases linearly with the field strength to pressure ratio.

Numerical results for helium and neon

To calculate the ratio $\frac{D}{\mu}$ for a particular gas the diffusion cross section must be known as a function of energy. Barbiere [16] calculated Q_D from the measurement data of Ramsauer and Kollath [17] as a function of energy for helium from 1,8 eV to 19,2 eV and for neon from 0,99 eV to 15,9 eV. As we wish to calculate $\frac{D}{\mu}$ starting from very low electric field strength to pressure ratio, we need Q_D from zero energy up. O'Malley [18] applied the modified effective range theory to develop a relationship for Q_D for the case of low electron energies (from 0 to 1—2 eV) for helium and neon gases. The results show a fair agreement with Barbiere's calculations up to 1—2 eV.

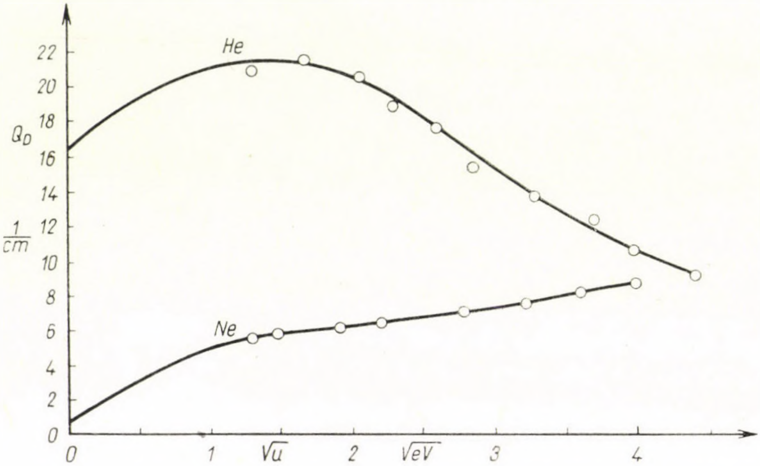

Fig. 1

O'Maalley's formula is

$$Q_D = 16{,}1 + 12{,}4u + 2{,}13u \ln u - 7{,}73u \tag{11}$$

for helium and

$$Q_D = 0{,}653 + 4{,}91u + 0{,}170u \ln u - 0{,}604u \tag{12}$$

for neon.

The dimension of Q_D in both instances is $\frac{1}{cm}$, for the case of 300° K temperature and 1 Torr pressure.

Figure 1 shows Q_D as a function of energy for helium and neon gases. The full line represents Q_D calculated from 0 to 1,8 eV from relationship (11), and from 0 to 0,99 eV from relationship (12). For higher energies **Barbiere**'s data applied to 300° K were used. These data are shown on the continuous curves with circles.

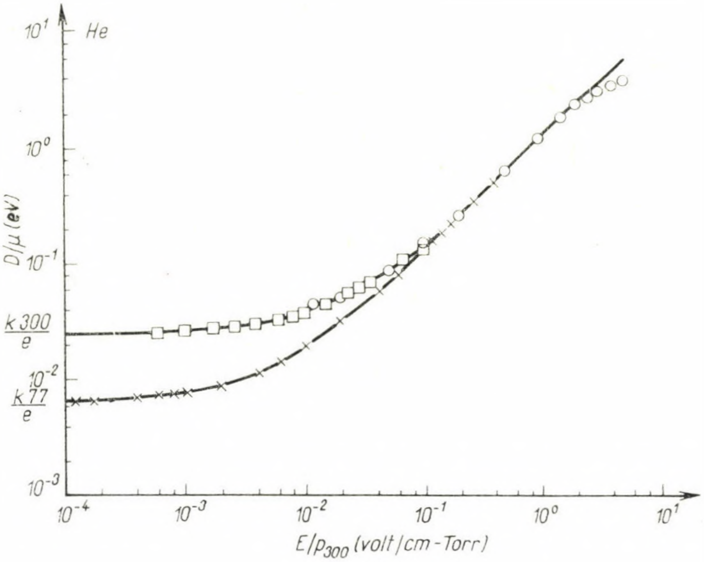

Fig. 2

In the knowledge of the function Q_D, using relationship (7), for helium the ratio $\frac{D}{\mu}$ was calculated as a function of the electric field strength to pressure ratio by numerical integration for 300° K and 77° K. The results are represented in Figure 2 by a full line. Along the horizontal axis the values of $\frac{E}{p_{300}}$ referred to pressure normalized for 300° K temperature are shown. Corresponding to this pressure at 77° K, $p_{77} = \frac{77}{300} p_{300}$, the number of gas atoms per cubic centimetre does not change with temperature and therefore Q_D does not vary either.

In the case of helium Q_D is energy-dependent only to a slight extent. Assuming the diffusion cross section to be constant $Q_D = 19{,}5 \frac{1}{cm}$, the ratio

$\frac{D}{\mu}$ as a function of the electric field strength to pressure ratio was calculated also from equation (9). The departure from the results of relationship (7) for each value $\frac{E}{p_{300}}$ remains below 2 per cent. Considering relationship (10) from the value of $\frac{E}{p_{300}} = \frac{V}{\text{cm Torr}}$ on, the ratio $\frac{D}{\mu}$ is increasing linearly with a fair approximation.

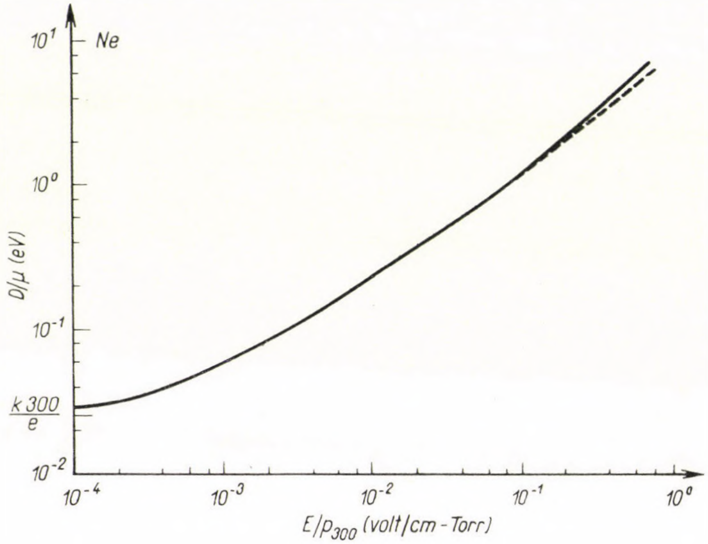

Fig. 3

Figure 2 shows also the measured results. The results of **Warren** and **Parker** [10] related to a gas temperature of 77° K are indicated by crosses, those referred to 300° K by squares. The results of **Townsend** and **Bailey** [19] referred to 288° K are indicated by circles. The theoretical curve shows a very good agreement with the measurements up to $\frac{E}{p_{300}} = 2\ \frac{\text{Volt}}{\text{cm Torr}}$.

For neon gas of 300° K temperature the ratio $\frac{D}{\mu}$ as the function of electric field strength to pressure ratio, calculated by the numerical integration of relationship (7) is represented in Figure 3 by a full line. In this case Q_D, as a function of energy, cannot be considered constant. Measurements [5] are represented by a dotted line. The disagreement of calculated and measured values increases with the electric field strength to pressure ratio.

In our calculation inelastic collisions have been neglected. For this reason our results hold true only up to an electric field strength to pressure ratio, at which only a negligibly small number of electrons reaches the energy of the first excitation. This can be assumed if the equilibrium energy distribution function of the electrons is calculated from relationship (2) for various values $\frac{E}{p}$. Figure 4 shows the equilibrium energy distribution function for $\frac{E}{p} = 2 \frac{\text{Volt}}{\text{cmTorr}}$. At this stage only very few electrons reach the level of 19,2 eV corresponding to the first excitation energy. When $\frac{E}{p}$ is larger than that, in accordance with the equilibrium energy distribution functions, the number of electrons that reach the first excitation energy is increasing. Owing to this the discrepancy between calculated values and measured results is increasing from $\frac{E}{p} = 2 \frac{\text{Volt}}{\text{cmTorr}}$ up. The equilibrium energy distribution function referred to $\frac{E}{p} = 2 \frac{\text{Volt}}{\text{cmTorr}}$ shows a fair agreement with BARBIERE's calculations [16] in which inelastic collisions were taken into consideration. The effect of inelastic collisions has proved negligible also in this case.

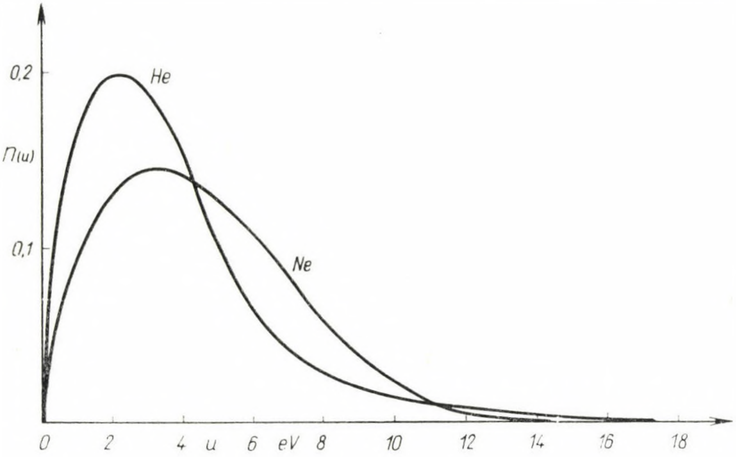

Fig. 4

From the examination of the equilibrium energy distribution for neon gas it is seen that up to $\frac{E}{p} = 0{,}4 \frac{\text{Volt}}{\text{cmTorr}}$ a negligibly small amount of electrons possesses the energy of 15,9 eV needed for the first excitation. Figure 4 also shows the equilibrium energy distribution referred to $\frac{E}{p} = 0{,}4 \frac{\text{Volt}}{\text{cmTorr}}$.

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ОПРЕДЕЛЕНИЕ ОТНОШЕНИЯ КОЭФФИЦИЕНТОВ ДИФФУЗИИ И ПОДВИЖНОСТИ ЭЛЕКТРОНОВ В СЛУЧАЕ БЛАГОРОДНЫХ ГАЗОВ

О. ОРИЭНТ

Резюме

На основе уравнения переноса Больцмана, исходя из упругого рассеяния и пренебрегая неупругимии столкновениями, в работе вычисляется функция равновесного распределения электронов, учитывая зависимость диффузионного поперечного сечения от энергии. Функции равновесного распределения использованы для определения частного $\frac{D}{\mu}$, то есть отношения коэффициента диффузии к подвижности электронов. Полученная функция равновесного распределения в случае очень слабых электрических полей соответствует распределению Максвелла—Больцмана, и $\frac{D}{\mu} = \frac{kT}{e}$. С увеличением напряженности электрического поля функция распределения через переходное распределение перейдет в равновесное распределение, определенное Морзе, Эллисом и Ламаром. Отношение $\frac{D}{\mu}$ с увеличением напряженности электрического поля увеличивается. Если диффузионное эффективное сечение считать независимым от энергии при больших напряженностях, то отношение $\frac{D}{\mu}$ линейно возрастает с напряженностью электрического поля. Результаты вычислений применяются в случае газов гелия и неона для определения зависимости отношения $\frac{D}{\mu}$ от напряженности электрического поля. Вычисленные данные сравниваются с результатами измерений.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3—4), pp. 303—310 (1966)

DISINTEGRATION OF N^{14} BY FAST NEUTRONS

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(Presented by A. Szalay. — Received 31. III. 1966)

The energy spectrum and angular distribution of alpha particles from the reaction $N^{14}(n, \alpha) B^{11}$ measured at $E_n = 14{,}7$ MeV with a cloud chamber are well described by the statistical model. A nuclear temperature of $2{,}0 \pm 0{,}1$ MeV has been deduced. The cross-sections for the reactions $N^{14}(n, p) C^{14}$ and $N^{14}(n, np) C^{13}$ are 77 ± 14 and 46 ± 13 mb, respectively. The measured cross-section ratio for the emission of protons and alpha particles and the ratio calculated with the statistical model are in good agreement.

1. Introduction

The study of the energy spectrum and the angular distribution of charged particles emitted in nuclear reactions provides information about the reaction mechanism. Only a few (n, α) and (n, p) reactions on light elements ($A \leq 20$) have been investigated with 14,7 MeV neutrons. Some of the measurements of the energy spectra and angular distributions support direct interaction and another the compound nucleus mechanism [1—4]. To obtain additional information fast neutron reactions with N^{14} were investigated using a cloud chamber. This method makes it possible to distinguish between processes in which one or two particles are emitted, e.g. the (n, p) and (n, np) reactions.

2. Experimental procedure

An expansion cloud chamber of 28 cm diam. and 5 cm depth was used for the measurements [5, 6]. It was filled with nitrogen gas; a water and alcohol mixture was used as condensable vapour. The total pressure was 490 mm Hg. Neutrons of 14,7 MeV were made in the $D + T$ reaction with the 300 kV cascade generator [7] of ATOMKI. The generator worked as a pulsed neutron source synchronized to the sensitive time of the cloud chamber. The tracks were measured by the reprojection method through the same optical system. The ranges of the emitted particle and the recoil nucleus, and their angles with respect to the neutron beam were measured. One can easily distinguish between the processes with emissions of one or two particles since in the first case the momenta of the emitted particle, the recoil nucleus and the bombarding neutron are in the same plane. In the case of two-particle emission, the process takes place in three dimensions. To evaluate the experimental data and to discriminate between the particles, it is necessary to know the range-energy relations for alpha particles, protons and recoil nuclei. For protons and alpha particles, the range-energy relation measured in air [8] was used and normalized at one point for the gas filling using a Po^{210}-alpha source. The range-energy relation for recoil nuclei was determined experimentally by reaction kinematics from processes in which the range of the emitted charged particle was within the illuminated part of the cloud chamber. Knowing the range-energy relation for the recoil nuclei we could evaluate events where the range of emitted particles was not measurable. Particle discrimination was possible by reaction kinematics.

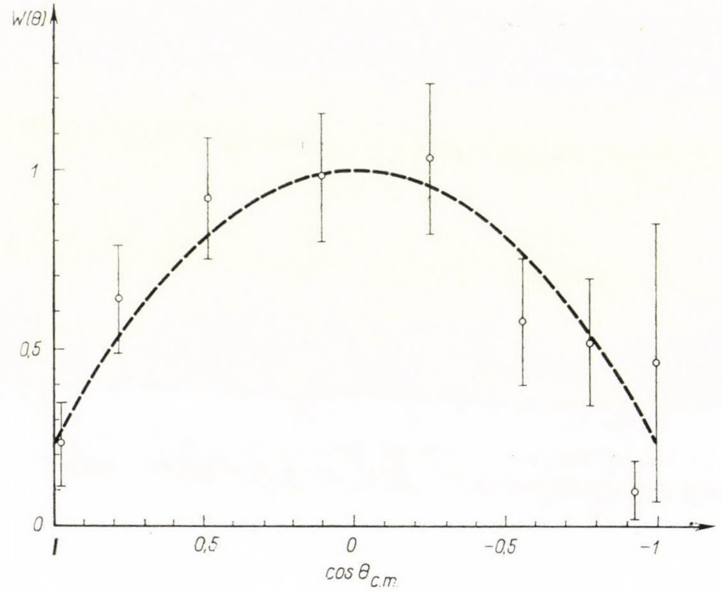

Fig. 1

3. Results and discussion

In relation to the total alpha spectrum, the angular distribution in the centre-of-mass system is symmetrical around 90° for the $N^{14}(n, \alpha)B^{11}$ reaction (Fig. 1). This angular distribution is in agreement with an earlier measurement [9] performed with poorer statistics and within a narrower range of angles. A least squares fit of the experimental angular distribution to the formula

$$W(\Theta) = 1 + b \cdot \cos^2 \Theta \tag{1}$$

yields $b = -0{,}76 \pm 0{,}25$. According to **Ericson** [10] the maximum at 90° shows a complete decoupling of I and l (I being the spin of the compound nucleus, and l the orbital angular momentum of the emitted particles). The dependence of the penetration factor $T_l(E)$ on the orbital angular momentum of the emitted particle, plays an important role in determining the form of angular distribution.

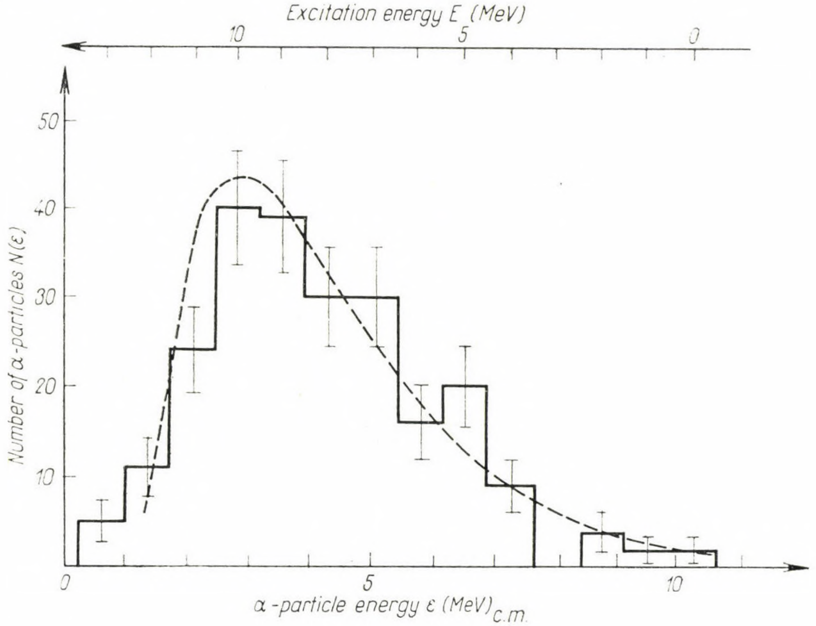

Fig. 2

Fig. 2 shows the energy spectrum of alpha particles in the c. m. system emitted over all angles. The errors stated represent statistical errors only. The energy distribution from N^{14} has the typical form of an evaporation spectrum with a maximum at about 3 MeV alpha energy.

From the results obtained for the angular distribution and energy spectrum it can be assumed that the statistical model may be used for the analysis of the reaction. The evaporation spectrum is given by the **Weisskopf—Ewing** [11] formula:

$$N(\varepsilon)\,d\varepsilon \sim \varepsilon\sigma_c(\varepsilon)\,\omega(E)\,d\varepsilon\,, \tag{2}$$

where ε = the kinetic energy of the alpha particles,

$\sigma_c(\varepsilon)$ = the inverse cross section,

$\omega(E)$ = the level density of the product nucleus at the excitation energy E,

$N(\varepsilon)d\varepsilon$ the number of alpha particles emitted with energies between ε and $\varepsilon + d\varepsilon$.

For the cross section, $\sigma_c(\varepsilon)$ data are available only for $Z \geqslant 10$ in the various Tables [12—14]; therefore the simple analytic expression [15] was used:

$$\sigma_c(\varepsilon) = \gamma_\alpha \pi R^2 (1 - V'_\alpha/\varepsilon), \tag{3}$$

where V'_α = the effective Coulomb barrier height,
R = the nuclear radius,
γ_α = an empirical parameter.

The Coulomb barrier is

$$V_\alpha = \frac{2{,}058(Z-2)}{(A-3)^{1/3} + 4^{1/3}} \text{ MeV}. \tag{4}$$

According to GOVE and NAKASIMA [16], the effective barrier is

$$V'_\alpha = V_\alpha \left(1 - \frac{1{,}13}{(A-3)^{1/3}}\right). \tag{5}$$

For alpha particles the nuclear radius parameter $r_0 = 1{,}7$ fm was taken from [17].

For the energy dependence of the level density $\omega(E)$ three approximate forms (given by the Fermi gas model) were adopted:

$$\omega(E) \sim E^{-2} \exp\left(2\sqrt{aE}\right), \tag{6}$$

$$\omega(E) \sim \exp\left(2\sqrt{aE}\right), \tag{7}$$

$$\omega(E) \sim \exp(E/T). \tag{8}$$

T in Eq. (8) is the nuclear temperature which by definition is connected with the level density in the following way:

$$\frac{1}{T} = \frac{d[\ln \omega(E)]}{dE}. \tag{9}$$

From Eqs. (2), (6) and (7) it follows that the logarithm of the reduced spectrum plotted as a function of $\sqrt{E}$ exhibits a straight line for an evaporation spectrum. As Fig. 3 shows, the experimental points lie in good approximation on a straight line in the case of the $N^{14}(n, \alpha)B^{11}$ reaction. The gradient of the straight line has a value $2\sqrt{a}$. For the value of the level density parameter $a = 4{,}4 \pm 0{,}2$ MeV^{-1} and $a = 1{,}14 \pm 0{,}05$ MeV^{-1} were obtained according to Eqs. (6) and (7), respectively. The results demonstrate that the value of the parameter a in the low level density region is largely dependent on the accepted form of level density. The value obtained from Eq. (6) is in better agreement with those determined in other ways on light nuclei [19]. Using Eqs. (2) and (8) the logarithm of the reduced spectrum as a function of E gives a straight line. As can be seen in Fig. 4 most of the experimental points in the total region of the spectrum define a straight line. From the gradient of the straight line a value of $T = 2{,}0 \pm 0{,}1$ MeV was deduced. Fig. 2 (dashed curve) represents the spectrum calculated with this temperature by means of Eqs. (2) and (8). As can be seen, the constant temperature model describes the spectrum fairly well. Substituting the level densities (6) and (7) in Eq. (9), the nuclear temperature is given by the following expressions:

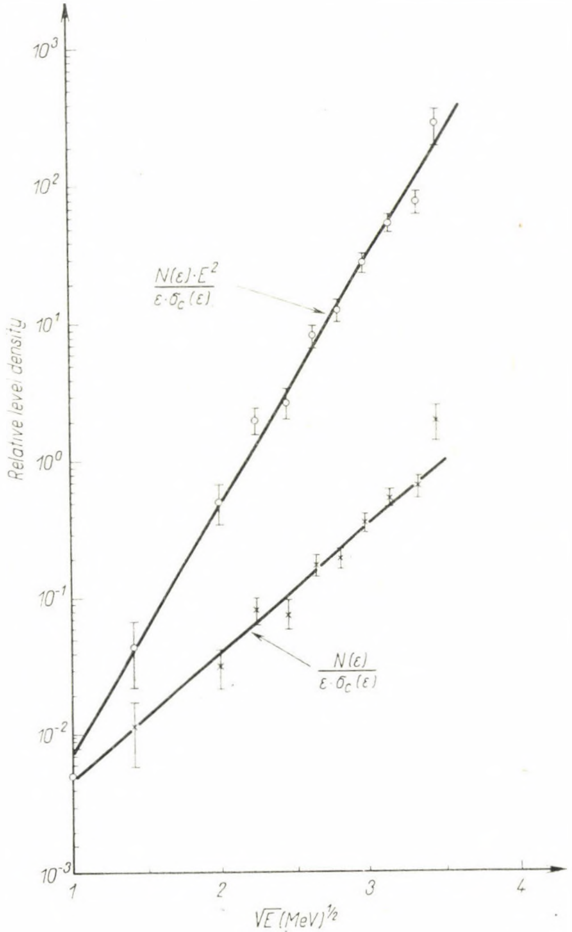

Fig. 3

$$\frac{1}{T} = \sqrt{\frac{a}{E}} - \frac{2}{E}\,; \qquad \frac{1}{T} = \sqrt{\frac{a}{E}}\,.$$

Using the average residual energy ($E = 8{,}6$ MeV), and the level density parameter a, obtained by Eqs. (6) and (7) the nuclear temperatures were found to be $T = 2{,}1$ MeV and $T = 2{,}7$ MeV, respectively. The data suggest that the nuclear temperature is not very sensitive to the choice of the level density formula. The nuclear temperature of the average excitation energy is in good agreement with that given by the constant temperature model, if the value $a = 4{,}4$ MeV^{-1} [Eq. (6)] is accepted. The T-value measured by us closely follows the tendency observed in the mass number dependence of nuclear temperature [20]. At $A \leq 20$, no earlier data are to be found for nuclear temperature. The energy spectrum and the angular distribution for the N^{14} $(n, \alpha)B^{11}$ reaction can be explained by the statistical model.

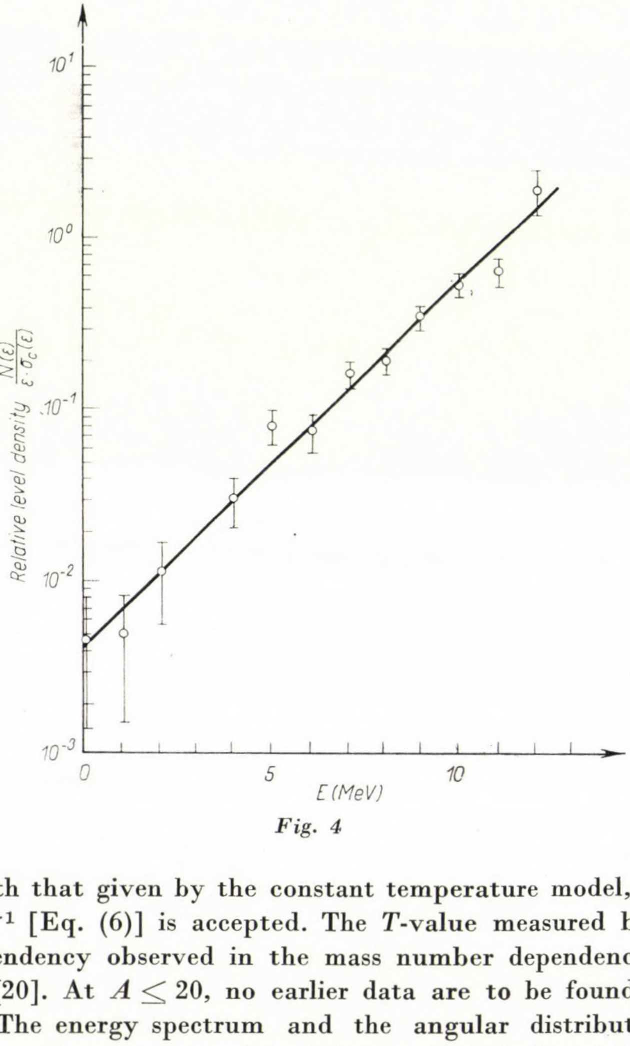

Fig. 4

The experiment also made it possible to determine the cross-section ratio of (n, α) and (n, p) reactions on the N^{14} nucleus. The experimental value is

$$\frac{\sigma(n, \alpha)}{\sigma(n, p)} = 1{,}3 \pm 0{,}2 \,.$$

Accepting for $\sigma(n, \alpha) = 100$ mb [21], our measurement gives $\sigma(n, p) = 77 \pm \pm 14$ mb.

It was assumed that all processes with emissions of two particles are attributed to (n, np) reaction because of the high negative Q-value of the $(n, n\alpha)$ reaction. ($Q(n, n\alpha) = -11{,}46$ MeV; $Q(n, np) = -7{,}55$ MeV; all Q-values in this article are taken from the tables of Kunz et al. [22]).

Starting from this assumption, the cross-section ratio of (n, np) and (n, p) reactions on the N^{14} nucleus could be determined. Its value is

$$\frac{\sigma(n, np)}{\sigma(n, p)} = 0{,}60 \pm 0{,}09\,.$$

Accepting $\sigma(n, \alpha) = 100$ mb (ref. [21]) we obtain from the measured cross-section ratios $\sigma(n, np) = 46 \pm 13$ mb.

In our investigations it was found that the number of protons from the $(n, p\gamma)$ process nearly equals the (n, np) and (n, pn) reaction yield in the energy region where second particle emission is allowed energetically. This means that de-excitation with gamma particles as a concurrent process cannot be neglected. In the proton spectrum in this energy region, 93 (n, p) and 104 $(n, np + n, pn)$ events were observed. (The high-energy part of the proton spectrum could be determined by the range-energy relation of recoil nuclei, but unfortunately this lacks the precision of direct measurement. Therefore, the form of the spectrum was not analysed theoretically.)

A comparison of measured and calculated cross-section ratios yields information about reaction mechanisms. The cross-section ratio of alpha and proton emissions on the N^{14} nucleus has the experimental value

$$\frac{\sigma(n, \alpha)}{\sigma(n, p) + \sigma(n, np)} = 0{,}83 \pm 0{,}09\,.$$

For the calculation of the ratio of the reaction yield, an approximate relation is given by Bodansky [15]:

$$\frac{\Gamma_\alpha}{\Gamma_p} = \frac{(2s_\alpha + 1)\, M_\alpha \gamma_\alpha R_\alpha^2}{(2s_p + 1)\, M_p \gamma_p R_p^2} \exp\left[(S_p - S_\alpha) + (V_p' - V_\alpha')\right]/T\,, \tag{10}$$

where S_p, S_α, M_p, M_α are the spins and masses for protons and alpha particles, $\gamma_\alpha = 1{,}1$, $\gamma_p = 1{,}75$, R_p and R_α the interaction radii, S_p and S_α separation energies, V_p' and V_α' effective barrier heights and T the nuclear temperature (with the value 2 MeV measured by us). The value of V_p' was calculated similarly to that of V_α' ($r_0 = 1{,}25$ fm). The calculations of separation energies were based on the data of Kunz et al. [22]. The ratio $\Gamma_\alpha/\Gamma_p = 1{,}16$ obtained from the approximate expression (10) can be regarded as in good agreement with that measured i.e. 0,83.

We are indebted to Professor A. **Szalay** for his interest in the present work and for the excellent working conditions he secured. We also thank Mr. L. **Bunkóczi** and Mrs. G. **Sepsy** for their assistance in operating the accelerator and scanning the photographs.

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РАСПАД N^{14} БЫСТРЫМИ НЕЙТРОНАМИ

Й. ЧИКАИ и Ш. НАДЬ

Резюме

Энергетический спектр и угловое распределение альфа-частиц в реакции $N^{14}(n, \alpha)B^{11}$, измеренные при $E_n = 14{,}7$ Мэв в камере Вильсона, хорошо описываются со статистической моделью. Выводится ядерная температура 2,0 ± 0,1 Мэв. Поперечное сечение для реакций $N^{14}(n, p)C^{14}$ и $N^{14}(n, np)C^{13}$ составляет 77 ± 14 и 46 ± 13 мбарн соответственно. Измеренное соотношение поперечное сечения для эмиссии протонов и альфа-частиц и вычисленное на основе статистической модели значение удовлетворительно согласуются.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3—4), pp. 311—320 (1966)

ON THE ELASTIC MODULI OF ALKALINE AND NOBLE METALS I

By

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(Presented by A. Kónya. — Received 5. IV. 1966)

An approximate expression on the basis of GOMBÁS's theory of monovalent metals is derived for the energy of the Wigner—Seitz cell of alkaline and noble metals in the case of elastic deformation, approximating the cell by a rotation ellipsoid instead of a sphere. From the energy minimum principle one obtains the ratio of the ellipsoidal axes, which yields the Poisson ratio in the vicinity of unstrained equilibrium, while from GOMBÁS's results the compressibility is known. With these two quantities it is possible to calculate the elastic moduli c_{11} and c_{12}.

1. GOMBÁS's theory of monovalent metals [1], [2] accounts for the cohesion of the alkaline, alkaline earth and noble metals on a purely theoretical basis, without introducing any empirical or semiempirical parameter and at the same time yielding numerical results for cell energy as a function of the cell radius. The minimum of this energy and the proper stationary radius give very excellent values for the cell energy and the equilibrium lattice constant compared with the experimental results taken at an adequately low temperature or even extrapolated to absolute zero. It is very remarkable that the compressibility calculated from the energy vs. cell radius function agrees very well with the experimental results, and this reflects even the curvature of the energy curve about the minimum to be very near to the actual value of the crystal cell.

The theory treats the metal as a system of a positive metal ion lattice and a practically free "gas" of valence electrons. The most characteristic feature of the theory is that it deals with valence electrons and ion core electrons separately. The latter are taken into account in some of the customary ways, while the former are treated in a modified potential of the ion core lattice.

This modified potential consist of the electrostatic potential of the ion core and a nonclassical pseudopotential, which is the result of the Pauli principle. When this pseudopotential is introduced it is no longer necessary to orthogonalize the eigenfunctions of the valence electrons to those of the core electrons. At the same time, naturally, the deepest possible energy states for the valence electrons are obtained.

In the course of the computation the elementary cell is approximated by a sphere of radius R and the cell-energy is taken as

$$U = E_C + E_A + E_W + E_F + W_C + W_E + W_A + W_W + W_K + H\,, \qquad (1)$$

where E always stands for the different parts of the self-energy of the valence electrons, W for the interaction energy of the valence electron with the ion cores and H for the interaction of the cores. The indices are C for Coulomb type, A for exchange, W for correlational, F for zeropoint, E for non Coulomb-type electrostatic energy, and K represents the energy resulting from the pseudo-potential. The valence electron gas density is assumed to be constant as

$$\nu = \frac{3}{4\pi R^3} . \tag{2}$$

As for the actual form of the different energy terms and pseudo-potentials above we refer to the original publications of GOMBÁS [3, 4].

The methods outlined above were applied to some alkaline and noble metals by GOMBÁS. Here, we quote his results for potassium and silver [5, 6]. The numerical results can be approximated in an analytical form. The cell-energy for potassium is

$$U_K = -\frac{1{,}4083}{R} + \frac{21{,}633}{R^3} \tag{3}$$

and for silver

$$U_{Ag} = -\frac{1{,}26604}{R} + \frac{154{,}687}{R^{7{,}677}} , \tag{4}$$

where U and R are given in $\frac{e^2}{a_0}$ and a_0 atomic units, respectively, e being the elementary electrical charge and a_0 the first Bohr radius of the hydrogen atom.

2. Let the cell-energy be given in general as a function of the radius R of the elementary sphere in the following form:

$$U = -\frac{A}{R} + \frac{B}{R^n} , \tag{5}$$

where A, B and n are constants. Then in the equilibrium-state the energy is a minimum:

$$\left(\frac{dU}{dR}\right)_{R_0} = 0 \tag{6}$$

and the minimum value is:

$$U_0 = U(R_0). \qquad 7)$$

Using (6), (5) and (7) one obtains:

$$A = \frac{nU_0 R_0}{1-n}\,, \tag{8}$$

$$B = \frac{U_0 R_0^n}{1-n} \tag{9}$$

or using the minimum energy U_0 and the equilibrium radius R_0 instead of A and B:

$$U = \frac{U_0}{1-n}\left[-n\left(\frac{R_0}{R}\right)+\left(\frac{R_0}{R}\right)^n\right]. \tag{10}$$

Owing to the energy minimum the second derivative in the equilibrium is positive:

$$\left(\frac{d^2 U}{dR^2}\right)_{R_0} = \gamma > 0\,. \tag{11}$$

So in the vicinity of the equilibrium the energy of the elementary sphere of radius $(R_0 + \delta R)$ is given by

$$U = U_0 + \frac{1}{2}\,\gamma(\delta R)^2\,. \tag{12}$$

Meanwhile the equilibrium volume V_0 is changed by δV, which is given as

$$\delta V = \frac{3V_0}{R_0}\,\delta R \tag{13}$$

neglecting the higher order terms in δR.

The change in equilibrium energy:

$$\delta U = U - U_0 = \frac{\gamma}{2}\,(\delta R)^2 \tag{14a}$$

is equal to the work necessary to produce the volume change of the elementary cell. This (static) work is

$$\delta U = \frac{1}{2}\,\delta p \cdot \delta V\,, \tag{14b}$$

where δp must be first order in δR, too, and can be introduced formally as "normal stress" using (14a), (14b) and (13) as:

$$\delta p = \frac{R_0 \gamma}{3V_0}\,\delta R. \tag{15}$$

The compressibility $\varkappa$ is then defined as

$$\frac{1}{\varkappa} = V_0 \frac{\delta p}{\delta V} = \frac{\gamma}{12\pi R_0} . \tag{16}$$

Let us introduce the absolute value of the equilibrium energy of unit volume as w_0

$$w_0 = - \frac{U_0}{V_0} \tag{17}$$

then using (10), (11), (16) and (17) the compressibility is:

$$\frac{1}{\varkappa} = \frac{n w_0}{9} \tag{18}$$

and for the normal stress introduced

$$\delta p = \left(\frac{3}{\varkappa} \right) \frac{\delta R}{R_0} . \tag{19}$$

3. While the energy function gives the work required for a spherically symmetric deformation (14a) correctly, in other non spherically symmetric deformations the original energy expression (1) should again be computed for the specific deformation. This would be rather a lengthy and laborious procedure because of the lack of spherical symmetry. For such cases, however, when the deformed cell can be approximated by a rotational ellipsoid for small deformation very near to the equilibrium state it is possible to give the deformation work as a first approximation as follows.

Let Λ be a small quantity:

$$\Lambda \ll 1 \tag{20}$$

and approximate the deformed cell by a rotational ellipsoid with the axis (up to the first order in Λ)

$$a = R_0 (1 + \Lambda) , \tag{21}$$

$$b = R_0 (1 + \mu \Lambda) , \tag{22}$$

where μ is another quantity. Evidently if $\Lambda \to 0$, a and $b \to R_0$ if μ is finite.

The contour curve of the ellipsoid in some plane (having the rotational axis in it) in (r, φ) polar-coordinates, (the central point of the ellipsoid being the origin of the coordinate system) is given by the equation:

$$r^2 = \frac{a^2}{1 + \varepsilon^2 \sin^2 \varphi} , \tag{23}$$

where

$$\varepsilon^2 = \frac{a^2}{b^2} - 1 . \tag{24}$$

Taking into account the fact that $\Lambda \ll 1$ and $\varepsilon^2 \ll 1$ one obtains from (21), (22), (23) and (24) (see Appendix):

$$\frac{\delta R}{R_0} = \Lambda[1 - (1 - \mu)\sin^2 \varphi] , \tag{25}$$

where

$$\delta R = r - R_0 . \tag{26}$$

If e.g. $\varphi = 0$, $\delta R = \Lambda R_0$ and $r(\varphi = 0) = a$, while $\varphi = \frac{\pi}{2}$, $\delta R = \mu \Lambda R_0$ and so $r\left(\varphi = \frac{\pi}{2}\right) = b$ as stated above.

As a further approximation we will use (19) for a stress even in the case where spherical symmetry is absent. By remaining only in the very close vicinity of the equilibrium sphere we do not expect to cause too large errors, at least in this nominal stress value introduced. This approximation, however, neglects at the same time, all the energy terms, which will be brought about by the lack of spherical symmetry and so are zero in the spherical equilibrium state. Certainly there are such terms, on which we shall report in a subsequent paper.

Reverting, however, to the former approximation, one gets for the stress

$$\delta p = \left(\frac{3}{\varkappa}\right)[1 - (1 - \mu)\sin^2 \varphi]\, \Lambda . \tag{27}$$

To obtain the deformation work, instead of (14b) we must integrate for the volume changed because δp is a function of the polar angle φ. After integration, we get for the deformation work (see Appendix):

$$\delta U = - U_0 \frac{3}{10 \varkappa w_0} (3 + 4\mu + 8\mu^2)\, \Lambda^2 \tag{28}$$

or

$$U = U_0 (1 - \varphi_\mu \Lambda^2) , \tag{29}$$

where

$$\varphi_\mu = \frac{3}{10 \varkappa w_0} (3 + 4\mu + 8\mu^2) \tag{30}$$

or

$$\varphi_\mu = \frac{n}{30}(3 + 4\mu + 8\mu^2) \tag{30a}$$

because of (18).

In spherical symmetric deformation i.e. $\mu = 1$

$$\varphi_1 = \frac{n}{2} \tag{31}$$

and

$$U_1 = U_0\left(1 - \frac{n}{2}\Lambda^2\right) \tag{32}$$

$$= U_0 - \frac{1}{2}\left(\frac{nU_0}{R_0^2}\right)(\delta R)^2, \tag{32a}$$

so

$$\gamma = -\frac{nU_0}{R_0^2} \tag{33}$$

in agreement with (10), (11) and (12).

Up to now no specific value of μ has been given except for the spherical case. Owing to this we take a ratio of axis in the rotational ellipsoid, when the deformation work should be minimum in the closest vicinity of the equilibrium sphere, i.e.

$$\left(\frac{\partial U}{\partial \mu}\right)_\Lambda = 0, \tag{34}$$

$$\left(\frac{d\varphi_\mu}{d\mu}\right)_{\mu_0} = 0\,, \tag{35}$$

$$\mu_0 = -\frac{1}{4} \tag{36}$$

or

$$\varphi_{-\frac{1}{4}} = \frac{n}{12} \tag{37}$$

and finally

$$U_{-\frac{1}{4}} = U_0\left(1 - \frac{n}{12}\Lambda^2\right). \tag{38}$$

4. It is known from the theory of elasticity that the deformation work of unit volume by a spherically symmetric deformation of $\Lambda = \frac{\delta R}{R_0}$ is for a cubic lattice

$$\delta E_1 = \frac{3}{2}(c_{11} + 2c_{12})\Lambda^2, \tag{39}$$

where c_{11} and c_{12} are the proper elastic moduli. Using (32) and (39)

$$c_{11} + 2c_{12} = \frac{w_0 n}{3} . \tag{40}$$

Applying a uniaxial tension stress only in one (axial) direction in the perpendicular plane it follows that

$$c_{12} \Lambda + (c_{11} + c_{12}) \mu\Lambda = 0 , \tag{41}$$

i.e.

$$\frac{c_{12}}{c_{11}} = - \frac{\mu}{1 + \mu} . \tag{42}$$

Combining (40) and (42)

$$c_{11} = \frac{1 + \mu}{1 - \mu} \frac{n w_0}{3} , \tag{43}$$

$$c_{12} = - \frac{\mu}{1 + \mu} \frac{n w_0}{3} . \tag{44}$$

Finally, using (36)

$$c_{11} = \frac{n w_0}{5} , \tag{45}$$

$$c_{12} = \frac{n w_0}{15} . \tag{46}$$

In Table I theoretical and experimental values of $\frac{1}{\varkappa}$, μ_0, c_{11} and c_{12} are given for potassium and silver.

It can be seen that the compressibilities have very accurate values, while the Poisson ratios are rather inaccurate. The c_{11} and c_{12} are of the correct order of magnitude, but the c_{11} are rather high, and the c_{12} somewhat low.

In spite of the very approximate nature of this procedure, the results obtained are of the order of magnitude and even the numerical values within a factor of 2 compared with the experimental results.

In a following paper we shall extend the present method taking into account the energy term resulting from the nonspherical deformation of the elementary cell. This will result in better Poisson ratio and elastic moduli values.

Table I

c_{11}, c_{12} in 10^{11} dyn/cm^2

	Potassium		Silver		Ref.
	theoretical	experimental	theoretical	experimental	
$\frac{1}{\varkappa}$	0,4086	0,40	10,79	10,8	[7]
c_{11}	0,735	0,457*	19,45	12,40	[8]
c_{12}	0,245	0,374*	6,48	9,34	[8]
μ_0	0,25	—	0,25	0,37	[9]

* Measured at 83° K.

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Appendix

As already defined in (21) and (22) if

$$a = R_0 (1 + \Lambda)\,, \tag{A.1}$$

$$b = R_0 (1 + \mu\Lambda)\,, \tag{A.2}$$

then

$$r^2 = \frac{a^2}{1 + \varepsilon^2 \sin^2 \varphi}\,, \tag{A.3}$$

$$\varepsilon^2 = \frac{a^2}{b^2} - 1\,. \tag{A.4}$$

Assuming $\Lambda \ll 1$ and $\varepsilon^2 \ll 1$

$$r = a \left[1 - \frac{1}{2} \varepsilon^2 \sin^2 \varphi + \ldots \right]. \tag{A.5}$$

If

$$\delta R = r - R_0 , \tag{A.6}$$

$$\frac{\delta R}{R_0} = \frac{a}{R_0}\left(1 - \frac{\varepsilon^2}{2}\sin^2\varphi\right) - 1 . \tag{A.7}$$

We need to obtain $\frac{\delta R}{R_0}$ as the function of Λ up to the first order in

$$\begin{aligned}\varepsilon^2 &= \left(\frac{1+\Lambda}{1+\mu\Lambda}\right)^2 - 1 ,\\ &\approx (1+2\Lambda)(1-2\mu\Lambda) - 1 ,\\ \varepsilon^2 &\approx 2(1-\mu)\Lambda .\end{aligned} \tag{A.8}$$

Using (A.1), (A.7) and (A.8)

$$\frac{\delta R}{R_0} = (1+\Lambda)\left[1-(1-\mu)\sin^2\varphi\Lambda\right] - 1 ,$$

$$\frac{\delta R}{R_0} = \Lambda\left[1-(1-\mu)\sin^2\varphi\right] \tag{A.9}$$

as stated in (25).

In computing the deformation work (28)

$$\delta U = \frac{1}{2}\int_0^{(\Lambda)} \delta p \, d(\delta V) , \tag{A.10}$$

where, as in (27),

$$\delta p = \left(\frac{3}{\varkappa}\right)\left[1-(1-\mu)\sin^2\varphi\right]\Lambda , \tag{A.11}$$

while

$$d(\delta V) = 2\pi r^2 \sin\varphi \, dR \cdot d\varphi . \tag{A.12}$$

Now

$$r = R_0 + dR = R_0\left(1 + \frac{dR}{R_0}\right) , \tag{A.13}$$

$$r^2 \, dR \approx R_0^2 \, dR \tag{A.14}$$

up to the first order in Λ, because of (A.9)

$$\delta R \sim \Lambda$$

and

$$r^2\, dR = R_0^3 \left[1 - (1 - \mu) \sin^2 \varphi\right] \Lambda\,.$$

So the volume element is

$$d(\delta V) = 2\pi\, R_0^3 \left[1 - (1 - \mu) \sin^2 \varphi\right] \sin\, \varphi\; \Lambda\; d\varphi \tag{A.13a}$$

and the deformation work:

$$\delta U = \frac{1}{2} \int\limits_0^{(\Lambda)} \delta p \cdot d(\delta V) = \frac{6\pi\, R_0^3}{\varkappa}\, \Lambda^2 \int\limits_0^{\pi/2} \left[1 - (1 - \mu) \sin^2 \varphi\right]^2 \sin\, \varphi\; d\varphi \tag{A.15}$$

$$= \frac{3 V_0 \Lambda^2}{10\varkappa} (3 + 4\mu + 8\mu^2)\,,$$

$$\delta U = -\, U_0\, \varphi_u\, \Lambda^2\,, \tag{A.16}$$

where

$$\varphi_\mu = \frac{3}{10 \varkappa w_0} (3 + 4\mu + 8\mu^2) \tag{A.17}$$

as stated in (30).

О МОДУЛЕ УПРУГОСТИ ЩЕЛОЧНЫХ И БЛАГОРОДНЫХ МЕТАЛЛОВ I.

Я. АНТАЛ

Резюме

На основе теории одновалентных металлов Гомбаша выводится приближенная формула для энергии ячеек Вигнера—Зейтца для щелочных и благородных металлов в случае упругой деформации. Принимается приближение ячейки эллипсоидом вращения вместо сферы. Из принципа минимума энергии выводится соотношение оси эллипсоида, результирующее соотношение Пуассона в области ненапряженного равновесия. В то же время из результатов Гомбаша известна сжимаемость. С помощью этих величин имеется возможность для определения модуля упругости c_{11} и c_{12}.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3—4), pp. 321—327 (1966)

ON THE ELASTIC MODULI OF ALKALINE AND NOBLE METALS II

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(Presented by A. Kónya. — Received 5. IV. 1966)

Following a previous paper [1] for nonspherically symmetric deformation of the elementary cell of a monovalent metal, a new term is introduced into the energy-expression of the elementary cell approximated by a rotational ellipsoid, due to the quadrupole moment of the valence electrons brought about by the nonspherically symmetric shape of the deformed unit cell. This procedure leads to a better Poisson ratio and more reliable values being obtained for c_{11} and c_{12}.

1. In the first part of this paper [1] (referred to below as [I]) the author has outlined a method for obtaining some elastic moduli of alkaline and noble metals using the theory of monovalent metals developed by Gombás (see references in [I]). However, this method can be regarded only as a first approximation as the Poisson ratio and the values of the elastic constants are not very reliable. This is chiefly due to the lack of terms in the energy expression normally absent in the spherically symmetric state, which is the equilibrium state of the unit cell of the crystals treated.

We have to investigate this problem in some detail and in order to do so it is necessary to revert to the original energy expression of Gombás presented in [I] restating here again:

$$U = E_C + E_A + E_W + E_F + W_C + W_E + W_A + W_W + W_K + H, \qquad (1($$

where U = the energy of the elementary cell at absolute zero temperature;
E_C = the energy term of the Coulomb-type interaction;
E_A and E_W = the energy terms of the exchange and of the correlation of the valence electrons, respectively;
E_F = their zero point energy;
W_C = the Coulomb-type interaction energy between the positive (point-like) nuclei and the valence electrons;
W_E = the electrostatic energy terms due to the overlapping of the electron cloud of the valence and ion core electrons;
W_A = the exchange energy term for the same overlapping;
W_W = the correlation energy between the valence and ion core electrons;
W_K = a term which takes into account in some manner the Pauli principle and is due to a pseudo-potential introduced by Gombás

(see ref. in [I]);

H = the interaction energy of the ion cores.

For alkaline metals

$$W_w = 0 \tag{2}$$

and

$$H = 0 \tag{3}$$

with very good approximation.

GOMBÁS has shown further [2] that at equilibrium and in its rather large vicinity

$$E_C + E_A + E_W + E_F + W_A = 0\,, \tag{4}$$

$$U = W_C + W_E + W_K\,. \tag{5}$$

This can be given even in an analytical form as:

$$U = -\frac{C_1}{R} + \frac{C_2}{R^3} \tag{6}$$

for alkaline metals. The constants C_1 and C_2 can be calculated directly from the theory [2]:

$$C_1 = \frac{3e^2}{2}\,, \tag{7}$$

$$C_2 = 3e^2 (I_K - I_E)\,, \tag{8}$$

where

$$I_K = \frac{\pi^2 a_0}{8} \int_0^\infty D^2 r^2 \, dr \tag{9}$$

and

$$I_E = \frac{1}{e} \int_0^\infty \left(V - \frac{e}{r} \right) r^2 \, dr\,, \tag{10}$$

where D = the radial density function of the valence electrons;

V = the potential of the ion core;

e = elementary electric charge;

a_0 = the first Bohr radius of the hydrogen atom.

It can be seen that this approximation dispenses completely with the self-energy of the valence electrons in the equilibrium state because of (4), so (6) contains only the energy terms W_C, W_E and W_K, which are all terms of the interaction between the valence electrons and the ion core.

In [I] we have used an analytical form for U very similar to (6). As a matter of fact (I.3) is for alkaline metals completely equivalent to (6). As far as a spherically symmetric deformation is concerned, no further difficulties arise from this approximation. In the non-spherically symmetric deformation, however, (4) will no longer be satisfied because of some characteristic changes in the self-energy of valence electrons even of the assumed constant density. This effect gives rise to a new energy term, which of course disappears in the spherically symmetric case.

2. To obtain this new term we recall at first the well known results for the self-energy E_0 of a sphere with radius R homogeneously charged with a constant ν_e charge density

$$E_0 = \frac{3}{5} \frac{e^2}{R}, \tag{11}$$

where, obviously,

$$e = \nu_e \frac{4\pi R^3}{3} \tag{12}$$

the integral charge is equal to one electron charge.

This energy can be calculated for a rotational ellipsoid of axis a, b according to FLÜGGE [3] ($a > b$) as

$$E_E = \frac{3}{5} e^2 \frac{\operatorname{Arch} \frac{a}{b}}{\sqrt{a^2 - b^2}}. \tag{13}$$

If

$$a = b = R$$

(13) goes over (11), so the necessary correction term will be:

$$E_Q = E_E - E_0 \tag{14}$$

or

$$E_Q = \frac{3}{5} e^2 \left[\frac{\operatorname{Arch} \frac{a}{b}}{\sqrt{a^2 - b^2}} - \frac{1}{(ab^2)^{1/3}} \right], \tag{15}$$

because of splitting down the energy change due to spherically symmetric deformation it is necessary to have:

$$\frac{4\pi R^3}{3} = \frac{4\pi ab^2}{3}. \tag{16}$$

Using (I.24), (15) can be written as

$$E_Q = \frac{3}{5}\,\frac{e^2}{a}\left[\frac{\sqrt{1+\varepsilon^2}}{\varepsilon}\,\mathrm{Arch}\,\varepsilon - (1+\varepsilon^2)^{1/3}\right]. \tag{17}$$

In the immediate vicinity of equilibrium this can again be simplified to a great extent in the same way as in (I) to

$$E_Q = -\frac{4e^2}{75\,R_0}(1-\mu)^2 \Lambda^2 . \tag{18}$$

Λ and μ are the same as in [I], i.e. they are defined by

$$\left.\begin{aligned} a &= R_0(1+\Lambda) \\ b &= R_0(1+\mu\Lambda) \end{aligned}\right\}. \tag{19}$$

From (I.29) and (18), for the cell energy one obtains

$$U = U_0(1 - \Phi_\mu \Lambda^2), \tag{20}$$

where

$$\Phi_\mu = \varphi_\mu + \frac{4e^2}{75\,R_0\,U_0}(1-\mu)^2, \tag{21}$$

while φ_μ as defined in (I.30a)

$$\varphi_\mu = \frac{n}{30}(3 + 4\mu + 8\mu^2) \tag{22}$$

and

$$n = \frac{9}{\varkappa w_0}, \tag{23}$$

$\varkappa$ being the compressibility and w_0 the absolute value of the equilibrium energy per unit volume.

Introducing

$$h = -\frac{4e^2}{75\,R_0\,U_0}, \tag{24}$$

which can be calculated from the equilibrium state values, finally

$$\Phi_\mu = \frac{n}{30}(3 + 4\mu + 8\mu^2) - h(1-\mu)^2 . \tag{25}$$

Now minimum conditions in the vicinity of the equilibrium are:

$$\left(\frac{\partial U}{\partial \Lambda}\right)_{\Lambda \to 0} = 0 \tag{26}$$

and

$$\left(\frac{\partial U}{\partial \mu}\right)_{\Lambda} = 0\,. \tag{27}$$

Using (25) and (27) one gets for the near-equilibrium Poisson constant:

$$\mu_0 = -\frac{1}{4}\,\frac{1+\dfrac{15h}{n}}{1-\dfrac{15h}{4n}}\,. \tag{28}$$

It is somewhat more convenient to introduce $\varkappa$ into the equations taking

$$g\varkappa = \frac{15h}{4n} = -\frac{e^2}{5n\,U_0\,R_0}\,, \tag{29}$$

where g is another constant, i.e. by (23)

$$g = \frac{e^2}{60\pi R_0^4}\,. \tag{30}$$

In view of this:

$$\mu_0 = -\frac{1}{4}\,\frac{1+4g\varkappa}{1-g\varkappa}\,. \tag{31}$$

In just the same way as in [I] we get finally:

$$c_{11} = \frac{3}{5\varkappa}(3-8g\varkappa) \tag{32}$$

and

$$c_{12} = \frac{3}{5\varkappa}(1+4g\varkappa) \tag{33}$$

for cubic lattices.

3. In Table I we give c_{11}, c_{12} and μ_0 for potassium and silver calculated by a) the results of [I] using equation (I.45, I.46); b) using the methods of the present paper by equations (30), (31), (32), (33); c) the Fuchs values [4] and finally d) the experimental values already presented in [I].

Table I

c_{11} and c_{12} in 10^{11} dyn/cm^2

	Potassium			Silver		
	c_{11}	c_{12}	$-\mu_0$	c_{11}	c_{12}	$-\mu_0$
a) by I	0,735	0,245	0,25	19,45	6,48	0,25
b) by II	0,593	0,315	0,347	18,63	7,25	0,28
c) by FUCHS' method	0,440	0,38	—	—	—	—
d) experimental	0,457*	0,374*	—	12,4	9,34	0,37

* Measured at 73° K (ref. see in [I]).

It can be seen that results obtained with the corrected energy expression of the present paper do not differ greatly from the experimental values as far as potassium is concerned, while in the case of silver the results are somewhat better than those in [I], but the discrepancies are rather considerable. The results of FUCHS' calculation are far better, but it must be realized that the present calculation makes no use of any data taken from experiment nor has it any adjustable parameter. It is based only on the theoretical assumptions and procedures of the monovalent metal model and theory referred to.

In view of (30), (31), (32), (33) using the theoretical values of R_0, U_0 and $\varkappa$ one can calculate c_{11}, c_{12} and μ_0 for different alkaline and noble metals (those referred to below all have cubic lattices). These are given in Table II, for K, Rb, Cs, Ag and Cu with the experimental values (if available). For some elements the values calculated by FUCHS are also included [5].

The results are again somewhat better for alkaline metals, while they are not so good for others. In any case, they are the worst for noble metals. This is chiefly due to the fact that the present correction term is most effective for alkaline metals. For noble metals on the other hand the situation is much more

Table II

All data in 10^{11} dyn/cm^2

		K	Rb	Cs	Ag	Cu
c_{11}	by II	0,593	0,475	0,412	18,63	23,79
	exp.	0,457	—	—	12,4	17,88
	FUCHS	0,44	0.33	0,245	—	17,5
c_{12}	by II	0,315	0,246	0,217	6,98	9,27
	exp.	0,374	—	—	9,34	12,6
	FUCHS	0,38	0,286	0,208	—	12,4

complicated. There is a remarkable overlapping even of ion cores and so some basic assumptions regarding the spherical symmetry of the ion core of the elementary cell at equilibrium are not satisfied. For the equilibrium state these effects can be compensated for by a more appropriate choice of the pseudo potential [6], but for the deformed state the present rather simple suggestions do not make it possible for these further interactions to be taken into account.

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О МОДУЛЕ УПРУГОСТИ ЩЕЛОЧНЫХ И БЛАГОРОДНЫХ МЕТАЛЛОВ II.

Я. АНТАЛ

Резюме

Согласно работе I в данной статье для деформации элементарных ячеек одновалентных металлов, не обладающих сферической симметрией, в выражение энергии элементарных ячеек, представленных в форме эллипсоида вращения, вводится новый член, обусловленный квадрупольным моментом валентного электрона, вызванным несферической формой деформированной единичной ячейки. Приемом, изложенным в статье I, выводится более точное соотношение Пуассона, и для величин c_{11} и c_{12} получены более надежные результаты.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3—4), pp. 329—344 (1966)

THE LORENTZ PRINCIPLE AND THE GENERAL THEORY OF RELATIVITY III

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(Received 31. III. 1966)

The connection between the propagation tensor **g** and the sources of the gravitational field is investigated. It is shown that supposing light to be propagated isotropically with the velocity depending upon gravitational potential, two of the three relativistic effects can be accounted for. The usual interpretation of the deflection of light is only obtained if one supposes that the propagation of light to be unisotropic in a gravitational field. EINSTEIN's equations for the gravitational fields are derived from the point of view of the LORENTZ principle.

Connection between the propagation of light and the gravitational field

§ 1. So as to be able to apply the equations for the geodetical orbits which we gave in Part II to actual physical problems it is necessary to determine the tensor **g** and with its help the Christoffel brackets.

The connection between the tensor **g** and the sources of the gravitational field were given by EINSTEIN. We shall discuss here how EINSTEIN's equations of the gravitational field are obtained using our concepts based on the generalized LORENTZ principle.

§ 2. So as to approach the problem we consider to begin with a particular form of the tensor **g**. We consider thus

$$\mathbf{g} = \mathbf{\Gamma}(\mathbf{r}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & g_{44} \end{pmatrix}, \tag{1}$$

where we suppose g_{44} to be a function of coordinates, we shall suppose $g_{44} = g_{44}(\mathbf{r})$ and $\partial g_{44}/\partial x_4 = 0$. It follows from previous considerations that $g_{44} < 0$ and we shall also write

$$\sqrt{-g_{44}} = c(\mathbf{r})\,. \tag{2}$$

The tensor defined by (1) corresponds to a state of affairs where light is propagated isotropically but the velocity of propagation varies from point to point.

The velocity of propagation at large distances from the gravitational centres we shall consider to be homogeneous and we may denote by c the velocity of light in such distant regions. Thus we suppose

$$c(\mathbf{r}) \rightarrow c \quad \text{if} \quad r \rightarrow \infty . \tag{3}$$

The latter supposition is made purely for convenience and the $r \rightarrow \infty$ must not be taken too seriously. We may e.g. suppose that in the vicinity of the Sun $c(\mathbf{r})$ varies with r the distance from the Sun. At large distances as compared with the measures of the solar system but still at small distances as compared with the distances between the fixed stars we have a region where light may be taken to be propagated in a good approximation both isotropically and homogeneously with the velocity c of relation (3).

§ 3. From (1) we may calculate the Christoffel brackets. We find

$$\begin{Bmatrix} 44 \\ k \end{Bmatrix} = -\frac{1}{2} \frac{\partial g_{44}}{\partial x_k} , \qquad \begin{Bmatrix} 4k \\ 4 \end{Bmatrix} = \begin{Bmatrix} k4 \\ 4 \end{Bmatrix} = -\frac{1}{2} \frac{\partial g_{44}}{\partial x_k} g_{44} \tag{4}$$

all the others being zero.

The equations of a geodetic orbit using the values (4) for the Christoffel brackets (eliminating the parameters p) according to equ. (39) of Part II are thus found

$$\frac{d\mathbf{v}}{dt} = \frac{1}{2} \operatorname{grad} g_{44} + \frac{(\mathbf{v} \operatorname{grad} g_{44})\, \mathbf{v}}{g_{44}} . \tag{5}$$

Considering (2) we see that the second term on the right side of (5) is small provided we consider motions with velocities much smaller than that of light. Neglecting the small terms we find in a first approximation

$$\frac{d\mathbf{v}}{dt} = -\operatorname{grad} \Phi , \tag{6}$$

where

$$\Phi = \left(\text{const} - \frac{1}{2} g_{44} \right) .$$

We see thus that (6) reduces to NEWTON's equations provided

$$g_{44} = -c^2 - 2\Phi , \tag{7}$$

or if we neglect further terms in v^2/c^2 we may also suppose

$$c(r) = \sqrt{-g_{44}} = c + \frac{\Phi}{c} , \tag{8}$$

where Φ is the usual gravitational potential. E.g. in the vicinity of the Sun we may suppose

$$\Phi = -\frac{\alpha}{r}, \qquad \alpha = GM\,, \tag{9}$$

where G is the gravitational constant and M the mass of the Sun.

Introducing (8) and (9) into (1) we find the form of the tensor **g** which gives in NEWTON's approximation the orbits of the planets.

§ 4. From the tensor **g** thus obtained the deflection of light passing the Sun can also be derived. With the help of (2) we have

$$\mathrm{grad}\, g_{44} = -\,\mathrm{grad}\, c^2(\mathbf{r})\,.$$

Multiplying (5) with $2\mathbf{v}$ we find further

$$\frac{d}{dt}v^2 = -\,\mathbf{v}\,\mathrm{grad}\, c^2(r)\left(1 - \frac{2v^2}{c(\mathbf{r})^2}\right). \tag{10}$$

If in a point $\mathbf{r}$ the velocity of the orbit $v = c(\mathbf{r})$ is equal to the velocity of light, then for such a point the above relation reduces to

$$\left(\frac{d}{dt}\,v^2\right)_{v=\,(\mathbf{r})} = \mathbf{v}\,\mathrm{grad}\, c^2(\mathbf{r})\,.$$

The above relations show that along a path $\delta\mathbf{r} = \mathbf{v}\delta t$ the square of the velocity changes by

$$\delta v^2 = \mathrm{grad}\, c^2(\mathbf{r})\,\delta\mathbf{r}\,,$$

i.e. exactly by the same amount as the local velocity of light. We see thus that if the initial velocity of a point is equal to the local light velocity $c(\mathbf{r})$ and if the point proceeds along a geodetic orbit, its velocity will be always equal to the local velocity of light in the points which it passes.

We may therefore assume that a signal of light itself is proceeding along a geodetic orbit.

§ 5. So as to obtain the deflection of a beam of light when passing the Sun we consider an orbit which lies in one plane with the Sun; (there exist such orbits as can be seen directly examining (5)). For such an orbit we may write for the angle of deflection in a time dt, $d\varphi = dt\,|\mathbf{v}\times\dot{\mathbf{v}}|/v^2$, thus with the help of (5) introducing the g_{44} from (8) and (9) remembering also that $v = c(r)$

$$\left|\frac{d\varphi}{dt}\right| = |\mathbf{v}\times\mathbf{r}|/c(\mathbf{r})^2\,. \tag{11}$$

Neglecting the change of $c(\mathbf{r})$ with $\mathbf{r}$ on the right hand expression and supposing further that the orbit in a first approximation moves along a straight line we may write

$$\mathbf{r}(t) \sim \mathbf{a} + \mathbf{v}_0 t\,, \qquad v_0 = c\,, \tag{12}$$

where $\mathbf{a}$ is a vector perpendicular to $\mathbf{v}_0$, its absolute value a giving the closest approach of the beam to the gravitating centre resting in the point $\mathbf{r} = 0$. Introducing (11) into (10) and integrating we find for the relative deflection

$$\varphi = \int\limits_{-\infty}^{+\infty} \frac{GMa/c^2}{(a^2 + c^2 t^2)^{3/2}}\, dt = \frac{2GM}{ac^2}\,. \tag{13}$$

The above value for the deflection is equal to that found long ago by LAPLACE — but it is by a factor 2 smaller than the value given by EINSTEIN. Taking the value given by EINSTEIN as the correct one, we see that the assumptions (1) and (8) giving the connection between propagation of light and gravitational field lead in first approximation to NEWTON's theory of the planetary motion and given at the same time one half of the value (predicted by EINSTEIN) for the deflexion of light near the Sun.

The perihelion motion of the planets

§ 6. The second term on the right hand side of (5) gives a small correction only for the motion of systems with velocities $v \ll c$.

We note by the way that for large velocities the second term of (5) becomes as important as the first.

As can be seen from (10) for velocities $v > c/\sqrt{2}$ the gravitational force changes its sign — and the force between systems moving with such velocities becomes *repulsive*. The latter effect accounts for the fact that the velocity of light decreases when light is approaching the Sun. Roughly speaking the light approaching the Sun with the velocity c is repelled and thus slows down.

So as to obtain the correction caused by the second term of (5) on NEWTON's law in the case of small velocities, we express grad $c^2(\mathbf{r})$ in terms of the gravitational potential. We may write thus in place of (5) and of (10)

$$\dot{\mathbf{v}} = -\frac{\alpha \mathbf{r}}{r^3}\left(1 - \frac{2\alpha}{rc^2}\right) + \frac{2\alpha(\mathbf{v}\mathbf{r})\,\mathbf{v}}{c^2 r^3}\,, \tag{14a}$$

$$\frac{dv^2}{dt} = -2\frac{\alpha}{r^3}(\mathbf{v}\mathbf{r})\left(1 - \frac{2\alpha}{rc^2} - \frac{2v^2}{c^2}\right). \tag{14b}$$

Eliminating **vr** from (14a) and (14b) we find

$$\dot{\mathbf{v}} = -\frac{\alpha \mathbf{r}}{r^3}\left(1-\frac{2\alpha}{rc^2}\right) - \frac{\mathbf{v}\,\dfrac{dv^2}{dt}\Big/c^2}{1-\dfrac{2\alpha}{rc^2}-\dfrac{2v^2}{c^2}}\,. \tag{15}$$

Multiplying (15) by **v** we have

$$\frac{\dot{\mathbf{v}}\,\mathbf{v}}{1-\dfrac{2\alpha}{rc^2}-\dfrac{2v^2}{c^2}} = -\frac{\alpha r}{r^2}\,.$$

Neglecting the dependence of c upon **r** and some higher order terms in v^2/c^2 we obtain total differentials. Integrating we have

$$-\frac{c^2}{4}\ln\left(1-\frac{2v^2}{c^2}\right) = A + \frac{\alpha}{r}\left(1+\frac{\alpha}{rc^2}\right),$$

where A is a constant of integration. Developing in powers of v^2/c^2 and neglecting higher powers we have thus

$$\frac{1}{2}\left(v^2+\frac{v^4}{c^2}\right) = A + \frac{\alpha}{r}\left(1+\frac{\alpha}{rc^2}\right),$$

or neglecting further small terms we have

$$v^2 = 2\left[A+\frac{\alpha}{r}\left(1+\frac{\alpha}{c^2 r}\right)\right] - \frac{4}{c^2}\left(A+\frac{\alpha}{r}\right)^2. \tag{16}$$

So as to obtain the angular momentum integral we multiply (15) by **r** and obtain as the result of a simple calculation

$$\mathbf{r}\times\dot{\mathbf{r}} = \mathbf{a}\,e^{-2\alpha/rc^2}, \tag{17}$$

where **a** is a constant of integration. Remembering the general relations

$$v^2 = \dot{r}^2 + (\mathbf{r}\times\dot{\mathbf{r}})^2/r^2\,, \qquad \left(\frac{d\varphi}{dt}\right)^2 = ((\mathbf{r}\times\dot{\mathbf{r}})/r^2)^2\,,$$

we find from (16) and (17) when introducing $1/r = s$

$$d\varphi = -\frac{ds(1-2\alpha s/c^2)}{\sqrt{2(A+\alpha s)/\mathbf{a}^2 - s^2 - \dfrac{2}{c^2}\left[2(A+\alpha s)^2(\mathbf{a}^2-\alpha^2 s^2)\mathbf{a}^2 - 2\alpha s^3\right]}}\,.$$

Neglecting terms in $1/c^2$ integrating the above relation over the whole period we find

$$\oint d\varphi = 2\pi + \text{terms in} \frac{1}{c^2} .$$

Thus apart from the terms of the order of $1/c^2$ the motion is periodic. Retaining the terms in $1/c^2$ one finds in a first approximation (see e.g. [1] p. 221.)

$$\int d\varphi = 2\pi + \varepsilon ,$$

where

$$\varepsilon = + 6\pi \frac{\bar{v}^2}{c^2} , \tag{18}$$

where $\bar{v}^2 = (\alpha/a)^2$; the latter expression gives the average square of the orbital velocity of the planet. Expression (18) is identical with the value obtained by EINSTEIN and seems to be in good agreement with observation.

The gravitational red shift

§ 7. Consider an atom at rest near $\mathbf{x}$. The velocity of the atom can be represented by a four-vector

$$\mathbf{v} = 0,\ 0,\ 0,\ \dot{x}_4 .$$

The atom should oscillate with a period T; the latter oscillation can also be expressed by a time-like four-vector

$$\mathbf{T} = 0,\ 0,\ 0,\ T .$$

If we subject the system to a parallel shift from $\mathbf{x}$ to $\mathbf{x} + \mu$ the vectors $\mathbf{v}$ and $\mathbf{T}$ change into $\mathbf{v}^*$ and $\mathbf{T}^*$ which vectors can be determined with the help of equ. (18) Part II. However, if $\mathbf{g}$ is of the form (1) we have

$$\mathbf{S} = \mathbf{g}^{-1/2} (\mathbf{x} + \mu)\, \mathbf{g}^{1/2} (\mathbf{x}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \dfrac{c(\mathbf{x})}{c(\mathbf{x}+\mu)} \end{pmatrix}$$

and thus we find

$$\mathbf{v}^* = 0,\ 0,\ 0,\ \dot{x}_\nu^*,$$

$$\mathbf{T}^* = 0,\ 0,\ 0,\ Tc(\mathbf{x})/c(\mathbf{x} + \mu) .$$

We see that the system after the parallel shift is still at rest and its period is changed by a factor

$$T^*/T = c(\mathbf{x})/c(\mathbf{x} + \mu)\,.$$

The above change in the period of an oscillating atom when shifted adiabatically from $\mathbf{x}$ to $\mathbf{x} + \mu$ gives exactly the gravitational red shift as found in terms of the general theory of relativity.

Considering thus an atom brought adiabatically from the Earth to the Sun, the time of one oscillation of the system changes inversely with the local velocity of light. Since the velocity decreases near the Sun as can be seen from equs. (8) and (9) the period increases and the frequency decreases.

We note that for the decrease of frequency to take place it is not necessary to transport the atom from the Earth to the Sun. Indeed during such a transport the atom adjusts itself continuously to the local conditions and the transport of the atom from the Earth to the Sun represents merely an ideal experiment with the help of which we can clear up the difference in behaviour of the atoms in different parts of a gravitational field.

We note further that the red shift has been directly verified with the help of the MÖSSBAUER effect shifting atoms on the Earth between points of different gravitational potential [2].

Einstein's gravitational equations

§ 8. We have seen that the greater part of the general relativistic effects can be accounted for by assuming the tensor **g** to be of the form (1), where the expression for g_{44} has to be adjusted so as to give in first approximation the correct law for the planetary motion — this procedure gives automatically the relativistic correction to NEWTON's law.

Postulating the tensor **g**(**x**) it appears unsatisfactory that the connection between gravitational field and masses is only given for masses *at rest* and it is desirable to find the connection between arbitrarily moving masses and their gravitational field.

So as to obtain the connection between **g** and the gravitational field, we remember that in the case of truly inhomogeneous propagation of light there exists no coordinate transformation such that

$$\mathbf{g}'(\mathbf{x}') = \tilde{\mathbf{S}}(\mathbf{x})\, g(\mathbf{x})\, \mathbf{S}(\mathbf{x}) = \text{constant}$$

therefore it is not unreasonable to suppose that the gravitational field in the vicinity of **x** is connected with those covariant features of **g**(**x**) which cannot be transformed away by coordinate transformations.

The first derivatives of $\mathbf{g}(\mathbf{x})$ can be transformed away, therefore they cannot be taken to characterize the gravitational field. The second derivatives cannot, however, all be made to vanish by a coordinate transformation. Indeed, the ten functions $g_{\nu\mu}(\mathbf{x})$ have each ten second derivatives and thus the tensor $\mathbf{g}(\mathbf{x})$ has altogether onehundred second derivatives. If we want to make the second derivatives of the transform of $\mathbf{g}(\mathbf{x})$ to disappear, we obtain thus 100 conditions on the third derivatives of the four transformation functions $f_\nu(\mathbf{x})$; the latter possess 20 third derivatives each thus altogether 80 third derivatives. We thus obtain 100 equations for 80 quantities which can be disposed of. We expect thus that there exist $100 - 80 = 20$ expressions containing the second derivatives of $\mathbf{g}(\mathbf{x})$ which are invariant to coordinate transformations — the latter quantities may be supposed to be connected with the gravitational field.

The Riemann—Christoffel tensor

§ 9. A representation of the RIEMANN—CHRISTOFFEL tensor can be obtained when looking for the invariant expressions built of the second derivatives of $\mathbf{g}$.

Let us for this purpose consider such a representation $\mathbf{g}'$ of the tensor $\mathfrak{g}$ in which all the first derivatives are zero, i.e. $\mathbf{g}'$ should be such that

$$\frac{\partial \mathbf{g}'(\mathbf{x}' + \boldsymbol{\xi}')}{\partial \boldsymbol{\xi}} = 0 \qquad \text{for} \qquad \boldsymbol{\xi}' = 0\,. \tag{19}$$

By a suitable transformation we can obtain another representation $\mathbf{g}''$ of $\mathfrak{g}$ such that

$$\mathbf{x}' = \mathbf{x}'',\ \mathbf{g}'(\mathbf{x}') = \mathbf{g}''(\mathbf{x}'') \quad \text{and} \quad \frac{\partial \mathbf{g}''}{\partial \xi''} = 0 \quad \text{for} \quad \boldsymbol{\xi}'' = 0\,. \tag{20}$$

The transformation leading from $\mathbf{g}'$ to $\mathbf{g}''$ can be obtained by putting

$$\mathbf{x}' + \boldsymbol{\xi}' = \mathbf{f}^{-1}(\mathbf{x}'' + \boldsymbol{\xi}'')\,, \tag{21}$$

and the components f_ν^{-1} of $\mathbf{f}^{-1}$ have the following form

$$f_\nu^{-1}(\mathbf{x}'' + \boldsymbol{\xi}'') = x_\nu'' + \xi_\nu'' + \frac{1}{2} \sum_{\varkappa\lambda\mu} \xi_\varkappa'' \xi_\lambda'' \xi_\mu'' F_{\varkappa\lambda\mu}^{(\nu)} \tag{22}$$

$+$ terms of higher order in $\boldsymbol{\xi}''$.

So as to show that the transformation defined by (21) and (22) satisfies the conditions (20) indeed we note that

$$S'_{\nu\mu} = \frac{\partial f_\nu^{-1}}{\partial \xi''_\mu} = \delta_{\nu\mu} \qquad \text{for} \qquad \boldsymbol{\xi}'' = 0\,, \tag{23}$$

further

$$\frac{\partial S'_{\nu\mu}}{\partial \xi''_\varkappa} = 0, \qquad \frac{\partial S'_{\nu\mu}}{\partial \xi''_\varkappa \partial \xi''_\lambda} = F^{(\nu)}_{\mu\varkappa\lambda} \qquad \text{for} \qquad \boldsymbol{\xi}'' = 0\,. \tag{24}$$

Noting that the transformed $\mathbf{g}''$ can be written as

$$\mathbf{g}''(\mathbf{x}'' + \boldsymbol{\xi}'') = \tilde{\mathbf{S}}'(\mathbf{x}'' + \boldsymbol{\xi}'')\,\mathbf{g}'(\mathbf{x}' + \boldsymbol{\xi}')\,\mathbf{S}'(\mathbf{x}'' + \boldsymbol{\xi}'')\,. \tag{25}$$

We see with the help of (23) that the first and second conditions (20) are satisfied. So as to show that the third condition (20) is also fulfilled we note that

$$\frac{\partial \mathbf{g}'}{\partial \xi''_\varkappa} = \sum_{\varkappa'} \frac{\partial \mathbf{g}'}{\partial \xi'_{\varkappa'}} \frac{\partial \xi'_{\varkappa'}}{\partial \xi''_\varkappa} = \frac{\partial \mathbf{g}''}{\partial \xi''_\varkappa} \qquad \text{for} \qquad \boldsymbol{\xi}'' = 0, \tag{26}$$

thus differentiating (25) into $\xi''_\varkappa$ and inserting $\boldsymbol{\xi}'' = 0$ we obtain with the help of (26) an expression equivalent to the third condition (20), thus we see that the latter is also fulfilled.

So as to investigate second derivatives, we note that we have with the help of (19), (21), (23) and (24)

$$\frac{\partial^2 \mathbf{g}'}{\partial \xi''_\varkappa \partial \xi''_\lambda} = \sum_{\varkappa'\lambda'} \left(\frac{\partial^2 \mathbf{g}'}{\partial \xi'_{\varkappa'} \partial \xi'_{\lambda'}} \frac{\partial \xi'_{\varkappa'}}{\partial \xi''_\varkappa} \frac{\partial \xi'_{\lambda'}}{\partial \xi''_\lambda} + 2 \frac{\partial \mathbf{g}'}{\partial \xi'_{\varkappa'}} \frac{\partial^2 \xi'_{\varkappa'}}{\partial \xi''_\varkappa \partial \xi''_\lambda} \right). \tag{27}$$

Differentiating thus (25) into $\xi''_\varkappa$ and ξ''_λ we find with the help of (23), (24), (26) and (27)

$$\frac{\partial^2 \mathbf{g}''}{\partial \xi''_\varkappa \partial \xi''_\lambda} = \frac{\partial^2 \mathbf{g}'}{\partial \xi'_\varkappa \partial \xi'_\lambda} + \tilde{\mathbf{F}}^{(\varkappa\lambda)} \mathbf{g}' + \mathbf{g}' \mathbf{F}^{(\varkappa\lambda)} \qquad \text{for} \qquad \boldsymbol{\xi}'' = 0\,, \tag{28}$$

where $\mathbf{F}^{(\varkappa\lambda)}$ for $\varkappa\lambda = 1, 2, 3, 4$ are matrices with component

$$F^{(\varkappa\lambda)}_{\nu\mu} = F^{(\nu)}_{\mu\varkappa\lambda} \qquad \nu, \mu = 1, 2, 3, 4.$$

Relation (28) can be brought into a simpler form by writing down (28) for the cyclic permutation of $\nu\mu\varkappa\lambda$, and taking the consecutive permutated expressions with opposite sign and adding the expressions thus obtained. Thus we introduce a summation $\sum\limits_{c.p}$ which may be defined as

$$\sum_{c.p} A(\nu\mu\varkappa\lambda) = A(\nu\mu\varkappa\lambda) - A(\lambda\nu\mu\varkappa) + A(\varkappa\lambda\nu\mu) - A(\mu\varkappa\lambda\nu)\,, \tag{29}$$

where $A(\nu\mu\varkappa\lambda)$ is some function of the four suffices ν, μ, $\varkappa$, λ.

Applying the summation defined by (29) to both sides of (28) we find

$$\sum_{c.p} \frac{\partial^2 \mathbf{g}''}{\partial \xi''_\varkappa \partial \xi''_\lambda} = \sum_{c.p} \frac{\partial^2 \mathbf{g}'}{\partial \xi'_\varkappa \partial \xi'_\lambda}\,, \qquad \boldsymbol{\xi}'' = 0\,. \tag{30}$$

Thus we may define a quantity $R'^{(\varkappa\lambda)}$ with components

$$R'^{(\varkappa\lambda)}_{\nu\mu} = \sum_{c.p} \frac{\partial^2 g'_{\nu\mu}}{\partial \xi'_\varkappa \partial \xi'_\lambda} \qquad \boldsymbol{\xi} = 0\,. \tag{31}$$

The components of the latter quantity do not change when the variables are subjected to a transformation of the form given by (21) and (22).

We thus see that the $R'^{(\varkappa\lambda)}_{\nu\mu}$ give the components of a four-dimensional tensor in the representation K'. The latter representation is, however, a restricted one as it is a representation in which the first derivatives of $\mathbf{g}'$ are zero at $\boldsymbol{\xi}' = 0$.

So as to obtain the general form of the representation of $\mathbf{R}^{(\varkappa\lambda)}$ consider a system of reference K in which $\mathfrak{g}$ is represented by a tensor $\mathbf{g}$ such that

$$\mathbf{g}(\mathbf{x}) = \mathbf{g}'(\mathbf{x}') = \mathbf{g}''(\mathbf{x}'')\,,$$

and

$$\mathbf{x} = \mathbf{x}' = \mathbf{x}''\,,$$

but K is such that in general $\partial\mathbf{g}/d\mathbf{x} \neq 0$ for $\boldsymbol{\xi} = 0$. Using the results of Part II we find that the transformation $\mathbf{g} \rightarrow \mathbf{g}'$ may have the form

$$\mathbf{g} = \widetilde{\mathbf{S}}\mathbf{g}'\,\mathbf{S}\,, \tag{32}$$

where

$$\mathbf{S} = \mathbf{1} - \sum_{\varkappa} \xi_\varkappa \mathfrak{G}^{(\varkappa)}\,, \tag{33}$$

with

$$\mathfrak{G}^{(\varkappa)} = -\,\mathbf{g}^{-1}\mathbf{C}^{(\varkappa)}\,, \tag{33a}$$

and

$$C^{(\varkappa)}_{\nu\mu} = \frac{1}{2}\left(\frac{\partial g_{\nu\mu}}{\partial \xi_\varkappa} + \frac{\partial g_{\nu\varkappa}}{\partial \xi_\mu} - \frac{\partial g_{\mu\varkappa}}{\partial \xi_\nu}\right), \qquad \boldsymbol{\xi} = 0\,. \tag{33b}$$

That the transformation (33) has indeed the required properties can be seen by differentiating (32) into $\xi_\varkappa$ and introducing for the derivatives $\partial \mathbf{S}/\partial \xi_\varkappa$ expressions obtained from (33).

Differentiating (32) into $\xi_\varkappa$ and ξ_λ we find with the help of relations

$$\frac{\partial^2 \mathbf{g}'}{\partial \xi_\varkappa \partial \xi_\lambda} = \sum_{\varkappa'\lambda'} \left(\frac{\partial^2 \mathbf{g}'}{\partial \xi'_{\lambda'} \partial \xi'_{\varkappa'}} \frac{\partial \xi'_{\lambda'}}{\partial \xi_\lambda} \frac{\partial \xi'_\varkappa}{\partial \xi_\varkappa} + 2 \frac{\partial \mathbf{g}'}{\partial \xi'_{\varkappa'}} \frac{\partial^2 \xi'_{\varkappa'}}{\partial \xi_\lambda \partial \xi_\varkappa} \right) = \frac{\partial^2 \mathbf{g}'}{\partial \xi'_\varkappa \partial \lambda'_\lambda}$$

which are valid for $\boldsymbol{\xi}' = 0$ that

$$\frac{\partial^2 \mathbf{g}}{\partial \xi_\varkappa \partial \xi_\lambda} = \frac{\partial^2 \mathbf{g}'}{\partial \xi'_\varkappa \partial \xi'_\lambda} + 2 \left(\widetilde{\mathfrak{C}}^{(\varkappa)} \mathbf{g}' \, \mathfrak{C}^{(\lambda)} + \widetilde{\mathfrak{C}}^{(\lambda)} \mathbf{g}' \, \mathfrak{C}^{(\varkappa)} \right) \qquad \text{for} \quad \boldsymbol{\xi} = 0 \,.$$

Summing the above expression alternating the sign over cyclic permutation we find thus remembering for

$$\sum_{c.p} \left(\frac{\partial^2 \mathbf{g}}{\partial \xi_\varkappa \partial \xi_\lambda} + 2 \left(\widetilde{\mathfrak{C}}^{(\varkappa)} \mathbf{C}^{(\lambda)} + \widetilde{\mathfrak{C}}^{(\lambda)} \mathbf{C}^{(\varkappa)} \right) \right) = 2 \mathbf{R}'^{(\varkappa\lambda)} \qquad \text{for} \quad \boldsymbol{\xi} = 0 \,.$$

Changing the notation and writing

$$\left(\frac{\partial^2 \mathbf{g}}{\partial \xi_\varkappa \partial \xi_\lambda} \right)_{\xi = 0} = \frac{\partial^2 \mathbf{g}}{\partial x_\varkappa \partial x_\lambda} \,,$$

we may thus introduce the quantities

$$\mathbf{R}^{(\varkappa\lambda)} = \sum_{c.p} \left(\frac{1}{2} \frac{\partial^2 \mathbf{g}}{\partial x_\varkappa \partial x_\lambda} - \mathbf{g}^{-1} \left(\widetilde{\mathbf{C}}^{(\varkappa)} \mathbf{C}^{(\lambda)} + \widetilde{\mathbf{C}}^{(\lambda)} \mathbf{C}^{(\varkappa)} \right) \right) \tag{34}$$

we find that

$$\mathbf{R}'^{(\varkappa\lambda)} = \mathbf{R}^{(\varkappa\lambda)} \,.$$

Adding to the type transformations $\mathbf{S}$ and $\mathbf{S}'$ so far considered also the linear transformations with constant matrices $\mathbf{S}_0$ such that

$$\frac{\partial \mathbf{S}_0}{\partial \boldsymbol{\xi}} = 0 \qquad \text{for any value of } \xi \,.$$

We may build up any coordinate transformation from transformations of the types $\mathbf{S}_0$, $\mathbf{S}$ and $\mathbf{S}'$. We can thus show that the quantities $\mathbf{R}^{(\varkappa\lambda)}$ can be regarded as the components

$$R_{\varkappa\lambda\nu\mu} = R^{(\varkappa\lambda)}_{\nu\mu} \,,$$

of a four-dimensional tensor. The latter is the socalled RIEMANN—CHRISTOFFEL tensor.*

§ 10. It follows from the definition of the tensor $\mathbf{R}^{(\varkappa\lambda)}$ that in a region where the propagation of light is truly homogeneous in the sense of Part II § 8, we have

$$\mathbf{R}^{(\varkappa\lambda)} = 0\,, \tag{35}$$

and it is also true, that provided (35) is valid for an extended (four-dimensional) region thus the propagation of light is homogeneous in the latter region.

We note that if we try to introduce normal coordinates in the vicinity of a four-point $\mathfrak{x}$ using light signals for to determine coordinate measures in a manner not unlike that described in Part II, then we may obtain coordinates in terms of which the propagation of light appears practically homogeneous in a sufficiently small vicinity of $\mathfrak{x}$. Extending our region further, we find in general that the measures of the four coordinates of points somewhat farther away from $\mathfrak{x}$ cannot anymore be determined consistently supposing $\mathbf{g}$ to be constant.

Supposing, however, $\mathbf{g}$ to vary slightly with distance, we find that making suitable corrections, we can extend the region in which we can obtain consistent coordinate measures. The corrections thus obtained define in a unique way the components of the RIEMANN—CHRISTOFFEL tensor. We conclude therefore, that observing return times of signals between points in an inhomogeneous region, we can determine from the measured return times the components of the RIEMANN—CHRISTOFFEL tensor — the latter seem therefore to be really characteristic for the mode of propagation of light.

Taking still greater regions, we may have to introduce corrections of the third orders apart from those of the first and second orders so as to obtain consistent coordinates. These corrections determine the components of invariants of higher dimensions than the RIEMANN—CHRISTOFFEL tensor. The propagation of light in gravitational fields as it could be practically observed, was always very nearly homogeneous. The RIEMANN—CHRISTOFFEL tensor gives the biggest order deviation from homogeneity — and this deviation could just be observed. Higher order deviations are too small to be observable under circumstances which were accessible to observations so far and therefore the higher order invariants can thus not be determined practically by measurement.

The condition (35) cannot be supposed to be valid in the regions surrounding gravitating masses as in such regions the gravitational action produces inhomogeneous propagation of light.

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* The form (34) of the RIEMANN—CHRISTOFFEL tensor was given by BIEBERBACH quoted by LAUE [3].

A condition which is weaker than (25) and which according to EINSTEIN can be supposed to hold in empty space surrounding gravitating masses can be obtained with the help of the tensor

$$\mathbf{R} = \sum_{\varkappa\lambda} g^{+}_{\varkappa\lambda} \mathbf{R}^{(\varkappa\lambda)} = \mathrm{spur}\,(\mathbf{g}^{-1}\mathbf{R})\,. \tag{35a}$$

The relation thus postulated is

$$\mathbf{R} = 0\,. \tag{36}$$

So as to see the content of (36) we express the components of $\mathbf{R}^{(\varkappa\lambda)}$ in terms of **g** as given by equ. (1). The Christoffel brackets obtained from (1) are given in eq. (4) inserting these values into (34) we find

$$\begin{gathered} R^{(kl)}_{44} = -R^{(l4)}_{k4} = R^{(44)}_{lk} = -R^{(4k)}_{4l} = \\ = \frac{1}{2}\,\frac{\partial^2 g_{44}}{\partial x_k\,\partial x_l} - \frac{1}{8 g_{44}}\,\frac{\partial g_{\cdot 4}}{\partial x_k}\,\frac{\partial g_{44}}{\partial x_i} \qquad k, l = 1, 2, 3. \end{gathered} \tag{37}$$

Writing $g_{44} = -c^2(\mathrm{r})$ we have also

$$R_{44} = -c(\mathbf{r})\,\nabla^2 c(\mathbf{r}) + \frac{1}{2}\,(\nabla\, c(\mathbf{r}))^2\,. \tag{37a}$$

The remaining components are obtained as

$$\left.\begin{aligned} R_{lk} &= \frac{1}{g_{44}}\,R^{(44)}_{lk}\,, \\ R_{4l} &= -\frac{1}{g_{44}}\,R^{(44)}_{4l}\,. \end{aligned}\right\} \tag{38}$$

We see thus that the components of **R** other than R_{44} are of the order of R_{44}/c^2 thus they are small. Thus the equation (36) reduces in a first approximation to

$$\nabla^2 c(\mathbf{r}) = 0\,. \tag{39}$$

Connecting $c(\mathbf{r})$ with the gravitational potential according to relation (8) we see that (39) in a good approximation reduces to the LAPLACE—POISSON equation for empty space.

§ 11. So as to obtain the connection between gravitating masses and the propagation tensor **g** we have to determine **R** also in regions where there are sources of gravitation.

In the approximation of NEWTON's theory we have to replace (39) by

$$\nabla^2 \Phi = -4\pi\,Gm\,, \tag{40}$$

where m is the density of gravitating matter. The latter relation is obtained from (28) if we suppose

$$\mathbf{R} = \varkappa \mathbf{T}, \tag{41}$$

where **T** is the energy momentum tensor of matter and thus

$$T_{44} = u = mc^2,$$

and $\varkappa$ is taken

$$\varkappa = -\, 4\pi G/c\,.$$

However, relation (41) is contradictory because the right hand expression (as known from relativistic mechanics) obeys $\Box\mathbf{T} = 0$, while in general $\Box\mathbf{R} \neq 0$ as can be shown.

Relation (41) has thus to be replaced by

$$\mathbf{R} - \frac{1}{2}\,\mathbf{g}\,R = \varkappa\mathbf{T}, \tag{41a}$$

where

$$R = \sum_{\nu\mu} g^{+}_{\nu\mu} R_{\nu\mu} = \operatorname{spur} \mathbf{g}^{-1}\,\mathbf{R}\,.$$

Both sides of the left hand expression are free of divergence. For free space where $\mathbf{T} = 0$ we have identically $R = 0$ and thus (41a) reduces also to (41) in regions without matter.

Equations (41a) were solved by SCHWARZSCHILD for the field of a point mass. Thus the rotational symmetric solution of (41a) was obtained when $\mathbf{T} = 0$ for $r > 0$ and **T** having a regularity at $\mathbf{r} = 0$.

The latter solutions give for **g** expressions which differ by small terms from the form given in (1). In the latter solution the g_{ik} $i \neq k = 1, 2, 3$ differ from zero by small amounts thus the SCHWARZSCHILD solution predicts anisotropic propagation of light in the vicinity of the gravitating centre.

Determining the orbit of a beam of light from relations (39) of Part II and using for **g** the values given by SCHWARZSCHILD, the value of the deflection is obtained having twice the value obtained from a tensor **g** of the form (1).

It is seen thus that the deflection of light in a gravitational field gives an effect with the help of which it is possible to decide whether the propagation of light can be described by a tensor of the simple form (1) or whether **g** obeys a differential equation of the form (41a).

The experimental results seem to confirm the latter alternative.

§ 12. Thus the gravitational equations (41a) seem to give correct results at least inside the margin of error of the observation.

Nevertheless the question was raised whether relations (41a) can be generalized?

One possible generalization was already given by EINSTEIN introducing the "λ-term". I.e. it was suggested that (41) might be replaced by

$$\mathbf{R} - \frac{1}{2}\,\mathbf{g}\;R = \varkappa T - \lambda \mathbf{g}\,. \tag{42}$$

This latter relation might be interpreted by supposing that $-\lambda \mathbf{g}/\varkappa$ represent the energy momentum tensor of the ether. Taking the 44 — component of (42) we may suppose that $-\lambda g_{44}/\varkappa = \mu_E$ is the energy density of the stressed ether and that this energy density gives also a contribution to the gravitational field.

Multiplying (42) by $\mathbf{g}^{-1}$ and forming the spur we find for regions with $\mathbf{T} = 0$

$$R = 4\lambda\,,$$

and thus we may write for free space

$$R_{44} = \lambda g_{44}\,. \tag{43}$$

Introducing R_{44} from (37) we find the asymptotic solution of (43) of the form

$$g_{44} = c\,\frac{e^{-\sqrt{\lambda} r}}{r}\,.$$

Thus for $\lambda > 0$ we obtain solutions in which the gravitational field of a mass is shielded by the gravitational polarization of the ether and thus the potential decreases more rapidly to $\sim 1/r$. Whether such an effect exists or not is at present a purely speculative question.

We note further that the gravitational equations (41) or (41a) make use only of the second derivatives of $\mathbf{g}$. There exist covariants containing higher order derivatives than the seconds and thus it might be possible that (41) or (41a) represent only the first terms of some series, the further terms containing higher derivatives.

Of course even if the correct relations contained such terms, inside the accuracy of the present observations, neither the existence or non-existence of such terms can be ascertained. Such terms might be of importance in strong gravitational fields — thus they might play a role e.g. in the phenomena connected with gravitational collapse. It is not impossible that the recent discovery of new stellar objects with extreme densities will lead to phenomena which might give information on possible higher order terms of the gravitational equations.

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ПРИНЦИП ЛОРЕНЦА И ОБЩАЯ ТЕОРИЯ ОТНОСИТЕЛЬНОСТИ

Часть III

Л. ЯНОШИ

Резюме

Рассматривается связь между тензором распространения **g** и источниками гравитационного поля. Доказывается, что при предположении изотропного распространения света со скоростью, зависящей от гравитационного потенциала, два из трёх релятивистских эффектов может быть объяснено. Обычное истолкование отклонения света получается лишь при предположении неизотропного распространения света в гравитационном поле. Уравнения Эйнштейна для гравитационных полей выводятся с точки зрения принципа Лоренца.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3—4), pp. 345—365 (1966)

HIGHER MESON RESONANCES IN THE SU(6) SYMMETRY

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(Presented by K. Novobátzky. — Received 21. IV. 1966)

The mass values of positive parity meson resonances are compared in $\underline{189}$ and $\underline{405}$ with predictions of simple SU(6) mass formulae. It turns out that the 2^+ mesons alone can be assigned to both $\underline{189}$ and $\underline{405}$. Nevertheless $\underline{405}$ seems to be more promising, for it allows to include all well established positive parity mesons.

1. Introduction

The discovery of new boson resonances made it possible to compare the predications of different symmetry schemes with the measured experimental values. Therefore a considerable number of theoretical works dealt lately with these and related questions. E.g. a possibility for describing these meson resonances is offered by the quark models where they appear as bound-states of a quark (q) and an antiquark ($\bar{q}$) in p-states [1]. On the other hand the assignment of particles and resonances to different SU(6) representations corresponds to systems of quarks (and antiquarks) in s-state.

It is known that in the SU(6) theory the ordinary 0^- and 1^- mesons belong to $\underline{35} \oplus \underline{1}$, the baryons to $\underline{56}$, [2] the known negative parity baryon resonances can be assigned to $\underline{70}$ [3] and the $\underline{189}$- and $\underline{405}$-dimensional representations are the candidates for the positive parity mesons [4]:

$$
\begin{array}{lll}
f = 1253 \pm 20\,\mathrm{MeV}, & & I\,(J^P)^C = 0\,(2^+)^+ \\
D = 1286 \pm 6 & , & 0\,(1^+)^+ \\
f' = 1500 \pm & , & 0\,(2^+)^+ \\
A_1 = 1072 \pm 8 & , & 1\,(1^+)^+ \\
A_2 = 1324 \pm 9 & , & 1\,(2^+)^+ \\
H = 725 \pm 2 & , & 1/2\,(0^+) \\
K = 1405 \pm 8 & , & 1/2\,(2^+)
\end{array}
$$

Both representations correspond to $qq\bar{q}\bar{q}$ states.

The main task of the present paper is to compare the consequences of the assignment of the 2^+ meson nonet (composed of f', f, A_2, K^*) to $\underline{189}$ and $\underline{405}$. Our considerations are based on a simplified, "semiempirical" mass formula which is very well established in the $\underline{35}$ and $\underline{56}$ dimensional representations (see Section 2). The most important results of our investigations were published elsewhere [5].

2. Mass formulae in SU(6)

A mass formula was written down by **Gürsey**, **Radicati** and **Pais** in [2], on the basis of physical intuition. Namely one can expect that within an SU(3) multiplet the SU(6) theory reproduces the SU(3) mass formulae and gives a definite, simple spin-dependence of masses. Such a simple mass-formula is for example

$$\mu^2 = \mu_0^2 + \varkappa J(J+1) + \gamma\left[I(I+1) - \frac{1}{4}Y^2\right] \tag{1}$$

for the mesons and

$$M = M_0 + aJ(J+1) + bY + c\left[I(I+1) - \frac{1}{4}Y^2\right] \tag{2}$$

for baryons. From eqs. (1) and (2) it follows that the "physical" states diagonalizing the mass operator are the states in the SU(3) ⊗ SU(2) reduction of SU(6). It is known, however, that for mesons the octet and singlet states are "mixed". Therefore **Gürsey**, **Pais** and **Radicati** proposed the mass operator to be diagonal on the states of an SU(4) ⊗ SU(2) reduction of SU(6) [6]. (See below the so-called U-chain.)

The systematic study of mass operators in SU(6) can be carried out as in SU(3), namely by investigating the SU(6) transformation properties of the symmetry breaking. In this context T. K. **Kuo** and T. **Yao** [7] considered the most simple case, when the symmetry breaking term of the mass operator transforms like the $I = 0$, $Y = 0$, $J = 0$ member of the $\underline{35}$ representation. However, this choice turned out to be rather inadequate since the spin degeneracy is not lifted at all and for baryons also the isospin degeneracy remains. It was shown by **Baqi Bég** and **Singh** [8], that one must take the symmetry breaking term as a linear combination of different tensor operators. Using the reduction chain (the so called *physical chain* or P-chain):

$$SU(6) \supset SU(2)_J \otimes SU(3) \supset SU(2)_J \otimes U(1)_Y \otimes SU(2)_I \tag{3}$$

and the *unphysical chain* (U-chain):

$$SU(6) \supset U(1)_Y \otimes SU(2)_S \otimes SU(4) \supset U(1)_Y \otimes SU(2)_S \otimes SU(2)_I \otimes SU(2)_N \tag{4}$$

the appropriate tensor operators can be easily written down in such representations α, where in $a \otimes \alpha^*$ $\underline{189}$ and $\underline{405}$ occur no more than once. Indicating by $M^{(m)}_{(n)}$ the mass operator $I = Y = J = 0$ containing a symmetry breaking term transforming like an SU(6) tensor of multiplicity n and an SU(3) tensor of multiplicity m, we have (see [8]):

$$M^{(8)}_{(35)} = a_1 + b_1 Y + c_1 \left[2S(S+1) - C_2^{(4)} + \frac{1}{4} Y^2\right], \tag{5}$$

$$M^{(1)}_{(189)} = a_2 + b_2 \left[2J(J+1) - C_2^{(3)}\right], \tag{6}$$

$$\begin{aligned} M^{(8)}_{(189)} = a_3 + b_3 \Bigl\{ &\left[2J(J+1) - C_2^{(3)}\right] + \\ &+ 3\left[2I(I+1) - \frac{1}{2} Y^2 - 2N(N+1) + 2S(S+1)\right] - \\ &- \frac{3}{4}\left[2S(S+1) - C_2^{(4)} + \frac{1}{4} Y^2\right]\Bigr\}, \end{aligned} \tag{7}$$

$$M^{(1)}_{(405)} = a_4 + b_4 \left[2J(J+1) + C_2^{(3)}\right], \tag{8}$$

$$\begin{aligned} M^{(8)}_{(405)} = a_5 + b_5 \Bigl\{ &\left[2J(J+1) + C_2^{(3)}\right] - \\ &- \frac{21}{8}\left[2S(S+1) - C_2^{(4)} + \frac{1}{4} Y^2\right] - \\ &- 3\left[2I(I+1) - \frac{1}{2} Y^2 + 2N(N+1) - 2S(S+1)\right]\Bigr\}. \end{aligned} \tag{9}$$

Here the coefficients $a_1, a_2, \ldots, b_5, c_1$ are constant within an SU(6) multiplet. If the actual mass operator contains all the five terms listed above then the mass formula is the following:

$$\begin{aligned} M = a + bc_2^{(3)} + cJ(J+1) + dY + e\left[2S(S+1) - C_2^{(4)} + \frac{1}{4} Y^2\right] + \\ + f\left[N(N+1) - S(S+1)\right] + g\left[I(I+1) - \frac{1}{4} Y^2\right]. \end{aligned} \tag{10}$$

In [8] **Baqi Bég** and **Singh** have shown that in order to explain the observed masses in the $\underline{35}$ and $\underline{56}$ it is enough to take only $M^{(8)}_{(35)}$, $M^{(1)}_{(189)}$, $M^{(1)}_{(405)}$ and $M^{(8)}_{(405)}$. In this case the mass operator is:

$$\begin{aligned} M = a + bc_2^{(3)} + cJ(J+1) + dy + e\left[2S(S+1) - C_2^{(4)} + \frac{1}{4} Y^2\right] + \\ + f\left[N(N+1) - S(S+1) + I(I+1) - \frac{1}{4} Y^2\right]. \end{aligned} \tag{11}$$

Naturally the question arises, whether the choice of the above tensor operators is necessary or they can be replaced by others. It was shown by ACHASOV, KADISHEVSKIJ and MURADYAN [9] that instead of $M^{(8)}_{(405)}$ it is possible to take

$$M^{(84)}_{(405)} = a_6 + b_6 \left[I(I+1) + N(N+1) - \frac{4}{5} C_2^{(4)} \right], \tag{12}$$

where the upper index indicates that this tensor operator transforms as the appropriate member of the 84 dimensional SU(4) representation in the U-chain reduction. In this case the mass formula reads [9]

$$M = a + bC_2^{(3)} + cJ(J+1) + dY + e\left[2S(S+1) - C_2^{(4)} + \frac{1}{4} Y^2\right] + \\ + f\left[I(I+1) + N(N+1) - \frac{4}{5} C_2^{(4)}\right]. \tag{13}$$

Analyzing this mass formula in $\underline{35}$ and $\underline{56}$ it turns out that, beside the results given by (11), small corrections appear and this in the right direction. An analogue of the more general formula (10) can be written down also here, namely one can add to $M^{(8)}_{35}, M^{(8)}_{(189)}, M^{(1)}_{405}, M^{(84)}_{(405)}$ a term $M^{(20)}_{(189)}$ beloing to the U-chain instead of the earlier $M^{(1)}_{(189)}$. Taking into account

$$M^{(20)}_{(189)} = a_7 + b_7 [N(N+1) - I(I+1)] \tag{14}$$

we get from (5), (6), (8), (12) and (14) the mass formula

$$M = a + bC_2^{(3)} + cJ(J+1) + dY + \\ + e\left[2S(S+1) - C_2^{(4)} + \frac{1}{4} Y^2\right] + \\ + f\left[N(N+1) - \frac{2}{5} C_2^{(4)}\right] + g\left[I(I+1) - \frac{2}{5} C_2^{(4)}\right]. \tag{15}$$

It must be emphasized once more that the mass formulae given above are valid only in representations α such that $\alpha \otimes \alpha^*$ contains $\underline{189}$ and $\underline{405}$ not more than once. Therefore they cannot be used in the case of $\underline{189}$ or $\underline{405}$, because

$$\underline{189} \otimes \underline{189} = \underline{6720} \oplus \underline{5670} \oplus \underline{5670}^* \oplus \underline{3969} \oplus 2 \cdot \underline{3675} \oplus 2(\underline{896} \oplus \underline{896}^*) \oplus \\ \oplus \underline{490} \oplus \underline{490}^* \oplus \underline{405} \oplus \underline{280} \oplus \underline{280}^* \oplus 3 \cdot \underline{189} \oplus \underline{175} \oplus 2 \cdot \underline{35} \oplus \underline{1} \tag{16}$$

and

$$\begin{aligned}\underline{405} \oplus \underline{405} = {} & \underline{29700} \oplus \underline{19845} \oplus \underline{19845}^{*} \oplus \underline{14175} \oplus \underline{14175}^{*} \oplus \underline{12740} \oplus \underline{9625} \oplus \\ & \oplus \underline{9625}^{*} \oplus \underline{6720} \oplus 2 \cdot \underline{3675} \oplus 2 \cdot (\underline{3200} \oplus \underline{3200}^{*}) \oplus 2 \cdot \underline{2695} \oplus 3 \cdot \underline{405} \oplus \\ & \oplus \underline{280} \oplus \underline{280}^{*} \oplus \underline{189} \oplus 2 \cdot \underline{35} \oplus \underline{1}\,. \end{aligned} \tag{17}$$

In this case it is possible to work out special formulae, valid only in $\underline{189}$ or $\underline{405}$. For $\underline{189}$ such a formula was derived by CHIA-HWA CHAN and NGUYEN-HUU XUONG [10]. This mass formula in $\underline{189}$ reads

$$\begin{aligned} M = a + bC_2^{(3)} + cJ(J+1) + e\left[2S(S+1) + \frac{1}{4}Y^2 - C_2^{(4)}\right] + \\ + f\left[N(N+1) - S(S+1) + I(I+1) - \frac{1}{4}Y^2\right] + \\ + h\left[2J(J+1) + 22C_2^{(3)} - \{J(J+1)\}^2 - \right. \\ \left. - J(J+1)\,C_2^{(3)} - \{C_2^{(3)}\}^2\right]. \end{aligned} \tag{18}$$

The same problem was attacked by ROBASHIK and UHLMANN in a different way [11], resulting also in a six-parameter mass formula for $\underline{189}$. The problem for $\underline{405}$ is somewhat more complicated for the corresponding mass formula contains 7 parameters. On the basis of Wigner—Eckhart theorem and taking into account that in meson representations the mass of particle and antiparticle must be the same, the number of parameters in the different representations is the following:

	35	56	70	189	405
in (10) or (15)	6	4	7	8	8
in (11) or (13)	5	4	6	6	7

In the representations 35 and 56 the given mass formulae agree very well with the experimental data. It is a remarkable fact, however, that there exist simpler mass formulae, which are true both in 35 and 56 with a high accuracy. Such formulae can be obtained from (10) or (16) by putting b and f equal to zero, i.e. neglecting the dependence on $C_2^{(3)}$ and $N(N+1)$. These formulae are

$$\begin{aligned} M = a + cJ(J+1) + dY + e\left[2S(S+1) - C_2^{(4)} + \frac{1}{4}Y^2\right] + \\ + g\left[I(I+1) - \frac{1}{4}Y^2\right] \end{aligned} \tag{19}$$

and

$$M = a + cJ(J+1) + dY + e\left[2S(S+1) - C_2^{(4)} + \frac{1}{4}Y^2\right] +$$

$$+ g\left[I(I+1) - \frac{2}{5}C_2^{(4)}\right], \tag{20}$$

respectively. The dropping of $C_2^{(3)}$ means that the mass operator becomes diagonal on the U-chain.

It is possible to consider (19) and (20) as "semiempirical" mass formulae. The fact that (19) and (20) cannot be obtained directly from (11) or (13) shows perhaps that it is not allowed to drop the $M_{(189)}^{(8)}$ or $M_{(189)}^{(20)}$ contributions from the symmetry breaking term. Throughout this paper we apply these "semi-empirical" mass formulae as probably good approximations. The results given by (19) and (20) do not differ very much from each other. We shall give always both values. Now we summarize for convenience the consequences of (19) and (20) in the $\underline{56}$, $\underline{35}$ and $\underline{70}$.

The 56 baryons

In $\underline{56}$ there exist the following identities (see [8] and [9]):

$$2J(J+1) - C_2^{(3)} = -\frac{9}{2},$$

$$2S(S+1) - C_2^{(4)} + \frac{1}{4}Y^2 = -8Y - \frac{15}{2},$$

$$I(I+1) - \frac{1}{4}Y^2 - N(N+1) + S(S+1) = -Y + \frac{3}{4}, \tag{21}$$

$$N(N+1) + I(I+1) - \frac{2}{3}C_2^{(4)} = 2\left[I(I+1) - \frac{1}{4}Y^2\right] - 4Y - 6,$$

$$C_2^{(4)} = \frac{3}{4}Y^2 + 6Y + 9.$$

Thus here (10), (11) and (19) are simplified to

$$M = a + dY + cJ(J+1) + g\left[I(I+1) - \frac{1}{4}Y^2\right] \tag{22}$$

and (13), (15) and (20) give

$$M = a + cJ(J+1) + dY + g\left[I(I+1) - \frac{3}{10}Y^2\right]. \tag{23}$$

Using the Table given in [8] we can easily calculate the masses from (22):

$$\begin{aligned} \Lambda &= a + \frac{3}{4} c , & N^* &= a + \frac{15}{4} c + d + \frac{7}{2} g , \\ \Sigma &= a + \frac{3}{4} c + 2g , & Y_1^* &= a + \frac{15}{4} c + 2g , \\ N &= a + \frac{3}{4} c + d + 1/2\, g , & \Xi^* &= a + \frac{15}{4} c - d + \frac{1}{2} g , \\ \Xi &= a + \frac{3}{4} c - d + 1/2\, g, & \Omega &= a + \frac{15}{4} c - 2d - g . \end{aligned} \tag{24}$$

This gives for example the following mass relations:

$$\begin{gathered} 3\Lambda + \Sigma - 2(N + \Xi) = 0 , \\ Y_1^* - N^* = \Xi^* - Y_1^* = \Omega - \Xi^* , \\ \frac{1}{3} (\Omega - N^*) = \frac{3}{2} \Lambda - \frac{1}{2} \Sigma - N . \end{gathered} \qquad (25$$

On the other hand (23) gives

$$\begin{aligned} \Lambda &= a + \frac{3}{4} c , & N^* &= a + \frac{15}{4} c + d + \frac{69}{20} g , \\ \Sigma &= a + \frac{3}{4} c + 2g , & Y_1^* &= a + \frac{15}{4} c + 2g , \\ N &= a + \frac{3}{4} c + d + \frac{9}{20} g , & \Xi^* &= a + \frac{15}{4} c - d + \frac{9}{20} g , \\ \Xi &= a + \frac{3}{4} c - d + \frac{9}{20} g, & \Omega &= a + \frac{15}{4} c - 2d - \frac{6}{5} g \end{aligned} \tag{26}$$

and hence the mass relations are

$$\begin{gathered} 3\Lambda + \Sigma - 2 (N + \Xi) = \frac{1}{10} (\Sigma - \Lambda) , \\ Y_1^* - N^* = \Xi^* - Y_1^* + \frac{1}{20} (\Sigma - \Lambda) , \\ \Omega - \Xi^* = \Xi^* - Y_1^* - \frac{1}{20} (\Sigma - \Lambda) , \\ \frac{1}{3} (\Omega - N^*) = \frac{3}{2} \Lambda - \frac{1}{2} \Sigma - N + \frac{1}{20} (\Sigma - \Lambda) . \end{gathered} \tag{27}$$

(for mesons particle label denotes the squared mass).

The 35 mesons

Here (19) gives

$$\begin{aligned} \pi &= a - 8e + 2g , & \varrho &= a + 2c - 8e + 2g , \\ K &= a - 2e + \frac{1}{2} g , & K^* &= a + 2c - 2e + \frac{1}{2} g , \\ \eta &= a , & \varphi &= a + 2c + 4e , \\ & & \omega &= a + 2c - 8e \end{aligned} \tag{28}$$

and therefore we have the following mass relations

$$\begin{aligned} 4 K &= 3\eta + \pi , \\ 4K^* &= 2\varphi + \omega + \varrho , \\ K - \pi &= K^* - \varrho . \end{aligned} \tag{29}$$

The application of (20) leads now to

$$\begin{aligned} \pi &= a - 8e - \frac{6}{5} g , & \varrho &= a + 2c - 8e - \frac{6}{5} g , \\ K &= a - 2e - \frac{3}{4} g , & K^* &= a + 2c - 2e - \frac{3}{4} g , \\ \mu &= a , & \varphi &= a + 2c + 4e , \\ & & \omega &= a + 2c - 8e - \frac{16}{5} g \end{aligned} \tag{30}$$

and hence

$$\begin{aligned} 4 K &= 3\eta + \pi + \frac{9}{10} (\omega - \varrho) , \\ 4K^* &= 2\varphi + \omega + \varrho - \frac{7}{10} (\omega - \varrho) , \\ K^* - \varrho &= K - \pi . \end{aligned} \tag{31}$$

The 70 (negative parity) baryon resonances

Using the Table given in [3] we can evaluate the coefficients in (19) and (20) (in parentheses we give the coefficient of g in (20)).

$$\begin{aligned}
N_\gamma &= a + \frac{15}{4}c + d - \frac{19}{2}e + \frac{1}{2}g && \left[-\frac{63}{20}\right],\\
\Sigma_\gamma &= a + \frac{15}{4}c - \frac{15}{2}e + 2g && \left[-\frac{8}{5}\right],\\
\Lambda_\gamma &= a + \frac{15}{4}c - \frac{7}{2}e && [-2]\,,\\
\Xi_\gamma &= a + \frac{15}{4}c - d + \frac{1}{2}e + \frac{1}{2}g && \left[-\frac{3}{4}\right],\\
\Lambda' &= a + \frac{3}{4}c - \frac{15}{2}e && \left[-\frac{18}{5}\right],\\
\tilde{N} &= a + \frac{3}{4}c - \frac{19}{2}e + d + \frac{1}{2}g && \left[-\frac{63}{20}\right],\\
\Sigma &= a + \frac{3}{4}c - \frac{15}{2}e + 2g && \left[-\frac{8}{5}\right],\\
\tilde{\Lambda} &= a + \frac{3}{4}c - \frac{7}{2}e && [-2]\,,\\
\tilde{\Xi} &= a + \frac{3}{4}c - d - \frac{7}{2}e + \frac{1}{2}g && \left[-\frac{3}{4}\right],\\
\tilde{N}^* &= a + \frac{3}{4}c + d - \frac{19}{2}e + \frac{7}{2}g && \left[-\frac{3}{20}\right],\\
\tilde{Y}^* &= a + \frac{3}{4}c - \frac{7}{2}e + 2g && [0]\,,\\
\tilde{\Xi}^* &= a + \frac{3}{4}c - d + \frac{1}{2}e + \frac{1}{2}g && \left[-\frac{3}{4}\right],\\
\tilde{\Omega} &= a + \frac{3}{4}c - 2d + \frac{5}{2}e - g && [0]\,.
\end{aligned} \tag{32}$$

3. 2^+ mesons in $\underline{189}$

In this section we apply the mass formulae (19) and (20) in the 189 dimensional representation. In the P-chain reduction we have

$$\underline{189} = (27,1)^+ \oplus [(10,3) + (10^*,3)]^+ \oplus [(10,3) - (10^*,3)]^- \oplus (8,5)^+ \oplus \oplus (8_F,3)^+ \oplus (8_D,3)^- \oplus (8,1)^+ \oplus (1,5)^+ \oplus (1,1)^+\,. \tag{33}$$

Here we have given also the C-parity of the $[\mathrm{SU}(3) \otimes \mathrm{SU}(2)]$ representations, therefore instead of $(10, 3)$ and $(10^*, 3)$ the combinations $(10, 3) \pm (10^*, 3)$ appear. The C-parity of the different representations can be calculated with the help of the tensor reduction given in Table I of the Appendix, where $M^{a\alpha,b\beta}_{c\gamma,d\delta}$ denotes the $\underline{189}$ tensor $[a, b, c, d = 1, 2, 3;\ \alpha, \beta, \gamma, \delta = 1, 2]$.

The C-conjugation interchanges quark $(q^{a\alpha})$ and antiquark $(q_{a\alpha})$ and leaves the spin unaltered. That is

$$Cq^{a\alpha} = \varepsilon^{\alpha\varrho}\, q_{a\varrho} \quad \text{and} \quad Cq_{a\alpha} = \varepsilon_{\alpha\varrho}\, q^{a\varrho}\,, \tag{34}$$

where $\varepsilon_{\alpha\beta} = \varepsilon^{\alpha\beta}$ is the Levi—Civita symbol. From (34) follows that

$$CM^{a\alpha,b\beta}_{c\gamma,d\delta} = \varepsilon^{\alpha\varrho}\, \varepsilon^{\beta\sigma}\, \varepsilon_{\gamma\tau}\, \varepsilon_{\delta\omega}\, M^{c\tau,d\omega}_{a\varrho,b\sigma}\,. \tag{35}$$

This definition of C corresponds to determining it as a certain outer automorphism of SU(6). (See for example [12]).

For the "recoupling" transformations between the P-chain and U-chain we need the reduction of the $\underline{189}$ tensor in the P-chain (see Table II) and the tensors in the U-chain, where $\underline{189}$ is reduced like

$$\begin{aligned} \underline{189} = {} & (6,1)^2 \oplus (20^*, 2)^1 \oplus (4,2)^1 \oplus (20', 1)^0 \oplus (15,3)^0 \oplus (15,1)^0 \oplus \\ & \oplus (1,1)^{\circ} \oplus (20,2)^{-1} \oplus (4^*, 2)^{-1} \oplus (6,1)^{-2}\,. \end{aligned} \tag{36}$$

In (36) also the Y values are written out. The corresponding tensors are given in Table III, in the $\mathrm{SU}(2)_S \otimes \mathrm{SU}(2)_I \otimes \mathrm{SU}(2)_N$ decomposition. In Table III the notation $|N_{\mathrm{SU}(4)}, 2S+1 \,|\, 2I + 1,\ Y \,|\, 2N + 1)$ is used for the $\mathrm{SU}(2)_S \otimes \mathrm{SU}(2)_I \otimes \mathrm{SU}(2)_N$ tensors. The indices k, l, m, n, o, p belong to the group $\mathrm{SU}(2)_I$; $\alpha, \beta, \gamma, \delta, \varrho, \sigma$ to $\mathrm{SU}(2)_N$ and $3\alpha, 3\beta, 3\gamma, 3\delta, 3\varrho, 3\sigma$ to $\mathrm{SU}(2)_S$.

Using Tables II and III the recoupling transformations can be accomplished. Our mass operators are diagonal on the U-chain, thus the observable states correspond to the states in the U-chain tabulated in Table IV. Table IV contains also the mass values calculated from the mass formulae (19) and (20).

In $\underline{189}$ there are 25 different masses and (19) or (20) contains 4 parameters (for mesons $d = 0$), therefore it is possible to derive also plets. In the case of (19) and using the particle labelling introduced in Table IV these mass relations are:

$$2\tau_0 = \pi'_0 + \eta''_0\,, \qquad 4\delta_0 = \pi'_0 + \eta''_0 + 2\lambda_0,$$

$$4K'_0 + \lambda_0 = 4\pi'_0 + \eta''_0\,, \qquad \pi'_0 - \eta''_0 = \frac{4}{3}(\pi_0 - \varkappa_0)\,,$$

$$2\pi'_0 + \eta'_0 = 2\pi_0 + \eta''_0\,, \qquad 3\pi'_0 + \eta'_0 = 3\eta''_0 + \lambda_0\,,$$

$$3\pi'_0 = 2\eta_0 + \lambda_0\,,$$

$$\begin{aligned}
&2\,(\pi'_D - \varkappa_1) = 2\,(\delta_1 - \pi'_D) = \pi'_F - \xi_1 = 6\,(\varkappa_D - \eta_D)\,,\\
&3\eta_D + 2\pi'_F = 3\pi'_D + 2\xi_1\,, \qquad\qquad \pi_D = \pi'_F\,,\\
&4\varkappa_2 = \pi_2 + 2\eta'_2 + \eta_2\,,\\
&\pi_F + 2\eta_2 = \pi_2 + \eta_F + \eta'_2\,, \qquad\qquad \varkappa_F - \eta_F = \frac{1}{4}\,(\pi_2 - \eta'_2)\,,\\
&\pi'_0 - \eta''_0 = \frac{2}{3}\,(\pi'_F - \xi_1) = \pi_2 - \eta_2\,,\\
&\pi'_0 - \pi_0 = \pi'_F - \pi'_D = \frac{1}{2}\,(\eta_2 - \eta'_2)\,,\\
&9\,(\pi'_0 - \eta''_0) + 8\,(\eta_D - \pi_D) + \eta_F - \pi_F = 4\,(\varkappa_D - \varkappa_F)\,,\\
&2\varkappa'_0 - \tau_0 = \frac{1}{2}\,(3\eta_F - \eta'_2)\,.
\end{aligned} \tag{37}$$

The experimental values show that identifying K^* as K_2, f' as η'_2, f as η_2 and A_2 as π_2, the mass relation between the 2^+ mesons,

$$4K^* = 2f' + f + A_2 \tag{38}$$

is well satisfied. The corresponding mass relation obtained from (20) is

$$4K^* = 2f' + f + A_2 + \frac{7}{10}\,(\pi_2 - \eta_2)\,. \tag{39}$$

This is still better obeyed by the present experimental data [4]. Therefore the 2^+ mesons *alone* can be assigned to $\underline{189}$. The mixing angle for the 2^+ nonet is $\sim 35°$ (ideal mixing) as shown by Table IV. This value does not differ very much from the "experimental" one ($\sim 30°$), obtained by GLASHOW and SOCOLOW [13] on the basis of SU(3) (i.e. the GELL—MANN—OKUBO mass formula). Taking into account the experimental errors, the value given by us cannot be excluded either: this is in accordance with the fact that (38) is also true within the experimental errors. In the case of the more exact formula (39) the usual definition of the mixing angle cannot be applied since the diagonal elements of the mass operator on the SU(3) states are not OKUBO-type expressions. Therefore in our treatment the obtained value of the mixing angle does not at all exclude the possibility of assigning 2^+ mesons to $\underline{189}$ as was stated, on different grounds, in the work of HORN et al. [14].

The other conclusion which can be drawn from Table IV is that one can not assign 2^+ and 1^+ or 0^+ mesons *together* to $\underline{189}$. (See also the work of DAO-WONG DUC and PHAM-QUI TU [15], who arrived at the same conclusion.) The most unpleasant feature is that the well established A_1 resonance has no place in this scheme. The chance for the identification of other resonances is also poor. Another strange property of $\underline{189}$ is that the spin dependence is relatively small and negative (the parameter c is negative), so 0^+ mesons have large masses. (See also [11].)

4. 2^+ mesons in $\underline{405}$

The calculation in $\underline{405}$ can be carried out in the same way as in $\underline{189}$. The Tables V, VI, VII in the Appendix contain the tensor reductions corresponding to the reduction of $\underline{405}$,

$$\begin{aligned}\underline{405} &= (27,5)^+ \oplus (27,3)^- \oplus (27,1)^+ \oplus [(10,3) + (10^*,3)]^- \oplus \\ &\oplus [(10,3) - (10^*,3)]^+ \oplus (8,5)^+ \oplus (8_F,3)^+ \oplus (8_D,3)^- \oplus (8,1)^+ (1,5)^+ \oplus (1,1)^+\end{aligned} \tag{40}$$

in the P-chain and

$$\begin{aligned}\underline{405} &= (10,3)^2 \oplus (36,2)^1 \oplus (4,4)^1 \oplus (4,2)^1 \oplus (84,1)^0 \oplus (15,3)^0 \oplus (15,1)^0 \oplus \\ &\oplus (1,5)^0 \oplus (1,3)^0 \oplus (1,1)^0 \oplus (36^*,2)^{-1} \oplus (4^*,4)^{-1} \oplus (4^*,2)^{-1} \oplus (10^*,3)^{-2}\end{aligned} \tag{41}$$

in the U-chain. The quantum numbers of the observable states and the mass values calculated from (19) and (20) are given in Table VIII. The occurrence of (27, 5) and (27, 3) representations causes in $\underline{405}$ an additional difficulty, namely the identification of observed particles is not unambigous. Fitting for example the masses of $K^*(1405)$, $A_2(1324)$, $f(1253)$ and $D(1286)$ one has 12 different possibilities. But from these 12 choices only 3 gives the right mass formula (38) (or 39)), and only the one given in Table VIII has *positive spin dependence* ($c > 0$). This motivates the identification of K_2 with K^*, π_2 with A_2, η_2 with f and η_F with D.

As can be seen from Table VIII in this way almost every known positive parity meson can be identified. Only the $\varkappa(725)$ and the K^+K^+ (1055) resonance can not be fitted in the scheme. We remark, however, that taking into account the errors of the masses of K^*, A_2, f and D it is not possible to *exclude* the identification $\tau_0 = K^+K^+$ (1055) and $\varkappa_0 = \varkappa$ (725). It is remarkable that also the recently reported *So* (700) and the K^+K^+ (1280) [$I = 1$, $S = 2$] resonance can be included. The latter one is a typical member of an SU(3) 27-plet and has no extremely high mass at all as was expected in [14].

A very essential consequence of the mass operator being diagonal on the U-chain is that the symmetry breaking destroys very much the SU(3) ⊗ SU(2) multiplet structure of $\underline{405}$ and a considerable mixing of SU(3) states takes place. This fact can be directly seen from our mass relations derived from (19)

$$\begin{array}{ll}
2\pi_2' = \varkappa_2' + \delta_2\,, & 2\delta_2 = \lambda_2 + \tau_2\,, \\
2\varkappa_2' = \eta_2' + \tau_2\,, & 2\tau_2 + \eta_2 = 2\eta_2' + \pi_2\,, \\
\lambda_2 + 2\eta_2 = 3\pi_2\,, & \eta_2'' + \eta_2 = 2\eta_2'\,, \\
4\varkappa_2 = 2\eta_2' + \pi_2 + \eta_2\,, & \\
2\pi_1 = \delta_1' + \varkappa_1^{**}\,, & 2\delta_1' = \lambda_1 + \tau_1\,, \\
3\pi_1 = 2\eta_D' + \lambda_1\,, & \tau_1 - \eta_D' = \dfrac{1}{2}\,(\pi_F - \eta_F)\,, \\
\tau_1 + 2\varkappa_1 = \pi_F + 2\eta_F\,, & \lambda_1 + 4\varkappa_1 = 2\tau_1 + 3\pi_F\,, \\
\delta_1 + 2\xi_1 = \varkappa_1 + 3\eta_F\,, & 2\varkappa_1 = \xi_1 + \pi_F\,, \\
\varkappa_1^* - \varkappa_1 = \dfrac{5}{8}\,(\pi_F' - \pi_F)\,, & 4\eta_D + \pi_D' = 4\varkappa_1 + \eta_F\,, \\
4\pi_D = \pi_F' + 2\delta_1 + \xi_1\,, & \varkappa_1^* - \pi_F' = \dfrac{1}{2}\,(\xi_1 - \pi_D)\,, \\
\varkappa_1' = \varkappa_1\,, & \pi_D' = \pi_F\,, \\
3\tau_0 = 2\varkappa_0' + \pi_0'\,, & 2\delta_0 = \lambda_0 + \tau_0\,, \\
\delta_0 - \pi_0' = \dfrac{1}{4}\,(\lambda_0 - \eta_0'')\,, & \lambda_0 + 4\eta_0 = 4\tau_0 + \pi_0\,, \\
5\eta_0'' = 4\eta_0 + \eta_0'\,, & \tau_0 + \eta_0' = 2\varkappa_0\,, \\
2\tau_0 = \eta_0'' + \pi_0\,, & \\
\varkappa_2 - \varkappa_1 = \pi_2 - \pi_F = \eta_2' - \eta_F\,, & 4\eta_0 + \eta_2 + \eta_2' = 6\eta_F\,, \\
\eta_0 - \eta_0' = \dfrac{5}{4}\,(\eta_2' - \eta_2)\,, & \tau_0 - \eta_0'' = \dfrac{1}{2}\,(\pi_2 - \eta_2)\,, \\
\multicolumn{2}{l}{\tau_2 - \tau_1 = \delta_2 - \delta_1' = \varkappa_2' - \varkappa_1^{**} = \lambda_2 - \lambda_1 = \pi_2' - \pi_1 = 2(\tau_1 - \tau_0) =} \\
\multicolumn{2}{l}{\quad = 2(\delta_1' - \delta_0) = 2(\lambda_1 - \lambda_0) = 2(\delta_1 - \delta_0) = 2(\pi_D - \pi_0') =} \\
\multicolumn{2}{l}{\quad = 2(\varkappa_1^* - \varkappa_0') = \varkappa_2 - \varkappa_1' = \pi_2 - \pi_F = \varkappa_2 - \varkappa_1 =} \\
\multicolumn{2}{l}{\quad = 2(\varkappa_1 - \varkappa_0) = 2(\pi_F' - \pi_0)\,.}
\end{array} \tag{42}$$

It is remarkable that we obtained the mass relation (38) — or using (20) — the relation (39) which is confirmed by present experimental data with an accuracy better than 0,5%. Therefore 2^+ mesons *alone* fit in $\underline{405}$ as well as in $\underline{189}$. The occurrence of (27,5), however, has the consequence that in $\underline{405}$ there are six further 2^+ isomultiplets, with masses about 1500—1600 MeV.

The comparison of Table IV and Table VIII shows that the mass formulae (19) and (20) favour $\underline{405}$ against $\underline{189}$ as relevant for the known positive parity meson resonances. However, the 2^+ nonet alone cannot distinguish between $\underline{405}$ and $\underline{189}$. This conclusion agrees with the suggestion of $U(6,6)$ as a spectrum generating algebra [16]. (Namely $\underline{405}$ is a "ladder representation", while $\underline{186}$ is not.) The same conclusion was drawn also by Horn et al. in reference [14], but from different considerations. There are also works dealing with the different decay modes of positive parity mesons [17]. The question of identification of these meson resonances in $\underline{189}$ or in $\underline{405}$ can be decided only by taking into account also these results.

Acknowledgment

The authors are indebted to Prof. G. Marx for his kind interest in this work.

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ВЫСШИЕ МЕЗОННЫЕ РЕЗОНАНСЫ В SU(6) СИММЕТРИИ

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Резюме

Величина масс мезонных резонансов положительной четности сравнивается в $\underline{189}$ и $\underline{405}$ с предсказаниями простой массовой формулы SU(6). Оказывается, что оба 189 и 405 определяются самим мезоном 2+. Тем не менее $\underline{405}$ проявляет себя более надежным, так как оно может содержать все хорошо известные мезоны положительной четности.

Appendix

Table I

$$(\underline{27},\underline{1}) : h^{ab}_{cd} = \frac{1}{2\sqrt{2}} \left(M^{a\varrho,b\sigma}_{c\varrho,d\sigma} + M^{b\varrho,a\sigma}_{c\varrho,d\sigma}\right) - \text{Trace SU(3)} ,$$

$$(\underline{10},\underline{3}) : t^{abc,\alpha}{}_{\beta} = \frac{1}{6} \left[\varepsilon^{rsc} \left(M^{a\alpha,b\varrho}_{r\beta,s\varrho} + M^{b\alpha,a\varrho}_{r\beta,s\varrho}\right) + \varepsilon^{rsa} \left(M^{b\alpha,c\varrho}_{r\beta,s\varrho} + M^{c\alpha,b\varrho}_{r\beta,s\varrho}\right) + \right.$$

$$\left. + \varepsilon^{rsb} \left(M^{a\alpha,c\varrho}_{r\beta,s\varrho} + M^{c\alpha,a\varrho}_{r\beta,s\varrho}\right)\right] ,$$

$$(\underline{10^*},\underline{3}) : t^{*}_{abc,}\frac{\alpha}{\beta} = - \frac{1}{6} \left[\varepsilon_{rsc} \left(M^{r\alpha,s\varrho}_{a\beta,b\varrho} + M^{r\alpha,s\varrho}_{b\beta,a\varrho}\right) + \varepsilon_{rsa} \left(M^{r\alpha,s\varrho}_{b\beta,c\varrho} + M^{r\alpha,s\varrho}_{c\beta,b\varrho}\right) + \right.$$

$$\left. + \varepsilon_{rsb} \left(M^{r\alpha,s\varrho}_{a\beta,c\varrho} + M^{r\alpha,s\varrho}_{c\beta,a\varrho}\right)\right],$$

$$(\underline{8},\underline{5}) : m^{a,\alpha\beta}_{b,\gamma\delta} = - \frac{1}{2} \left[M^{a\alpha,r\beta}_{r\gamma,b\delta} + M^{r\alpha,a\beta}_{c\gamma,r\delta} + M^{a\beta,r\alpha}_{r\gamma,b\delta} + M^{r\beta,a\alpha}_{b\gamma,r\delta}\right] - \text{Trace SU(3)} \otimes \text{SU(2)} ,$$

$$(\underline{8}_F,\underline{3}) : f^{a,\alpha}_{b,\beta} = \frac{1}{\sqrt{3}} \left(M^{a\alpha,r\varrho}_{r\beta,b\varrho} - M^{r\alpha,a\varrho}_{b\beta,r\varrho}\right) ,$$

$$(\underline{8}_D,\underline{3}) : d^{a,\alpha}_{b,\beta} = \frac{2\sqrt{3}}{5} \left(M^{a\alpha,r\varrho}_{r\beta,b\varrho} + M^{r\alpha,a\varrho}_{b\beta,r\varrho}\right) - \frac{4}{5\sqrt{3}} M^{r\alpha,a\varrho}_{r\beta,b\sigma} - \text{Trace SU(3)} \otimes \text{SU(2)} ,$$

$$(\underline{8},\underline{1}) : n^{a}_{b} = \frac{2}{\sqrt{15}} \left(M^{a\varrho,r\sigma}_{r\varrho,b\sigma} - \frac{1}{3} \delta^{a}_{b} M^{r\varrho,s\sigma}_{s\varrho,r\sigma}\right) .$$

$$(\underline{1},\underline{5}) : u^{\alpha\beta}_{\gamma\delta} = \frac{1}{6} \left(M^{r\alpha,s\beta}_{r\gamma,s\delta} + M^{r\beta,s\alpha}_{r\gamma,s\delta}\right) - \text{Trace SU(2)} ,$$

$$(\underline{1},\underline{1}) : \ s = - \frac{\sqrt{5}}{12\sqrt{3}} M^{r\varrho,s\sigma}_{r\sigma,s\varrho} .$$

Table II

$$M^{a\alpha,b\beta}_{c\gamma,d\delta} = \frac{1}{\sqrt{2}} h^{ab}_{cd} \left(\delta^{\alpha}_{\gamma} \delta^{\beta}_{\delta} - \delta^{\alpha}_{\delta} \delta^{\beta}_{\gamma}\right) +$$

$$+ \frac{1}{4} \varepsilon_{cds} \left(t^{abs,\alpha}{}_{\gamma} \delta^{\beta}_{\delta} - t^{abs,\beta}{}_{\gamma} \delta^{\alpha}_{\delta} + t^{abs,\alpha}{}_{\delta} \delta^{\beta}_{\gamma} - t^{abs,\beta}{}_{\delta} \delta^{\alpha}_{\gamma}\right) +$$

$$+ \frac{1}{4} \varepsilon^{abs} \left(t^{*}_{cds,\gamma}{}^{\alpha} \delta^{\beta}_{\delta} - t^{*}_{cds,\delta}{}^{\alpha} \delta^{\beta}_{\gamma} + t^{*}_{cds,\gamma}{}^{\beta} \delta^{\alpha}_{\delta} - t^{*}_{cds,\delta}{}^{\beta} \delta^{\alpha}_{\gamma}\right) +$$

$$+ \frac{1}{2} \left(\delta^{a}_{c} m^{b,\alpha\beta}_{d,\gamma\delta} - \delta^{b}_{c} m^{a,\alpha\beta}_{d,\gamma\delta} + \delta^{b}_{d} m^{a,\alpha\beta}_{c,\gamma\delta} - \delta^{a}_{d} m^{b,\alpha\beta}_{c,\gamma\delta}\right) +$$

$$+ \frac{1}{4\sqrt{3}} \delta^{b}_{c} \delta^{\beta}_{\delta} f^{a,\alpha}_{d,\gamma} - \delta^{a}_{d} \delta^{\beta}_{\delta} f^{b,\alpha}_{c,\gamma} - \delta^{b}_{d} \delta^{\beta}_{\gamma} f^{a,\alpha}_{c,\delta} + \delta^{a}_{c} \delta^{\beta}_{\gamma} f^{b,\alpha}_{d,\delta} -$$

$$- \delta^{a}_{c} \delta^{\alpha}_{\delta} f^{b,\beta}_{d,\gamma} + d^{b}_{d} \delta^{\alpha}_{\delta} f^{a,\beta}_{c,\gamma} + \delta^{a}_{d} \delta^{\alpha}_{\gamma} f^{b,\beta}_{c,\delta} - \delta^{b}_{c} \delta^{\alpha}_{\gamma} f^{a,\beta}_{d,\delta}) +$$

$$+ \frac{1}{2\sqrt{3}} [\delta^{b}_{c} \delta^{\beta}_{\delta} \delta^{a,\alpha}_{d,\gamma} + \delta^{a}_{d} \delta^{\beta}_{\delta} d^{b,\alpha}_{c,\gamma} - \delta^{b}_{d} \delta^{\beta}_{\gamma} d^{a,\alpha}_{c,\delta} - \delta^{a}_{c} \delta^{\beta}_{\gamma} d^{b,\alpha}_{d,\delta} -$$

$$- \delta^{a}_{c} \delta^{\alpha}_{\delta} d^{b,\beta}_{d,\gamma} - \delta^{b}_{d} \delta^{\alpha}_{\delta} d^{a,\beta}_{c,\gamma} + \delta^{a}_{d} \delta^{\alpha}_{\gamma} d^{b,\beta}_{c,\delta} + \delta^{b}_{c} \delta^{\alpha}_{\gamma} d^{a,\beta}_{d,\delta} +$$

Table II (continued)

$$+\frac{1}{2}\,(\delta^a_c\,\delta^\alpha_\gamma\,d^{b,\beta}_{d,\delta}+\delta^b_d\,\delta^\beta_\delta\,d^{a,\alpha}_{c,\gamma}-\delta^a_d\,\delta^\alpha_\delta\,d^{b,\beta}_{c,\gamma}-\delta^b_c\,\delta^\beta_\gamma\,d^{a,\alpha}_{d,\delta})]+$$

$$+\frac{1}{\sqrt{15}}\left[(\delta^b_c\,n^a_d+\delta^a_d\,n^b_c)\left(\delta^\alpha_\gamma\,\delta^\beta_\delta+\frac{1}{4}\,\delta^\alpha_\delta\,\delta^\beta_\gamma\right)-\right.$$

$$\left.-(\delta^a_c\,n^b_d+\delta^b_d\,n^a_c)\left(\delta^\alpha_\delta\,\delta^\beta_\gamma+\frac{1}{4}\,\delta^\alpha_\gamma\,\delta^\beta_\delta\right)\right]+\frac{1}{2}\,u^{\alpha\beta}_{\gamma\delta}\,(\delta^a_c\,\delta^b_d-\delta^a_d\,\delta^b_c)+$$

$$+\frac{\sqrt{5}}{4\sqrt{3}}\,s\left[\frac{1}{5}\,(\delta^a_c\,\delta^\alpha_\gamma\,\delta^b_d\,\delta^\beta_\delta-\delta^a_d\,\delta^\alpha_\delta\,\delta^b_c\,\delta^\beta_\gamma)+(\delta^\alpha_\gamma\,\delta^\beta_\delta\,\delta^a_d\,\delta^b_c-\delta^\alpha_\delta\,\delta^a_c\,\delta^\beta_\gamma\,\delta^b_d)\right]$$

Table III

$$|6,1|1,2|3)^{\alpha\beta}=\varepsilon_{op}\,\varepsilon^{\varrho\sigma}\,(M^{o\alpha,p\beta}_{3\varrho,3\sigma}+M^{o\beta,p\alpha}_{3\varrho,3\sigma}),$$

$$|6,1|3,2|1)^{kl}=\varepsilon_{\varrho\sigma}\,\varepsilon^{\tau\omega}\,(M^{k\varrho,l\sigma}_{3\tau,2\omega}+M^{l\varrho,k\sigma}_{3\tau,3\omega}),$$

$$|20^*,2|2,1|2)^{k\alpha}_{3\beta}=M^{o\alpha,k\varrho}_{o\varrho,3\beta},$$

$$|20^*,2|2,1|4)^{\alpha\beta,k}_{\gamma,3\delta}=M^{o\alpha,k\beta}_{o\gamma,3\delta}+M^{o\beta,k\alpha}_{o\gamma,3\delta}-\text{Trace SU(2)}_S\otimes\text{SU(2)}_I\otimes\text{SU(2)}_N,$$

$$|20^*,2|4,1|2)^{kl,\alpha}_{m,3\beta}=M^{k\varrho,l\alpha}_{m\varrho,3\beta}+M^{l\varrho,k\alpha}_{m\varrho,3\beta}-\text{Trace SIN},$$

$$|4,2|2,1|2)^{k\alpha}_{3\beta}=M^{k\alpha,3\varrho}_{3\beta,3\varrho},$$

$$|15,3|1,0|3)^{\alpha,3\beta}_{\gamma,3\delta}=M^{o\alpha,3\beta}_{o\gamma,3\delta}-\text{Trace SN},$$

$$|15,3|3,0|1)^{k,3\alpha}_{l,3\beta}=M^{k\varrho,3\alpha}_{l\varrho,3\beta}-\text{Trace SI},$$

$$|15,3|3,0|3)^{k\alpha,3\beta}_{l\gamma,3\delta}=M^{k\alpha,3\beta}_{l\gamma,3\delta}-\text{Trace SIN},$$

$$|20',1|3,0|3)^{k\alpha}_{l\beta}=M^{k\alpha,o\varrho}_{l\varrho,o\beta}-\text{Trace IN},$$

$$|20',1|1,0|5)^{\alpha\beta}_{\gamma\delta}=M^{o\alpha,p\beta}_{o\gamma,p\delta}+M^{o\beta,p\alpha}_{o\gamma,p\delta}-\text{Trace N},$$

$$|20',1|5,0|1)^{kl}_{mn}=M^{k\varrho,l\sigma}_{m\varrho,n\sigma}=M^{l\varrho,k\sigma}_{m\varrho,n\sigma}-\text{Trace I},$$

$$|20',1|1,0|1)=M^{o\varrho,p\sigma}_{o\sigma,p\varrho},$$

$$|15,1|1,0|3)^{\alpha}_{\beta}=M^{o\alpha,3\varrho}_{o\beta,3\varrho}-\frac{1}{2}\,\delta^\alpha_\beta\,M^{o\varrho,3\sigma}_{o\varrho,3\sigma},$$

$$|15,1|3,0|1)^{k}_{l}=M^{k\sigma,3\varrho}_{l\sigma,3\varrho}-\frac{1}{2}\,\delta^k_l\,M^{o\varrho,3\sigma}_{o\varrho,3\sigma},$$

$$|15,1|3,0|3)^{k\alpha}_{l\beta}=M^{k\alpha,3\varrho}_{l\beta,3\varrho}-\text{Trace IN},$$

$$|1,1|1,0|1)=\varepsilon^{\varrho\sigma}\,\varepsilon_{\tau\omega}\,M^{3\tau,3\omega}_{3\varrho,3\sigma},$$

$$|20,2|2,-1|2)^{3\alpha}_{k\beta}=M^{o\varrho,3\alpha}_{o\beta,k\varrho},$$

$$|20,2|2,-1|4)^{\alpha,3\beta}_{\gamma\delta,k}=M^{o\alpha,3\beta}_{o\gamma,k\delta}+M^{o\alpha,3\beta}_{o\delta,k\gamma}-\text{Trace SIN},$$

$$|20,2|4,-1|2)^{k,3\alpha}_{lm,\beta}=M^{k\varrho,3\alpha}_{l\varrho,m\beta}+M^{k\varrho,3\alpha}_{m\varrho,l\beta}-\text{Trace SIN},$$

$$|4^*,2|2,-1|2)^{3\alpha}_{k\beta}=M^{3\alpha,3\varrho}_{k\beta,3\varrho},$$

$$|6,1|1,-2|3)_{\alpha\beta}=(M^{3\varrho,3\sigma}_{o\alpha,p\beta}+M^{3\varrho,3\sigma}_{o\beta,p\alpha})\,\varepsilon_{\varrho\sigma}\,\varepsilon^{op},$$

$$|6,1|3,-2|1)_{kl}=\varepsilon_{\varrho\sigma}\,\varepsilon^{\omega\tau}\,(M^{3\varrho,3\sigma}_{k\omega,l\tau}+M^{3\varrho,3\sigma}_{l\omega,k\tau}).$$

Table IV

Symbol	SU (4) states	J	C_n	I	Y	$C_2^{(4)}$	S	N	M_{I}(Mev)	M_{II}	M_{exp}
$\varkappa_2$	$\vert 8>$	2		$\frac{1}{2}$	± 1	$\frac{39}{4}$	$\frac{1}{2}$	$\frac{3}{2}$	1405*	1405*	$K^*(1405)$
π_2	$\vert 8>$	2	+	1	0	8	1	1	1324*	1324*	$A_2(1324)$
η_2	$\vert 8 > + \sqrt{2}\vert 1>$	2	+	0	0	8	1	1	1253*	1253*	$f(1253)$
η_2'	$-\sqrt{2}\vert 8 > + \vert 1>$	2	+	0	0	12	0	2	1520	1500	$f'(1500)$
ξ_1	$\vert 10>$	1		0	± 2	5	0	1	1250	1330	
δ_1	$\vert 10>$	1		$\frac{3}{2}$	± 1	$\frac{39}{4}$	$\frac{1}{2}$	$\frac{1}{2}$	1520	1530	
$\varkappa_1$	$2\vert 8_F> \mp 2\vert 8_D> + \vert 10>$	1		$\frac{1}{2}$	± 1	$\frac{39}{4}$	$\frac{1}{2}$	$\frac{1}{2}$	1430	1430	
$\varkappa_F$	$2\vert 8_F > \pm \vert 8_D > - 2\vert 10>$	1		$\frac{1}{2}$	± 1	$\frac{15}{4}$	$\frac{1}{2}$	$\frac{1}{2}$	1240	1290	C (1215)
$\varkappa_D$	$\vert 8_F > \pm 2\vert 8_D > + 2\vert 10 >$	1		$\frac{1}{2}$	± 1	$\frac{39}{4}$	$\frac{1}{2}$	$\frac{3}{2}$	1430	1430	
π_F	$2\vert 8_F > + \vert 10 > + \vert 10^* >$	1	+	1	0	12	0	1	1580	1580	
π_F'	$\vert 8_F > - \vert 10 > - \vert 10^* >$	1	+	1	0	8	1	1	1350	1350	
π_D	$2\vert 8_D > + \vert 10 > - \vert 10^*>$	1	—	1	0	8	1	0	1350	1350	
π_D'	$\vert 8_D > - \vert 10 > + \vert 10^* >$	1	—	1	0	8	0	1	1470	1500	
η_F	$\vert 8_F >$	1	+	0	0	8	1	1	1286*	1286*	$D(1286)$
η_D	$\vert 8_D >$	1	—	0	0	8	0	1	1410	1430	$E(1410)$
τ_0	$\vert 27 >$	0		1	± 2	5	0	0	1330	1410	
δ_0	$\vert 27 >$	0		$\frac{3}{2}$	± 1	$\frac{39}{4}$	$\frac{1}{2}$	$\frac{1}{2}$	1530	1540	
$\varkappa_0$	$\vert 27 > - 2\vert 8 >$	0		$\frac{1}{2}$	± 1	$\frac{39}{4}$	$\frac{1}{2}$	$\frac{1}{2}$	1440	1440	
$\varkappa_0'$	$2\vert 27 > + \vert 8 >$	0		$\frac{1}{2}$	± 1	$\frac{15}{4}$	$\frac{1}{2}$	$\frac{1}{2}$	1250	1300	
λ_0	$\vert 27 >$	0	+	2	0	12	0	0	1700	1700	
π_0	$\sqrt{2}\vert 27 > - \sqrt{3}\vert 8 >$	0	+	1	0	8	0	0	1490	1510	
π_0'	$\sqrt{3}\vert 27 > \sqrt{2}\vert 8 >$	0	+	1	0	8	1	1	1370	1370	
η_0	$\sqrt{6}\vert 27 > + 2\vert 8 > + \sqrt{2}\vert 1 >$	0	+	0	0	0	0	0	1160	1250	
η_0'	$\sqrt{3}\vert 27 > - 4\sqrt{2}\vert 8 > + 5\vert 1 >$	0	+	0	0	12	0	0	1530	1540	
η_0''	$3\sqrt{3}\vert 27 > - 2\sqrt{2}\vert 8 > - 5\vert 1 >$	0	+	0	0	8	1	1	1300	1300	

Table V

$$(\underline{27},\underline{5}) : \varkappa^{ab,\alpha\beta}_{cd,\gamma\delta} = \frac{1}{4}\,(M^{a\alpha,b\beta}_{c\gamma,d\delta} + M^{a\alpha,b\beta}_{c\delta,d\gamma} + M^{a\beta,b\alpha}_{c\gamma,d\delta} + M^{a\beta,b\alpha}_{c\delta,d\gamma}) - \text{Trace SU(3)} \otimes \text{SU(2)}\,,$$

$$(\underline{27},\underline{3}) : \lambda^{ab,\alpha}_{cd,\beta} = \frac{1}{4}\,(M^{a\alpha,b\varrho}_{c\beta,d\varrho} + M^{a\alpha,b\varrho}_{d\beta,c\varrho} + M^{b\alpha,a\varrho}_{c\beta,d\varrho} + M^{b\alpha,a\varrho}_{d\beta,c\varrho}) - \text{Trace SU(3)} \otimes \text{SU(2)}\,,$$

$$(\underline{27},\underline{1}) : \chi^{ab}_{cd} = \frac{1}{2\sqrt{6}}\,(M^{a\varrho,b\sigma}_{c\varrho,d\sigma} + M^{a\varrho,b\sigma}_{d\varrho,c\sigma}) - \text{Trace SU(3)},$$

$$(\underline{10},\underline{3}) : \tau^{abc,\alpha}{}_{\beta} = \frac{1}{6}\,[\varepsilon^{rsc}\,(M^{a\alpha,b\varrho}_{r\beta,s\varrho} + M^{b\alpha,a\varrho}_{r\beta,s\varrho}) + \varepsilon^{rsa}\,(M^{b\alpha,c\varrho}_{r\beta,s\varrho} + M^{c\alpha,b\varrho}_{r\beta,s\varrho}) +$$
$$+ \varepsilon^{rsb}\,(M^{c\alpha,a\varrho}_{r\beta,s\varrho} + M^{a\alpha,c\varrho}_{r\beta,s\varrho})]\,,$$

$$(\underline{10}^*,\underline{3}) : \tau^{*}{}_{abc,\beta}{}^{\alpha} = -\,\frac{1}{6}\,[\varepsilon_{rsc}\,(M^{r\alpha,s\varrho}_{a\beta,b\varrho} + M^{r\alpha,s\varrho}_{b\beta,a\varrho}) + \varepsilon_{rsa}\,(M^{r\alpha,s\varrho}_{b\beta,c\varrho} + M^{r\alpha,s\varrho}_{c\beta,b\varrho}) +$$
$$+ \varepsilon_{rsb}\,(M^{r\alpha,s\varrho}_{c\beta,a\varrho} + M^{r\alpha,s\varrho}_{a\beta,c\varrho})]\,,$$

$$(\underline{8},\underline{5}) : \mu^{a,\alpha\beta}_{b,\gamma\delta} = \frac{1}{2\sqrt{5}}\,[M^{a\alpha,r\beta}_{r\gamma,b\delta} + M^{a\beta,r\alpha}_{r\gamma,b\delta} + M^{a\alpha,r\beta}_{r\delta,b\gamma} + M^{a\beta,r\alpha}_{r\delta,b\gamma}] - \text{Trace SU(3)} \otimes \text{SU(2)},$$

$$(\underline{8}_F,\underline{3}) : \varphi^{a,\alpha}_{\beta,\beta} = \frac{1}{\sqrt{3}}\,(M^{a\alpha,r\varrho}_{r\beta,b\varrho} - M^{r\alpha,a\varrho}_{b\beta,r\varrho}),$$

$$(\underline{8}_D,\underline{3}) : \delta^{a,\alpha}_{b,\beta} = 2\sqrt{\frac{6}{5}}\left(M^{a\alpha,r\varrho}_{r\beta,b\varrho} + M^{r\alpha,a\varrho}_{b\beta,r\varrho} - \frac{2}{3}\,M^{r\alpha,a\varrho}_{r\beta,b\varrho}\right) - \text{Trace SU(3)} \otimes \text{SU(2)}\,,$$

$$(\underline{8},\underline{1}) : \nu^{a}_{b} = 2\sqrt{\frac{2}{15}}\left(M^{a\delta,r\sigma}_{r\varrho,b\sigma} - \frac{1}{3}\,\delta^{a}_{b}\,M^{r\varrho,s\sigma}_{s\varrho,r\sigma}\right),$$

$$(\underline{1},\underline{5}) : \omega^{\alpha\beta}_{\gamma\delta} = \frac{1}{6\sqrt{2}}\,(M^{r\alpha,s\beta}_{r\gamma,s\delta} + M^{r\alpha,s\beta}_{r\delta,s\gamma}) - \text{Trace SU(2)}\,.$$

$$(\underline{1},\underline{1}) : \sigma = \frac{\sqrt{7}}{12\sqrt{3}}\,M^{r\varrho,s\sigma}_{r\sigma,s\varrho}.$$

Table VI

$$M^{a\alpha,b\beta}_{c\gamma,d\delta} = \varkappa^{ab,\alpha\beta}_{cd,\gamma\delta} +$$
$$+ \frac{1}{4}\,[\delta^{\beta}_{\delta}\,\lambda^{ab,\alpha}_{cd,\gamma} + \delta^{\beta}_{\gamma}\,\lambda^{ab,\alpha}_{cd,\delta} + \delta^{\alpha}_{\delta}\,\lambda^{ab,\beta}_{cd,\gamma} + \delta^{\alpha}_{\gamma}\,\lambda^{ab,\beta}_{cd,\delta}] +$$
$$+ \frac{1}{\sqrt{6}}\,(\delta^{\alpha}_{\gamma}\,\delta^{\beta}_{\delta} + \delta^{\alpha}_{\delta}\,\delta^{\beta}_{\gamma})\,\chi^{ab}_{cd} +$$
$$+ \frac{1}{4}\,[\varepsilon_{cds}\,(\delta^{\beta}_{\delta}\,\tau^{abs,\alpha}{}_{\gamma} - \delta^{\beta}_{\gamma}\,\tau^{abs,\alpha}{}_{\delta} + \delta^{\alpha}_{\delta}\,\tau^{abs,\beta}{}_{\gamma} - \delta^{\alpha}_{\gamma}\,\tau^{abs,\beta}{}_{\delta})] +$$
$$+ \frac{1}{4}\,\varepsilon^{abs}\,(\delta^{\alpha}_{\gamma}\,\tau^{*}{}_{cds,\delta}{}^{\beta} - \delta^{\beta}_{\gamma}\,\tau^{*}{}_{cds,\delta}{}^{\alpha} + \delta^{\alpha}_{\delta}\,\tau^{*}{}_{cds,\gamma}{}^{\beta} - \delta^{\beta}_{\delta}\,\tau^{*}{}_{cds,\gamma}{}^{\alpha}) +$$
$$+ \frac{1}{2\sqrt{5}}\,(\delta^{a}_{c}\,\mu^{b,\alpha\beta}_{d,\gamma\delta} + \delta^{a}_{d}\,\mu^{b,\alpha\beta}_{c,\gamma\delta} + \delta^{b}_{c}\,\mu^{a,\alpha\beta}_{d,\gamma\delta} + \delta^{b}_{d}\,\mu^{a,\alpha\beta}_{c,\gamma\delta}) +$$
$$+ \frac{1}{4\sqrt{3}}\,(\delta^{b}_{c}\,\delta^{\beta}_{\delta}\,\varphi^{a,\alpha}_{d,\gamma} - \delta^{a}_{d}\,\delta^{\beta}_{\delta}\,\varphi^{b,\alpha}_{c,\gamma} + \delta^{b}_{d}\,\delta^{\beta}_{\gamma}\,\varphi^{a,\alpha}_{c,\delta} - \delta^{a}_{c}\,\delta^{\beta}_{\gamma}\,\varphi^{b,\alpha}_{d,\delta} +$$

$$+ \delta^a_c \, \delta^\alpha_\delta \, \varphi^{b,\beta}_{d,\gamma} - \delta^b_d \, \delta^\alpha_\delta \, \varphi^{a,\beta}_{c,\gamma} + \delta^a_d \, \delta^\alpha_\gamma \, \varphi^{b,\beta}_{c,\delta} - \delta^b_c \, \delta^\alpha_\gamma \, \varphi^{a,\beta}_{d,\delta}) +$$

$$+ \frac{1}{\sqrt{30}} \, [\delta^b_c \, \delta^\beta_\delta \, \delta^{a,\alpha}_{d,\gamma} + \delta^a_d \, \delta^\beta_\delta \, \delta^{b,\alpha}_{c,\gamma} + \delta^b_d \, \delta^\beta_\gamma \, \delta^{a,\alpha}_{c,\delta} + \delta^a_c \, \delta^\beta_\gamma \, {}^{b,\alpha}_{d,\delta} +$$

$$+ \delta^a_c \, \delta^\alpha_\delta \, \delta^{b,\beta}_{d,\gamma} + \delta^b_d \, \delta^\alpha_\delta \, \delta^{a,\beta}_{c,\gamma} + \delta^a_d \, \delta^\alpha_\gamma \, \delta^{b,\beta}_{c,\delta} + \delta^b_c \, \delta^\alpha_\gamma \, \delta^{a,\beta}_{d,\delta} -$$

$$- \frac{5}{4} \, (\delta^a_c \, \delta^\alpha_\gamma \, \delta^{b,\beta}_{d,\delta} + \delta^a_d \, \delta^\alpha_\delta \, \delta^{b,\beta}_{c,\gamma} + \delta^b_c \, \delta^\beta_\gamma \, \delta^{a,\alpha}_{d,\delta} + \delta^b_d \, \delta^\beta_\delta \, \delta^{a,\alpha}_{c,\gamma})] +$$

$$+ \sqrt{\frac{2}{15}} \left[\left(\delta^a_c \, \nu^b_d + \delta^b_d \, \nu^a_c \right) \left(\delta^\alpha_\delta \, \delta^\beta_\gamma - \frac{7}{8} \, \delta^\alpha_\gamma \, \delta^\beta_\delta \right) + \right.$$

$$\left. + (\delta^a_d \, \nu^b_c + \delta^b_c \, \nu^a_d) \left(\delta^\alpha_\gamma \, \delta^\beta_\delta - \frac{7}{8} \, \delta^\alpha_\delta \, \delta^\beta_\gamma \right) \right] +$$

$$+ \frac{1}{2\sqrt{2}} \, (\delta^a_c \, \delta^b_d + \delta^a_d \, \delta^b_c) \, \omega^{\alpha\beta}_{\gamma\delta} +$$

$$+ \frac{\sqrt{7}}{4\sqrt{3}} \, \sigma \left[\delta^\alpha_\gamma \, \delta^\beta_\delta \, \delta^a_d \, \delta^b_c + \delta^\alpha_\delta \, \delta^\beta_\gamma \, \delta^a_c \, \delta^b_d - \frac{5}{7} \left(\delta^\alpha_\gamma \, \delta^\beta_\delta \, \delta^a_c \, \delta^b_d + \delta^\alpha_\delta \, \delta^\beta_\gamma \, \delta^a_d \, \delta^b_c \right) \right] .$$

Table VII

$$|10,3|3,2|3)^{k\alpha,l\beta}_{3\gamma,3\delta} = M^{k\alpha,l\beta}_{3\gamma,3\delta} + M^{l\alpha,k\beta}_{3\gamma,3\delta} ,$$

$$|10,3|1,2|1)_{3\gamma,3\delta} = \varepsilon_{op} \, \varepsilon_{\varrho\sigma} \, (M^{o\varrho,p\sigma}_{3\gamma,3\delta} - M^{o\sigma,p\varrho}_{3\gamma,3\delta}) ,$$

$$|4,4|2,1|2)^{k\alpha,3\beta}_{3\gamma,3\delta} = M^{k\alpha,3\beta}_{3\gamma,3\delta} - \text{Trace SIN} ,$$

$$|36,2|2,1|2)^{k\alpha}_{3\delta} = M^{k\varrho,o\alpha}_{o\varrho,3\delta} - \frac{4}{5} \, M^{o\varrho,k\alpha}_{o\varrho,3\delta} ,$$

$$|36,2|2,1|4)^{k,\alpha\beta}_{3\delta,\gamma} = M^{k\alpha,o\beta}_{o\gamma,3\delta} - \text{Trace SIN} ,$$

$$|36,2|4,1|2)^{\alpha,kl}_{3\delta,m} = M^{k\sigma,l\varrho}_{m\varrho,3\delta} - \text{Trace SIN} ,$$

$$|36,2|4,1|4)^{k\alpha,l\beta}_{m\gamma,3\delta} = M^{k\alpha,l\beta}_{m\gamma,3\delta} + M^{k\beta,l\alpha}_{m\gamma,3\delta} - \text{Trace SIN} ,$$

$$|4,2|2,1|2)^{k\alpha}_{3\gamma} = M^{k\alpha,3\varrho}_{3\gamma,3\varrho} ,$$

$$|1,5|1,0|1)^{3\alpha,3\beta}_{3\gamma,3\delta} = M^{3\alpha,3\beta}_{3\gamma,3\delta} - \text{Trace S} ,$$

$$|15,3|1,0|3)^{\alpha,3\beta}_{\gamma,3\delta} = M^{o\alpha,3\beta}_{o\gamma,3\delta} - \text{Trace SN} ,$$

$$|15,3|3,0|1)^{k,3\beta}_{l,3\delta} = M^{k\varrho,3\beta}_{l\varrho,3\delta} - \text{Trace SI} ,$$

$$|15,3|3,0|3)^{k\alpha,3\beta}_{l\gamma,3\delta} = M^{k\alpha,3\beta}_{l\gamma,3\delta} - \text{Trace SIN} ,$$

$$|1,3|1,0|1)^{3\beta}_{3\delta} = M^{o\varrho,3\beta}_{o\varrho,3\delta} - \frac{1}{2} \, \delta^\beta_\delta \, M^{o\varrho,3\sigma}_{o\varrho,3\sigma} ,$$

$$|84,1|5,0|1)^{kl}_{mn} = M^{k\varrho,\ \sigma}_{m\varrho,n\sigma} + M^{l\varrho,k\sigma}_{m\varrho,n\sigma} - \text{Trace I} ,$$

$$|84,1|5,0|3)^{kl,\alpha}_{mn,\beta} = M^{k\alpha,l\varrho}_{m\beta,n\varrho} + M^{k\alpha,l\varrho}_{n\beta,m\varrho} + M^{l\alpha,k\varrho}_{m\beta,n\varrho} + M^{l\alpha,k\varrho}_{n\beta,m\varrho} - \text{Trace IN} ,$$

$$|84,1|5,0|5)^{k\alpha,l\beta}_{m\gamma,n\delta} = M^{k\alpha,l\beta}_{m\gamma,n\delta} + M^{k\alpha,l\beta}_{m\delta,n\gamma} + M^{l\alpha,k\beta}_{m\gamma,n\delta} + M^{l\alpha,k\beta}_{m\delta,n\gamma} - \text{Trace IN} ,$$

$$|84,1|1,0|5)^{\alpha\beta}_{\gamma\delta} = M^{o\alpha,p\beta}_{o\gamma,p\delta} + M^{o\beta,p\alpha}_{o\gamma,p\delta} - \text{Trace N} ,$$

Table VII (continued)

$$|84,1|3,0|5)^{\alpha\beta,k}_{\gamma\delta,l} = M^{k\alpha,o\beta}_{l\gamma,o\delta} + M^{k\alpha,o\beta}_{l\delta,o\gamma} + M^{k\beta,o\alpha}_{l\gamma,o\delta} + M^{k\beta,o\alpha}_{l\delta,o\gamma} - \text{Trace IN}\,,$$

$$|84,1|3,0|3_\varphi)^{k\alpha}_{l\beta} = M^{k\alpha,p\varrho}_{p\beta,l\varrho} - M^{p\alpha,k\varrho}_{l\beta,p\varrho}\,,$$

$$|84,1|1,0|1) = M^{o\varrho,p\sigma}_{o\sigma,p\varrho} - \frac{4}{5} M^{o\varrho,p\sigma}_{o\varrho,p\sigma}\,,$$

$$|84,1|3,0|3_\delta)^{k\alpha}_{l\beta} = M^{p\alpha,k\varrho}_{p\beta,l\varrho} - \frac{1}{3} M^{o\varrho,k\alpha}_{o\varrho,l\beta} - \text{Trace IN}\,,$$

$$|15,1|1,0|3)^{\alpha}_{\beta} = M^{o\alpha,3\varrho}_{o\beta,3\varrho} - \frac{1}{2}\,\delta^{\alpha}_{\beta}\, M^{o\varrho,3\sigma}_{o\varrho,3\sigma}\,,$$

$$|15,1|3,0|1)^{k}_{l} = M^{k\varrho,3\sigma}_{l\varrho,3\sigma} - \frac{1}{2}\,\delta^{k}_{l}\, M^{o\varrho,3\sigma}_{o\varrho,3\sigma}\,,$$

$$|15,1|3,0|3)^{k\alpha}_{l\beta} = M^{k\alpha,3\varrho}_{l\beta,3\varrho} - \text{Trace IN}\,,$$

$$|1,1|1,0|1) = M^{o\varrho,3\sigma}_{o\varrho,3\sigma}\,,$$

$$|4^*,4|2,-1|2)^{3\alpha,3\beta}_{k\gamma,3\delta} = M^{3\alpha,3\beta}_{k\gamma,3\delta} - \text{Trace SIN}\,,$$

$$|36^*,2|2,-1|2)^{3\beta}_{k\gamma} = M^{o\varrho,3\beta}_{k\varrho,o\gamma} - \frac{4}{5} M^{o\varrho,3\beta}_{o\varrho,k\gamma}\,,$$

$$|36^*,2|2,-1|4)^{3\delta,\gamma}_{k,\alpha\beta} = M^{o\gamma,3\delta}_{k\alpha,o\beta} - \text{Trace SIN}\,,$$

$$|36^*,2|4,-1|2)^{3\alpha,k}_{\beta,lm} = M^{k\varrho,3\alpha}_{l\beta,m\varrho} - \text{Trace SIN}\,,$$

$$|36^*,2|4,-1|4)^{k\alpha,3\beta}_{l\gamma,m\delta} = M^{k\alpha,3\beta}_{l\gamma,m\delta} + M^{k\alpha,3\beta}_{l\delta,m\gamma} - \text{Trace SIN}\,,$$

$$|4^*,2|2,-1|2)^{3\alpha}_{k\beta} = M^{3\alpha,3\varrho}_{k\beta,3\varrho}\,,$$

$$|10^*,3|3,-2|3)^{3\alpha,3\beta}_{k\gamma,l\delta} = M^{3\alpha,3\beta}_{k\gamma,l\delta} + M^{3\alpha,3\beta}_{l\gamma,k\delta}\,,$$

$$|10^*,3|1,-2|1)^{3\alpha,3\beta} = \varepsilon^{op}\,\varepsilon^{\varrho\sigma}\,(M^{3\alpha,3\beta}_{o\varrho,p\sigma} - M^{3\alpha,3\beta}_{o\sigma,p\varrho})\,.$$

Table VIII

Symbol	SU (4) states	J	C_n	I	Y	$C_2^{(4)}$	S	N	M_{I}(Mev)	M_{II}	M_{exp}
τ_2	$\|27\rangle$	2		1	± 2	9	1	1	1550	1545	
δ_2	$\|27\rangle$	2		$\frac{3}{2}$	± 1	$\frac{55}{4}$	$\frac{1}{2}$	$\frac{3}{2}$	1500	1500	
$\varkappa_2$	$\sqrt{2}\|27\rangle - \sqrt{3}\|8\rangle$	2		$\frac{1}{2}$	± 1	$\frac{55}{4}$	$\frac{1}{2}$	$\frac{3}{2}$	1405*	1405*	$K^*(1405)$
$\varkappa_2'$	$\sqrt{3}\|27\rangle + \sqrt{2}\|8\rangle$	2		$\frac{1}{2}$	± 1	$\frac{15}{4}$	$\frac{3}{2}$	$\frac{1}{2}$	1650	1650	
λ_2	$\|27\rangle$	2	+	2	0	20	0	2	1460	1460	
π_2	$\|27\rangle - 2\|8\rangle$	2	+	1	0	20	0	2	1324*	1324*	$A_2(1324)$
π_2'	$2\|27\rangle + \|8\rangle$	2	+	1	0	8	1	1	1580	1550	
η_2	$\|27\rangle - 2\|8\rangle + \sqrt{5}\|1\rangle$	2	+	0	0	20	0	2	1253*	1253*	$f(1253)$
η_2'	$3\|27\rangle - \|8\rangle - \sqrt{5}\|1\rangle$	2	+	0	0	8	1	1	1520	1500	$f'(1500)$
η_2''	$3\|27\rangle + 4\|8\rangle + \sqrt{5}\|1\rangle$	2	+	0	0	0	2	0	1750	1660	$\pi^+\pi^-$ (1670)?
τ_1	$\|27\rangle$	1		1	± 2	9	1	1	1320	1340	K^+K^+ (1280)?

Symbol	SU (4) states	J	C_n	I	Y	$C_2^{(4)}$	S	N	M^{I}(Mev)	M_{II}	M_{exp}
ξ_1	$\vert 10\rangle$	1		0	± 2	9	1	0	1250	1270	
δ_1	$\vert 27\rangle + \sqrt{2}\vert 10\rangle$	1		$\frac{3}{2}$	± 1	$\frac{55}{4}$	$\frac{1}{2}$	$\frac{3}{2}$	1265	1290	K^* (1270)?
δ_1'	$\sqrt{2}\vert 27 - \vert 10\rangle$	1		$\frac{3}{2}$	± 1	$\frac{55}{4}$	$\frac{1}{2}$	$\frac{1}{2}$	1265	1290	
$\varkappa_1$	$\sqrt{2}\vert 27\rangle \mp \sqrt{5}\vert 8_F\rangle - 2\sqrt{2}\vert 8_D\rangle$	1		$\frac{1}{2}$	± 1	$\frac{55}{4}$	$\frac{1}{2}$	$\frac{3}{2}$	1150	1180	$C(1215)$
$\varkappa_1'$	$\sqrt{2}\vert 27\rangle - 3\sqrt{5}\vert 10 \pm$ $\pm 2\sqrt{5}\vert 8_F\rangle - 2\sqrt{2}\vert 8_D\rangle$	1		$\frac{1}{2}$	± 1	$\frac{55}{4}$	$\frac{1}{2}$	$\frac{1}{2}$	1150	1180	
$\varkappa_1^*$	$12\vert 27\rangle + 2\sqrt{10}\vert 10\rangle \pm$ $\pm 2\sqrt{10}\vert 8_F\rangle + \vert 8_D\rangle$	1		$\frac{1}{2}$	± 1	$\frac{15}{4}$	$\frac{1}{2}$	$\frac{1}{2}$	1340	1380	$K\pi\pi$ (1320)?
$\varkappa_1^{**}$	$3\vert 27\rangle - \sqrt{10}\vert 10\rangle \mp$ $\pm\sqrt{10}\vert 8_F\rangle + 4\vert 8_D\rangle$	1		$\frac{1}{2}$	± 1	$\frac{15}{4}$	$\frac{3}{2}$	$\frac{1}{2}$	1440	1410	
λ_1	$\vert 27\rangle$	1	$-$	2	0	20	0	1	1210	1240	
π_F	$\vert 10\rangle - \vert 10^*\rangle + 2\vert 8_F\rangle$	1	$+$	1	0	20	0	1	1040	1080	$A_1(1072)$
π_F'	$\vert 10\rangle - \vert 10^*\rangle - \vert 8_F\rangle$	1	$+$	1	0	8	1	1	1350	1350	
π_D	$2\sqrt{6}\vert 27\rangle + \sqrt{10}\vert 10\rangle +$ $+ \sqrt{10}\vert 10^*\rangle - \vert 8_D\rangle$	1	$-$	1	0	8	0	1	1280	1330	$B(1220)$
π_D'	$\sqrt{3}\vert 27\rangle - \sqrt{5}\vert 10\rangle -$ $- \sqrt{5}\vert 10^*\rangle - 4\sqrt{2}\vert 8_D\rangle$	1	$-$	1	0	20	0	1	1040	1080	$K\bar{K}$ (1025)?
π_1	$2\sqrt{3}\vert 27\rangle - \sqrt{5}\vert 10\rangle - \sqrt{5}\vert 10^*\rangle +$ $+ 2\sqrt{2}\vert 8_D\rangle$	1	$-$	1	0	8	1	0	1350	1350	
η_F	$\vert 8_F\rangle$	1	$+$	0	0	8	1	1	1286*	1286*	$D(1286)$
η_D	$\sqrt{2}\vert 27\rangle - \sqrt{3}\vert 8_D\rangle$	1	$-$	0	0	8	0	1	1210	1260	
η_D'	$\sqrt{3}\vert 27\rangle + \sqrt{2}\vert 8_D\rangle$	1	$-$	0	0	0	1	0	1420	1435	$E(1410)$
τ_0	$\vert 27\rangle$	0		1	± 2	9	1	1	1190	1225	K^+K^+ (1280)?
δ_0	$\vert 27\rangle$	0		$\frac{3}{2}$	± 1	$\frac{55}{4}$	$\frac{1}{2}$	$\frac{1}{2}$	1130	1170	
$\varkappa_0$	$\vert 27\rangle - 2\sqrt{6}\vert 8\rangle$	0		$\frac{1}{2}$	± 1	$\frac{55}{4}$	$\frac{1}{2}$	$\frac{1}{2}$	1000	1050	
$\varkappa_0'$	$2\sqrt{6}\vert 27\rangle + \vert 8\rangle$	0		$\frac{1}{2}$	± 1	$\frac{15}{4}$	$\frac{1}{2}$	$\frac{1}{2}$	1210	1240	
λ_0	$\vert 27\rangle$	0	$+$	2	0	20	0	0	1060	1110	
π_0	$\vert 27\rangle + 2\vert 8\rangle$	0	$+$	1	0	8	1	1	1225	1240	
π_0'	$2\vert 27\rangle - \vert 8\rangle$	0	$+$	1	0	8	0	0	1150	1220	
η_0	$3\sqrt{7}\vert 27\rangle + \sqrt{7}\vert 8\rangle + \sqrt{5}\vert 1\rangle$	0	$+$	0	0	0	0	0	1230	1300	
η_0'	$\vert 27\rangle - 8\vert 8\rangle + \sqrt{35}\vert 1\rangle$	0	$+$	0	0	20	0	0	760	820	$S^0(700)$?
η_0''	$3\sqrt{27}\rangle - 4\vert 8\rangle - \sqrt{35}\vert 1\rangle$	0	$+$	0	0	8	1	1	1150	1160	

Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3—4) pp. 367—371 (1966)

COMMUNICATIONES BREVES

EINWIRKUNG DER HILFSELEKTRODEN AUF DIE KATHODE UND DIE KATHODENDUNKELRÄUME

Von

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(Eingegangen: 20. I. 1966.)

Wie bekannt, können die in der Nähe der Gasentladungselektroden angeordneten Hilfselektroden den Potentialablauf der Räume dieser Elektroden beeinflussen [1, 2]. Gleichzeitig ändern sie aber auch die Temperatur dieser Elektroden selbst, doch kann all dies z. B. auch durch Änderung der Lage der Hilfselektroden erzielt werden.

Die vorliegende Arbeit berichtet über die Ergebnisse von Prüfungen dieser Art, die bei Gleich- und Wechselstrom Hg-Ar-Entladungen mit einem Entladungsstrom von 430 mA durchgeführt wurden. Bei den Prüfungen wurde ein Gasentladungsrohr mit einem lichten Durchmesser von 36 mm verwendet. Seine Füllung bestand aus Argon mit einem Druck von 3 Torr und aus Quecksilberdampf mit einem Druck von $6 \pm 0{,}5 \cdot 10^{-3}$ Torr. Der Abstand zwischen den Hauptelektroden, gleichmässig ausgeführten Elektroden aus Wolfram-Doppelspiralen mit einem Emissionsüberzug, betrug 1090 mm. Zwei, je 0,1 mm starke, 7×12 mm grosse Nickelplättchen waren parallel zueinander und zur Achse der einen Elektrodenspirale angeordnet. Die beiden Plättchen waren voneinander unabhängig in radialer Richtung bewegbar. Die Entladung stabilisierte sich bis etwa 20 Minuten vor Beginn der Messungen.

Ein Teil der Ergebnisse der unter Gleichstrom-Entladungsbedingungen durchgeführten Kathodeneingriffe sind in Abb. 1 dargestellt. Auf der Abszisse sind die getrennt errechneten Abstände d der Hilfselektroden von der Spiralenachse, auf der Ordinate hingegen die Kathodentemperatur T_f und der Abstand l_d des kathodenseitigen Endes der positiven Säule sowie der Abstand d_g des Glimmentladungsraumes rings um die Kathode aufgetragen.

Im Verlauf der Messungen bewegten sich die Hilfselektroden relativ zur Kathode zusammen, wobei sie entweder ausserhalb des Entladungsraumes an das eine oder das andere Ende der Kathode gebunden waren (in der Abbildung mit dem Index h bezeichneter Zustand) oder ein vom Kathodenpotential abweichendes Wandpotential besassen (Zustand ohne Index). Aus der Abbildung ist ersichtlich, dass die Bewegung der Hilfselektroden sowohl den Glimmraum als auch über diesen hinaus die Lage der Grenze des bis zur positiven Säule reichenden Dunkelraumes beeinflusst. Sobald die Hilfselektrode das Potential des einen Endes der Spirale aufnimmt, verschieben sich der Glimmraum und die Grenzen des Dunkelraumes näher an die Kathodenspirale heran. Gleichzeitig aber ändern sich die Ausmasse des Glimmraumes auch in radialer Richtung, und zwar gleichzeitig mit der längs der Entladungsachse vor sich gehenden Schrumpfung. Im hier beschriebenen Falle war der Aufbau des Glimmraumes äusserst komplex und wegen des Erscheinens der für den Elektronemissionsüberzug an der Kathodenfläche charakteristischen Spektrallinien konnten auch die einzelnen Entladungsräume voneinander nicht getrennt werden. Diese Spektrallinien verwischen die Dunkelräume innerhalb des Glimmraumes und deren Grenzen.

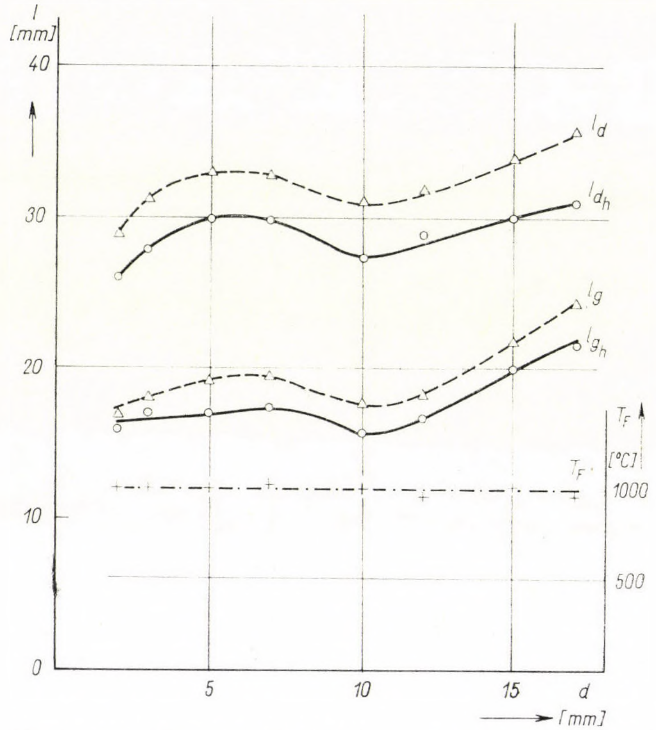

Abb. 1. Einfluss der im Kathodenraum der Gleichstromentladung bewegten Hilfselektroden auf die Abstände l_d, bzw. l_{dh} der kathodenseitigen Enden der positiven Säule von der Kathode sowie auf die Verschiebung der Grenzen der kathodischen Glimmbereiche l_g, bzw. l_{gh} in Richtung zur positiven Säule und auf die Kathodenflecktemperatur T_f. Der Index *h* steht für die mit den Kathodenenden verbundenen Hilfselektroden, die Bezeichnungen ohne Index betreffen die Messungen mit an Wandpotential liegenden Hilfselektroden

Sobald sich die Hilfselektroden in radialer Richtung der Kathode nähern, ändern sie die Ausmasse des Glimmraumes. Diese Wirkung tritt am kräftigsten in Erscheinung, wenn die Hilfselektroden die Potentiale der Kathodenenden besitzen. Die Änderung des Hilfselektrodenpotentials selbst vom Wandpotential auf Kathodenpotential, ändert die Ausmasse der Räume vor der Kathode durchschnittlich um 3 mm, höchstens aber um 5 mm. Dadurch ergibt sich ein Bild, als erhöhte eine dieses Potential besitzende Hilfselektrode die Wirtschaftlichkeit der im Kathodenraum vor sich gehenden Entladungsvorgänge und als ermöglichte sie damit eine Verminderung der axialen Ausmasse des Glimmraumes, was auf Grund der hier beschriebenen Vorgänge eine Möglichkeit zur Vergrösserung der positiven Säule böte. Nach den Messungen war die Kathodenflecktemperatur im Verlauf dieser Eingriffe von der Lage der Hilfselektroden unabhängig. Auch die gleichzeitig ermittelten Kathodenfallwerte zeigten keine wesentliche Änderungen abgesehen von einem Sprung von etwa 0,5 V, der sich bei einem Abstand von 10 mm ergab. Während jedoch die Flecktemperatur auch von der hier beschriebenen Änderung des Hilfselektrodenpotentials nicht beeinflusst wurde, sank unter ihrer Einwirkung der Kathodenfall um etwa 0,5 V. Um diesen Wert war der Kathodenfall geringer, wenn das Potential der Hilfselektroden dem der entsprechenden Kathodenenden gleich war. In Abb. 2 sind die Ergebnisse der Messungen dargestellt, die bei einer Wechselstromentladung von 50 Hz mit einem Ent-

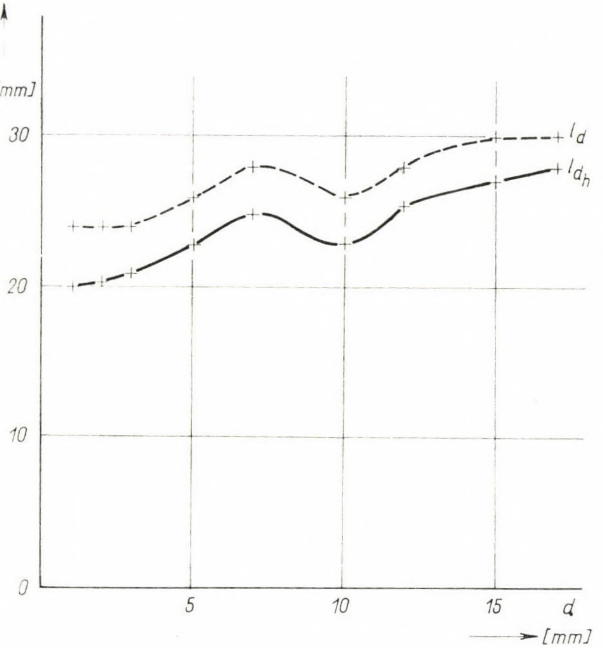

Abb. 2. Einfluss der bewegten Hilfselektrode im Raume der in der kathodischen Halbperiode befindlichen Elektrode bei Wechselstromentladung auf den von der Kathode gerechneten Abstand l_d, l_{dh} der kathodenseitigen Grenze der positiven Säule

ladungsstrom von gleichfalls 430 mA durchgeführt wurden. In diesem Falle ist bloss der Abstand des kathodenseitigen Endes der positiven Säule von der Kathodenspirale aufgetragen, da die Verschiebungen der Glimmraumgrenzen, die die Änderungen der Dunkelraumgrenzen verursachen, in genau der gleichen Weise vor sich gehen. Die hier gezeigten Kurven wurden mit Hilfe eines von einem Phasenschieber gesteuerten Stroboskops aufgenommen. Entsprechend sind die hier angegebenen Dunkelraumwerte auf Halbperioden bezogene Durchschnittswerte, die bei je einem gegebenen Hilfselektrodenabstand ermittelt wurden. Wie ersichtlich, beeinflusst das Potential der Hilfselektroden auch hier die Lage des kathodenseitigen Endes der positiven Säule, in erster Linie durch Verkleinerung des mit »Glimmraum« bezeichneten leuchtenden Raum-

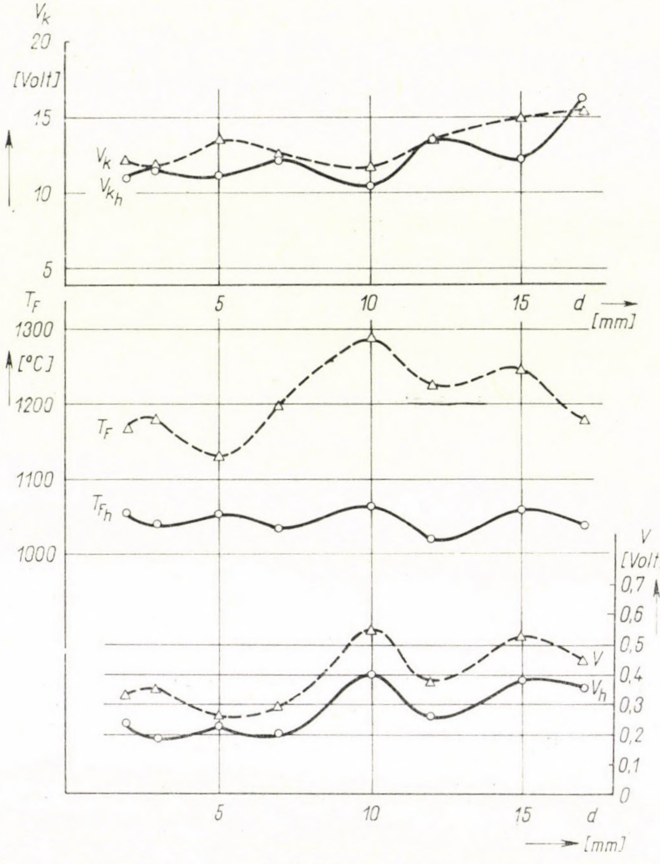

Abb. 3. Einfluss der bewegten Hilfselektrode im Raume der in der kathodischen Halbperiode befindlichen Elektrode bei Wechselstromentladung auf den Kathodenfall V_k, V_{kh}, auf die Flecktemperature T_f, T_{fh} und auf die Grösse der zwischen den Kathodenenden gemessenen, Gleichspannungsunterschiede V, V_h

komplexes. Die derart nachweisbare Raumänderung verlängert die positive Säule um etwa 3—4 mm.

An den Kurven der Abb. 2 ist weiterhin ersichtlich, dass die Länge der Kathodenräume in einem Zustand gegebenen Potentials um so mehr abnimmt, je näher die Hilfselektroden an die Kathode heranrücken. Dies hängt aller Wahrscheinlichkeit nach damit zusammen, dass von den Hilfselektroden als Verlust erhebliche Mengen des Ladungsträgers abgeführt werden, sowie mit den Vorgängen, die zum Ausgleich dieses Verlustes einsetzen. Das Minimum der Kurven bei 10 mm weist auf einen ausgezeichneten Zustand hin, zu dessen Deutung auch die Kurven des Kathodenfalles V_k und der Flecktemperatur T_f in Abb. 3 berücksichtigt werden müssen. Diese Kurven wurden bei den vorangegangenen Messungen, d. h. unter gleichen Versuchsbedingungen aufgenommen. Bei den Temperaturmessungen war vorausgesetzt, dass die so gemessenen Temperaturen der Kathodenflecktemperatur zumindest proportional sind und deren Änderungen folgen.

Bei einem Hilfselektrodenabstand von 10 mm tritt bei beiden ein Potential besitzenden Lagen der Ansatzstücke ein ausgesprochenes Kathodenfallminimum V_k und gleichzeitig ein Flecktemperaturmaximum auf. Diese Erscheinung lässt sich mit den Eigenschaften des aus den Ansatzstücken und der Spirale gebildeten elektronenoptischen Systems erklären. Aller Wahrscheinlichkeit nach ergeben sich für die der Kathode zustrebenden positiven Ionen so optimale Beschleunigungsverhältnisse, dass die zuvor bei anderen Hilfselektrodenabständen noch bestandenen Kathodenfallwerte überflüssig werden. Andererseits kann sich auch die Länge des Beschleunigungsraumes vor der Kathode vermindern, und die Kathodenflecktemperatur vermag auch so noch verhältnismässig hohe Werte anzunehmen.

Gleichfalls in Abb. 3 ist der in diesem Falle zwischen den beiden Kathodenenden gemessene Gleichspannungsunterschied aufgetragen. Er folgt den Schwankungen der Flecktemperatur gut, ändert sich verhältnisgleich mit dieser, was eine weitere Möglichkeit bietet, nach geeigneter Eichung die Flecktemperatur unabhängig vom optischen Verfahren fallweise einfacher und schneller zu bestimmen.

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Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3—4), pp. 373—376 (1966)

CHARACTERISTIC DISTANCES IN CLUSTERS OF GALAXIES

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(Received: 3. II. 1966)

There are 7 clusters of galaxies for which the red shift values z and the numbers of member galaxies N (in some not too large magnitude intervals Δm) as functions of the angular diameter of the counting circle 2ϑ are available in the literature [1—5]. The corresponding diagrams $N(\vartheta)$, corrected for the field, are represented in Fig. 1.

It is seen that these curves show at least two sudden changes of slope at values ϑ belonging to the inner parts of the clusters. Using the National Geographic Society-Palomar Sky Atlas the existence of similar remarkable changes is established for a number of other clusters by the author. Considering, however, that the latter examinations will be completed by extending the counts to all clusters available for observation only during the following years, the present preliminary communication is restricted to the study of clusters for which counts have already been published. Although it is premature to give any numerical value of the statistical significance of the phenomenon because the sample size will be increased at least threefold in the course of the work in progress, it is evident on the basis of Fig. 1 that the significance will be satisfactory for the practical purposes discussed below. The author's unpublished investigations reveal the important fact, partially confirmed by the similarity of the curves in Fig. 1a, c, e, that by repeating the counts a change of slope on the diagram $N(\vartheta)$ of a given cluster is to be observed at the same values ϑ whatever the spectral sensitivity of the plate-filter combination (blue or red), the adopted magnitude interval* and the field correction may be (cp. [6]), provided the centre of the counting circle is kept unchanged. Therefore, in the case of a regular cluster of galaxies with a definite centre, the angular distances of the first and second changes of slope, ϑ_1 and ϑ_2, are real characteristics of the cluster. For the clusters represented in Fig. 1 the values ϑ_1 and ϑ_2 are listed in Table 1 whereas the values $\log \vartheta_1$ and $\log \vartheta_2$ are plotted against the logarithms of the mean corrected red shifts in Fig. 2.

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* There is an upper limit: the effect disappears at very large magnitude intervals and counted numbers, especially in the case of a high field density.

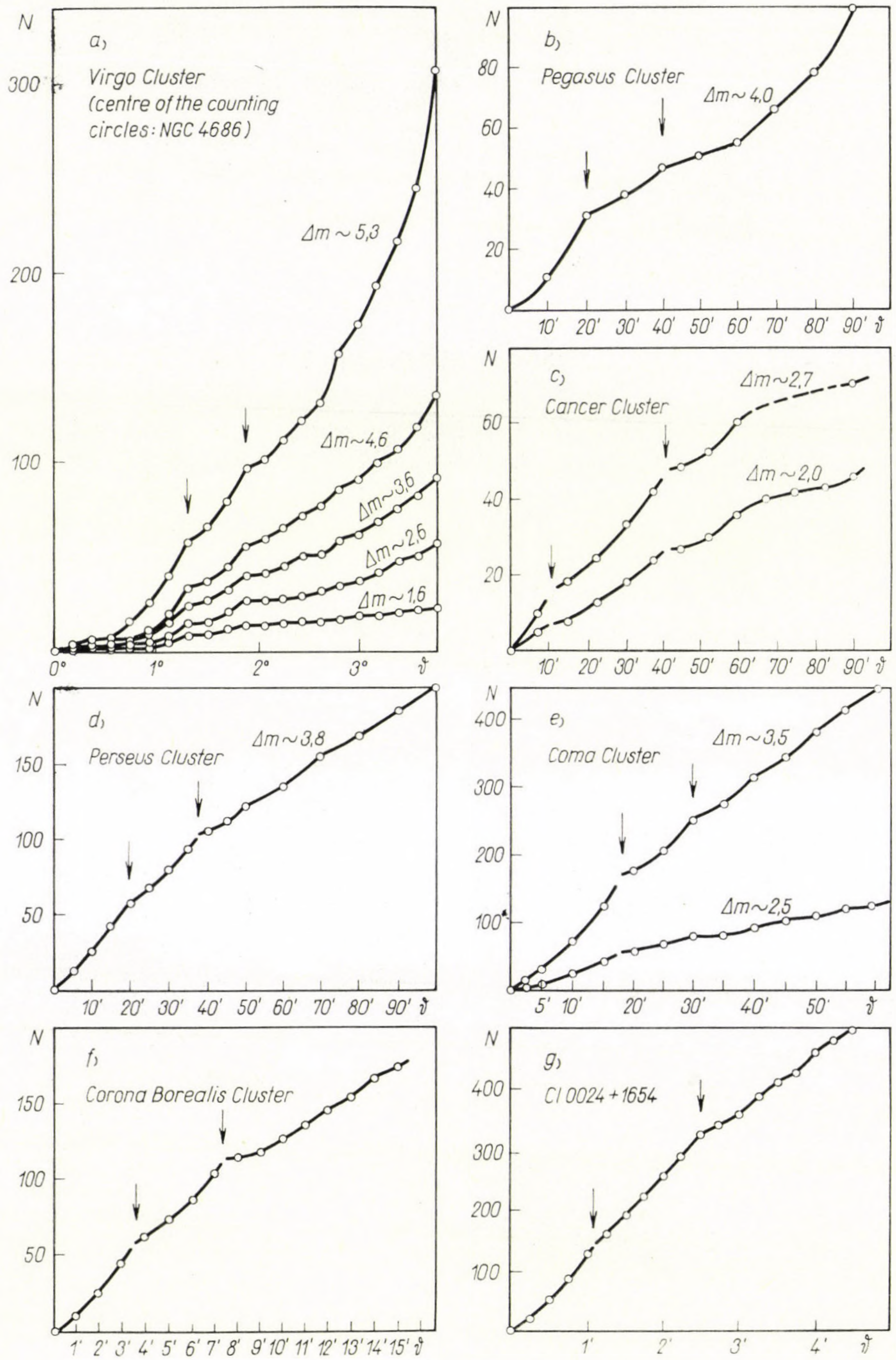
a)
Virgo Cluster
(centre of the counting circles: NGC 4686)
N
300
200
100
0°
1°
2°
3°
ϑ
Δm ~ 5,3
Δm~4,6
Δm~3,6
Δm~2,6
Δm~1,6
b)
Pegasus Cluster
Δm~4,0
N
80
60
40
20
10'
20'
30'
40'
50'
60'
70'
80'
90'
ϑ
c)
Cancer Cluster
Δm~2,7
Δm~2,0
N
60
40
20
10'
20'
30'
40'
50'
60'
70'
80'
90'
ϑ
d)
Perseus Cluster
Δm~3,8
N
150
100
50
10'
20'
30'
40'
50'
60'
70'
80'
90'
ϑ
e)
Coma Cluster
Δm~3,5
Δm~2,5
N
400
300
200
100
5'
10'
20'
30'
40'
50'
ϑ
f)
Corona Borealis Cluster
N
150
100
50
1'
2'
3'
4'
5'
6'
7'
8'
9'
10'
11'
12'
13'
14'
15'
ϑ
g)
Cl 0024+1654
N
400
300
200
100
1'
2'
3'
4'
ϑ

Fig. 1

Table I

Name or designation	ϑ_1	ϑ_2
	in minutes of arc	
Virgo Cluster	80	110
Pegasus Cluster	20	40
Cancer Cluster	11	40
Perseus Cluster	20	38
Coma Cluster	18	30
Corona Borealis Cluster	3,7	7,4
Cl 0024 + 1654	1,1	2,5

Fig. 2 suggests the presence of two correlations $\vartheta_1(z)$ and $\vartheta_2(z)$, the second one being perhaps the more reliable. It is highly probable that the scatter of the points on the diagram might be reduced by examining further clusters with known red shifts and selecting those which have similar diagrams $N(\vartheta)$ or similar physical and morphological properties. This would indicate the approximate identity of the characteristic linear sizes for the central parts of the clusters of galaxies of any given type. (A similar statistical phenomenon is likely to exist for some star clusters too. — Dr. P. N. KHOLOPOV's private communication).

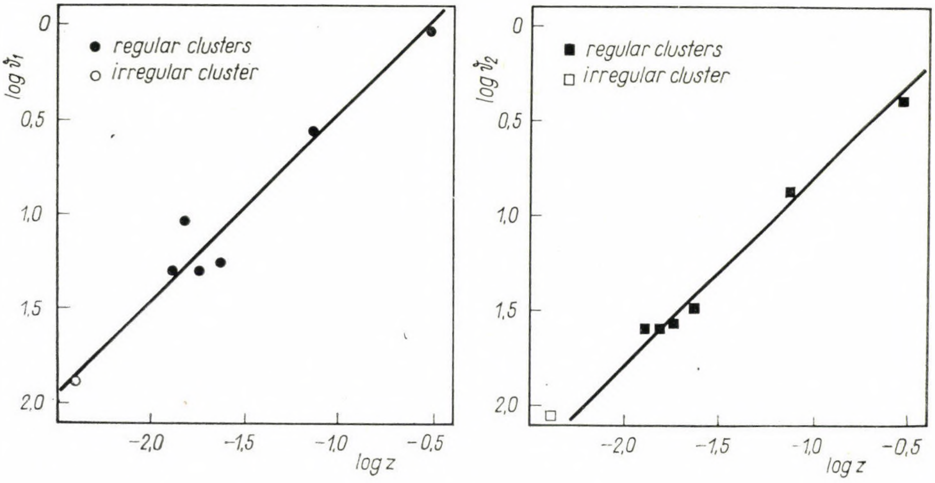

Fig. 2

A standard diagram $N(\vartheta)$ — derived by normalization of the arguments — seems to provide new statistical distance-parameters by its sudden changes of slope and new means of classifying regular clusters of galaxies by its general form. When better known it may well prove as valuable a guide in investigating the distance and the physical type of clusters of galaxies as the HR diagram has proved to be in the case of star clusters. On the other hand the comparison of the correlation $\vartheta_2(z)$ with the theoretically expected one for the "metric angular diameters" [7—9] and the investigation of the dependence of the ratio ϑ_1/ϑ_2 on the distance of the clusters may largely contribute to our knowledge on the evolution of galaxy clusters and the Metagalaxy taken as a whole.

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Acta Physica Academiae Scientiarum Hungaricae, Tomus 21 (3—4), pp. 377—379 (1966)

VARIATIONAL PROBLEM IN THE SCHRÖDINGER THEORY*

By

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(Received 31. III. 1966)

With integrated forms of the one particle Schrödinger equation a variational principle is presented and applied to some simple problems.

Armstrong [1] has discussed an interesting special form of the integrated Schrödinger equation. In the following we would like to generalize this idea and discuss a variational principle for the determination of the wave function and energy eigenvalue. To avoid some problems at the beginning we restrict our discussion to a one particle theory leaving the many-body problems for a forthcoming paper.

If the Hamiltonian of an atomic system is

$$H = -\frac{1}{2}\Delta + V \tag{1}$$

(in the following we use atomic units in which $e = m = \hbar = 1$ i.e. the units are the elementary charge, the mass of the electron and Planck's constant divided by 2π. The energy is measured in double Rydbergs) with bound state ψ_i and energy E_i, then

$$H\psi_i = E_i\,\psi_i\,. \tag{2}$$

Using Green's theorem Armstrong converted $\int\limits_{\Omega} \Delta\psi\, dv$ into $\int\limits_{F} \Delta\psi\, dS$ with Ω a large volume and F its surface. For bound states the latter integral vanishes and he got

$$E_i \int \psi_i\, dv = \int V\psi_i\, dv\,. \tag{3}$$

By a repeated application of the arguments we may arrive to a very similar equation in the following manner. By using (2) and (3) we get

$$E_i^2 \int \psi_i\, dv = E_i \int V\psi_i\, dv = \int VH\,\psi_i\, dv\,. \tag{4}$$

---

* This work was begun at the Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, Colorado while the author was a Visiting Fellow.

With the detailed form of the Hamiltonian and using Green's theorem and taking into account that

$$\Delta V = f(\mathbf{r}) \tag{5}$$

in the space between surfaces surrounding the singularities of the potential and a large surface very far away from the singularities we get

$$\begin{aligned} \int V \left(-\frac{1}{2} \Delta \right) \psi_i \, dv = -\frac{1}{2} \Bigg\{ \sum_l \int\limits_{fl} \left[V \frac{\partial \psi_i}{\partial n} - \psi_i \frac{\partial V}{\partial n} \right] d f_l + \\ + \int\limits_F \left[V \frac{\partial \psi_i}{\partial n} - \psi_i \frac{\partial V}{\partial n} \right] dF + \int f(\mathbf{r}) \, \psi_i \, dv \Bigg\} . \end{aligned} \tag{6}$$

The sum within the curly bracket is over the singularities. Assume F to be so large that the second term may be neglected. This is reasonable because for bound states ψ_i and $\frac{\partial \psi_i}{\partial n}$ tend to zero fast enough far from the singularities. f_l is a small sphere with radius r_l around the singularity l. df_l is a surface element on the sphere f_l. If r_l is small enough V is spherically symmetrical around the singularity for point charges with singularity like $1/r_l$.

In the following we shall restrict our discussion to potentials with singularities like those of point charges. For other type potentials the discussion may be led along similar lines.

Because $\psi_i \sim r^a \; a \geqslant 0$ near each point charge and $df = r^2 d\Sigma$, where $d\Sigma$ is the solid angle of df seen from the point charge, the first terms in the square brackets vanish and we get for the other terms

$$\int V \left(-\frac{1}{2} \Delta \right) \psi_i \, dv = -2\pi \sum_l Z_l \, \psi_i \, (r_l = 0) , \tag{7}$$

where Z_l is the atomic number of the point charge at $r_l = 0$.

By collecting the terms and rearranging we get

$$E_i^2 \int \psi_i \, dv = \int V^2 \, \psi_i \, dv - 2\pi \sum_l Z_l \, \psi_i \, (r_l = 0) . \tag{8}$$

Let us try to substitute into (3) and (8) a trial function φ_i instead of ψ_i; Then we get $\overline{\varepsilon}_i$ from (3) and $\overline{\varepsilon_i^2}$ from (8) and we have that

$$\overline{\varepsilon_i^2} \neq (\overline{\varepsilon}_i)^2 \tag{9}$$

in general. If $\varphi_i \equiv \psi_i$ then naturally $\overline{\varepsilon_i^2} = \overline{\varepsilon}_i^2$.

The quantity

$$\delta^2 \varepsilon = \left| \overline{\varepsilon_i^2} - |\overline{\varepsilon_i}|^2 \right| \tag{10}$$

minimized will lead us to the true wave function.

For the hydrogen atom with the trial function $\varphi_i = \exp(-\lambda r)$ we easily get from (10) $\lambda = 1$.

The application to other simple problems as harmonic oscillator, etc. is also straightforward.

This variational principle cannot be applied to many-particle Fermion systems because of the antisymmetry of the wave function both the left side and the right one of (3) and (8) vanish. But the generalization of this theorem is easy and will be the subject of a forthcoming paper.

Acknowledgement

The author is grateful to the staff at Lockheed Research Laboratories, Palo Alto and especially to Dr. STEPHAN ORMONDE for hospitality.

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RECENSIONES

The Origin of Cosmic Rays

by V. L. Ginzburg and S. I. Syrovatskii (translated from Russian), Pergamon Press, Oxford—London—Edinburg—New York—Paris—Frankfurt 1964

Although this book has the title "The Origin of Cosmic Rays" it would perhaps have been more correct to call it "The Astrophysics of Cosmic Rays", as is pointed out by the authors in the Preface. The subject of this book is much broader than "the origin of cosmic rays" used in its narrow sense.

The cosmos was investigated until the fourties of this century almost entirely by optical methods. The most important recent feature of modern astronomy is, however, the development of two new research fields: radio astronomy and the investigation of the astrophysical aspects of cosmic rays. This monograph deals with the latter rapidly developing scientific subject in detail, and problems of radio astronomy are touched upon only insofar as they are connected with cosmic rays.

The main subjects studied are the following: 1) Primary cosmic rays on the Earth (composition, energy spectrum, spatial distribution); 2) Cosmic rays beyond the solar system (in the Galaxy and Metagalaxy) and the effect of the interstellar medium and interstellar magnetic fields on them; 3) The origin of cosmic rays.

In the English edition some new results partly published at the International Conference on Cosmic Rays, Jaipur 1963 are also added. The excellent monograph which can already be considered as a classical summary of this subject was translated by H. S. H. Massey and edited by D. ter Haar.

E. Fenyves

Physical Acoustics

(Edited by Warren P. Mason) Vol. I. Part A and Part B. Academic Press, New York, London 1964

The first two volumes of this large encyclopedia include 14 major papers of a general character. All the authors are Americans, most of them research workers in the Bell Telephone Laboratories. The Editor has broken with classical traditions and introduces in the first two parts the physics and excitation methods of ultrasounds. The idea being very fascinating its continuation is awaited with much interest.

Though the structure of the whole work is warranted by the widespread technical knowledge and the rich experience of W. P. Mason, we are not quite sure whether it is entirely suitable for such a general work, to be written by a group which group is rather restricted, after all. The European scientific literature shows many examples of good encyclopedias (Ergebnisse der exakten Naturwissenschaften, Handbuch der Physik etc.) from which we realize that the best surveys of any special scientific field are given by the most competent researchers with the widest knowledge and experience. These conditions can be satisfied more easily when the authors are chosen from all over the international scientific range.

All this does not refer to the value of the separate papers, each chapter giving a good picture of the results in its special field. Yet there are, in our opinion, chapters of extreme importance (e.g. the four treatises on semiconductors appearing in part B; Chapters 10—13) and there are also some which seem superfluous (e.g. Chapter 8 which is of only industrial interest, or Chapter 14 which cannot be compared in importance with the others). We must point out the uniformly comprehensive bibliographies and the references gathered from a central viewpoint (900 references) which really make this standard work an encyclopedia.

The two volumes include the following chapters:

A Chapter 1. R. N. Thurston, Wave Propagation in Fluids and Normal Solids. Phenomena of wave propagation, with rather more mathematics than in other chapters.

Chapter 2. T. R. Mecker—A. H. Meitzler, Guided Wave Propagation in Elongated Cylinders and Plates. Modern treatise of wave propagation in limited spaces with hints for applications.

Chapter 3. D. A. Berlincourt—D. R. Curran—H. Jaffe, Piezoelectric and Piezomagnetic Materials and Their Function in Transducers. A detailed survey not only of the physical characteristics of materials but also of the circuit solutions to applications.

Chapter 4. H. J. McSkimin, Ultrasonic Methods for Measuring the Mechanical Properties of Liquids and Solids. Considering the width of the subject, this is a very short summary of the application of passive ultrasounds in measuring technique.

Chapter 5. W. P. Mason, Use of Piezoelectric Crystals and Mechanical Resonators in Filters an Oscillators. A survey of the author's wide experience in this field including practical aspects.

Chapter 6. J. E. May *Jr.*, Guided Wave Ultrasonic Delay Lines. Theoretical and technological treatment of the guided-type propagation of various mechanical waves.

Chapter 7. W. P. Mason, Multiple Reflection Ultrasonic Delay Lines. A short reference on reflection delay systems which are, today, of only historical importance.

B Chapter 8. B. Carlin, The Use of High- and Low-Amplitude Ultrasonic Waves for Inspection and Processing. A short treatise of an industrial nature.

Chapter 9. H. G. Flynn, Physics of Acoustic Cavitation in Liquids. An objective and possibly rather too lengthy discussion of the physical phenomenon of cavitation which is not yet completely clarified.

Chapter 10. W. P. Mason, Semiconductor Transducers — General Considerations. The first clear survey on the application of semiconductors as electromechanical transducers.

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Chapter 12. M. E. Sikorski, Use of $p - n$ Junction Semiconductor Transducers in Pressure and Strain Measurements. Describes in detail the efforts of the author and others to elaborate a completely modern semiconductor transducer for pressure measurements.

Chapter 13. D. L. White, The Depletion Layer and Other High-Frequency Transducers Using Fundamental Modes. Suitability of layer semiconductors for the production of hypersonic frequencies.

Chapter 14. E. Eisner, The Design of Resonant Vibrators. A quite short treatise (10 pp) on a special method of amplitude-transformation.

Both parts are completed by separate indices of authors and subject. The books are well produced and typographically excellent.

T. Tarnóczy

J. R. Frederick: **Ultrasonic Engineering**

J. Wiley & Sons, New York, 1965. 379 pp.

Ultrasonics is a modern branch of acoustics. Scientific research was begun in the twenties of this century and by the end of the World War II actually all basic phenomena had been investigated. After the war technical and medical applications were being realized. In many fields ultrasonic technology proved to be the best or unique solution of some problems in measuring techniques, biology or medicine. There are some cases yet where the application of ultrasounds has proved to be less successful and less economical than other ways of processing.

So an objective opinion about a new branch of engineering — ultrasonic technology — arose at the beginning of the sixties. It can be stated that though American scientists did not take part in research until relatively recently (mainly only in the last 20...25 years) and medical experiments were forbidden in the USA for some time, yet in aspects of technology they joined forces with European development. In some respects, such as industrial production and application of cleaning equipments and ultrasonic brain operations the European level has even been surpassed.

Thus, many summarizing books — written by European and American authors — have been published in the last five years. This book by **Frederick** is intended for engineering purposes and introduces a minimum of basic theoretical considerations and no mathematics at all. The layout is based on the results of the scientific literature from 1948 to 1962 and recent experiences of technology. The following enumeration of the 9 chapters also shows that efforts were made to summarize each of the fields where ultrasounds are applied in practice.

The chapters are:

1. Introduction 11 pp.
2. Basic Principles of Acoustics 32 pp.
3. Introduction to Ultrasonic Processing 8 pp.
4. Ultrasonic Transducers for Industrial Processing 73 pp.
5. Application of Ultrasonics to Processing 73 pp.
6. Uses of Ultrasonics in Measurement and Control 47 pp.
7. Flaw Detection 65 pp.
8. Applications of Ultrasonics to Biology 10 pp.
9. Medical Ultrasonics 43 pp.

The subject matter of Chapters 4 and 5 is treated very thoroughly; a good summary is given in Chapter 7; but Chapter 8 seems to be rather short. Unfortunately, this book, like almost all other American books, is found to be lacking in references except those in the English language. This is the more regrettable in ultrasonic technology as in this scientific field the non-English literature is more important both qualitatively and quantitatively. Only "Soviet Physics: Acoustics" and "Soviet Physics: Doklady", which are translated into English, are referred to, but these do not give a complete survey of the abundant Western and Eastern European (German, French, Russian etc.) literature of the last 10 years. So it may often occur that a certain paper of any author — quoted by chance — is not his most important work nor does it contain his most recent results.

Apart from these weaknesses the publication of such interesting new industrial techniques (as applied to cleaning, welding, etc.) — which until now were not widely known must be acknowledged and appreciated. The method of treatment is clear and easy to understand both for engineers and also for students.

T. Tarnóczy

T. S. Littler: The Physics of the Ear

Pergamon Press, Oxford, 1965 (International Series of Monographs on Physics. Vol. 3.) 378 pp.

It is by no means merely an accident that this well-known firm of Publishers has included a psychoacoustical book as the third in this Series of Monographs. The close connections between acoustics, information theory and telecommunication techniques have led to profound interest in acoustical research. Within the field of physics, acoustics is much more important today than it was 30 years ago, and it represents 8—10% of the whole of the international scientific literature of physics and of those who are occupied in research work and engineering.

In addition to the increasing importance of the whole scientific field of acoustics some internal adjustment is to be observed concerning the interest shown in research on specific problems. A survey of the acoustical literature of the last 5 years (some 5000 papers) shows that about 30% of the total material belongs to psychoacoustics and of this at least two-thirds deals with hearing research. General works used to appear, therefore, again and again particularly to summarize new results.

The present book by **Littler** is such a general work and was destined primarily to supplement obsolescent university text books. In accordance with the purpose of the book the author demonstrates the physical principles of the hearing mechanism by experimental results. Great importance is attached to the exact analysis of experimental conditions and the results of various authors are compared in an instructive manner. Practical applications of theoretical and experimental results (hearing protection, communication techniques) are also mentioned.

Contents of the book:

- I Anatomy and Physiology of the Ear
- II The Nature of Nerve Conduction
- III The Conductive Mechanism
- IV The Analytical Mechanism: its Dynamics by Direct Observations
- V Electrical Activity of the Auditory System
- VI The Dynamics of the Ear as Deduced from Electrical Observations
- VII Sensitivity Range of the Ear: Objective and Subjective Investigations
- VIII Physical Characteristics of Speech
- IX Binaural Hearing
- X Music
- XI Audiometry
- XII Auditory Adaptation and Fatigue
- XIII Defects of Hearing and Their Measurements
- XIV The Alleviation of Deafness
- XV Theory of Hearing

The book is completed by Appendices containing important physical data and mathematical apparatus. There is also a selected bibliography.

This well composed monograph brings its own results, too. The author always stresses that the hearing process in the ear consists of two parts: the first being a Fourier-type analysis occurring in the cochlea; the second a phase analysis resulting from identifications of pulse-time patterns which are in extraordinarily complicated connections with each other and are transferred by nerve pathways. Thus, the author not only has in view a new chapter of hearing theory of growing importance but also lays the foundations for an understanding of the general common mechanism of sensory nerve pathways.

An attractive feature of the book is that relations with other psycho-acoustical phenomena are not neglected. Thus, the physical characteristics of speech, binaural hearing and musical acoustics are dealt with, too. In the chapter on audiometry technical methods are also mentioned.

If any criticism can be made at all, it is that there is insufficient adaptation of recent results in the scientific literature. The references of the book — published in 1965 — are dated actually up to 1957/58. Only some sporadic later dates are to be found, the investigations (1955/56) concerning critical bands are not mentioned in the book at all, and sometimes (e.g. the physical characteristics of speech) its point of view is that of 20 years ago. This does not detract from the value of the methodological structure of the book, or from some excellent chapters summarizing the material.

Altogether, the book is a standard work that gives a clear survey of the state and results of modern hearing research and will be very profitable for physicists.

T. Tarnóczy

L. Prandtl: Führer durch die Strömungslehre

6. Auflage. Neubearbeitet und herausgegeben von K. Oswatitsch und K. Wieghardt.
Verlag von Fr. Vieweg und Sohn, Braunschweig, 1965. XII + 523. S. u. 449 Abb.

Jeder technisch oder naturwissenschaftlich Interessierte wird es mit Freude begrüssen, dass das weltberühmte Lehrbuch von Prandtl über die Strömungstheorie jetzt, völlig modernisiert, in sechster Auflage wieder vorliegt. Die Theorie ist in dem Buch von den ersten Anfängen an aufgebaut, so dass ihre Aneignung dem Studierenden keinerlei Schwierigkeiten bereitet. Doch auch sonst ist das Werk so klar und schön verfasst, dass es auch ältere, auf anderen Gebieten arbeitenden Physiker oder Ingenieure mit wirklichem Genuss lesen werden.

Das erste einleitende Kapitel handelt von den Eigenschaften der Flüssigkeiten und Gase. Das zweite bespricht die Kinematik der Flüssigkeiten und die Dynamik der reibungsfreien Flüssigkeiten. Das dritte Kapitel ist der Gasdynamik gewidmet, die entsprechend ihrer heutigen grossen Bedeutung schon hier behandelt wird. Das vierte erörtert die Bewegung der zähen Flüssigkeiten, die Turbulenz und die technischen Anwendungen. Dieser Teil wurde von

J. C. Rotta bearbeitet. Das fünfte Kapitel behandelt die konvektive Wärme- und Stoffübertragung sowie das Problem der Grenzschichten bei hochen Geschwindigkeiten. (Die letzteren zwei Kapitel besprechen die Prandtlsche Grenzschichttheorie.) Das sechste handelt von der experimentellen Technik der Aero- und Hydrodynamik. Im siebenten werden die Flugkörper, die Antriebe und die Strömungsmaschinen erörtert. Dieser Teil umfasst das grosse Lebenswerk des Verfassers (Prandtlsche Tragflügeltheorie). Ergänzt wurde dieses Kapitel von D. Küchemann und W. Dettmering. Das achte Kapitel befasst sich mit den meteorologischen Anwendungen, das neunte endlich mit verschiedenen Einzelproblemen. Bemerkt sei noch, dass die Abschnitte über Wärmeübergang, über Hochgeschwindigkeitsgrenzschichten, über das Versuchswesen und über die meteorologischen Anwendungen von H. Schuh, H. Ludwieg und E. Kleinschmidt neu verfasst wurden.

In dem Werk werden die Probleme der Bewegungen mit Überschallgeschwindigkeit ausführlich besprochen. Abschliessend findet sich auch die Ableitung der Grundgleichungen der Magnetohydrodynamik, an die sich Darlegungen über zwei Anwendungen dieser Gleichungen anschliessen. Unberücksichtigt bleiben dagegen die in hochverdünnten Gasen auftretenden Erscheinungen. Dieses Gebiet der sogenannten freien Molekülbewegung, das beim Fliegen in sehr grossen Höhen eine Rolle spielt, gehört auch tatsächlich eher in das Gebiet der kinetischen Gastheorie. Ähnliches gilt auch für die Knudsenströmung in Röhren, die ebenfalls unberücksichtigt bleibt. Das Werk enthält ausserdem sehr ausführliche Literaturhinweise, die nicht nur für den Studierenden, sondern auch für den wissenschaftlich arbeitenden Fachmann von grossem Wert sind. Ein sehr ausführliches Sachregister erleichtert die Benützung des Buches.

Es ist selbstverständlich weitgehend Sache der individuellen Beurteilung, was alles ein solches Lehrbuch enthalten soll. Der Referent könnte sich z. B. denken, dass es bei der Besprechung des Vogelfluges (Tragflügel und Luftschraube in einem Organ vereinigt) für den Studierenden interessant sein könnte, zum Vergleich den viel primitiveren Insektenflug heranzuziehen, der einem Nurpropeller-Modell oder, richtiger ausgedrückt, dem Modell zweier in entgegengesetztem Drehsinn rotierender und ineinandergeschobener Luftsschrauben entspricht. (Nur einige grosse Tagfalter bilden eine gewisse Ausnahme, weil sie auch segeln können.) Ebenso liefern die Körper der Schwärmer eines der schönsten Beispiele für das Strebenprofil. Nun kann aber ein Lehrbuch natürlich nicht alles enthalten. Das Literaturverzeichnis ergänzend möchten wir kurz bemerken, dass beide Bände der Theoretischen Hydromechanik von Kotschin, Kibel und Rose in deutscher Übersetzung vorliegen (Berlin 1954 und 1955). Ausserdem mag es selbst für deutsche Leser interessant sein, wenn wir hier erwähnen, dass die zwei anderen von Tietjens veröffentlichten Hauptwerke von Prandtl in englischer Übersetzung in einer ganz billigen »Paperbound« — Ausgabe 1957 bei Dover in New York erschienen und somit leicht zugänglich sind.

Th. Neugebauer

I. Ye. Irodov: **A Collection of Problems in Atomic and Nuclear Physics**

(Edited by S. Doniach) Pergamon Press, Oxford, —London—Edinburgh—New York—
—Paris—Frankfurt 1966.

This edition is a translation of the second edition of I. Ye. Irodov's book entitled Sbornik zadach po atomnoi fizike, published in Moscow by Gosatomizdat. It is translated by Stevan Dedijer. About 850 problems taken from a wide field of atomic and nuclear physics are contained in this book. They are intended for students who are beginning their study of atomic and nuclear physics and for students taking physics as an ancillary subject.

The problems are arranged in 15 chapters, each of which starts with a short summary of fundamental concepts and formulae needed for the solution of the problems contained in it. There are questions on the thermodynamics of radiation, the quantum nature of light, photoelectric and Compton effect, Rutherford's scattering formula, Bohr theory of the atom, De Broglie relation and uncertainty relations, the Schrödinger equation, spectra of the alkali metals, the fine structure and natural width of spectral lines, Zeeman effect, Stern—Gerlach experiment, dia- and paramagnetism, X-ray diffraction and absorption; some questions about many electron atoms and molecules, the rotation and vibration of molecules, the Raman scattering of light, radioactivity, nuclear reactions and fission; several questions connected with the utilization of nuclear energy, and the properties of the nucleus; a few questions about elementary particles; and many questions concerning experimental methods used in atomic physics such as mass spectrometer, Wilson cloud chamber, ionization chamber, GM counter and the several particle accelerators.

The answers occupying the second half of the book are very comprehensive and include some derivations of the important theoretical formulae. At the end of the book there are several tables including work function and density of metals, ionization potentials of atoms and molecules, constants of diatomic molecules, properties of certain isotopes and the elementary particles, and the table of atomic and nuclear physics constants. This has the advantage of accustoming the student to the use of tables. At the end of the chapters there are references to textbooks dealing with the topic in greater detail. Indeed, this book will prove a useful adjunct to the standard textbooks at the introductory level.

ÉVA KISDI-KOSZÓ

INDEX

COMMUNICATIONES BREVES

RECENSIONES

Acta Phys. Hung. XXI. Fasc. 3—4, Budapest, 5. XII. 1966.

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15. XII. 1966

Index: 26.022