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L. JÁNOSSY, I. KOVÁCS, K. NAGY, A. SZALAY

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INVESTIGATIONS OF γ SPECTRA OF CERTAIN (p, γ) RESONANCES

By

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(Received 20. I. 1970)

The investigation of γ spectra of the isobaric analogue resonances gives useful information about the structure of the nuclei. Our original aim was to look for isobaric analogue resonances in (p, γ) reactions on several nuclei, and to study the systematics of their γ spectra.

Experimental

The experiments were performed with the proton beam of the 2.5 MeV Van de Graaff generator with an energy spread and calibration uncertainty of about 1 keV. The excitation functions were measured with a $3'' \times 3''$ NaJ(Tl) scintillation counter while the γ spectra were taken by a 15 cm^3 Ge(Li) detector located at 90°. The targets were evaporated on thick Ta and Au backings from natural metals, except ^{44}Ca when the target material was enriched $^{44}CaCO_3$. The thickness of the targets was about 1—2 keV, for 2 MeV protons.

$^{44}Ca(p, \gamma)^{45}Sc$

This reaction has been investigated by several authors [1, 2]. Surprisingly, the measured excitation functions did not show any striking resonance in the region of bombarding proton energy corresponding to the position of the isobar analogue of the $E_x = 1904$ keV $(3/2^-)$ state in the ^{45}Ca nucleus. From (d, p) stripping measurements [3] it is known that this level has a relatively large spectroscopic factor, namely $(2J + 1)S_n = 2.56$. This fact suggests the idea that the isobaric analogue of this level should be found in the ^{45}Sc nucleus. From the estimation of the Coulomb displacement energy, the expected position of the IAR is about 1670 keV bombarding proton energy. We have also measured the excitation function (Fig. 1) in the 1550—1750 keV proton energy region, in 2 keV steps with an overall resolution of about 3 keV. As is seen

from Fig. 1 it is very difficult to decide on the basis of intensities, which of the peaks belong to the IAR. It can be expected that the structure of the γ-spectra of the different resonances makes it possible to find out their features. So we have measured the γ-spectra on the different peaks, with a Ge(Li) detector. The results on the high energy part of the γ-spectra are summarised in Table I.

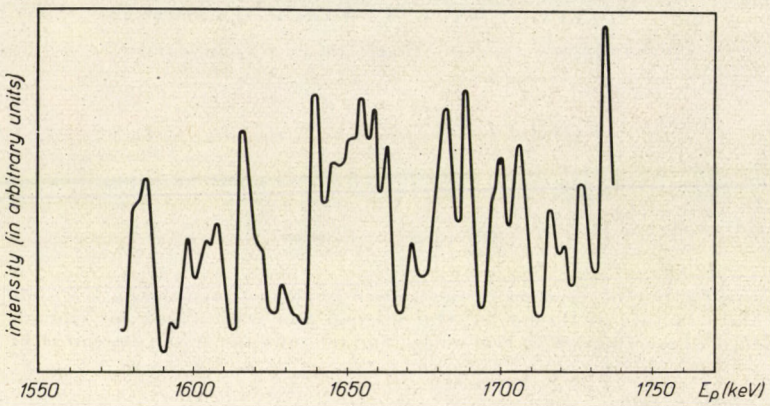

Fig. 1. The excitation function of the reaction $^{44}Ca(p, \gamma)^{45}Sc$ taken with $E_\gamma > 3.5$ MeV energy γ rays

The N_γ/N_p relative intensities displayed on it show the characteristics of γ-transitions leading to the 376 keV $(3/2^-)$ second excited state of the ^{45}Sc. At $E_p = 1640$, 1650, and 1658 keV resonances there are relatively strong transitions to this level in comparison with the $E_p = 1583$ and 1619 keV resonances.

Table I

γ yields from the reaction $^{44}Ca(p, \gamma)^{45}Sc$
N_γ/N_p in 10^{-12} units

^{45}Sc E_x	E_p keV / J^π	1583	1619	1640	1650	1658	1757
0	$7/2^-$	5	13	14	21	9	20
12	$3/2^+$	5	39	—	—	18	20
376	$3/2^-$	7	14	36	36	31	22
541		12	9	—	—	—	—
719		—	—	34	22	3	—
940	$1/2^+$	—	24	—	—	—	—
973		—	23	—	—	—	11
1065		—	27	—	—	—	—

After the appearance of [4] it became certain that the resonances found at $E_p = 1640$, 1650 and 1658 keV are the fine structure members of the isobaric analogue of the $3/2^-$ level in ^{45}Ca. On the basis of this work it was possible to evaluate the radiation width at $E_p = 1640$ keV for some of the transitions.

$$\Gamma_{\gamma_0}^{1640\text{ keV}} = 0.06 \pm 0.02 \text{ eV} \quad \text{and} \quad \Gamma_{\gamma\,376\text{ keV}}^{1640\text{ keV}} = 0.15 \pm 0.05 \text{ eV}$$

were obtained. The Weisskopf estimations for these transitions are $\Gamma_{\gamma_0}(\text{E2}) = 0.1$ eV and $\Gamma_{\gamma\,376\text{ keV}}$ (M1) = 1.63 eV. However, the strength of the γ transition leading to the 376 keV level is only of the order 0.1 Weisskopf unit; its relative large intensity at the members of IAR in comparison with the other resonances suggests that the 376 keV level in ^{45}Sc may be a member of the fragmented anti-analogue state. ENDT has called attention to this type of M1 γ transitions [5] in the s—d shell, where these transitions between the analogue and anti-analogue are very intensive and can be assumed to be pure single particle transitions. In the heavier nuclei e.g. in the $f_{7/2}$ shell it can be expected that the strength of the anti-analogue state is fragmented. So the M1 transition strength will be distributed over the fragments. More detailed investigations of γ spectra of better statistics would be necessary to determine the whole fragmentation pattern of the anti-analogue state.

$^{48}Ti(p, \gamma)^{49}V$

The reaction has also been measured [6, 7] recently. Detailed measurements were made at $E_p = 1007$, 1013 keV and 1362 keV resonances. From these experiments it turned out that the referred resonances are the isobaric analogues of the 1384 keV ($3/2^-$) and 1724 keV ($1/2^-$) states in ^{49}Ti.

The aim of this work was to extend the investigated region of excitation function to higher bombarding energies. We have measured the excitation function between 1320 keV—2140 keV proton energy in 2 keV steps, including γ rays above 3.5 MeV energy. Fig. 2 shows the excitation function. There are 85 resonances. Some of them are of remarkably higher intensity than the average. The $E_p = 1362$ keV, 1925 keV and 2077 keV are supposed to be isobaric analogues. It is striking that in the bombarding energy region between 1400 keV and 1900 keV there is an intensive resonance at $E_p = 1566$ keV. In the corresponding energy region there is no known level in the ^{49}Ti parent nucleus. We have measured the γ spectra of the resonances at $E_p = 1566$ keV, 1579 keV and $E_p = 1392$ keV. The γ yields for the high energy transitions are collected in Table II. It can be seen from the Table that in the case of the 1566 keV resonance there is a very strong transition to the 753 keV level in contrast to the investigated analogue resonances. It is known from [8] that the 753 keV level in ^{49}V is a $d_{3/2}$ hole state. This may suggest that the $E_p =$

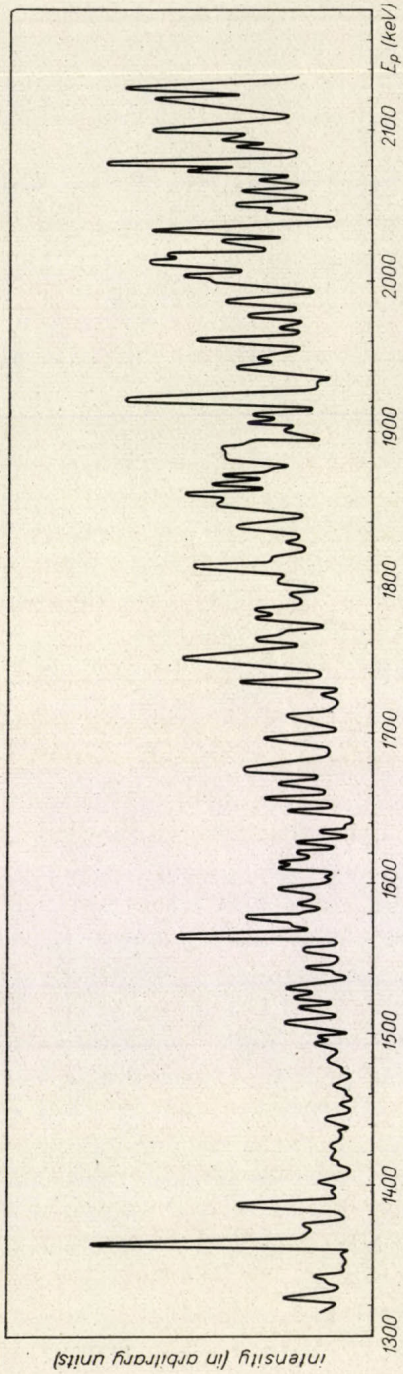

Fig. 2. The excitation function of the reaction $^{48}Ti(p, \gamma)^{49}V$ taken with $E_\gamma > 3.5$ MeV energy γ rays

Table II

γ yields from the reaction $^{48}Ti(p, \gamma)^{49}V$ N_γ/N_p in 10^{-12} units

^{49}V E_x	E_p keV / J^π	1392	1566	1579
0	$7/2^-$	3	20	20
90	$5/2^-$	6	6	32
153	$3/2^-$	47	27	11
753	$3/2^+$	21	126	18
1139	$7/2^-$	18	61	35
1639	$1/2^+$	14	25	—

= 1566 keV resonance has a similar configuration. So one could assume that this resonance may be an isobaric analogue resonance as well, but its parent state according to its peculiar structure cannot be excited in (d, p) reaction. If it exists at all it can be found in proton pick-up reaction e.g. $^{50}V(d, ^3He)^{49}Ti$.

The γ spectra of the 1392 keV and 1579 keV resonances do not show any characteristic feature to give any indication of their origin.

$^{51}V(p, \gamma)^{52}Cr$

This reaction was studied by TERANISHI and FURUBAYASHI [9, 10, 11]. They measured the excitation function in $E_p = 0.7$—2.6 MeV bombarding energy range and identified 13 resonances as isobaric analogues of the low lying levels of ^{52}V nucleus. The identification was made only on the basis of resonance energies.

Our aim was to study the γ spectra and some angular distributions at certain resonances, to obtain further evidence concerning their origin. Resonances at $E_p = 1217$; 1559; 1568; 1629 and 2333 keV were studied. The results of the evaluation of the γ spectra are summarized in Table III. The results of recent investigations [12, 13] on the level structure of ^{52}Cr differ somewhat from earlier ones [14]. The present work is in a good agreement with the results of [12, 13]. As is seen from Table III the structure of γ spectra of 1559 keV and 1568 keV resonances are very different. These resonances have been assumed to be fine structure splitting. Since the γ spectra themselves cannot give sufficient information about this question, it seemed necessary to make angular distribution measurements. The angular distribution of γ transition leading to 1.434 MeV(2^+) excited state gives the following A_2 values assuming that the transitions are of E2 + M1 type:

$$E_p = 1559 \text{ keV}; \qquad A_2 = +0.19 \pm 0.06;$$
$$E_p = 1568 \text{ keV}; \qquad A_2 = +0.09 \pm 0.05.$$

Table III

Final state energies and widths of γ-transitions of $^{51}V(p, \gamma)^{52}Cr$ reaction

Katsanos, Huizenga [12]		Macgregor, Brown [13]	$E_p = 1217$ keV 2+		$E_p = 1559$ keV 3+		$E_p = 1568$ keV 3+		$E_p = 1629$ keV 4+		$E_p = 2333$ keV 4+	
E_x MeV		E_x MeV	E_x MeV	Γ_γ eV	E_x MeV	Γ_γ eV	E_x MeV	$\Gamma_\gamma\Gamma_p/\Gamma_t$ eV	E_x MeV	$\Gamma_\gamma\Gamma_p/\Gamma_t$ eV	E_x MeV	$\Gamma_\gamma\Gamma_p/\Gamma_t$ eV
1.434	2+	1.437	1.434	0.23	1.434	0.085	1.434	0.23	1.434	0.026	1.434?	0.007
2.371	4+	2.372	2.368	0.054	2.369	0.16	2.370	0.35	2.366	0.15	2.369	0.12
2.650	0+	2.650										
2.767	4+	2.768			2.765	0.2	2.767	0.095	2.765	0.04	2.766?	0.015
2.965	2+	2.964			2.965	0.013	2.965	0.07	2.966	0.013	2.965?	0.015
3.114	6+	3.119					3.114?	0.02	3.115?	0.01		
3.163	2+	3.162	3.165	0.03			3.163	0.13	3.162?	0.01		
3.416		3.413			3.412	0.14	3.414	0.042	3.409	0.053	3.418	0.04
3.472		3.470			3.469	0.08	3.473	0.078	3.471	0.026	3.467	0.03
3.619	5+	3.617					3.622	0.025	3.615	0.026	3.615	0.07
3.772	2+	3.772	3.762	0.01								
3.947		3.944	3.927?	0.01	3.947	0.02	3.949	0.02	3.943	0.03	3.945	0.02
4.016		4.013	3.986?	0.01	4.022	0.008	4.018	0.02	4.013	0.04		
4.040		4.038	4.023?	0.01	4.037	0.012	4.044?	0.01	4.037	0.042		
4.563		4.563										
4.630		4.630			4.630	0.08	4.630	0.02	4.630	0.062	4.630	0.04
4.706		4.706									4.704?	0.015
4.743		4.741	4.731	0.024			4.743?	0.014	4.738	0.01	4.740?	0.015
4.808		4.807										
4.837		4.838			4.838	0.024	4.841	0.048	4.831	0.01		

These values are not contradictory to the assumption that both the resonances have 3^+ spin and parity.

Returning to the discussion of the γ spectra, it is interesting that ground state transition cannot be found even in the case of the 2^+ resonance. No γ transitions were observed to the 2.650 keV (0^+) excited level either. This latter fact can be explained by the $2p$—$2h$ character of this level [15]. Furthermore, in most of the γ spectra the levels of $J^\pi = 2^+, 4^+$ dominated by the configuration of seniority $v = 2$ are preferred to those dominated by $v = 4$.

$^{59}Co(p, \gamma)^{60}Ni$

Earlier, BUTLER and GOSSET have dealt with this reaction and, recently, ARAI and MIESSNER [16, 17] have also measured the excitation function, between 1.5 MeV and 2.3 MeV. They [17] claimed to have found the isobaric analogues on the bases of the positions of the resonances. The two published excitation functions are very different.

We have also repeated this measurement and we have taken the excitation function in the $E_p = 1.3$ MeV—2.5 MeV region in 1 keV steps. Our result was very similar to that of [16] and contradictory to [17], even if we averaged our excitation function over 5 and 10 keV. There were no prominent resonances in this energy range which could have been concerned as isobaric analogue resonances. There were in the excitation function, however, relatively intensive

Table IV

γ yields from the reaction ^{59}Co(p, γ)^{60}Ni
N_γ/N_p 10^{-12} units

^{60}N E_x	$J\pi$ \ E_p keV		1537	2114	2150	2206	2448
0	0^+	—	—	—	—	—	—
1332	2^+	3.3	2.8	5.8	5.3	5.0	3.9
2159	2^+	2.9	7.9	8.7	7.7	3.0	4.0
2285	0^+	—	—	—	—	—	—
2505	4^+	17.9	8.6	17.3	10.5	25.0	17.7
2626	3^+	13.2	7.3	10.2	14.5	14.4	5.4
3124	2^+	6.0	6.3	13.5	9.0	33.8	12.7
3190	1^+	4.6	6.3	3.7	6.7	15.9	3.1
3269		2.0	2.5	3.0	13.4	3.0	—
3390		—	2.3	—	—	—	—
3618		3.6	2.2	4.5	1.6	6.6	5.5
3671		3.8	1.7	2.6	4.4	15.4	18.7
3732		1.0	2.1	4.3	5.2	7.1	17.0

peaks which seemed to be interesting to investigate. Therefore, we have measured the γ spectra on certain resonances to look for systematics in their structure. Table IV shows the strength of the primary transitions. The main features of the spectra are the following: there is no ground state transition from any of the resonances; nor is the second 0^+ state at 2285 keV populated at all. The states at 2.505 MeV and 2.624 MeV excitation energy in ^{60}Ni are relatively strongly populated in the decay of every resonance. These levels were found in proton and neutron transfer reactions and proton and deuteron scattering as well [18, 19, 20]. This fact refers to the complicated structure of these final states, so the transitions cannot give any information about the structure of the initial states. On the other hand, the resonance at $E_p = 2448$ keV bombarding proton energy shows appreciably strong transitions to final states above 3.5 MeV, too. It is well known from [18] that these levels are of a relatively simple $1p$—$1h$ character. Therefore, the strength of the above mentioned transitions might indicate that a similar simple component exists in this resonance. Furthermore, its position corresponds within the limits of the Coulomb-energy estimation to the position of the isobaric analogue of the 1006 keV level in ^{60}Co; this level seems to be of relatively simple structure from (*dp*) spectroscopic data [21]. Summing up, one can suppose that the 2448 keV resonance may be the isobaric analogue of the 1006 keV level of the ^{60}Co. The certain identification of this resonance as an isobaric analogue seems to be very difficult because the spin assignment of the parent state is not known yet.

It can be seen from these experiments that more detailed investigations could give very important information about the nature of isobaric analogues and about the nuclear structure. The measurements described above must be taken as preliminary results.

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ИССЛЕДОВАНИЕ γ-СПЕКТРА НЕКОТОРЫХ (p, γ) РЕЗОНАНСОВ

И. ДЕМЕТЕР, И. ФОДОР, Л. КЕСТХЕИ, И. СЕНТПЕТЕРИ, Й. СЮЧ, З. СЁКЕФАЛВИ-НАДЬ, Л. ВАРГА, Й. ЗИМАНИ, Г. У. ГЕРШ и В. РУДОЛЬФ

Р е з ю м е

Исследование γ-спектра изобарных аналоговых резонансов дает полезные информации о структуре ядер. Наша цель была найти изобарные аналоговые резонансы в реакциях (p, γ) в случае некоторых ядер и изучать систематику их γ-спектра.

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A SIMPLE THOMAS—FERMI MODEL FOR NUCLEI WITH DIFFERENT PROTON AND NEUTRON NUMBER

By

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(Received 24. II. 1970)

Starting from realistic two-body potentials, and using the results of nuclear many body calculations for infinite nuclei, a modified Thomas—Fermi theory is developed for nuclei with different proton and neutron number. Coupled non-linear integral equations are deduced to determine the proton and neutron density distributions separately. The method is applied for a simplified case with rectangular density distribution. The range of neutron and proton density distributions turns out to be equal.

I. Introduction

The Thomas—Fermi theory has been used for a long time to determine the properties of finite nuclei. The original simple methods [1] consisted of expressing the energy of finite nuclei as a function of the density, and its derivatives. Minimizing the total energy as the function of the density, we can determine the equilibrium density distributions and some overall properties of large finite nuclei.

In recent years the Thomas—Fermi theory of large nuclei has been further developed by BETHE [2]. Starting from realistic nuclear forces, and using the results of the nuclear many-body approximations applied for infinite nuclear matter, it was found that the local density approximation of BRUECKNER et al. [3] is valid, with certain corrections. The theory was applied for semi-infinite [4] and finite [5] nuclei, and the results for surface energy and surface thickness were in good agreement with the experimental values.

In the previous calculations the theory was applied for nuclei with equal neutron and proton number, and the Coulomb energy was neglected. In the present article we intend to extend the previous theory for realistic heavy nuclei with different neutron and proton number, and to include the Coulomb energy in the calculations. We shall apply the theory for a special simplified case with rectangular proton and neutron distributions, and consider the qualitative properties of the results. The more exact solutions will be published in a following article [6].

II. The extended Thomas—Fermi theory

The extended Thomas—Fermi theory for the $N = Z$ case can be found in previous articles [2, 4, 7, 8]. The same method can be applied for nuclei with $N \neq Z$, with some modifications.

The energy of a system with N neutrons and Z protons can be written in first order BRUECKNER approximation as

$$W = \sum_m \langle \Phi_m | T | \Phi_m \rangle + \frac{1}{2} \sum_{m=0}^{k_N} \sum_{n=0}^{k_N} \langle \Phi_m \Phi_n | G_{NN}(k_N k_p) | \Phi_m \Phi_n \rangle +$$
$$+ \frac{1}{2} \sum_{m=0}^{k_P} \sum_{n=0}^{k_P} \langle \Phi_m \Phi_n | G_{PP}(k_N k_P) | \Phi_m \Phi_n \rangle + \tag{2,1}$$
$$+ \sum_{m=0}^{k_N} \sum_{n=0}^{k_P} \langle \Phi_m \Phi_n | G_{NP}(k_N k_P) | \Phi_m \Phi_n \rangle + \frac{1}{2} \sum_{m=0}^{k_P} \sum_{n=0}^{k_P} \langle \Phi_m \Phi_n | V_c | \Phi_m \Phi_n \rangle ,$$

where V_C is the Coulomb interaction and G_{NN}, G_{NP} and G_{PP} are the neutron-neutron, neutron—proton and proton—proton interaction contributions to the G matrix, respectively:

$$G_{PP}(k_N k_P) = \sum_{sm_s} G(sm_s ,\ T = 1, T_3 = -1;\ k_N k_P) ,$$
$$G_{NP}(k_N k_P) = \frac{1}{2} \sum_{sm_s} [G(sm_s , T = 1, T_3 = 0;\ k_N k_P) +$$
$$+ G(sm_s, T = 0 , T_3 = 0;\ k_N k_P)] , \tag{2.2}$$
$$G_{NN}(k_N k_P) = \sum_{sm_s} G(sm_s, T = 1,\ T_3 = 1;\ k_N k_P) ,$$

where k_N is the neutron, k_P the proton Fermi momenta, s, m_s is the spin and its third component. T, T_3 the isospin and its third component, and the $|\Phi_m \Phi_n >$ are the finite unperturbed single-particle wave functions. G satisfies the usual matrix equation:

$$\langle \Phi_{m'} \Phi_{n'} | G | \Phi_m \Phi_n \rangle = \langle \Phi_{m'} \Phi_{n'} | v | \Phi_m \Phi_n \rangle - \tag{2,3}$$
$$- \sum_{ab} \langle \Phi_m \Phi_{n'} | v | \Phi_a \Phi_b \rangle \frac{Q(ab)}{E(a) + E(b) - E(m) - E(n)} \langle \Phi_a \Phi_b | G | \Phi_m \Phi_n \rangle ,$$

where v is the realistic two-body potential, Q is the Pauli operator and the E are the single particle and hole energies. BETHE has shown in his paper [2], that we can separate the G matrix elements into a local and a non-local part, where the non-local part includes the long range central and the density

dependent effective long range tensor forces. The local part of the matrix elements can be determined from the nuclear matter calculations, including, however, the corrections arising from the fact that in Eq. (2, 3) the single hole energies are those for finite nuclei, not for an infinite system, as in the case of the matrix elements of nuclear matter. Taking into account all these considerations, the (2, 3) matrix elements can be written as (see Eq. (2, 11), [7]):

$$\begin{aligned}&\langle \Phi_m \Phi_n | G_F | \Phi_m \Phi_n \rangle \sim \langle \Phi_m \Phi_n | v_l | \Phi_m \Phi_n \rangle - \\ &- \langle mn | v_l | mn \rangle + \langle mn | G_{NM} | mn \rangle - 2\Delta U \langle \xi_{mn} | \xi_{mn} \rangle\end{aligned} \tag{2,4}$$

where v_l is the long range part of the nuclear forces, G_{NM} is the nuclear matter G matrix, G_F the finite one,

$$\xi_{mn} = |mn> - \psi_{mn} = \frac{Q}{e} G_{NM} |mn> \tag{2,5}$$

is the deviation wave function for nuclear matter, and ΔU is the difference between infinite and finite single hole energies. ΔU can be considered momentum independent with good approximation, as BETHE has shown [2]. With the above (2,4) approximation the energy of a system with equal numbers of protons and neutrons can be written in the Thomas—Fermi approximation as

$$\begin{aligned}W = &\int W_{NM}(\varrho(r))\, d^3 r + \frac{1}{2}\int v_l^D(r\varrho)\,[\varrho(r_1)\,\varrho(r_2) - \varrho(r_1)^2]\, d^3 r_1\, d^3 r_2 + \\ &+ \frac{1}{2}\int v_l^x(r\varrho)\,[|\varrho(r_1 r_2)|_F^2 - |\varrho(r_1 r_2)|_{NM}^2]\, d^3 r_1\, d^3 r_2 - \\ &- \int \Delta U(r)\,\tau(r)\, d^3 r + W_c\,,\end{aligned} \tag{2,6}$$

where

$$\tau(r) = \sum_{nm} \int d^3 r' |\xi_{mn}(r')|^2\,, \tag{2,7}$$

W_{NM} is the nuclear matter energy as a function of the density, W_C the Coulomb energy, and v_l^D and v_l^x are those parts of the nuclear forces which give a direct and an exchange term, respectively.

If we accept the result of BETHE [2] and NÉMETH and BETHE [4], that the exchange term is, in good approximation, a local one, then the finite and infinite exchange terms cancel each other in [2,6].

If the proton and neutron numbers are not equal, the total energy of the system can be written as

$$W = \int W_{NM}(\varrho_N, \varrho_P) d^3r + 1/2 \int V_1(r_1 \varrho_N) [\varrho_N(r_1) \varrho_N(r_2) - \varrho_N(r_1)^2] d^2 r_1 d^3 r_2 +$$
$$+ \frac{1}{2} \int V_1(r, \varrho_P) [\varrho_P(r_1) \varrho_P(r_2) - \varrho_P(r_1)^2] d^3 r_1 d^3 r_2 +$$
$$+ \int V_2(r, \varrho_N, \varrho_P) [\varrho_N(r_1) \varrho_P(r_2) - \varrho_N(r_1) \varrho_P(r_1)] d^3 r_1 d^3 r_2 + \tag{2,8}$$
$$+ \frac{1}{2} e^2 \int \frac{\varrho_P(r_1) \varrho_P(r_2)}{|r_1 - r_2|} d^3 r_1 d^3 r_2 - \int [\Delta U_N(r) \tau_N(r) + \Delta U_P(r) \tau U_P(r)] d^3 r,$$

where

$$\tau_N = \tau_{NN} + \tau_{NP}, \qquad \tau_P = \tau_{PP} + \tau_{NP}, \tag{2,9}$$

$$\tau_{NN} = \frac{1}{\Omega} \sum_{m=0}^{k_N} \sum_{n=0}^{k_N} \int d^3 r' |\xi_{NM}(r', r, |k_n - k_m|)|^2,$$
$$\tau_{NP} = \frac{1}{\Omega} \sum_{m=0}^{k_N} \sum_{n=0}^{k_P} \int d^3 r' |\xi_{NP}(r', r, |k_n - k_m|)|^2, \tag{2,10}$$

and $V_1(r, \varrho_N)$ is the neutron—neutron, $V_1(r, \varrho_P)$ the proton—proton and $V_2(r, \varrho_N, \varrho_P)$ the neutron—proton effective long range interaction occurring in the direct term. Knowing the ϱ dependence of W_{NM}, τ_N, τ_P and of the effective forces, we have expressed the total energy of the system as a function of the neutron and proton density. Minimizing W according to ϱ_N and ϱ_P, we can determine these functions, and the total energy of the nucleus.

III. Density dependence of the different terms in the energy

a) Nuclear matter energy

The calculations of SPRUNG [9] and BETHE and NÉMETH [10] have shown that the nuclear matter G matrix elements can be written as:

$$G_{PP}(k) = 4a_1 + 4b_1 k/k_F,$$
$$G_{NN}(k) = 4a_2 + 4b_2 k/k_F, \tag{3,1}$$
$$G_{NP}(k) = 2(a_3 + \alpha) + 2(b_3 + \beta) k/k_F,$$

where a and b are the $T = 1$ interaction contributions and α and β are the $T = 0$ ones to the G matrix. In the $0.1\varrho_0 - 2\varrho_0$ density domain, where ϱ_0 is the nuclear matter equilibrium density, a, b, α and β can be represented with the following curves in MeV units [10]:

$$a = -1/y - 1.13 - 1.07y + 0.25\,y^2,$$
$$b = (0.16 + 1.05y + 0.36y^2)k_F/y, \qquad (3,2)$$
$$\alpha = -8.26/y - 0.51 - 2.61y + 1.1y^2,$$
$$\beta = (1.66 + 5.04y - 0.27y^2)k_F/y,$$

where

$$y = \begin{cases} k_N \\ k_F \\ k_P \end{cases} \qquad \text{for} \qquad T_3 = \begin{cases} 1 \\ 0 \\ -1\,. \end{cases} \qquad (3,3)$$

With the help of (3,1) we can determine the total energy of the infinite system at a given density. Since the nuclear matter calculations give too little binding, we multiply the potential energy by a factor 1.22 to get the correct infinite nuclear matter binding energy for the $N = Z$ case. The total energy after this correction is:

$$W_{NM} = \frac{c}{2}\varrho_0^2[\hat{\varrho}_N^2(1.62/\hat{\varrho}_N^{1/3} - 0.88 - 0.62\hat{\varrho}_N^{1/3} + 0.72\hat{\varrho}_N^{2/3}) +$$
$$+ \hat{\varrho}_P^2(1{,}62/\hat{\varrho}_P^{1/3} - 0{,}88 - 0{,}62\,\hat{\varrho}_P^{1/3} + 0{,}72\,\hat{\varrho}_P^{2/3}) + \qquad (3,4)$$
$$+ \hat{\varrho}_N\hat{\varrho}_P(-5{,}55/\hat{\varrho}^{1/3} - 0{,}60 - 0{,}65\,\hat{\varrho}^{1/3} + 2{,}30\,\hat{\varrho}^{2/3})],$$

where $\hat{\varrho} = \varrho/\varrho_0$, and

$$\varrho_0 = 0.1855\ \text{fm}^{-3}. \qquad (3,5)$$

b) Effective long range forces

We have to deduce the effective $v_l(r\varrho)$ long range forces from realistic two-nucleon potentials. As a starting point we shall use the soft core REID potentials [11]. For even singulet forces we accept the ^1S force and for odd singulet forces the ^1P force. Since the nuclear matter calculations have shown that the ^3P state contribution to the nuclear matter energy is negligible for every density, we take the form of the triplet odd forces as the sum of the one-pion exchange potential and a term as Ae^{-3x}/x, where A is determined from the requirement that the total ^3P energy should be zero, just as in [4]. The effective force has been determined from the nuclear matter calculations of SIEMENS [12] in [7] as a density dependent expression, and we can take into account the effect of the ^1D—^1S forces acting only in the d-state as a density dependent force, acting in every even state.

Taking into account all the above considerations, the effective forces acting in the different states are given in Eqs. (3,2)—(3,7) of [7]. The direct

contribution of the $T = 1$ forces can be written as

$$\frac{1}{4}\left[{}^1\text{Even} + 3 \cdot {}^3\text{Odd} + ({}^1D - {}^1S)_{\text{eff}}\right], \tag{3,6a}$$

and that of the $T = 0$ forces

$$\frac{3}{4}\left[{}^3\text{Even} + \frac{1}{3}\,{}^1\text{Odd} + ({}^3D - {}^3S)_{\text{eff}}\right]. \tag{3,6b}$$

As a result, the density dependent effective long range forces can be written as:

$$\begin{aligned} v^D_{\substack{NN\\PP}} = \frac{1}{4x}\{[&-7.501e^{-2x} - 228.72e^{-3x} - 1928.8e^{-4x} + \\ &+ 908.4e^{-6x} + 5768.2e^{-7x}] - k^2_{\substack{N\\P}}(R)\,[-3.762e^{-2x} + \\ &+ 91.51e^{-3x} - 458.84e^{-4x} + 2917.8e^{-6x} - 3561e^{-7x}]\} = \\ &= v_1(r) - \varrho_{\substack{N\\P}}(R)^{2/3}\, v_2(r)\,, \end{aligned} \tag{3,7a}$$

$$\begin{aligned} v^D_{NP} = \frac{1}{4x}\{[&-284.523e^{-2x} + 2542.81e^{-3x} - 15\,002.93e^{-4x} + \\ &+ 70\,584.96e^{-6x} - 66\,399.1e^{-7x}] - k_N(R)\,k_P(R)[-0.86e^{-2x} + \\ &+ 467.463e^{-3x} - 4353.4e^{-7x} + 43\,000.9e^{-6x} - 60\,939.3e^{-7x}]\} = \\ &= v_3(r) - \varrho_N(R)^{1/3}\,\varrho_P(R)^{1/3}\, v_4(r)\,, \end{aligned} \tag{3,7b}$$

where

$$x = \mu r, \qquad \mu = 0.7 fm^{-1}. \tag{3,8}$$

The effective long range forces are no longer central forces, because of the tensor forces. It does not make much difference if instead of $\varrho^{2/3}(R)$ we use rather $\varrho(r_1)^{1/3}\varrho(r_2)^{1/3}$, and the calculations are much easier, so in the following we shall use this approximation.

c) Determination of τ

The derivation wave function as a function of the relative momenta has been calculated by SIEMENS [12] for nuclear matter at different densities. His data can be approximated in the important density domain with a polynomial:

$$W_{NN}(k) = \int |\xi_{NN}(r')|^2 \, d^3 r' = a(\varrho_N) + b(\varrho_N) k + c(\varrho_N) k^2 + d(\varrho_N) k^3$$
$$W_{NP}(k) = \int |\xi_{NP}(r')|^2 \, d^3 r' = \alpha(\varrho_N, \varrho_P) + \tag{3,9}$$
$$+ \beta(\varrho_N, \varrho_P) k + \gamma(\varrho_N, \varrho_P) k^2 + \delta(\varrho_N, \varrho_P) k^3 .$$

From (3,9) τ can be determined by integration over k:

$$\tau_N = \sum_{m=0}^{k_N} \sum_{n=0}^{k_N} W_{NN} |(k_n - k_m)|^2 + \sum_{m=0}^{k_N} \sum_{n=0}^{k_P} W_{NP}(|k_n - k_m|) =$$
$$= \frac{1}{18\pi^4} [0{,}7\, k_N^5 + 5\, k_N^2 k_P^2] = B \varrho_N^{5/3} + C \varrho_N^{2/3} \varrho_N^{2/3},$$
$$\tau_P = \sum_{m=0}^{k_P} \sum_{n=0}^{k_P} W_{PP}(|k_n - k_m|) + \sum_{m=0}^{k_N} \sum_{n=0}^{k_P} W_{NP}(|k_n - k_m|) = \tag{3,10}$$
$$= \frac{1}{18\pi^4} [0{,}7\, k_P^5 + 5\, k_N^2 k_P^2] = B \varrho_P^{5/3} + C \varrho_N^{2/3} \varrho_P^{2/3} .$$

IV. The equations determining the densities

With the results of Section III we are already able to determine the total energy of the nucleus as a function of the neutron and proton density:

$$W = \int W_{NM}(\varrho_N, \varrho_P) \, d^3 r + \frac{1}{2} \int v_1(r) [\varrho_N(r_1) \varrho_N(r_2) - \varrho_N(r_1)^2 +$$
$$+ \varrho_P(r_1) \varrho_P(r_2) - \varrho_P(r_1)^2] \, d^3 r_1 \, d^3 r_2 -$$
$$- \frac{1}{2} \int v_2(r) [\varrho_N(r_1)^{4/3} \varrho_N(r_2)^{4/3} - \varrho_N(r_1)^{8/3} + \varrho_P(r_1)^{4/3} \varrho_P(r_2)^{4/3} - \tag{4,1}$$
$$- \varrho_P(r_1)^{8/3}] \, d^3 r_1 \, d^3 r_2 + \int v_3(r) [\varrho_N(r_1) \varrho_P(r_2) - \varrho_N(r_1) \varrho_P(r_1)] \, d^3 r_1 \, d^3 r_2$$
$$+ \int v_4(r) [\varrho_N(r_1)^{7/6} \varrho_N(r_2)^{1/6} \varrho_P(r_1)^{1/6} \varrho_P(r_2)^{7/6} -$$
$$- \varrho_N(r_1)^{4/3} \varrho_P(r_1)^{4/3}] \, d^3 r_1 \, d^3 r_2 + \frac{1}{2} e^2 \int \frac{\varrho_P(r_1) \varrho_P(r_2)}{|r_1 - r_2|} d^3 r_1 \, d^3 r_2 +$$
$$- \int [\Delta U_N(r) \tau_N(r) + \Delta U_P(r) \tau_P(r)] \, d^3 r .$$

ΔU_N and ΔU_P in (4,1) are exactly the differences between the finite and infinite single particle energies of a neutron and a proton, respectively. Minimizing with the subsidiary condition

$$\int \varrho_N \, d^3 r + \int \varrho_P \, d^3 r = A, \tag{4,2}$$

we obtain the following equations:

$$E_N = \frac{\partial W}{\partial \varrho_N} = \frac{\partial W_{NM}}{\partial \varrho_N} + K_N,$$
$$E_P = \frac{\partial W}{\partial \varrho_P} = \frac{\partial W_{NM}}{\partial \varrho_P} + \frac{\partial W_c}{\partial \varrho_P} + K_P. \tag{4,3}$$

Here E_N and E_P are the Fermi energy of a neutron and a proton, respectively. From Eqs. (4,3) we can determine the ΔU:

$$\Delta U_N = K_n, \quad \Delta U_P = \frac{\partial W_c}{\partial \varrho_P} + K_P. \tag{4,4}$$

From (4,1) and (4,3), (4,4) it is clear that ΔU is the solution of an integral-differential equation. Since the last term in (4,1) is small, we can solve this equation system by iteration. In first order

$$\begin{aligned} U_N^{(1)}(r_1) = {} & \int v_1(r)\,[\varrho_N(r_2)-\varrho_N(r_1)]\,d^3r_2 - 4/3\,\varrho_N(r_1)^{1/3}\int v_2(r)[\varrho_N(r_2)^{4/3} - \\ & - \varrho_N(r_1)^{4/3}]\,d^3r_2 + \int v_3(r)\,[\varrho_P(r_2)-\varrho_P(r_1)]\,d^3r_2 - \\ & - 7/6\,\varrho_N(r_1)^{1/6}\,\varrho_P(r_1)^{1/6}\int v_4(r)\,[\varrho_N(r_2)^{1/6}\,\varrho_P(r_2)^{7/6} - \varrho_N(r_1)^{1/6}\,\varrho_P(r_1)^{7/6}]\,d^3r_2 - \\ & - 1/6\,\varrho_N(r_1)^{-5/6}\varrho_P(r_1)^{7/6}\int v_4(r)\,[\varrho_N(r_2)^{7/6}\,\varrho_P(r_2)^{1/6} - \varrho_N(r_1)^{7/6}\,\varrho_P(r_1)^{1/6}]\,d^3r_2, \end{aligned} \tag{4,5}$$

and we get a similar equation for $U_N^{(1)}(r_1)$. Substituting this first order expression back into (4,1), we get $U_N^{(2)}$ and $U_P^{(2)}$. In this way we get two coupled non-linear integral equations for ϱ_N and ϱ_P. Putting these back into (4,1), we get the total energy:

$$\begin{aligned} W = {} & \int W_{NM}(\varrho_N, \varrho_P)\,d^3r + 1/2\int v_1(r)\,[\varrho_N(r_2)-\varrho_N(r_1)][\varrho_N(r_1) - \\ & - 2B\varrho_N^{5/3}(r_1) - 2C\varrho_N(r_1)^{2/3}\,\varrho_P(r_1)^{2/3}]\,d^3r_1\,d^3r_2 + \\ & + 1/2\int v_1(r)\,[\varrho_P(r_2)-\varrho_P(r_1)][\varrho_P(r_1) - 2B\varrho_P(r_1)^{5/3} - \\ & - 2C\varrho_N(r_1)^{2/3}\,\varrho_P(r_1)^{2/3}]\,d^3r_1\,d^3r_2 - \\ & - 1/2\int v_2(r)\,[\varrho_N(r_2)^{4/3}-\varrho_N(r_1)^{4/3}]\,[\varrho_N(r_1)^{4/3} - 8/3\,B\varrho_N(r_1)^2 - \\ & - 8/3\,C\varrho_N(r_1)\,\varrho_P(r_1)^{2/3}]\,d^3r_1\,d^3r_2 - 1/2\int v_2(r)\,[\varrho_P(r_2)^{4/3} - \\ & - \varrho_P(r_1)^{4/3}]\,[\varrho_P(r_1)^{4/3} - 8/3\,B\varrho_P(r_1)^2 - 8/3\,C\varrho_P(r_1)\,\varrho_N(r_1)^{2/3}]\,d^3r_1\,d^3r_2 + \\ & + 1/2\int v_3(r)\,[\varrho_N(r_2)-\varrho_N(r_1)]\,[\varrho_P(r_1) - 2B\varrho(r_1)^{5/3} - \\ & - 2C\varrho_P(r_1)^{2/3}\,\varrho_N(r_1)^{2/3}]\,d^3r_1\,d^3r_2 + 1/2\int v_3(r)\,[\varrho_P(r_2)-\varrho_P(r_1)]\cdot \\ & \cdot\,[\varrho_N(r_1) - 2B\varrho_N(r_1)^{5/3} - 2C\varrho_N(r_1)^{2/3}\,\varrho_P(r_1)^{2/3}]\,d^3r_1\,d^3r_2 - \end{aligned}$$

$$
\begin{aligned}
&- 1/2 \int v_4(r)\,[\varrho_N(r_2)^{1/6}\,\varrho_P(r_2)^{7/6} - \varrho_N(r_1)^{1/6}\,\varrho_P(r_1)^{7/6}]\,[\varrho_N(r_1)^{7/6}\,\varrho_P(r_1)^{1/6} - \\
&- 7/3\,B\varrho_N(r_1)^{11/6}\varrho_P(r_1)^{1/6} - 7/3\,C\varrho_N(r_1)^{5/6}\varrho_P(r_1)^{5/6} - 1/3\,B\varrho_P(r_1)^{5/6}\varrho_N(r_1)^{7/6} - \\
&- 1/3\,C\varrho_P(r_1)^{-1/6}\,\varrho_N(r_1)^{11/6}]\,d^3 r_1\,d^3 r_2 - \\
&- 1/2 \int v_4(r)\,[\varrho_P(r_2)^{1/6}\,\varrho_N(r_2)^{7/6} - \varrho_P(r_1)^{1/6}\,\varrho_N(r_1)^{7/6}]\,[\varrho_P(r_1)^{7/6}\,\varrho_N(r_1)^{1/6} - \\
&- 7/3\,B\varrho_P(r_1)^{11/6}\,\varrho_N(r_1)^{1/6} - 7/3\,C\varrho_P(r_1)^{5/6}\,\varrho_N(r_1)^{5/6} - \\
&- 1/3\,B\varrho_N(r_1)^{5/6}\,\varrho_P(r_1)^{7/6} - 1/3\,C\varrho_N(r_1)^{-1/6}\,\varrho_P(r_1)^{11/6}]\,d^3 r_1\,d^3 r_2 + \\
&+ 1/2 \int \frac{\varrho_P(r_2)}{|r_1 - r_2|}\,[\varrho_P(r_1) - B\varrho_P(r_1)^{5/3} - C\varrho_N(r_1)^{2/3}\,\varrho_P(r_1)^{2/3}]\,d^3 r_1\,d^3 r_2 .
\end{aligned}
$$

Solving the equations as a function of E_N and E_P, we can determine the density distribution of nuclei with given N and Z. Since for stable nuclei the energy of the last neutron and proton is the same, $E_N = E_P$ in our calculations. From the total energy (4,1a) we can determine the effective long range two-body forces in a given nucleus:

$$
\begin{aligned}
(v^l_{NN})_{\text{eff}} = &\{v_1(r)\,[1 - B\varrho_N(r_1)^{2/3} - B\varrho_N(r_2)^{2/3} - C\varrho_P(r_1)^{1/3} - C\varrho_P(r_2)^{1/3}] - \\
&- v_2(r)\,\varrho_N(r_1)^{1/3}\,\varrho_N(r_2)^{1/3}\,[1 - 4/3\,B\varrho_N(r_1)^{2/3} - \\
&- 4/3\,B\varrho_N(r_2)^{2/3} - 4/3\,C\varrho_P(r_1)^{1/3} - 4/3\,C\varrho_P(r_2)^{1/3}]\}\left(\frac{1+P_{NM}}{2}\right),
\end{aligned}
\tag{4,6a}
$$

$$
\begin{aligned}
(v^l_{PP})_{\text{eff}} = &\, v^l_{NN}\,(\varrho_N \to \varrho_P,\, \varrho_P \to \varrho_N)_{\text{eff}} + \\
&+ \frac{e^2}{|r_1 - r_2|}\,[1 - B\varrho_P(r_1)^{2/3} - C\varrho_N(r_1)^{2/3}\,\varrho_P(r_1)^{-1/3}] ,
\end{aligned}
\tag{4,6b}
$$

$$
\begin{aligned}
(v^l_{NP})_{\text{eff}} = &\{v_3(r)\,[1 - B\varrho_N(r_1)^{2/3} - B\varrho_P(r_1)^{2/3} - C\varrho_N(r_1)^{-1/3}\,\varrho_P(r_1)^{2/3} - \\
&- C\varrho_P(r_1)^{-1/3}\,\varrho_N(r_1)^{2/3}] - v_4(r)\,\varrho_N(r_1)^{1/6}\,\varrho_P(r_1)^{1/6}\,\varrho_N(r_2)^{1/6}\,\varrho_P(r_2)^{1/6} \cdot \\
&\cdot [1 - 4/3\,B\varrho_N(r_1)^{2/3} - 4/3\,B\varrho_P(r_1)^{2/3} - 4/3\,C\varrho_N(r_1)^{-1/3}\,\varrho_P(r_1)^{2/3} - \\
&- 4/3\,C\varrho_P(r_1)^{-1/3}\,\varrho_N(r_1)^{2/3}]\}\left(\frac{1+P_{NM}}{2}\right).
\end{aligned}
\tag{4,6c}
$$

The total effective force can be written as:

$$
[v(r, \varrho)_{AB}]_{\text{eff}} = G_{AB}(\varrho)\,\delta(r) + (v^l_{AB})_{\text{eff}} , \tag{4,7}
$$

where P_{NM} is the operator projecting into nuclear matter state.

V. Rectangular density distribution model

Let us assume a simple rectangular density distribution with ϱ_N and ϱ_P heights and a and b ranges, respectively. The total energy can be written as

$$
W = W_{NM} + D + W_c - \Delta , \tag{5,1}
$$

where W_{NM} is the nuclear matter, D the surface; W_c the Coulomb energy, and Δ the correction term. The calculations were performed for three nuclei, $A = 64$, 125, 216. The results for the densities can be seen in Table I. The range of the neutron and proton distribution turned out to be the same:

Table I

Parameters of the rectangular density distribution

	ϱ in fm^{-3}	r_0 in fm	x	E_F	ϱ_c' in fm^{-3}	r_0' in fm	E_p'
$A = 64$	0.151	1.16	0.095	—8.32	0,138	1.19	—7.61
$A = 125$	0.135	1.20	0.123	—7.65	0.132	1.21	—6.14
$A = 216$	0.124	1.24	0.174	—6.92	0.122	1.24	—4.17

$$a = b = r_0 A^{1/3}, \tag{5,2}$$

where r_0 increases slightly with increasing mass number, while the central density decreases. The neutron and proton central density was written as:

$$\begin{aligned} 2\varrho_c &= \varrho_N + \varrho_P, \\ x &= \frac{\varrho_N - \varrho_P}{\varrho_N + \varrho_P}. \end{aligned} \tag{5,3}$$

The calculations were made beside the minimizing x values for the $x = 0$ case as well, to see the effect of the symmetry terms on the density distribution. E_F is the Fermi energy of the nucleons.

Table II

Energy values for rectangular density distributions in MeV

	$A = 64$		$A = 125$		$A = 216$	
	$x = 0.095$	$x = 0$	$x = 0.123$	$x = 0$	$x = 0.174$	$x = 0$
W_{NM}/A	—13.312	—13.530	—13.667	—13.961	—13.806	—14.166
D/A	5.795	5.790	5.231	5.127	5.041	4.507
W_c/A	2.037	2.547	3.308	4.270	4.333	6.255
Δ_1/A	— 1.347	— 1.338	— 1.243	— 1.231	— 1.256	— 1.103
Δ_2/A	— 0.553	— 0.629	— 0.930	— 1.062	— 1.309	— 1.574
Δ/A	— 1.900	— 1.967	— 2.173	— 2.293	— 2.565	— 2.677
D'/A	4.448	4.452	3.998	3.896	3.785	3.403
W_c'/A	1.520	1.918	2.379	3.208	3.024	4.681
W/A	— 7.344	— 7.160	— 7.300	— 6.857	— 6.997	— 6.093

The results concerning the energies are shown in Table II. It is easy to see that the energy per particle is slightly too high, which is not surprising, since the minimizing density is not the correct one. It is interesting to note that the effect of the correction term is very important. The nuclear matter energy term is much less than for an infinite system. The reason for this is that the Coulomb energy decreases the central densities, and increases the range of the distributions. The value of the Coulomb energies are the correct ones, but the surface terms are a little too big, owing to the rectangular density distributions.

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ПРОСТАЯ МОДЕЛЬ ТОМАСА-ФЕРМИ ДЛЯ ЯДЕР С РАЗЛИЧНЫМ КОЛИЧЕСТВОМ ПРОТОНОВ И НЕЙТРОНОВ

Й. НЕЙМЕТ

Р е з ю м е

Исходя из реального двухчастичного потенциала и используя результаты вычислений задачи многих тел для бесконечных ядер, выводится модифицированная теория Томаса—Ферми для ядер с различным числом протонов и нейтронов. Выведены связанные нелинейные интегральные уравнения для определения распределения плотности протонов и нейтронов в отдельности. Метод применяется в упрощенном случае прямоугольного распределения плотности. Область распределения плотности нейтронов и протонов оказывается равной.

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ON THE BREAKDOWN MECHANISM OF EXTERNAL ELECTRODE DISCHARGES AT LOW FREQUENCY

By

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The breakdown phenomena, taking place between metal plates, placed outside the discharge space under the influence of voltage at 50 cps, without an external magnetic field in the case of argon and mercury vapour, are interpreted by us through a statistical description on the basis of a theoretical model elaborated by us. The pressure of the discharge space in our experiments was carried out with argon, 2.5 mmHg, and with mercury vapour, $6 \cdot 10^{-3}$ mmHg. The distance between the external electrodes was 20 mm. The breakdown process and the current peaks following this process are interpreted.

1. Introduction

The assurance of a clean working space containing the gas or vapour to be ionized is a basic requirement both for the fusion experiments and the discharges brought about for spectroscopic purposes. Therefore, external electrode discharges are often employed, in such a way that the breakdown is capacitative. Contamination of the discharge space with the material of the electrodes can be prevented in this way.

In connection with this more treatises are known (Dawidow [1], Fridkin [2], Goldstein [3], Granowski [4], Grinberg [5], Hale [6], Hertz [7], Kapzow [8] and von Engel [9]). In the case of the model examined by Hale [6] it was presupposed that the energy necessary for ionization is taken up by the electron during the movement on the mean free path. This model was developed further by Fridkin [2] in so far that he took the collisions into account and so extended the adaptability of the model to higher pressures. Grinberg [5], Goldstein [3] and Kapzow [8] applied further refinements with the consideration of the diffusion processes by the characterization of the phenomena.

By the examination of the stationary case, von Engel and Steenbeck [9] and also Hertz [7] established an energy balance for the characterization of these discharges.

In the case of low and intermediate frequencies the discharges were characterized by Granowski [4] with the setting up of the equation characterizing the energy balance. The energy balance equation determined in this way was not used for the characterization of the breakdown process, but for

the description of the microphysical parameters of the discharge. Such a description which discusses a breakdown phenomenon of this type on the basis of the energy balance has not yet been published.

In the following, the breakdown process will be treated in the case of low frequency, taking into account the time and space dependences. The discussion will deal with argon and mercury vapours, with the determination of the energy balance.

2. Capacitive breakdown in argon

In the description of both the argon and mercury vapour processes the discharge between the copper plates of 30 mm diameter, and at 20 mm distance from each other was examined in a working space of about 14 cm^3, at 50 cps frequency. An external magnetic field was not taken into account and the argon pressure was taken as 2.5 mmHg.

The description was made with the presumption of the Maxwell—Boltzmann distribution and with the presumption that at the moment of the breakdown the average electron energy is not less than the first ionization energy characteristic for argon. We presupposed on the basis of our previous calculations that the mean random velocity of the electrons is $2 \cdot 10^8$ cm/sec. Taking the cylindric coordinate system as a starting point, we discuss by description only the changes occurring in the direction preferred by the direction of the external electric field. The number of collisions, occurring in the half period is, in our case, of 10^5 order.

For the average velocity — drift velocity — of the electrons an upper limit can be given, with the assumption of a constant electric field strength and with the application of the relation:

$$\bar{u}_d = \frac{e}{m} \frac{L}{\bar{v}} E, \tag{1}$$

where e is the charge of the electron, m is the mass of the electron, L is the mean free path of the electron, E is the potential gradient, v is the average random velocity of the electron.

The value of E was taken on the basis of our previous experiments for 0.1 e. s. u. In this case, the value of the drift velocity u_d is

$$\bar{u}_d = 7 \cdot 10^6 \text{ cm/sec}. \tag{2}$$

Because

$$\frac{u_d}{\bar{v}} = \frac{7 \cdot 10^6}{2 \cdot 10^8} < 1 \tag{3}$$

as well as the quotient of the breakdown distance D and of the mean free path L is:

$$\frac{L}{D} = \frac{3 \cdot 10^{-2}}{2} < 1 \tag{4}$$

by the division of the perturbated distribution function into a stationary and an other, by the electric field perturbated member we can apply the following extension:

$$f_e(v) = f_0(v) + \frac{u_d}{v} f_1(v) + \left(\frac{3}{2} \frac{u_d^2}{v^2} - \frac{1}{2} \right) f_2(v) \tag{5}$$

where $f_e(v)$ is the complete distribution function, $f_0(v)$ is the stationary member of the distribution function $f_e(v)$, in our case the Maxwell—Boltzmann distribution $\cos \varphi = u_d/v$, $f_1(v)$, $f_2(v)$ are the perturbated members of the complete distribution function.

As was shown by DAWIDOW [1] if we stop by the extension at f_1, we still get a very good approximation. The members of higher order were not taken into account in the following.

In our case, the expression proposed by DAWIDOW [1] was applied instead of the collision integral in the Boltzmann equation, and in accordance with our initial experiments, we do not deal with the power effect produced by the external magnetic field:

$$\frac{\partial (n_e f_0)}{\partial t} + \frac{v}{3} \nabla (n_e f_1) + \frac{1}{3} \frac{e}{m} E n_e \frac{1}{v^2} \frac{\partial}{\partial v} (v^2 f_1) - \\ - \frac{n_e}{v^2} \frac{m}{M} \frac{\partial}{\partial v} \left[\frac{v^3 k T_g}{m L(v)} \frac{\partial f_0}{\partial v} + \frac{v^4 f_0}{L(v)} \right] = 0 \tag{6}$$

$$\frac{\partial (n_e f_1)}{\partial t} + v \nabla (n_e f_0) + \frac{e}{m} E n_e \frac{\partial f_0}{\partial v} + \frac{n_e}{L(v)} f_1 = 0 \tag{7}$$

where n_e is the electron concentration, M is the mass of the neutral atom, k is the Boltzmann constant, T_g is the gas temperature, $L(v)$ is the free path of the electrons.

With the application of value $f_1(v)$ the $\bar{u}_d$ average of the drift velocity of the electrons is as follows:

$$\bar{u}_d = \frac{4\pi}{3} \int_0^\infty f_1(v)\, v^3\, dv \,. \tag{8}$$

From Eqs. (6) and (7) it is enough to take into consideration equation (7), because it was assumed previously that $f_0(v)$ is a Maxwell—Boltzmann

distribution. Taking the time dependence as a factor $e^{-i\omega t}$ into account, the value of $f_1(v)$ is as follows:

$$f_1 = -\frac{\frac{e}{m} E \frac{\partial f_0}{\partial v}}{\nu(v) - i\omega}, \tag{9}$$

where $\nu(v) = v/L(v)$ and $\nu(v)$ is the collision frequency.

Inserting the value of $f_1(v)$ from Eq. (9) in relation (8), integrating partially and presupposing that the $\nu(v)$ can be considered as changing slowly compared with stationary distribution function $f_0(v)$, for the value of $\bar{u}_d$ we obtain:

$$\bar{u}_d = \frac{e}{m} \frac{E}{\bar{\nu} - i\omega}, \tag{10}$$

where $\bar{\nu} = v_{\max}/L(v_{\max})$ and $v_{\max}$ is the maximum velocity of the stationary distribution function.

The P_1 energy, taken up by the electrons with the help of average drift velocity is as follows:

$$P_1 = \frac{e^2}{m} \frac{E^2}{\bar{\nu} - i\omega} dt. \tag{11}$$

The P_2 energy taken up by the excited atoms through secondary collisions is as follows:

$$P_2 = \bar{\nu} n_a S_a e \bar{U}_a \, dt, \tag{12}$$

where n_a is the concentration of the excited argon atoms, S_a is the cross-section of the collision energy transfer in the case of collisions of the second kind, $\bar{U}_a$ is the average excitation energy of the argon atoms.

The N_1 member of the negative energy transport, which may be attributed to elastic losses is

$$N_1 = -\frac{2m}{M} e (U_e - U_g) n_g S \sqrt{\frac{8 e U_e}{\pi m}} dt, \tag{13}$$

where U_e is the potential of electrons (energy equivalent), U_g is the potential of the gas atoms (energy equivalent), n_g is the concentration of the gas atoms, S is the elastic cross-section of collision of the electron-gas atom.

The loss which may be attributed to the inelastic collisions N_2 is

$$N_2 = -\bar{\nu} n_g e \sum_i S_i U_i \, dt, \tag{14}$$

where S_i is the cross-section of the inelastic collisions, U_i are the excitation and ionization potentials of the argon atom.

With their application the energy balance equation is as follows:

$$\frac{dU_e}{dt} = \frac{2}{3}\frac{e}{m}E^2\frac{1}{\bar{\nu}-i\omega} - \frac{2}{3}\bar{\nu}\,n_g\,S\times \\ \times\left[\frac{2m}{M}(U_e-U_g)+\sum_i\frac{S_i}{S}U_i-\frac{n_a}{n_g}\frac{S_a}{S}\bar{U}_a\right], \tag{15}$$

where d/dt is the total differential, but the space dependence may be neglected with a good approximation. Averaging for a half period we get the following relation:

$$U_e = \frac{4}{3\pi}E^2\frac{e}{m}\left[\frac{1}{\bar{\nu}\omega}+i\frac{1}{\bar{\nu}^2}\right]-\frac{8}{3\pi}\sqrt{\frac{8}{\pi}}\sqrt{\frac{e}{m}}\frac{m}{M}\frac{U_e^{3/2}}{L}[1+i]- \\ -\frac{4}{3\pi}\sqrt{\frac{8}{\pi}}\sqrt{\frac{e}{m}}\frac{1}{L}\frac{S_i}{S}U_i\,U_e^{1/2}[1+i]+\frac{4}{3\pi}\sqrt{\frac{8}{\pi}}\sqrt{\frac{e}{m}}\frac{\bar{U}_a}{L}\frac{n_a}{n_g}\frac{S_a}{S}U_e^{1/2}[1+i]\,, \tag{16}$$

where the energy dependence of the cross-sections is taken in a linear shape. If the relation is divided into real and imaginary parts, we get

$$U_e = \frac{4}{3\pi}\frac{e}{m}\frac{1}{\bar{\nu}\omega}E^2-\frac{8}{3\pi}\sqrt{\frac{8}{\pi}}\sqrt{\frac{e}{m}}\frac{m}{M}\frac{U_e^{3/2}}{L}- \\ -\frac{4}{3\pi}\sqrt{\frac{8}{m}}\sqrt{\frac{e}{m}}\frac{1}{L}\frac{S_i}{S}U_i\,U_e^{1/2}+\frac{4}{3\pi}\sqrt{\frac{8}{\pi}}\sqrt{\frac{e}{m}}\frac{\bar{U}_a}{L}\frac{n_a}{n_g}\frac{S_a}{S}U_e^{1/2}\,, \tag{17}$$

$$0 = \frac{4}{3\pi}\frac{e}{m}\frac{1}{\bar{\nu}^2}E^2-\frac{8}{3\pi}\sqrt{\frac{8}{\pi}}\sqrt{\frac{e}{M}}\frac{m}{M}\frac{U_e^{3/2}}{L}- \\ -\frac{4}{3\pi}\sqrt{\frac{8}{\pi}}\sqrt{\frac{e}{m}}\frac{1}{L}\frac{S_i}{S}U_i\,U_e^{1/2}+\frac{4}{3\pi}\sqrt{\frac{8}{\pi}}\sqrt{\frac{e}{m}}\frac{\bar{U}_a}{L}\frac{n_a}{n_g}U_e^{1/2}. \tag{18}$$

The suffix, characteristic for the excitation phenomena may be neglected on account of magnitude, when we insert the value of the constants and we are confined only to the processes preceding the breakdown. In addition to this the value of the negative energy transport, taking place by the inelastic collisions, must be taken into account, completed with a probability factor.

By the division of the equation into real and imaginary terms it is evident that in the expression for the energy taken up by the electrons from space, the periodicity of the field strength supplying the energy is not to be found in the imaginary term. Therefore, the more complete expressions of the

real part may give us fuller information. In this case, we get from Eq. (17), containing the real term:

$$E \geq 2.2 \cdot 10^{-1} \tag{19}$$

the field strength, expressed in e. s. u., which in practical units is:

$$E \geq 66\ V/\text{cm}.$$

It must be mentioned that this criterion has the character of the lower limit, exactly because of the way it was treated and because of our initial conditions.

3. Capacitive breakdown in mercury

We must start with a given mercury vapour pressure, in our case from the following microparameters:

Table I

mean free path for electrons (cm):	8.7
average random velocity of electrons (cm.sec^{-1}):	$2 \cdot 10^8$
average drift velocity of electrons (cm.sec^{-1}):	greater than 10^9

On the basis of the above data it is evident that the criteria of the statistical description, applied in the case of argon [Eq. (3) and (4)] are not fulfilled. The energy transport may be analysed independently from this: in this case, however, the collision frequency must be given on the basis of elementary considerations. The equation of motion is, in our case:

$$m \frac{d^2 x}{dt^2} = eE + \nu \frac{dx}{dt}, \tag{20}$$

where x is the coordinate, preferred by the direction of the electric field, ν is the coefficient of viscosity.

In this case the mobility will be

$$b = \frac{e}{m} \frac{1}{\nu - i\omega} \tag{21}$$

together with which the energy balance with the previously considered terms will be

$$\frac{dU_e}{dt} = \frac{2}{3} \frac{e}{m} E^2 \frac{1}{\nu - i\omega} - \frac{2}{3} \bar{v}\, n_g\, S \times$$
$$\times \left[\frac{2m}{M} (U_e - U_g) + \sum_i \frac{S_i U_i}{S} - \frac{n_a}{n_g} \frac{S_a}{S} \bar{U}_a \right], \tag{22}$$

where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \bar{u}_d \frac{\partial}{\partial x} . \tag{23}$$

Taking an average, applied also for the half period — as previously — and neglecting the transport of the inelastic and second kind collisions, we get the relation:

$$U_e + \frac{2}{\pi\omega} \bar{u}_\alpha \frac{dU_e}{dx} [1+i] = \frac{3}{\pi\omega} E \bar{u}_\alpha [1+i] - \frac{8}{3\pi} \frac{\bar{v}}{L} \frac{m}{M} \frac{U_e}{\omega} [1+i] \tag{24}$$

in which the space dependence is taken into account with a linear energy dependence, substituting $U_e = U_i$:

$$\begin{aligned} &\frac{U_i}{2} + \frac{2}{\pi\omega} \frac{e}{m} \frac{E}{\nu - i\omega} \frac{U_i}{D} [1+i] = \\ &= \frac{3}{\pi\omega} E^2 \frac{e}{m} \frac{1}{\nu - i\omega} [1+i] - \frac{16}{15\pi} \sqrt{\frac{8}{\pi}} \sqrt{\frac{e}{m}} U_i^{3/2} . \end{aligned} \tag{25}$$

Dividing the relation so obtained into real and imaginary terms, we get the following equations:

$$\begin{aligned} &\frac{U_i}{2} + \frac{2}{\pi\omega} \frac{e}{m} \frac{E(\nu - \omega)}{\nu^2 + \omega^2} \frac{U_i}{D} = \\ &= \frac{3}{\pi\omega} E^2 \frac{e}{m} \frac{\nu - \omega}{\nu^2 + \omega^2} - \frac{16}{15\pi} \sqrt{\frac{8}{\pi}} \sqrt{\frac{e}{m}} \frac{U_i^{3/2}}{L} \frac{m}{M} \frac{1}{\omega} , \end{aligned} \tag{26}$$

$$\frac{2}{\pi\omega} \frac{e}{m} \frac{E(\nu + \omega)}{\nu^2 + \omega^2} \frac{U_i}{D} = \frac{3}{\pi\omega} E^2 \frac{e}{m} \frac{\nu + \omega}{\nu^2 + \omega^2} - \frac{16}{15\pi} \sqrt{\frac{8}{\pi}} \sqrt{\frac{e}{m}} \frac{U_i^{3/2}}{L} \frac{m}{M} \frac{1}{\omega} . \tag{27}$$

If the viscosity coefficient is considered as a specific viscosity, for a non-closed, infinite space, we get relatively low critical field strength, from both equations. One possible method for the closing of the model is weighting according to the u_d/v and L/D. In the case of the closed model we then get the following expression as the breakdown criterion having the character of the lower limit:

$$E > 6, \tag{28}$$

which is expressed in practical units:

$$E > 1800 \ V/\text{cm}. \tag{29}$$

By the treatment of the model, concerning the processes immediately preceding the breakdown and characteristic for the "reflection time", we have left out of consideration, as well as in the case of argon, the positive energy transport representing only a very small amount of energy and depending on the presence of excited atoms.

4. Further characteristic current peaks

In the equations, characteristic for the energy balance (15), (22) in the indication of the energy transport there is a sum, attributable to inelastic collisions. The coefficients belonging to the single terms of this sum characterize the cross-section of all processes, produced by the inelastic collision.

In the description of this method a recursive correction must be made, however, which mainly affects the first term in the energy balance equation — the energy quantity taken up from the electric field. The correction must be made according to a distribution function, changing in the course of the discharge, e.g. with the application of an iteration method or by a successive approximation.

For the analyses of the current peaks, manifesting themselves at the capacitive discharge it is suitable to use a method carried out over a greater time interval and describing the elementary time dependences more minutely instead of by the averaging applied so far for the half period. It is imaginable that the energy accumulation, starting at this time with the population of the excited and metastable atomic levels, which may have been neglected in the description of the breakdown, alters the energy transport more considerably.

The detailed analysis and description of these phenomena and of the behaviour of the transient processes in gas mixtures outlined will be the subjects of our further examinations.

5. Experimental references

The relations established for the state preceding the transient period and obtained theoretically were checked experimentally with the realization of the formerly outlined arrangements. It has been found that the given breakdown criteria can be proved experimentally and the described model is suitable for further development.

The accuracy of the measurements was ± 0.5 V, the calculated values and their equivalents determined experimentally are shown in Table II.

Table II

	breakdown voltage (V)	
	calculated	measured
2.5 mmHg argon	132	156
$6 \cdot 10^{-3}$ mmHg mercury	1800	below 1800 there is no breakdown

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О МЕХАНИЗМЕ ПРОБОЯ НИЗКОЧАСТОТНЫХ РАЗРЯДОВ В СЛУЧАЕ ВНЕШНИХ ЭЛЕКТРОДОВ

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Р е з ю м е

На основе разработанной нами статистической модели интерпретируются явления пробоя, возникающие под действием напряжения с частотой 50 гц в аргоне и парах ртути, причем электроды располагаются вне области разряда и магнитное поле отсутствует. Давление в рабочей области при экспериментах с аргоном 2,5 мм р. ст., при экспериментах с парами ртути $6 \cdot 10^{-3}$ мм р. ст., расстояние между внешними электродами составляет 20 мм. Объясняется процесс пробоя и следующие за этим скачки тока.

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IMPURITY INDUCED $T_C = 0\,°K$ SUPERCONDUCTIVITY

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Our earlier result, representing the dependence of critical temperature of superconducting transition on the concentration of dia- and paramagnetic impurities is applied to the case when T_c approaches absolute zero owing to impurities. We calculated the rate of spin flip scatterings $\Delta\Gamma_{s0}$ for an electron at the Fermi surface, when either the scattering processes or the change in the Fermi surface topology have a dominant role. The expressions obtained were verified by a comparison with experimental data and by numerical estimation.

Introduction

In a previous paper [1] we examined the effect of para- and diamagnetic impurities on the temperature of superconducting transition. Assuming a Lifshitz singularity in the density of normal single-electronic states, we obtained the next equation for the determination of the critical temperature T_c

$$\lambda\nu_0(\varepsilon_F^0)\,\mathrm{Re}\int_0^{\omega_D} d\omega\,\frac{\mathrm{th}\dfrac{\omega}{2T_c}}{\omega+i\Gamma_s}-\lambda M\,\mathrm{Re}\int_0^{\omega_D} d\omega\,\frac{\mathrm{th}\dfrac{\omega}{2T_c}}{\omega+i\Gamma_s}\left(\sqrt{\alpha-\omega}-\sqrt{\alpha^*-\omega}\right)=1, \tag{1}$$

where the first term is the result of the ABRIKOSOV—GORKOV theory [2] and the second term is due to the singularity. In this formula the symbols mean: λ the potential of electron—electron interaction, $\nu_0(\varepsilon_F^0)$ the density of the regular normal single-electronic states on the Fermi surface of the pure metal ε_F^0, ω_D the Debye frequency, Γ_n and Γ_s are the rates of normal and spin flip scatterings for an electron at the Fermi surface (proportional to the impurity concentration), M is a constant depending on the effective mass of electron:

$$M=\frac{m_1\sqrt{2m_3}}{2\pi^2}$$

and

$$\begin{aligned}\alpha&=\gamma_d\Delta Z_d\,\Gamma_{nd}+\gamma_p\Delta Z_p\,\Gamma_{np}-i\frac{\Gamma_n+\Gamma_s}{2}+\varepsilon_F^0-\varepsilon_c\,,\\ \alpha^*&=\gamma_d\Delta Z_d\,\Gamma_{nd}+\gamma_p\Delta Z_p\,\Gamma_{np}+i\frac{\Gamma_n+\Gamma_s}{2}+\varepsilon_F^0-\varepsilon_c\,,\end{aligned} \tag{2}$$

where m_1 and m_3 are the diagonal elements of the effective mass tensor, ΔZ_d and ΔZ_p are the differences in the valence of dia- and paramagnetic impurities and the normal metal, γ_d and γ_p are constants, ε_c is the critical value of electron energy.

Superconductivity at $T_c = 0$ °K

The value of T_c may be decreased to absolute zero owing to the effects of impurities. This is due to paramagnetic impurities. In this case, in Eq. (1) we have

$$\operatorname{th} \frac{\omega}{2\,T_c} = 1 . \tag{3}$$

If $\Gamma_s = \Gamma_{s0}$, where Γ_{s0} is the value at which $T_c = 0$ according to ABRIKOSOV—GORKOV theory, then

$$\lambda \nu_0(\varepsilon_F^0) \operatorname{Re} \int_0^{\omega_D} \frac{d\omega}{\omega + i\Gamma_{s0}} = 1 . \tag{4}$$

Writing $\Gamma_s = \Gamma_{s0} + \Delta\Gamma_{s0}$ and using the iteration method we have, in an approximation of first order,

$$\Delta\Gamma_{s0} = C \operatorname{Re} \left\{ - \int_0^{\omega_D} d\omega \frac{i(\Gamma_n + \Gamma_s) + 2\,\omega}{(\omega + i\,\Gamma_{s0})(\sqrt{\alpha_0 - \omega} + \sqrt{\alpha_0^* + \omega})} \right\}, \tag{5}$$

where

$$C = - \frac{M}{\nu_0(\varepsilon_F^0)} \frac{\Gamma_{s0}(\omega_D^2 + \Gamma_{s0}^2)}{\omega_D^2} .$$

Taking into account that $\Gamma_{n0}/\omega_D \sim 1$, the absolute values of square roots in the denominator of Eq. (5) are large, we may write, approximately,

$$\Delta\Gamma_{s0} = C \operatorname{Re} \left\{ \frac{-i(\Gamma_{n0} + \Gamma_{s0}) \ln(\omega + i\Gamma_{s0}) - 2\omega + 2i\Gamma_{s0}(\omega + i\Gamma_{s0})}{\sqrt{\alpha_0 - \omega} + \sqrt{\alpha_0^* + \omega}} \Bigg|_0^{\omega_D} \right\} . \tag{6}$$

The value of $\Delta\Gamma_{s0}$ we calculate in two important limiting cases of experimental interest.

a) If the *scattering processes* dominate, e.g. $\gamma_p \ll 1$, and assuming, that $\Gamma_{nd} = 0$, then expression (6) has the form

$$\Delta\Gamma_{s0} = C \operatorname{Re} \left\{ \frac{i(\Gamma_{s0} - \Gamma_n) \ln(\omega_D + i\Gamma_{s0}) - 2\omega_D}{(1+i)\sqrt{\omega_D + \frac{1}{2} i(\Gamma_n + \Gamma_{s0})}} - \frac{i(\Gamma_{s0} - \Gamma_n) \ln i\Gamma_{s0}}{\sqrt{2}\,i \sqrt{\frac{1}{2}(\Gamma_n + \Gamma_{s0})}} \right\} . \tag{7}$$

Separating the real part, after some calculation we have

$$\Delta\Gamma_{s0} = C \frac{\left\{(\Gamma_{s0} - \Gamma_{np0})\left[\ln(\omega_D^2 + \Gamma_{s0}^2) - 2 \arctan \frac{\Gamma_{s0}}{\omega_D}\right] - 4\omega_D\right\} \cos\beta}{4\left[\omega_D^2 + \frac{(\Gamma_{s0} + \Gamma_{np0})^2}{4}\right]^{1/4}} + \tag{8}$$

$$= C \frac{\left\{(\Gamma_{s0} - \Gamma_{np0})\left[\ln(\omega_D^2 + \Gamma_{s0}^2) + 2 \arctan \frac{\Gamma_{s0}}{\omega_D}\right] + 4\omega_D\right\} \sin\beta}{4\left[\omega_D^2 + \frac{(\Gamma_{s0} + \Gamma_{np0})^2}{4}\right]^{1/4}} +$$

$$+ C \frac{\Gamma_{s0} - \Gamma_{np0}}{(\Gamma_{s0} + \Gamma_{np0})^{1/2}} \ln \Gamma_{s0},$$

where

$$\beta = \frac{1}{2} \arctan \frac{\Gamma_{s0} + \Gamma_{np0}}{2\omega_D}.$$

According to this relation if $M > 0$ (and consequently $C < 0$), then $\Delta\Gamma_{s0} > 0$, but if $M < 0$ (and therefore $C > 0$), then $\Delta\Gamma_{s0} < 0$. In the first case we can conclude that an electron group is generated in the Brillouin zone

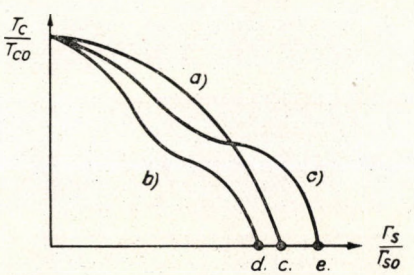

Fig. 1

independently of the fact that other mechanisms may also contribute to the decrease of the critical temperature. But if $\Delta\Gamma_{s0} < 0$, then we cannot reach such a direct and definite conclusion.

Curve a) in Fig. 1 represents the ABRIKOSOV—GORKOV theory and on comparing the experimental curve b) [3] with our result we find a good agreement. The curve c) would represent an alloy which has a positive effective mass. The point c corresponds to $\Gamma_s = \Gamma_{s0}$, and the points d and e stand for $M < 0$ and $M > 0$, respectively.

We can make a numerical estimate to verify our results. We shall use data for In:

$$T_{c0}=3{,}4\,^\circ\mathrm{K},\ \omega_D=109\ ^\circ\mathrm{K},\ \Gamma_{s0}=\frac{\pi}{2}\,\frac{T_{c0}}{\gamma},\ \gamma=3{,}5\cdot10^{-4}\,\mathrm{cal/grad^2\,mol},$$

$$\nu^\circ(\varepsilon_F^0)=9{,}2\cdot10^{33}\,\mathrm{erg^{-1}\,cm^{-3}},\ m^*=1{,}4\,m_e,$$

$$M=\frac{m^{*3/2}}{1{,}41\pi^2}=\frac{27\cdot10^{-42}}{14}=2\cdot10^{-42}\,\mathrm{gr^{3/2}},$$

where m_e is the electronic mass, γ is the electronic specific heat constant, and the effective mass of electron is assumed to be isotropic and assuming $\Gamma_{np0}\sim10^2\Gamma_{s0}$. Comparing the BCS-formula for T_c

$$T_c=1{,}2\,\omega_D\cdot e^{-\frac{1}{\lambda\nu_0(\varepsilon_F^0)}}$$

with the ABRIKOSOV—GORKOV expression for Γ_{s0}

$$\lambda\nu_0(\varepsilon_F^0)\int_0^{\omega_D}d\omega\,\frac{\omega}{\omega^2+\Gamma_{s0}^2}=1$$

and hence

$$\Gamma_{s0}\approx\omega_D\,e^{-\frac{1}{\lambda\nu_0(\varepsilon_F^0)}},$$

we see that $\Gamma_{s0}\sim1{,}2T_c$. From these data we obtained $\Delta\Gamma_{s0}/\Gamma_{s0}\sim0{,}1\div0{,}3$.

b) If the change in the *Fermi surface topology* has a dominant role e.g. $\gamma_p\gg1$, and assuming that $\Gamma_{nd}\approx0$ and $\Delta Z_p>0$, then Eq. (6) has the form (after neglecting the imaginary part):

$$\Delta\Gamma_{s0}=\frac{M}{\nu_0(\varepsilon_F^0)}\,\frac{\Gamma_{s0}(\omega_D^2+\Gamma_{s0}^2)}{\omega_D^2}\times\left\{\frac{(\Gamma_{s0}-\Gamma_{np0})\arctan\dfrac{\Gamma_{s0}}{\omega_D}+2\,\omega_D}{\sqrt{\alpha_0-\omega_D}+\sqrt{\alpha_0+\omega_D}}-\frac{\pi}{4}\,\frac{\Gamma_{s0}-\Gamma_{np0}}{\sqrt{\alpha_0}}\right\}\tag{9}$$

where

$$\alpha_0=\gamma_p\,\Delta Z_p\,\Gamma_{np0}>\omega_D\quad\text{and}\quad\varepsilon_F^0=\varepsilon_c.$$

But if $\Delta Z_p<0$, after similar calculation we have

$$\Delta\Gamma_{s0}=\frac{M}{\nu_0(\varepsilon_F^0)}\,\frac{\Gamma_{s0}(\omega_D^2+\Gamma_{s0}^2)(\Gamma_{s0}-\Gamma_{np0})}{2\,\omega_D^2}-\left[\frac{\ln\Gamma_{s0}}{\sqrt{|\alpha_0|}}-\frac{\ln(\omega_D^2+\Gamma_{s0}^2)}{\sqrt{|\alpha_0|+\omega_D}+\sqrt{|\alpha_0|-\omega_D}}\right].\tag{10}$$

With respect to experimental situations we notice that the decrease in the critical temperature owing to the change in the nature of the Fermi surface topology can be measured independently of other mechanisms. Namely, adding diamagnetic impurities with $+\Delta Z_d$ and $-\Delta Z_d$ to the pure superconductor we can make the potential of electron – electron interaction isotropic and therefore the KADANOFF—MARKOWITZ mechanism [4] does not contribute with a further increase of impurities.

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СВЕРХПРОВОДИМОСТЬ ПРИ $T_c = 0$ °К ВСЛЕДСТВИЕ ПРИМЕСЕЙ

И. КИРШНЕР и А. ШТАРК

Р е з ю м е

Ранее полученный нами результат для определения зависимости критической температуры от концентрации диа- и парамагнитных примесей применяется к случаю, когда T_c стремится к нулю вследствие влияния примесей. Вычисляется число столкновений в единицу времени с переворотом спина для электрона на поверхности Ферми $\Delta\Gamma_{s0}$, когда главную роль играют либо процессы рассеяния, либо изменение топологии поверхности Ферми. Полученные результаты проверены сравнением с опытными данными и численной оценкой.

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THE EFFECT OF THE DENSITY DEPENDENCE OF THE FORCES ON FIRST ORDER FINITE NUCLEAR CALCULATIONS

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Hartree—Fock type of calculations are made with density dependent forces, and we examine the effect of density dependence on the results. The single particle and total energies and the average radii of spherical nuclei are determined. The results are compared with other calculations. Good agreement is found between theoretical and experimental values.

I. Introduction

The most usual method to determine properties of finite nuclei is the Hartree—Fock approximation. It is applicable only for weak forces. Phase shift analysis shows, however, that the two-body forces are not weak forces. There are two ways of avoiding this difficulty. One is to deduce from the two-body scattering some weak force which fits the scattering data relatively well, and which are already applicable in first order calculations [1, 2]. The other possibility is to use BRUECKNER Hartree—Fock calculations [3, 4]. There one rearranges the perturbation series by running up the ladder graphs, and in this way a new first order term is deduced which already gives a better first order approximation.

The biggest problem with the BRUECKNER Hartree—Fock calculations is the double self-consistency. One determines first a single particle potential, from this the single particle wave functions by solving the Schrödinger equation, then one determines the G matrix elements, and from this again the single-particle potential, and so on. The single particle potential is non-local, because of the exchange term, which makes the whole calculation process even longer. One can make a short cut by using harmonic oscillator wave functions, as the real one, and forgetting about the Hartree—Fock self-consistency, keeping only the BRUECKNER one; this is, however, a bad approximation for heavier nuclei.

A new way of dealing with this problem has been developed in recent years. Using the original local density approximation of BRUECKNER [3], one can develop it further by applying certain corrections [5] and as a result one can deduce an effective two-nucleon force, which is density dependent [6—9] and which gives quite good results for first order calculations [8—10].

In this work we examine in detail the solution of the Hartree—Fock equations for different density dependent forces. A short report of the following results has been already published [10] in the Physics Letters. In the second section we deduce the Hartree—Fock equations for our density dependent force; in the third we examine the method for their solutions, and in the fourth we discuss the results.

II. Hartree—Fock equation with density dependent forces

The density dependent force we use for the $\varrho_N = \varrho_P$ case can be written as [7, 8]

$$v = f(\varrho(R))\ \delta(r_1 - r_2) + v_e(r, \varrho)\, g(\varrho)\,, \tag{2,1}$$

where $f(\varrho)$ can be obtained from the nuclear matter energy density, and $v_e = 0$ if $r < 1\,fm$. The density dependence of the long range forces can be written as

$$v_e(r, \varrho) = v_1(\varrho) - \varrho(r_1)^{1/3}\, \varrho(r_2)^{1/3}\, v_2(r), \tag{2,2}$$

$$g(\varrho) = 1 - 2B\varrho^{2/3} - 2C\varrho^{1/3}. \tag{2,3}$$

B and C are constants, and v_e is different for the different partial waves, and is the sum of Yukawa terms.

The total energy can be written as

$$\begin{aligned} W = W_{\text{kin}} &+ \int w(\varrho(R)) d^3R + \frac{1}{2}\int v_1^D(r)\, g(\varrho(r_1))\ \cdot \\ &[\varrho(r_1)\varrho(r_2) - \varrho(r_1)^2] d^3r_1 d^3r_2 - \\ &- \frac{1}{2}\int v_2^D(r)\, g(\varrho(r_1))\, [\varrho(r_1)^{4/3}\, \varrho(r_2)^{4/3} - \varrho(r_1)^{8/3}]\, d^3 r_1\, d^3 r_2 + \\ &+ \frac{1}{2}\int v_1^x(r)\, g(\varrho(r_1))\, [\varrho(r_1 r_2)^2 - \tau(r_1\, \varrho(R))^2]\, d^3 r_1\, d^3 r_2 - \\ &- \frac{1}{2}\int v_2^x(r)\, g(\varrho(r_1))\, [\varrho(r_1 r_2)^2\, \varrho(r_1)^{1/3}\, \varrho(r_2)^{1/3} - \\ &- \tau(r, \varrho(R))^2\, \varrho(R)^{2/3}]\, d^3 r_1\, d^3 r_2 + \\ &+ \frac{c}{2}\int \frac{1 + g(\varrho(r_1))}{2}\, \frac{\varrho(r_1)\, \varrho(r_2)}{|\mathbf{r}_1 - \mathbf{r}_2|}\, d^3 r_1\, d^3 r_2\,, \end{aligned} \tag{2,4}$$

and τ is the nuclear matter exchange density

$$\tau = \frac{2}{\pi^2}\, \frac{\sin k_F(R)\, r - k_F(R)\, r \cos k_F(R)\, r}{r^3}\,. \tag{2,5}$$

k_F is the Fermi momentum, v^D, v^X are the direct and exchange combinations of the total forces, respectively, W_{kin} is the kinetic energy and the last term the Coulomb energy, corrected by a factor arising from the local density approximation [6, 7, 8]. For the $\varrho_n \neq \varrho_p$ case the energy is a much longer expression and can be found in [7].

From (2,5) we can get the Hartree—Fock equations

$$\begin{aligned} &-\frac{\hbar^2}{2m}\nabla^2\varphi_i(r_1) + \alpha(\varrho(r_1))\varphi_i(r_1) + \\ &+\int \beta(\varrho(r_1), \varrho(r_2), r_1, r_2)\, d^3 r_2 \varphi_i(r_1) + \\ &+\int \gamma(\varrho(r_1 r_2), \varrho(r_1), \varrho(r_2), r_1, r_2) d^3 r_2 \varphi_i(r_1) + \\ &+\int \delta(\varrho(r_1 r_2), \varrho(r_1), \varrho(r_2), r_1, r_2)\varphi_i(r_2)\, d^3 r_2 = e_i \varphi_i(r_1)\,, \end{aligned} \tag{2,6}$$

where the various terms are given in the Appendix.

The Hartree—Fock equations can be solved in coordinate space or on a harmonic oscillator wave function basis. In our case the last method is very difficult in practice, because we have $\varrho^{1/3}$, $\varrho^{2/3}$ in our calculation. We used the coordinate space solution method of VAUTHERIN and VENERONI [2] who substituted the non-local potential with an equivalent local potential, namely after integrating out for the angle the remaining

$$\int k(r_1 r_2) u_i(r_2)\, d^3 r_2 \tag{2,7}$$

integral is replaced by an equivalent local expression

$$\frac{1}{u_i(r_1)}\int k(r_1 r_2)\, u_i(r_1)\, u_i(r_2)\, d^3 r_2\,, \tag{2,8}$$

and we avoid the poles of $u_i(r_1)$ at $r_1 = r_0$ by calculating (2,8) for $r_0 - \varepsilon$ and $r_0 + \varepsilon$ values, and linearly connecting the two terms ($\varepsilon \ll$).

Because of the ϱ dependence of the effective forces, in (2,6) we have terms coming from $\dfrac{\partial v}{\partial \varrho}$ so we get the so called rearrangement expressions. This arises because when we change the wave function, the total density also changes and, therefore, so does the effective force. The effect of the rearrangement term is very important. For density independent forces the total energy can be written as

$$E = \frac{1}{2}\sum_i (t_i + e_i) \tag{2,9}$$

where t_i is the kinetic, e_i the single particle energy. From known e_i - s we can roughly determine E, because t_i is almost the same for the known models.

We obtain $|E|$ as smaller than its experimental value. For density dependent forces the total energy can be written as

$$E = \frac{1}{2} \sum (t_i + e_i) - \frac{1}{2} \sum_{ij} \left\langle ij \left| \frac{\partial v}{\partial \varrho} \delta \varrho_i \right| ij \right\rangle \tag{2,10}$$

instead of as in (2,9), and the rearrangement term corrects the above mentioned contradiction. This means that first order calculation cannot give well all the experimental results, but the density dependence of the forces, which comes from the inclusion of higher order terms, can provide good results.

III. Solution of the Hartree—Fock equations

The solution of the Hartree—Fock equations was carried out only for spherical nuclei, with the method of VAUTHERIN and VENERONI [2].

If we write the long range forces in the form

$$v = f(\varrho)\, \delta(r_1 - r_2) + W(r, \varrho) + B(r, \varrho) P_\sigma - H(r, \varrho) P_\tau - M(r, \varrho)\, P_\sigma\, P_\tau, \tag{3,1}$$

where

$$P_\sigma = \frac{1 + \sigma_1 \sigma_2}{2}, \quad P_\tau = \frac{1 + \tau_1 \cdot \tau_2}{2} \tag{3,2}$$

are the spin and isospin projection operators, and we expand the Yukawa terms as

$$v(|r_1 - r_2|) = \sum_B v_B(r_1 r_2) P_k(\cos \delta_{12}), \tag{3,3}$$

the Hartree—Fock equation can be written as

$$-\frac{\hbar^2}{2m} \left(u_\alpha'' + \frac{l(l+1)}{r^2} u_\alpha \right) + V_\alpha(r)\, u_\alpha(r) = e_\alpha\, u_\alpha(r), \tag{3,4}$$

where V_α is the total equivalent local potential

$$V_\alpha(r) = \frac{1}{u_d(r)} \int_0^\infty rr'\, U_\alpha(rr')\, dr'\, u_\alpha(r') \tag{3,5}$$

and for density independent forces

$$\begin{aligned} U_\alpha(r_1 r_2) = {} & \frac{4\pi}{r_1^2} \delta(r_1 - r_2) \int_0^\infty \varrho(r_3)\, v_0(r_1 r_3)\, d^3 r_3 - \\ & - (2l_\alpha + 1) \sum_{k\beta} (2 l_\beta + 1)(2_{\alpha\beta} + 1 \begin{pmatrix} l_a & l_\beta & k \\ 0 & 0 & 0 \end{pmatrix}^2 \\ & \Gamma_{k\alpha\beta}(r_1 r_2)\, \varrho_\beta(r_1 r_2)\, d^3 r_2, \end{aligned} \tag{3,6}$$

where α, β denotes the j_α, l_α, q_α quantum number set,

$$v_0 = 3W_0 + \frac{2}{3}B_0 - \frac{3}{4}H_0 - M_0\,,$$
$$\Gamma_{\alpha\alpha\beta} = \begin{Bmatrix} l_\alpha & j_\alpha & 1/2 \\ j_\beta & l_\beta & k \end{Bmatrix}^2 [W_k\,\delta_{q_\alpha q_\beta} - H_k] + B_k\,\delta_{q_\alpha q_\beta} - M_k\,. \tag{3,7}$$

$\begin{pmatrix} l_\alpha & l_\beta & k \\ 0 & 0 & 0 \end{pmatrix}$ is the Clebsch—Gordon and

$\begin{Bmatrix} l_\alpha & j_\alpha & 1/2 \\ j_\beta & l_\beta & k \end{Bmatrix}$ the Racach coefficient.

In the case of density dependent forces the whole calculation becomes more complicated, because W, B, H, and M now depend on the density. In this case in (3,6) instead of v_0 and $\Gamma_{k\alpha\beta}$ we have to substitute

$$v_0' = v_0 + 2\,\varrho(r_1)\,\frac{\partial v_0\,(r_1\,r_3\,\varrho(r_1)\,\varrho(r_3))}{\partial\varrho(r_1)} \tag{3,7a}$$

and

$$\Gamma'_{k\alpha\beta} = \Gamma_{k\alpha\beta} + 2\,\delta(r_1 - r_2)\,\varrho_\beta(r_1\,r_3)\,\frac{\partial\Gamma_{k\alpha\beta}(r_1\,r_3\,\varrho(r_1)\,\varrho(r_3))}{\partial\varrho(r_1)}\,. \tag{3,8a}$$

To get good numerical results we have to introduce a single particle spin-orbit force

$$v_{LS} = c_{LS}\,\mathbf{ls}, \tag{3,9}$$

where c is determined from experimental fitting, because theoretical calculations cannot be carried out if one approximates the tensor force with a density dependent effective force.

The numerical solution of the equations (3,4) consists of the following steps:

a) First we determine the

$$v_k(r_1\,r_2) = \int v(\mathbf{r}_1 - \mathbf{r}_2)P_k(\cos\Theta)d\Omega$$

expressions, where $v(\mathbf{r}_1 - \mathbf{r}_2)$ is the sum of Yukawa terms

$$v(\mathbf{r}_1 - \mathbf{r}_2) = \sum_i A_i\,\frac{e^{-\mu_i|r_1 - r_2|}}{|\mathbf{r}_1 - \mathbf{r}_2|}\,.$$

We determine $v_k(r_1, r_2)$ for every k, μ, r_1 and r_2 values, and the results are put on a drum for every r_1 value as a function of μ, k and r_2.

b) We solve the single-particle Schrödinger equation for given initial conditions and equivalent local potential. For the first iteration the starting potential is a Saxon—Wood one. In this way we get the single particle energies and wave functions.

c) Knowing the wave functions we determine the neutron and proton densities and mean square root radii.

d) We calculate the Coulomb potential, the spin-orbit potential, and the local density dependent potential coming from the direct terms.

e) We determine in a sub-programme the integrals for every μ, k, α, β and r_1 value. For heavy nuclei (like lead) $k = 13$, α, $\beta = 38$ and r_1 has a value of 150 so that this is by far the longest part of the calculations.

f) We determine in a sub-programme the Racach and Clebsch—Gordon coefficients needed for the exchange potential.

g) We calculate the non-local exchange potential, and express it with the help of an equivalent local potential.

h) From the Coulomb, spin orbit, direct and equivalent exchange potentials we construct the total single particle potential for every state as a function of r_1.

i) We calculate the total energy. This is now not such a simple calculation as in the usual Hartree—Fock case, because of the rearrangement term.

j) With the new potential we again solve the Schrödinger equation and repeat the whole programme.

Since the exchange energy calculations are very long, for the first eight iterations we used the Slater approximation, and only in the last five did we use the total exchange programme.

IV. The results

The calculations were carried out for two different cases. In one case in the long range forces and in the $g(\varrho)$ correction factor we suppressed the density dependence for which we substituted its nuclear matter value. In the other case the long range density dependence was taken into account. We also examined the effect of the different terms on the radii and energies, so for this reason we changed the values of the different parts of the forces.

a) The mean square root radii

Table I shows the neutron and proton radii of the spherical nuclei. With r_c we note the charge radius

$$r_c^2 = r_p^2 + 0.6.$$

We also show the radii for the long range density independent case. It can be seen that for the density dependent case the radii decrease. The reason for this is that the density becomes bigger at the centre and smaller at the sur-

Table I

The average neutron, proton, and charge radii of spherical nuclei. The $r^{(1)}$- s are the results of the density dependent, the $r^{(2)}$- s the density independent long range force calculations. $r_{c\exp}$ is the experimental charge density, $r_c^{(3)}$ the results of DAVIES and TARBUTTON [4], $r_c^{(4)}$ the results of KERMANN et al. [1] and $r_c^{(5)}$ the results of VAUTHERIN and VENERONI [2]

	$r_n^{(1)}$	$r_p^{(1)}$	$r_c^{(1)}$	$r_n^{(2)}$	$r_p^{(2)}$	$r_c^{(2)}$	$r_{c\exp}$	$r_c^{(3)}$	$r_c^{(4)}$	$r_c^{(5)}$
^{16}O	2.63	2.66	2.75	2.69	2.72	2.81	2.73	2.67	2.39	2.77
^{40}Ca	3.30	3.36	3.45	3.36	3.42	3.59	3.50	3.30	2.89	3.52
^{48}Ca	3.66	3.43	3.52	3.69	3.50	3.57	3.49	3.34	2.79	3.60
^{90}Zr	4.23	4.16	4.23	4.28	4.22	4.29	4.30	3.03		4.32
^{208}Pb	5.53	5.38	5.44	5.58	5.42	5.48	5.52	5.14		5.50

face. For comparison, in Table I we also show the experimental values and the results of some theoretical calculations [1, 4, 2].

If we slightly decrease the total value of the forces or decrease the saturation density of the nuclear matter, the mean square root radii will increase. If we increase the attraction in the longest part of the long range forces and decrease it in the medium, the radii will again increase. The reason

Table II

The energies per particles of spherical nuclei (1), (2), (3), (4), (5) are the same as in Table I, E_D and E_X can be seen from (4, 2), and E_R is the rearrangement energy

	E/A		E_R		E_D	
	1	2	1	2	1	2
^{16}O	—7.73	—7.60	—4.89	—4.65	3.33	3.52
^{40}Ca	—8.32	—8.25	—5.65	—5.42	2.57	2.31
^{48}Ca	—8.02	—7.9	—5.43	—5.25	2.32	2.12
^{90}Zr	—8.20	—8.02	—6.05	—5.83	1.50	1.23
^{208}Pb	—7.45	—7.21	—7.63	—7.37	1.46	1.19

	E_X		$(E/A)_{\exp}$	$E/A^{(3)}$	$E/A^{(4)}$	$E/A^{(5)}$
	1	2				
^{16}O	0.54	0.70	—7.98	—4.81	—2.94	—6.05
^{40}Ca	0.62	0.82	—8.55	—5.64	—3.96	—6.43
^{48}Ca	0.67	0.90	—8.67	—5.3	—3.41	—6.10
^{90}Zr	1	1.15	—8.71	—5.99		—6.28
^{208}Pb	0.82	1.00	—7.87	—5.20		—5.52

Table III

The single particle energies of ^{16}O, ^{40}Ca and ^{48}Ca for density-dependent (1) and density-indepen-

	^{16}O					
	1		2		1	
	neutron	proton	neutron	proton	neutron	proton
$1s\,^1/_2$	—34.26	—30.53	—33.80	—30.40	45.25	—37.74
$1p\,^3/_2$	—19.39	—15.85	—19.21	—15.92	—33.19	—25.97
$1p\,^1/_2$	—14.76	—11.25	—14.85	—11.55	—33.06	—22.84
	(—15.67)	(—12.15)				
$1d\,^5/_2$					—20.77	—13.81
$2s\,^1/_2$					—16.85	— 9.83
$1d\,^3/_2$					—15.53	— 8.61
					(—15.62)	(— 8.33)
$1f\,^7/_2$						

for this is clear: in our case the attractive long range part acts as a repulsive force, because

$$\int \alpha \frac{e^{-\mu r}}{r} [\varrho(r_2) - \varrho(r_1)]\, d^3 r_2 \tag{4,1}$$

is positive for negative α.

b) The energies of nuclei

As can be seen in (2,4), the total energy can be written as

$$\frac{E}{A} = E_{NM} + E_D + E_X + E'_{\text{coul}}\,, \tag{4,2}$$

where E_{NM} are the first two terms in (2,4), E_D direct, E_X the exchange corrections and E'_{coul} the Coulomb energy. In Table II we can find the energies per particle of different nuclei and the different terms in (4,2). One can also see from Table II the importance of the rearrangement energy. In Tables III and IV we can find the single particle energies of different nuclei. In each Table we also show the energy values for the density-independent long range forces. One can see that the deep single particle energies become more bounded for the density dependent case, and the total binding increases. The results are in very good agreement with experiments, as can be seen from Tables II, III, IV (the experimental values are put in brackets). We also compared our energy results with other calculations.

The density dependent effective forces give very good results in first order calculations. The single particle and total energies and the radii are in very good agreement with experiments. It seems to us that by deducing our effective forces with the help of the modified local density approximation we

dent (2) long range forces. The values in parentheses mean the last nucleon's separation energies

^{40}Ca		^{48}Ca			
2		1		2	
neutron	proton	neutron	proton	neutron	proton
—44.70	—37.26	—42.89	—41.03	—43.40	—41. 87
—32.73	—25.32	—31.30	—31	—31.75	—31.68
—32.41	—22.16	—29.49	—28.86	—29.93	—29.51
—20.32	—13.51	—19.66	—20.11	—19.82	—21.93
—16.53	— 9.63	—16.77	—16.50	—16.91	—17.15
—15.45	— 8.70	—16.11	—15.08	—16.13	—15.72
			(—15.60)		
		— 7.97		— 8.12	
		(— 9.94)			

have succeeded in finding a way to take into account the biggest contribution of the higher order perturbative terms in first order calculations.

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Appendix

If we minimize the (2,7) energy as a function of we get the equation (2,8) where

$$\alpha = \frac{\partial w(\varrho(r_1))}{\partial \varrho(r_1)} \tag{A,1}$$

$$\beta = v_1^D(r)\, g(\varrho(r_1)\,[\varrho(r_2) - \varrho(r_1)] + \frac{1}{2}\, v_1^D(r)\, \frac{\partial g\,(\varrho(r_1))}{\partial \varrho(r_1)}\, \varrho(r_1)\,[\varrho(r_2) - \varrho(r_1]\times$$

$$\times \frac{4}{3}\, v_2^D(r)\,(g(\varrho_1))\,[\varrho(r_2)^{4/3} - \varrho(r_1)^{4/3}]\,\varrho(r_1)^{1/3} -$$

$$- \frac{1}{2}\, v_2^D(r)\, \frac{\partial g\,(\varrho(r_1))}{\partial \varrho(r_1)}\,[\varrho(r_2)^{4/3} - \varrho(r_1)^{4/3}]\,\varrho(r_1)^{4/3} -$$

$$- v_1^x(r)\left[\frac{1}{2}\, \frac{\partial g\,(\varrho(r_1))}{\partial \varrho(r_1)}\, \tau^2\,(r_1\,\varrho(r_1)) + \right. \tag{A,2}$$

Table IV

The single particle energies of ^{208}Pb, ^{90}Zr for density-dependent (1) and density-independent (2) long range forces. The values in parentheses mean the last nucleon's separation energies

	^{90}Zr				^{208}Pb			
	1		2		1		2	
	neutron	proton	neutron	proton	neutron	proton	neutron	proton
$1s\ ^1/_2$	—50.02	—42.92	—49.82	—42.70	—50.61	—40.28	—51.02	—39.29
$1p\ ^3/_2$	—40.75	—34.72	—40.51	—34.17	—44.97	—35.78	—42.21	—34.57
$1p\ ^1/_2$	—38.99	—32.75	—38.73	—32.23	—44.37	—35.14	—44.82	—34.39
$1d\ ^5/_2$	—30.32	—25.37	—30.11	—24.76	—38.56	—29.82	—38.97	—28.81
$2s\ ^1/_2$	—27.42	—21.33	—27.23	—20.87	—36.19	—26.92	—36.65	—24.95
$1d\ ^3/_2$	—27.60	—22.30	—27.41	—21.76	—38.35	—28.51	—38.77	—27.50
$1f\ ^7/_2$	—20.39	—15.94	—20.18	—15.21	—31.55	—23.21	—31.97	—21.13
$2p\ ^3/_2$	—16.40	—10.36	—16.21	— 9.67	—28.09	—19.15	—28.51	—18.07
$1f\ ^5/_2$	—15.96	—11.11	—15.77	—10.52	—29.51	—20.97	—30.08	—20.03
$2p\ ^1/_2$	—14.60	— 8.57	—14.42	— 8.13	—27.12	—18.14	—27.87	—16.12
		(— 8.36)						
$1g\ ^9/_2$	—10.20		—10.03		—24.10	—15.82	—24.53	—14.57
	(—12)							
$2d\ ^5/_2$					—19.86	—11.12	—20.31	—10.35
$1g\ ^7/_2$					—21.02	—12.54	—21.76	—11.78
$3s\ ^1/_2$					—17.93	— 8.83	—18.52	— 7.67
$2d\ ^3/_2$					—18.16	— 9.40	—18.78	
$1h\ ^{11}/_2$					—15.95	— 7.89	—15.95	— 8.53
						(—8.03)		
$2f\ ^7/_2$					—11.50		—12.03	— 7.30
$1h\ ^9/_2$					—11.77		—11.77	
$3p\ ^3/_2$					— 8.99		— 9.57	
$2f\ ^5/_2$					— 9.18		— 9.72	
$1i\ ^{13}/_2$					— 8.13		— 8.23	
$3p\ ^1/_2$					— 7.62		— 8.21	
					(—7.37)			

$$+ g(\varrho(r_1))\,\tau(r,\varrho(r_1))\,\frac{\partial\tau\,(r_1\,\varrho(r_1))}{\partial\varrho\,(r)}\Big] +$$

$$+ v_2^x(r)\Big[\frac{1}{2}\,\frac{\partial g\,(\varrho(r_1))}{\partial\varrho(r_1)}\,\varrho(r_1)^{2/3}\,\tau^2(r_1\,\varrho(r_1)) +$$

$$+ \frac{1}{3}\,g(\varrho(r_1))\,\varrho(r_1)^{-1/3}\,\tau^2\,(r_1\,\varrho(r_1)) +$$

$$+ g\,(\varrho(r_1))\,\varrho(r_1)^{2/3}\,\tau\,(v_1\,\varrho(r_1))\,\frac{\partial\tau\,(r_1\,\varrho(r_1))}{\partial\varrho(r_1)}\Big],$$

$$\gamma = \frac{1}{2}\,v_1^x(r)\,\frac{\partial g\,(\varrho(r_1))}{\partial\varrho(r_1)}\,\varrho(r_1\,r_2)^2 -$$

$$- \frac{1}{2}\,v_2^x(r)\Big[\frac{\partial g\,(\varrho(r_1))}{\partial\varrho(r_1)}\,\varrho(r_1)^{1/3}\,\varrho(r_2)^{1/3} + \qquad \text{(A,3)}$$

$$+ \frac{2}{3}\,\varrho(r_1)^{-2/3}\,\varrho(r_2)^{1/3}\,g\,(\varrho\,(r_1))\Big]\varrho(r_1\,r_2)^2,$$

$$\delta = \left[v_1^x(r) - v_2^x(r)\,\varrho(r_1)^{1/3}\,\varrho(r_2)^{1/3}\right] g\,(\varrho(r_1))\,\varrho(r_1\,r_2)\,. \qquad \text{(A,4)}$$

If we have different neutron and proton densities, the total energy can be written as

$$W = W_{kin} + \int w\,(\varrho_n(R),\,\varrho_P(R))\,d^3R +$$

$$+ \frac{1}{2}\int v_\varrho^{1D}(r_1\,\varrho_n)\,g_1(\varrho_n(r_1))\,[\varrho_n(r_2) - \varrho_n(r_1)]\,\varrho_n(r_1)\,d^3r_1\,d^3r_2 +$$

$$+ \frac{1}{2}\int v_1^{1D}(r_1\,\varrho_P)\,g_1(\varrho_P)\,[\varrho_P(r_2)\,\varrho_P(r_1) - \varrho_P(r_1)^2]\,d^3r_1\,d^3r_2 +$$

$$+ \int v_2^{1D}(r,\varrho_n,\varrho_P)\,g_2(\varrho_n\,\varrho_P)\;[\varrho_n(r_2) - \varrho_n(r_1)]\;\varrho_P(r_1)\,d^3r_1\,d^3r_2 +$$

$$+ \frac{1}{2}\int v_1^{1x}(r_1\,\varrho_p)\,g_1(\varrho_n)\,[\varrho_n(r_1\,r_2)^2 - \tau_n^2(r\varrho_n)]\,d^3r_1\,d^3r_2 + \qquad \text{(A,5)}$$

$$+ \frac{1}{2}\int v_1^{1x}(r\varrho_P)\,g_1(\varrho_P)\,[\varrho_P(r_1\,r_2)^2 - \tau_p^2(r\varrho_P)]\,d^3r_1\,d^3r_2 +$$

$$+\int v_2^{1x}(r\varrho_n\,\varrho_P)\,g_2(\varrho_n\,\varrho_P)\,[\varrho_n(r_1\,r_2)\,\varrho_P(r_1\,r_2)-$$

$$-\tau_n(r\varrho_n)\,\tau_P(r\varrho_P)]\,d^3r_1\,d^3r_2+$$

$$+\frac{c}{8}\int\frac{1+g_1(\varrho_P)}{2}\,\frac{\varrho_P(r_1)\,\varrho_P(r_2)}{|\mathbf{r}_1-\mathbf{r}_2|}\,d^3r_1\,d^3r_2$$

and from this we get a coupled differential-integral equation system for ϱ_n, ϱ_p

$$-\hbar^2/2m\,\Delta\varphi_i^n(r_1)+\alpha_1\big(\varrho_n(r_1),\varrho_P(r_1)\big)\varphi_i^n(r_1)+$$

$$+\int\beta_1\big(\varrho_n(r_1)\,\varrho_P(r_1)\,\varrho_n(r_2)\,\varrho_P(r_2)\,r_1\,r_2\big)\,d^3r_2\,\varphi_n^i(r_1)+ \qquad \text{(A,6)}$$

$$+\int\gamma_1\big(\varrho_n(r_1\,r_2)\,\varrho_P(r_1\,r_2)\,\varrho_n(r_1)\,\varrho_n(r_2)\,\varrho_P(r_1)\,\varrho_P(r_2)\big)\,d^3r_2\,\varphi_i^n(r_1)+$$

$$+\int\delta\big(\varrho_n(r_1\,r_2)\,\varrho_P(r_1\,r_2)\,\varrho_n(r_1)\,\varrho_n(r_2)\,r_1\,r_2\big)\,\varphi_i^n(r_2)\,d^3r_2=e_i^n\,\varphi_i^n(r_1)$$

and a similar equation for $\varphi^P(r_1)$. We can solve the system by iteration.

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ВЛИЯНИЕ ЗАВИСИМОСТИ СИЛ ОТ ПЛОТНОСТИ ПРИ РАСЧЕТАХ СВОЙСТВ КОНЕЧНЫХ ЯДЕР В ПЕРВОМ ПОРЯДКЕ ПРИБЛИЖЕНИЯ

Й. НЕЙМЕТ

Резюме

Проведены вычисления типа Хартри—Фока с учетом сил, зависящих от плотности и исследовано влияние зависимости плотности от сил. Определены полная и одночастичная энергия, средний радиус сферического ядра. Получено удовлетворительное согласие теоретических и экспериментальных данных.

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THE GLOBAL STRUCTURE OF THE UNIVERSE AND THE DISTRIBUTION OF QUASI-STELLAR OBJECTS

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Periodicities in the frequency distribution of quasars according to their redshifts (as well as other proposed regularities in their distribution on the sky) are shown to be compatible with the cosmological interpretation of the redshifts: they may be apparent geometrical phenomena in world models with multiply connected space sections. It is therefore a misconception that significant regularities would necessarily imply the existence of intrinsic redshift components in the spectra of quasars — as generally stated in the astronomical literature. Some further remarks on the connectivity properties of cosmological models are also made.

There are a number of arguments to indicate that the redshifts of QSOs are cosmological [1, 2]. On the other hand it has been argued recently that QSOs appear to exhibit such a non-random character in their distribution both according to redshift and position which could only mean that the redshifts are an intrinsic property of the QSOs [3]. Certain suggested properties of the distribution have since failed to pass the significance tests, but, of course, have not been disproved in this way [4]. Others seem likely to be of some importance, while most of them have remained without due analysis. Putting aside the issue of statistics, this note aims at calling attention to the fact, apparently unrecognized by both sides of the debate, that regularities in quasars' distribution admit the cosmological interpretation of the redshifts in a wide class of cosmological models.

Let us consider a space-time described by a Robertson—Walker metric. We then have, with the usual notations,

$$ds^2 = dt^2 - R^2(t)[d\chi^2 + S^2(\chi)(d\Theta^2 + \sin^2\Theta d\Phi^2)].$$

This line element for $t = \text{const}$ is compatible with infinitely many topologically different space forms of constant curvature [5]. Clearly some cosmological models with multiply connected space sections automatically produce apparent periodicities in the distribution of sufficiently old objects — regarded as negligible test particles — which are distributed in a not strictly homogeneous manner, i.e. which constitute large-scale "clouds" in a universe otherwise homogeneous in first approximation. Essentially the same clouds — seen at different stages of their evolution — could be observed repeatedly in the models

under consideration. In reality the clouds may be "local" (in the sense of being situated at the distance of their first appearance) yet the route covered by their light may be measured approximately by their redshifts in suitably chosen models (see later). In this connection two points are to be noticed. Firstly, contrary to the case of a simply connected spherical space, in our models the

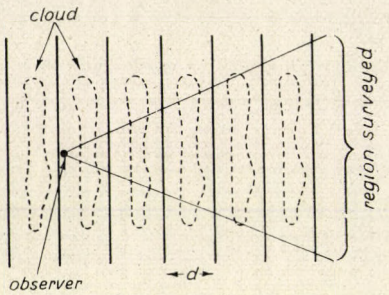

Fig. 1

frequency of light revolution has nothing to do with the curvature of the space in question. (Cf. the analogy of the surface of any infinitely long cylinder, which has zero Gaussian curvature just like the Euclidean plane.) Secondly, the light travel time for a revolution may well be more than the age of individual objects, if the cloud, as such, outlives them. — We see no strong reason why the latter assumption should not apply to "clusters" of QSOs.

It is known from the elements of geometry [6] that any space form of constant curvature can be derived from a simply connected spherical, flat or hyperbolic "universal covering space" by introducing into the latter a discontinuous group of fixed point free isometric transformations and identifying its points which correspond to each other according to the transformations of the group. — For example by the group of parallel translations (n times a given length d) a cylinder is obtained from the two-dimensional Euclidean space. (See Fig. 1). As a consequence one finds that the observable properties of a multiply connected model universe of the considered type are identical with those of a corresponding "universal covering model" populated by equal configurations in strictly congruent cells and all the known formulae of observational cosmology hold in this crystal-like covering. These models naturally show periodicities in the spatial coordinate distance, χ. However, when they are applied to the real universe, evolutionary effects and observational selections have to be accounted for, which may make the periodicities obscure. Although it is premature to discuss the question of the best fitting model on the basis of the inadequate information available, there are still some remarks relating these models to observations which seem to be pertinent.

One easily finds models in which the period is "normal" in one region of the sky and "doubled" in an antipodal region, as suggested by BELL [3]. Such a phenomenon can be found both in some Euclidean space versions — orientables and non-orientables alike — and in some of the simplest spherical space forms with cyclic fundamental groups. The tendency for the redshifts to increase outwards from the "central" point of a cloud (admitting to draw spiral joining lines in it with increasing redshifts) may be due to a nearly orthogonal view on a flattened cloud or to secondary intrinsic redshift components. The existence of apparently associated objects with different redshifts near to one line of sight [3] is a general property of models with multiply connected spaces. The angular sizes of the parts of the cloud-images situated within the region of the sky surveyed (see Fig. 1) may be roughly equal for different redshifts, as proposed by BELL, especially in an expanding model where the angular sizes of distant objects remain relatively large. Nevertheless, the advantage of spherical spaces in interpreting this phenomenon is obvious. Our conception is likely to be most vulnerable in the transition from periodicities in χ to those in the redshift. These distance parameters are convertible only in models with a nearly exponential expansion law and with a deceleration parameter $q_0 = -(\ddot{R}_0 R_0)/\dot{R}_0^2 \sim -1$, which is not a good fit to recent Hubble diagrams [7], provided our theories on galaxy evolution prove correct. It must be pointed out, however, that changing periods in χ can be found in some models, thus q_0 may be higher. Note also that this difficulty disappears in some "non-Doppler cosmologies". Summing up, we may say that at the moment no conclusive argument from regularities in the distribution of QSOs against their "Hubble distance" appears to be possible.

Apart from the applicability or otherwise of multiply connected spaces to the QSO problem it is worth mentioning that a search for apparent recurrences in the distribution of observable objects on a cosmological scale is an empirical approach to the topology of the universe (cf. [5a]). A direct observation concerning the global structure of the universe might have far-reaching consequences. For example to observe that the space is not orientable is to exclude spaces of constant positive curvature. This hints at a possibility of an absolute delimitation of the space curvature by topological means. Furthermore, the same global experience would imply that the CP symmetry breaking in elementary particle interactions is not true at least everywhere in the universe [8]. (Some related inferences might be the existence of mirror-particles or that of galaxies made up of antimatter.) An observed multiply connectedness of the space would require that the field equations of physics show periodicities both in a geometrical sense and in matter distribution which is possible in special cases [9] but is by no means self-evident in general. This would provide a method of testing field equations that is sensitive to the higher order terms undetectable in laboratories. Finally both homogeneity and isotropy

of the universe might have a completely new interpretation in a "crystal model" [10]. It is clearly a promising task to study the global aspects of cosmology in more detail.

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ГЛОБАЛЬНАЯ СТРУКТУРА ВСЕЛЕННОЙ И РАСПРЕДЕЛЕНИЕ КВАЗИЗВЁЗДНЫХ ОБЪЕКТОВ

Г. ПААЛ

Р е з ю м е

Показано, что периодичности в распределении частот квазаров по красному смещению (а также и другие предложенные регулярности в их распределении на небе) совместимы с космологической интерпретацией красного смещения: регулярности такого типа могут быть кажущиеся геометрические явления в моделях Вселенной с многосвязными пространственными сечениями. Таким образом получено опровержение обычного в астрономической лутературе вывода о том, что обнаружение статистически значимых регулярностей безусловно означало бы существование собственных компонентов красного смещения в спектре квазаров. Сделаны некоторые дальнейшие замечания по поводу свойств связности космологических моделей.

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CALCULATION OF ELECTRON SCATTERING USING THE STATISTICAL ATOM MODEL INCLUDING THE INHOMOGENEITY CORRECTION

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The cross-sections for scattering of low energy electrons are calculated using the statistical atom model including the inhomogeneity correction. Results are compared with the empirical data.

It is well known that if we incorporate the inhomogeneity correction of GOMBÁS [1] in the statistical atom model we arrive at an atom model, which besides its simplicity describes many features of atoms in a very good approximation [2]. The electron density of this model approximates the wave mechanical Hartree—Fock distribution better than the original model including WEIZSÄCKER'S [3] correction and it behaves exactly like the wave-mechanical distribution at the nucleus and at large distances from the nucleus.

As is known, the calculation of the atomic cross-sections of the collision of low energy electrons can be treated by the method of partial waves.

The differential cross-section is determined by the following expression:

$$|f(\vartheta)|^2 = \frac{1}{k^2}\left|\sum_l (2l+1)e^{i\delta_l}\sin\delta_l P_l(\cos\vartheta)\right|^2, \tag{1}$$

where k is the wave number, which is proportional to the square root of the energy of the incident beam of electrons, l is the angular momentum quantum number, δ_l is the phase shift of the l-th partial wave. The total cross-section is given by

$$\sigma(\vartheta) = \int |f(\vartheta)|^2 \, d\Omega = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\delta_l. \tag{2}$$

Concrete calculations have been made referring to the cross-section for scattering of 0.2 keV electrons by Kr atoms. For the purpose of determining phase-shift, first of all we have to solve the radial Schrödinger equation, which is given in atomic units:

$$\frac{d^2R_l}{dr^2} + \frac{2}{r}\frac{dR_l}{dr} + 2[E-V(r)] - \frac{1}{2}\frac{l(l+1)}{r^2}R_l = 0. \tag{3}$$

If we introduce the wave number defined by $k^2 = 2E$ and replace the radial wave function R_l by the function

$$f_l(r) = \frac{1}{r} R_l(r)$$

then

$$\frac{d^2 f_l(r)}{dr^2} + \left(k^2 + 2V(r) - \frac{l(l+1)}{r^2}\right) f_l(r) = 0. \tag{4}$$

For the equation (4) to be soluble, we have to know the potential $V(r)$.

The well-known equation is valid between the potential and density

$$V(r) = e^2 \int \frac{\varrho(\bar{r}')}{|\bar{r} - \bar{r}'|} dv', \tag{5}$$

where $\varrho(r)$ has been calculated by GOMBÁS [2]. We have put that density in (5) and have performed the integration numerically. The results are given in Table I.

Table I

The potential function

r	$V(r)$	r	$V(r)$
0.0005	71 836.58	0.024	1343.84
10	35 836.58	28	1131.44
15	23 836.39	32	972.664
20	17 836.39	36	849.615
25	14 236.66	40	751.556
30	11 836.69	44	671.674
35	10 122.46	48	605.410
40	8 836.80	52	549.601
45	7 836.88	56	502.000
50	7 036.95	60	460.963
0.006	5 837.14	0.068	393.908
7	4 980.21	76	341.547
8	4 337.60	84	299.652
9	3 837.88	92	265.458
0.010	3 438.17	0.100	237.087
		0.108	213.223
0.012	2 838.82		
14	2 410.97	0.124	175.468
16	2 090.32	140	147.098
18	1 841.16	156	125.143
20	1 642.02	172	107.747
		188	93.7009

Table Ia

The potential function

r	$V(r)$	r	$V(r)$
0.204	82.1764	1.212	1.52804
220	72.5946		
236	64.5348	1.340	1.09878
252	57.6892	1.468	0.799905
268	51.8235	1.596	0.587895
284	46.7576	1.724	0.435458
		1.852	0.323391
0.316	38.5108	1.980	0.240732
348	32.1336	2.108	0.179554
380	27.1061	2.236	0.133318
412	23.0778	2.364	0.098807
444	19.8057	2.492	0.072002
476	17.1168	2.620	0.052183
508	14.8836	2.748	0.036779
		2.876	0.024965
0.572	11.4412	3.004	0.016305
636	8.95300	3.132	0.009358
700	7.10342	3.260	0.002
764	5.70296	3.388	0.000334
828	4.62796	3.644	
892	3.78890		
956	3.12540		
1.020	2.59270		
1.084	2.16211		
1.148	1.81398		

As the potential is given in the form of a numerical table, the Schrödinger equation also has to be solved with the method of numerical integration. In the point $r = 0$, the initial condition is $f_l(r) = 0$, because the radial wave function $R_l(r)$ must be free from singularities. As the second initial condition we have to give the function $f_l'(r)$ at the point $r = 0$. Since the function $f_l(r)$ is determined only up to a normalisation factor, therefore $f_l'(0)$ can be chosen arbitrarily. We have chosen it as $f_l'(0) = 1$. Starting from that initial data, we have computed the functions $f_l(r)$ by the method of Runge-Kutta. For that purpose, so that the phase-shift can be determined, we have to carry out these calculations up to such large values of r, where the potential disappears, as is

Table II

l	tg δ_l	δ_l
0	11.130	1.481
1	—0.61147	2.593
2	0.14136	0.1404
3	2.4999	1.190
4	0.57154	0.5192
5	0.27362	0.2671
6	0.29026	0.2825
7	0.12502	0.1244
8	0.08722	0.0870
9	0.018836	0.0188
10	0.013692	0.0137
11	0.0012470	0.00125
12	0.0012470	0.00125
13	0.00125	0.00125
14	0.0012220	0.00122
15	0.0011704	0.00117
16	—0.0029548	0.
17	0.	

well known from the method of partial waves. At least, the cross-section has been obtained from Eq. (1) having a knowledge of the phase-shift. In order to determine the phase-shift the most simple method is to seek that value of r_0 at which point the radial wave function would disappear, in the asymptotic domain of large values of r. In that domain the solution of Eq. (3) is of the form:

$$R_l(r) = a_l\, j_l(kr) + b_l\, n_l(kr), \tag{6}$$

where a_l and b_l are integration constants, j_l and n_l are the spherical Bessel functions. According to the expression (6) when $R_l(r_0) = 0$

$$\frac{b_l}{a_l} = -\frac{j_0(kr_0)}{n_l(kr_0)}\,. \tag{7}$$

Let us introduce the terms α_l and δ_l instead of the integration constants a_l and b_l, in the following manner:

$$a_l = i^l(2l+1)\,\alpha_l \cos\delta_l\,,$$

$$b_l = -i^l(2l+1)\,a_l \sin\delta_l\,,$$

Table III

Differential cross-section as a function of angle

ϑ	$\sigma(\vartheta)$
0°	28.120
10°	17.371
20°	4.0825
30°	1.2516
40°	1.1412
50°	0.15962
60°	0.26174
70°	0.075764
80°	0.003335
90°	0.16522
100°	0.51587
110°	0.74094
120°	0.59230
130°	0.62942
140°	0.02740
150°	0.22784
160°	0.68326
170°	1.3518
180°	1.7610

then we shall get this expression:

$$\tan \delta_l = \frac{j_l(kr_0)}{n_l(kr_0)} . \tag{8}$$

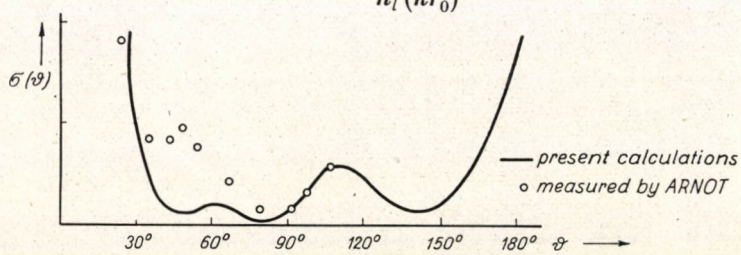

Fig. 1. Differential cross-section for scattering of 200 eV electrons by Kr atoms

Table II contains our results obtained for the scattering of 0.2 keV electrons by Kr atoms. From the phase-shift given in Table II, we can easily obtain the cross-section for scattering electrons according to (1). Our results are given in Table III. The mesh of ϑ used was 10°. The cross-sections as a function of angle ϑ are shown in Fig. 1. We compared our results with the data measured

by Arnot, which are plotted by small circles. We can see that the data agree with our result. It is quite satisfying especially for all the maxima. The experimental points of Arnot do not extend over the values of $\vartheta = 100°$. According to our results a hard backward scattering had been obtained as is shown in Fig. 1. From this it can be concluded from our calculations that the statistical atom model including the inhomogeneity correction gives a good approximation to a description of such a complicated phenomenon as the angular distribution of the cross-section for scattering of low energy of electrons.

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РАСЧЕТ РАССЕЯНИЯ ЭЛЕКТРОНОВ НА ОСНОВЕ СТАТИСТИЧЕСКОЙ МОДЕЛИ АТОМА, СОДЕРЖАЩЕЙ ПОПРАВКУ НА НЕОДНОРОДНОСТИ

А. ДОБАИ-СЕГЛЕТ

Резюме

Вычисляется поперечное сечение рассеяния электронов низкой энергии, применяя статистическую модель атома с поправкой на неоднородность. Результаты сравниваются с экспериментальными данными.

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STABILITY OF STATIONARY THERMODYNAMIC STATES

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The stability of stationary thermodynamic states will be examined by means of a variation principle. The Euler—Lagrange equations, existing as the necessary condition of the extremum, provide the total stationary balance equation of the entropy production where — beside the spontaneous entropy production — the source terms also appear. This method is equally suitable for describing stable and unstable stationary states, moreover it contains the total stationariness. It will be shown that the stability of the stationary equilibrium is secured by the positive definite character of the conductivity matrix. Applying this principle for the interaction of homogeneous bodies we get the simplest model and stability criteria for stationariness.

Introduction

The thermodynamic interpretation of stationary states according to PRIGOGINE and DE GROOT [1], can be given as follows. If a system is characterized by n independent general thermodynamic forces $X_1, X_2, \ldots, X_n$ and is kept in a state with fixed $X_1, X_2, \ldots, X_k$ $(k < n)$ and minimum entropy production σ, the "current" density $\dot{\alpha}_i = j_i$ belonging to the indices $i = k+1$, $k+2, \ldots, n$ disappear. Here α_i is the deviation of the i-th extensive parameter x_i from the equilibrium:

$$\alpha_i = \frac{x_i - (x_i)_0}{x_{n+1}}, \quad i = 1, 2, \ldots, n; \tag{1}$$

where the starting point of the scale of the extensive parameter x_i is related to the state of equilibrium. $(x_i)_0$ denotes the equilibrium value of the i-th extensive variable while x_{n+1} the volume V or mass m of the body. (Correspondingly, α_i is density or any specific quantity, and therefore of intensive character.)

According to the interpretation above, those currents will be zero which as conjugate variables correspond to the forces $X_{k+1}, X_{k+2}, \ldots, X_n$ not being fixed. Such a state is called stationary of k-th order. (It must be remarked that here entropy production means the spontaneous one which is independent from the accidental source of the extensive quantities characterizing the interactions.)

The entropy production belonging to this state can easily be computed. Namely, the necessary minimum condition for the indices $i = k + 1, k + 2, \ldots, n$

$$\frac{\partial \sigma}{\partial X_i} = \frac{\partial}{\partial X_i} \sum_{i,j=1}^{n} L_{ij} X_i X_j = 2 \sum_{j=1}^{n} L_{ij} X_j = 2 \dot{\alpha}_i = 0 , \tag{2}$$

where L_{ij} are the elements of the conductivity matrix.

It follows from this that if among the fixed X_i belonging to the indices $i = 1, 2, \ldots, k$ there is one which is not zero for these indices $\dot{\alpha}_i \neq 0$, $i = 1, 2, \ldots, k$. Thus the minimal entropy production will be

$$\sum_{i=1}^{k} \sum_{j=1}^{n} L_{ij} X_i X_j = \sum_{i=1}^{k} \dot{\alpha}_i X_i = \sigma_{\min} . \tag{3}$$

It can also be seen that because of $\dot{\alpha}_i \neq 0$, $i = 1, 2, \ldots, k$ the stationariness is only partial and can relate only to stable states, namely if $L = L[L_{ik}] > 0$. In the vicinity of a non stable state, equation $\dot{\alpha} = LX$ is not even valid, so the minimal entropy production can characterize a stable state only.

It should be mentioned that if we consider the equation $X = -g\alpha$ too, then we reach a contradiction, since

$$\begin{aligned} \dot{\alpha} &= LX, \\ X &= -g\alpha, \end{aligned} \tag{4}$$

simultaneously describe the non-stationary process only, the decay of the non-equilibrium state without external constraint. Even the conditions of their deduction exclude stationariness. Here g is the entropy matrix

$$-g_{ik} = \left(\frac{\partial^2 \alpha_s}{\partial \alpha_i \partial \alpha_k} \right)_0 = \left(\frac{\partial^2 \alpha_s}{\partial \alpha_k \partial \alpha_i} \right)_0 = -g_{ki} ,$$

where α_s is the α-parameter of entropy.

PRIGOGINE and GLANSDORFF [2], [3] later generalized the minimum principle of entropy production in such a way that for a stationary process in the case of a boundary condition being constant in time:

$$\int_V \sum_i j_i \, dX_i \, dV \leqq 0 . \tag{5}$$

Completing this they have shown [4] that for macroscopic mechanical changes the total differential

$$d\Phi = \int_V \sum_i j_i' \, dX_i' \, dV \leqq 0 \tag{6}$$

exists near the state of equilibrium. They denoted this inequality as the genera evolution criterion.

The principle can be used if the conductivity coefficients L_{ik} can depend on place and time only but are independent of the thermodynamical parameters. Though the authors pointed out that in a state near the stationary equilibrium the L_{ik} can be taken as belonging to the supposedly known stationary distribution of the y_i:

$$L_{ik} = L_{ik}(y_{i0}(r, t))$$

but, since y_{i0} is known, the L_{ik} are still given as functions of place and time, where y_i are intensive parameters characterizing the interactions.

The general investigation of stationariness

A variation principle [5, 6] can be applied for the general description of stationary states. The exact equations of the stationary state will be derived therefrom. The expedient variation principle is:

$$\int_t \iiint_V \mathfrak{L}(r_1, r_2, r_3, t; y_1, y_2, \ldots, y_n; \nabla y_1, \nabla y_2, \ldots, \nabla y_n) dr_1, dr_2, dr_3\, dt = \text{extr.}, \tag{7}$$

where the variables of the Lagrange function $\mathfrak{L}$ are the space coordinates r_1, r_2, r_3, the time t, their functions to be determined $y_1, y_2, \ldots, y_n$ and the gradients $\nabla y_1, \nabla y_2, \ldots, \nabla y_n$, it does not, however, contain $\partial y_i/\partial t$. Using the notation $\partial y_i/\partial r_k = y_i^{(r_k)}$, $k = 1, 2, 3$ the Euler—Lagrange equations of the variation problem will be

$$\frac{\partial}{\partial r_1}\frac{\partial \mathfrak{L}}{\partial y_i^{(r_1)}} + \frac{\partial}{\partial r_2}\frac{\partial \mathfrak{L}}{\partial y_i^{(r_2)}} + \frac{\partial}{\partial r_3}\frac{\partial \mathfrak{L}}{\partial y_i^{(r_3}} - \frac{\partial \mathfrak{L}}{\partial y_i} = 0\,. \tag{8}$$

$$i = 1, 2, \ldots, n$$

Applying these for the stationary thermodynamical Lagrange function:

$$\mathfrak{L} = \sum_i y_i q_i + \frac{1}{2}\sum_i (\nabla y_i, j_i)\,, \tag{9}$$

where q_i is the source density of the i-th extensive quantity, $\nabla y_i = X_i$ is the i-th component of the general force, and thus

$$j_i = \sum_k L_{ik} \nabla y_k = \sum_k L_{ik} X_k \tag{10}$$

that is

$$\sum_i (\nabla y_i, j_i) = \sum_{i,k} L_{ik}(\nabla y_i, \nabla y_k) = \sum_{i,k} L_{ik}(X_i, X_k)\,. \tag{11}$$

Taking these into consideration

$$\begin{aligned}
\frac{\partial \mathfrak{L}}{\partial y_i^{(r_1)}} &= L_{i1} y_1^{(r_1)} + \ldots + L_{in} y_n^{(r_1)} = j_{i(r_1)}\,, \\
\frac{\partial \mathfrak{L}}{\partial y_i^{(r_2)}} &= L_{i1} y_1^{(r_2)} + \ldots + L_{in} y_n^{(r_2)} = j_{i(r_2)}\,, \\
\frac{\partial \mathfrak{L}}{\partial y_i^{(r_3)}} &= L_{i1} y_1^{(r_3)} + \ldots + L_{in} y_n^{(r_3)} = j_{i(r_3)}
\end{aligned} \tag{12}$$

and

$$\frac{\partial \mathfrak{L}}{\partial y_i} = q_i\,. \tag{13}$$

Here the L_{ik} and q_i are given function of r_1, r_2, r_3 and t, but they are independent from the y_i and from the derivatives of these.

Using (12) and (13) according to (8) we get

$$\operatorname{div} j_i - q_i = 0, \qquad i = 1, 2, \ldots, n \tag{14}$$

which represent the stationary variety of the continuity equations, as the differential equations of the irreversible thermodynamics for the stationary case. Multiplying (14) by y_i

$$y_i \operatorname{div} j_i = y_i q_i,$$

where

$$y_i \operatorname{div} j_i = \operatorname{div} y_i j_i - (\nabla y_i, j_i),$$

that is

$$\operatorname{div} y_i j_i = y_i q_i + (\nabla y_i, j_i).$$

Summing for i and using $j_s = \sum_i y_i j_i$ we get the stationary balance equation of entropy:

$$\operatorname{div} j_s = \sum_i y_i q_i + \sum_i (\nabla y_i, j_i). \tag{15}$$

The stationary "motion equations" (14) and the entropy balance equation (15) — which we have got from it — correspond to the validity of the following equations:

$$\frac{\partial \varrho_i}{\partial t} = 0\,, \quad i = 1, 2, \ldots, n \tag{16}$$

and

$$\frac{\partial \varrho_s}{\partial t} = \sum_i y_i \frac{\partial \varrho_i}{\partial t} = 0\,, \tag{17}$$

which are just the conditions of stationariness. (Here ϱ_i is the density of the i-th extensive quantity, and ϱ_s that of the entropy.) If all $q_i = 0$, $i = 1, 2, \ldots n$, which occurs in some cases, then expression (15) represents the spontaneous entropy production

$$\operatorname{div} j_s = \sum_i (\nabla y_i, j_i) = \sum_{i,k} L_{ik} X_i X_k = \sigma = \text{const} \tag{18}$$

since — because of the ϱ_i being constant in time — the $y_i = y_i(\varrho_1, \varrho_2, \ldots, \varrho_n)$ and ∇y_i are also constant.

The physical meaning of this is that entropy is being produced at each place and in each moment of time at a constant velocity and in such a way that:

$$\left| \int \mathfrak{L}\, dt \right|_{\text{instac}} > \left| \int \mathfrak{L}\, dt \right|_{\text{stac}}\,,$$

that is

$$\int \left(\frac{\partial \varrho_s}{\partial t} + \operatorname{div} j_s + \sum_i y_i q_i \right) dV\, dt > \int \left(\operatorname{div} j_s + \sum_i y_i q_i \right) dV\, dt, \tag{19}$$

respectively

$$\int \frac{\partial \varrho_s}{\partial t}\, dV\, dt \geqq 0\,, \tag{20}$$

where the sign of equality corresponds just to the stationary state. According to this non-stationary entropy production is always bigger than that belonging to the stationary state.

Let us examine whether the extremum (7) really means a minimum. In order to simplify the computations two independent intensive quantities y_1 and y_2 will be considered. Then (9) will be

$$\mathfrak{L} = y_1 q_1 + y_2 q_2 + \frac{1}{2} L_{11}(\nabla y_1)^2 + L_{12}(\nabla y_1, \nabla y_2) + \frac{1}{2} L_{22}(\nabla y_2)^2, \tag{9'}$$

where

$$\begin{aligned} j_1 &= L_{11} \nabla y_1 + L_{12} \nabla y_2, \\ j_2 &= L_{21} \nabla y_1 + L_{22} \nabla y_2, \end{aligned} \tag{21}$$

and

$$\begin{aligned} \operatorname{div} j_1 &= q_1, \\ \operatorname{div} j_2 &= q_2. \end{aligned} \tag{22}$$

The Euler—Lagrange equations have been obtained by varying y_i in the form:

$$\bar{y}_i + \varepsilon_i \eta_i(r, t) = \bar{y}_i, \tag{23}$$

where r now denotes the space coordinates r_1, r_2, r_3.

By means of this the Lagrange function can be constructed

$$\bar{\mathfrak{L}} = \mathfrak{L}(r, t; \bar{y}_1, \bar{y}_2; \nabla\bar{y}_1, \nabla\bar{y}_2) \tag{24}$$

and the integral (7)

$$I(\varepsilon_1, \varepsilon_2) \equiv \int \bar{\mathfrak{L}}\, dr\, dt\,. \tag{25}$$

These are completed by a given boundary condition, that is, no variation has occurred on the boundary where $y_1 = \bar{y}_1$, $y_2 = \bar{y}_2$ and so $\eta_1 = \eta_2 = 0$.

Therefore, the total second derivative of I is:

$$I^{(2)} = \int [L_{11}(\nabla\eta)^2 + 2L_{12}(\nabla\eta_1, \nabla\eta_2) + L_{22}(\nabla\eta_2)^2]\, dr\, dt. \tag{26}$$

$I^{(2)}$ is positive if the matrix L is positive definite. Thus, in the case of a stationary state it follows that

$$\int \mathfrak{L}\, dr\, dt = \min. \tag{27}$$

As a result of our computations we stress that g and L must equally be positive definite to secure the stability of the static equilibrium while the stability of the stationary state is secured if matrix L alone is positive definite.

It can be seen that the thoughts followed here are general since they contain the case of *total* stationariness. Further *no extra* subsidiary conditions are necessary to (9). The meaning of the variation principle is also different. Namely, spontaneous entropy production is in accord with that from the Lagrange function only when each of the extensive quantities is source-free. This is not the case, for instance, in chemical reactions where each component of matter has its source. Thus, beside spontaneous entropy production the part originating from these *sources* also appears. A further noteworthy difference is that now stationariness — in compliance with the facts — is not connected with *stability*, which is an essential condition in the interpretation in physics literature since there the matrix L must be assumed to be positive definite, whereas the motion equations which can be obtained from the Lagrange functions are equally valid for stable and unstable stationariness since the Euler—Lagrange equations are only necessary conditions of the extremum. The q_i and L_{ik} together determine what sort of state sets in, in a particular case.

The interaction of homogeneous bodies

If a homogeneous system R — being investigated — has the volume V and is confined with the surface F, the non-stationary macroscopic balance of the change of the i-th extensive quantity is

$$\frac{d}{dt}\int_V \varrho_i \, dV + \int_F (j_i, dF) - \int_V q_i \, dV = 0 , \tag{28}$$

that is, the change $\dot{\alpha}_i$ per unit time is put together partly from the current I_i through the confining surface and partly from the source Q_i inside the body. Consequently

$$\dot{\alpha}_i = -I_i + Q_i . \tag{29}$$

The condition of stationariness is that $\dot{\alpha}_i = 0$. This can be realized if

$$I_i = Q_i \tag{30}$$

that is, the current from the chosen body R into another R^1 (or into the surroundings of R) is equal with the source inside of R. As homogeneous systems are being considered, I_i is determined by the forces on the boundary of the

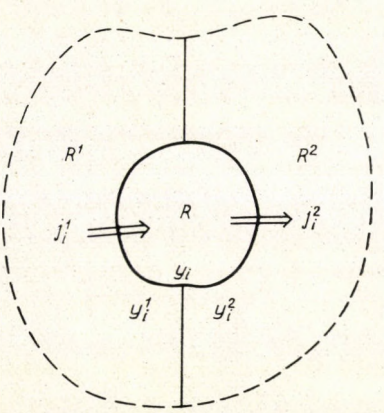

Fig. 1

two systems, Q_i, on the other hand by the inner structure of R. Hence the correspondence of I_i and Q_i, so this stationariness can be considered only as random. The case when it sets in may occur but is not from necessity. For the unconditional securing of the stationary state at least three bodies R^1, R, R^2 are needed (Fig. 1).

In this case $I_i^2 = I_i^{R \to R^2}$ can always be covered by means of $I_i^1 = I_i^{R^1 \to R}$ and Q_i. In general, this arrangement can be taken for the simplest model of stationariness but in this case Eqs. (4) need some modification

$$\dot{\alpha}_i = I_i^1 - I_i^2 + Q_i = \dot{\alpha}_i^1 - \dot{\alpha}_i^2 + Q_i = 0, \tag{31}$$

where any of the currents present can be taken for external generation $G_i(t)$ [7]. If

$$I_i^2 = \sum_k L_{ik}^2 X_k^2 = G_i(t),$$

then

$$\dot{\alpha}_i = \sum_k L_{ik}^1 X_k^1 - G_i(t) + Q_i(t) \tag{32}$$

and the balance equations for the extensive parameters are

$$-\dot{\alpha}_i^1 + \dot{\alpha}_i + \dot{\alpha}_i^2 = -I_i^1 + I_i^1 - I_i^2 + Q_i + I_i^2 = Q_i. \tag{33}$$

Information about entropy production is given by means of the equation $\alpha_s = \alpha_s(\alpha_1, \alpha_2, \ldots, \alpha_n)$:

$$\dot{\alpha}_s = \sum_i \frac{\partial \alpha_s}{\partial \alpha_i} \dot{\alpha}_i = \sum_i y_i \dot{\alpha}_i . \tag{34}$$

Since all the three bodies taking part in the process are homogeneous there is no inhomogeneity in R^1, R and R^2, but only on the boundaries. Thus, the boundaries isolating the bodies and having intensive parameters $y_i^1 \neq y_i$ and $y_i \neq y_i^2$ on their two sides, are responsible for the irreversibility. This fact can be expressed with the respective general forces which give information about the jump on the two boundaries. Then the entropy production balance according to (33) and (34) will be

$$\begin{aligned} -\dot{\alpha}_s^1 + \dot{\alpha}_s + \dot{\alpha}_s^2 &= \sum_i (-y_i^1 \dot{\alpha}_i^1 + y_i \dot{\alpha}_i + y_i^2 \dot{\alpha}_i^2) = \\ &= \sum_i (\dot{\alpha}_i^1 X_i^1 - \dot{\alpha}_i^2 X_i^2 + y_i Q_i) = \sum_i (I_i^1 X_i^1 - G_i X^2{}_i + y_i Q_i) \end{aligned} \tag{35}$$

in accordance with (15) which was deduced from the variation principle. Since the state of R is stationary, in (35) $\dot{\alpha}_s = 0$ and so $\dot{\alpha}_s^2 - \dot{\alpha}_s^1$ will be equal to the right side of the equation.

Returning to (32) and omitting the superscripts with the matrix formalism we have

$$\dot{\alpha} = LX - G(t) + Q(t). \tag{36}$$

If we consider the state equation $X = -g\alpha$ too, we get the motion equations describing the complete stationary state:

$$\dot{X} = -gLX + gG(t) - gQ(t), \tag{37}$$

$$\dot{\alpha} = -Lg\alpha - G(t) + Q(t). \tag{38}$$

From the point of the investigation of the stability of states we take the external generation for a disturbance by means of which a stationary state can be maintained.

In the case of $G(t) = G_0 = \text{const}$ and $Q(t) = Q_0 = \text{const}$, the solutions of these equations are:

$$X(t) = e^{-gLt}(-L^{-1}G_0 + L^{-1}Q_0 + X_{\text{initial}}) + L^{-1}G_0 - L^{-1}Q_0, \tag{39}$$

$$\alpha(t) = e^{-Lgt}(g^{-1}L^{-1}G_0 - g^{-1}L^{-1}Q_0 + \alpha_{\text{initial}}) - g^{-1}L^{-1}G_0 + g^{-1}L^{-1}Q_0. \tag{40}$$

These formulae show that both X and α contain a term constant in time, and another which decreases exponentially with time provided $gL > 0$. After a sufficiently long time has passed e.g. $t \to \infty$, remaining deviations α_i and forces X_i form a non-equilibrium ground level of constant value

$$X_{\text{ground}} = X(\infty) = L^{-1}G_0 - L^{-1}Q_0 = \text{const}, \tag{41}$$

$$\alpha_{\text{ground}} = \alpha(\infty) = -g^{-1}L^{-1}G_0 + g^{-1}L^{-1}Q_0 = \text{const}. \tag{42}$$

This is just the stationary limit case which sets in at $t = \infty$.

Turning the order of ideas, in the stationary state:

$$\dot{X} = -gLX + gG(t) - gQ(t) = 0, \tag{43}$$

$$\dot{\alpha} = -Lg\alpha - G(t) + Q(t) = 0, \tag{44}$$

from which we get

$$G(t) = LX + Q(t) = -Lg\alpha + Q(t) \tag{45}$$

as the general condition of stationariness for the expression of $G(t)$ provided the determinant of g-matrix is not zero. (45) shows directly that the value of the external generation securing the stationary state is constant:

$$G(t) = G_0 = \text{const}. \tag{46}$$

Choosing the value of the constant G_0 in (39) and (40) according to (45)

$$G_0 = LX_{\text{initial}} + Q_0 = -Lg\alpha_{\text{initial}} + Q_0 \tag{47}$$

or in the case $Q(t) = Q_0 = 0$

$$G_0 = LX_{\text{initial}} = -Lg\alpha_{\text{initial}} \tag{48}$$

the state will be stable stationary from the beginning. Namely, if we substitute this form of G_0 into (39) and (40) we get the results: $X = \text{const}$ and $\alpha = \text{const}$, and the magnitude of the resulting parameters is in accordance with (41) and (42).

It should be noticed that (45) is formally similar to the equation $\dot{\alpha} = LX$. This is the reason why the latter equation is also suitable for describing station-

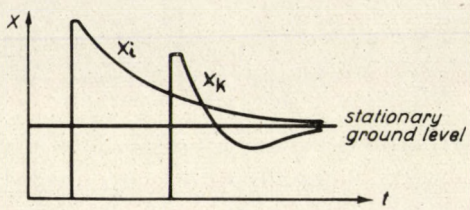

Fig. 2

ary processes. This correspondence is, however, only formal since — as we have seen — G_0 and $\dot{\alpha}$ have quite another meaning. Therefore, only a partial stationariness can be characterized with the relation $\dot{\alpha} = LX$.

If the established stationary state is perturbed with an external disturbance then it will be superposed upon this ground level.

Moreover, after the disturbance introduced has decayed in the way outlined, the system will return (possibly with oscillation) to this stable stationary state — as shown in Fig. 2.

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УСТОЙЧИВОСТЬ СТАЦИОНАРНЫХ ТЕРМОДИНАМИЧЕСКИХ СОСТОЯНИЙ

И. КИРШНЕР

Р е з ю м е

Рассматривается устойчивость стационарных термодинамических состояний с помощью вариационного принципа. Уравнения Эйлера—Лагранжа вытекающие как необходимые условия экстремума, дают полное стационарное уравнение баланса производства энтропии, где кроме спонтанного производства энтропии появляются также источные члены. Этот метод в одинаковой мере годится для описания устойчивых и неустойчивых стационарных состояний, и к тому же содержит полную стационарность. Показывается, что устойчивость стационарного равновесия обеспечивается уже положительно определённым характером матрицы проводимости. Применяя этот принцип к взаимодействию однородных тел, мы получим простейшую модель и критерии устойчивости стационарности

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INVESTIGATION OF $^{27}Al(d, \alpha)^{25}Mg$ NUCLEAR REACTION IN THE ENERGY RANGE $E_d = 650-540$keV USING A PLASTICS TRACK DETECTOR

By

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The angular distributions of the α_0 and α_1 groups from the $^{27}Al(d, \alpha)^{25}Mg$ nuclear reaction have been measured at deuteron energies $E_d = 650$, 585 and 540 keV using plastics track detector techniques. The angular distributions which are nearly isotropic have been analysed in terms of the Legendre polynomials. Assuming statistical compound reaction mechanism the relative intensity ratio of the two measured alpha groups could be reproduced by a simple calculation giving the statistical weight factors for the alpha transitions concerned.

1. Introduction

Recently the extensive study of the properties of plastics track detectors leads to their increasing use in experimental nuclear physics. In certain plastics the track diameter of charged particles entering the detectors at right angles — under suitable etching conditions — depends strongly on the energy and type of particles [1, 2]. By measuring the diameter distribution of the track holes an energy resolution of 200 keV can be reached for monoenergetic alpha particles under optimal conditions.

A possible use of these detectors, as recommended by us earlier, is the measurement of angular distribution of alpha particles emitted in nuclear reactions. A complete angular distribution can be measured by a single irradiation using bent plastics sheets around the target. This method enables experimental investigations of very low yield nuclear reactions emitting alpha particles to be made. By using proper etching techniques it is possible to distinguish the desired groups of α-particles from the unwanted ones (p, t, d) emitted from the background reactions. In our previous work we have already proved the utility of this detection method in the case of $^{19}F(d, \alpha)^{17}O$ nuclear reaction [3, 4]. In this paper, we describe a further use of this method in the study of $^{27}Al(d, \alpha)^{25}Mg$ reaction.

The measurements of angular distributions and excitation functions of α-groups emitted in the $^{27}Al(d, \alpha)^{25}Mg$ nuclear reaction below 5 MeV, at bom-

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barding energies 1.2—2.0 MeV [5], 1.4—2.3 MeV [6], 1.5—2.3 MeV [7], 1.5—2.6 MeV [8], 2.0—5.0 MeV [9] and 2.4—2.6 MeV [10], give results characteristic of the statistical compound reaction mechanism. For individual α-groups the excitation functions show resonance like maxima and the shape of angular distributions varies strongly with the bombarding energy. Generally these results have been analysed on the basis of the statistical compound reaction theory.

Below 1.2 MeV bombarding deuteron energy no data are available for ^{27}Al(d, α)^{25}Mg nuclear reaction. Owing to the low bombarding energy compared with the Coulomb barrier, the cross-sections in this region become so low that the measurement of angular distribution by the traditional methods becomes practically impossible. Using plastics track detectors we have been able to measure the angular distributions of the α_0 and α_1-groups from the ^{27}Al(d, α)^{25}Mg nuclear reaction even in the bombarding energy range 650—540 keV.

2. Experimental method

Deuterons were accelerated by the cascade generator of the Institute of Nuclear Research, Debrecen. The high voltage of the cascade generator was measured to 1% accuracy with a rotary-type voltmeter calibrated with (p, γ) resonances on ^{7}Li, ^{19}F and ^{27}Al. After passing through a 12° magnetic analyzer and collimating system, the ion beam hit the target placed in the centre of the vacuum chamber used for angular distribution measurements [11].

The aluminium target was evaporated on to copper backing foils of about 0.3 mg/cm^2 thickness. The target thickness was determined by measuring the shift of the 340 keV ^{19}F(p, $\alpha\gamma$) resonance line. Under suitable geometrical conditions the aluminium was evaporated from a point source on to the copper backings and copper backings having a thin ($\sim 5\mu$g/cm^2) CaF_2 film. In the latter case the energy shift of the 340 keV ^{19}F(p, $\alpha\gamma$) resonance line corresponding to the energy loss of protons in the aluminium layer was measured. The number of target nuclei per cm^2 was determined by using the dE/dx tables given by C. F. WILLIAMSON et al. [12]. The thickness of the aluminium targets was 25—30 keV.

The bombarding ion current was measured with a current integrator connected to a Faraday cup.

The cellulose acetate (T-Cellit) plastics detectors were irradiated in the reaction chamber mentioned. Two detector sheets, one in the angular range 20°—90° and the other in the range 90°—165° were fixed on the outer side of the curved wall of a stainless-steel cylindrical holder of diameter 90 mm having circular openings of 4.5 mm diameter at the desired angles. The emitted alpha particles passing through the openings entered perpendicularly in the surface of the plastics detectors.

The energy dependence of the emitted alpha groups on laboratory angles was eliminated within an accuracy of ± 0.1 MeV by using suitable Al-degrading foils on the inner side of the cylindrical holder in the position of the circular openings.

The ^{3}He particles emitted from the d + d reaction produced a track density on the entering surface of the detectors about three order of magnitude higher than the examined α-groups from the $^{27}Al(d, \alpha)^{25}Mg$ nuclear reaction. The tracks of the low energy ^{3}He particles having a range of only a few microns in the detector material appeared after a very short etching time. The large track density of the ^{3}He particles resulted in circular opal spots on the irradiated surface of the detectors marking the exposed areas at various angles.

Owing to nitrogen contamination on the targets, only the α_0 and α_1-groups from the $^{27}Al(d, \alpha)^{25}Mg$ reaction could be distinguished from the disturbing α_1 and α_2-groups of the $^{14}N(d, \alpha)^{12}C$ nuclear reaction by etching the plastics detectors from the back surface. In this case, detectors of a thickness equal to the range of the α_0-group in the detector material had to be chosen. As the T-Cellit available in our laboratory had a thickness of about 100 μ, it was reduced to the required thickness by etching it in the following solution at 60° C:

$$30 \text{ g } K_2Cr_2O_7 + 95 \text{ cm}^3 H_2SO_4 + 120 \text{ cm}^3 H_2O.$$

In this solution the thickness of T-Cellit reduced uniformly at quite a fast rate (21 μ/h) but according to our experience the thickness reducing process had to be stopped before about 5 μ of the required thickness. The remaining layer had to be removed by etching in the track revealing solution [3]. This change was needed because the dichromate solution was found to diffuse a few microns in the detector surface and change its track revealing features as compared with the rest of the material.

Using the above mentioned process the thickness of the detector was reduced to such an extent that almost the whole of the etchable part of the α_1-groups from the $^{14}N(d, \alpha)^{12}C$ reaction passed through the detector thickness. On etching the detector from the back the tracks of the α_0 and α_1-groups from the $^{27}Al(d, \alpha)^{25}Mg$ reaction appeared in succession and they could be distinguished from each other owing to the difference in their appearance time and diameters.

It should be mentioned here that the detectors were first etched from both sides for a short time and when the dense ^{3}He tracks marked the boundary of openings on the irradiated surface of the plastics sheets then the etching was continued only from their back by fixing them in a suitable plexi frame in order to avoid too much thinning of the detectors.

3. Results and discussion

Fig. 1 shows the measured absolute differential cross-sections of the α_0 and α_1-groups from the $^{27}Al(d, \alpha)^{25}Mg$ nuclear reaction in the centre-of-mass system at $E_d = 650$, 585 and 540 keV bombarding energies. The bars in the figure represent the error of the relative angular distribution. According to the uncertainty in the target thickness determination the errors in the absolute

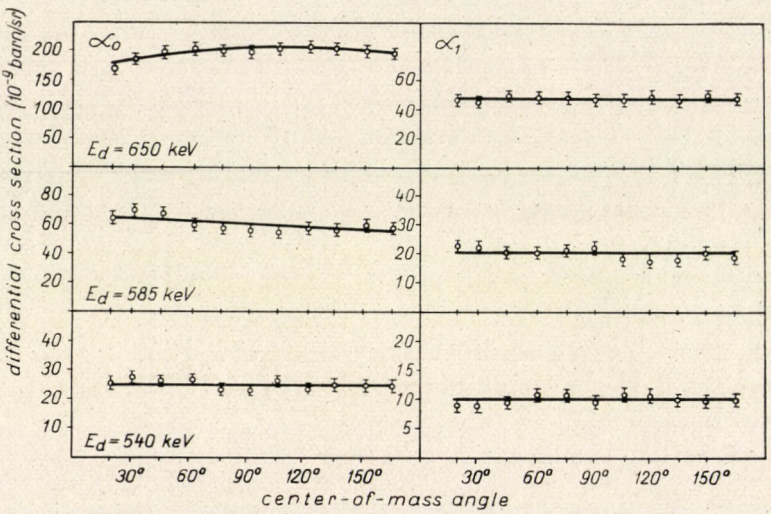

Fig. 1. The angular distributions of the α_0 and α_1 groups of the $^{27}Al(d, \alpha)^{25}Mg$ nuclear reaction $E_d = 650—540$ keV

cross-sections are estimated to be 35% in general. The curves in the Figure are the least square fits of the experimental points to a series of Legendre polynomials.

Table I contains the A_0, A_1, . . . etc. Legendre coefficients with their errors and the calculated χ^2 values. The experimental angular distributions were analyzed up to P_l needed for the best fit in accordance with the experimental errors. Therefore, the Table contains only those coefficients for which the normalized χ^2 values are near unity.

From the results it can be seen that the angular distributions are nearly isotropic as expected at such low bombarding energies. At $E_d = 650$ and 585 keV, however, a small anisotropy can be seen in the case of α_0-group, but the angular distribution of this group averaged over the examined energy range also becomes isotropic.

These results are in accordance with the previous works at higher energies ($E_d < 5$ MeV) and suggest the assumption of statistical compound reaction mechanism for the $^{27}Al(d, \alpha)^{25}Mg$ nuclear reaction. It is, therefore, worth while

Table I

Coefficients of the Legendre polynomials

$$\frac{d\sigma}{d\Omega} = \sum_{l=0}^{n} A_l P_l(\cos\Theta)$$

E_d (keV)	A_0	A_1	A_2	χ^2
α_0 650	199.6±2	−9.7±2.9	−13.2±3.9	0.97
585	60.1±1.1	4.8±1.7		0.80
540	24.9±0.5			0.70
α_1 650	49.7±0.5			0.54
585	20.6±0.5			0.70
540	10.0±0.2			0.60

to see if the intensities of the observed alpha groups correspond to the $(2I + 1)$ rule characterizing the statistical compound reaction mechanism. The $(2I + 1)$ rule cannot be applied directly in our case because the conditions for its applicability as given by MAC DONALD [13] are, obviously, not satisfied. However, with the simplifying condition introduced by our experimental conditions it is possible to follow in detail the formation of the statistical weight factors for the two measured alpha transitions.

At these low bombarding energies in the incoming deuteron channel $l = 0$ is most probable. Therefore, in the ^{29}Si compound nucleus only those states can be excited which have spins equal to the possible channel spin values 3/2, 5/2 and 7/2 and have positive parities. The transition from a certain excited level of the ^{29}Si compound nucleus to the 5/2 and 1/2 states of the residual nucleus can take place with different l' values, where l' is the orbital angular momentum carried by the emitted alpha particle. (For example the $7/2 \rightarrow 5/2$ transition can take place with $l' = 1, 2, \ldots 6$, in total $2 \cdot 5/2 + 1 = 6$, and the $7/2 \rightarrow 1/2$ transition with $l' = 3, 4$, in total $2 \cdot 1/2 + 1 = 2$ possible orbital angular momentum values.) According to the parity conservation rule l' must be even and this further limits the possible values of l'. The possible l' values corresponding to the different transitions are given in Table II.

Table II

The possible l' values in the transitions from the $7/2^+$, $5/2^+$ and $3/2^+$ levels of the ^{29}Si compound nucleus to the $5/2^+$ ground state and $1/2^+$ first excited state of ^{25}Mg

I \ J	$7/2^+$	$5/2^+$	$3/2^+$
$5/2^+$	2, 4, 6	0, 2, 4	2, 4
$1/2^+$	4	2	2

It can be seen from this Table that with these values of l' the transition from the excited states of the compound nucleus to the $5/2^+$ ground state and $1/2^+$ first excited state of the residual nucleus can take place in eight and three different ways, respectively. If the penetration factors in the outgoing channels are neglected, then — because of the assumed statistical character of the process — the transitions with each possible l' value have equal probabilities. Further, if the spin dependence of level density is also neglected then the intensity ratio of the α_0 and α_1 transitions can be expected to be 8/3. However, taking into account the penetration factors of the outgoing alpha particles this ratio will change. The penetration factors for the emitted alpha energies were determined by interpolation for $l' = 0, 2, 4$ using the Tables given by J. R. HUIZENGA and G. J. IGO [14]. (The penetration factor for $l' = 6$ was taken to be zero.) A more correct calculation of the ratio of alpha group intensities was made by summing up the weighted relative frequency of occurrence of the possible l' values by their respective penetration factors leading to the ground state and the first excited state of the residual nucleus. As a result, for the intensity ratio of the two alpha groups a value of 3.04 was derived.

If the spin dependence of the level density in the usual form $F_\nu = (2J + 1) \exp[-(J + 1/2)^2/\sigma^2]$ was also taken into account then only less than 4% change of the above mentioned intensity ratio was obtained.

In the latter calculation a value of the spin cut-off parameter $\sigma^2 = 6$ was used which reproduced satisfactorily the results of $^{27}Al(d, \alpha)^{25}Mg$ nuclear reaction at higher bombarding energies [13].

Table III

The measured and calculated relative intensities of the α_0 and α_1 groups

E_d (keV)	α_0 $5/2^+$	α_1 $1/2$
650	1	0.24
585	1	0.34
540	1	0.40
Mean	1	0.327
Relative intensities calculated without penetration factor	1	0.375
Relative intensities calculated with penetration factor	1	0.328

In Table III the relative intensities of the measured alpha groups integrated over the 0°—180° angular region and their mean values are shown. This Table also contains the relative intensities calculated by neglecting and

by taking into account the effect of the penetration factors. For ease of comparison the intensity of the α_0-group is normalised to unity.

Although the experimental relative intensities change with the bombarding energy, their mean values are found to be in agreement with those calculated, when the effect of penetration is included. This agreement between the experimental result and the former simple calculation for the statistical weight factors supports the validity of the statistical compound reaction mechanism assumption for the $^{27}Al(d, \alpha)^{25}Mg$ nuclear reaction in the examined energy region.

We wish to thank Prof. A. SZALAY, Director of the Institute of Nuclear Research, Debrecen, for his constant interest in our work, Dr. B. GYARMATI for valuable discussions and the members of the cascade and photo-emulsion groups for their help in the measurements. One of us (D.S.S.) acknowledges with thanks the special-duty leave granted by the Aligarh Muslim University, Aligarh, India.

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ИССЛЕДОВАНИЕ ЯДЕРНОЙ РЕАКЦИИ $^{27}Al(d, \alpha)^{25}Mg$ В ИНТЕРВАЛЕ ЭНЕРГИИ $E_d = 650-540$ КЭВ ПОСРЕДСТВОМ ПЛАСТИКОВОГО ТРЕКОВОГО ДЕТЕКТОРА

И. ХУНЯДИ, Б. ШЛЕНК, Г. ШОМОДИ и Д. С. СРИВАСТАВА

Резюме

Измеряются угловые распределения групп α_0 и α_1 в ядерной реакции ^{27}Al (d, $\alpha)^{25}Mg$ при энергиях дейтерия $E_d = 650$, 585 и 540 КЭВ с помощью пластикового трекового детектора. Угловые распределения, которые почти изотропны, разлагаются в ряд при помощи полиномов Лежандра. Предполагая статистический составной механизм реакции, соотношение относительной интенсивности двух измеренных альфа—групп можно воспроизводить простым вычислением, задавая статистические веса для рассмотренных альфа-переходов.

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COMMUNICATIONES BREVES

ON THE MOMENTUM DEPENDENCE OF THE $\pi\varrho\omega$-VERTEX

By

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1. In the GELL-MANN—SHARP—WAGNER model [1] the ratios $\Gamma(\omega \to \to \pi^\circ \gamma)/\Gamma(\pi^\circ \to 2\gamma)$ and $\Gamma(\omega \to \pi^\circ \gamma)/\Gamma(\omega \to 3\pi)$ are independent of the $\pi\varrho\omega$-vertex and they depend only on the leptonic decays of ϱ and ω, and $g_{\varrho\pi\pi}$. This idea could be tested in the new colliding beam experiments [2] with the result that there is an enormous contradiction between the above predictions of the GSW-model and the experimental partial widths. A possible way out of this situation is to assume that the $\pi\varrho\omega$-vertex function defines a momentum dependent coupling [3, 4]. Starting from this idea we want to show that in the current algebra a possibility exists for explaining the ratio $\Gamma(\omega \to \pi^\circ \gamma)/\Gamma(\pi^\circ \to 2\gamma)$.

2. In order to find the ratio of parameters of the $\pi\varrho\omega$-vertex function, we recall an approximate sum rule [5] derived from the assumption of c-number Schwinger terms, namely:

$$M(k^2)\,M(l^2)\left[\mathbf{p}_2^2-(\mathbf{p}_2^2+\mathbf{q}^2)\,\frac{P_{20}}{P_{20}}\right]+M(\bar{k}^2)\,M(\bar{l}^2)\left[\mathbf{p}_2^2+(\mathbf{p}_2^2+\mathbf{q}^2)\,\frac{P_{20}}{P_{20}}\right]=0\,, \qquad (1)$$

where $M\big((p-p')^2\big)$ is the invariant function of the matrix element

$$\langle\pi_t(p)|V_\mu\cdot(0)_a|\omega(p',\gamma)\rangle;$$

p_1, p_2 are pion four-momenta, $p_i^2 = m_\pi^2$ and

$$\begin{aligned} P_{20} &= (\mathbf{p}_2^2+\mathbf{q}^2+m_\omega^2)^{1/2},\\ k^2 &= (p_{10}-P_{20})^2-(\mathbf{p}_1-\mathbf{p}_2-\mathbf{q})^2,\\ l^2 &= (p_{20}-P_{20})^2-\mathbf{q}^2, \qquad (2)\\ \bar{k}^2 &= (p_{10}+P_{20})^2-(\mathbf{p}_1-\mathbf{p}_2-\mathbf{q})^2,\\ \bar{l}^2 &= (p_{20}+P_{20})^2-\mathbf{q}^2. \end{aligned}$$

(1) is valid under the conditions $\mathbf{p}_1 \neq 0$, $\mathbf{p}_i\mathbf{q} = 0$, $\mathbf{p}_1\mathbf{p}_2 = 0$ [5]. The second term of (1) represents some disconnected contributions derived from the inter-

mediate state $|2\pi\omega>$, while the $\pi\varrho\varphi$-vertex and higher-order terms are neglected.

For small values of $\mathbf{p}_i^2$, $\mathbf{q}^2$ ($\lesssim (3—4)m_\varrho^2$) we approximate M by a ϱ-pole dominated form

$$M(p^2) = \frac{a}{m_\varrho^2 - p^2} + b \tag{3}$$

with a, b constants. To evaluate (1) it is worth while to introduce dimensionless parameters x, y, z: $q^2 = zm_\pi^2$, $\mathbf{p}_1^2 = ym_\pi^2$, $\mathbf{p}_2^2 = xm_\pi^2$. By substituting (3) into (1) we get a quadratic equation for b/a. The corresponding solutions were studied numerically in the domain x, y, $z = [10 — 100]$. We obtained that real roots are present only for $z \geq 25$. Furthermore, the one root is $b = 0$ [5], almost independently of x, y, z, reproducing the wrong form of the GSW-model. The other root changes slightly with x, y, z. Typical curves are indicated in [6]. According to our calculations the average value of b/a over x, y, z is $(b/a)_{av} = 1.4\ \mathrm{GeV}^{-2}$.

On the other hand, b/a determines the ratio $\Gamma(\omega \to \pi^\circ\gamma)/\Gamma(\pi^\circ \to 2\gamma)$. Now, if we use our $(b/a)_{av}$ and other data from [2, 7], the ratio $1.9 \cdot 10^5$ is obtained while the experimental value is $1.6 \cdot 10^5$.

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ON THE IMPORTANCE OF USING EXACT FORMS FOR SCATTERING AMPLITUDE IN REGGE POLE THEORY

By

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Almost as soon as it had been proposed to describe the elastic scattering in terms of a single Regge pole, the so-called vacuum or Pomeranchuk pole, A. L. READ, I. OREAR and H. A. BETHE [1] suggested the use of exact, instead of asymptotic forms for the Legendre functions involved in the expression for scattering amplitude, giving simultaneously the computer plots of these functions. Nevertheless, in the calculations reported to date the asymptotic forms are used almost exclusively because of the usually high energy values and the poor experimental accuracy of the data.

Considering the data of a reported experiment [2], chosen as an example because of its high accuracy, it will be shown that the asymptotic forms may lead, in some cases, to substantially different results from those obtainable using forms which agree in the critical regions with the exact values within 1%. The measurement in question covered the differential cross-section for p—p elastic scattering observed at a fixed angle of 90° in the centre of mass system as a function of the squared 4-momentum transfer $-t$, at large values of $-t$, when the angular momentum of the incoming protons varied from 5 to 13.4 GeV/c.

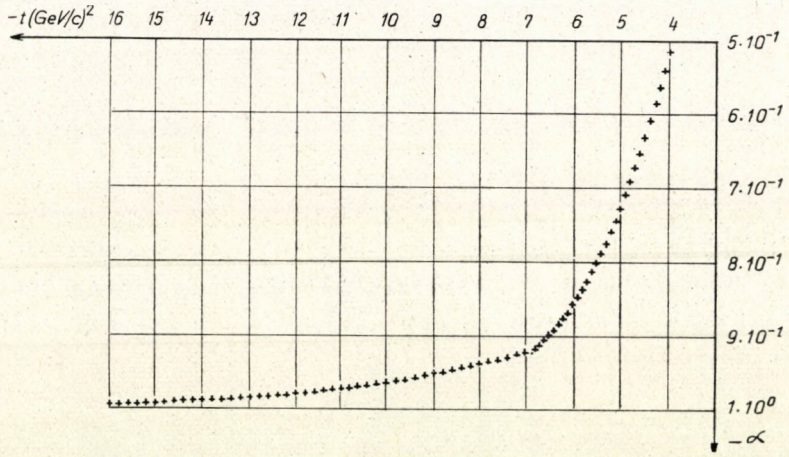

Fig. 1

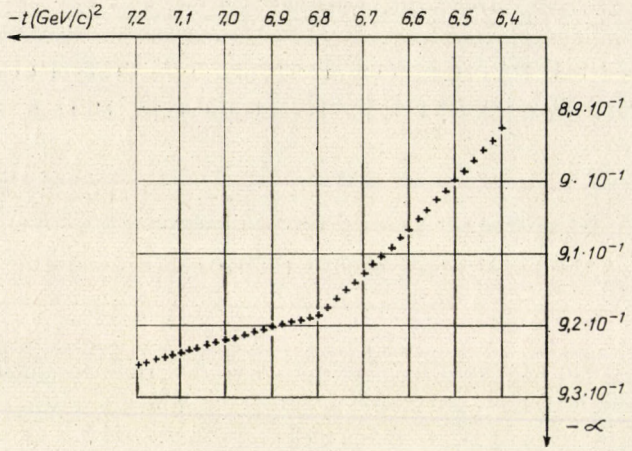

Fig. 2

The calculation serves merely for the illustration of the method without any discussion of the physical implications. For simplicity, instead of the experimental data shown in Fig. 2, we shall use the points of the two straight lines which are seen to fit the measured values fairly well owing to the small error of the latter.

The angular momentum values $\alpha(t)$ will be determined from the experimental data in terms of the vacuum pole model using for the scattering amplitude at $\alpha < 0$ the form

$$\bar{A}(s, t) = \beta(t)\alpha(2\alpha + 1)(1 + \exp[-i\pi\alpha])\frac{Q_{-\alpha-1}(z)}{\pi\cos\pi\alpha}, \tag{1}$$

where $z = \cos\Theta_t$ and the index t stands for the channel t. In the present case we have

$$z = \frac{2S}{2M^2 - t} - 1$$

with M being the proton mass and s the squared total energy in the centre of mass. In the analyzed experiment the value of z lies in the region $2 \geq Z \leq < 2.5$ and the function $Q_{-\alpha-1}$ is the Legendre function of second kind with non-integral index and positive argument. This function is usually approximated by its asymptotic form

$$Q_{-\alpha-1}(z) \approx \sqrt{\pi}\,\frac{\Gamma(-\alpha)}{\Gamma(-\alpha+1/2)}\,(2z)^{\alpha}. \tag{2}$$

Calculating the differential cross-section $d\sigma/dt$ from (1) and putting $\beta^2(t)/\beta^2(0) = 1$ and $\sigma_{\mathrm{Tot}} = 40$ mb, we get the expression

$$-2{,}70748 \cdot 10^{-4} \frac{d\sigma}{dt} \left(\frac{3z-1}{3-z}\right)^2 + \left[\alpha(2\alpha+1) \frac{\cos(\pi/2)\,\alpha}{\cos \pi\alpha} Q_{-\alpha-1}(z)\right]^2 = 0 \qquad (3)$$

which allows $\alpha(t)$ to be evaluated from the measured value of the differential cross-section at a given value of t (in the present case $-t = 2p_{cM}^2$).

Instead of the usual approximation (2) we use the form

$$Q_{-\alpha-1}(z) = \sqrt{\pi} \frac{\Gamma(\alpha)}{\Gamma\left(\frac{1}{2} - \alpha\right)} (2z)^{\alpha} + \sqrt{\pi} \frac{\Gamma(2-\alpha)}{\Gamma\left(\frac{3}{2} - \alpha\right)} (2z)^{\alpha-2} \sum_{j=0}^{3} c_j q_j^{(\alpha)} w^j, \qquad (4)$$

where

$$q_0^{(\alpha)} = 1 \qquad q_j^{(\alpha)} = \frac{j - \frac{\alpha}{2}}{j + \frac{1}{2} - \alpha} \frac{j + \frac{1}{2} - \frac{\alpha}{2}}{j+1} q_{j-1}^{(\alpha)} \quad j = 1, 2 \ldots$$

$w = 2/z^2$

$-1 < \alpha < 1$

j	c_j
0	0.997
1	0.576
2	—0.056
3	0.480

If $z \geq \sqrt{2}$ this form yields the values of $Q_{-\alpha-1}$ with a maximum error of 1%.

The values of $\alpha(t)$ calculated from the expression (3) are plotted in Fig. 1. With an appropriate transformation of scale and by increasing the number of points in the critical region, the break in curve 1 at $-t = 6.8(\mathrm{GeV/c})^2$ becomes well apparent (Fig. 2) and is seen to reproduce fairly well the break observable in the original data ($P_{CM}^2 = 3.4\,(\mathrm{GeV/c})^2$). Fig. 1 clearly shows that α is a single valued function of t and tends asymptotically to $\alpha = -1$ at large values of $-t$. It becomes evident from a simple numerical example why it is necessary to use Eq. (4).

Taking $\alpha = -0.95$ the ratio of expression (4) to (2) is 1.1985 if $z = 2$ and 1.1437 if $z = 2.5$ while with $\alpha = -0.985$ these ratios become 1.2146 and 1.1289, respectively. Thus, it can be seen that the conventional formula introduces in the present case a multiplication factor between 1.2 and 1.1 into the value of the scattering amplitude. It follows that e.g. the value of the cross-section of physical interest determined from the conventional formula is from 40% to 20% lower compared with that obtained from the more accurate form (4) used in our calculations.

If the values of $-t$ are small, the scattering amplitude in terms of the vacuum pole model is given by

$$A^+(s, t) = \beta(t)\alpha(2\alpha + 1)(1 + \exp[-i\pi\alpha])\frac{P_\alpha(z)}{\sin \pi\alpha}, \tag{5}$$

where $P_\alpha(z)$ is the Legendre function of the first kind with non-integral index and positive argument and the generally used asymptotic form is

$$P_\alpha(z) \approx \frac{\Gamma\left(\alpha+\frac{1}{2}\right)}{\sqrt{\pi}\,\Gamma(\alpha+1)}(2z)^\alpha.$$

This form is obviously inappropriate, if one wishes to describe a process with z in the region $0 \leq z \leq 2$. This is the case e.g. in diffraction dissociation experiments with π-mesons and heavy nuclei. Then, owing to the large nuclear mass and the small value of $-t$, at the currently used not too high energies, z is close to zero.

The form of P_α which should be used in this case, is

$$P_\alpha(z) = \sum_{j=0}^{5} a_j P_j^{(\alpha)} \mu^j \qquad \mu = 1 - z$$

j	a_j
0	1.000
1	0.500
2	0.243
3	0.122
4	0.088
5	0.044

$$P_0^{(\alpha)} = 1$$

$$P_j^{(\alpha)} = \frac{j+\alpha}{j}\,\frac{j-1-\alpha}{j}\,P_{j-1}^{(\alpha)} \qquad j = 1, 2, \ldots$$

For measurements performed with high accuracy, if $Z \geq 2$ we recommend the formula

$$P_{(\alpha)}(z) = \frac{\Gamma\left(\alpha+\frac{1}{2}\right)}{\Gamma(\alpha+1)\pi^{1/2}}(2z)^\alpha + \sum_{j=0}^{2} b_j R_j^{(\alpha)} \sigma^j,$$

$$\sigma = \frac{4}{z^2}, \qquad R_j^{(\alpha)} = \varrho_j^{(1)} + \varrho_j^{(2)},$$

$$\varrho_0^{(1)} = -\frac{\Gamma\left(\alpha-\frac{1}{2}\right)}{\Gamma(\alpha-1)\pi^{1/2}}(2z)^{\alpha-2},$$

$$\varrho_0^{(2)} = \frac{\Gamma\left(-\alpha-\frac{1}{2}\right)}{\Gamma(-\alpha)\pi^{1/2}}(2z)^{-\alpha-1},$$

$$\varrho_j^{(1)} = \frac{j-\frac{\alpha}{2}}{j+\frac{1}{2}-\alpha} \frac{j+\frac{1}{2}-\frac{\alpha}{2}}{j+1} \varrho_{j-r}^{(1)},$$

$$\varrho_j^{(2)} = \frac{j+\frac{\alpha}{2}}{j+\frac{1}{2}+\alpha} \frac{j-\frac{1}{2}+\frac{\alpha}{2}}{j} \varrho_{j-1}^{(2)},$$

$$b_0 = 1.001, \quad b_1 = 0.236, \quad b_2 = 0.096.$$

Summarizing what has been said it is advisable to establish the possible values of Z before choosing the formula used for the fit. Z being dependent only on s, t and the four masses involved (in the example chosen for illustration the four masses were, of course, equal), it can be calculated explicitly or from a given formula (e.g. [3]). If Z lies in the critical regions investigated above, it is preferable to use the forms suggested here. They are easy to handle both analytically and by computer. In multipole approximations the scattering amplitude has to be written as the sum of the contributions defined by (1) or (5) when the summation index concerns obviously α, β with the sign of the exponent varying according to the sign of the pole. The use of the suggested more accurate forms seems to be even more important in the multipole approximation.

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COMPOSITE SPHERE IN GENERAL RELATIVITY

By

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1. Introduction

Only a few solutions [1] describing the gravitational field inside a composite sphere are currently available in the general theory of relativity. This paper describes a solution of the field equations of general relativity which gives the internal structure of a composite sphere having a core of radius a and of density $\varrho = \varrho_0(1 - r^2/R^2)$ surrounded by a shell of outer radius R and of density $\varrho_1 = K/k^2$ where ϱ_0 is the density at the centre, and constant K is to be taken as $\varrho_0 a^2(1 - a^2/r^2)$ to make the density continuous at the interface.

2. Field equations and boundary conditions

We take the line element as

$$ds^2 = -e^{\lambda} dr^2 - r^2 d\Theta^2 - r^2 \sin^2 \Theta d\Phi^2 + e^{\nu} dt^2, \tag{2.1}$$

where λ and ν are functions of r alone. The field equations for this line element are [2]

$$8\pi p = e^{-\lambda}\left(\frac{\nu'}{r} - \frac{1}{r^2}\right) - \frac{1}{r^2}, \tag{2.2}$$

$$8\pi p = e^{-\lambda}\left(\frac{\nu''}{2} - \frac{\lambda'\nu'}{4} + \frac{\nu'^2}{4} + \frac{\nu' - \lambda'}{2r}\right), \tag{2.3}$$

$$8\pi\varrho = e^{-\lambda}\left(\frac{\lambda'}{r} - \frac{1}{r^2}\right) + \frac{1}{r^2}, \tag{2.4}$$

where prime denotes the differentiation with respect to r.

The following conditions must be satisfied to obtain a solution with physical significance:

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(i) The pressures e^{λ} and e^{r} are continuous at the interface of the core and the shell.

(ii) The pressure is zero at the surface of the sphere and beyond.

(iii) e^{λ} and e^{r} are continuous at the surface of the sphere.

3. Solution of the field equations

The field equations (2,2), (2,3) and (2,4) can be solved for the core [3] to give

$$e^{-\lambda} = 1 - \pi\varrho_0\left(5r^2 - \frac{3r^4}{R^2}\right), \tag{3.1}$$

$$e^{r} = [c_1 \cos z/2 + c_2 \sin z/2]^2, \tag{3.2}$$

$$8\pi p = \frac{4}{R}\left(\frac{2\pi\varrho_0}{5}\right)^{1/2}\left[1 - \frac{8\pi R_2\varrho_0}{15}(5\varkappa - 3\varkappa^2)\right]^{1/2} \times \times\left[\frac{c_2 - c_1\tan z/2}{c_1 + c_2\tan z/2}\right] - \frac{8\pi\varrho_0}{15}(5 - 3\varkappa), \tag{3.3}$$

where c_1 and c_2 are constants of integration and $\varkappa = r^2/R^2$ and

$$z = \log\left|\varkappa - \frac{5}{6} + \left(\varkappa^2 - \frac{5}{3}\varkappa + \frac{5}{8\pi R^2\varrho_0}\right)^{1/2}\right|.$$

We now solve the field equations for the shell where density varies as K/r^2. Eq. (2,4) can be easily integrated to give

$$e^{-\lambda} = 1 - 8\pi k + \frac{c}{r}, \tag{3.4}$$

where c is a constant of integration. Eliminating p from Eq. (2.2) and (2.3) and assuming $e^{\nu/2} = y$, we get

$$r^2[(1 - 8\pi k)r + c]\,Y'' - r\left[(1 - 8\pi k)r + \frac{3c}{2}\right]Y' + \left(8\pi kr - \frac{3c}{2}\right)Y = 0. \tag{3.5}$$

Substituting $x = 8\pi k - 1/c\ r$, Eq. (3.5) reduces to the differential equation of hypergeometric form

$$x^2(1-x)\frac{d^2y}{dx^2} + x\left(x - \frac{3}{2}\right)\frac{dy}{dx} + \left(\frac{8\pi k}{8\pi k - 1} - \frac{3}{2}\right)y = 0. \tag{3.6}$$

Solution of Eq. (3,6) is

$$y = \frac{1}{x}\left[AF(\alpha, \beta; \nu; x) + Bx^{5/2} E(\alpha+1-\nu, \beta+1-\nu; 2-\nu; x)\right], \quad (3.7)$$

where A and B are constants of integration. The symbols E and F stand for hypergeometric functions. The values of α, β and ν are

$$\left(-1+\frac{1}{\sqrt{1-8\pi k}}\right), \quad \left(-1-\frac{1}{\sqrt{1-8\pi k}}\right)$$

and $-3/2$, respectively. To get real values for α and β we must have $8\pi k < 1$. Eq. (3.7) can be re-written as

$$e^{\nu} = \frac{1}{x^2}\left[AF + Bx^{5/2}E\right]^2. \quad (3.8)$$

Eqs. (2.2) and (3.8) are used to obtain pressure at a point inside the shell which is given by

$$8\pi p = c\left(\frac{8\pi k-1}{cx}\right)^3 (1-x)\left[\frac{A(2xF'-F)+2Bx^{5/2}(2E+xE')}{AF+Bx^{5/2}E} - \frac{x}{(8\pi k-1)(1-x)}\right]. \quad (3.9)$$

The exterior solution ($r > R$) of the field equations (2.2), (2.3) and (2.4) is known as the Schwarzschild exterior solution which is given by

$$e^{-\lambda} = e^{\nu} = 1 - \frac{2m}{r}, \quad p = 0, \quad (3.10)$$

where m is a constant of integration.

4. Determination of the constants

Applying the condition of continuity of e^{λ} at $r = a$ and $r = R$, we get

$$c = \frac{16\pi\varrho_0 a^2}{15}\left(5 - \frac{6a^2}{R^2}\right), \quad (4.1)$$

$$m = 4\pi\varrho_0 a^2\left(\frac{4a^2}{5R^2} - \frac{2a}{3} + R - \frac{a^2}{R}\right). \quad (4.2)$$

The constant m, therefore, is identifiable as the mass of the sphere. The continuity of e^{ν} and zero pressure at $r = R$ give us

$$A = \frac{x_R\left(1-\frac{2m}{R}\right)^{1/2}}{F_R}\left[1-\frac{2x_R F'_R - F_R\left(1+\frac{x_R}{(8\pi k-1)(1-x_R)}\right)}{2x_R(F'_R E_R - E'_R F_R) - 5E_R F_R}\right], \tag{4.3}$$

$$B = \frac{\left(1-\frac{2m}{R}\right)^{1/2}\left[2x_R F'_R - F_R\left(1+\frac{x_R}{(8\pi k-1)(1-x_R)}\right)\right]}{x_R^{3/2}[2x_R(F'_R E_R - E'_R F_R) - 5E_R F_R]}, \tag{4.4}$$

where x_R, F_R and E_R denote values corresponding to $r = R$. The constants c_1 and c_2 are calculated by applying the continuity conditions of e^{ν} and p at $r = a$. The values of c_1 and c_2 are:

$$c_1 = \cos\frac{z_a}{2}\left(\frac{AF_a + Bx_a^{5/2}E_a}{x_a}\right)\left[1 - J\cdot\tan\frac{z_a}{2}\right], \tag{4.5}$$

$$c_2 = \cos\frac{z_a}{2}\left(\frac{AF_a + Bx_a^{5/2}E_a}{x_a}\right)\left(J + \tan\frac{z_a}{2}\right), \tag{4.6}$$

where x_a, F_a, E_a and z_a denote values corresponding to $r = a$ and

$$J = \frac{\frac{8\pi\varrho_0}{15}\left(5-\frac{3a^2}{R^2}\right) - \frac{1}{a^2} + \frac{c[A(2x_aF'_a - F_a) + 2Bx_a^{5/2}(2E_a + x_aE'_a)](1-x_a)}{a^3(AF_a + Bx_a^{5/2}E_a)}}{\frac{4}{R}\left(\frac{2\pi\varrho_0}{5}\right)^{1/2}\left[1-\frac{8\pi\varrho_0 a^2}{15}\left(5-\frac{3a^2}{R^2}\right)^{1/2}\right]}.$$

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EFFECT OF FORM FACTORS ON HIGH ENERGY NEUTRINO REACTIONS

By

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1. Introduction

The theory of weak interaction which is formulated in terms of the current—current interaction [2] with universal coupling constant, has received considerable support from the conserved vector current hypothesis [3]. The hypothesis was originally postulated in analogy to electromagnetic interaction and was shown to be true by means of the β-ray spectra [4] with larger energy release.

Another theory assumes that the weak interactions are mediated by a weak boson field with heavy quanta [1]. This can only be demonstrated by means of high energy experiments, because at low energies the detection of any non-locality is impossible. Also, the possible weak non-locality is made unobservable by the strong non-locality coming from the pionic form factors of the nucleons [5].

Our aim is to study the effect of different form factors on the following reaction

$$\bar{\nu} + p \rightarrow n + \mu^+ \tag{1}$$

by the weak boson theory. If we accept the hypothesis of the conserved vector current, we have [6]

$$F_1(q^2) = F_2(q^2) = F_A(q^2) = \left(1 + \frac{lq^2}{M^2}\right)^{-n}. \tag{2}$$

2. Weak boson

If we consider that the weak interactions are mediated by weak bosons, we can write the interaction Hamiltonian as follows

$$H = gJ_\mu \varphi_\mu + gj_\mu \varphi_\mu . \tag{3}$$

Here g is the coupling constant, φ_μ is the wave function for the W boson, J_μ and j_μ are the strangeness — conserving baryon currents and lepton currents,

respectively. Applying this Hamiltonian for the reaction (1) we get the following relation between the Fermi constant f and the coupling constant g of weak bosons.

$$f = \frac{\sqrt{2}\, g^2}{M_\omega^2} \,. \tag{4}$$

3. Form factors

In this section we study the effect of different form factors on the total cross-section for high energy antineutrinos, on the basis of the conserved vector current hypothesis and intermediate vector boson. We consider the fol-

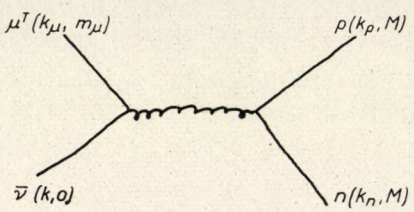

Fig. 1

owing Feynman diagram and assign the masses and momenta of the particles as indicated in Fig. 1.

The most general form of the S-matrix element of the four fermion interaction following from Fig. 1 is:

$$S_{if} = \frac{-ig^2}{4\hbar c M_w^2} \frac{(2\pi)^2}{V^2} \bar{u}_n \left[F_1(q^2)\, \gamma_\alpha - \frac{\mu}{2M} F_2(q^2)\, \sigma_{\alpha\beta} q_\beta + \right.$$
$$\left. + \lambda F_A(q^2)\, \gamma_\alpha \gamma_5 \right] u_p \frac{1}{1 + (q/M_w)^2} \bar{v}_\nu \gamma_\alpha (1+\gamma_5)\, v_e \tag{5}$$
$$\delta(k_p - k_n + k_\nu - k_e) \,,$$

where $F_1(q^2)$ and $F_2(q^2)$ are both equal to the isovector nucleon electromagnetic form factor, μ is equal to the difference of anomalous magnetic moment between proton and neutron and, F_A is the axial vector form factor.

After tedious calculations the total cross-section for the absorption of antineutrinos according to (5) in the laboratory system is given by the following:

$$\sigma(E) = \frac{\sigma_0}{2} \int_{K_{\min}}^{K_{\max}} F(K, E)\, dK \,, \tag{6}$$

where

$$F(K,E)=\left[\frac{A_0+A_1K+A_2K^2}{E^2(K+\alpha)^{2n}(K+\beta)^2}\right]\alpha^{2n}\beta^2, \tag{7}$$

$$A_0=4(1+\lambda^2)E^2, \tag{8}$$

$$A_1=-E(4+4\lambda^2+8\lambda+8\mu\lambda)+\mu^2E^2+2(\lambda^2-1), \tag{9}$$

$$A_2=-\mu^2E+(2+2\lambda^2+4\lambda+4\mu\lambda+4\mu+\mu^2), \tag{10}$$

$$\sigma_0=\frac{f^2M^2}{2\pi\hbar^2c^2}=1\cdot6\times10^{-38}\,\mathrm{cm}^2,$$

$$K_{\max}=\frac{2E^2-\dfrac{m_\mu^2}{2M^2}}{1+2E}, \tag{11}$$

$$K_{\min}=-\frac{m_\mu^2}{2M^2}, \tag{12}$$

$$\lambda=1.25, \qquad \mu=3.71, \tag{13}$$

$$\alpha=\frac{1}{2l} \quad \text{and} \quad \beta=\frac{M_w^2}{2M^2}. \tag{14}$$

Here E is the energy of the incident antineutrino, K the kinetic energy of the recoil neutron, all measured in nucleon mass units. M^{-1} is the Compton wave length of the nucleon.

Assuming that all form factors are the same analytical functions of q^2, i.e.

$$F_1(q^2)=F_2(q^2)=F_A(q^2)=\left(1+\frac{lq^2}{M^2}\right)^{-n}, \tag{15}$$

where l and n are parameters. For the parameter n, it was mentioned by GALILIO and CHILTON [7] that the total cross-section diverges for $n=0$ and $n=1$ but approaches a constant value for $n\geqslant 2$ when the energy E of the incident antineutrino approaches ∞.

First we take $n=2$, and study the effect of the parameter l on the cross-section. The total cross-sections were calculated for three values of l as follows:

a) Taking $l=0$, and $M_w=\sqrt{2}M$ Eq. (6) becomes

$$\sigma(E)=\frac{\sigma_0}{2}\int_{K_{\min}}^{K_{\max}}\frac{\beta^2(A_0+A_1K+A_2K^2)}{E^2(K+\beta)^2}\,dK.$$

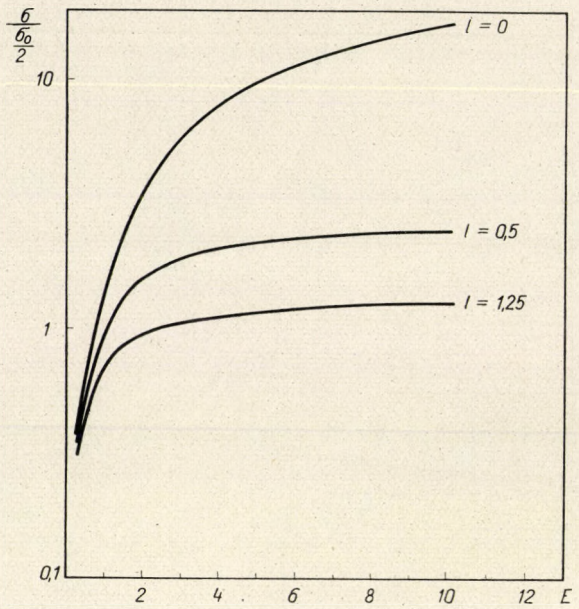

Fig. 2

Integrating we obtain,

$$\sigma(E) = \frac{\sigma_0}{2}\,\frac{\beta^2}{E^2}\left[A_2 K - \frac{A_0 - A_1\beta + A_2\beta^2}{(K+\beta)} + (A_1 - 2A_2\beta)\,ln\,(K+\beta)\right]_{K_{min}}^{K_{max}}. \quad (16)$$

b) Taking $l = 1/2$ and $M_w = \sqrt{2}\,M$, i.e. $\alpha = \beta$ Eq. (6) becomes

$$\sigma(E) = -\frac{\sigma_0}{2}\,\frac{\alpha^6}{E^2}\left[\frac{A_0 - A_1\alpha + A_2\alpha^2}{5\,(K+\alpha)^5} + \frac{A_1 - A_2\alpha}{4(K+\alpha)^4} + \frac{A_2}{3\,(K+\alpha)^3}\right]_{K_{min}}^{K_{max}}. \quad (17)$$

c) Taking $l = 1.25$ and $M_w = \sqrt{2}\,M$, i.e. $\alpha \neq \beta$, the total cross-setion becomes

$$\begin{aligned}\sigma(E) = -\frac{\sigma_0}{2}\,\frac{\alpha^4\beta^2}{E^2}\Bigg[&\frac{10^2(A_0 - \alpha A_1 + \alpha^2 A_2)}{3\,(K+\alpha)^3} + \\ &+ 10^3\,\frac{(-2A_0 + A_1(2\alpha+0.1) - 2\alpha A_2(0.1+\alpha)}{2\,(K+\alpha)^2} + \\ &+ 10^4[3A_0 - A_1(0.2+3\alpha) + A_2(0.01+0.4\alpha+3\alpha^2)]/(K+\alpha) + \\ &+ 10^4(A_0 - A_1\beta + A_2\beta^2)/(K+\beta) - [-4A_0 + A_1(0.3+4\alpha) - \\ &- A_2(0.02+0.6\alpha+4\alpha^2)]10^5\,\ln\,(K+\alpha) - [4A_0 + A_1(0.1-4\beta) + \\ &+ 2\beta A_2(-0.1+2\beta)]10^5\,\ln\,(K+\beta)\Bigg]_{K_{min}}^{K_{max}}\end{aligned} \quad (18)$$

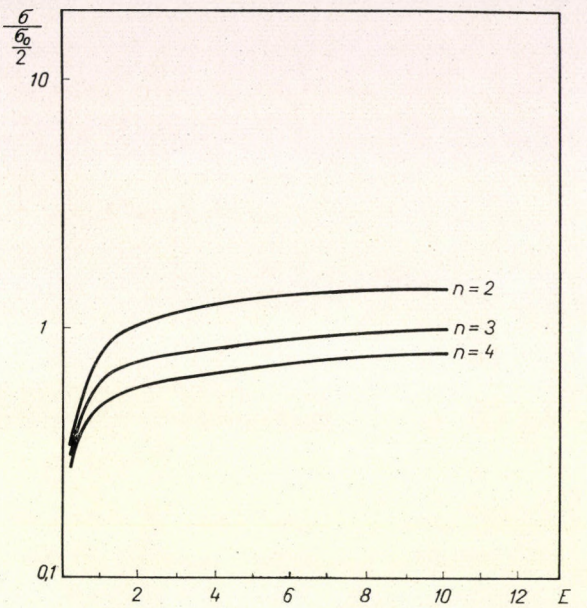

Fig. 3

The dependence of the total cross-section on the parameter l is shown in Fig. 2. Secondly, we shall study the effect of the parameter n on our cross-section by taking $l = 5/4$.

The cross-sections were calculated numerically by a 1905 E ICL computer for values of n equal to 2, 3 and 4. The effect is shown in Fig. 3 where the mass of the vector intermediate boson is taken to be $2M$. From the Figure it is evident that the cross-section decreases with increasing values of n.

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INVESTIGATION OF THE CURRENT DEPENDENCE OF "VOLUME-GRADIENT" E.M.F. IN SEMICONDUCTORS

By

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The experimental investigations of inhomogeneous semiconductors have shown [1—4] that the voltage difference measured between two point contacts depends on the direction of the current. This effect could be explained by the so-called distributed injection of minority carriers from the high resistivity to the low resistivity part of the sample.

In [5] a theoretical treatment of the problem was given, assuming the following distribution of impurities (donors):

$$N_d = \begin{cases} N_{d0}(1 + a'x) & \text{if } x_0 \leqslant x < \infty, \\ N_{d0}(1 + a'x_0) = \text{const.} & \text{if } -\infty < x \leqslant x_0. \end{cases}$$

For low values of the current, the algebraic sum of the voltages measured at different directions of the current density e* was explicitly determined. e* is known as the "volume-gradient" e.m.f. [1]. The experimental investigations of e*(i) characteristics show that it is interesting to investigate those impurity distributions for which the function e*(i) can be given explicitly for the whole range of current density i.

In the present work, the following types of impurity distributions are investigated:

a) sinus-like distribution along the x axis ($-\infty < x < +\infty$):

$$N_d = N_{d0}\left[1 + \eta \sin\left(\frac{2\pi}{T_i} x\right)\right]; \tag{1}$$

b) distribution composed of exponents:

$$N_d = \begin{cases} N_{d0}[1 + \eta(e^{ax} - 1)] & \text{if} \quad x \leqslant 0, \ a > 0, \\ N_{d0}[1 + \eta(1 - e^{-ax})] & \text{if} \quad 0 \leqslant x, \ a > 0. \end{cases} \tag{2}$$

The calculations are carried out using the following assumptions:

(i) the amplitude of the impurity inhomogeneity is small: $\eta \ll 1$;
(ii) the impurity atoms are fully ionized;

(iii) surface recombination can be neglected;
(iv) the assumption of quasi-neutrality is valid.

Using the usual notation, the equations describing the problem in question are:

I. The steady-state equations of charge continuity:

$$\frac{\partial}{\partial t} n, p = -\operatorname{div} \bar{j}_{n,p} - (pn - n_i^2)/[(n+n_1)/C_p+(p+p_1)/C_n] \equiv 0\,, \quad (3)$$

where C_n, C_p, n_1, p_1 are the parameters of the Shockley—Read—Hall model [7].

It is obvious from Eq. (3) that the total current density i is constant: $e(\bar{j}_p - \bar{j}_n) = \bar{i}$.

II. The phenomenological expressions for the electron and hole particle current densities:

$$\begin{aligned} \bar{j}_n &= -D_n \operatorname{grad} n - n\mu_n \bar{E}, \\ \bar{j}_p &= -D_p \operatorname{grad} p + p\mu_p \bar{E}. \end{aligned} \quad (4)$$

III. The Poisson's equation:

$$\operatorname{div} \bar{E} = \frac{e}{\varepsilon}(p + N_d - n)\,. \quad (5)$$

The numerical estimates show that, in our case, the semiconductor remains electrically neutral to a very good approximation. Thus, instead of Eq. (5), the condition of electrical neutrality can be used:

$$n = p + N_d. \quad (6)$$

With this remark, the complete set of differential equations to be solved is:

$$\begin{aligned} &dn/dx = -(j_n + n\mu_n E)/D_n; \quad dp/dx = -(j_p - p\mu_p E)/D_p\,, \\ &dj_n/dx = -(pn - n_i^2)/[(n+n_1)/C_p+(p+p_1)/C_n]; \; n = p+N_d. \end{aligned} \quad (7)$$

To make the calculations more concise, dimensionless quantities will be introduced:

$$\begin{aligned} &\xi = x/L; \; N = n/(n_0+Kp_0); \; P = p/(n_0+Kp_0); \; N_D = N_d/(n_0+Kp_0)\,; \\ &\Theta = -ej_n/i; \; Y = -[e\mu_n (n_0 + Kp_0)/i]\, E; \\ &K = 1/b = \mu_p/\mu_n; \; \lambda = [L/eD_n(n_0+Kp_0)]i; \; A = KL^2/L_{p0}^2\,, \end{aligned} \quad (8)$$

where L is the characteristic length of the impurity distribution: $T_i/2\pi$ for case a) and $1/a$ for case b) $L_{p0}^2 = D_p\tau_{p0} = D_p/C_p$. Using the dimensionless quantities (8), the differential equation system (7) is linearized with respect to the variables N^*, P^*, Θ^*, Y^* originating just from the varying part of impurity distribution. The decomposition of variables N, P, Θ, Y into two parts ($N = N_0 + N^*$, $P = P_0 + P^*$, etc.) is justified by the assumption $\eta \ll 1$ which leads to the conditions $N^* \ll N_0$, $P^* \ll P_0$.

The actual calculation will be repeated here briefly for the sine like distribution. Based on equation system (7), for the hole concentration P^* originating from the inhomogeneity one obtains:

$$[1+P_0(1-K)]\frac{d^2P^*}{d\xi^2} - [1-P_0(1+K)]\lambda\frac{dP^*}{d\xi} - \frac{A'}{K}[1+P_0(1-K)]P^* = \\ = \left(1+\frac{A'}{K}\right)P_0 N_{D0}\eta\sin\xi - \lambda P_0 N_{D0}\eta\cos\xi\,, \tag{9}$$

where $A' = A/[N_0 + N_1 + (P_0 + P_1)C_p/C_n]$.

Without essential restriction of generality an n-type material can be supposed, where

$$N_0 \gg P_0,\ N_1,\ P_1. \tag{10}$$

The dimensionless field strength Y can now be determined, using the periodic solution of Eq. (9) and taking condition (10) into account:

$$\lambda Y = -\lambda + \lambda\eta\sin\xi + \eta\cos\xi + \lambda(1+K)P^* + (1-K)\frac{dP^*}{d\xi}\,. \tag{11}$$

With the definitions given by (8) we obtain:

$$E = -\frac{2\pi}{T_i}\frac{kT}{e}\lambda Y\,. \tag{12}$$

Following [5], the "volume-gradient" e.m.f. is defined as:

$$\mathcal{E}^* = \Delta U_+ + \Delta U_- = \int_{x-\Delta l/2}^{x+\Delta l/2}(E_+ - E_i)\,dx + \int_{x-\Delta l/2}^{x+\Delta l/2}(E_- - E_i)\,dx, \tag{13}$$

where $E_\pm$ — is the electrical field at different direction of the current, E_i — is the internal field at zero current and Δl — is the distance between the probes.

It is worth noting that the electrical field E_i should be subtracted because the voltage difference caused by this term will always be compensated for during the measurements by the contact potential differences of the circuit.

Using Eqs. (11), (12) and (13) we obtain

$$e^* = -B_0 \frac{i^2\left[1+\frac{1+b}{2b}\left(\frac{T_i/2\pi}{L_{p0}}\right)^2\right]}{i^2+i_c^2\left[1+\left(\frac{T_i/2\pi}{L_{p0}}\right)^2\right]^2}\left[\sin\left(\frac{2\pi}{T_i}\left(x+\frac{\Delta l}{2}\right)\right)-\sin\left(\frac{2\pi}{T_i}\left(x-\frac{\Delta l}{2}\right)\right)\right], \quad (14)$$

where

$$B_0 = 8kT/e\,\frac{b^2}{(1+b)^2}(\sigma_i/\sigma_0)^2\,\eta;\quad \sigma_i = e(\mu_n+\mu_p)\,n_i;\quad i_c = \frac{\sigma_0\,kT/e}{T_i/2\pi}\,.$$

If the condition $\Delta l/(T_i/\pi) \ll 1$ is valid, Eq. (14) can further be simplified as follows:

$$e^* = -B_0\,\frac{\Delta l}{T_i/2\pi}\,\frac{i^2\left[1+\frac{1+b}{2b}\left(\frac{T_i/2\pi}{L_{p0}}\right)^2\right]}{i^2+i_c^2\left[1+\left(\frac{T_i/2\pi}{L_{p0}}\right)^2\right]^2}\cos\left(\frac{2\pi}{T_i}\,x\right)\,. \quad (15)$$

A similar calculation can be applied for case b).[+] After tedious calculations one obtains:

$$e^* = F\left\{C_0\exp(-a|x|)+\left(F_1\,\mathrm{sh}\,\frac{ia|x|}{2\,i_m}+F_2\,\mathrm{ch}\,\frac{ia|x|}{2\,i_m}\right)\exp(-Ha|x|)\right\} \quad (16)$$

where i is the absolute value of current density

$$F = -8kT/e\,\frac{b^2}{(1+b)^2}(\sigma_i/\sigma_0)^2\,\frac{\Delta l}{1/a}\,\eta\,\frac{i^2}{i^2-i_m^2\left[1-\left(\frac{1/a}{L_{p0}}\right)^2\right]^2};$$

$$F_1 = \frac{i}{i_m}\,\frac{1+b}{2b}+\frac{i_m}{i}\,\frac{b-1}{2b}\left[1-\left(\frac{1/a}{L_{p0}}\right)^2\right];$$

$$F_2 = \frac{1+b}{4b}\left[\left(\frac{i}{i_m}\right)^2-\frac{1+3b}{1+b}+\frac{3+b}{1+b}\left(\frac{1/a}{L_{p0}}\right)^2\right]/H;$$

$$H = \left[\left(\frac{i}{2i_m}\right)^2+\left(\frac{1/a}{L_{p0}}\right)^2\right]^{1/2};$$

$$C_0 = 1-\frac{1+b}{2b}\left(\frac{1/a}{L_{p0}}\right)^2;\quad \sigma_i = e(\mu_n+\mu_p)\,n_i;\quad i_m = \frac{\sigma_0 kT/e}{1/a}\,.$$

[+] Here the boundary conditions differ from those of case a. It follows from the physical picture, that if $x \to \pm\infty$, P^* tends to the equilibrium concentration, while at $x = 0$, P^* and its derivative must be continuous.

The results of the calculations will now be discussed briefly. Eqs. (15), (16) show that e* cannot generally be given by the local values of σ and $d\sigma/dx$ even for small current densities. This is the case, however, if the characteristic length is large and the current is small [see, e.g. the denominator of Eq. (15)]. For this limiting case, Eq. (15) reduces to the expression (32) in [5].

It is interesting to compare the current dependences of Eqs. (15) and (16). For sine like distribution e* shows a saturation, while in case b) for a fixed value of x, one finds a linear current dependence, similarly to the results of [5]. The above calculation can be applied also for the more general case when the impurity distribution is given by

$$N_d = N_{d0}\left\{1 + \eta \sum_{n=1}^{N}\left[A_n \sin\left(n\frac{2\pi}{T_i}x\right) + B_n \cos\left(n\frac{2\pi}{T_i}x\right)\right]\right\}. \tag{17}$$

It can be seen that if the conditions (i)—(iv) are still valid,

$$e^* = \sum_{n=1}^{N}\left[A_n\, e_n^*\left(\sin\left(n\frac{2\pi}{T_i}x\right)\right) + B_n\, e_n^*\left(\cos\left(n\frac{2\pi}{T_i}x\right)\right)\right], \tag{18}$$

where

$$e_n^*\left(\sin\left(n\frac{2\pi}{T_i}x\right)\right) \quad \text{and} \quad e_n^*\left(\cos\left(n\frac{2\pi}{T_i}x\right)\right)$$

can be determined with Eq. (14).

As for the comparison of theory with the experimental results, the analysis of experimental data of [1] shows that for the nearly sine-like distribution of Fig. 2, we actually meet the large current case. Comparing the measured value of e* with the theoretical expression (15), we obtain:
e^*_{meas} ($x = 9$ mm) = 3.1 mV, e^*_{theor} = 4.1 mV, (From Fig. 2 we read $\eta \approx 0.5$; T_i = = 1.8 cm, $\Delta l = 0.1$ cm and $\tau_{po} = 100$ μsec is supposed).
Taking into account that the sample has a finite length, and also the condition $\eta \ll 1$ is not satisfied, the agreement is satisfactory. The investigation of e* vs i characteristics at higher current densities, using the pulse method proposed in [6], is in progress.

The authors are indebted to Mr. F. Beleznay for his valuable remarks.

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RECENSIONES

I. E. McCARTY: Nuclear Reactions

Pergamon Press, Oxford, 1970

Nowadays there is a tendency for undergraduate students to learn physics completely from textbooks, without becoming acquainted with the original literature and therefore not realizing how the subject grew and developed.

Keeping in mind this tendency, a few years ago the Commonwealth and International Library started to publish a new series of books under the heading: "Selected Readings in Physics." The purpose of the series in which Professor McCARTHY's work on Nuclear Reactions was published is to present a set of books which give, for a particular subject or a particular physicist, reprints of those papers which record the development of new ideas. The preprints are preceded by a careful introduction which places the papers in the context of present-day physics.

The idea of this series is very welcome both to students and teachers all over the world. Reading only textbooks the student may acquire a considerable knowledge of his special field, but without reading well-selected original papers the secrets of the creative human mind remain hidden from him and to become an active worker in the field is almost impossible. "Nuclear Reactions" the latest volume of "Selected Readings in Physics", was written and selected by Professor McCARTHY with a deep understanding of the purpose of this series.

The first part of the book starts with the "Early Successes and Difficulties" in the field of nuclear reactions. In the subsequent chapters the author summarises very clearly and economically the main points referring to "The Compound Nucleus", "The Optical Model", "Nuclear Structure and Nuclear Forces" and "Direct Interactions".

This introductory part of the book provides a firm basis for the understanding of the original papers contained in the second part of the book. It seems to be best to list the papers selected by Professor McCARTHY in order to give a general idea of the book:

1. "Discussion on the Structure of Atomic Nuclei", Sir ERNEST RUTHERFORD, O. M., F. R. S. (1929).
2. "The Theory of the Effect of Resonance Levels on Artificial Disintegration", N. F. MOTT (1931).
3. "Neutron Capture and Nuclear Constitution", NIELS BOHR (1936).
4. "Capture of Slow Neutrons", G. BREIT and E. WIGNER (1936).
5. "Fluctuations of Nuclear Reaction Widths", E. E. PORTER and R. G. THOMAS (1956).
6. "The Scattering of High-energy Neutrons by Nuclei", S. FERNBACH, R. SERBER and T. B. TAYLOR (1949).
7. "Regularities in the Total Cross-sections for Fast Neutron", H. H. BARSCHALL (1952).
8. "Model for Nuclear Reactions with Neutrons", H. FESHBACH, C. E. PORTER and V. F. WEISSKOPF (1954).
9. "Nuclear Reactions at High Energies", R. SERBER (1947).
10. "Angular Distribution in (d, p) and (d, n) Reactions", A. B. BHATIA, K. HUANG, R. HUBY and H. C. NEWNS (1952).
11. "Elastic and Inelastic Diffraction Scattering", J. S. BLAIR (1960).
12. "Information Obtainable from (p, 2p) Reactions", I. E. McCARTHY (1965).

Finally one should note if it is worth while, as it is, to publish such books in English then it would be even more worth while to publish them in other languages, since the foreign language entails a barrier especially for undergraduate students which can be surmounted only by additional effort.

I. LOVAS

L. D. Landau, A. I. Akhiezer and E. M. Lifschitz: General Physics, Mechanics and Nuclear Physics

Übersetzt aus dem Russischen von J. B. Sykes, A. D. Petford und C. L. Petford, VIII + 372 p., Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967

This is a general physics textbook covering mechanics, symmetry theory, thermodynamics and solid state physics. The book emphasizes the close relationship of physics to physical chemistry, crystallography and properties of matter to a greater extent than in usual textbooks.

It contains the following chapters: Particle Mechanics, Fields, Motion of a Rigid Body; Oscillations, The Structure of Matter; The Theory of Symmetry; Heat; Thermal Processes; Phase Transitions; Solutions; Chemical Reactions; Surface Phenomena; Mechanical Properties of Solids; Diffusion and Thermal Conduction and Viscosity.

P. Gombás

Gyo Takeda and A. Fujii: Elementary Particle Physics

1966 Tokyo Summer Lectures in Theoretical Physics, Part II. VI + 209 p., Syokabo Tokyo and W. A. Benjamin, Inc. New York, 1967

This volume contains the second part of the second Tokyo Summer Lectures. It contains the texts of the twelve principal lectures delivered during the second period. It covers the following five main topics: Regge pology; the quark model of elementary particles; higher symmetries, weak interactions and a new approach to field theory. It can be recommended to everybody who is interested in this field.

P. Gombás

M. Born u. E. Wolf unter Mitwirkung von A. B. Bhatia, P. C. Clemmow, D. Gabov, A. R. Stokes, A. M. Taylor, P. A. Wyman und W. L. Wilcock: Principles of Optics, Electromagnetic Theory of Propagation, Interference and Diffraction of Light

4. Auflage, XXVIII + 808 S., Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1970

Alle die Vorzüge, die in den Referaten der früheren Auflagen dieses weltbekannten Werkes schon öfters gewürdigt wurden, sind auch dieser neusten Auflage eigen. Die Verfasser haben mit äußerster Präzision und Sorgfalt eine gründliche Darlegung der gesamten optischen Erscheinungen gegeben, wobei für die Materie eine kontinuierliche Verteilung zugrunde gelegt wurde. Dieses Werk, das in den weitesten Kreisen der Physiker durch ihre früheren Auflagen bestens bekannt ist, bedarf keiner Würdigung. Es wurde zu einem Standardwerk, das für jeden Physiker, der sich mit Optik befasst unentbehrlich ist. Diese neuste Auflage begrüssen wir wärmstens und wünschen dieser denselben Erfolg wie den früheren Auflagen.

P. Gombás

M. A. Preston: Physics of the Nucleus

X + 661 p. Addison-Wesley Publishing Comp., Inc., Reading, Massachusetts, Palo-Alto, London, 1962, $ 15

Dieses Buch von Preston ist auch heute noch, nach dem Erscheinen vor rund 8 Jahren, ein Werk das allen denjenigen, die sich mit Atomkernen befassen, wärmstens empfohlen werden kann. Es ist weder rein experimentell noch rein theoretisch; der Author hat es ver-

standen die beiden Gebiete in einander zu verschmelzen und meisterhaft darzustellen und den Leser mit einem möglichst geringen mathematischen Apparat in die Theorie der Kerne einzuführen.

Das Buch enthält 5 Kapitel. Das erste behandelt die grundlegenden Eigenschaften der Kerne, das zweite die verschiedenen Kernmodelle, das dritte die elektromagnetischen Eigenschaften der Kerne, das vierte die Radioaktivität und schliesslich das letzte die Kernreaktion. In einem Anhang bringt der Autor mathematische Ergänzungen zu mehreren im Text vorkommenden Grössen, Begriffen und zur Theorie der Streuung.

P. GOMBÁS

K. GOTTFRIED: Quantum Mechanics Vol. I: Fundamentals

XVII + 494 p., W. A. Benjamin, Inc., New York, Amsterdam, 1966, $. 13.50

Wie schon aus dem Untertitel zu sehen ist, behandelt dieser erste Band die Grundlagen der Quantenmechanik und zwar befassen sich die insgesamt 9 Kapitel mit den folgenden Gebieten: Kapitel I: Unbestimmtheit und Komplementarität. Kap. II: Wellenmechanik, Kap. III: Lösungen der Schrödinger Gleichung für einige Probleme, Kap. IV: Der Prozess des Messens in der Interpretation der Quantenmechanik, Kap. V: Transformationstheorie, Kap. VI: Symmetrien, Kap. VII: Störungsrechnung für stationäre Zustände, Kap. VIII: Das elektromagnetische Feld, Kap. IX: Störungsrechnung zeitabhängiger Systeme.

Das Buch setzt ziemlich viel mathematische Kenntnisse voraus und kann all' denen empfohlen werden, die eine mehr abstrakte und wenig anschauliche Weise der Quantenmechanik vorziehen.

P. GOMBÁS

A. VISCONTI: Quantum Field Theory

Vol. 1, XI + 289 p., Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1969

Dies Buch enthält den ersten Teil der ins Englische übersetzten Vorträge, die der Verfasser an verschiedenen französischen Universitäten unter diesen auch an der Faculté des Sciences d'Aix-Marseille gehalten hat. Der vorliegende erste Band befasst sich mit den Grundlagen und behandelt nach deren Darlegung die Skalaren und Pseudoskalaren Felder, das Diracsche Feld, das Maxwellsche Feld und das Proca—de Broglie Feld.

Die Behandlung des bearbeiteten Gebietes ist auf hohem Niveau gehalten und erfordert seinem Wesen nach einen beträchtlichen mathematischen Apparat. Das Buch kann all' denen, die sich für Feldtheorie interessieren bestens empfohlen werden.

P. GOMBÁS

R. H. FURTH: Fundamental Principles of Modern Theoretical Physics

XV + 351 p., Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1970

Das Buch enthält die erweiterten Vorlesungen, die der Verfasser für die Studenten im letzten Jahr zur Erreichung des Grades B. Sc. im Birbeck College gehalten hat. Die fundamentalen Prinzipien der modernen Physik sind für die folgenden drei Hauptteile der Physik hergeleitet und ausführlich diskutiert: für die Quantenmechanik, die Relativitätstheorie und die statistische Mechanik. Es enthält auch eine grössere Anzahl Anwendungen und am Ende von jedem Kapitel Aufgaben, deren Lösung zum Selbststudium anregen.

Der Inhalt zergliedert sich folgendermassen. Im ersten Teil: Quantenmechanik, werden zuerst die grundlegenden Prinzipien der klassischen Physik behandelt, dann folgt ein kurzer Überblick der Entwicklung der Quantentheorie. Danach bringt der Verfasser die Prinzipien der Wellenmechanik mit den meist in jedem Buch über Wellenmechanik vorfindbaren Anwendungen. Dem folgt die Operator- und Matrixmechanik ebenfalls mit mehreren Anwendungen. Im zweiten Teil: Relativitätstheorie, befasst sich der Verfasser zunächst mit dem klassischen Relativitätsprinzip und danach mit den Prinzipien der Einsteinschen speziellen Relativitätstheorie und ganz kurz mit der allgemeinen Relativitätstheorie. Daneben wird noch der Zusammenhang zwischen der speziellen Relativitätstheorie und Quantentheorie behandelt. Im dritten Teil: Statistische Mechanik, werden zunächst die grundlegenden Prinzipien dieses Gebietes gebracht, dem dann Anwendungen auf die idealen Gase, auf den idealen Festkörper, auf die Hohlraumstrahlung und die Fluktuationen folgen.

Den Abschluss des Werkes bildet eine Zusammenstellung der Lösungen der Aufgaben.

P. GOMBÁS

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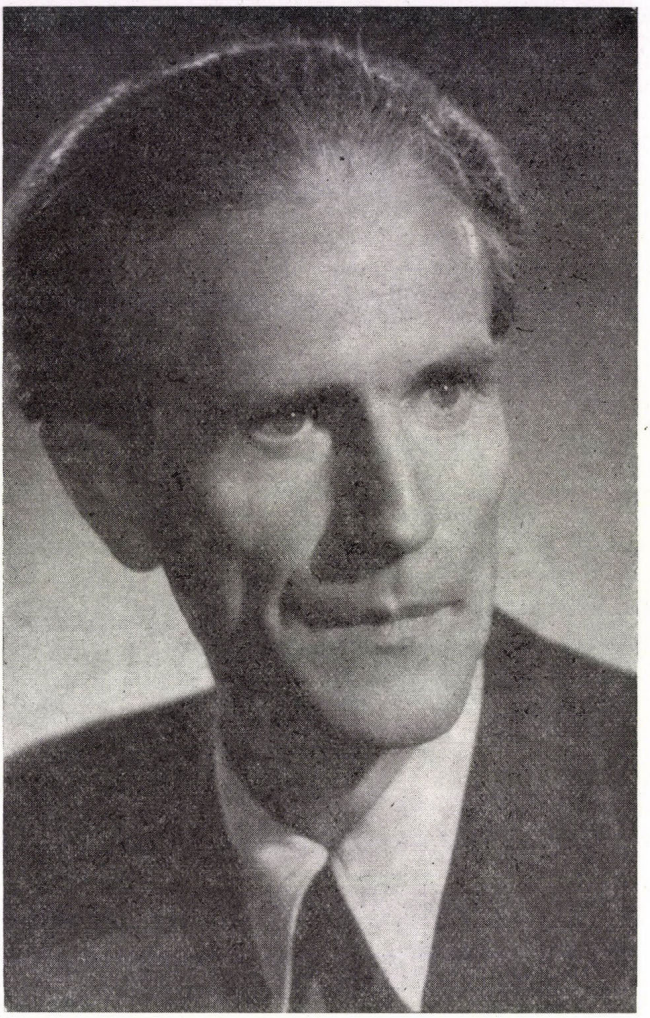

PÁL GOMBÁS
1909—1971

The unexpected death of Professor PÁL GOMBÁS, Member of the Hungarian Academy of Sciences and Director of the Academy's Research Group for Theoretical Physics, is a great loss to Hungarian scientific life.

Professor GOMBÁS's life was one of incessant work and through his scientific activities over nearly forty years he rose to the first rank of Hungarian physicists. His youth was, however, full of hardship. After obtaining the Ph. D. degree in physics in 1932 at the University of Budapest, he was appointed to the Insti-

tute of Theoretical Physics — very characteristically of those times — to an unpaid post. It was his undaunted will and deep attachment for physics that helped him weather out this very difficult period, during which, besides doing scientific and educational work, he had to give private lessons to earn a livelihood for himself and his family. In 1938 he became Privatdocent and worked for a year as assistant professor at the University of Budapest. His career then took a sudden turn upwards: his internationally recognized scientific activities brought him an appointment to an associate professorship at the University of Szeged, then to full professorship and directorship of the Institute of Theoretical Physics at the University of Kolozsvár (1941). In 1944 he was invited to take up the post of Head of the Institute of Physics at the Budapest Polytechnical University, where to his death he was to pay great attention to the training and education of mechanical and electrical engineers.

In the early fifties Hungarian physics was granted significant state subsidies. It was then that the Central Research Institute for Physics was founded and Prof. GOMBÁS took charge of the Department of Theoretical Physics. From 1954 he was Director of the Research Group for Theoretical Physics of the Hungarian Academy of Sciences, which afforded an appropriate medium for his work. This was the place where he worked and taught till his death.

His scientific activities were manifold. At the very beginning of his career his attention was directed towards the statistical theory of the atom. While still an undergraduate he had witnessed the splendid achievements of FERMI and DIRAC, and following JENSEN's work he started further development and application of the statistical theory. As a first step he worked out the statistical model generalized for correlation, now referred to as the THOMAS—FERMI—DIRAC—GOMBÁS model, which proved to be much more convenient than previous models in interpreting the average properties of valence electrons. He also elaborated the perturbation calculation of the statistical model of the atom for the consideration of the effect of both the outer field and an outer perturbing atom. He was long concerned with the possibilities of obtaining a better consideration of kinetic energy. The correction for inhomogeneity elaborated by him and his co-workers allows the determination of very good total energy values and density distributions. He worked a great deal on a generalization of the statistical model able to describe the shell structure of the atomic core. His investigations resulted in atomic models operating with electrons arranged according to principal and azimuthal quantum numbers, which constituted a considerable advance.

From the beginning GOMBÁS had been aware that statistical theory, with its comprehensive possibilities, enables us to treat a number of problems that can hardly or not at all be approximated by the methods of wave mechanics. The theoretical analysis of experimental studies on the inner structure

of the Earth, for example, cannot be performed without a knowledge of the behaviour of matter at high pressures. GOMBÁS demonstrated the suitability of the statistical model for such analysis by working out a realistic model that yielded the pressure — density relation. Another essential property of the statistical method is its descriptive power. The basis of any modern investigation of the structure of matter, the Schrödinger equation, can be applied without any difficulty to systems of particles interacting by Coulomb forces. It is a much more difficult problem to find the wave functions for many-particle systems and their interpretation, since these are defined in a multi-dimensional configurational space. The statistical theory operates with a density function interpreted in a three-dimensional space, is extremely descriptive and very effective in explaining the properties of atoms, ions, molecules and solids.

The completion of the first developmental stage of the statistical theory was marked by GOMBÁS's book "Die statistische Theorie des Atoms und ihre Anwendungen", published by Springer Verlag, Vienna, 1949. This book clearly sets out the fundamentals of statistical theory, analysing its applications and giving detailed critical remarks. A whole generation of physicists acquired their knowledge of statistical theory from this book, to which the revival of the theory is actually due. The number of papers using this work as starting point and reference amounts to several thousand. One of the greatest achievements of GOMBÁS in this field is his brilliant monograph in the 36th volume of "Handbuch der Physik" (Springer Verlag, Berlin, 1956) published under the title "Die statistische Behandlung des Atoms".

GOMBÁS very early recognized the possibility of studying the valence and core electrons of atomic systems detached from one another. For the consideration of core electrons this possibility is yielded by a pseudopotential, for the local form of which he derived several formulae. The pseudopotential takes into account part of the kinetic energy of valence electrons in potential form and greatly simplifies the investigation of valence electrons, partly because the dimension of the configurational field in which operations must be carried out, is decreased by several orders of magnitude, partly because convergence is accelerated due to the reduction of the singularity of the potential fields. From the physicist's standpoint the greatest advantage of this method is that the phenomena become more easily surveyable and demonstrable. Through GOMBÁS's pioneering studies during the past 30 years, a whole series of investigations have been initiated and have gained recognition by physicists. Here reference should be made to his work "Pseudopotentiale" (Springer Verlag, Vienna, 1967) which gives an excellent survey of previous investigations and contributes to their further development.

At the beginning of his career GOMBÁS carried out investigations on the structure of ionic crystals, then established a unified theory of alkali- and alkaline earth metal cohesions. One of his significant observations was that

outside the core the wave function of the electrons of these metals, in respect of the cohesion, can be described by the free electron wave function. He succeeded in extending this theory to noble metals. The most general basis for the explanation of metallic cohesion and the corresponding metallic properties is even today given by GOMBÁS's theory.

The statistical theory of the nucleus was established, after the partially successful experiments of renowned researchers, by GOMBÁS, who succeeded in pointing out that the average properties of the nucleus can be interpreted by the statistical theory even on the basis of very simple assumptions. In his studies he also pointed out that besides the strongly singular Yukawa-type interaction it is worth paying attention to other, e.g. exponential or Gauss-type, interactions too. Quite recently he carried out research of great interest on the structures of pseudo-nuclear molecules and neutron stars.

Professor GOMBÁS's scientific career was, in fact, accompanied throughout by investigations on atomic structures. His first work dealt with the interpretation of the diamagnetic susceptibility of the atoms. After establishing the pseudopotentials, he was highly successful in investigating, together with his collaborators, the optical terms of atoms with one and two valence electrons, and theoretically determined their electron affinity. With the collaboration of the members of his Research Group he developed several atomic models, which excelled in the simplicity and relative unostentatiousness of numerical calculations. The last of these models, published in his book "Solutions of the simplified self-consistent field for all atoms of the periodic system of elements from $Z = 2$ to $Z = 92$", despite its simplicity, amazingly well reproduces the results of the "self-consistent field".

GOMBÁS has always followed with great attention the investigations concerning molecular structure, and with active work he himself promoted development in this field. His most prominent work on the subject is his book "Theorie und Lösungsmethoden des Mehrteilchenproblems der Wellenmechanik" (Birkhäuser, Basel, 1950), which was later published in Russian in the Soviet Union. In this work he gives a crystal-clear analysis of the quantum mechanical methods known at that time for the treatment of the structure of atoms and molecules. The value of the book is further increased by the fact that the author calls attention to methods of the field theoretical many-body problem that were only later included in the armoury of atomic and molecular physics.

Besides his books, GOMBÁS published more than 130 papers, all written in that lucid style so characteristic of him. It can be stated that on the basis of his publications, he has become the internationally best-known and most widely cited Hungarian physicist of our days.

Another important field of GOMBÁS's activities was teaching and education. His thoroughness and love of precision fitted him outstandingly for this

role. He always had a deep feeling of responsibility. His university lectures were easy to understand and rich in inner content. His special lectures were true sources of inspiration for research work. His educational activities can be appreciated best by surveying the books he wrote for this purpose. As early as 1943, during his years in Kolozsvár, he published the monograph: "Bevezetés az atomfizikai többtestprobléma kvantummechanikai elméletébe" (Introduction to the Quantummechanical Theory of the Atomic Many-body Problem) as the 14th volume of the Proceedings of the University of Kolozsvár. Very important means of scientific education are his books "Bevezetés az atomelméletbe" (Introduction to the Theory of the Atom) (Mérnöktovábbképző Intézet, Budapest, 1947) as well as "Bevezetés a hullámmechanikába és alkalmazásaiba" (Introduction to Wave Mechanics and its Applications) (Akadémiai Kiadó, Budapest, 1967). The German and English editions of these latter are in the press. It is a great pity he did not live to see the publication of his monograph on theoretical physics currently in press.

After the end of the Second World War appreciation of GOMBÁS's scientific work deepened very quickly. In 1946 he became in quick succession corresponding member, then ordinary member of the Hungarian Academy of Sciences and between 1949—1958 served as the Academy's Vice-President. He was awarded the Kossuth Prize twice, in 1948 and 1950, in recognition of his work. In 1951 he was decorated with the 3rd grade of the Order of the Hungarian People's Republic and in 1969, on the occasion of his 60th birthday, with the golden grade of the Order of Labour.

He took an active part in the work of the Hungarian Mathematical and Physical Society, and later, when the Society was divided, he participated in the foundation of the Eötvös Loránd Physical Society as Chairman.

He was Editor-in-Chief of this journal from the year of its foundation (1949) to his death and was highly attentive, solicitous and careful in directing the editorial work.

Professor GOMBÁS's scientific activities attracted considerable numbers of young researchers around him. In his school, his many disciples have learnt from his example the necessity of hard work and high scientific standards and could always rely on him, whether they needed generous aid or firm and outspoken criticism. A man of special personal charm he always regarded his colleagues as close friends. Despite his fragile bodily constitution he worked with ceaseless energy; neither ill health nor pain diverted him from creative work. To the immense scientific activity of the last year of his life was added too much other strain and the organism was unable to counteract this multiple burden. The great number of his friends and disciples can hardly believe that Prof. GOMBÁS with his boundless energy is no longer with us.

R. GÁSPÁR

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SEARCH FOR TRENDS IN TOTAL NEUTRON CROSS SECTIONS*

By

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A survey of total neutron cross sections at 14 MeV suggests the existence of different trends in the data. In order to determine the reliability of data given by different authors, a statistical evaluation has been carried out. It was found that the deviation in the data, measured in different laboratories for the same nuclei, is about one per cent higher than the given limits of error. A simple empirical expression is given to describe the smooth oscillating deviations of measured values from the "black-nucleus" formula as a function of mass number. Experiments were performed under the same circumstances to search for the possible fine trends or systematic behaviour in the cross-sections, e.g. $N—Z$ dependence, odd—even effect, correlation between nuclear radii and binding energies.

The experiments were carried out in the "good geometry" arrangement at 14,7 MeV neutron energy. Total neutron cross-sections were determined for N, O, Ar, Ca, Co, Ni, Cu, Zn, Ga, Ge, J, Cs, Ce, Pb, Bi.

1. Introduction

Among fast neutron data the total cross sections are the most complete and accurate, so they give reliable information about the average properties of nuclei. In fast neutron reaction cross-sections several trends have been observed [1—5]. Therefore, it seems worth while to search for systematic behaviour in total cross sections. In our investigations total neutron cross-sections at 14 MeV were measured under the same circumstances to avoid systematic errors, and the best averages of the literature data for the 13—15 MeV interval were calculated using a statistical procedure. The deadline date for the literature survey was March 1970.

2. Experimental method and results

Neutrons from the $^3H(d,n)^4He$ reaction were produced by deuterons striking a thick tritiated titanium target. The samples were approximately 2 cm in diameter. The lengths were chosen so that the transmissions were about

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50%. Stilbene crystals were used as detector and monitor using pulse-shape discrimination against gamma background. To eliminate instability effects the "bias window" method [6] was used. The measurements were performed in a "good geometry" arrangement. The target—detector distance was 60 cm and the sample was placed midway between them.

Only one of the samples deserves special attention: the argon sample was a solid argon crystal grown in liquid nitrogen. After a few attempts, it was possible to find the conditions under which a clear uniform argon crystal filled the glass holder. The metallic Ca sample was measured in a similar glass holder. The sample out runs were measured with similar empty holders. Background and in-scattering corrections were taken into account.

Table I

Experimental total cross section values at 14.7 MeV

Element	Sample	σ_T(b)	$\pm \Delta\sigma_T$(b)
N	$C_6H_{12}N_4$	1.56	0.03
O	H_2O	1.58	0.025
Ar	Ar(solid)	1.95	0.04
Ca	Ca	2.12	0.04
Co	Co	2.66	0.06
Ni	Ni	2.76	0.08
Cu	Cu	2.83	0.03
Zn	Zn	2.91	0.03
Ga	Ga	3.06	0.03
Ge	Ge	3.12	0.05
I	I	4.89	0.05
Cs	CsCl	5.01	0.07
Ce	$Ce_2(CO_3)_3$	5.16	0.10
Pb	Pb	5.34	0.04
Bi	Bi	5.33	0.04

The measured total cross section values are shown in Table I. In calculating the errors, we used the standard deviations instead of the statistical values. For each sample 15—20 runs were taken. The measurements for Ca and I were repeated on different samples to control the reproducibility of the data. One of the Ca measurements was carried out under the same conditions as for Ar.

3. Statistical treatment of literature data

For fast neutrons most of the total cross-sections data can be found in the interval of 13—15 MeV. Therefore this region was considered in our survey [7—37]. The averaging procedure was similar to that described in [38].

First, data measured at different energies by the same author were averaged. The energy dependence of σ_T was taken into account by adding 1% to the error of this average. The "grand mean" for a given element was calculated using the weighted average of the mean values mentioned above, using as weights the inverse square errors of the means. The error of the grand mean was determined in two ways: by the propagation of errors and by the standard deviation of the means around the grand mean; the larger was accepted. The total cross section data measured by different authors are approximately consistent with the given errors. Although there are some exceptions, on the average the inconsistency does not exceed 1%. The grand means and their errors for various elements and isotopes are indicated in Table II. For each atomic number the first line refers to the natural element.

4. Conclusions

The total neutron cross sections can be approximated by the "black nucleus" formula

$$\sigma_T = 2\pi(r_0 A^{1/3} + \lambda\!\!\!^{-})^2. \tag{1}$$

In order to search for fine structure in the mass number dependence of the cross-sections, the experimental data were divided by values calculated from (1) accepting $r_0 = 1.4$ fm and $\lambda\!\!\!^{-} = 1.22\,(A+1)/A$ fm. The results are shown in Fig. 1 (crosses, present work; circles, averages of literature data). As can be seen, the reduced cross-section values show a sinusoidal form as a function of $A^{1/3}$.

It was found that the data in Fig. 1 can be well described by the following empirical expression (dashed curve):

$$\frac{\sigma_T^{\text{exp.}}}{2\pi(R+\lambda\!\!\!^{-})^2} = 1{,}021 - 0{,}104\cos(2{,}18A^{1/3} - 1{,}25). \tag{2}$$

In our experiments the choice of the samples was subordinated to the aim of observing possible N—Z or odd—even effects. In Table III the ratio of measured total cross-section values and those calculated by the empirical expression are presented. Although there are significant deviations in the ratio for some pairs, these cannot be definitely attributed to odd—even or N—Z effect. The A—Ca isobaric pair seemed to be the most suitable for checking the N—Z dependence.

Table II

Averages of total cross section data for the energy interval from 13 to 15 MeV

Atomic number	Mass number	σ_T(b)	$\pm\Delta\sigma_T$(b)	Atomic number	Mass number	σ_T(b)	$\pm\Delta\sigma_T$(b)
1	1.0010	0.6935	0.0049	24	52.0555	2.4185	0.0222
1	2.0000	0.8021	0.0149	24	52.0000	2.4500	0.0645
1	3.0000	0.9776	0.0110	25	55.0000	2.5820	0.0327
2	4.0000	1.0356	0.0162	26	55.9101	2.5754	0.0179
2	3.0000	1.1400	0.0714	27	59.0000	2.6940	0.0276
3	6.9225	1.4089	0.0290	28	58.7716	2.6815	0.0209
3	6.0000	1.4465	0.0160	28	58.0000	2.7010	0.0350
3	7.0000	1.4526	0.0206	28	60.0000	2.7440	0.0364
4	9.0000	1.4772	0.0097	28	62.0000	2.7960	0.0380
5	10.8097	1.3736	0.0123	28	64.0000	2.8340	0.0383
5	10.0000	1.4601	0.0149	29	63.6154	2.9270	0.0184
5	11.0000	1.4149	0.0204	30	65.4517	2.9908	0.0214
6	12.0109	1.3268	0.0085	30	64.0000	2.9650	0.0396
7	14.0036	1.5721	0.0164	30	66.0000	3.0110	0.0401
8	16.0043	1.6008	0.0170	30	67.0000	2.9900	0.0599
8	18.0000	1.4215	0.1848	30	68.0000	3.0510	0.0405
9	19.0000	1.7599	0.0131	30	70.0000	3.1160	0.0492
10	20.1758	1.5520	0.0826	31	69.7933	3.1392	0.0360
11	23.0000	1.7257	0.0133	32	72.6990	3.2357	0.1106
12	24.3232	1.7664	0.0088	33	75.0000	3.4954	0.1008
13	27.0000	1.7412	0.0127	34	79.0959	3.4793	0.0391
14	28.1067	1.8308	0.0231	35	79.9872	3.4920	0.0462
15	31.0000	1.9459	0.0374	36	83.8846	3.7767	0.0786
16	32.0914	1.9189	0.0116	37	85.5552	3.9000	0.1390
17	35.2449	2.0211	0.0173	38	87.7092	3.6800	0.0755
18	39.9850	2.0018	0.0553	39	89.0000	3.8646	0.0487
19	39.1370	2.1155	0.0273	40	91.3125	3.7441	0.2007
19	39.0000	2.2900	0.0729	41	93.0000	4.0033	0.0444
20	40.1123	2.1790	0.0178	42	95.9691	4.0128	0.0346
20	42.0000	2.6814	0.0426	42	96.0000	4.0400	0.1204
20	44.0000	2.1614	0.0374	43	99.0000	4.1964	0.0601
21	45.0000	2.1791	0.0339	46	106.6244	4.2798	0.0406
22	47.9227	2.3000	0.0159	47	107.9712	4.3237	0.0367
23	50.9976	2.3421	0.0311	47	107.0000	4.3400	0.0734
				47	109.0000	4.3800	0.0638

Table II (continued)

Atomic number	Mass number	σ_T(b)	$\pm\Delta\sigma_T$(b)	Atomic number	Mass number	σ_T(b)	$\pm\Delta\sigma_T$(b)
48	112.5139	4.4485	0.0399	60	144.3205	5.0140	0.0549
48	106.0000	4.2900	0.1129	61	148.0000	5.5992	0.1426
48	108.0000	4.3300	0.1133	62	150.0000	5.1756	0.0602
48	110.0000	4.3400	0.0834	63	152.0434	5.1992	0.0809
48	111.0000	4.4400	0.0844	64	157.3281	5.2311	0.0484
48	112.0000	4.5300	0.0753	65	159.0000	5.2036	0.0762
48	113.0000	4.5000	0.0750	66	162.5703	5.2650	0.0716
48	114.0000	4.5400	0.0654	67	165.0000	5.2647	0.0503
48	116.0000	4.5600	0.0756	68	167.3271	5.3644	0.0641
49	114.9151	4.5303	0.0352	69	169.0000	5.3045	0.0711
50	118.8763	4.6063	0.0331	70	173.0952	5.5350	0.0784
50	116.0000	4.4300	0.1243	71	175.0260	5.3282	0.0774
50	117.0000	4.6400	0.0964	72	178.5506	5.3447	0.0696
50	118.0000	4.7500	0.1175	73	181.0000	5.2357	0.0473
50	119.0000	4.4600	0.1446	74	183.8881	5.3655	0.0552
50	120.0000	4.6600	0.0866	74	182.0000	5.4267	0.0774
50	122.0000	4.6900	0.0869	74	186.0000	5.5191	0.0793
50	124.0000	4.7100	0.1071	75	186.2577	5.1964	0.0821
51	121.8535	4.6647	0.0382	76	190.2763	5.1545	0.0817
51	121.0000	4.6600	0.0666	77	192.2291	5.2364	0.0825
51	123.0000	4.6800	0.0768	78	195.1177	5.3701	0.0728
52	127.7164	4.8732	0.0545	79	197.0000	5.3188	0.0452
52	122.0000	4.6500	0.0865	80	200.6251	5.3473	0.0602
52	124.0000	4.6000	0.0960	81	204.4092	5.4124	0.0491
52	125.0000	4.6900	0.0869	82	207.2419	5.4006	0.0305
52	126.0000	4.7300	0.0673	82	204.0000	5.4949	0.0934
52	128.0000	4.7600	0.0776	82	206.0000	5.4154	0.0649
52	130.0000	4.8100	0.0681	82	207.0000	5.3488	0.0847
53	127.0000	4.8203	0.0431	82	208.0000	5.2950	0.0812
54	131.3835	5.0400	0.1320	82	206.3000	5.2945	0.0667
55	133.0000	5.0012	0.1090	83	209.0000	5.4090	0.0355
56	137.4206	5.0998	0.0509	90	232.0000	5.6344	0.1296
57	138.9991	4.9143	0.0750	92	237.9783	5.7493	0.0549
58	140.2081	5.0165	0.0478	92	235.0000	5.7900	0.1279
59	141.0000	4.9381	0.0574	94	239.0000	5.8300	0.1383

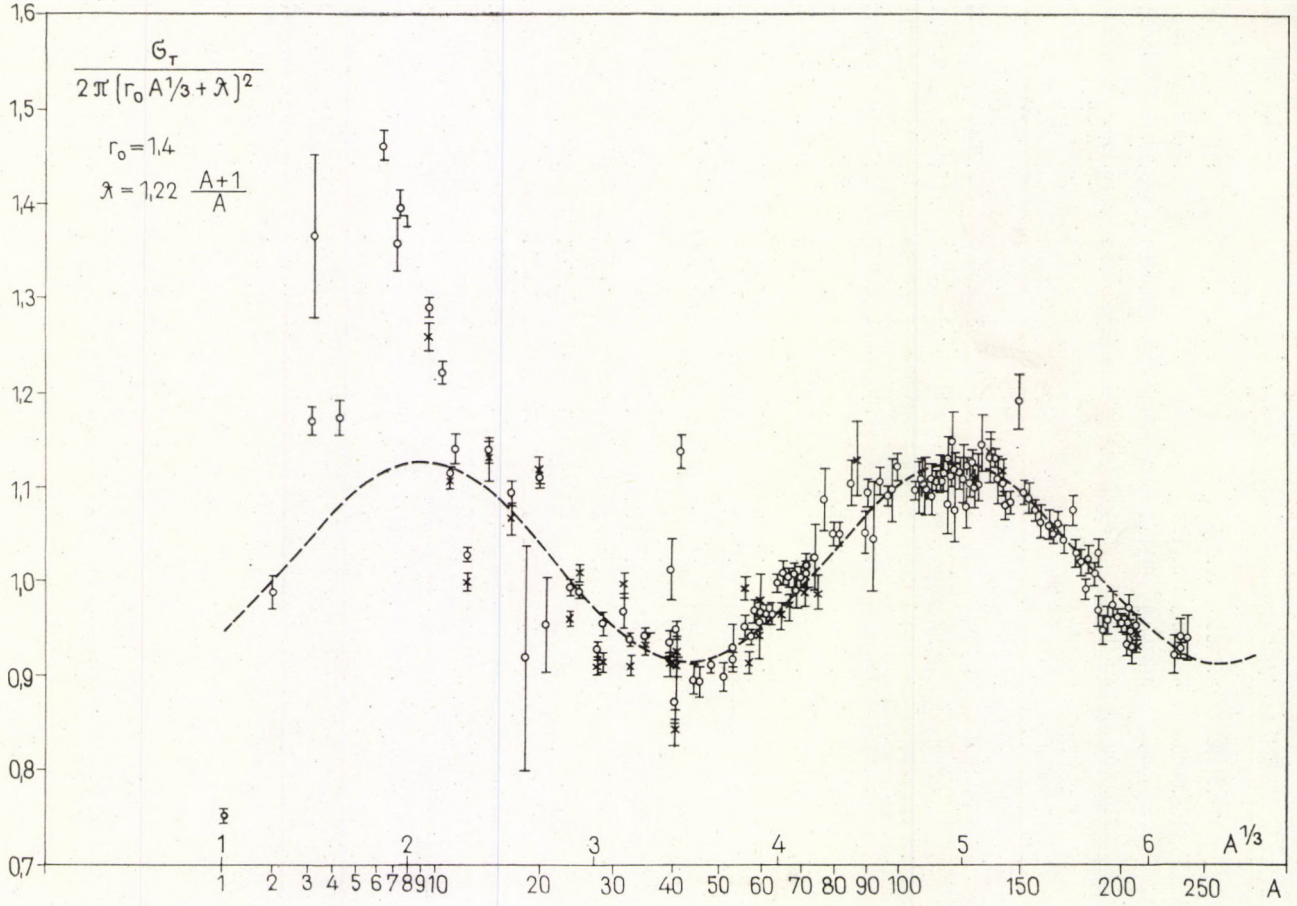

Fig. 1. The 14 MeV neutron total cross sections divided by $2\pi(R+\lambda)^2$ as a function of $A^{1/3}$

Table III

Ratio of measured and calculated cross sections for the nuclei investigated

Odd	Even	$N-Z$	N	$\frac{\sigma_{exp}}{\sigma_{calc}}$
B		1		1.00±0.01
			6	
	C	0		0.90±0.01
N		0	7	1.04±0.02
	O	0	8	1.01±0.02
Na		1		0.97±0.01
			12	
	Mg	0		1.03±0.01
Al		1		0.95±0.01
			14	
	Si	0		0.96±0.01
P		1		1.07±0.01
			16	
	S	0		0.98±0.01
	Ar	4	22	0.93±0.02
	Ca	0	20	1.01±0.02
Mn		5		1.05±0.01
			30	
	Fe	4		0.97±0.01
Co		5	32	0.98±0.02
	Ni	2—3	30	1.02±0.03
Cu				0.99±0.01
	Zn	—	—	0.99±0.01
Ga				0.99±0.01
	Ge	—	—	0.97±0.02
I		21		1.01±0.01
	Te	22—26		1.00±0.01
Bi		—	—	0.98±0.01
	Pb			0.98±0.01

In general, the good fit of this simple formula to the experimental data for medium and heavy nuclei suggests that if any systematic trend in total neutron cross sections exists, its magnitude does not exceed a few per cent. Expression (2) can be used for the calculation of unknown total cross sections in the mass number region mentioned above.

As for light nuclei, expression (2) does not describe well the variation of reduced cross sections, although its shape is similar. As was shown in our earlier paper [36, 37] a correlation exists between r_0 and the binding energy per nucleon. This suggests that the higher r_0 values in this region are connected with a loose nuclear structure, giving a higher cross section. The deviations or pairs in Table III can be mainly explained by the binding energy effect.

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ИССЛЕДОВАНИЕ ЗАВИСИМОСТИ ПОЛНЫХ НЕЙТРОННЫХ СЕЧЕНИЙ ОТ РАЗНЫХ ЯДЕРНЫХ ПАРАМЕТРОВ

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Резюме

Сравнение полных нейтронных сечений при 14 Мэв указывает на существование зависимости этих данных от разных ядерных характеристик. С целью проверки надежности результатов, полученных разными авторами, была проведена статистическая обработка данных. Оказалось, что данные, полученные разными лабораториями для одного и того же ядра дают отклонения на один процент выше чем пределы ошибок указанные авторами.

В статье дается простая эмпирическая формула для описания гладкого осциллирующего отклонения измеренных значений от рассчитанных по модели черного ядра, в зависимости от массового числа. Измерения были выполнены при одинаковых условиях чтобы найти возможные плавные зависимости или систематическое поведение в ходе сечений, например зависимость от $N - Z$, нечетно-четные эффекты, корреляцию между радиусами ядер и энергиями связи.

Измерения были выполнены при «хорошей геометрии» и нейтронной энергии 14,7 Мэв. Полные нейтронные сечения были определены для N, O, Ar, Ca, Co, Ni, Cu, Zn, Ga, Ge, J, Cs, Ce, Pb, Bi.

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SUM RULE FOR THE VERTICES $K^* \to K\pi$ AND $K_A \to K_\pi^*$

By

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The method, based on the techniques of current algebra and dispersion relations, is used for calculating the ratio of the d and s wave coupling of the vertex $<K_A|J_\pi|K^*>$. We obtain a limitation for the pole approximation and applying the general results of LAI [1] the $\Gamma(K^* \to K\pi)$ and $\Gamma(K_A \to K^*\pi)$ decay widths are calculated in good agreement with recent experimental data. In our calculation we apply the Weinberg broken sum rules.

I. Introduction

In connection with current algebra two approaches have been advanced to calculate the form factors of the vector and axial vector mesons, within a single framework [1]. Although the arguments used in these two methods are different, they lead to exactly the same results. One is based on the the technique of dispersion relations, and the other involves the use of Ward identities for vertex functions. The extension of the latter method to the entire SU(3) octet of current was not lucky, because this extension produced the self-consistency relation $F_K/F_\pi = m_\pi/m_K$. It is, however, possible to generalise the dispersion method, namely, LAI [1] has proved that the assumption of soft mesons may not be essential in the determination of the subtraction constant. So, using the divergence conditions for the currents the form factors of the matrix-elements $<\pi^0 \mid V_\mu^{K^-}(C) \mid K_A>$ and $<\pi^0 \mid A_\mu^{K^-}(C) \mid K^*>$ can be parametrised as functions of an unknown parameter δ_1 [1]. Our aim is to determine the value of δ_1 merely with the input values of the masses of the mesons.

In Section II we describe the derivation of the sum rule, while in Section III we evaluate the sum rule. Finally, in Section IV we discuss the result of our calculation.

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II. Restriction for δ_1 from four-point function sum rule

Our basic equation in the usual notation is the following:

$$\langle\pi^0(p)|[A_4^{K^-}(x), A_\pi^{K^+}(y)]_{x_0=y_0}|\pi^0(p)\rangle = \\ = \langle\pi^0(p)|\pi^0(p)\rangle\langle 0|[A_4^{K^-}(x)|A_\lambda^{K^+}(y)]_{x_0=y_0}|0\rangle, \tag{1}$$

where $\lambda = 1,2,3$. (A similar sum rule was derived in [2].) (1) follows from c-number Schwinger terms and C-invariance.

Now, we carry out a Fourier transform on both sides of (1) in the form $1/(2\pi)^3 \int d^3(\boldsymbol{x}-\boldsymbol{y})\, e^{iq(x-y)}$, and in the spirit of FUBINI and FURLAN's method [3] decompose the left hand side of (1) with respect to the singularity structure: the first term (W_I) ist the direct graph, the second and third terms correspond to the "mass singularities", the fourth one (W_IV) contains the so called Z graphs. Finally, the last contribution (W_V) is due to the disconnected diagrams; it is equal to the righ-hand side of (1). For the sake of simplicity we do not take into account the second and third graps. Thus, in the place of (1) we write the sum rule:

$$W_\mathrm{I} + W_\mathrm{IV} = 0. \tag{2}$$

Here, we are dealing only with low-lying states:

$$W_\mathrm{I} = \sum_\gamma [\int d^3\boldsymbol{k}\big(\delta^3(\boldsymbol{q}+\boldsymbol{k}-\boldsymbol{p}) - \delta^3(\boldsymbol{q}+\boldsymbol{p}-\boldsymbol{k})\big)\langle\pi^0(p)\,|A_4^{K^-}(0)|K^{*+}(k,\varepsilon)\rangle \cdot \\ \cdot \langle K^{*+}(k,\varepsilon)\,|A_\lambda^{K^+}(0)\,|\pi^0(p)\rangle],$$

$$W_\mathrm{IV} = \sum_\gamma [\int d^3\boldsymbol{k}\big(\delta^3(\boldsymbol{q}+\boldsymbol{k}+\boldsymbol{p}) - \delta^3(\boldsymbol{q}-\boldsymbol{k}-\boldsymbol{p})\big)\langle 0\,|\,A_4^{K^-}(0)\,|\,\pi^0(p)\,K^{*+}(k,\varepsilon)\rangle \cdot \\ \cdot \langle\pi^0(p)\,K^{*+}(k,\varepsilon)\,|\,A_\lambda^{K^+}(0)\,|\,0\rangle],$$

where the invariant decomposition

$$\langle\pi^0(k)|A_\mu^{K^-}(0)|K^{*+}(\varepsilon,p)\rangle\, N_0 = \\ = i\varepsilon_\nu\,[K_1(t^2)\,\delta_{\nu\mu} + K_2(t^2)\,k_\nu(p+k)_\mu + K_3(t^2)\,k_\nu(p-k)_\mu] \tag{4}$$

can be used. $N_0 = (4p_0\,k_0)^{1/2}\,(2\pi)^3$ and $K_i(t^2)$ $(i = 1,2,3)$ are invariant functions. Applying (2) and (3), instead of (2) we can write:

$$A_1(t^2) - C_1(l^2) + \frac{k_0}{p_0}\,[A_2(t^2) + C_2(l^2)] = 0 \tag{5}$$

provided $\boldsymbol{p}\cdot\boldsymbol{q} = 0$, $\boldsymbol{p}^2 \neq 0$, $\boldsymbol{q}^2 \neq 0$, where

$$A_1(t^2) = \frac{(k_\mu p_\mu)}{m^2 K^*}\,(K_2 - K_3)[K_1 + (k_\varrho p_\varrho)(K_2 + K_3)] + K_1(K_2 + K_3)\,,$$

$$A_2(t^2) = \frac{1}{m_{K^*}^2}[K_1+(k_\mu p_\mu)(K_2+K_3)]^2,$$

$$k_0 = \sqrt{\boldsymbol{p}^2+\boldsymbol{q}^2+m_{K^*}^2} \quad ; \quad p_0 = \sqrt{\boldsymbol{p}^2+m_\pi^2},$$

$$t^2 = \boldsymbol{q}^2 - (p_0-k_0)^2 \quad ; \quad l^2 = \boldsymbol{q}^2 - (p_0+k_0)^2.$$

$C_i(l^2)$ can be obtained from $A_i(t^2)$, $(i = 1,2)$ by replacing $\boldsymbol{p} \to -\boldsymbol{p}$. Terms multiplied by m_π^2 are negligible.

III. Evaluation of the sum rule

To evaluate Eq. (5), we use the parametrised form of the form factors K_i which is derived in [1] but with the following modification: the leptonic coupling constants $g_{K^*}, g_{K_A}, F_K F_\pi$ are taken from the broken Weinberg sum rules (CLEYMANS [4]) based on the SUGAWARA model [5]. So, on the one hand these are in better agreement with recent experiments, and on the other hand, their predictions for F_K/F_π and for the form factor $f_+(0)$ of the decay K_{l3} are in accordance both with experiments and with the Adamello-Gatto theorem.

The broken Weinberg sum rules (we neglect F_x^2, because $F_x^2 \ll F_K^2$, [4]) are

$$\frac{g_{K_A}^2}{m_{K_A}^2} + F_K^2 = \frac{g_{K^*}^2}{m_{K^*}^2} = 2\frac{m_{K^*}^2}{m_\varrho^2} F_\pi^2 \; ; \; g_{K_A}^2 = g_{K^*}^2 .$$

Thus, we can write the form factors K_i in the following modified form

$$K_1(x) = \sqrt{2}\, m_{K^*}\left[\frac{1}{f_1} - \frac{d}{f_2}\left(1+\frac{1}{2}\delta_1\right)\frac{x+1}{x+f_2^2}\right],$$

$$K_2(x) = -\frac{\sqrt{2}}{m_{K^*}}\frac{d}{f_2}\frac{\delta_1}{2(x+f_2^2)}, \tag{7}$$

$$K_3(x) = \frac{\sqrt{2}}{m_{K^*}}\left\{\frac{1}{f_1(x+f_3^2)}\left[1-\frac{1}{f_2^4}(1+\delta_1)\right] - \right.$$

$$\left. - \frac{d}{f_2(x+f_2^2)}\left[\left(1+\frac{1}{2}\delta_1\right) - \frac{1}{f_2^2}(1+\delta_1)\right]\right\},$$

where we had used the definitions:

$$\frac{m_\varrho}{m_{K^*}} = f_1\,; \; \frac{m_{K_A}}{m_{K^*}} = f_2\,; \; \frac{m_K}{m_{K^*}} = f_3\,; \; d = \left(\frac{m_{K^*}^2}{m_\varrho^2} - \frac{F_K^2}{2F_\pi^2}\right)^{1/2} \approx$$

$$\approx 0.81 \left(\text{if } \frac{F_K}{F_\pi} = 1.18, \text{ see [4]}\right)$$

$$\text{and } t^2 = m_{K^*}^2\, x.$$

We solved Eq. (5) numerically. First, we studied the roots of (5) whilst p^2, q^2 were changing, secondly we compared (5) to 0 putting in the physically possible values δ_1. The two programmes led to the same result. We could establish that both the real roots of Eq. (5) and their least deviation from 0 were obtainable for those values of t^2, l^2 which are inside a circle with radius 6 m^2_{pole} (both for K and K_A poles). The average value of the roots of Eq. (5):

$$\delta_1 = -0.44 \pm 0.06. \tag{8}$$

With this result, we can easily calculate the decay widths (according to the formulae of [1]):

$$\Gamma(K^* \to K\pi) = [51 \pm 3]\ \text{MeV}; \quad \Gamma(K_A \to K^*\pi) = (70 \pm 8)\ \text{MeV}. \tag{9}$$

The experimental values [6]:

$$\Gamma(K^* \to K\pi) = [50.1 \pm 0.8]\ \text{MeV};$$

$$\Gamma(K_A \to K^*\pi, K\varrho, \omega K, \eta K) = (90 \pm 40)\ \text{MeV}.$$

The partial widths of K_A are not known because of their overlapping, but it is known that the $K_A \to K^*\pi$ decay mode is dominant (the others are less than a few percent), so the agreement with experiment is good.

IV. Discussion

In deriving our results, the use of the broken Weinberg sum rules played an important role. It caused a deviation from the calculations made by LAI [1], but our results are in better agreement with experiments.

We learned from the results of the evaluation that the pole approximation cannot be applied to arbitrary values of t^2, l^2. A six-times neighbourhood of the poles, where the approximation was still valid, was unambiguously chosen by the different methods of evaluation; our method was able to test the limit of the pole approximation, too.

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ПРАВИЛО СУММ ДЛЯ ВЕРШИН $K^* \to K\pi$ И $K_A \to K^*\pi$

Г. ФЕРЕНЦИ

Резюме

Для вычисления соотношения d и s волновой связи вершины $\langle K_A | J_\pi | K^* \rangle$ применяются техника алгебры токов и дисперсионные соотношения. Получено ограничение для полюсного приближения. Применяя общие результаты Лаи [1], вычислялись ширины распадов $\Gamma(K^* \to K\pi)$ и $\Gamma(K_A \to K^*\pi)$, находящиеся в хорошем согласии с опытными данными. В вычислениях использовано нарушенные правила сумм Вейнберга.

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THE HYDRODYNAMICAL MODEL OF WAVE MECHANICS VII

THE STERN—GERLACH EFFECT OF THE H-ATOM

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It is shown that treating the Stern—Gerlach effect as a one-body wave mechanical problem — i.e. supposing the nucleus to behave classically — the treatment leads to the incorrect classical result. The splitting of the beam is only obtained in the many-body treatment.

§ 1. A beam of neutral atoms is passed through an inhomogeneous magnetic field. The field strength **B** is about perpendicular to the beam. If the atoms possess magnetic moments **M** a force

$$\mathbf{F} = \operatorname{grad}(\mathbf{MB}) \tag{1}$$

acts on them and passing through the region of the field they are deflected and they obtain a transversal momentum

$$\mathbf{p} = \int \mathbf{F}\, dt. \tag{2}$$

The experiments of Stern and Gerlach showed that such a beam is indeed deflected by the inhomogeneous magnetic field; the beam is found to be split into a number of discrete components.

§ 2. The classical treatment of the effect leads to expect, that contrary to the experimental result, the beam should be smeared out continuously. This treatment can be summarized briefly as follows. Supposing the atoms to be rotating solids of spherical symmetry with magnetic moment **M** and angular momentum π so that

$$\mathbf{M} = \alpha\dot{\pi}, \tag{3}$$

where α is a characteristic of the structure of the atom. The equation of motion of the rotational part of the motion can be written

$$\dot{\pi} = \mathbf{B} \times \mathbf{M}. \tag{4}$$

Eliminating π with the help of (3) we obtain as the equation of motion of the magnetic moment

$$\dot{\mathbf{M}} = \alpha(\mathbf{B} \times \mathbf{M}).$$

While the atom is passing through the inhomogeneous region the field strength **B** acting on the atom changes in time. We may thus write $\mathbf{B}(t)$ for the field strength acting at the time t on the atom. Denote the unit vector pointing in the direction of $\mathbf{B}(t)$

$$\varkappa(t) = \mathbf{B}(t)/B(t).$$

Further write

$$\alpha B(t) = \omega(t),$$

where $\omega(t)$ is a quantity with the dimension of a frequency. The equation of motion can thus be written

$$\dot{\mathbf{M}} = \omega(t)\,(\varkappa(t) \times \mathbf{M}). \tag{5}$$

§ 3. Multiplying (5) by **M** we find

$$\mathbf{M}\dot{\mathbf{M}} = 0 \text{ thus } M = \text{const.} \tag{6}$$

Thus the total magnetic moment and angular moment remains constant.

Multiplying (5) by $\varkappa(t)$ we find

$$\varkappa(t)\,\dot{\mathbf{M}} = 0\,. \tag{7}$$

If we suppose that the magnetic field changes only slowly, i.e. its change in an interval $\Delta T = 1/\omega(t)$ is small, then we can neglect terms proportional to $\dot{\varkappa}(t)$ and $\dot{\omega}(t)$ and we find

$$\frac{d}{dt}\,(\varkappa(t)\,\mathbf{M}) = 0\,,$$

thus

$$|\mathbf{M}^{(1)}| = \varkappa(t)\,\mathbf{M} \approx \text{const.},$$

where $\mathbf{M}^{(1)}$ is the component of **M** parallel to **B**. In the same approximation we find also

$$\ddot{\mathbf{M}}^{(2)} = -\,\omega^2(t)\,\mathbf{M}^{(2)},$$

where $\mathbf{M}^{(2)}$ is the component of **M** perpendicular to **B**. Thus in this approximation the vector **M** precesses with a frequency $\omega(t)$ around **B**.

Since the component $\mathbf{M}^{(1)}$ of **M** parallel to **B** remains constant, therefore an atom moving across the field suffers a deflection proportional to $\mathbf{M}^{(1)}$ in accord with (1) and (2).

Considering a beam of atoms passing through the field one must expect that the initial directions of **M** were distributed at random. Therefore the atoms

are expected to enter the field with various inclinations of **M** with respect to **B**. Thus the values of $M^{(1)}$ for the individual atoms must be expected to be distributed continuously between $-M$ and $+M$ and therefore the deflections are expected to be distributed continuously between two extreme values.

The experimental results can only be explained if one assumes that for some reason the atoms when entering the magnetic field orient themselves into specified direction. E. g. hydrogen atoms in ground state orient themselves parallel or antiparallel to the direction of the magnetic field.

We see thus that — as it is well-known — the classical treatment does not lead to the correct result.

It seems to us important, however, to discuss two classical effects which have a tendency to produce a splitting of the beam. We show that neither of the effects is sufficient to explain the observed splitting of the beam.

§ 4. Firstly, we note that we have given only the approximate solution of the equations of motion (5) having neglected terms of the order of $\dot{\varkappa}(t)$, $\dot{\omega}(t)$. Although neglecting such terms causes only a small error, the motion is to be considered for the duration of very large numbers of periods of the precession and it is not obvious whether or not the errors accumulate. Thus it must be investigated whether or not the accumulation of small perturbations can cause a systematic change of $M^{(1)}$?

In particular one might raise the following question. The inhomogeneous magnetic field which was used in the actual experiments of the Stern—Gerlach type are strongly concentrated into the vicinity of the pole pieces of the permanent magnet. It could be imagined that the atom, when it enters through the boundary of the magnetic field, suffers a sudden impact which impact makes it to orient itself parallel or antiparallel to the field. The "impact" thus mentioned is taken as a period when $\dot{\varkappa}(t)$ is comparatively large and thus the accumulating perturbation might also become large.

The above processes do not lead, however, to the observed orientation of the magnetic moments. This was shown by a mathematical analysis carried out together with BÉKÉSSY [1]. In the latter analysis we have shown that the approximate solutions neglecting $\dot{\varkappa}$, $\dot{\omega}$ give an adequate description of the motion of the rotating magnetic dipole and the errors caused by neglecting such terms do not accumulate sufficiently to produce any observable effects.

Secondly, we have neglected in our treatment that the precessing magnetic dipole emits radiation and therefore it loses energy until a stationary state is obtained. The stationary states are e.g. those where the magnetic dipole is parallel or antiparallel to the field **B** and in such states no radiation is emitted. The rate of emission of energy of a rotating magnetic dipole is, however, negligibly small and thus no noticeable change of orientation of the dipoles caused by radiation reaction can be expected in the period the atoms pass through the deflecting field.

§ 5. The splitting of the beam as observed in the Stern – Gerlach effect can only be accounted for by the quantum mechanical treatment. A problem nevertheless arises if we remember that the Pauli equation can be rewritten and replaced by a set of hydrodynamical equations which give a mathematical description of the atom equivalent with the classical description [2] which we have shown above do not lead to the correct result.

So as to see the problem more clearly we refer to the treatment of the Stern—Gerlach effect found in some text books, where it is suggested, that because of its comparatively large mass, the motion of the atomic nucleus can be treated classically and it is sufficient to treat the motion of the electrons in accord with quantum mechanics.

Let us consider a hydrogen atom passing through an inhomogeneous magnetic field. If we treat the nucleus classically then we have a one body problem. The electron cloud can be considered as being under the influence of the Coulomb field of the moving nucleus and the outside magnetic field. The nucleus moves under the influence of the outside field and the electrostatic field of the electron cloud.

Rewriting the Pauli equation in the form of the hydrodynamical equations we find that the electron behaves like a charged cloud rotating freely around the nucleus. The cloud is kept together by the Coulomb attraction which is compensated by the inner forces arising from the quantummechanical potential. These forces are much stronger than the forces produced by the outer magnetic field. Thus the system as a whole behaves like a very hard rotating magnetized and charged solid body and is expected to behave in accord with classical physics.

The body carries out a precession and also it is pulled away by the inhomogeneous magnetic field. Because of the Coulomb interaction between electron cloud and nucleus, the nucleus is dragged away from the straight path by the electron cloud. The motion can be described exactly by the classical equations which we have discussed further above.

§ 6. Since the hydrodynamical equations are exactly equivalent to the Pauli equation, the exact solution of the time dependent Pauli equation must necessarily lead to the same incorrect result as the classical treatment sketched above. This discrepancy arises because the assumption to the effect, that the nucleus can be treated classically, is incorrect. The correct result is obtained only if we treat the problem as a many body problem — in the case of the hydrogen atom as a two body problem.

In the correct quantum mechanical treatment we have to solve the Schrödinger equation

$$H\psi = i\hbar\dot{\psi},$$

where

$$\psi = \psi(\mathbf{r}_1, \mathbf{r}_2, t)$$

$\mathbf{r}_1$ is the coordinate vector of the proton, $\mathbf{r}_2$ that of the electron. H contains the inhomogeneous magnetic field.

In the usual treatment of the effect the wave function is taken as the superposition of two particular solutions, thus

$$\psi(\mathbf{r}_1, \mathbf{r}, t) = c_1 \psi_+(\mathbf{r}_1, \mathbf{r}_2, t) + c_2 \psi_-(\mathbf{r}_1, \mathbf{r}_3, t).$$

The particular solutions ψ_+ and ψ_- are solutions corresponding to spin orientations parallel and antiparallel to **B**.

Often ψ_+ and ψ_- are taken as plane wave solutions and it is shown that the plane waves change their directions — the outcoming beam can thus be described as the superposition of the plane waves.

This treatment is, however, not satisfactory. Indeed, infinite plane waves do not separate at all and the splitting of the beam can only be obtained if we were to treat the problem in terms of plane waves the cross section of which is appreciably smaller than the distance of separation of the beams.

In a satisfactory treatment of the effect one must thus show the following: describing the incoming beam as a superposition of wave packets each packet having polarization in a direction inclined to **B**. It must be shown that such packets when passing through the field split into two packets each with opposite polarizations. One must show further that those fractions of the original packet proceed along the two extreme paths.

The latter statement is certainly correct. Indeed, if we take ψ_+ and ψ_- not to be plane waves, but wave functions describing parallel and anti parallel polarized packets — then it follows from the wave equation that both of the polarized packets proceed along the extreme orbits in accord with observation.

The following question remains, however. The function ψ could also be decomposed into two components ψ_1 and ψ_2 the polarizations of which are somehow inclined relative to **B**. Why can one assume that the packets which are polarized parallel or anti parallel remain together and those polarized into inclined directions split up?

So as to answer this question it must be remembered that every packet diffuses along its path. If this diffusion is too strong then it blurs the effect to be observed. This is the reason why no Stern—Gerlach effect can be observed on a beam of free electrons.

The diffusion of an electron cloud in the atom, when the polarization is parallel to the magnetic field, is found from the hydrodynamical equation to be the normal diffusion to be expected without magnetic field. If, however, a packet is polarized in a direction inclined to **B**, then another diffusion process sets in which may lead eventually to separation of the packet. We discuss this process presently.

§ 7. We give thus a qualitative explanation why a packet with magnetic moment inclined to the direction of the magnetic field is separated into components. Consider for this purpose an electron cloud with polarization into a direction **T**. If the cloud enters a magnetic field it starts a precession round **B** with an angular velocity proportional to **B**. If the field strength varies across the atom then the angular velocity of the precession will also change with the coordinates and thus as an effect of the non uniform precession the state of polarization becomes inhomogeneous. From the hydrodynamical equations of motions we find that as a result of the inhomogeneous polarization torques appear which try to make polarization homogeneous again.

The total torque being zero, there appears thus a tendency to make parts of the cloud to rotate more quickly, others to slow down the rotation. A stationary state can be achieved if, as a result of the inner forces, the motion is separated into two parts. The first part of the cloud is made to be polarized parallel, the second part antiparallel to **B**. In the latter case the precession ceases in both separated parts.

We note, that for the process described above the inhomogeneity of the field which causes the separation is not the inhomogeneity across the atomic radius, thus it is not simply the change of field across a distance of the order of the hydrogen radius, i.e. of the order of 1 Å. Indeed, describing the atom e.g. with a two body wave function, we obtain a packet which diffuses very strongly if it is orientated into a region with dimenions of the hydrogen radius. It seems more reasonable to take the packets of the order comparable with the cross section of the atomic beam. Such packets show only negligible diffusion and thus if orientated parallel or anti parallel to **B**, they proceed practically along the classical orbit. — Such a large packet if its orientation is inclined to **B** will show the effect discussed above and thus split into parts polarized parallel to **B**.

§ 8. The question can also be answered how does it mathematically come about that packets appear to remain together if their motion is treated with the help of the one body wave equation?

The answer to the question is simple. In the one body treatment the elements of the electron cloud are kept together by the (supposed classically behaving) point nucleus. The Coulomb attraction is, in this treatment much stronger than the magnetic forces and thus even if there is a tendency to separate the cloud — this tendency is compensated by the Coulomb attraction.

In the two body treatment the Coulomb force does not prevent the splitting up of a wave packet. Indeed, the wave function ψ can be written in the following form

$$\psi(\mathbf{r}_1, \mathbf{r}_2, t) = a\left(\frac{M\mathbf{r}_1 + m\mathbf{r}_2}{m+M}\right) b(\mathbf{r}_1 - \mathbf{r}_2, t). \tag{8}$$

The function b is the wave function of the one body problem only, m is to be replaced by the reduced mass

$$m' = \frac{mM}{m+M} .$$

The function a is a slowly varying function of its first variable, it gives the distribution of the wave packet representing the H-atom as a whole.

According to a previous publication [3] the wave function (8) corresponds to two densities

$$\left.\begin{aligned} \varrho_1(\mathbf{r}) &= \int \psi(\mathbf{r}, \mathbf{r}_2)\, d\tau_2, \\ \varrho_2(\mathbf{r}) &= \int \psi(\mathbf{r}_1, \mathbf{r})\, d\tau_1 . \end{aligned}\right\} \tag{9}$$

Considering (8) we find — provided the packet as a whole is much larger than the radius r_H of the H-atom — that

$$\varrho_1(\mathbf{r}) \approx \varrho_2(\mathbf{r}) .$$

Thus the electron and the proton are forming clouds of about equal densities. The cloud is therefore about neutral and there are no strong Coulomb forces which prevented the separation of the cloud.

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ГИДРОДИНАМИЧЕСКАЯ МОДЕЛЬ ВОЛНОВОЙ МЕХАНИКИ, VII

Л. ЯНОШИ

Резюме

Доказывается, что толкование эффекта Штерна—Герлаха квантово-механическим методом «одного тела», т. е. методом, при котором ядро вводится классически, приводит к неправильному классическому результату. Дискретное разложение луча получается толкованием, соответствующим проблеме «многих тел».

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THE HYDRODYNAMICAL MODEL OF WAVE MECHANICS VIII

SOME LIMITATIONS OF THE ONE BODY TREATMENT

By

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As we have shown in a previous publication the quantum mechanical treatment of the Stern—Gerlach effect of the H-atom leads to an incorrect result if we treat it as a one body problem. Here it is shown by further examples that the characteristic quantum mechanical results are obtained only when considering many body problems in wave mechanics. The schematized treatment of certain problems as one body problems leads to classical results.

§ 1. In a previous publication [1] we have shown that the wave mechanical treatment of the Stern—Gerlach effect leads to the incorrect classical result if the motion of the nucleus is treated classically. The correct result is obtained if we use the many body wave function for the atoms and take the nucleus as one of the bodies described by the wave function.

The result obtained for the Stern—Gerlach effect is a typical one. The specifically quantum mechanical features of physical systems present themselves only in the many body treatment. We illustrate this with one more example.

§ 2. Considering a H-atom we have shown [2] that the distribution of the electron is such that

$$\oint \mathbf{v}\, d\mathbf{s} = \frac{k\hbar}{m} + \text{terms depending on } \mathbf{B} \text{ and spin}, \qquad (1)$$

$$k = 0, \pm 1, \ldots$$

the line of integration is to be taken so as to avoid singular points where $\varrho = 0$. If the path of integration is taken to move together with the flow of the electron, then $\mathbf{v}$ changes continuously on every point of the line of integration. Therefore, whatever external perturbations are acting on the system, the value of the integral will change continuously.

A change of k from one integer value to another would correspond to a discontinuous change of the value of the integral, such a change can therefore not occur as the result of finite perturbations.

In the ground state of the H-atom $k = 0$ therefore we see that there exists no perturbation which can produce a state with $k \neq 0$ if we consider only changes in accord with the Schrödinger equation of the one body problem.

§ 3. Wave functions for which $k = 0$ along any closed line of integration represent the S-states of the H-atom. Wave functions where $|k| > 0$ for some line of integration represent $P, D, \ldots$ states or combinations containing such states. The latter states correspond to atoms with orbital spin and orbital magnetic moments.

The H-atom possesses stationary states with wave function (neglecting spin)

$$\psi_{\pm 1} = C_1 r \exp\left\{-\frac{1}{4}\alpha r \pm i\varphi - iE_1 t/\hbar\right\} . \tag{2}$$

The latter states correspond to values $k = \pm 1$ for paths of integration taken around the z-axis. Starting from the ground state with the wave function

$$\psi_0 = C_0 \exp\left\{-\alpha r - iE_0 t/\hbar\right\} , \tag{3}$$

no perturbation can cause a change from a state ψ_0 to ψ_{+1} or ψ_{-1}. Changes can, however, be produced into mixed states of the form

$$\psi = \frac{1}{\sqrt{2}}(e^{i\gamma}\psi_1 + e^{-i\gamma}\psi_{-1}) = 2C_1 r \cos(\varphi+\gamma)\exp\left\{-\frac{1}{4}\alpha r - iE_1 t/\hbar\right\} . \tag{4}$$

The latter wave function is real therefore it corresponds to a distribution $\mathbf{v} = 0$ and $k = 0$. Such a state possesses thus no orbital magnetic moment.

The above results do not reflect the experimental results. Indeed, it is possible to excite the atoms of a gas, e.g. with the help of light of suitable frequency and thus to produce atoms with states possessing orbital magnetic moments. That the excited gas contains atoms with orbital magnetic moments can be shown experimentally. Indeed, the atoms brought into such states can be selected with the help of a magnetic separator and thus it can be established which fraction of the atoms of the excited gas possessed specified non-vanishing orbital magnetic momentum.

§ 4. The apparent contradiction between theory and experiment is solved immediately if we treat the problems as many body problems.

We note, that an atom the electron of which is brought into a mixed state of the form (4) can be separated into components of the form (3) by a suitable magnetic deflection. The separation is of the type of the Stern—Gerlach effect — and the separation can be understood if we consider the system in terms of the two body wave function which contains coordinates of both electron and nucleus.

The production of $P,D, \ldots$ electron states can also be understood if we consider the collision of atoms. Consider for this purpose two electron packets which are represented by wave functions $\psi_1(\mathbf{r}_1)$ and $\psi_2(\mathbf{r}_2)$. (These functions may contain also the coordinates of the nuclei holding the packets together but this circumstance is not important for our analysis). If the atoms are

situated at a sufficient distance from each other, then the packets practically do not overlap; we can suppose that

$$\psi_1(\mathbf{r}) \neq 0 \text{ only if } \mathbf{r} \text{ inside } \mathfrak{R}_1,$$
$$\psi_2(\mathbf{r}) \neq 0 \text{ only if } \mathbf{r} \text{ inside } \mathfrak{R}_2,$$

where $\mathfrak{R}_1$ and $\mathfrak{R}_2$ are non overlapping regions. In this approximation ψ_1 and ψ_2 both obey one body wave equations of the type

$$H_1 \psi_1 = i\hbar\dot{\psi}_1, \qquad H_2 \psi_2 = i\hbar\dot{\psi}_2,$$

and therefore if we express these equations in terms of the hydrodynamical variables, we find

$$\oint \mathbf{v}_1 \, d\mathbf{s}_1 = 2\pi \frac{k_1 \hbar}{m}, \quad \oint \mathbf{v}_2 \, d\mathbf{s}_2 = 2\pi \frac{k_2 \hbar}{m}, \tag{5}$$

where

$$\left.\begin{aligned} \mathbf{v}_1 &= \frac{\hbar}{m} \operatorname{grad} S_1, & \mathbf{v}_2 &= \frac{\hbar}{m} \operatorname{grad} S_2, \\ \text{and} & & & \\ \psi_1 &= R_1 e^{iS_1}, & \psi_2 &= R_2 e^{iS_2}. \end{aligned}\right\} \tag{6}$$

In particular, if both atoms are in the ground state we have

$$k_1 = k_2 = 0.$$

The two electron wave function can be written

$$\psi(\mathbf{r}_1, \mathbf{r}_2, t) = \psi_1(\mathbf{r}_1, t)\, \psi_2(\mathbf{r}_2, t) \tag{7}$$

as long as the interaction between the atoms can be neglected. In place of (7) we should write

$$\psi(\mathbf{r}_1, \mathbf{r}_2, t) = \frac{1}{\sqrt{2}} \left(\psi_1(\mathbf{r}_1)\, \psi_2(\mathbf{r}_2) \pm \psi_2(\mathbf{r}_1)\, \psi_1(\mathbf{r}_2)\right) \tag{8}$$

because of the Pauli principle, however, our considerations are not affected if — for the sake of simplicity — we use the asymmetric wave function (7).

The initial conditions (5) are to be replaced [3] in the two body problem by a condition

$$\oint \mathfrak{v}(\mathbf{r}_1, \mathbf{r}_2)\, d\mathfrak{s} = 2\pi \frac{k\hbar}{m}, \tag{9}$$

where $\mathfrak{v}$ is a six component vector and $d\mathfrak{s}$ is the length of the six dimensional element of arc. Using the formalism given in [3] we find

$$\oint \operatorname{grad}_1 \mathrm{S}(\mathbf{r}_1, \mathbf{r}_2, t)\, d\mathbf{s}_1 + \oint \operatorname{grad}_2 \mathrm{S}(\mathbf{r}_1, \mathbf{r}_2, t)\, d\mathbf{s}_2 = 2\pi k. \tag{10}$$

If the wave function

$$\psi(\mathbf{r}_1, \mathbf{r}_2, t) = Re^{iS}$$

is of the form (7) then we have

$$S(\mathbf{r}_1, \mathbf{r}_2, t) = S_1(\mathbf{r}_1, t) + S_2(\mathbf{r}_2, t).$$

Thus

$$\left.\begin{aligned} \mathfrak{v}_1(\mathbf{r}_1, \mathbf{r}_2) &= \mathbf{v}_1(\mathbf{r}_1), \\ \mathfrak{v}_2(\mathbf{r}_1, \mathbf{r}_2) &= \mathbf{v}_2(\mathbf{r}_2), \end{aligned}\right\} \tag{11}$$

where $\mathfrak{v}_1$ and $\mathfrak{v}_2$ stand for the first three and the last three of the six components of $\mathfrak{v}$. In this way we find in place of (9)

$$\oint \mathbf{v}_1 \, d\mathbf{s}_1 + \oint \mathbf{v}_2 \, d\mathbf{s}_2 = 2\pi \frac{k\hbar}{m}. \tag{12}$$

Relation (12) is compatible with (5) if we put

$$k = k_1 + k_2.$$

We see therefore that as long as the two wave packets are separated the two body wave function can be taken as a product of two one body wave functions each obeying an initial condition of the form (5).

If the atoms collide an interaction between the two electrons sets in. For the period of the interaction the wave function has not any more the form of a product. During the period of the collision the (six dimensional) condition (9) remains correct but this condition cannot any more be separated into two conditions (5). Thus the condition (5) which can be regarded as three dimensional projections of (9) are not valid in the course of the collision.

If the atoms separate again after the collision, then a state establishes itself in which the wave function becomes again of the form (7) (or (8)). In the latter state the conditions (5) become valid again. Thus if before the collision we had a state such that

$$k_1 = k_2 = 0 \quad \text{and thus} \quad k = 0,$$

then during the collision we have a state where k_1 and k_2 are not defined (the three dimensional integrals $\oint v_l \, ds_l$, $l = 1,2,3$ can have arbitrary values during the period) but $k = 0$ remains satisfied. After the collision when the atoms have separated we obtain a state where

$$k = k_1 + k_2 = 0,$$

but

$$k_1 = -k_2 = 0 \pm 1, \pm 2$$

thus during the interaction of the two electrons, states with non vanishing orbital magnetic moments can be established. Thus the interactions of the two electrons can produce transitions which cannot be produced by the perturbation of outside fields on one electron alone.

§ 5. Another aspect of the same problem arises in connection with interference patterns shown by atomic beams falling on a crystal lattice. Taking the atomic beam to consist of single atoms these are often considered as electron shells surrounding the comparatively small nuclei. If an atom of such structure is taken to collide with the lattice, it is difficult to understand how it is possible, that the de Broglie wave length should play an important role in the collision — this wave length is mainly determined by the mass of the nucleus — and the collision takes place effectively between the electron shell and the lattice, the nucleus playing only a passive role in the collision.

The question becomes immediately clear — if we drop the inaccurate picture of atom consisting of a shell around a small nucleus. Indeed, in terms of the many body wave function the nucleus is spread over the whole of the region of the atom and a medium consisting of smeared out electrons and nuclear matter falls upon the lattice. The density of the latter medium is practically the density of the nucleus matter and therefore it is easy to understand that the characteristic wave length is also mainly determined by the mass of the nucleus.

A further aspect is how to imagine e.g. a gas closed into a container? As the quantum mechanical diffusion of the single gas atoms is limited only by the walls of the container it is reasonable to suppose that each of the gas atoms diffuses until it extends over the whole of the volume. Effects of density fluctuation and Brownian motion can be understood as interference effects.

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ГИДРОДИНАМИЧЕСКАЯ МОДЕЛЬ ВОЛНОВОЙ МЕХАНИКИ, VIII

Л. ЯНОШИ

Резюме

В нашей предыдущей статье было доказано, что квантово-механическое толкование эффекта Штерна—Герлаха приводит к неправильному результату, если применяется метод квантово-механической проблемы «одного тела». Приводятся другие примеры для доказательства того, что упрощенное толкование, соответствующее квантово-механической проблеме «одного тела» приводит к классическому результату, а результаты, характерные для квантовой механики, получаются только методом квантово-механической проблемы «многих тел».

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THEORY OF THE INFLUENCE OF CONCENTRATION ON THE LUMINESCENCE OF SOLID SOLUTIONS

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In the theory presented the following phenomena have been analysed from a uniform point of view: 1) concentration quenching 2) quenching by foreign absorbing substances 3) concentration depolarization of photoluminescence. The participation of primarily unexcited molecules of the donor in the process of energy transfer to the molecules of the acceptor as well as the remigration of excitation energy have been considered in the theory. It has been accepted that in case 1) the role of the molecules of the acceptor is carried out by dimers. Expressions for the quantum yield as well as emission anisotropy of photoluminescence have been obtained. It has been proved that the expression for yield, describing the process of quenching by foreign absorbing substances in the particular case when $\gamma_D \ll \gamma_A$ turns into the expression which was previously obtained by FÖRSTER. The expression for emission anisotropy which also takes into account the self-quenching of photoluminescence describes the effect of repolarization appearing in the range of large concentrations. A discussion of the results obtained is presented.

1. Introduction

An increase in the concentration of the luminescent substance in solutions leads to substantial changes in the properties of the emitted radiation. These changes appear in depolarization and in concentration quenching (self-quenching) of photoluminescence as well as in shortening the mean life-time of the excited state of the luminescent molecules. In some cases one can also notice considerable changes of absorption and sometimes even of luminescence spectra of the investigated solutions, particularly in a range of large concentrations [1, 2]. These concentration effects are mainly explained by resonance transfer of the electronic excitation energy from the excited molecule (the donor of energy —D) to the unexcited one (the acceptor of energy —A) as well as by molecules association of the solute [3, 4]. (We are dealing with non-radiative excitation energy transfer neglecting emission and reabsorption of photons [5]).

It is to be stressed that the non-radiative energy transfer is usually accompanied by radiative transfer. Under laboratory conditions the influence of reabsorption and secondary fluorescence can sometimes be eliminated, when investigating the substance in small concentrations and in sufficiently thin layers, or by making the appropriate corrections while elaborating the results [6—11].

In the case of solid or very viscous[1] solutions in which dimers appear it is assumed [4] that concentration quenching may take place by:

1 — direct inactive absorption of exciting light by dimers;

2 — energy transfer from excited monomers to dimers by quantum-mechanical resonance as a result of a single act of exchange (simple resonance quenching);

3 — energy transfer from excited monomers to dimers by means of primarily unexcited molecules of the monomer as a result of successive acts of energy exchange (migration — resonance quenching);

4 — quenching of the excitation energy, occurring during its transfer from the molecule of one monomer to another.

The influence of concentration upon the luminescence of solutions has been the object of numerous experimental works for nearly 50 years [1,12—20]. The theory of quenching by foreign absorbing substances [23—28] has been worked out comparatively well mainly owing to elaborating the idea of resonance transfer of energy by FÖRSTER [3], DEXTER [29], GALANIN [30] and KETSKEMÉTY [31]. These authors have proved that the rate constant for energy transfer (probability per time unit) may be associated with the absorption and luminescence spectra of the interacting D and A molecules. It is, however, to be stressed that the results obtained are based in most cases on the assumption that the excitation energy is transferred only to the nearest neighbours [24, 25].

In the case of concentration quenching the main results, as far as the explanation of this phenomenon on the basis of the above mentioned forms of quenching is concerned, have been achieved by LEVSHIN et al. [5, 32].

As for the existing theories of concentration depolarization [12, 3, 33, 14, 34, 21, 22] they are in agreement only for small ranges of concentration of the solute. For greater concentrations depolarization is less than one would expect from the theory. This fact may be explained by the influence of self-quenching on polarization of photoluminescence [14, 35]. In the theories quoted this effect is either entirely neglected, or self-quenching is considered in an appropriate way [18, 36].

In this work we present the theory of concentration influence upon photoluminescence of solid or very viscous solutions. We shall consider from a uniform point of view the problem of quenching by foreign absorbing substances and concentration quenching as well as concentration depolarization, taking into account the last three of the above mentioned forms of quenching.

[1] It is assumed that the viscosity of the solution is so large that

$$\sqrt{\langle r^2 \rangle} \ll R_0 \tag{1}$$

where $\sqrt{\langle r^2 \rangle}$ is the mean displacement of the luminescent molecule in Brownian diffusion movement during the mean life-time of the monomer molecule in the excited state, R_0 is the critical distance (cf. Section 2 for definition).

2. Assumptions and notations

A system is being considered which consist of two types of molecules: donor (D) and acceptor (A) of energy, distributed at random in an inactive medium (not participating in the process of energy transfer). It is assumed that the system is of finite volume V and possesses a number N_D of donor and N_A of acceptor molecules. Moreover, the luminescence spectrum of D molecules and absorption spectrum of A molecules partly overlap. This overlapping of spectra conditions the nonradiative energy transfer from the D^* molecule which is in the first excited singlet state to the A molecule which is in the ground state. According to FÖRSTER [3] the rate constant for the energy transfer from D^* to A (the probability per time unit) is:

$$k_{DA} = k_F(R_0/r)^6, \tag{2}$$

where $k_F = 1/\tau_0$ is the rate constant for the photoluminescence emission, τ_0 the mean life-time of the molecule of the donor in the excited state if $N_A = 0$, r the distance between D^* and A, R_0 the critical distance for energy transfer i. e. such that:

$$k_{DA}(R_0) = k_F = 1/\tau_0.$$

In elaborating the theory by considering the case of concentration quenching we restrict ourselves to that concentration range only at which the appearance of trimmers and higher associates may be neglected, whereas in the case of quenching by foreign absorbing substances to that range of concentration at which the associates do not appear at all.

The process of deactivation of the excited D^* molecule depends essentially on the distribution of D and A molecules in the neighbourhood of D^*. It is assumed that the configuration is invariant and the energy transfer from D^* to A, or D may occur by quantum-mechanical resonance. The configuration which is being discussed here is completely determined by giving $(N_D - 1) + N_A$ numbers r_j and $r_l, j = 1,2, \ldots, N_D - 1$; $l = 1,2, \ldots N_A$ denoting the distances of the j-th D molecule and the l-th A molecule from D^*, respectively.

In the theoretical considerations below we have assumed the possibility of the following elementary processes occurring:

Elementary process	Designation of process	Rate constant for the process
2a) Luminescence of D molecule	$D^* \rightarrow D + h\nu_D$	$k_{DF} \equiv k_F$
2b) Luminescence of A molecule	$A^* \rightarrow A + h\nu_A$	k_{AF}
2c) Inner quenching in D molecule	$D^* \rightarrow D$	$k_{Dq} \equiv kq$
2d) Inner quenching in A molecule	$A^* \rightarrow A$	k_{Aq}
2e) Nonradiative transfer of excitation energy from D^* to A	$D^* + A \rightarrow D + A^*$	$k_{DAEt} \equiv k_{DA}$
2f) Nonradiative transfer of excitation energy from D^* to D	$D^* + D \rightarrow D + D^*$	$k_{DDEt} \equiv k_{DD}$

We shall not, take into account the transfer of energy between A molecules:

$$A^* + A \rightarrow A + A^*$$

or that from A molecules to D molecules

$$A^* + D \rightarrow A + D^*.$$

The acceptance of the processes 2e) and 2f) is equivalent to acceptance of the process of energy transfer from D^* to A by means of primarily unexcited D molecules, i.e.

$$D^* + D + \ldots + D + A \rightarrow D + D^* + \ldots + D + A \rightarrow \ldots \rightarrow D + D + \ldots D + A^*. \quad (3)$$

In the case of concentration quenching and depolarization having only one type of dissolved molecules the dimers (D'') may be the molecules of the energy acceptor. Then, we assume that the above elementary processes 2a) — 2f) occur, but in the designation of the above processes D'' should be substituted for A. Moreover we introduce the following denotations:

2.1. Upper index (m) denotes order of molecules, namely: $D^{(m)}$ is D molecule of m-th order, i.e. that which has obtained excitation energy after its m nonradiative transfers: e.g. $D^{(0)}$ is a molecule of order zero, i.e. excited directly by absorption of exciting radiation.

2.2. Symbol $N^{(m)}_{(p)(s)}$ denotes number of $D^{(m)}$ molecules, i.e. of D^* molecules of order m, for which the j-th D molecule is situated at distance r_j, while the l-th A molecule is at distance r_l; at the same time r_j and r_l satisfy the inequalities:

$$x_j < r_j \leq x_j + dx_j \quad ; \quad y_l < r_l \leq y_l + dy_l.$$

Indices (p) and (s) denote appropriate systems of bi-indices (x_j,dx_j) and (y_l,dy_l), where $j = 1,2,3,\ldots, N_D - 1; l = 1,2,\ldots, N_A$. Moreover the following assumptions have been introduced:

2.3. The viscosity of the medium is large enough to fulfil conditions (1)(cf.[1]). This means that the process of energy transfer takes place at fixed distances between D^* and D and also A molecules.

2.4. Nonradiative transfer of excitation energy occurs as a result of dipole — dipole interaction. The rate constants for the process fulfil (2) for both 2e) and 2f) processes. The values R_0 for processes 2e) and 2f) are quite different. We shall designate them by R_{0D} and R_{0A}, respectively.

2.5. Constants k_{DA} and k_{DD} are independent from mutual orientation of the transition-moments of interacting molecules. This simplifying assumption is admissible only when condition (1) has been fulfilled and the viscosity of the medium is so small that the speed of Brownian molecular rotation may be considered as very large in comparison with the rate constant for energy transfer. If solid systems are considered the above assumption is not fulfilled because the spatial directions of all molecules remain unchanged during τ_0. In such a situation the dependence of the luminescence yield η on the concentration is somewhat different [37]. Recently, various cases of the influence of correlation between the directions of the transition-moment vectors of the interacting unmoveable molecules upon luminescence yield [27] have been analysed.

2.6. The rate constants for the elementary processes may have various values for molecules of different order. Thus, e.g. constant k_F for molecules of m-th order will be designated by $k_F^{(m)}$. We must explain that the above assumption is treated in our work purely formally and by no means affects the correctness of the theoretical considerations accomplished.[2] If we assume the dependence of rate constants on m then, according to 2.4., we shall obtain:

$$k_{DD}^{(m)}(x_j) = k_F^{(m)}(R_{OD}^{(m)})^6 x_j^{-6}, \tag{4'}$$

$$k_{DA}^{(m)}(y_l) = k_F^{(m)}(R_{OA}^{(m)})^6 y_i^{-6}, \tag{4''}$$

where $R_{OD}^{(m)}$ and $R_{OA}^{(m)}$ are "critical distances" for the energy transfer from $D^{(m)}$ molecule appropriately to molecules D and A. Magnitudes $k_{DD}^{(m)}(x_j)$ and $k_{DA}^{(m)}(y_l)$ mean the rate constants for the energy transfer from $D^{(m)}$ molecule to a D molecule which is at distance x_j and to an A molecule which is at distance y_l, respectively.

[2] Assumption of dependence of rate constants of order of molecules includes, of course, cases when they are molecular constants. Moreover, it appears that by assuming the independence of these constants of order of molecules in the final formulae containing $k^{(m)}$ one can obtain the same results as would be obtained assuming this right from the beginning. The accepted assumption 2.6 will allow us, however, to draw the conclusion concerning the "mechanism" of quenching which we shall present in Section 4, case (B. 2).

2.7. The final formule are obtained as limit values of appropriate magnitudes computed for a model of a finite number fo molecules placed in a finite volume (assumptions 2.3.—2.6. satisfied). This means that, finally, we pass with V, N_D and N_A to ∞, by fulfilling the following conditions:

$$\lim_{V\to\infty} \frac{N_A}{V} = n_A \; ; \; \lim_{V\to\infty} \frac{N_D}{V} = n_D . \tag{5}$$

3. Basic equations

We shall compute the photoluminescence yield of a two-component system containing D and A molecules (active ones) taking into account the elementary processes from 2a) to 2f). The excited molecule can emit its energy in the form of luminescence (process 2a) or lose it in some other way (processes 2c), 2e) and 2f)). The probability of any elementary process taking place depends essentially on the configuration of the unexcited D and A molecules in the neighbourhood of $D^{(m)}$. For this reason all the luminescent centres are divided into groups characterized by indices (p) and (s) (cf. 2.2).

The probability that a D molecule chosen at random belongs to the group of centres (p) (s) is:

$$P\left(D\varepsilon\{D_{(p)(s)}\}\right) \equiv P(D = D_{(p)(s)}) = \prod_{j=1}^{N_D-1} \frac{4\pi x_j^2\, dx_j}{V} \prod_{l=1}^{N_A} \frac{4\pi y_l^2\, dy_l}{V} . \tag{6}$$

It is to be noted that molecules $D^{(m)}_{(p)(s)}$ may transfer their excitation energy to $D^{(m+1)}$ only, or possibly lose it in one of the processes 2a), 2c) or 2e).

Consequently we obtain the following "final conditions":

$$N^{(m)}_{(s)(p)}(t) \to 0, \quad \text{when } t \to \infty \tag{7}$$

We assume that the changes of numbers $N^{(m)}_{(p)(s)}(t)$, after an impulsive excitation of the system in $t = 0$, are described by the following system of equations[3]:

$$\frac{dN^{(0)}_{(p)(s)}(t)}{dt} = -k^{(0)}_{(p)(s)} N^{(0)}_{(p)(s)}(t) , \tag{8'}$$

$$\frac{dN^{(m)}_{(p)(s)}(t)}{dt} = -k^{(m)}_{(p)(s)} \cdot N^{(m)}_{(p)(s)}(t) + \left(\sum_{(p')(s')} k^{(m-1)}_{(p')(s')} N^{(m-1)}_{(p')(s')}(t) \right) \cdot P(D = D_{(p)(s)}) , \tag{8''}$$

for $m = 1,2,3, \ldots ,$

[3] It is worthwhile to notice that the system of Eqs. (8) is a set of linear equations with three parameters — one discrete (m) and two continuous (p) and (s). For this reason expression $\sum_{(p)(s)}$, which appears in Eqs. (8) (10) and in the others, is to be understood as an abbreviated form of an appropriate integral (cf. (24)).

where

$$k^{(m)}_{(p)(s)} = k^{(m)}_{DD(p)(s)} + k^{(m)}_{DA(p)(s)} + k^{(m)}_F + k^{(m)}_q, \tag{9'}$$

$$k^{(m)}_{DD(p)(s)} = \sum_{j=1}^{N_D - 1} k^{(m)}_{DD}(x_j) \; ; \; k^{(m)}_{DA(p)(s)} = \sum_{l=1}^{N_A} k^{(m)}_{DA}(y_l) \, . \tag{9''}$$

Eq. (8′) describes the decrease in time of the number of $D^{(0)}_{(p)(s)}$ — molecules caused by emission of photoluminescence ($k^{(0)}_F$), nonradiative deactivation ($k^{(0)}_q$), transfer of excitation energy to D molecules ($k^{(0)}_{DD(p)(s)}$) or to A molecules ($k^{(0)}_{DA(p)(s)}$). Numbers $N^{(m)}_{(p)(s)}$ of $D^{(m)}_{(p)(s)}$ molecules for $m = 1,2,3, \ldots$ decrease for the same reasons (Eq. (8″), the first term on the left-hand side). The latter term of Eq. (8″) represents the increase of number of $D^{(m)}_{(p)(s)}$ per unit time, conditioned by nonradiative energy transfer from $D^{(m-1)}$ molecules to $D^{(m)}$, according to the definition of order of molecule (cf. 2.1). The sum from expression (8″) has been multiplied by $P(D = D_{(p)(s)})$ since only some of the nonradiative transfers from $D^{(m-1)}$ to $D^{(m)}$ will be conveyed to the molecules of donor with distribution of neighbours determined by parameters (p) (s). This means that $P(D = D_{(p)(s)})$ is treated here as a conditional probability that molecule $D^{(m)}_{(p)(s)}$ will be excited provided that molecule $D^{(m)}$ has been excited.

4. Quantum yield

In order to calculate the quantum yield of the solution photoluminescence the following additional magnitudes will be introduced:

4.1. Symbol $N^{(m)}_F$ denotes the number of photons emitted by $D^{(m)}$ over the time interval $(0, \infty)$, computed according to the formula

$$N^{(m)}_F = \sum_{(p)(s)} \int_0^\infty k^{(m)}_F \, N^{(m)}_{(p)(s)}(t) \, dt \, , \qquad m = 0,1,2, \ldots \tag{10}$$

4.2. The symbol $\eta^{(m)}$ denotes the photoluminescence yield of $D^{(m)}$ molecules, defined as follows:

$$\eta^{(m)} = N^{(m)}_F / N_0 \quad \text{for} \quad m = 0,1,2, \ldots, \tag{11}$$

where $N_0 = N^{(0)}(0)$ is the number of photons absorbed at the moment $t = 0$ (i.e. the moment of impulsive excitation of the system).

4.3. The photoluminescence yield η of the whole system is

$$\eta = \sum_{m=}^{\infty} \eta^{(m)} \, , \tag{12}$$

To calculate the efficiency of the quantum photoluminescence η of the whole system by means of expressions (10), (11) and (12) there is no need to solve the set of Eqs. (8), i.e. the determination of $N^{(m)}_{(p)(s)}(t)$ can be omitted, because it is possible to calculate the particular integrals (10) directly from (8). In order to compute them let us introduce some auxiliary denotations:

$$L^{(m)}_{(p)(s)} = \int_0^\infty N^{(m)}_{(p)(s)}(t)\, dt\,, \tag{13}$$

$$P^{(m)}_F = \sum_{(p)(s)} k^{(m)}_F [k^{(m)}_{(p)(s)}]^{-1} \cdot P(D = D_{(p)(s)})\,, \tag{14}$$

$$P^{(m)}_q = \sum_{(p)(s)} k^{(m)}_q [k^{(m)}_{(p)(s)}]^{-1} \cdot P(D = D_{(p)(s)})\,, \tag{15}$$

$$P^{(m)}_{DA} = \sum_{(p)(s)} k^{(m)}_{DA(p)(s)} [k^{(m)}_{(p)(s)}]^{-1} \cdot P(D = D_{(p)(s)})\,, \tag{16}$$

$$P^{(m)}_{DD} = \sum_{(p)(s)} k^{(m)}_{DD(p)(s)} [k^{(m)}_{(p)(s)}]^{-1} \cdot P(D = D_{(p)(s)})\,. \tag{17}$$

On account of (9′)

$$P^{(m)}_F + P^{(m)}_q + P^{(m)}_{DA} + P^{(m)}_{DD} = 1\,. \tag{18}$$

The above values are the probabilities of the appearance of the elementary processes denoted by 2a), 2c), 2e) and 2f) for molecules of m-th order.

In order to calculate $\eta^{(m)}$ we integrate both sides of Eq. (8) with respect to t in the interval $< 0, \infty)$: and then we obtain

$$N^{(0)}_{(p)(s)}(t)\Big|_{t=0}^{t=\infty} = -\, k^{(0)}_{(p)(s)} \cdot L^{(0)}_{(p)(s)}\,,$$

$$N^{(m)}_{(p)(s)}(t)\Big|_{t=0}^{t=\infty} = -\, k^{(m)}_{(p)(s)} \cdot L^{(m)}_{(p)(s)} + \left(\sum_{(p')(s')} k^{(m-1)}_{DD(p')(s')} \cdot L^{(m-1)}_{(p')(s')} \right) \cdot P(D = D_{(p)(s)})$$

$$\text{for} \qquad m = 1,2, \ldots .$$

Taking into account the initial conditions

$$N^{(m)}_{(p)(s)}(0) = \begin{cases} N_0 \cdot P(D = D_{(p)(s)}), & \text{for} \quad m = 0 \\ 0 \qquad\qquad\qquad\quad , & \text{for} \quad m = 1, 2, \ldots \end{cases}$$

as well as the final conditions (7) we obtain

$$N^{(0)}_{(p)(s)}(0) \equiv N_0 \cdot P(D = D_{(p)(s)}) = k^{(0)}_{(p)(s)} \cdot L^{(0)}_{(p)(s)}\,, \tag{19′}$$

$$\left[\sum_{(p')(s')} k^{(m-1)}_{DD(p')(s')} \cdot L^{(m-1)}_{(p')(s')} \right] P(D = D_{(p)(s)}) = k^{(m)}_{(p)(s)} \cdot L^{(m)}_{(p)(s)},\ m = 1,2,3,\ldots . \tag{19″}$$

After multiplying the above formulae by $k^{(0)}_{DD(p)(s)}/k^{(0)}_{(p)(s)}$ and $k^{(m)}_{DD(p)(s)}/k^{(m)}_{(p)(s)}$

respectively, summing up both sides of (19) with respect to $(p)(s)$ and considering (17) we can rewrite them in the form of

$$\sum_{(p)(s)} k^{(0)}_{DD(p)(s)} L^{(0)}_{(p)(s)} = N_0 \cdot P^{(0)}_{DD} ,$$

$$\sum_{(p)(s)} k^{(m)}_{DD(p)(s)} L^{(m)}_{(p)(s)} = \left(\sum_{(p')(s')} k^{(m-1)}_{DD(p')(s')} L^{(m-1)}_{(p')(s')} \right) P^{(m)}_{DD} .$$

Hence

$$\sum_{p\,)(s} k^{(m)}_{DD(p)(s)} L^{(m)}_{(p)(s)} = N_0 \prod_{j=0}^{m} P^{(j)}_{DD} . \tag{20}$$

If we multiply Eqs. (19′) and (19″) by $k^{(0)}_F / k^{(0)}_{(p)(s)}$ and $k^{(m)}_F / k^{(m)}_{(p)(s)}$, respectively, then, taking into account (20), we obtain

$$\frac{k^{(0)}_F L^{(m)}_{(p)(s)}}{N_0} = \frac{k^{(0)}_F}{k^{(0)}_{(p)(s)}} \cdot P(D = D_{(p)(s)}) \tag{21′}$$

$$\frac{k^{(0)}_F L^{(m)}_{(p)(s)}}{N_0} = \left(\prod_{j=0}^{m-1} P^{(j)}_{DD} \right) \frac{k^{(m)}_F \, P(D = D_{(p)(s)})}{k^{(0)}_{(p)(s)}} . \tag{21″}$$

Summing up both sides of (21) with respect to $(p)(s)$ and then applying Eqs. (11), (10), (13) and (14) we obtain

$$\eta^{(m)} = \begin{cases} P^{(0)}_F & , \text{ if } m = 0 \\ P^{(m)}_F \prod_{j=0}^{m-1} P^{(j)}_{DD} , & \text{if } m = 1,2,3, \ldots \end{cases} \tag{22}$$

Relations (22) are of a basic significance for describing the concentration dependence of photoluminescence quantum yield as well as the degree of polarization of the whole system. To make use of the above relations it is necessary to compute explicitly the magnitudes $P^{(m)}_F$ and $P^{(m)}_{DD}$ as solute concentration functions. It turns out that in the case of dipole-dipole interaction (assumption 2.4. and also 2.6.) such computations are possible.

Now, we shall compute the quantities $P^{(m)}_F$ and $P^{(m)}_{DD}$ as functions of donor and acceptor molecules concentrations, n_D and n_A, respectively.

5. Concentration dependence of $P^{(m)}_F$ and $P^{(m)}_{DD}$

According to note 2.7. we shall first compute $P^{(m)}_F(V)$ and $P^{(m)}_{DD}(V)$, where V is the volume of the sample, and then pass over with V and numbers N_D and N_A to infinity in an appropriate way (cf. (5)). The limit values of $P_F(V)$ and $P_{DD}(V)$ determined in this way will be denoted by

$$P_F = \lim_{V \to \infty} P_F(V) \quad ; \quad P_{DD} = \lim_{V \to \infty} P_{DD}(V) . \tag{23}$$

For the sake of simplicity, the upper index m will be neglected.

5.1. *The computation of* $P_F(V)$ and P_F

Taking into consideration Eqs. (14), (6) and (9) as well as the note[3] concerning the symbol $\sum_{(p)(s)}'$ we can write

$$P_F(V) \equiv \sum_{(p)(s)}' (k_F/k_{(p)(s)}) \cdot P(D = D_{(p)(s)}) =$$

$$= \underbrace{\int_0^R \cdots \int_0^R}_{N_D-1} \underbrace{\int_0^R \cdots \int_0^R}_{N_A} \frac{k_F \dfrac{4\pi x_1^2\, dx_1}{V} \cdots \dfrac{4\pi x_{N_D-1}^2\, dx_{N_D-1}}{V} \cdot \dfrac{4\pi y_1^2}{V} \cdots \dfrac{4\pi y_{N_A}^2}{V}}{k_F + k_q + k_{DD(p)(s)} + k_{DA(p)(s)}} \tag{24}$$

where $V = 4/3 \cdot \pi R^3$. The introduction of new variables

$$X_j = \frac{4}{3}\pi x_j^3 \quad \text{for} \quad j = 1,2, ..., N_D-1\,; \quad Y_l = \frac{4}{3}\pi y_l^3 \quad \text{for} \quad l = 1,2, ..., N_A \tag{25}$$

and also the denotations

$$v_{OD} = \frac{4}{3}\pi R_{OD}^3 \quad , \quad v_{OA} = \frac{4}{3}\pi R_{OA}^3 \tag{26}$$

as well as considering (9″) give us:

$$P_F(V) = \underbrace{\int_0^V \cdots \int_0^V}_{N_D-1+N_A} \frac{k_F \dfrac{dx_1}{V} \cdots \dfrac{dX_{N_D-1}}{V} \cdot \dfrac{dY_1}{V} \cdots \dfrac{dY_{N_A}}{V}}{k_F + k_q + k_F(v_{OD}^2 \sum_j' X^{-2} + v_{OA} \sum_l' Y_l^{-2}}\,.$$

Further on, we shall use the following identity

$$\frac{k_F}{k_F + k_q + k_F(a+b)} = k_F \int_0^\infty \exp\left\{-[k_F + k_q + k_F(a+b)]\, t\right\} dt\,, \tag{27'}$$

where

$$a = v_{OD}^2 \sum_{j=1}^{N_D-1} X_j^{-2} \quad ; \quad b = v_{OA}^2 \sum_{l=1}^{N_A} Y_l^{-2}. \tag{27''}$$

We shall then obtain:

$$P_F(V) = \int_0^\infty k_F \exp\left[-(k_F + k_q)\, t\right] \cdot \prod_j \left(\frac{\int_0^V \exp\left(-k_F\, v_{OD}^2\, X_j^{-2}\, t\right) dx_j}{V} \right) \cdot$$
$$\cdot \prod_l \left(\frac{\int_0^V \exp\left(-k_F\, v_{OA}^2\, Y_l^{-2}\, t\right) dY_l}{V} \right) dt \tag{28}$$

The above integrals over X_j are all identical as also are the integrals over Y_l. Substituting u for X_j and Y_l in Eq. (28) and denoting

$$\alpha_D = k_F\, v_{OD}^2\, t \quad , \quad \alpha_A = k_F\, v_{OA}^2\, t \tag{29}$$

we obtain

$$P_F = \int_0^\infty k_F \exp\left[-(k_F + k_q)\, t\right] \cdot \lim_{V\to\infty} \left(\frac{\int_0^V \exp\left(-\alpha_D\, u^2\right) du}{V} \right)^{N_D-1} \cdot$$
$$\cdot \lim_{V\to\infty} \left(\frac{\int_0^V \exp\left(-\alpha_A\, u^2\right) du}{V} \right)^{N_A} dt\,. \tag{30}$$

The limits appearing in (30) can be calculated in the following way

$$\frac{\int_0^V \exp(-\alpha u^2)\,du}{V} = 1 - \frac{\int_0^V [1-\exp(-\alpha u^2)]\,du}{V} = 1 - \frac{\sqrt{\alpha}\sqrt{\pi} + 0\left(\frac{1}{V}\right)}{V}.$$

Hence,

$$\lim_{V\to\infty}\left(\frac{\int_0^V \exp(-\alpha_D u^2)\,du}{V}\right)^{N_D-1} = \lim_{V\to\infty}\left[1 - \frac{\sqrt{\alpha_D}\cdot\sqrt{\pi}}{\quad}\right]^{N_D-1} = \tag{31}$$

$$= e^{-\sqrt{\pi\alpha_D}\cdot\lim\limits_{V\to\infty}(N_D-1/V)} = e^{-\sqrt{\pi\alpha_D}\cdot n_D}.$$

An analogous formula is true for the second limit

$$\lim_{V\to\infty}\left(\frac{\int_0^V \exp(-\alpha_A u^2)\,du}{V}\right)^{N_A} = e^{-\sqrt{\pi\alpha_A}\cdot n_A}. \tag{32}$$

The substitution of Eqs. (31) and (32) into (30) and taking into account denotation (29) yield

$$P_F = \int_0^\infty k_F \exp[-(k_F+k_q)\,t]\exp\left[-\sqrt{\pi k_F\,t}\,(v_{OD}\,n_D + v_{OA}\,n_A)\right]dt. \tag{33}$$

The computation of integral (33) leads to

$$P_F = \frac{k_F}{k_F+k_q}\,[1-f(\gamma)], \tag{34}$$

where

$$f(\gamma) = \sqrt{\pi}\,\gamma e^{\gamma^2}(1-erf\gamma), \tag{35}$$

$$erf\gamma = \frac{2}{\sqrt{\pi}}\int_0^\gamma \exp(-y^2)\,dy, \tag{36}$$

$$\gamma = \gamma_D+\gamma_A = \frac{\sqrt{\pi}}{2}\sqrt{\frac{k_F}{k_F+k_q}}\,(n_D\,v_{OD}+n_A\,v_{OA}). \tag{37}$$

Introducing a full set of indices the expressions (34) and (37) obtained for $P_F^{(m)}$ and $\gamma^{(m}$ respectively, may be written as follows

$$P_F(\gamma^{(m)}) = \frac{k_F^{(m)}}{k_F^{(m)}+k_q^{(m)}}\,[1-\sqrt{\pi}\,\gamma^{(m)}\exp(\gamma^{(m)})^2(1-erf\gamma^{(m)})] \tag{34'}$$

$$\gamma^{(m)} = \frac{\sqrt{\pi}}{2}\cdot\sqrt{\frac{k_F^{(m)}}{k_F^{(m)}+k_q^{(m)}}}\,(n_D\,v_{OD}^{(m)}+n_A\,v_{OA}^{(m)}). \tag{37'}$$

5.2. *Computation of $P_{DD}(V)$ and P_{DD}*

On account of (17), (6), (9), (25), (26) we have

$$P_{DD}^{(m)}(v) = \sum_{(p)(s)}\frac{k_{DD(p)(s)}\cdot P(D=D_{(p)(s)})}{k_F+k_q+k_{DD(p)(s)}+k_{DA(p)(s)}} =$$

$$= \underbrace{\int_0^V\cdots\int_0^V}_{N_D-1+N_A}\frac{k_F\,v_{OD}^2\left(\sum_j{}' X_j^{-2}\right)\frac{dX_1}{V}\cdots\frac{dX_{N_D-1}}{V}\cdot\frac{dY_1}{V}\cdots\frac{dY_{N_A}}{V}}{k_F+k_q+k_F\left(v_{OD}^2\sum_j{}' X_j^{-2}+v_{OA}^2\sum_l{}' Y_l^{-2}\right)}. \tag{38}$$

Making use of the relation

$$\frac{k_F \cdot a}{k_F+k_q+k_F(a+b)} = -\int_0^\infty \exp\left[-(k_F+k_q)\,t\right] \cdot \frac{d}{dt} \exp\left(-k_F\,at\right) \cdot \exp\left(-k_F\,bt\right) dt\,,$$

where a and b are determined in (27″) we obtain

$$P_{DD}(V) = -\int_0^\infty \exp\left[-(k_F+k_q)\,t\right] \cdot$$

$$\cdot \frac{d}{dt}\left[\underbrace{\int_0^V \cdots \int_0^V}_{N_D-1} \exp\left(-k_F+v_{OD}^2\,t \sum_j X_j^{-2}\right) \frac{dX_1}{V} \cdots \frac{dX_{N_D-1}}{V}\right] \cdot$$

$$\cdot \left[\underbrace{\int_0^V \cdots \int_0^V}_{N_A} \exp\left(-k_F\,v_{OA}^2\,t \sum Y^{-2}\right) \frac{dY_1}{V} \cdots \frac{dY_{N_A}}{V}\right] dt\,.$$

As in case 5.1.

$$P_{DD} = \lim_{V\to\infty} P_{DD}(V).$$

Putting the limit under the sign of the integral and making use of relations (31) and (32) we obtain

$$P_{DD} = -\int_0^\infty \exp\left[-(k_F+k_q)\,t\right] \cdot \frac{d}{dt} \exp\left(\sqrt{\pi k_F\,t}\,v_{OD}\,n_D\right) \cdot$$

$$\cdot \exp\left(-\sqrt{\pi k_F\,t}\,v_{OA} n_A\right) dt.$$

Calculating this integral gives

$$P_{DD} = \frac{\gamma_D}{\gamma_D+\gamma_A} \cdot f(\gamma)\,, \tag{39}$$

where $f(\gamma)$ is determined by (35), and γ, γ_D and γ_A by formula (37). Expression (39) written with all the indices takes the form of

$$P_{DD}^{(m)}(\gamma_D^{(m)}, \gamma^{(m)}) = \sqrt{\pi}\,\gamma_D^{(m)} \exp\left(\gamma^{(m)}\right) \cdot \left[1-erf(\gamma^{(m)})\right], \tag{39'}$$

where $\gamma^{(m)}$ is determined by (37′).

6. Examples of applying the results obtained

On the basis of the relations (12) and (22) as well as of the concentration dependences of P_F and P_{DD} we shall consider the following cases of photoluminescence quenching of solutions:

(A) Quenching by foreign absorbing substances

(B) Concentration quenching (self-quenching) conditioned exclusively by: (B.1) — dimers, (B.2) — the dependence of magnitudes $B^{(m)} = k_F^{(m)}/(k_F^{(m)} + k_q^{(m)})$ on the order of molecules, (B.3) — molecules of monomer which are "unable" for luminescence.

Cases (A), (B.1) and (B.2) will be considered with the assumption of independence of the appearance in the theory parameters of the order of molecules.

We shall also consider the concentration dependence of the degree of photoluminescence polarization when taking self-quenching into account as well as the general case of quenching and depolarization with a simultaneous occurrence of the last three forms of quenching (cf. Section 1).

(A) *Quenching by foreign absorbing substances*[4]

Let us assume that parameters $k_F^{(m)}$, $k_q^{(m)}$, $V_{OD}^{(m)}$, $V_{OA}^{(m)}$ and, hence, the magnitudes $P_F^{(m)}$, $P_{DD}^{(m)}$ and $\gamma^{(m)}$ do not depend on the order of the molecules, i.e.:

$$k_F^{(m)} = k_F^{(0)} = k_F\,;\; k_q^{(m)} = k_q^{(0)} = k_q\,;\; v_{OD}^{(m)} = v_{OD}^{(0)} = v_{OD}\,;\; v_{OA}^{(m)} = v_{OA}^{(0)} = v_{OA}$$

and

$$P_F^{(m)} = P_F^{(0)} = P_F\,;\; P_{DD}^{(m)} = P_{DD}^{(0)} = P_{DD}\,;\; \gamma^{(m)} = \gamma^{(0)} = \gamma,$$

where P_F and γ are determined by Eqs. (34) and (37) resp. while P_{DD}, on the basis of (39), may be presented as

$$P_{DD} = \frac{n_D v_{OD}}{n_D v_{OD} + n_A v_{OA}} \cdot f(\gamma). \tag{40}$$

Substituting the expressions (34), and (40) found for P_F and P_{DD} into formulae (12) and (22) we obtain

$$\eta = \sum_{m=1}^{\infty} P_F \prod_{j=1}^{m-1} P_{DD} + P_F = P_F \sum_{m=0}^{\infty} (P_{DD})^m.$$

Since $P_{DD} < 1$ (cf. (18)) then

$$\eta(\gamma) = \frac{P_F}{1-P_{DD}} = \frac{k_F}{k_F + k_q} \cdot \frac{1-f(\gamma)}{1 - \frac{\gamma_D}{\gamma_D+\gamma_A} \cdot f(\gamma)}.$$

Let us notice that $f(\gamma) \to 0$ if $\gamma \to 0$, hence:

$$\eta_0 \equiv \lim_{\gamma \to 0} \eta(\gamma) = \frac{k_F}{k_F + k_q} \equiv B^{(0)}.$$

[4] See also [38]

Ultimately we have

$$\frac{\eta}{\eta_0} = \frac{1-f(\gamma)}{1-\dfrac{\gamma_D}{\gamma_D+\gamma_A}\cdot f(\gamma)}, \tag{41}$$

where

$$f(\gamma) = \sqrt{\pi}\,\gamma e^{\gamma^2}\,[1-erf\,\gamma], \tag{35}$$

$$\gamma = \gamma_D+\gamma_A = \frac{\sqrt{\pi\eta_0}}{2}\,(n_D\,v_{OD}+n_A\,v_{OA}). \tag{37'}$$

If $\gamma_D \ll \gamma_A$ expression (41) becomes

$$\frac{\eta}{\eta_0} = 1-f(\gamma_A) = 1-\sqrt{\pi}\,\gamma_A\,e^{\gamma}\;[1-erf\,\gamma_A]. \tag{42}$$

An expression for quantum yield of photoluminescence of the donor in the form of (42) has been derived by FÖRSTER (24) and later on in another way also by other authors [30, 26, 27].

Expression (41) contrary to expression (42) takes into account the participation of D molecules in the process of energy transfer from D^* to A (cf. case 3 in Section 1, and also (3)). The effectiveness of this participation depends on the ratio

$$\frac{\gamma_D}{\gamma_A} \equiv \frac{n_D}{n_A}\cdot\frac{v_{OD}}{v_{OA}} = \frac{n_D}{n_A}\left(\frac{I_{\tilde{\nu}D}}{I_{\tilde{\nu}A}}\right)^{1/2}$$

i.e. on the ratio of concentrations as well as of overlapping integrals $I_{\tilde{\nu}}$[1].

For quenching by foreign absorbing substances this kind of energy transfer has been proved experimentally [30, 40] recently. The natural conditions for multistage excitation transfer occur in photosynthetic systems, as well as in chromoproteins [37, 41].

(B.1.) *Concentration quenching conditioned exclusively by dimers*

As in (A) it is assumed that parameters and magnitudes appearing in the theory do not depend on the order of molecules, and quenching is conditioned exclusively by the presence of dimers, which are considered as acceptor molecules. In this situation quenching by dimers is simply the case of quenching by foreign absorbing substances considered above.

Consequently, we obtain for relative yield of photoluminescence of the solution

$$\frac{\eta}{\eta_0} = \frac{1-f(\gamma)}{1-\dfrac{\gamma_{D'}}{\gamma_{D'}+\gamma_{D''}}\cdot f(\gamma)}, \tag{41'}$$

where

$$\gamma = \gamma_{D'}+\gamma_{D''} = \frac{\sqrt{\pi\eta_0}}{2}\,(n_{D'}\,v_{OD'}+n_{D''}\,v_{OD''}), \tag{37''}$$

at the same time molecules of monomers and dimers have been denoted by D' and D'', respectively. Note that $\gamma_{D'}/(\gamma_{D'}+\gamma_{D''})$ is now a function of the solution concentration (because of the relation (44) between the concentrations). On the contrary the ratio $\gamma_D/(\gamma_D+_A)$ for a two-component solution may be constant if one considers solutions of a fixed donor and acceptor concentration ratio n_D/n_A.

The consideration of the participation of primarily unexcited D' molecules in the process of energy transfer from D'^* to D'' is necessary in the case (B.1), because $n_{D''} < n_{D'}$ generally, at least over a very large range of concentrations.

Let us denote the concentration of the solution by n, calculated with the assumption that all the D molecules are monomers. Then

$$n = n_{D'} + 2\, n_{D''}, \tag{43}$$

where $n_{D'}$ and $n_{D''}$ denote the concentrations of monomers and dimers, respectively. Moreover,

$$n_{D''} = K n_{D'}^2, \tag{44}$$

where K is the equilibrium constant in the process of dimer formation. From formulae (43) and (44) it is possible to compute $n_{D'}$, as well as $n_{D''}$ if K and n are known, or, knowing K to express $n_{D'}$ and $n_{D''}$ as functions of n. Moreover, knowing $v_{0D'}$ and $v_{0D''}$ we can express (cf. (37″)) γ, $\gamma_{D'}$, $\gamma_{D''}$ as functions of n and, in this way, by means of (41′) determine the concentration dependence of the relative quantum yield of photoluminescence η.

(B.2) *Concentration quenching conditioned by dependence $B^{(m)}$ on order of molecules*

If dimers do not appear in the solution ($n_{D''} = 0$) then one may attempt to explain the concentration quenching assuming that $k_F^{(m)}/k_q^{(m)}$ depends on m.

We assume that

$$\begin{aligned} k_F^{(m)} &= k_F^{(0)} \qquad \text{for} \quad m = 0, 1, 2, \ldots, \\ k_q^{(m)} &= k_q^{(1)} > k_q^{(0)} \quad \text{for} \quad m = 1, 2, 3, \ldots . \end{aligned} \tag{45}$$

We shall prove that assumption (45) also leads to an expression which will describe the yield's drop with the increase of the solution concentration.

If we substitute the assumption (45) into (34′), (39′) and (37′), then we obtain

$$P_F^{(0)} = B^{(0)}[1 - f((\gamma)^{(0)})]\,; \; P_{DD}^{(0)} = f(\gamma^{(0)}) \tag{46}$$

and

$$P_F^{(m)} = P_F^{(1)} = B^{(1)}[-f(\gamma^{(1)})]\,; \; P_{DD}^{(m)} = P_{DD}^{(1)} = f(\gamma^{(1)}) \tag{47}$$

for $m = 1,2,3, \ldots$, where

$$B^{(0)} = \frac{k_F^{(0)}}{k_F^{(0)} + k_p^{(0)}}; \quad B^{(1)} = \frac{k_F^{(0)}}{k_F^{(0)} + k_q^{(1)}};$$

$$\gamma^{(0)} = \gamma = \frac{\sqrt{\pi}}{2} n_D v_{OD} \sqrt{B^{(0)}}; \quad \gamma^{(1)} = \frac{\sqrt{\pi}}{2} n_0 v_{OD}^{(1)} \sqrt{B^{(1)}}.$$

On the basis of (12) and (22) as well as (46) and (47) we have

$$\eta = \eta^{(0)} + \sum_{m=1}^{\infty} \eta^{(m)} = P_F^{(0)} + \sum_{m=1}^{\infty} P_F^{(m)} \prod_{j=0}^{m-1} P_{DD}^{(j)} =$$

$$= B^{(0)}[1 - f(\gamma)] + f(\gamma) B^{(1)}[1 - f(\gamma^{(1)})] \cdot \sum_{m=1}^{\infty} [f(\gamma^{(1)}]^{m-1}.$$

Ultimately,

$$\eta(\gamma) = B^{(0)} - [B^{(0)} - B^{(1)}] f(\gamma). \tag{48}$$

It appears that

$$\eta_0 \equiv \lim_{\gamma \to 0} \eta(\gamma) = B^{(0)}; \quad \lim_{\gamma \to \infty} \eta(\gamma) = B^{(1)}. \tag{49}$$

Since $f(\gamma)$ is a monotonically increasing function ($0 < f(\gamma) < 1$, cf. (35)) and because of our assumption (45) $B^{(1)} < B^{(0)}$, $\eta(\gamma)$ is a decreasing function of concentration. If we assume $B^{(0)} = B^{(1)}$, then $\eta(\gamma) = B^{(0)}$, i. e. if the ratio $k_F^{(m)}/k_q^{(m)}$ is constant for molecules of arbitrary order then the yield is a constant magnitude independent of concentration, although k_{DD} and P_{DD} depend on the concentration. However, the yield decrease with the concentration increase requires the following inequality to be satisfied:

$$k_F^{(m)}/k_q^{(m)} < k_F^{(0)}/k_q^{(0)}$$

at least for one $m \geq 1$. Assumption (45) is one of many other possible assumptions concerning $k_F^{(m)}$ and $k_q^{(m)}$ fulfilling this condition.

Cases of other assumptions about $k_F^{(m)}$ and $k_q^{(m)}$ have been discussed in [42].

(B.3) *The quenching by monomer molecules "unable" of luminescence*

We shall present here another attempt to explain the concentration quenching when dimers do not appear in the solution ($n_{D''} = 0$). The present case as well as case (B.2) concerns the situation when quenching of photoluminescence takes place during the transfer of excitation energy between monomers (cf. case 4 of Section 1). This form of quenching has been accepted[5]

[5] Some less importance has lately been annotated to this form of quenching [5, 45], or it has been entirely neglected [50]. Since we share the opinion that so far sufficient proofs of a quantitative character have not yet been found which would determine whether energy quenching during its transfer between monomer molecules may be rejected, therefore we admit in our consideration a possibility of such a form of quenching occurring.

in many papers [4, 12, 23, 42—44]. According to the above remark the molecules of monomer have formally been classified into "able" and "unable" for luminescence [12, 20]. "Able" molecules will be treated as molecules of a donor, and "unable" ones as molecules of acceptor. Consequently, let $\gamma_D = \gamma'_D + \gamma''_D$ where γ'_D and γ''_D concern molecules "able" and "unable" for luminescence, respectively.

If we assume that

$$\gamma'_D/\gamma_D = \alpha_0 = \text{const.} \tag{50}$$

then for relative yield we shall obtain an expression formally identical to expression (41), namely

$$\frac{\eta}{\eta_0} = \frac{1-f(\gamma)}{1-\alpha_0 f(\gamma)} \,. \tag{41''}$$

At the same time the following meaning can be given to α_0: α_0 equals the probability that as a result of the energy transfer, an excitation of such a state will not occur which leads with probability 1 to the energy quenching.

(C) *Generalization of cases (A) and (B)*

From the cases considered concerning concentration quenching only case (B.1) has a clearly determined physical sense. Cases (B.2) and (B.3) offer some attempts for a formal explanation of concentration quenching of photoluminescence provided that dimers do not appear. Analysis of these cases seems us to be useful because it may appear that it will be impossible to explain the observed yield drop exclusively by dimers. Energy quenching during its transfer between monomers would then be the sole possibility of explaining the phenomenon. We hope that the yield drop is, on the whole, conditioned by all four types of quenching mentioned in Section 1 participating in the process to a various degree depending partly on the properties of the interacting molecules of donor and acceptor, their concentration as well as the properties of the medium itself. We present below a method of generalizing expressions (41), (41′) and (41″) for η/η_0 in such a way as to take into consideration the last three types of quenching[6] (cf. Section 1), i.e. to involve simultaneously cases (A) and (B.3) or (B.1) and (B.3). (As is shown below for these cases, cases (A), (B.1) and (B.3) may be combined).

In order to do this it is necessary to substitute factors

$$\frac{\gamma_D}{\gamma'_D + \gamma''_D + \gamma_A} = \alpha_0 \frac{\gamma_D}{\gamma_D + \gamma_A} \quad \text{or} \quad \frac{\gamma'_D}{\gamma'_D + \gamma''_D + \gamma_{D''}} = \alpha_0 \frac{\gamma'_D}{\gamma_{D'} + \gamma_{D''}}$$

[6] The first type of quenching may be taken into account experimentally according to method presented in [5, 20].

for factors

$$\frac{\gamma_D}{\gamma_D+\gamma_A} \quad \text{or} \quad \frac{\gamma_D}{\gamma_{D'}+\gamma_{D''}}$$

appearing in (41) and (41′), respectively, where α_0 is determined by (50).

In the case of concentration quenching for quantum yield of photoluminescence one obtains

$$\frac{\eta}{\eta_0} = \frac{1-f(\gamma)}{1-\alpha_0 \dfrac{\gamma_{D'}}{\gamma_{D'}+\gamma_{D''}} \cdot f(\gamma)} . \tag{41‴}$$

The above expression involves items (B.1) and (B.3) and differs from (41′) only by a constant factor α_0 in the denominator. If we substitute γ_A instead of $\gamma_{D''}$ and γ_D instead of $\gamma_{D'}$ in (41‴) we obtain a generalized expression for η/η_0 which involves items (A) and (B.3). When the energy quenching during its transfer between the molecules of donor does not take place, then $\alpha_0 = 1$, because $\gamma''_D = 0$, i.e. then the obtained expressions turn into (41) or (41′), respectively.

The analysis of case (B.2) leads to the following conclusion: If there are neither associates, nor molecules of a donor, which are "unable" for luminescence in the solution, then the relative yield of photoluminescence does not depend on concentration (in all the range of its changes) unless k_F/k_q depends on the order of the excited D molecules (provided that the appropriate corrections for the first type of quenching have been made). This conclusion is regarded as the main result of the analysis of item (B.2.).

(D) *Concentrational depolarization of photoluminescence*

The theory presented above also enables us to obtain an expression describing the concentrational dependence of polarization of photoluminescence of the solution. It is known that the degree of polarization P, with the assumption that only molecules originally excited by light absorption are responsible for the polarized luminescence emission, can be computed from the relation [21]

$$\frac{P}{P_0} = \frac{3\,\eta^{(0)}/\eta}{3-[1-\eta^{(0)}/\eta]\,P_0} , \tag{51}$$

where $\eta^{(0)}$ is the yield of photoluminescence of molecules of order zero (cf. 2.1), η is the overall quantum yield, P_0 is the fundamental degree of polarization.

Dependence (51) will be considerably simplified if we introduce emission anisotropy r which is connected with degree of polarization P as follows [46]:

$$r = \frac{2P}{3-P} . \tag{52}$$

From expressions (51) and (52) we have

$$r/r_0 = \eta^{(0)}/\eta ,$$

where r_0 is emission anisotropy corresponding to P_0.

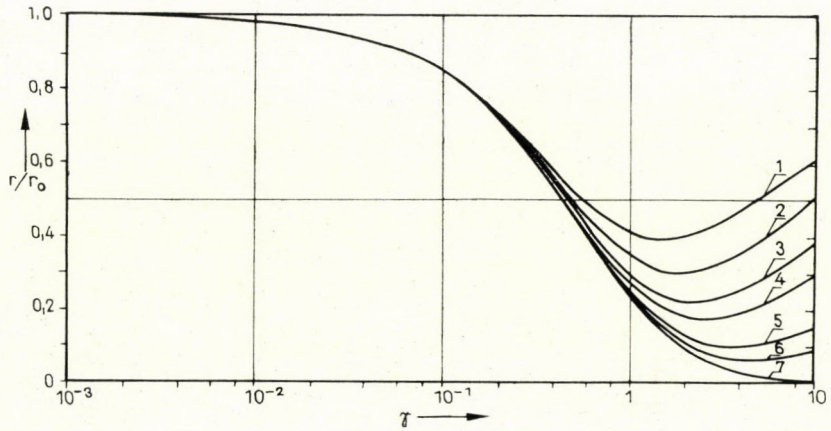

Fig. 1. Concentration dependence of the emission anisotropy of photoluminescence computed according to (53) for various values of equilibrium constants K_γ. 1—0.4; 2—0.2; 3—0.1; 4—0.06; 5—0.02; 6—0.01; 7—0.00

Let us assume that the last three types of quenching[7] (cf. Section 1) participate in the concentration quenching (case (B.2) excluded). Since, on the basis of (22), (46) and (49)

$$\eta^{(0)} = P_F^{(0)} = \eta_0[1 - f(\gamma)]$$

then, taking into account (41‴) we obtain

$$\frac{r}{r_0} = \frac{\eta^{(0)}}{\eta} = \frac{\eta^{(0)}/\eta_0}{\eta/\eta_0} = 1 - \alpha_0 \frac{\gamma_{D'}}{\gamma_{D'} + \gamma_{D''}} \cdot f(\gamma), \tag{53}$$

where $f(\gamma)$, γ, $\gamma_{D'}$, $\gamma_{D''}$ and α_0 are determined by (35), (37″) and (50), respectively.

Fig. 1 shows emission anisotropy of photoluminescence as a function of γ determined by (53) for $\alpha_0 = 1$, for various equilibrium constants K_γ in the process of dimer formation.[8] The given curves show minima depending on K_γ

[7] The nonactive absorption of exciting light by dimers does not influence the observed polarization.

[8] The constant K_γ is determined by dependence $\gamma_{D''} = K_\gamma \cdot \gamma_{D'}^2$; K_γ and K are related to each other by means of the dependence

$$K = K_\gamma \cdot v_{OD'}^2 (\pi\eta_0)^{1/2}/v_{OD''} .$$

only. It is worthwhile to notice that similar experimental curves have been obtained by SZALAY et al. [18] in the case of concentrational depolarization of photoluminescence of Na fluorescein in glycerine solutions of different viscosities. Similar results have also been obtained for glycerine solutions of tripaflavin [47, 17].

7. Final remarks

In the theory presented above the following phenomena have been described from a uniform aspect: quenching by foreign absorbing substances, concentrational quenching and also concentrational depolarization of photoluminescence of solutions with sufficiently large viscosity. The participation of unexcited donor molecules in the process of energy transfer from D^* to A or D'' has been taken into consideration in the theory. We hope that this fact will permit the theory to describe correctly the process of concentrationa l quenching of photoluminescent solutions in which dimers appear, as well as to describe the nonradiative energy transfer in some biological systems. The theory may be applied for describing the phenomenon of concentrational depolarization in a broad range of concentrations and at the same time takes into account the influence of concentrational quenching on this phenomenon.

There is a possibility for a further generalization of Eq. (53) for emission anisotropy for the case when molecules of order higher than zero are also contributing to the observed polarization.

The theory presented operates by means of microscopic constants.

The constants v_{OD}, v_{OA}, η_0, K appearing in the final formulas have a clearly determined physical meaning and may be determined from independent measurements. The theory is adequate to the generally accepted types of quenching with particular importance being paid to the role of dimers in the process of quenching. The possibility of excitation energy quenching during its transfer between the molecules of donor has also been considered; the process being treated purely formally. It seems that any attempt to describe the concentrational effects in luminescent solutions will fail without taking into account this type of quenching [42]. We think that concentrational quenching similar to the drop of yield in the anti-Stokes region [48] cannot be explained exclusively by means of quenching by dimers.

We also hope that the theory presented will help in making quantitative estimates of the share of particular types of quenching in the observed total quenching. The experimental verification of the theory requires an appropriate set of experimental data which is hard to find in the literature. Special experimental work is in progress.

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ТЕОРИЯ ВЛИЯНИЯ КОНЦЕНТРАЦИИ НА ЛЮМИНЕСЦЕНЦИЮ ТВЕРДЫХ РАСТВОРОВ

Ц. БОЯРСКИ и Й. ДОМСТА

Резюме

Представлена теория, в которой проанализированы с общей точки зрения следующие явления: 1) концентрационное тушение, 2) тушение посторонними веществами, 3) концентрационная деполяризация фотолюминисценции.

В теории учтено посредничество первоначально невозбужденных молекул донора в процессе переноса энергии на молекулы акцептора, а также реэмиграция энергии возбуждения. Считается, что в первом случае акцептором являются димеры. Получены выражения для квантового выхода и анизотропии эмиссии фотолюминесценции. Доказано, что полученное выражение для квантового выхода, описывающее тушение посторонними веществами в частном случае, когда $\gamma_D \ll \gamma_A$, переходит в выражение, ранее полученное Ферстером. Выражение анизотропии эмиссии, которое учитывает также самотушение фотолюминесценции, описывает эффект реполяризации, появляющийся в области больших концентраций. Представлена дискуссия полученных результатов.

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A STUDY OF INTERNAL CONVERSION AT TRANSITIONS OF HIGHER ENERGY IN THE DECAY ^{131}I

By

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The higher energy region of gamma-rays (from 480 to 810 keV) and conversion electrons (from 570 to 760 keV) was studied with a 20 cm^3 Ge(Li) and a 3 mm deep Si(Li) semiconductor spectrometer, respectively. For the conversion coefficients and for their ratio, $\alpha_K = (3{,}6 \pm \pm 0.5) \cdot 10^{-3}$ and $K/L = 5.3 \pm 1.6$ were obtained at the 636.3 keV transition as well as $\alpha_K = = (3.9 \pm 0.6) \cdot 10^{-3}$ and $K/L = 4.7 \pm 1{,}4$ at the 722.9 keV transition. On the basis of these and some other published data, the $5/2^+$ assignment for the 722.9 keV level and the $7/2^+$ one for the 636.3 keV level seem to be the most probable.

1. Introduction

^{131}I is one of the best known radioactive isotopes and its decay has been studied many times and by various methods (see e.g. in [1]—[5]). Several measurements have been carried out on the spectrum of the conversion electrons in this decay of which the latest are [6]—[9].

In spite of the considerable effort several problems still remain in connection with the parameters of the internal conversion especially at the transitions of higher energy (see the Tables). The measured values generally have large errors here and some of them are contradictory beyond the limits of the error (see e.g. the α_K for the 636 keV transition, Table III), but the data are very scanty for the K/LM ratio, (cf. Table V). Partly as a consequence of this situation, the spin and parity assignment at the higher energy levels of ^{131}Xe, populated in the decay of ^{131}I, are incomplete and problematic (see e.g. [3]). At the same time recent techniques of semiconductor beta-ray spectrometry have not yet been used for the study of the conversion electron spectrum in the decay of ^{131}I.

In the present study the highest energy transitions (636,3 and 722,9 keV) in the decay under consideration have been investigated with Ge(Li) and Si(Li) semiconductor gamma- and beta-ray spectrometers, respectively, to determine the a/K and K/LM values for the above two transitions.

2. Experimental details

The gamma-ray spectrum was studied with a coaxial type 20 cm³ Ge(Li) detector (EFKI, Budapest) having a resolution (FWHM) 4,7 keV at 661,6 keV (^{137}Cs). The spectrum in the region from 460 to 810 keV was recorded in a 512-channel pulse-height using a window-amplifier.

The energy and efficiency calibration of the Ge(Li) spectrometer were carried out using absolutely calibrated sources of ^{22}Na, ^{137}Cs and ^{54}Mn from the IAEA, Vienna.

In the semiconductor beta ray spectrometer the detector was Si(Li) type (Simtec LC 200—300—120) whose area was 2 cm² and sensitive thickness 3 mm. The details of the Si(Li) semiconductor will be published elsewhere [10]. The resolution (FWHM) was 5,6 keV for 624,2 keV (^{137}Cs) conversion electrons.

The carrier-free radioactive preparation of ^{131}I was supplied by the Isotope Institute, Budapest and the source for the measurement was made by evaporation of a droplet on a cellux tape ($\sim$ 6 mg/cm²).

The determination of α_K for the two studied transitions was performed by means of the so-called NPG method. Here the gamma- and beta-ray spectra of ^{137}Cs were measured under the same conditions as those of ^{131}I. Using the measured value of α_K for the 661.6 keV transition in the decay of ^{137}Cs taken from [11] (using the weighted average of the last four values in the Table) the gamma-, and beta-ray intensity values for ^{131}I can be normalized to each

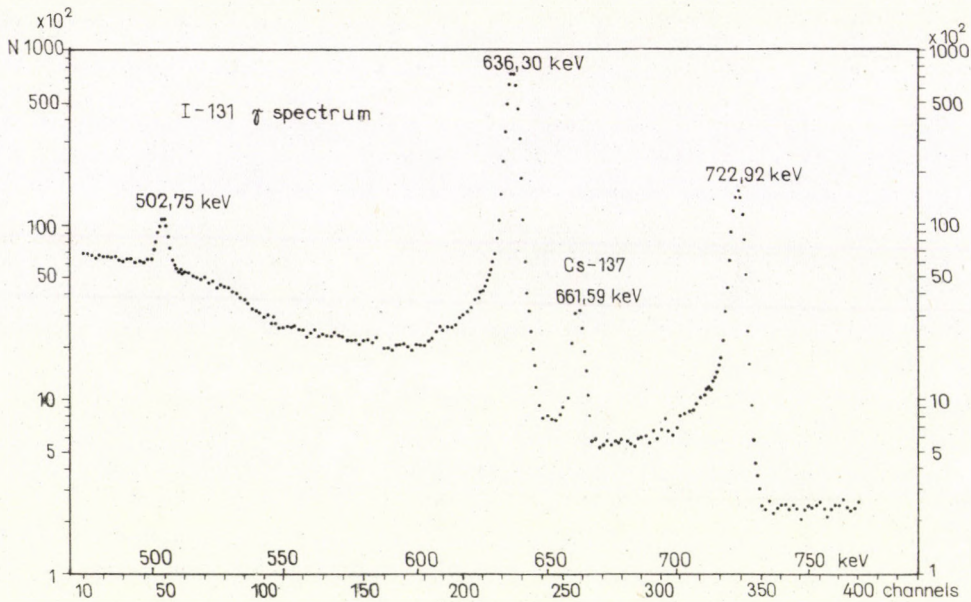

Fig. 1. The spectrum of gamma rays from ^{131}I in the region from 480 to 810 keV taken with a 20 cm³ Ge(Li) detector

Table I

The relative intensity* of 636.3 and 722.9 keV gamma-rays from the decay of ^{131}I

636.3 keV**	722.9 keV**	$\frac{I_\gamma(722.9}{I_\gamma(636.3)}$	Method***	Reference
20			sl pe	METZGER and DEUTSCH, 1948 [15]
17			sl pe	KERN et al., 1949 [16]
11.6±1.7	3.5±0.8	0.30	sl pe	BELL et al., 1953 [17]
10	3	0.30	sl pe	HASKINS and KURBATOV, 1952 [18]
13	1,7	0.31	sd	ROSE et al., 1952 [19]
10.2±1.2	2.8±0.4	0.27	s pe	WOLFSON, 1952 [20]
11.6±2.3	2.4±0.5	0.21	scin	MIJATOVIC and WINTERSTEIGER 1953 [21]
8.9±0.9	1.9±0.2	0.21	s Cp	DZHELEPOV et al., 1959 [22]
8.8±0.5	2.1±0.1	0.24	scin	HAGROVE et al., 1963 [23]
8.3±0.3	1.9±0.1	0.23	scin	DANIEL et al. 1964 [7]
9.1±0.9	2.1±0.2	0.23	semi	MOSS et al., 1966 [14]
8.2±0.8	1.8±0.2	0.22	semi	YTHIER et al., 1967 [29]
8.0±0.4	2.1±0.15	0.26	semi	GRAEFFE and WALTERS, 1967 [24]
9.1±0.9****	1.9±0.2	0.24	semi	Present work

* Intensities relative to 364.5 keV gamma ray
** The energy value taken from the work of Moss et al. [14]
*** The signs are the same as used in Nuclear Data Sheets
**** This value taken equal to the corresponding one in the work of Moss et al. [14]

other. In this way, the absolute intensity values for the conversion lines of ^{131}I under study are not needed, only the constancy of the conversion peak efficiency, i.e. absolute efficiency (peak + tail) of the beta-ray spectrometer and that of the peak-to-tail ratio have to be valid in the relevant energy region. These assumptions are true in a good approximation as is shown by experimental studies (e.g. [12], [13] and [28]).

3. Results and discussion

The gamma-ray spectrum of ^{131}I in the region from 480 to 810 keV is shown in Fig. 1. In Table I the present and the published experimental data for the relative intensity of the 636.3 and 722.9 keV gamma-rays are given. The agreement of our data with recent measurements of other authors on the intensity ratio of the two studied gamma rays is excellent (cf. Table I).

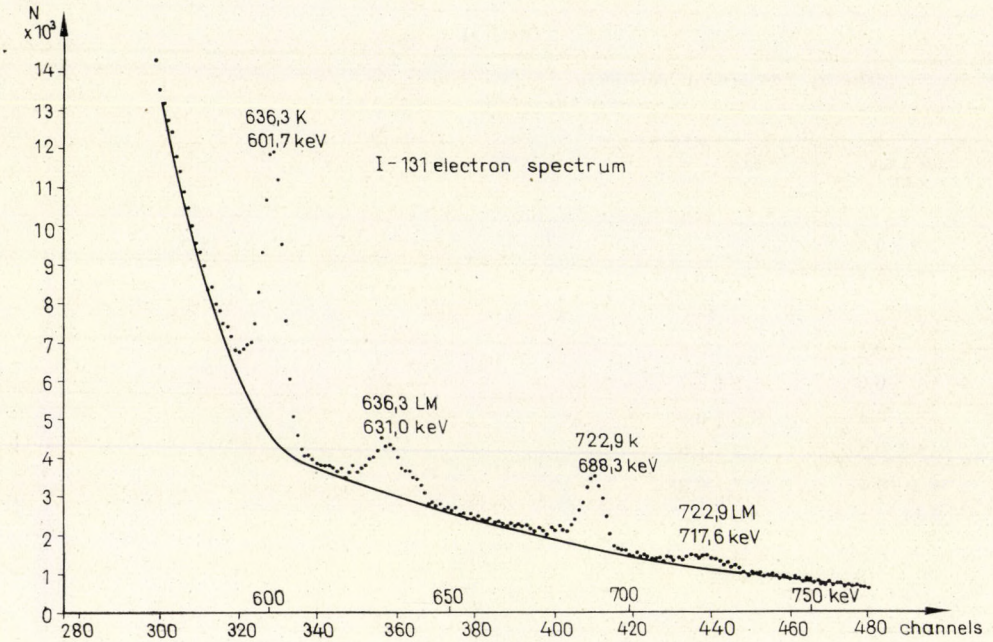

Fig. 2. The conversion electron spectrum from ^{131}I in the region from 570 to 760 keV taken with a 2 cm² area, 3 mm thick Si(Li) detector

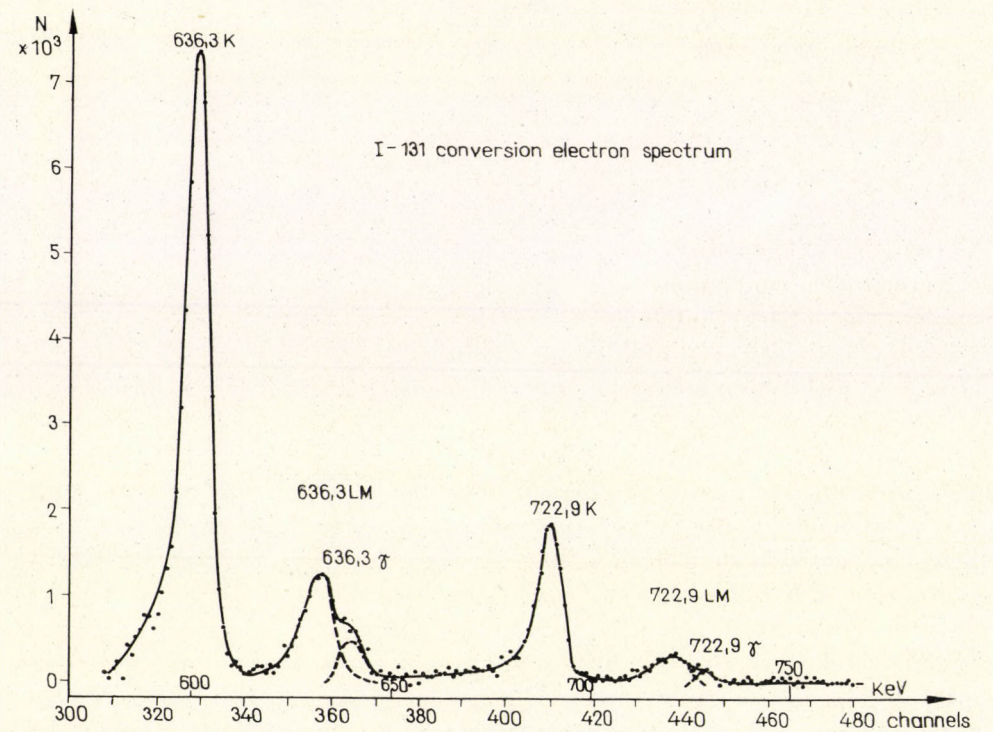

Fig. 3. The same spectrum as can be seen in Fig. 2 but after subtraction of the continuous beta-background

Table II

The α_K conversion coefficient for the 636.3 and 722.9 keV transitions in the decay of ^{131}I

636.3 keV $\times 10^{-3}$	722.9 $\times 1$	Method*	Reference
1.9 ± 0.2		sl pe ce	VERSTER et al., 1951 [25]
3.7 ± 0.9	2.8 ± 0.8	sl pe ce	BELL et al., 1952 [17]
4.0	3.4	sl pe ce	HASKINS and KURBATOV, 1952 [18]
2.1 ± 0.1	3.7 ± 0.5	sd ce	ROSE et al., 1952 [19]
4.0 ± 0.6	3.1 ± 0.7	s pe ce	WOLFSON, 1952 [20]
3.9 ± 0.4	3.8 ± 0.7	scin	HAGROVE et al., 1963 [23]
3.9 ± 0.3	3.7 ± 1.0	sd ce	DANIEL et al., 1964 [7]
4.3 ± 0.4	3.7 ± 0.35	semi***	GRAEFFE and WALTERS, 1967 [24]
3.6 ± 0.5	3.9 ± 0.6	semi	Present work
4.0 ± 0.2**	3.6 ± 0.2		Weighted average
5.40	3.97	M1	
15.3	10.8	M2	Theoretical values HAGER and SELTZER,
38.2	25.1	M3	1967 [26]
1.46	1.11	E1	
4.06	2.96	E2	

* The signs are the same as used in Nuclear Data Sheets
** Here the 1.9 and 2.1 values were not taken into consideration
*** The conversion electron intensities here were taken from WOLFSON et al. [30]

In Figs. 2 and 3 the conversion electron spectrum and the same spectrum corrected for the continuous beta background can be seen in the energy region studied. The intensity of the 636,3 K line is to that of the 722.9 K line as 1.9 ± 0.57 is to 0.49 ± 0.15. The same figures of WOLFSON et al. [6] are 1.9 ± 0.13 and 0.43 ± 0.5, respectively. In Table II the α_K value obtained for the 636.3 keV and the 722.9 keV gamma rays are given in comparison with similar data published in literature. The data on the K/LM ratio obtained in this study and those published by other authors are tabulated in Table II.

It should be noted here that there was a correction made for the decay of the ^{131}I source in the calculation of the α_K values. Furthermore, for the determination of K/LM ratios, the gamma-ray sensitivity of the Si(Li) detector was also corrected.

As can be seen from the Tables the present value for α_K well agrees with recent data in the case of both transitions and the agreement is also good with the other figures for the K/LM ratios within the limit of errors. From compari-

Table III

The *KL/M* intensity ratios for the 636.3 and 722.9 keV transitions in the decay of ^{131}I

636.3 keV		722.9 keV	Reference
9.0±1.8		8.0±2.4	BELL et al., 1952 [17]
5.2±0.9			ROSE et al., 1952 [19]
9±5			DANIEL et al., 1964 [7]
5.3±0.7		4.7±1.4	Present work
5.9±0.7		5.5±1.2	Weighted average
5.93	M1	7.18	
5.22	M2	6.75	
4.73	M3	6.31	Theoretical values*
6.19	E1	7.30	
5.50	E2	7.03	

* The α_K and α_L values were taken from HAGER and SELTZER [26], the α_M value was taken from ROSE [31]. (We took half of ROSE's value)

son with the theoretical values it can be stated that the 363.3 keV transition is mostly E2 and the 722.9 keV transition is mostly M1.

All the authors agree that the 636.3 and 722.9 keV transitions start from the 636.3 and 722.9 keV level of ^{131}Xe, respectively, and both end on its ground level. As to the spin and parity assignments to the 636.3 and 722.9 keV levels, even recent works are rather uncertain and contradictory (see Fig. 4). At the same time the theory cannot say discouragingly anything (see KISSLINGER and SORENSEN's results on the levels of ^{131}Xe in [24]).

Using the data for the log ft value on beta decays populating the levels under consideration (7,1 [7], 7.1 [14], 7.0 [24] and 6.9 [7], 6.8 [14], 6.9 [24]), which are in an excellent agreement with each other, and using the propositions for spin and parity assignments of Nuclear Data Sheets (see e.g. in [27]), $7/2^+$, $5/2^+$, $9/2^+$, $3/2^-$ and $11/2^-$ are the possible values for both levels considering

$5/2^+$	$(5/2^+)$ $(7/2^+)$	$5/2^+$	$5/2^+$
$5/2^+$ $(7/2^+)$	$(5/2^+)$	$7/2^+$	$7/2^+$
DANIEL et al. [7]	MOSS et al. [14]	GRAEFFE and WALTERS [24]	present work

Fig. 4. Spin and parity assignment to the 636,3 and 722.9 keV levels of ^{131}Xe in recent works on the decay scheme of ^{131}I

the $7/2^+$ assignment to the ground state of ^{131}I. On the other hand, the M1 multipolarity of 722.9 keV gamma rays and the E2 one of 636.3 keV gamma rays suggest $1/2^+$ or $5/2^+$ for the 722.9 keV and $7/2^+$ for the 636.3 keV level, respectively. In this way, the most probable assignment for their higher level is $5/2^+$ and for the lower one $7/2^+$. These assignments agree with those of GRAEFFE and WALTERS [24].

Finally, it should be noted here that the experimental data on the parameters of the level seem to be particularly important in that region of the nuclei where the theoretical prediction and interpretation is so hopeless for the moment.

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ИЗУЧЕНИЕ ВНУТРЕННЕЙ КОНВЕРСИИ ПРИ ПЕРЕХОДАХ ВЫСОКОЙ ЭНЕРГИИ В РАСПАДЕ ^{131}I

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Резюме

Изучалась область высоких энергий гамма лучей (от 480 до 810 кэв) и конверсионных электронов (от 570 до 760 кэв) полупроводниковым детектором 20 см^3 Ge(Li) и Si(Li) с толщиной 3 мм. Для коэффициентов конверсий и для их отношения получены следующие значения: в случае перехода 636,3 кэв $\alpha_K = (3{,}6 \pm 0{,}5) \cdot 10^{-3}$ и $K/L = 5{,}3 \pm 1{,}6$, а в случае перехода 722,9 кэв $\alpha_K = (3{,}9 \pm 0{,}6) \cdot 10^{-3}$ и $K/L = 4{,}7 \pm 1{,}4$. На основе наших и некоторых опубликованных результатов можно заключить, что величины $5/2^*$ для уровня 722,9 кэв и $7/2^+$ для уровня 636, 3 кэв оказываются наиболее вероятными.

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SIMPLE AB-INITIO METHOD OF CALCULATING THE COHESIVE PROPERTIES OF ALKALI METALS

By

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The quantum-statistical model of a free atom in which electrons are grouped in shells according to the principal quantum number has been applied to the calculations of the cohesive properties of alkali metals. The cohesive energies and radii of metal cells obtained for Li, Na, and K differ from the experimental values by less than 30%.

Introduction

In parallel with those methods whose aim is to reproduce cohesive energies and other properties of solids as exactly as possible, simple methods of an ab-initio type have been developed based on the quantum-statistical model of the atom [1—3]. The purpose of these methods is to exclude the use of empirical parameters and to obtain the simple treatment of solids even at the expense of the exactitude of the results. The statistical model of the free atom in which electrons are grouped in shells according to the principal quantum number, developed by GOMBÁS [4, 5] makes it possible to refine the quantum-statistical model of solids. In the present work, we have taken advantage of GOMBÁS's model in calculations of the cohesive properties of alkali metals.

Description of the method

An atom in a solid is considered here as in the cellular method. Thus, the energy of an atom in a solid is defined by the energy functional and the boundary condition which must be obeyed by the wave function or by the electronic density distribution. In the case of the alkali metals we can assume that only the valence electron density ϱ_v is affected by the boundary conditions in the solid and replace the atomic polyhedron by the sphere of equal volume. With these assumptions, the boundary correction

$$E_b = E(r_0) - E(r_\infty) \tag{1}$$

(e.g. the difference between the energy of the atom in a metal cell with the valence electron in the lowest electron state, and the energy of the free atom $E(r_\infty)$) is determined by the energy functional and the boundary condition

$$\frac{\partial \varrho_v}{\partial r}\Big|_{r=r_0} = 0\,,$$

$$\varrho_v(r_0) \neq 0, \tag{2}$$

which is fulfilled by ϱ_v on the surface of the sphere.

The energy functional suggested by GOMBÁS [4, 5] for free atoms is assumed to be valid also for atoms of finite radii in solids. Only the form of the valence electron radial density is changed to obey the boundary condition (2) and the form of the inner-shell electron radial densities is left the same as in the case of free atoms. This is:

$$\varrho_n(r) = \frac{1}{4\pi} N_n A_n^2 r^{2\varkappa_n - 2} e^{-2\lambda_n r}\,, \tag{3}$$

where N_n is the number of electrons in the n-shell, $\varkappa_n$ and λ_n are the variational parameters, A_n is the normalization constant

$$A_n = \left[\int_0^{r_0} r^{2\varkappa_n} e^{-2\lambda_n r}\, dr\right]^{-1/2}. \tag{4}$$

In (3) only the normalization constant A_n is influenced by the boundary conditions for a solid because in this case the normalization integral is extended over the sphere of finite radius r_0. The valence electron density ϱ_v has been assumed to be of the form

$$\varrho_v(r) = \frac{1}{4\pi} N_v r^{2\varkappa_v - 2} (A_v e^{-2\lambda_v r} - B_v e^{\lambda_v r})^2\,. \tag{5}$$

The boundary conditions (2) give the requirement:

$$B_v = A_v e^{-2\lambda_v r_0} \frac{\varkappa_v - 1 - r_0 \lambda_v}{\varkappa_v - 1 + r_0 \lambda_v}\,, \tag{6}$$

where r_0 is the radius of the sphere and the constant A_v is determined by the normalization condition

$$A_v = \left[\int_0^{r_0} r^{2\varkappa_v} \left(e^{-\lambda_v r} - \frac{\varkappa_v - 1 - r_0 \lambda_v}{\varkappa_v - 1 + r_0 \lambda_v} e^{-2\lambda_v r_0} e^{\lambda_v r}\right)^2 dr\right]^{-1/2}. \tag{7}$$

The energy functional can be expressed in terms of ϱ_n as follows

$$E = \sum_{n=1}^{v} E^{(n)}, \tag{8}$$

where

$$E^{(n)} = E_i^{(n)} + E_k^{(n)} + E_\varphi^{(n)} + E_g^{(n)} + E_{ce}^{(n)} + E_e^{(n)}, \tag{9}$$

$$E_{ce}^{(n)} = e^2 \sum_{n'=1}^{n-1} \int \frac{\varrho_{n'}(r')\,\varrho_n(r)}{|\vec{r}' - \vec{r}|}\, dv'\, dv, \tag{10}$$

$$E_e^{(n)} = \frac{1}{2}\,\frac{N_n - 1}{N_n}\, e^2 \int \frac{\varrho_n(r)\,\varrho_n(r')}{|\vec{r}' - \vec{r}|}\, dv\, dv' \tag{11}$$

and the other symbols have the same meaning as in [5].

Now we seek to establish the parameters $\varkappa_n$ and λ_n from the condition of the minimum of the energy. However, the minimalization procedure for solids is much more complicated than for free atoms. To avoid too many difficulties we have fixed the values of $\varkappa_n$ in (3) and (5) which are put as equal to their values for free atoms [6]. Then, the $E^{(n)}$ have been minimalized with respect to λ_n successively for $n = 1,2, \ldots v$, in the same way as in [7]. One can expect for two reasons that the simplification of the minimalization procedure will not influence the boundary corrections considerably. First, it was checked that the $E(r_\infty)$ values obtained in this manner are close to the atomic energies given in [6]. Second, this procedure was used for obtaining $E(r_\infty)$ and $E(r_0)$ in Eq. (1), and neither value reached the complete minimum.

In the cellular method the cohesive energy is usually assumed to be equal to the sum

$$E_{\mathrm{coh}} = E_b + E_{el} + E_F + E_c, \tag{12}$$

where E_{el} is the interaction energy of the electron distribution in the valence band (electrostatic self-energy and exchange energy), E_F is the Fermi energy and E_c is the correlation energy per electron in the band.

We take E_{el} in the free-electron approximation

$$E_{el} = \frac{1.05}{r_0^2} \quad \text{a. u.} \tag{13}$$

The Fermi energy has been calculated from the expression

$$E_F = \frac{1}{m^*}\,\frac{1.105}{r_0^2} \quad \text{a. u,} \tag{14}$$

where m^* is the effective mass of an electron.

A simple formula given in [8] has been used for calculations of the effective mass. In terms of the valence electron density ϱ_v it may be expressed as

$$m^* = \left[\frac{4\pi}{3} r_0^3 \varrho_v(r_0)\right]^{-1}. \tag{15}$$

Both GOMBÁS's [9]

$$E_c = -\frac{\alpha_1}{\alpha_2 + n^{1/3}} n^{1/3} - \beta_1 \ln(1+\beta_2 n^{1/3}) \text{ a. u.} \tag{16}$$

$$n^{1/3} = \left(\frac{3}{4\pi}\right)^{1/3} r_0^{-1} \text{ and } \alpha_1 = 0.0357;\ \alpha_2 = 0.05625;\ \beta_1 = 0.0311;\ \beta_2 = 2.39,$$

and PINES's [10]

$$E_c = -0.0575 + 0.0155 \ln r_0 \text{ a. u.} \tag{17}$$

formulae have been used for the calculations of the correlation energy.

Results and discussion

Calculations were performed for lithium, sodium, and potassium. By means of the method described the cohesive energy has been found for each metal as a function of r_0. The values corresponding to minima of the curves or $E_{\text{coh}}(r_0)$ are shown in Table I. For comparative purposes the Table also

Table I

Quantum-statistical cohesive energies and cellular radii of alkali metals

	E_{coh}(in Kcal/mole)			r_0 (in a_0)		
	Theory	Experiment [11]	Difference experiment-theory %	Theory	Experiment [12]	Difference experiment-theory %
Li	29.1	36.5	20.3	4.13	3.18	29.9
Na	27.0	26.1	3.3	4.60	3.92	17.3
K	20.9	21.7	3.8	6.13	4.84	26.7

contains the experimental values for E_{coh} and r_0. The cohesive energies given in the Table were obtained with the PINES formula for the correlation energy (Eq. (17)). These energies calculated with Eq. (16) and the corresponding radii from the minima of $E_{\text{coh}}(r_0)$, are only slightly different from those given in the Table. With an accuracy to the first decimal place the values of E_{coh} are equal except for K; in this case Eq. (16) gives $E_{\text{coh}} = 21.0$ kcal/mole. The values of

r_0 (with an accuracy to the second decimal place) are equal for Na, whereas for Li, Eq. (16) gives $r_0 = 4.14\ a_0$ and $r_0 = 6.14\ a_0$ for K.

The cohesive energies obtained by the present method are generally quite close to the experimental values. The values of r_0 are too large but the

Table II

The results of the present theory as compared with those of more exact methods

	r_0 (in a_0)	E_b (in Ry)		m^* (in a. u.)		Source of more exact values for E_b and m^*
		Present method	More exact value	Present method	More exact value	
Li	3.21	—0.2850	—0.2869	0.902	1.376	[13]
Na	3.94	—0.2336	—0.2168	0.991	0.938	[14]
K	4.84	—0.1413	—0.1605	0.840	0.862	[15]

differences are not significant if the approximate character of the method is taken into account.

In order to estimate the inaccuracy involved in different components of E_{coh}, the calculations for the values of r_0 for which the comparison with a more exact method is possible have been performed. The results are given in Table II. The comparison shows the method to be very useful for the calculations of the boundary correction. The calculations of the effective mass seem to be the main source of the inaccuracy of the present method.

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ПРОСТОЙ МЕТОД ОПРЕДЕЛЕНИЯ ИЗ ПЕРВЫХ НАЧАЛ СВОЙСТВ СЦЕПЛЕНИЯ ЩЕЛОЧНЫХ МЕТАЛЛОВ

П. МОДРАК

Резюме

При вычислении свойств сцепления щелочных металлов применяется квантово-статистическая модель свободного атома, в которой электроны сгруппированы по главным квантовым числам. Энергии сцепления и радиусы металлических ячеек, определенные для Li, Na и K, отличаются от экспериментальных данных менее чем на 30 процентов.

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THEORY OF ANHARMONIC CRYSTALS IN PSEUDOHARMONIC APPROXIMATION

I. LINEAR CHAIN

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The properties of an anharmonic chain are considered in the pseudoharmonic approximation. The dependence of the instability temperature on the arbitrary external tension is investigated. It is shown that the instability region of the linear chain is limited by the critical temperature and the critical tension.

1. Introduction

Recently a theory of anharmonic crystals was developed which allows to take into account all the higher order anharmonic terms in a self-consistent manner (see [1—3] and the references cited in [3]) in the lower order perturbation theory. In [4]—[6] a simple model of the crystals, the linear chain with nearest neighbour interaction was investigated. Although this model is very far from real three-dimensional crystals, its investigation permits us to discuss qualitatively some properties of three-dimensional crystals. Also, in this case we can obtain a simple solution which helps to clarify some aspects of the theory.

It was shown in [4]—[6] that the chain under small external tension becomes unstable at sufficiently high zero-point energy or at a sufficiently high temperature. It was also shown in [4] that the damping of the self-consistent phonons is sufficiently small even near the instability temperature and, consequently, the most simple pseudoharmonic approximation [2] can be used. This allows the calculations to be simplified essentially and the properties of the anharmonic linear chain over a wide range of temperatures and coupling constant to be investigated. This investigation was made in [6] for small external tensions.

In the present paper we consider the properties of an anharmonic linear chain in pseudoharmonic approximation in the case of an arbitrary external tension. Some preliminary results were reported earlier in [7]. In Section 2 we obtain a self-consistent system of equations for the determination of the properties of the anharmonic chain. In Section 3 we investigate the behaviour of the self-consistent equation at the high temperature limit and we introduce the concept of the instability temperature and the critical temperature. These quantities are calculated in Section 4. In Section 5 we discuss the results.

2. Self-consistent system of equations in pseudoharmonic approximation

Let us consider a linear chain of length L which consists of $N+1$ identical atoms with mass M. We take into account only the nearest neighbour interaction which is described by the interaction potential denoted by $\varphi(R_n - R_{n-1})$. It is convenient to introduce the equilibrium separation between the neighbouring atoms and the relative displacement operators by the following definition:

$$R_n - R_{n-1} = <R_n - R_{n-1}> + u_n - u_{n-1} \equiv l + u_n - u_{n-1}. \tag{1}$$

The equilibrium separation l in the one-dimensional case can be obtained from the equation [3]:

$$P = -\frac{1}{2} < \frac{\partial}{\partial R_n} \varphi(R_n - R_{n-1}) > \tag{2}$$

which shows that the average force acting on the arbitrary atom in the equilibrium position is equal to zero.

Applying the method which was formulated in [2] a self-consistent system of equations for the investigation of a linear chain was obtained in [6]. It was shown that the renormalized frequency of vibrations takes the form:

$$\omega_k^2 = \frac{4f(\Theta, l)}{M} \sin^2 \frac{kl}{2} = \frac{f(\Theta, l)}{f} \omega_{0k}^2 \equiv \alpha^2 \omega_{0k}^2, \tag{3}$$

where ω_{0k} is the harmonic frequency of the vibrations and f stands for the harmonic strength constant. The pseudoharmonic strength constant $f(\Theta,l)$ can be written as:

$$f(\Theta, l) = \frac{1}{2} \tilde{\varphi}''(l), \tag{4}$$

where we introduce the self-consistent potential:

$$\tilde{\varphi}(l) = < \varphi(R_n - R_{n-1}) > = \sum_{s=0}^{\infty} \frac{1}{s!} \left(\frac{\bar{u}^2}{2} \right)^s \varphi^{(2s)}(l). \tag{5}$$

The mean square relative displacement of the neighbouring atoms can be written as:

$$\bar{u}^2 = <(u_n - u_{n-1})^2> = \frac{1}{Nf} \sum_k \frac{\omega_{0k}^2}{2\omega_k} \coth \frac{\omega_k}{2\Theta}. \tag{6}$$

In addition to the temperature $\Theta = kT$ the properties of the linear chain are also determined by the length of the chain $L = Nl$ or by the external tension P. According to (2), (5) these parameters satisfy the following equation:

$$P = -\frac{1}{2}\,\tilde{\varphi}'(l) \tag{7}$$

which is the thermal equation of state for the linear chain.

The caloric equation of state is obtained from the internal energy which is given in our approximation by the equation [6]:

$$\frac{1}{N}E = \frac{1}{2}\{\tilde{\varphi}(l) + f(\Theta, l)\,\bar{u}^2\}. \tag{8}$$

In this way we have a closed system of equations (3)—(8) which determine the properties of the anharmonic linear chain in the pseudoharmonic approximation. This self-consistent system of equations is determined by the self-consistent potential (5) which can be obtained if the potential $\varphi(R)$ is known. Let us take the Morse potential as a model:

$$\varphi(R) = D\{[e^{-a(R+r_0)} - 1]^2 - 1\}. \tag{9}$$

We note here after [1], that the deviation of a Lennard—Jones (12—6) interatomic potential from the Morse potential with $ar_0 = 6$ in the domain of the thermal expansion of the lattice is rather small. Therefore, we shall take further $ar_0 = 6$. Applying (5), (9) we get the following expression for the self-consistent potential:

$$\tilde{\varphi}(l, y) = D\left\{e^{-12\left(\frac{l}{r_0}-1\right)} e^{2y} - 2\,e^{-6\left(\frac{l}{r_0}-1\right)} e^{y/2}\right\} \tag{10}$$

where $y = a^2\bar{u}^2 = 36(\bar{u}^2/r_0^2)$.

Let us consider the case in which the external tension is fixed: $P = $ = const. but contrary to [5],[6] we do not assume that P is small. The length of the chain depends on the temperature of the system if we keep the external tension fixed. The equilibrium separation of neighbouring atoms l can be written as follows:

$$l(\Theta) = l_0 + \delta l = r_0\left\{1 + \frac{1}{4}\,y + \frac{\delta l}{r_0}\right\}, \tag{11}$$

where l_0 is the equilibrium separation at $P = 0$ which can be determined using Eq. (7) (10). It is convenient to introduce the reduced tension $P^* = P(r_0/D)$.

(We note here, that in [4]—[6] the dimensionless tension $p = P^*/2$ was used) Then Eq. (7) taking into account (10) (11) reads:

$$P^* = 6\, e^{-6\frac{\delta l}{r_0}} e^{y} \left(e^{-6\frac{\delta l}{r_0}} - 1 \right). \tag{12}$$

Using Eqs. (10), (11), (12) the pseudoharmonic strength constant α according to (3), (4) can be written as follows:

$$\alpha^2 = \frac{f(\Theta, l)}{f} = e^{-y} e^{-6\frac{\delta l}{r_0}} \left\{ 2\, e^{-6\frac{\delta l}{r_0}} - 1 \right\} = \\ = \frac{P^*}{3} + \frac{1}{2} \left\{ e^{-y} + \sqrt{e^{-2y} + \frac{2P^*}{3}\, e^{-y}} \right\}. \tag{13}$$

Solving the last equation for y we get:

$$y = \ln \frac{\alpha^2 - \dfrac{P^*}{6}}{\left(\alpha^2 - \dfrac{P^*}{3} \right)^2}. \tag{14}$$

Consequently the expressions for the self-consistent potential (10), the equilibrium separation of neighbouring atoms (11) and the internal energy (8) can be written as follows:

$$\tilde{\varphi}(l) = -D \left\{ \alpha^2 - \frac{P^*}{2} \right\}, \tag{15}$$

$$l = r_0 \left\{ 1 + \frac{1}{12} \ln \frac{\alpha^2 - \dfrac{P^*}{6}}{\left(\alpha^2 - \dfrac{P^*}{3} \right)^4} \right\}, \tag{16}$$

$$\frac{1}{N} E = \frac{D}{2} \left\{ \alpha^2 \ln \frac{\alpha^2 - \dfrac{P^*}{6}}{e \left(\alpha^2 - \dfrac{P^*}{3} \right)^2} + \frac{P^*}{2} \right\}. \tag{17}$$

Let us replace the sum over k by the integral over $\varphi = kl/2$ in Eq. (6). Taking into account (15) we can rewrite (6) as an equation for α:

$$\lambda \alpha\, y(\alpha) = \int_0^{\pi/2} d\varphi \sin \varphi \coth \frac{\alpha \sin \varphi}{2\tau}, \tag{18}$$

where $\omega_{0L} = (4f/M)^{1/2}$ is the maximum value for the vibrational frequency of the chain in harmonic approximation, $\lambda = (\pi D/\omega_{0L})$ is the dimensionless coupling constant and $\tau = (\Theta/\omega_{0L})$ is the dimensionless temperature.

It is worth while to note that the self-consistent equation (18) determines the properties of the anharmonic linear chain: when λ, τ and P^* are given, we can obtain the renormalization of the frequency α from Eq. (18) which according to (16), (17) determines the length of the chain and its internal energy. It is easy to see that all the equations obtained here for $P^* \ll 1$ coincide with those of paper [6].

3. Self-consistent equation in the high temperature limit

Let us now consider the self-consistent equation (18) in the high temperature limit ($\tau \gg 1$). In this case (18) can be rewritten in the following form:

$$\alpha^2 y(\alpha) = T^* \left\{1 + \frac{1}{24}\left(\frac{\pi\alpha}{\lambda T^*}\right)^2 + \ldots\right\}, \tag{19}$$

where we introduce the reduced temperature $T^* = (\Theta / D) = \tau\pi/\lambda$. Taking into account only the first term in the r.h.s. of (19) and using (12), (13), (14) the self-consistent equation can be written as follows:

$$F(y) = \left(1 - \frac{P^*}{3T^*} y\right)^2 e^y - \frac{y}{T^*}\left(1 - \frac{P^*}{6T^*} y\right) = 0 . \tag{20}$$

We point out here that (20) has different numbers of real solutions depending on the P^*, T^* values. The physical solution is that which coincides with the harmonic solution if the anharmonic terms tend to zero. The harmonic solution is given by

$$y_{\text{harm}} = \frac{T^*}{\alpha^2_{\text{harm}}} = \frac{2T^*}{1 + \frac{2}{3}P^* + \sqrt{1 + \frac{2}{3}P^*}} . \tag{21}$$

The dependence of the physical solution of Eq. (20) on the reduced temperature T^* and reduced tension P^* is given in Fig. 1. If the tension ($P^* < P_c^*$) and temperature [$T^* \leq T_s^*(P^*)$] are sufficiently low Eq. (20) has real solutions, and the smallest is the physical one. The temperature $T_s^*(P^*)$ is determined by the coincidence of two real solutions: $y_1(T_s^*) = y_2(T_s^*)$. Consequently the instability temperature $T_s^*(P^*)$ determined by this condition can be obtained by solving the following system of equations:

$$F(y) = 0; \quad F'(y) = 0. \tag{22}$$

For $T^* > T_s^*(P^*)$ the solutions y_1 and y_2 become complex conjugate. In the region $P^* < 0$ and $T^* > T_s^*(P^*)$ Eq. (20) has complex conjugate solutions only and consequently the linear chain has no stable state. The same situation occurs at all temperatures if $P^* < 0$ and $| P^* |$ are sufficiently high.

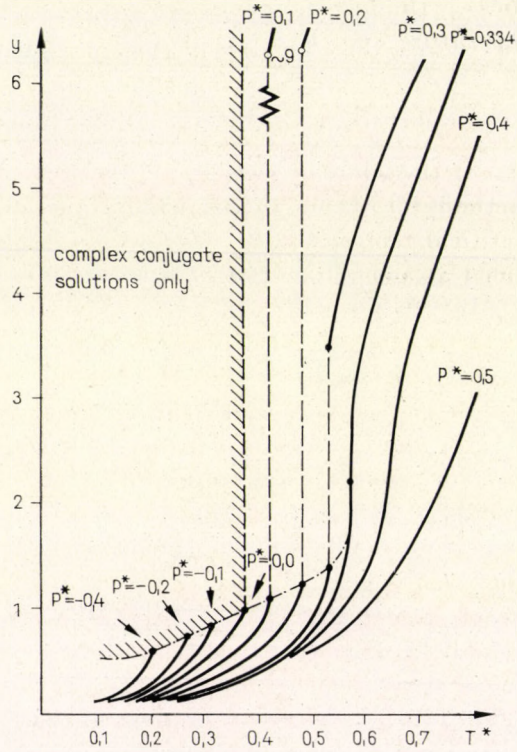

Fig. 1. The physical solution of the self-consistent equation in the high temperature limit

But when $P^* \geq 0$ there are real solutions $y_3 < y_4$ in addition to complex conjugate solutions. The smallest of these is the physical one. In this case at the temperature $T^* = T_s^*(P^*)$ the state of the chain changes by a jump from the state S_1(at $T^* \leq T_s^*$) to some new state S_2 which is stable at temperature $T^* \geq T_s^*(P^*)$. At the instability temperature $T_s^*(P^*)$ the length (16) and the internal energy (17) of the chain take a jump and their derivatives — the coefficient of the linear thermal expansion and the specific heat at constant pressure — tend to infinity as $T^* \to T_s^*(P^*)$.

In the region of sufficiently high tension or temperature, $P^* \geq P_c^*$ or $T^* \geq T_c^*$, Eq. (20) has always two real solutions, the smallest of which is the physical one. The critical temperature T_c^* and the critical tension P_c^* are determined by the coincidence of three real solutions of Eq. (20): $y_1(T_c^*, P_c^*) =$

$= y_2(T_c^*, P_c^*) = y_3(T_c^*, P_c^*)$. Consequently, they can be obtained from the solution of the following system of equations:

$$F(y) = 0; \qquad F'(y) = 0; \qquad F''(y) = 0. \tag{23}$$

In this region $P^* \geq P_c^*$ or $T^* \geq T_c^*$ the chain is always stable and its physical quantities — the internal energy and the length — are smooth functions of the temperature and the tension.

4. Instability temperature and critical temperature

The analysis of the solutions of the self-consistent equation (20) provides a convenient method for the determination of the instability temperature $\tau_s(P^*)$ and the critical temperature τ_c. According to (22) the instability temperature is obtained as a simultaneous solution of Eq. (18) and its derivative:

$$\lambda\{y(\alpha)+\alpha y'(\alpha)\} = -\frac{1}{2\tau}\int_0^{\pi/2} d\varphi \sin^2\varphi \, sh^{-2}\left(\frac{\alpha \sin\varphi}{2\tau}\right). \tag{24}$$

According to (23) the critical temperature is obtained as a simultaneous solution of Eqs. (18), (24) and the second derivative of (18):

$$\lambda\{2y'(\alpha)+\alpha y''(\alpha)\} = 2\left(\frac{1}{2\tau}\right)^2\int_0^{\pi/2} d\varphi \sin^3\varphi \, \mathrm{ch}\left(\frac{\alpha\sin\varphi}{2\tau}\right)\mathrm{sh}^{-3}\left(\frac{\alpha\sin\varphi}{2\tau}\right), \tag{25}$$

where the function $y(\alpha)$ is given by Eq. (14).

The results of numerical solutions of these systems of equations are given in Figs. 2 and 3. In Fig. 2 the dependence of the instability temperature $\tau_s = (\Theta_s/\omega_{0L})$ on the dimensionless coupling constant λ is given for some values of P^*. In Fig. 3 the dependence of the instability temperature on the reduced tension is shown for some values of λ. In both Figures the critical curves are denoted by a dotted line. We do not consider here the case of small values of $\lambda \lesssim 2$ which demands additional calculations. This will be discussed elsewhere.

In [5], [6] we obtain the following expressions for the instability temperature* for high ($\tau \gg 1$) and low ($\tau \ll 1$) temperatures:

$$\tau_s = \frac{\lambda}{\pi e}\left\{1 + \frac{e}{2}P^* - \frac{e}{24}\left(\frac{\pi}{\lambda}\right)^2\right\}; \tag{26}$$

$$(\tau \gg 1;\ P^* \ll 1)$$

$$\tau_s = \frac{1}{\pi e}\sqrt{\frac{6}{e}(\lambda-\lambda_0)};\ \lambda_0 = \frac{e}{2}\left\{1 - \left(\frac{e}{2}\right)^2 P^*\right\}. \tag{27}$$

$$(\tau \ll 1;\ P^* \ll 1).$$

* We note here that the instability temperature τ_s was called the critical temperature and denoted by τ_c in [4]—[6].

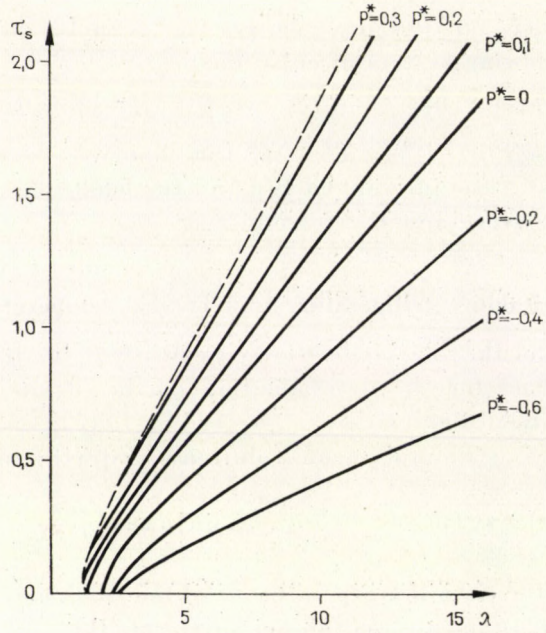

Fig. 2. The dependence of the instability temperature $\tau_s = (\Theta_s/\omega_{0L})$ on the dimensionless coupling constant $\lambda = (\pi D/\omega_{0L})$

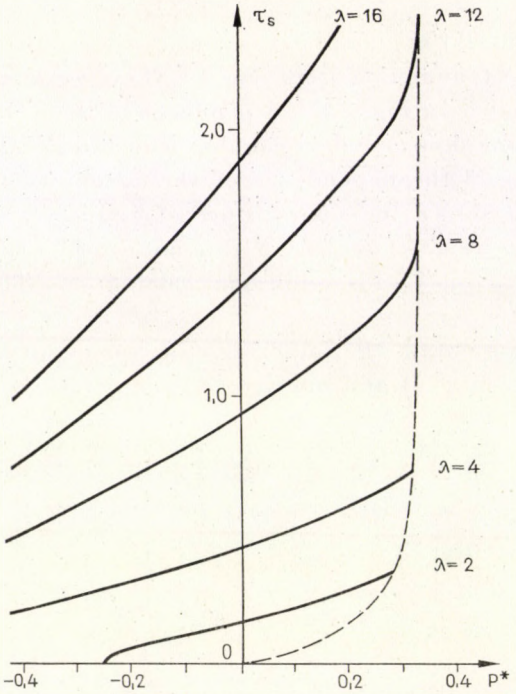

Fig. 3. The dependence of the instability temperature τ_s on the reduced tension P^*

The results of numerical solutions agree quite well with asymptotic expressions (26), (27) for $P^* \ll 1$.

We can also obtain the asymptotic expressions for the critical temperature for high temperatures ($\tau \gg 1$). In this case, Eqs. (18), (24), (25) read:

$$\alpha^2 \ln \frac{\alpha^2 - \frac{P^*}{6}}{\left(\alpha^2 - \frac{P^*}{3}\right)^2} = T^* + \frac{1}{24}\left(\frac{\pi}{\lambda}\right)^2 \frac{\alpha^2}{T^*}, \tag{18a}$$

$$\ln \frac{\alpha^2 - \frac{P^*}{6}}{\left(\alpha^2 - \frac{P^*}{3}\right)^2} - \frac{\alpha^4}{\left(\alpha^2 - \frac{P^*}{6}\right)\left(\alpha^2 - \frac{P^*}{3}\right)} = \frac{1}{24}\left(\frac{\pi}{\lambda}\right)^2 \frac{1}{T^*}, \tag{24a}$$

$$\alpha^4 - \alpha^2 P^* + \frac{(P^*)^2}{6} = 0 . \tag{25a}$$

Using (18a) and (24a) we obtain the instability temperature:

$$T_s^* = \frac{\alpha_s^6}{\left(\alpha_s^2 - \frac{P^*}{6}\right)\left(\alpha_s^2 - \frac{P^*}{3}\right)} . \tag{28}$$

The critical value of the renormalization parameter α_c is given by the solution of (25a) which reads:

$$\alpha_c^2 = \frac{P_c^*}{2}\left(1 + \frac{\sqrt{3}}{2}\right). \tag{29}$$

For the critical tension and critical temperature the calculations give the following approximate expressions:

$$P_c^* \approx 0{,}334\left\{1 - \frac{\sqrt{3}}{24}\left(\frac{\pi}{\lambda}\right)^2\right\}, \tag{30}$$

$$T_c^* \approx \sqrt{3}\, P_c^* \approx 0{,}575\left\{1 - \frac{\sqrt{3}}{24}\left(\frac{\pi}{\lambda}\right)^2\right\}, \tag{31}$$

where equations (29), (18a) and (28) have been used. The results of the numerical solutions agree quite well with the asymptotic expressions (30) and (31) for $\lambda \geq 2$.

5. Discussion

In this work the stability region of an anharmonic linear chain was investigated for arbitrary external tension over a wide range of temperature. It was found, contrary to [6], that the instability phenomenon vanishes at critical temperature T_c^* and critical tension P_c^*.

We make some remarks about the physical meaning of the instability temperature T_s and the critical temperature T_c. It is well known that though the fluctuation of the average position of the atoms in a linear chain is great: $\sqrt{<u_N^2>}/l \sim \sqrt{N} \gg 1$ the relative displacement of the neighbouring atoms is small: $[<(u_n - u_{n-1})^2>]^{1/2}/l \ll 1$. This fact shows the existence of the short range order in a linear chain, so that it can be considered as a bound state of N atoms, where collective excitations, the phonons, can exist [8]. If the temperature increases, the number of phonons also increases which means an increase in the amplitude of the relative displacement of the neighbouring atoms. At the temperature $T > T_s$ in the self-consistent equation (18) complex conjugate values of the vibrational frequency appear and, consequently, infinite relative displacement of atoms: $[<(u_n - u_{n-1})^2>]^{1/2} \sim e^{\gamma t}$ ($\gamma > 0$). This means that the linear chain becomes unstable in respect of the propagation of collective excitations which destroy the bound state of the atoms in the chain. On this basis the external tension can be considered as some external field which when $P > P_c$ limits the motion of the atoms in the linear chain.

The stability of the chain with fixed length found in [6] is not meaningless from the physical point of view as in this case the tension increases rather rapidly with the temperature: at $T \sim T_s$: $P \gtrsim P_c$ and it can stabilize the lattice. We think that the instability of the lattice at fixed volumes found in [1] is connected with the possibility of an exchange of the atoms situated in the neighbouring lattice sites which have not been taken into account here. To investigate this problem the hard core of the interatomic potential should be carefully taken into account.

The theory developed here does not take into account the damping of the phonons; its influence on the properties of the anharmonic linear chain will be considered elsewhere.

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ТЕОРИЯ АНГАРМОНИЧЕСКИХ КРИСТАЛЛОВ В ПСЕВДОГАРМОНИЧЕСКОМ ПРИБЛИЖЕНИИ

I. Линейная цепочка

Т. ШИКЛОШ

Резюме

Исследуются свойства ангармонической линейной цепочки в псевдогармоническом приближении. Получена зависимость температуры неустойчивости от произвольного внешнего натяжения. Показано, что область неустойчивости линейной цепочки ограничена значениями критической температуры и критического натяжения.

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THEORY OF ANHARMONIC CRYSTALS IN PSEUDOHARMONIC APPROXIMATION

II. THREE-DIMENSIONAL LATTICE

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The properties of the f.c.c. lattice with the central nearest neighbour interaction are considered in the pseudoharmonic approximation. The dependence of the instability temperature on the arbitrary external pressure is investigated. It is shown that the instability region of the crystal is limited by the critical temperature and the critical pressure.

1. Introduction

In our previous paper [1] the simple model of a crystal, the linear chain with nearest neighbour interaction, was investigated in pseudoharmonic approximation. The properties of the three-dimensional lattice, namely the face-centred cubic (f.c.c.) one with the nearest neighbour central force interaction was considered in pseudoharmonic approximation in paper [2] in the case of low pressure. It was shown that in this case the lattice becomes unstable at sufficiently high zero-point energy or temperature. It was shown also in [3] that the damping of the self-consistent phonons is sufficiently small even near the instability temperature and consequently the most simple pseudoharmonic approximation [4] can be used.

In the present paper we consider the properties of the f.c.c. lattice with the nearest neighbour central force interaction in the case of the arbitrary external pressure in pseudoharmonic approximation. In Section 2 we obtain a pelf-consistent system of equations for the determination of the physical proaerties of the crystal. In Section 3 the instability and the critical temperature cre calculated as functions of the external pressure and the dimensionless soupling constant of the atoms. In Section 4 we discuss the results.

2. Self-consistent system of equations in pseudoharmonic approximation

We consider a f.c.c. lattice consisting of N identical atoms of mass M. The Hamiltonian of a crystal with nearest neighbour central force interactions reads:

$$H = \sum_l \frac{\vec{P}_l^2}{2M} + \frac{1}{2} \sum_{l \neq m}{}' \varphi(|\vec{R}_l - \vec{R}_m|), \tag{1}$$

where $\vec{P}_l$ and $\vec{R}_l$ are the momentum and the position operators for the atom in the lattice site l, respectively. The interaction potential between neighbouring atoms is denoted by $\varphi(|\vec{R}_l - \vec{R}_m|)$. The prime on the summation means that the second summation is performed only over the z nearest neighbours (for f.c.c. $z = 12$).

We introduce the displacement operators u_l^α from the equilibrium positions l_α according to the definition:

$$R_l^\alpha = \langle R_l^\alpha \rangle + u_l^\alpha \equiv l_\alpha + u_l^\alpha. \tag{2}$$

The equilibrium lattice constant $d = l/\sqrt{2}$ can be obtained from the equation

$$P = -\frac{1}{6V} \sum_{\substack{l \neq m \\ \alpha}}{}' l_\alpha < \frac{\partial}{\partial R_l^\alpha} \varphi(|R_l^\alpha - R_m^\alpha|) >, \tag{3}$$

which shows that the average force acting on each atom in the equilibrium position is equal to zero [5]. In Eq. (3) the external pressure is denoted by P and $V = Nv = Nl^3/\sqrt{2}$ stands for the volume.

Applying the method formulated in [4], a self-consistent system of equations for the investigation of the f.c.c. lattice was obtained in [2]. It was shown that the renormalized frequency of vibrations takes the form:

$$\omega_{kj}^2 = \frac{f(\Theta, l)}{f} \omega_{0kj}^2 \equiv \alpha^2 \omega_{0kj}^2, \tag{4}$$

where ω_{0kj} is the harmonic frequency of the vibrations and $f = \varphi''(r_0)$ stands for the harmonic strength constant. The pseudoharmonic strength constant $f(\Theta, l)$ can be written as:

$$f(\Theta, l) = \tilde{\varphi}''s(l), \tag{5}$$

where we introduce the self-consistent potential which in a certain approximation can be written in the form [3]:

$$\tilde{\varphi}(l) \approx \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{2} \bar{u}^2\right)^n \varphi^{(2n)}(l). \tag{6}$$

The mean square relative displacement of neighbouring atoms can be written as:

$$\bar{u}^2 = \frac{1}{l^2} < [\vec{l}\,(\vec{u}_l - \vec{u}_0)]^2 > = \frac{1}{f(\Theta, l)} \frac{1}{zN} \sum_k \omega_{kj} \coth \frac{\omega_{kj}}{2\Theta}. \tag{7}$$

In addition to the temperature $\Theta = kT$, the properties of the crystal are also determined by the volume V of the crystal or by the external pressure. According to (3), (6) these parameters satisfy the following equation:

$$P = -\frac{zl}{6v}\,\tilde{\varphi}'(l) = -\frac{2\sqrt{2}}{l^2}\,\tilde{\varphi}'(l)\,. \tag{8}$$

The caloric equation of state is obtained from the internal energy which is given in our approximation by the equation

$$\frac{1}{N}E = \frac{z}{2}\left\{\tilde{\varphi}(l) + \frac{1}{2}f(\Theta, l)\,\bar{u}^2\right\}. \tag{9}$$

In this way we obtained a closed system of equations (4)—(9) which determine the properties of the anharmonic crystal in pseudoharmonic approximation. This self-consistent system of equations is determined by the self-consistent potential (6) which can be obtained if the potential $\varphi(\vec{R})$ is known. Let us take the Morse potential as a model:

$$\varphi(R) = \varepsilon\left\{[e^{-a(R-r_0)} - 1]^2 - 1\right\}. \tag{10}$$

As in [1] we take $ar_0 = 6$.

Let us consider the case in which the external pressure is fixed, $P = $ $= $ const., but contrary to [2] we do not assume that P is small. It is convenient to introduce the reduced pressure $P^* = P\,\sigma^3/\varepsilon$ where $\sigma^6 = r_0^6/2$ is the parameter of the Lennard-Jones (12—6) interaction potential. Then in the same way as in [1] we obtain the following expressions for the pseudoharmonic renormalization of the frequency α, the dimensionless mean square relative displacement of neighbouring atoms y, the self-consistent potential $\tilde{}(l)$, the equilibrium separations of neighbouring atoms l, and the internal energy $(1/N)E$:

$$\alpha^2 = \frac{P^*}{12}\left(\frac{l}{r_0}\right)^2 + \frac{1}{2}\left\{e^{-y} + \sqrt{e^{-2y} + \frac{P^*}{6}\left(\frac{l}{r_0}\right)^2 e^{-y}}\right\}, \tag{11}$$

$$y = a^2\,\bar{u}^2 = 36\,(\bar{u}^2/r_0^2) = \ln\frac{\alpha^2 - \dfrac{P^*}{24}\left(\dfrac{l}{r_0}\right)^2}{\left[\alpha^2 - \dfrac{P^*}{12}\left(\dfrac{l}{r_0}\right)^2\right]^2}\,, \tag{12}$$

$$\tilde{\varphi}(l) = -\varepsilon\left\{\alpha^2 - \frac{P^*}{8}\left(\frac{P^*}{r_0}\right)^2\right\}, \tag{13}$$

$$l = r_0 \left\{ 1 + \frac{1}{12} \ln \frac{\alpha^2 - \frac{P^*}{24}\left(\frac{l}{r_0}\right)^2}{\left[\alpha^2 - \frac{P^*}{12}\left(\frac{l}{r_0}\right)^2\right]^4} \right\}, \tag{14}$$

$$\frac{1}{N} E = 6\varepsilon \left\{ \alpha^2 \ln \frac{\alpha^2 - \frac{P^*}{24}\left(\frac{l}{r_0}\right)^2}{e\left[\alpha^2 - \frac{P^*}{12}\left(\frac{l}{r_0}\right)^2\right]^2} + \frac{P^*}{8}\left(\frac{l}{r_0}\right)^2 \right\}. \tag{15}$$

Let us replace the sum over $\vec{k}, j$ by the integral over frequency ω in Eq. (7) according to the formula:

$$\frac{1}{3N} \sum_{kj} (\ldots) = \int_0^{\omega_{0L}} g(\omega)\, d\omega (\ldots) = \frac{1}{2} \int_0^2 dx\, G(x) (\ldots),$$

where $x = 2(\omega/\omega_{0L})$; $\omega_{0L} = (8f/M)^{1/2}$ is the maximum value of the harmonic vibrational frequency, $G(x)$ is the distribution function which was obtained in [6]. Then equation (7) can be rewritten as an equation for α:

$$\lambda\alpha\, y(\alpha) = \frac{3}{8 \cdot 1{,}02} \int_0^2 dx\, G(x)\, x \coth \frac{\alpha x}{4\tau}, \tag{16}$$

where $\lambda = z\, \varepsilon/\varepsilon_0^{(0)}$ is the dimensionless coupling constant for atoms, $\varepsilon_0^{(0)} \approx \approx 1.02\, \omega_{0L}$ is the zero-point energy per atom in the harmonic approximation, $\tau = \Theta/\omega_{0L}$ is the dimensionless temperature. The function $y(\alpha)$ is given by (12), (14). It is easy to see that all the equations obtained here for $P^* \ll 1$ coincide with those of work [2].

Let us compare the self-consistent equation (16) and the expressions (11)—(15) with those obtained in [1] for the monatomic linear chain. It is easy to see that they have a similar form and consequently a similar analytical behaviour. Therefore, we shall not repeat here the discussions of Section 3 of [1] and we shall give the results only.

3. Instability temperature and critical temperature

According to [1] the instability temperature can be obtained as a simultaneous solution of Eq. (16) and its derivative:

$$\lambda\{y(\alpha) + \alpha y'(\alpha)\} = -0{,}3976 \frac{1}{4\tau} \int_0^2 dx\, G(x)\, x^2 \sinh^{-2}\left(\frac{\alpha x}{4\tau}\right). \tag{17}$$

The critical temperature can be obtained as a simultaneous solution of Eqs. (16), (17) and the second derivative of (16):

$$\lambda\{2y'(\alpha)+\alpha y''(\alpha)\} = 0{,}3676\left(\frac{1}{4\tau}\right)^2\int_0^2 dx\, G(x)\, x^3 \cosh\left(\frac{\alpha x}{4\tau}\right)\sinh^{-3}\left(\frac{\alpha x}{4\tau}\right), \quad (18)$$

where the function $y(\alpha)$ is given by (12), (14).

The results of numerical solutions of these systems of equations are given in Figs. 1—3. In Fig. 1 the dependence of the pseudoharmonic renormalization of the frequency $\alpha_s = \omega_{jk}/\omega_{0kj}$ at the instability temperature on the reduced pressure P^* is presented for some values of λ. In Fig. 2 the dependence of the instability temperature $\tau_s = \Theta_s/\omega_{0L}$ on the dimensionless coupling constant λ is given for some values of P^*. In Fig. 3 the dependence of the instability temperature on the reduced pressure is presented for some values of λ. In all Figures the critical curves are denoted by dot-and-dash lines. We do not consider here the case of small values of $\lambda \lesssim 2$ which demands additional calculations. That will be discussed elsewhere.

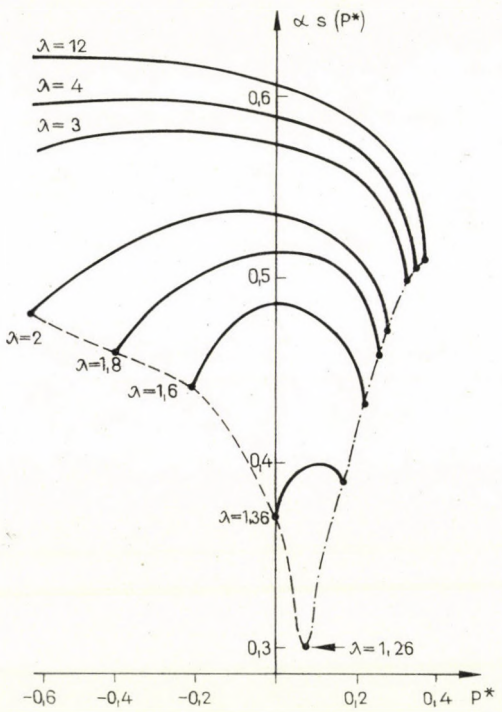

Fig. 1. The dependence of the pseudoharmonic renormalization of the frequency $\alpha_s = \omega_{kj}/\omega_{0kj}$ on the reduced pressure P^* at the instability temperature

For the values of $\lambda \geq 12$ we obtain the following values for the critical temperature $T_c^* \approx 1.56$ and the critical pressure $P_c^* \approx 0.37$ where $T^* = \Theta/\varepsilon = 11.76\ \tau/\lambda$ is the reduced temperature.

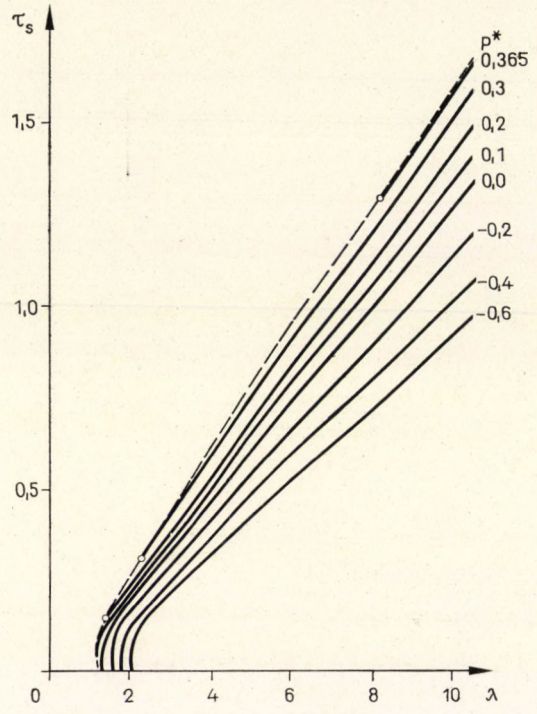

Fig. 2. The dependence of the instability temperature $\tau_s = \Theta_s/\omega_{0L}$ on the dimensionless coupling constant λ of the atoms

The following expressions were obtained in [2] for the instability temperature* for high ($\tau \gg 1$) and low ($\tau \ll 1$) temperatures:

$$\tau_s = \frac{1{,}02\lambda}{3e}\left\{1 + \frac{e}{5{,}1}P^* - \frac{e}{24}\left(\frac{3}{1{,}02\,\lambda}\right)^2\right\} \tag{19}$$

$$(\tau \gg 1;\ P^* \ll 1)$$

$$\tau_s = \frac{1{,}05}{\pi e}\left\{\frac{10}{3e}(\lambda - \lambda_0)\right\}^{1/4};\ \lambda_0 = \frac{e}{2}\left\{1 - \frac{e^2}{7{,}12}P^*\right\}. \tag{20}$$

$$(\tau \ll 1;\ P^* \ll 1)$$

* We note here that in [2] the instability temperature was called the critical temperature and denoted by τ_c.

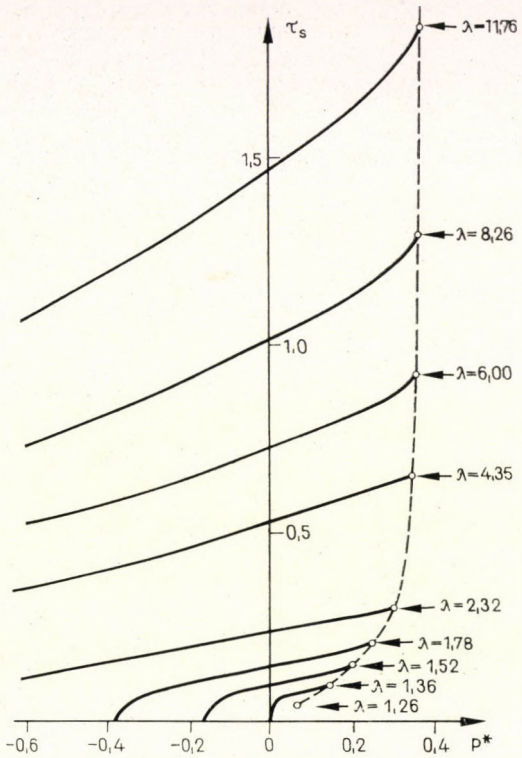

Fig. 3. The dependence of the instability temperature τ_s on the reduced pressure P^*

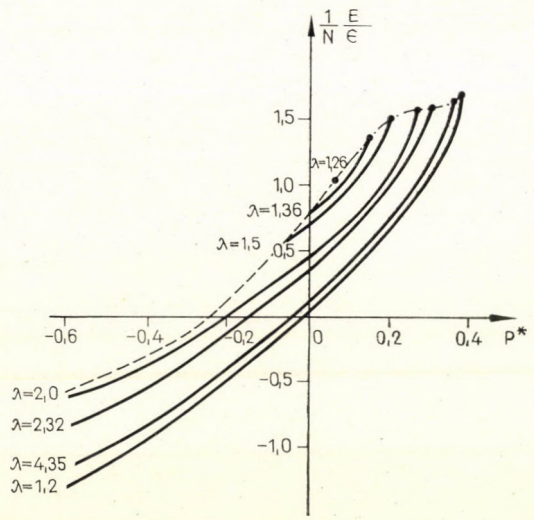

Fig. 4. The dependence of the internal energy $(1/N)\, E_s/\varepsilon$ on the dimensionless coupling constant λ at the instability temperature

The results of numerical solutions agree quite well with the asymptotic expressions (19), (20) for $P^* \ll 1$.

Using Eqs. (12)—(15) and the solution α_s of the Eqs. (16), (17), the dimensionless mean square relative displacement of the neighbouring atom y,

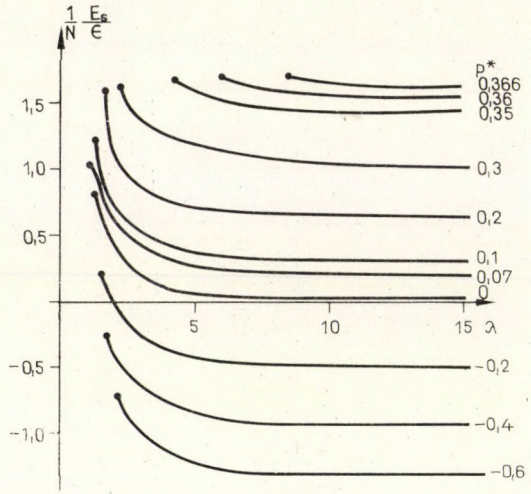

Fig. 5. The dependence of the internal energy on the reduced pressure P^* at the instability temperature

the self-consistent potential, the equilibrium separation of neighbouring atoms and the internal energy were calculated at the instability temperature. In Fig. 4 the internal energy of the crystal $(1/N)E/\varepsilon$ at the instability temperature is presented as a function of λ and in Fig. 5 as a function of P^*. The results of numerical calculations agree quite well with the results of [2] in the case of small pressures.

4. Discussion

In this work the behaviour of a three-dimensional f.c.c. lattice was investigated in the case of arbitrary external pressure in a wide range of temperatures. It was shown that the behaviour of a three-dimensional lattice does not differ qualitatively from the one-dimensional lattice discussed in [1].

It is also interesting to note that the reduced instability temperature $T_s^* = \Theta_s/\varepsilon$ as a function of the reduced pressure P^* qualitatively agrees with the reduced melting curves of the inert gas solids [7]. It seems, therefore, that the point of dynamic instability lies close to the melting point of the crystal. The critical temperature T_c^* and the critical pressure P_c^* found here limited the instability region of the crystal. But it should be noted that the damping

of phonons (the second order terms in the self-consistent theory [3]) should be taken into account in order to get more rigorous results. These will be considered in a separate paper.

Acknowledgement

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ТЕОРИЯ АНГАРМОНИЧЕСКИХ КРИСТАЛЛОВ В ПСЕВДОГАРМОНИЧЕСКОМ ПРИБЛИЖЕНИИ

II. Трехмерная решетка

Т. ШИКЛОШ

Резюме

Исследуются свойства ангармонической ГЦК решетки в псевдогармоническом приближении. Получена зависимость температуры неустойчивости от произвольного внешнего давления. Показано, что область устойчивости кристалла ограничена значениями критической температуры и критического давления.

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ÜBER DIE DURCH DEN KORRELATIONSFAKTOR ERWEITERTEN EIGENFUNKTIONEN

Von

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(Eingegangen: 20. X. 1970)

Auf Grund der Methode-LCAO-MO wurde die Elektronenergie des $1s\,3s\ ^1\Sigma_g^+$-Zustandes des Wasserstoffmoleküls berechnet. Es konnte weiterhin durch den Vergleich der Elektronener, giekorrektionen, die für den Grundzustand von FROST und BRAUNSTEIN und für die $1sns\ ^1\Sigma_g^+$-Zustände vom Verfasser mit der Hilfe der Methode-LCAO-CMO erhalten worden sind festgestellt werden, dass der Korrelationsfaktor bei den Berechnungen sowohl des Grundzustandes als der angeregten Zustände eine gleichwertige Rolle spielt.

Einleitung

Aus den zahlreichen quantenmechanischen Berechnungen des Wasserstoffmoleküls ist es wohlbekannt, dass jene Resultate, die sich auf Grund von Eigenfunktionen ergeben, die die Tendenz der Elektronen berücksichtigen, wegen ihrer gegenseitigen Abstossung voneinander entfernt zu bleiben, d. h. in welchen Eigenfunktionen Elektronenkorrelation vorhanden ist [1], [2], sich dem empirischen Wert besser nähern. Die Eigenfunktionen werden vom Gesichtspunkt der Elektronenkorrelation aus in die Gruppen der die Elektronenkorrelation explizit und implizit enthaltenden Eigenfunktionen eingeteilt. Werden die Resultate der quantenmechanischen Berechnungen des Wasserstoffmoleküls miteinander verglichen, kann man sich davon überzeugen, dass auf Grund der Rechenverfahren die mit solch zahlreichen Eigenfunktionen durchgeführt wurden, die nur implizite Elektronenkorrelation erhalten und physikalisch verschiedenartig interpretiert werden können, das beste Resultat für die Dissoziationsenergie des Wasserstoffmoleküls der von JAMES und COOLIDGE [3] erreichte Wert $D = 4.27$ eV ist.

In den auf Grund der Methode-MO durchgeführten Rechnungen ist die Aufhäufung der Elektronen, ohne Rücksicht auf die Atome im Molekül, möglich; die Elektronen bewegen sich nähmlich, der Annahme gemäss, in einem durchschnittlichen Potentialfeld, und die Wechselbeziehung zwischen den Elektronen, d. h. Korrelation, wird vernachlässigt, da in der Eigenfunktion die gegenseitige Entfernung der beiden Elektronen ($= r_{ik}$) fehlt. Die richtige Eigenfunktion hat also folgende Gestalt:

$$\Psi = \prod_{i=2}^{n} \psi_i \prod_{k<l} f(r_{kl}), \qquad 1)$$

wo ψ_i die von den Koordinaten des i-ten Elektrons abbhängige Molekülbahn bezeichnet; durch $f(r_{kl})$ wird die Wechselbeziehung zwischen den Elektronen berücksichtigt.

Die einfachste Gestalt der Funktion $f(r_{kl})$ ist $(1 + pr_{12})$, wo r_{12} die gegenseitige Entfernung der Elektronen bezeichnet und p ein Variationsparameter ist, welcher sich bei der Minimisierung der Energie immer positiv ergibt. Diese Tatsache spricht dafür, dass beim Bindungszustand die Elektronenkonfiguration, bei der die Elektronen voneinander weiter entfernt sind, mit einer grösseren Wahrscheinlichkeit auftritt, was die Möglichkeit keineswegs ausschliesst, dass die Elektronendichte bei der Molekülbindung zwischen den Kernen wesentlich zunimmt.

Die Molekülbahn wurde zuerst bei der Berechnung des Grundzustandes des Wasserstoffmoleküls von FROST und BRAUNSTEIN [4] durch den Korrelationsfaktor $(1 + pr_{12})$ erweitert und korrelationsmässige Molekülbahn genannt. Die wird mit CMO (Correlated Molecular Orbital) bezeichnet. Die Idee wurde von WIGNER [5] und von SEITZ [6] veranlasst, die die korrelationsmässige Bewegung der Elektronen in Metallen berücksichtigt haben.

In früheren Arbeiten des Verfassers [7], [8], [9] wurden die Molekülbahnberechnungen auf die $1sns\ ^1\Sigma_g^+$-Zustände $(n = 2,3)$ des Wasserstoffmoleküls ausgedehnt und dann mit Hilfe der Methode LCAO—CMO im Falle des $1s2s\ ^1\Sigma_g^+$-Zustandes des Wasserstoffmoleküls erweitert. In dieser Arbeit werden die korrelationsmässigen Molekülbahnberechnungen des $1s3s\ ^1\Sigma_g^+$-Zustandes des Wasserstoffmoleküls angegeben, sowie das FROST—BRAUNSTEINsche Resultat der Berechnung des Grundzustandes und die vom Verfasser erreichten Resultate der Berechnungen der angeregten Zustände des Wasserstoffmoleküls zur Prüfung der Rolle des Korrelationsfaktors, miteinander verglichen.

Die Rechenmethode

Bezeichnet man die Molekülbahnen der einzelnen, das Molekül aufbauenden Elektronen mit $\psi_1, \psi_2, \ldots, \psi_n$, so kann gemäss HUND [10], MULLIKEN [11], HÜCKEL [12] und LENNARD-JONES [13], die Eigenfunktion des Moleküls auf Grund des Modells der Eigenfunktionen der freien Systeme in folgender Weise konstruiert werden:

$$\Psi = \psi_1 \cdot \psi_2 \ldots \psi_n. \tag{2}$$

Die Molekülbahnen der einzelnen Elektronen lassen sich aber auf Grund der Methode LCAO (Linear Combination of Atomic Orbitals) [14] als Linearkombinationen der einzelnen Atombahnen aufschreiben. Die korrelationsmässige Molekülbahn ensteht dann durch Multiplikation mit dem Korrelationsfaktor $(1 + pr_{12})$.

Zur Berechnung des $1s3s\ ^1\Sigma_g^+$-Zustandes des Wasserstoffmoleküls wird es angenommen, dass sich das erste Elektron im Grundzustand und das zweite Elektron in angeregtem Zustand befindet. Demgemäss haben die Molekülbahnen der einzelnen Elektronen nach der LCAO-Methode die folgende Gestalt:

$$1\sigma_g(1) = [1s_A(1)+1s_B(1)]/\sqrt{2(1+S_1)}\,, \tag{3}$$

$$3\sigma_g(2) = [3s_A(2)+3s_B(2)]/\sqrt{2(1+S_2)}\,, \tag{4}$$

wo

$$S_i = <is_A \mid is_B>, \qquad i = 1,3, \tag{5}$$

und is_A und is_B die Wasserstoffeigenfunktionen der is-Zustände sind. Die Eigenfunktion des $1s3s\ ^1\Sigma_g^+$-Zustandes des Wasserstoffmoleküls nimmt also die folgende Gestalt an:

$$\Psi_{1s3s} = 1\sigma_g(1)\ 3\sigma_g(2)\,(1+pr_{12})\,\frac{1}{\sqrt{2}}\,(\alpha_1\beta_2-\beta_1\alpha_2)\,, \tag{6}$$

mit der sich die Elektronenergie auf Grund des Variationsverfahrens auf folgender Weise ergibt:

$$E_{1s3s} = \frac{\int \Psi_{1s3s} H \Psi_{1s3s}\, d\tau}{\int \Psi_{1s3s}^2\, d\tau}\,, \tag{7}$$

wo H der Hamilton-Operator des Wasserstoffmoleküls ist.

Die Ergebnisse der Berechnungen

In früheren Arbeiten [7], [8] wurde vom Verfasser die Elektronenergie der $1sns\ ^1\Sigma_g^+$-Zustände ($n = 2,3$) des Wasserstoffmoleküls auf Grund der Methode LCAO—MO berechnet. Um den Einfluss des Korrelationsfaktors auf die Berechnungen der $1sns\ ^1\Sigma_g^+$-Zustände des Wasserstoffmoleküls zu prüfen, wurden die vorigen Berechnungen mit der Methode LCAO—CMO wiederholt [9], (vorliegende Arbeit). Die für die Elektronenergie erreichten Resultate und die sich auf Grund der Erweiterung der Molekülbahn durch den Korrelationsfaktor ergebenden Energiekorrelationen befinden sich in der untenstehenden Tabelle:

Zustand	Methode	Elektronenergie at. Einheit	Energiekorrektion at. Einheit
$1s2s$ [7]	LCAO—MO	0,68086	0,02135
$1s2s$ [9]	LCAO—CMO	0,70221	
$1s3s$ [8]	LCAO—MO	0,63400	
$1s3s$ (in der vorliegenden Arbeit)	LCAO—CMO	0,65418	0,02018

Unsere Ergebnisse sollen mit den auf Grund der LCAO—MO- und LCAO—CMO-Methode im Falle des Grundzustandes des Wasserstoffmoleküls erreichten verglichen werden.

WEINBAUM berechnete [15] den Grundzustand des Wasserstoffmoleküls auf Grund der Methode LCAO—MO und erreichte eine Elektronenergie mit dem Wert von 1,12755 at. E., FROST und BRAUNSTEIN [4] wiederholten die vorige Berechnung auf Grund der Methode LCAO—CMO mit einem Resultat von 1,15107 at. E. für die Elektronenergie. Auf Grund der Erweiterung der Molekülbahn durch den Korrelationsfaktor ergibt sich also im Falle des Grundzustandes des Wasserstoffmoleküls eine Energiekorrektion mit dem Wert von 0,02352 at. E.

Wenn die von FROST und BRAUNSTEIN und vom Verfasser erhaltenen Energiekorrektionen miteinander verglichen werden, kann es festgestellt werden, dass die Energiekorrektionen grössenordnungsmässig gleich sind. Aus dieser Tatsache kann die Schlussfolgerung gezogen werden, dass der Korrelationsfaktor $(1 + pr_{12})$ bei den Berechnungen sowohl des Grundzustandes als der angeregten Zustände des Wasserstoffmoleküls, eine gleichwichtige Rolle spielt.

Ich danke auch an dieser Stelle Fräulein Á. DANKÓ für die Durchführung der Kontrollberechnungen der Integrale und Fräulein A. BOLDIZSÁR für die Hilfe bei den numerischen Rechnungen.

Anhang

Die Methode LCAO—CMO liefert zahlreiche Integrale, in welchen der Integrand $r_{12}^n (n = -1, 0, 1, 2)$ enthält. Diese seien folgendermassen bezeichnet:

$$I(\alpha, \beta, \gamma, \delta, i, j, k, m, n) = \frac{1}{\pi^2} \iint \exp(-\alpha r_{a1} - \beta r_{b1}) \times \times \exp(-\gamma r_{a2} - \delta r_{b2})\, r_{a1}^i\, r_{b1}^j\, r_{a2}^k\, r_{b2}^m\, r_{12}^n\, d\tau_1\, d\tau_2 . \tag{8}$$

Bei der Berechnung der Integrale wird die Methode von KOTANI [17] und seinen Mitarbeitern benutzt.

Unsere Integrale können der Gestalt der Exponentialfunktionen entsprechend in vier Gruppen eingeteilt werden:

$$\exp(-2r_{a1}) \exp\left(-\frac{2}{3} r_{a2}\right), \tag{9}$$

$$\exp(-2r_{a1}) \exp\left(-\frac{1}{3} r_{a2} - \frac{1}{3} r_{b2}\right), \tag{10}$$

$$\exp(-r_{a1}-r_{b1})\exp\left(-\frac{2}{3}r_{a2}\right), \tag{11}$$

$$\exp(-r_{a1}-r_{b1})\exp\left(-\frac{1}{3}r_{a2}-\frac{1}{3}\right). \tag{12}$$

Wegen der grossen Zahl der Molekülintegrale werden aus jeder Gruppe nur einige mitgeteilt: Es werden die folgenden Abkürzungen benutzt:

$(i/k) = H_k^i G_k^i G_k^i$ mit den Argumenten in den betreffenden Reihen,

$$C = 3\,(0/1) + 5\,(0/2) + 7\,(0/3) + 9\,(0/4)\,,$$

$$D = \frac{5}{18}\,(1/2) + \frac{7}{72}\,(1/3) + \frac{9}{200}\,(1/4)\,.$$

$$I\left(1, 1, \frac{1}{3}, \frac{1}{3}, 0, 0, 2, 2, 1\right) =$$

$$= \frac{R^{11}}{512}\Big\{4\,[H_0^0(4, R; 6, R/3) + H_0^0(2, R; 8, R/3)] -$$

$$- \frac{16}{3}\,H_0^0(2, R; 6, R/3) - \frac{8}{3}\,H_1^0(3, R; 7, R/3) +$$

$$+ \frac{8}{3}\,H_1^1(2, R; 6, R/3) -$$

$$- 4\,[H_0^0(4, R; 4, R/3) + H_0^0(2, R; 6, R/3)] +$$

$$+ \frac{64}{15}\,H_0^0(2, R; 4, R/3) - \frac{16}{15}\,(0/2) +$$

$$+ \frac{24}{5}\,H_1^0(3, R; 5, R/3) - \frac{8}{5}\,H_1^1(2, R; 4, R/3) +$$

$$+ \frac{12}{5}\,[H_0^0[4, R; 2, R/3) + H_0^0(2, R; 4, R/3)] -$$

$$- \frac{16}{7}\,H_0^0(2, R; 2, R/3) + \frac{32}{35}\,(0/2) -$$

$$- \frac{24}{7}\,H_1^0(3, R; 3, R/3) + \frac{24}{35}\,H_1^1(2, R; 2, R/3) -$$

$$- \frac{4}{7}\,[H_0^0(4, R; 0, R/3) + H_0^0(2, R; 2, R/3)] +$$

$$+ \frac{32}{63}\,H_0^0(2, R; 0, R/3) - \frac{16}{63}\,(0/2) +$$

$$+\frac{8}{9}H_1^0(3,R;1,R/3)-\frac{8}{63}H_1^1(2,R;0,R/3)-$$

$$-\frac{4}{3}[H_0^0(2,R;6,R/3)+H_0^0(0,R;8,R/3)]+$$

$$+\frac{64}{45}H_0^0(0,R;6,R/3)-\frac{16}{45}(0/2)+$$

$$+\frac{8}{5}H_1^0(1,R;7,R/3)-\frac{8}{15}H_1^1(0,R;6,R/3)+$$

$$+\frac{4}{3}[H_0^0(2,R;4,R/3)+H_0^0(0,R;6,R/3)]+\frac{16}{15}(0/2)-$$

$$-\frac{16}{15}H_0^0(0,R;4,R/3)-\frac{32}{105}(0/2)-$$

$$-\frac{72}{25}H_1^0(1,R;5,R/3)-\frac{96}{175}(0/3)+$$

$$+\frac{8}{25}H_1^1(0,R;4,R/3)+\frac{32}{525}(1/3)-$$

$$-\frac{4}{5}[H_0^0(2,R;2,R/3)+H_0^0(0,R;4,R/3)]-\frac{32}{35}(0/2)+$$

$$+\frac{96}{175}H_0^0(0,R;2,R/3)+\frac{62}{153}(0/2)-\frac{256}{3675}(0/4)+$$

$$+\frac{72}{35}H_1^0(1,R;3,R/3)+\frac{64}{105}(0/3)-$$

$$-\frac{24}{175}H_1^1(0,R;2,R/3)-\frac{64}{1575}(1/3)+$$

$$+\frac{4}{21}[H_0^0(2,R;0,R/3)+H_0^0(0,R;2,R/3)]+\frac{16}{63}(0/2)-$$

$$-\frac{112}{945}H_0^0(0,R;0,R/3)-\frac{1088}{14553}(0/2)+\frac{256}{8085}(0/4)-$$

$$-\frac{8}{15}H_1^0(1,R;1,R/3)-\frac{32}{165}(0/3)+$$

$$+\frac{8}{315}H_1^1(0,R;0,R/3)+\frac{32}{3465}(1/3)\Big\}.$$

$$I\left(1,1,\frac{1}{3},\frac{1}{3},0,0,2,2,2\right) =$$

$$= \frac{R^{12}}{1024}\Big\{4[A_4(R)\,A_6(R/3)+A_2(R)\,A_8(R/3)]-\frac{16}{3}A_2(R)\,A_6(R/3)-$$

$$-4[A_4(R)A_4(R/3)+A_2(R)A_6(R/3)]+\frac{64}{15}A_2(R)A_4(R/3)+$$

$$+\frac{12}{5}[A_4(R)A_2(R/3)+A_2(R)A_4(R/3)]-\frac{16}{7}A_2(R)A_2(R/3)-$$

$$-\frac{4}{7}[A_4(R)A_0(R/3)+A_2(R)\,A_2(R/3)]+\frac{32}{63}A_0(R)A_6(R/3)+$$

$$-\frac{4}{3}[A_2(R)A_6(R/3)+A_0(R)A_8(R/3)]+\frac{64}{45}A_2(R)A_6(R/3)+$$

$$+\frac{4}{3}[A_2(R)A_4(R/3)+A_0(R)A_6(R/3)]-\frac{16}{15}A_0(R)A_4(R/3)-$$

$$-\frac{4}{5}[A_2(R)A_2(R/3)+A_0(R)A_4(R/3)]+\frac{96}{175}A_0(R)A_2(R/3)+$$

$$+\frac{4}{21}[A_2(R)A_0(R/3)+A_0(R)A_2(R/3)]-\frac{784}{6613}A_0(R)A_0(R/3)\Big\}.$$

$$\left(2,0,\frac{1}{3},\frac{1}{3},0,0,2,2,1\right) =$$

$$= \frac{R^{11}}{512}\Big\{2[H_0^0(4,R;6,R/3)+H_0^0(2,R;8,R/3)]\,G_0^0(0,R)+$$

$$+2\,H_0^0(2,R;6,R/3)\,G_0^0(2,R)+$$

$$-\frac{10}{3}H_0^0(2,R;6,R/3)\,G_0^0(0,R)+\frac{4}{3}(0/2)-$$

$$-4\,H_1^0(3,R;7,R/3)\,G_1^0(1,R)+2\,H_1^1(2,R;6,R/3)\,G_1^1(0,R)-$$

$$-2\,[H_0^0(4,R;4,R/3)+H_0^0(2,R;6,R/3)]\,G_0^0(0,R)-4(0/2)-$$

$$-2\,H_0^0(2,R;4,R/3)\,G_0^0(2,R)-4(0/2)+$$

$$+\frac{14}{5}H_0^0(2,R;4,R/3)\,G_0^0(0,R)+\frac{32}{7}(0/2)-\frac{48}{35}(0/4)+$$

$$+\frac{36}{5}H_1^0(3,R;5,R/3)\,G_1^0(1,R)+\frac{24}{5}(0/3)-$$

$$-\frac{6}{5}H_1^1(2,R;4,R/3)\,G_1^1(0,R)-\frac{2}{15}(1/3)+$$

$$+\frac{6}{5}[H_0^0(4,R;2,R/3)+H_0^0(1,R;4,R/3)]\frac{24}{7}(0/2)+\frac{48}{35}(0/4)+$$

$$+\frac{6}{5}H_0^0(2,R;2,R/3)\,G_0^0(2,R)+(0/2)+\frac{48}{35}(0/4)-$$

$$-\frac{54}{35}H_0^0(2,R;2,R/3)\,G_0^0(0,R)-\frac{28}{7}(0/2)=\frac{336}{385}(0/4)-$$

$$-\frac{36}{7}H_1^0(3,R;3,R/3)\,G_1^0(1,R)-\frac{16}{3}(0/3)+$$

$$+\frac{18}{35}H_1^1(2,R;2,R/3)\,G_1^1(0,R)+\frac{4}{45}(1/3)-$$

$$-\frac{2}{7}[H_0^0(4,R;0,R/3)+H_0^0(2,R;2,R/3)]\,G_0^0(0,R)0/2)-$$

$$-\frac{20}{21}(0/2)-\frac{48}{77}(0/4)-$$

$$-\frac{2}{7}H_0^0(2,R;0,R/3)\,G_0^0(2,R)-\frac{20}{21}(0/2)-\frac{48}{77}(0/4)+$$

$$+\frac{22}{63}H_0^0(2,R;0,R/3)\,G_0^0(0,R)+\frac{760}{693}(0/2)+\frac{6336}{11011}(0/4)+$$

$$+\frac{4}{3}H_1^0(3,R;1,R/3)\,G_1^0(1,R)+\frac{56}{33}(0/3)-$$

$$-\frac{2}{21}H_1^1(2,R;0,R/3)\,G_1^1(4,R)-\frac{2}{99}(1/3)-$$

$$-2[H_0^0(2,R;6,R/3)+H_0^0(0,R;8,R/3)]\,G_0^0(2,R)-$$

$$-2H_0^0(0,R;6,R/3)\,G_0^0(0,R)+$$

$$+\frac{10}{3}H_0^0(0,R;6,R/3)\,G_0^0(2,R)-\frac{4}{3}(0/2)+$$

$$+4H_1^0(1,R;7,R/3)\,G_1^0(3,R)-2H_1^1(0,R;6,R/3)\,G_1^1(2,R)+$$

$$+2[H_0^0(2,R;4,R/3)+H_0^0(0,R;6,R/3)]\,G_0^0(2,R)+4(0/2)+$$

$$+2H_0^0(0,R;4,R/3)\,G_0^0(4,R)+(0/2)-$$

$$-\frac{14}{5}H_0^0(0,R;4,R/3)\,G_0^0(2,R)-\frac{32}{7}(0/2)+\frac{48}{35}(0/4)-$$

$$-\frac{36}{5}H_1^0(1,R;5,R/3)G_1^0(3,R)+\frac{24}{5}(0/3)+$$

$$+\frac{6}{5}H_1^1(0,R;4,R/3)G_1^1(2,R)+\frac{2}{15}(1/3)-$$

$$-\frac{6}{5}[H_0^0(2,R;2,R/3)+H_0^0(0,R;4,R/3)]G_0^0(2,R)-$$

$$-\frac{24}{7}(0/2)-\frac{48}{35}(0/4)-$$

$$-\frac{6}{5}H_0^0(0,R;2,R/3)G_0^0(4,R)-\frac{24}{7}(0/2)-\frac{48}{35}(0/4)+$$

$$+\frac{54}{35}H_0^0(0,R;2,R/3)G_0^0(2,R)+\frac{28}{7}(0/2)+\frac{336}{385}(0/4)+$$

$$+\frac{36}{7}H_1^0(1,R;3,R/3)G_1^0(3,R)+\frac{16}{3}(0/3)-$$

$$-\frac{18}{35}H_1^1(0,R;2,R/3)G_1^1(2,R)-\frac{4}{45}(1/3)+$$

$$+\frac{2}{7}[H_0^0(2,R;0,R/3)+H_0^0(0,R;2,R/3)]G_0^0(2,R)+$$

$$+\frac{20}{21}(0/2)+\frac{48}{77}(0/4)+$$

$$+\frac{2}{7}H_0^0(0,R;0,R/3)G_0^0(4,R)+\frac{20}{21}(0/2)+\frac{48}{77}(0/4)-$$

$$-\frac{22}{63}H_0^0(0,R;0,R/3)G_0^0(2,R)-\frac{760}{693}(0/2)-\frac{6336}{11011}(0/4)-$$

$$-\frac{4}{3}H_1^0(1,R;1,R/3)G_1^0(3,R)-\frac{56}{33}(0/3)+$$

$$+\frac{2}{21}H_1^1(0,R;0,R/3)G_1^1(2,R)+\frac{2}{99}(1/3)\Big\}.$$

$$I\left(2,0,\frac{1}{3},\frac{1}{3},0,0,2,2,2\right)=$$

$$=\frac{R^{12}}{1024}\Big\{2[A_4(R)A_6(R/3)+A_1(R)A_8(R/3)]\,B_0(R)+$$

$$+ 2\,A_2(R)A_6(R/3)\left[B_2(R) - \frac{5}{3}\,B_0(R)\right] -$$

$$- 2\,[A_4(R)A_4(R/3) + A_2(R)A_6(R/3)]\,B_0(R) -$$

$$- 2\,A_2(R)A_4(R/3)\left[B_2(R) - \frac{7}{5}\,B_0(R)\right] +$$

$$+ \frac{6}{5}\,[A_4(R)A_2(R/3) + A_2(R)A_4(R/3)]\,B_0(R) +$$

$$+ \frac{6}{5}\,A_2(R)A_2(R/3)\left[B_2(R) - \frac{9}{7}\,B_0(R)\right] -$$

$$- \frac{2}{7}\,[A_4(R)A_0(R/3) + A_2(R)A_2(R/3)]\,B_0(R) -$$

$$- \frac{2}{7}\,A_2(R)A_0(R/3)\left[B_2(R) - \frac{11}{9}\,B_0(R)\right] -$$

$$- 2\,[A_2(R)A_6(R/3) + A_0(R)A_8(R/3)]\,B_2(R) -$$

$$- 2\,A_0(R)A_6(R/3)\left[B_4(R) - \frac{5}{3}\,B_2(R)\right] +$$

$$- 2\,[A_2(R)A_4(R/3) + A_0(R)A_6(R/3)]\,B_2(R) +$$

$$+ 2A_0(R)A_4(R/3)\left[B_4(R) - \frac{7}{5}\,D_2(R)\right] -$$

$$- \frac{6}{5}\,[A_2(R)A_2(R/3) + A_0(R)A_4(R/3)]\,B_2(R) -$$

$$- \frac{6}{5}\,A_0(R)\,A_2(R/3)\left[B_4(R) - \frac{9}{7}\,B_2(R)\right] +$$

$$+ \frac{2}{7}\,[A_2(R)A_0(R/3) + A_0(R)A_2(R/3)]\,B_2(R) +$$

$$+ \frac{2}{7}\,A_0(R)\,A_0(R/3)\left[B_4(R) - \frac{11}{9}\,B_2(R)\right]\Bigg\}.$$

$$I\left(2, 0, \frac{2}{3}, 0, 0, 0, 1, 0, 1\right) =$$

$$= \frac{R^8}{64}\Big\{[H_0^0(4, R; 3, R/3) + H_0^0(2, R; 5, R/3)]\,G_0^0(0, R)\,G_0^0(0, R/3) + C +$$

$$+ H_0^0(2, R; 3, R/3)\,[G_0^0(2, R)\,G_0^0(0, R/3) + G_0^0(0, R)\,G_0^0(2, R/3)] + C -$$

$$
\begin{aligned}
&- 2\,H_0^0(3,R;4,R/3)\,G_0^0(1,R)\,G_0^0(1,R/3) - 2C - \\
&- 2\,H_0^0(2,R;3,R/3)\,G_0^0(0,R)\,G_0^0(0,R/3) - 2C + \\
&+ \frac{3}{2}\,H_1^1(2,R;3,R/3)\,G_1^1(0,R/3) + D + \\
&+ [H_0^0(4,R;2,R/3) + H_0^0(2,R;4,R/3)]\,G_0^0(0,R)\,G_0^0(1,R/3) + C + \\
&+ H_0^0(2,R;2,R/3)[G_0^0(2,R)\,G_0^0(1,R/3) + G_0^0(0,R)\,G_0^0(3,R/3) + C - \\
&- 2\,H_0^0(3,R;3,R/3)\,G_0^0(1,R)\,G_0^0(2,R/3) - 2C - \\
&- 2\,H_0^0(2,R;2,R/3)\,G_0^0(0,R)\,G_0^0(1,R/3) - 2C + \\
&+ \frac{3}{2}\,H_1^1(2,R;2,R/3)\,G_1^1(1,R/3) + D - \\
&- [H_0^0(2,R;1,R/3) + H_0^0(2,R;3,R/3)]\,G_0^0(0,R)\,G_0^0(2,R/3) - C - \\
&- H_0^0(2,R;1,R/3)\,[G_0^0(2,R)\,G_0^0(2,R/3) + G_0^0(0,R)\,G_0^0(4,R/3) - C + \\
&+ 2\,H_0^0(3,R;2,R/3)\,G_0^0(1,R)\,G_0^0(3,R/3) + 2C + \\
&+ 2\,H_0^0(2,R;1,R/3)\,G_0^0(0,R)\,G_0^0(2,R/3) + 2C - \\
&- \frac{3}{2}\,H_1^1(2,R;1,R/3)\,G_1^1(0,R)\,G_1^1(2,R/3) - D - \\
&- [H_0^0(4,R;0,R/3) + H_0^0(2,R;2,R/3)]\,G_0^0(0,R)\,G_0^0(3,R/3) - C - \\
&- H_0^0(2,R;0,R/3)\,[G_0^0(2,R)\,G_0^0(3,R/3) + G_0^0(0,R)\,G_0^0(5,R/3)] - C + \\
&+ 2\,H_0^0(3,R;1,R/3)\,G_0^0(1,R)\,G_0^0(4,R/3) + 2C + \\
&+ 2\,H_0^0(2,R;0,R/3)\,G_0^0(0,R)\,G_0^0(3,R/3) + 2C - \\
&- \frac{3}{2}\,H_1^1(2,R;0,R/3)\,G_1^1(0,R)\,G_1^1(3,R/3) - D - \\
&- [H_0^0(2,R;3,R/3) + H_0^0(0,R;5,R/3)]\,G_0^0(2,R)\,G_0^0(0,R/3) - C - \\
&- H_0^0(0,R;3,R/3)[G_0^0(4,R)\,G_0^0(0,R/3) + G_0^0(2,R)\,G_0^0(2,R/3)[-C + \\
&+ 2\,H_0^0(1,R;4,R/3)\,G_0^0(3,R)\,G_0^0(1,R/3) + 2C + \\
&+ 2\,H_0^0(0,R;3,R/3)\,G_0^0(2,R)\,G_0^0(0,R/3) + 2C - \\
&- \frac{3}{2}\,H_1^1(O,R;3,R/3)\,G_1^1(2,R)\,G_1^1(0,R/3) - D - \\
&- [H_0^0(2,R;2,R/3) + H_0^0(0,R;4,R/3)]\,G_0^0(2,R)\,G_0^0(1,R/3) - C - \\
&- H_0^0(0,R;2,R/3)[G_0^0(4,R)\,G_0^0(1,R/3) + G_0^0(2,R)\,G_0^0(3,R/3) - C + \\
&+ 2\,H_0^0(1,R;3,R/3)\,G_0^0(3,R)\,G_0^0(2,R/3) + 2C + \\
&+ 2\,H_0^0(0,R;2,R/3)\,G_0^0(2,R)\,G_0^0(1,R/3) + 2C -
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{3}{2} H_1^1(0, R; 2, R/3)\, G_1^1(2, R)\, G_1^1(1, R/3) - D + \\
&+ [H_0^0(2, R; 1, R/3) + H_0^0(0, R; 3, R/3)]\, G_0^0(2, R)\, G_0^0(2, R/3) + C + \\
&+ H_0^0(0, R; 1, R/3)[G_0^0(4, R)\, G_0^0(2, R/3) + G_0^0(2, R)\, G_0^0(4, R/3)] + C - \\
&- 2\, H_0^0(1, R; 2, R/3)\, G_0^0(3, R)\, G_0^0(3, R/3) - 2C - \\
&- 2\, H_0^0(0, R; 1, R/3)\, G_0^0(2, R)\, G_0^0(2, R/3) - 2C + \\
&+ \frac{3}{2} H_1^1(0, R, 1, R/3)\, G_1^1(2, R)\, G_1^1(2, R/3) + D + \\
&+ [H_0^0(2, R; 0, R/3) + H_0^0(0, R; 2, R/3)]\, G_0^0(2, R)\, G_0^0(3, R/3) + C + \\
&+ H_0^0(0, R; 0, R/3)[G_0^0(4, R)\, G_0^0(3, R/3) + G_0^0(2, R)\, G_0^0(5, R/3)] + C - \\
&- 2\, H_0^0(1, R; 1, R/3)\, G_0^0(3, R)\, G_0^0(4, R/3) - 2C - \\
&- 2\, H_0^0(0, R; 0, R/3)\, G_0^0(2, R)\, G_0^0(3, R/3) - 2C + \\
&+ \frac{3}{2} H_1^1(0, R; 0, R/3)\, G_1^1(2, R)\, G_1^1(3, R/3) + D \Big\}.
\end{aligned}
$$

$$
\begin{aligned}
&I\left(2, 0, \frac{2}{3}, 0, 0, 0, 1, 0, 2\right) = \\
&= \frac{R^q}{128} \Big\{ [A_4(R)A_3(R/3) + A_2(R)A_5(R/3) - 2A_2(R)A_3(R/3)]\, B_0(R)B_0(R/3) + \\
&+ A_2(R)A_3(R/3)\, [B_2(R)B_0(R/3) + B_0(R)B_2(R/3)] - \\
&- 2\, A_3(R)A_4(R/3)B_1(R)B_1(R/3) + \\
&+ [A_4(R)A_2(R/3) + A_2(R)A_4(R/3) - 2A_2(R)A_2(R/3)]\, B_0(R)B_2(R/3) + \\
&+ A_2(R)A_2(R/3)[B_2(R)B_1(R/3) + B_0(R)B_3(R/3)] - \\
&- 2\, A_3(R)A_3(R/3)B_1(R)B_2(R/3) - \\
&- [A_4(R)A_1(R/3) + A_2(R)A_3(R/3) - 2A_2(R)A_1(R/3)]B_0(R)B_2(R/3) - \\
&- A_2(R)A_1(R/3)[B_2(R)B_2(R/3) + B_0(R)B_4(R/3)] + \\
&+ 2\, A_3(R)A_2(R/3)B_1(R)B_3(R/3) - \\
&- [A_4(R)A_0(R/3) + A_2(R)A_2(R/3) - 2A_2(R)A_0(R/3)]B_0(R)B_3(R/3) - \\
&- A_2(R)A_0(R/3)[B_2(R)B_3(R/3) + B_0(R)D_6(R/3)] + \\
&+ 2A_3(R)A_1(R/3)B_1(R)B_4(R/3) - \\
&- [A_2(R)A_3(R/3) + A_0(R)A_5(R/3) - 2A_0(R)A_3(R/3)]B_2(R)B_0(R/3) - \\
&- A_0(R)A_3(R/3)[B_4(R)B_0(R/3) + B_2(R)B_2(R/3)] +
\end{aligned}
$$

$$+ 2\,A_1(R)A_4(R/3)B_3(R)B_1(R/3) -$$
$$-[A_2(R)A_2(R/3) - A_0(R)A_4(R/3) - 2A_0(R)A_2(R/3)]B_2(R)B_1(R/3) -$$
$$- A_0(R)A_2(R/3)[B_4(R)B_1(R/3) + B_2(R)B_3(R/3)] +$$
$$+ 2\,A_1(R)A_3(R/3)B_3(R)B_2(R/3) +$$
$$+[A_2(R)A_1(R/3) + A_0(R)A_3(R/3) - 2A_0(R)A_1(R/3)]B_2)R)B_3(R/3) +$$
$$+ A_0(R)A_1(R/3)[B_4(R)B_2(R/3) + B_2(R)B_4(R/4)] -$$
$$- 2A_1(R)A_2(R/3)B_3(R)B_3(R/3) +$$
$$+[A_2(R)A_0(R/3) + A_0(R)A_2(R/3) - 2A(R)A_0(R/3)]B^4(R)B_3(R/3) +$$
$$+ A_0(R)A_0(R/3)]C_4(R)B_3(R/3) + B_2(R)B_5(R/3)] -$$
$$- 2\,A_1(R)A_1(R/3)\,B_3(R)B_4(R/3)\Big\}.$$

$$I\left(2, 0, \frac{2}{3}, \frac{2}{3}, 0, 0, 1, 1, 1\right) =$$

$$= \frac{R^9}{60}\Big\{[H_0^0(4, R; 0, R/3) + H_0^0(2, R; 6, R/3)]\,G_0^0(0, R) -$$

$$- \frac{5}{3}\,H_0^0(2, R; 4, R/3)\,G_0^0(0, R) + \frac{2}{3}\,(0/2) +$$

$$+ H_0^0(2, R; 4, R/3)\,G_0^0(2, R) - 2\,H_1^0(3, R; 5, R/3)\,G_1^0(1, R) +$$

$$+ H_1^1(2, R; 4, R/3)\,G_1^0(0, R) -$$

$$- \frac{2}{3}\,[H_0^0(4, R; 2, R/3) + H_0^0(2, R; 4, R/3)]\,G_0^0(0, R) - \frac{4}{3}\,(0/2) +$$

$$+ \frac{14}{15}\,H_0^0(2, R; 2, R/3)\,G_0^0(0, R) + \frac{32}{21}\,(0/2) - \frac{16}{35}\,(0/4) -$$

$$- \frac{2}{3}\,H_0^0(2, R; 2, R/3)\,G_0^0(2, R) - \frac{4}{3}\,(0/2) +$$

$$+ \frac{12}{5}\,H_1^0(3, R; 3, R/3)\,G_1^0(1, R) + \frac{8}{5}\,(0/3) -$$

$$- \frac{2}{5}\,H_1^1(2, R; 2, R/3)\,G_1^1(0, R) - \frac{2}{45}\,(1/3) +$$

$$+ \frac{1}{5}\,[H_0^0(4, R; 0, R/3) + H_0^0(2, R; 2, R/3)]\,G_0^0(0, R) +$$

$$+ \frac{4}{7}\,(0/2) + \frac{8}{35}\,(0/4) -$$

$$-\frac{9}{35}H_0^0(2,R;0,R/3)\,G_0^0(0,R)-\frac{2}{3}(0/2)+\frac{24}{77}(0/4)+$$

$$+\frac{1}{5}H_0^0(2,R;0,R/3)\,G_0^0(2,R)+\frac{4}{7}(0/2)+\frac{8}{35}(0/4)-$$

$$-\frac{6}{7}H_1^0(3,R;1,R/3)\,G_1^0(1,R)-\frac{8}{9}(0/3)+$$

$$+\frac{3}{35}H_1^1(2,R;0,R/3)\,G_1^1(0,R)+\frac{2}{135}(1/3)-$$

$$-[H_0^0(2,R;4,R/3)+H_0^0(0,R;6,R/3)]\,G_0^0(2,R)+$$

$$+\frac{5}{3}H_0^0(0,R;4,R/3)\,G_0^0(2,R)-\frac{2}{3}(0/2)-$$

$$-H_0^0(0,R;4,R/3)\,G_0^0(4,R)+2H_1^0(1,R;6,R/3)\,G_1^0(3,R)-$$

$$-H_1^1(0,R;4,R/3)\,G_1^1(2,R)+$$

$$+\frac{2}{3}[H_0^0(2,R;2,R/3)+H_0^0(0,R;4,R/3)]\,G_0^0(2,R)+\frac{4}{3}(0/2)-$$

$$-\frac{14}{15}H_0^0(0,R;2,R/3)\,G_0^0(2,R)-\frac{32}{21}(0/2)+\frac{16}{35}(0/4)-$$

$$-\frac{2}{3}H_0^0(0,R;2,R/3)\,G_0^0(4,R)+\frac{4}{3}(0/2)-$$

$$-\frac{12}{5}H_1^0(1,R;3,R/3)\,G_1^0(3,R)-\frac{5}{8}(0/3)+$$

$$+\frac{2}{5}H_1^1(0,R;2,R/3)\,G_1^1(2,R)+\frac{2}{45}(1/3)-$$

$$-\frac{1}{5}[H_0^0(2,R;0,R/3)+H_0^0(0,R;2,R/3)]\,G_0^0(2,R)-$$

$$-\frac{4}{7}(0/2)-\frac{8}{35}(0/4)+$$

$$+\frac{9}{35}H_0^0(0,R;0,R/3)\,G_0^0(2,R)+\frac{3}{2}(0/2)-\frac{24}{77}(0/4)-$$

$$-\frac{1}{5}H_0^0(0,R;0,R/3)\,G_0^0(4,R)-\frac{4}{7}(0/2)-\frac{8}{35}(0/4)+$$

$$+\frac{6}{7}H_1^0(1,R;1,R/3)\,G_1^0(3,R)+\frac{8}{9}(0/3)-$$

$$-\frac{3}{35}H_1^1(0,R;0,R/3)\,G_1^1(2,R)-\frac{2}{135}(1/3)\Big\}.$$

$$I\left(2,0,\frac{2}{3},\frac{2}{3},0,0,1,1,2\right)=$$

$$=\frac{R^{10}}{228}\Big\{[A_4(R)A_4(R/3)+A_2(R)A_6(R/3)-2A_2(R)A_4(R/3)]\,B_0(R)+$$

$$+A_2(R)A_4(R/3)\left[B_2(R)+\frac{1}{3}B_0(R)\right]-$$

$$-\frac{2}{3}[A_3(R)A_2(R/3)+A_2(R)A_4(R/3)-2A_2(R)A_2(R/3)]\,B_0(R)-$$

$$-A_2(R)A_2(R/3)\left[\frac{2}{3}B_2(R)+\frac{2}{5}B_0(R)\right]+$$

$$+\frac{1}{5}[A_4(R)A_0(R/3)+A_2(R)A_2(R/3)-2A_2(R)A_0(R/3)]\,B_0(R)+$$

$$+A_2(R)A_0(R/3)\left[\frac{1}{5}B_2(R)+\frac{1}{7}B_0(R)\right]-$$

$$-[A_2(R)A_4(R/3)+A_0(R)A_6(R/3)-2A_0(R)A_4(R/3)]\,B_2(R)-$$

$$-A_0(R)A_4(R/3)\left[B_4(R)+\frac{1}{3}B_2(R)\right]+$$

$$+\frac{2}{3}[A_2(R)A_2(R/3)+A_0(R)A_4(R/3)-2A_0(R)A_2(R/3)]\,B_2(R)+$$

$$+A_0(R)A_2(R/3)\left[\frac{2}{3}B_4(R)+\frac{2}{5}B_2(R)\right]-$$

$$-\frac{1}{5}[A_2(R)A_0(R/3)+A_0(R)A_2(R/3)-2A_0(R)A_0(R/3)]\,B_2(R)-$$

$$-A_0(R)A_0(R/3)\left[\frac{1}{5}B_4(R)+\frac{1}{7}B_2(R)\right]\Big\}.$$

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О СОБСТВЕННЫХ ФУНКЦИЯХ, С ПОПРАВКОЙ НА КОРРЕЛЯЦИОННЫЕ ФАКТОРЫ

Ф. БЕРЕНЦ

Резюме

Определяются электронные энергии состояния $1s\,3s\,{}^1\Sigma_g^+$ молекулы водорода по методу LCAO—MO. Сопоставляя результаты расчета полученные по методу LCAO—CMO для основного состояния Фростом и Брауштейном, с результатами автора для состояний $1sns\,{}^1\Sigma_g^+$ ($n = 2,3$) определяются коррекции к энергии электронов и показывается, что корреляционный фактор при вычислениях энергий основного и возбужденного состояний играет довольно важную роль.

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COMMUNICATIONES BREVES

A NOTE ON THE ANOMALOUS SKIN EFFECT

By

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LANDAU [1], KURILKO and POPOV [2], GORMAN [3] and MASON [4] studied the penetration of an external longitudinal electric field into a semi-bounded plasma considering a fraction 'p' of all incident electrons reflecting specularly and the remaining portion diffusely. The authors [5] have calculated the penetration of transverse electromagnetic waves into a semibounded plasma and studied the specular reflection of electrons. Here we are using the results so obtained to discuss the phenomenon of anomalous skin effect.

In the case of specular reflection the field is expressed as

$$\tilde{E} = E_+(k)+E_-(k) = \frac{2iCB(O)U}{kD(k)}, \tag{1}$$

where

$$U = \frac{\omega}{k},$$

$$D(k) = U^2-C^2+\varepsilon(k),$$

$$\varepsilon(k) = \frac{i}{k} U\omega_P^2 \int_{-\infty}^{\infty} \frac{E(v_z)}{(-i\omega+ikv_z)} dv_z,$$

$$\omega_P^2 = \frac{4\pi e^2 n_0}{m},$$

On applying inverse Fourier transform for $z > 0$, we obtain

$$E(z>0) = \frac{iCB(0)}{\pi} \int_{-\infty}^{\infty} U \frac{e^{ikz}}{kD(k)} dk. \tag{2}$$

Eq. (2) can be written in more explicit form as

$$E(z>0) = \frac{i\omega cB(0)}{\pi} \int_{-\infty}^{\infty} \left[\omega^2-c^2k^2-\omega\omega_P^2 \int_{-\infty}^{\infty} \frac{F(v_z)}{(\omega_r-kv_z+i\sigma)} dv_z\right]^{-1} e^{ikz} dk, \tag{3}$$

where σ is the vanishingly small imaginary part of ω.

In the case of metals, the surface impedance Z is expressed as

$$Z = \frac{4\pi}{C} \frac{E(0)}{B(0)}, \tag{4}$$

in which the electric and magnetic fields are evaluated at the surface. The reflection from the surface of a metal may be expressed in terms of its surface impedance by

$$R = \frac{Z - \frac{4\pi}{C}}{Z + \frac{4\pi}{C}}. \tag{5}$$

The term $4\pi/C$ represents the impedance of free space.

The results of REUTER and SONDHEIMER [6] indicate that the electric field for intermediate frequencies does not die off exponentially in the metal but takes some complicated form. For this reason the usual definitions of the optical constants are not applicable and the surface impedance of the metal is calculated instead.

As the fields are continuous at $z = 0$, we get the following expression for surface impedance Z from Eq. (3) as

$$Z = 4i\omega \int_{-\infty}^{\infty} \left[\omega^2 - c^2 k^2 - \omega\omega_p^2 \int_{-\infty}^{\infty} \frac{F(v_z)}{(\omega_r - kv_z + i\sigma)} dv_z \right]^{-1} dk, \tag{6}$$

Our results are found to be in accordance with REUTER and SONDHEIMER's [6] results for the theory of anomalous skin effect in metals for the case of specular reflection.

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A REPLY TO JÁNOSSY'S TREATMENT OF THE AHARANOV-BOHM EFFECT AND THE MANY-BODY PROBLEM

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The questions raised by the AHARANOV—BOHM effect and the difficulties associated with the many-body problem are as will be shown intimately linked with the concepts present in quantum theory and physics in general. Any attempt to answer these questions or resolve the difficulties will, therefore, have to be directed towards the concepts underlying the problem. A satisfactory treatment of these questions must not appeal to those very concepts which are the cause of the trouble, otherwise nothing radically new can emerge. A purely mathematical treatment of a problem cannot radically alter its contents; the most it can achieve is a formalistic reformulation of the difficulty. This amounts to nothing more than a change of language, which may make the problem appear less urgent.

Seen in the above context, the hydrodynamical model, with its strong attachment to quantum theory, does not resolve radically either the AHARANOV—BOHM effect or the many-body problem. It merely reformulates them in terms of a different mathematical language.

The details of the AHARANOV—BOHM effect will be discussed first, and the discussion will be followed by an examination of the many-body problem.

(i) The Aharanov—Bohm effect [1,2]

AHARANOV and BOHM (from now on denoted AB) concluded from the experiment they suggested that the vector potential A has a more fundamental part in quantum mechanics than the auxiliary one it had in classical physics. The effect (which was predicted, and later observed) stated that the phase of the wave function describing electrons in a multiply-connected region, where curl $\mathbf{A} = 0$ but $\mathbf{A}$ is finite, changes by an amount equal to $\oint \mathbf{A} \cdot d\mathbf{l}$. This change results in changes of interference of electrons that have passed through regions at different $\mathbf{A}$. Now, physics, whether classical or quantum, is still based on concepts such as causality and locality of force. The electronic wave function, therefore, has to be linked causally to the current in the coil and influenced locally. The vector potential is the only physical quantity which does that.

It can be associated causally with the current in the coil through the relations $\mathbf{A} = \int \frac{i}{\mathbf{r}-\mathbf{r}'} d^3\mathbf{r}'$ and has a local finite value wherever the function is not zero. On the other hand, the magnetic field is zero where the wave function is non-zero and therefore the Lorentz force is zero.

It follows from the above that an explanation of the AB effect which does not grant the vector potential a more significant part than that of an auxiliary concept will have to be based on a theory which is radically different from all present theories. If a new theory depends in any way on one of the present ones (classical, quantum, relativistic, etc.) then causality and local theories become automatically relevant and in consequence the vector potential also. The hydrodynamical model depends heavily on quantum theory and it will be demonstrated that this dependence gives relevance to the vector potential.

The whole validity of the hydrodynamical model [4] rests on its ability to be translated back into wave mechanics at any time t. In mathematical terms, this means that if the wave function is written as $\psi = Re^{iS}$, then the following relations must be satisfied at all times:

$$\varrho = \psi^* \psi,$$
$$\mathbf{v} = \frac{\hbar}{m} \operatorname{grad} S - \frac{e}{mc} \mathbf{A}, \tag{1}$$

where ϱ is the hydrodynamical density distribution and $\mathbf{v}$ the velocity distribution. It is seen that $\mathbf{A}$ appears already in the Eqs. (1) which are the basis of the validity of the model. It would have been paradoxical if the hydrodynamical model could establish the unimportance of the vector potential and at the same time rely on $\mathbf{A}$ for its validity.

It has further been argued that $\mathbf{A}$ is of secondary importance [5] because, unlike the Schrödinger equation, the hydrodynamical equations of motion do not contain the vector potential explicitly, only the Lorentz force appears:

$$\operatorname{div} \varrho \mathbf{v} + \frac{\partial \varrho}{\partial t} = 0,$$
$$m \frac{d\mathbf{v}}{dt} = -\operatorname{grad}(Q+V) + \frac{e}{c}[\mathbf{E} - (\mathbf{v}\times\mathbf{B})], \quad [\mathbf{v}\times\mathbf{B}], \tag{2}$$
$$Q = \frac{-\hbar}{m} \frac{\nabla^2 \varrho^{1/2}}{\varrho^{1/2}}.$$

As pointed out above, these equations have to be equivalent to the Schrödinger wave equations for all time t. That is to say that substitution of the relation-

ships (1) in the Eqs. (2) must produce the Schrödinger equation for all t. It is found that the translation back into wave mechanics is possible only if the following boundary conditions are satisfied:

$$\int \varrho d\tau = 1$$

$$\oint \mathbf{v} \cdot d\mathbf{S} = 2\pi\hbar \frac{k}{m} - \frac{e}{mc} \int \mathbf{B} \cdot d\mathbf{S} = 2\pi\hbar \frac{k}{m} - \frac{e}{mc} \oint \mathbf{A} \cdot d\mathbf{l} \tag{3}$$

$$K = 0, \pm 1, \pm 2, \ldots$$

Any hydrodynamical problem has to satisfy Eqs. (2) which are independent of $\mathbf{A}$ and also the boundary conditions (3). Now the boundary conditions can be expressed either in terms of $\int \mathbf{B} \cdot d\mathbf{S}$ or $\oint \mathbf{A} \cdot d\mathbf{l}$. Because, however, $\mathbf{B} = 0$ everywhere along the path of the electrons, the physical meaning of the first integral is unclear. On the other hand, $\mathbf{A}$ is non-zero along the path and therefore $\oint \mathbf{A} \cdot d\mathbf{l}$ can meaningfully be evaluated in the same region as the wave function. So even though the hydrodynamic equations contain the Lorentz force instead of the vector potential, this force is zero in the AB experiment. It is the vector potential which will appear, through the *B.C.*'s, in the expression for ϱ. As pointed out above, this is the consequence of the requirement for correspondence with wave mechanics.

To conclude the discussion on the AB effect, the above observations are summarised as follows: $\mathbf{A}$ retains its physical importance even though it has been explicitly eliminated from the hydrodynamic equations of motion. The importance of the vector potential is established through its necessity for the validity of the model and also because of its appearance in the density distribution through the boundary conditions which are essential for the correspondence with wave mechanics. By eliminating $\mathbf{A}$ from the equations of motion, the model has merely obscured its significance.

(ii) The many-body problem

Some of the serious difficulties that wave mechanics encounters with the many-body problem arise because the theory still tacitly accepts the concept of a particle. Therefore, when presented with an ensemble of interacting particles, quantum theory has to resort to the solution of Schrödinger's equation for a $3N$ dimensional wave in configuration space. Such an approach is physically unsatisfactory, because it gives no concept of the structure of a system or its movement in a real three-dimensional space. Quantum theory, however, dismisses the idea of particles localised in a three-dimensional space, and adopts as basic the abstract configuration space formed out of all coordinates of the particles in physical space [6].

It seems reasonable to assume that any theory which aims at a more satisfactory solution than the quantum mechanical one will have to make use of concepts which are not linked to the current ideas of different particles interacting with each other, described only by a wave in $3N$ dimensional configuration space.

As with the case of the AB effect, the hydrodynamic model in the many-body problem is not free of the quantum ideas of individual particles. The requirement of its correspondence with wave mechanics has the same form as Eqs. (1) except that these relationships now have to occur in a $3N$ dimensional configuration space.

$$\begin{aligned} \varrho(\mathbf{r}, \ldots \mathbf{r}_N) &= R^2 , \\ \mathbf{v}_\nu(\mathbf{r}, \ldots \mathbf{r}_N) &= \frac{\hbar}{m_\nu} \operatorname{grad}_\nu S , \\ \psi_\nu(r, \ldots r_N) &= Re^{iS}, \qquad \nu = 1, 2, \ldots N. \end{aligned} \tag{4}$$

$\mathbf{r}_\nu = x_\nu, y_\nu, \xi_\nu$ is the position vector of the νth particle in configuration space. Eqs. (4) provide a hydrodynamical density distribution $\varrho(\mathbf{r}, \ldots \mathbf{r}_N)$ and a velocity distribution $\mathbf{v}_\nu(\mathbf{r}, \ldots \mathbf{r}_N)$ both in $3N$ dimensional space. These distributions obey hydrodynamical equations similar to (2) with one important difference. Whereas Eqs. (2) describe a fluid in 3 dimensional Euclidean space, the equations for the many-body problem describe a fluid in $3N$ dimensional configuration. This poses a conceptual problem because hydrodynamics was invented to describe real 3 dimensional fluids and not abstract multidimensional ones. Consequently, such an abstract fluid is not very useful as it is of no physical significance and, therefore, it is unclear how physical insight can be obtained from it. Quantum theoretical requirements therefore force the abstract configuration space into the context of hydrodynamics, making the latter physically quite meaningless.

In the hydrodynamic treatment of the many-body problem, the above conceptual difficulties can be removed by reducing the dimensionality of the hydrodynamic distributions from $3N$ to N three dimensional ones by forming averages of the following kind:

$$\begin{aligned} \varrho_\nu(\mathbf{r}) &= \int_{N-1} \cdots \int \varrho\,(\mathbf{r}, \ldots \mathbf{r}_{\nu-1}\, \mathbf{r}\mathbf{r}_{\nu+1} \ldots \mathbf{r}_N) \times \\ &\qquad \times d^3\mathbf{r}, \ldots d^3\mathbf{r}_{\nu-1}\, d^3\mathbf{r}_{\nu+1} \ldots d^3\mathbf{r}_N , \\ \varrho_\nu(\mathbf{r})\, \mathbf{v}_\nu(\mathbf{r}) &= \int_{N-1} \cdots \int \varrho\mathbf{v}(\mathbf{r}, \ldots \mathbf{r}_{\nu-1}\, \mathbf{r}\mathbf{r}_{\nu+1} \ldots \mathbf{r}_N) \times \\ &\qquad \times d^3\mathbf{r}, \ldots d^3\mathbf{r}_{\nu-1}\, d^3\mathbf{r}_{\nu+1} \ldots d^3\mathbf{r}_N . \end{aligned} \tag{5}$$

Thus by integrating the $3N$ dimensional distributions ϱ and $\varrho\mathbf{v}$ over the co-ordinates of each particle except the νth, say, three dimensional distribu-

tions for the νth particle are obtained. These correspond to as many averages of the type (5) as there are particles. The variables (5) are then shown to obey hydrodynamical equations of the same type as Eqs. (2). A conceptual problem however, still remains, because although relations (5) are three dimensional hydrodynamic distributions, the integrand on the right-hand side has no meaning in terms of three dimensional fluids. Moreover, averaging over coordinates of localised individual particles in physical space makes the meaning of $\varrho_\nu(\mathbf{r})$ and $\varrho_\nu(\mathbf{r})\,\mathbf{v}_\nu(\mathbf{r})$ even more obscure. The fact that quantities such as $e_\nu \mathbf{v}_\nu \varrho_\nu / c$ can be denoted by $\mathbf{i}_\nu$ and called current (just as $e_\nu \varrho_\nu$ is denoted by $\varrho_{el.\nu}$) and called charge density does not give a physical meaning to ϱ_ν and $\varrho_\nu v_\nu$. Rather it is just a question of linguistic convenience, in which abstract quantities are given names similar to those used in the hydrodynamics of real fluids.

If, for the sake of argument, one ignores the conceptual difficulties and pursues the formalism, it is seen that the equations for $\varrho_\nu(\mathbf{r})$ and $\varrho_\nu(\mathbf{r})\mathbf{v}_\nu(\mathbf{r})$ have to obey boundary conditions

$$\begin{aligned} \varrho_\nu(\mathbf{r}, 0) &= \varrho_\nu^0(\mathbf{r})\,, \\ \varrho_\nu(\mathbf{r}, 0)\,\mathbf{v}_\nu(\mathbf{r}, 0) &= \varrho_\nu^0(\mathbf{r})\,\mathbf{v}_\nu^0(\mathbf{r})\,. \end{aligned} \tag{6}$$

These conditions turn out to be inadequate for the unambiguous determination of $\varrho(\mathbf{r}, \ldots \mathbf{r}_\nu)$ and $\varrho\,\mathbf{v}(\mathbf{r}, \ldots \mathbf{r}_N)$ which in turn determine the $3N$ dimensional wave function $\psi(\mathbf{r}, \ldots \mathbf{r}_\nu)$. The need thus arises for a criterion that will decide which choice of distribution $\varrho_\nu(\mathbf{r})$ and $\varrho_\nu(\mathbf{r})\mathbf{v}_\nu(\mathbf{r})$ will produce an appropriate wave function. The many-body problem is therefore reformulated in a hydrodynamical context so as to find a way of picking out of a whole set of three dimensional solutions of hydrodynamic equations obeying boundary conditions (6), those distributions which can produce a "probable" wave function. Some rather rough quantum theoretic rules are necessary to define a probable wave function, as for example a function which is smooth, continuous and possesses a minimum property. It is then possible to choose N distributions $\varrho_\nu(\mathbf{r})$ and $\varrho_\nu(\mathbf{r})\mathbf{v}_\nu(\mathbf{r})$ from which $3N$ dimensional distributions $\varrho(\mathbf{r}), \ldots \mathbf{r}_N$ and $\varrho\mathbf{v}(\mathbf{r}, \ldots \mathbf{r}_N)$ can be constructed to finally give the "probable" wave function in configuration space $\psi(\mathbf{r}, \ldots \mathbf{r}_N)$.

Apart from the conceptual difficulties outlined above in connection with the meaning of configuration space and hydrodynamical multidimensional distributions, there exist serious doubts as to the effectiveness of the model in explaining the AB effect and the many-body problem. These doubts arise because of the inability of the model to provide its own explanation of some of the concepts that it makes use of. One case of such a failure was found in the last section where the decision of what constitutes a probable wave function s left to wave mechanics. The model does not prescribe its own rules for select-

ing the desirable solutions of its equations. Another case is the use of the potential term

$$Q = \frac{-\hbar}{m} \frac{\nabla^2 \varrho^{1/2}}{\varrho^{1/2}}$$

in Eqs. (2). In the AB effect where the quantum potential Q is associated with 3 dimensional distributions, it may be possible to give hydrodynamic explanations to the meaning of Q as originating from internal stresses in the fluid. Such suggestions have already been made in the past [7]. When, however, Q is associated with multi-dimensional distributions, then it is not clear how hydrodynamic explanations of its meaning could be provided. The final remark is in connection with the appearance of configuration space in the hydrodynamical model. Here again, the model does not explain why it is necessary to produce $3N$ dimensional distributions except in so far as is required by wave mechanics, but then this is not a hydrodynamical condition.

Because of the above mentioned failures of the hydrodynamical model to explain within its own framework some important ideas it makes use of, it can be concluded that the model is not a theory radical enough to cope in a satisfactory way with either the AB effect or the many-body problem. It reduces merely to a change of language which does not require explanation and which is constructed in a way that makes the central issues of the AB ffect and many-body problem seem less prominent.

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RECENSIONES

A. EARNSHAW: **Introduction to Magnetochemistry**

Academic Press, London and New York 1968

This book is a concise summary of magnetochemistry for research chemists who want an introduction into this field. The treatment is as simple as possible. The author uses many pictorial explanations to make his subject clear to the more practically minded readers, too.

In five chapters the author gives the theoretical basis of magnetism. After a short introduction dealing with the magnetic properties of materials in the second chapter the magnetic moment of free atoms and ions is treated using the classical atom model without any rigorous mathematical treatment, but always noticing the result of the quantum-mechanical treatment.

As transition metal complexes form one of the most interesting fields in chemistry, the third chapter deals with the magnetic moment of such complexes and with the connection between the structure of a transition metal compound and its magnetic moment.

The fourth chapter shows how to take account of spin-orbit coupling, the splitting of the spectroscopic terms into separate energy levels is worked out and the bulk susceptibility is calculated by considering the thermal distribution of ions within the various levels.

In the fifth chapter further such interesting topics are dealt with as the case of second and third row transition metal complexes or the co-operative or exchange phenomena, the result of which is ferromagnetism and antiferromagnetism.

The last chapter gives an account of the most important experimental methods and shows briefly how the problems of interpretation may be tackled.

References are given to some other works in this field, which provide access to the original literature. Some short notes between these references make one's way easier.

D. KISDI

C. M. H. SMITH: **A Textbook of Nuclear Physics**

Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfurt, 1965.

This book provides a general coverage of nuclear physics. The author has tried to make his book as self-contained as possible. For this reason, the first quarter of the book deals with those parts of atomic physics, relativity and quantum mechanics, which are necessary. It is, of course, impossible to give a comprehensive account of these branches of physics in single chapters so the reader has to have learnt these subjects already or to have read more detailed works about it.

The second part of the book, the bigger half, deals with low energy nuclear processes and nuclear structure. This part includes a chapter on the general properties of atomic nuclei, determinations of nuclear size, radioactive decay, detection of nuclear radiation, electronic techniques, alpha and gamma radiation, beta decay, the neutron, nuclear magnetism, nuclear fission, particle accelerators, nuclear forces and nuclear reactions and nuclear models.

The third part of the book is a chapter on high energy nuclear physics and elementary particles. The last chapter gives an account of thermonuclear reactions in stars and one of the theories of the origin of the elements.

Although nuclear physics is a very rapidly developing science, the advantage of this book is that it also contains many of the latest results. It is written for honours physics students but lecturers can also use it with good results as a handbook.

D. KISDI

Nuclear and Particle Physics

Editors: B. Margolis, C. S. Lam, W. V. Benjamin, Inc. Amsterdam, New York 1968

The book contains the lectures of the 1967 Summer Institute in Nuclear and Particle Physics, held at McGill University in August 1967. The lectures deal with current research topics in nuclear physics and elementary particle physics.

The first lecture given by K. GOTTFRIED treats of collision and decay phenomena. He gives some old scattering problems as scattering of an electron by an atom and shows how these problems can be related by a unifying treatment. Then he deals with resonance scattering of a particle by a bound system to study radiative decay.

S. KAHANA in his lecture about effective interactions in finite nuclei starts with the discussion of a typical shell model calculation. Then, he sets up a second quantized formalism for the many-body problem similar to that suggested by SCHWINGER and MARTIN to define within which approximations he is working. The formalism is used to perform a Brueckner-like calculation for a doubly magic core plus two valence nucleons.

G. KÄLLÉN gave a lecture about radiative corrections for weak interactions in which he discussed some old problems as well as new developments.

The next lecture, given by D. KURATH, deals with nuclear deformation in the shell model. He treats light nuclei with deformed single-particle orbitals in order to see how observable features depend on nuclear deformation.

W. A. BARDEEN and B. W. LEE dealing with chiral algebra and dynamics wanted to give a critical examination of this new method for treating particle phenomena. They made it clear through examples that the current algebra can only make definite predictions for off-shell amplitudes. Then they discuss the chiral dynamics method which gives the results of the current algebra rather easily.

B. MARGOLIS in his lectures on selected topics in nuclear reactions deals with resonance reactions, resonance scattering and nuclear structure, Feshbach's approach to resonance reactions, nuclear scattering and the Pauli principle, use of the eikonal approximation in nuclear reactions and nucleon—nucleus scattering in the eikonal approximation.

MANNQUE RHO gave lectures about muon-capture in nuclei and Migdal theory. He showed how to utilize information from elementary particle physics in the study of nuclear structure.

C. WILKIN spoke about high energy scattering from nuclei and about the investigation of nuclear structure with high energy protons.

J. SCHWINGER gave a new theory of particles, the theory of sources. This is a theory intermediate between field theory and S-matrix theory, which treats the localizability and energy momentum properties of a particle in an entirely symmetrical way.

D. KISDI

Readings from Scientific American: Lasers and Light

W. H. Freeman and Co., 1969

This is a collection of thirty two articles on lasers and related subjects originally published in the Scientific American. Eleven articles are reprinted from the issue for September, 1968, while the remaining items on various aspects of lasers and modern optics have also been previously published in the Scientific American. The material is arranged in seven sections: Light, Forming and Detecting Images, Chemical and Biological Effects of Light, Light and Vision, Beyond the Visible: X-Ray to Radio Waves, Lasers, Properties and Applications of Laser Light. Each article is reprinted with complete text and is fully illustrated. Many of the papers were written by outstanding experts in these fields, who played important roles in the development of the laser. The sections are introduced by A. L. SCHAWLOW. The material presented is quite up-to-date and covers a very broad field of modern optics and its applications. The book is well recommended as a supplementary reading for undergraduate physics courses.

J. ANTAL

D. TER HAAR: **Quantentheorie**

Einführung und Originaltexte (Wissenschaftliche Taschenbücher, Band 56; Vieweg und Sohn, Braunschweig, 1969; Übersetzung des Bandes "The Old Quantum Theory" aus der Reihe "Selected Readings in Physics", Pergamon Press, Oxford, 1967)

Der vorliegende Band behandelt die ältere Quantentheorie von PLANCK und EINSTEIN bis BOHR. Im Teil I des Buches erklärt der Autor die Strahlungsformel für den schwarzen Körper und führt die Idee der Lichtquanten ein, bespricht das RUTHERFORDsche und BOHRsche Atommodell und legt die Strahlungstheorie auf der Grundlage der älteren Quantentheorie dar. Im Teil II werden die wichtigsten Originaltexte von MAX PLANCK, A. EINSTEIN, E. RUTHERFORD, N. BOHR, J. FRANCK und G. HERTZ, sowie die etwas späteren Arbeiten von A. EINSTEIN und W. PAULI über die Quantentheorie der Strahlung bzw. über den Zusammenhang des Abschlusses der Elektronengruppen im Atom mit der Komplexstruktur der Spektren wiedergeben.

J. I. HORVÁTH

J. C. GIBBINGS: **Thermomechanics**

An introduction to the governing equations of thermodynamics and of the mechanics of fluids (Thermodynamics and Fluid Mechanics Division of the Commonwealth and Internationa Library; Pergamon Press, Oxford, 1970) XIX + 302 pages

Thermodynamics and the mechanics of fluids are usually taught in isolation from each other. So marked is this isolation that even excellent text-books ignore the whole extent of the mechanics of fluids in claiming the study of non-equilibrium thermodynamics as a recent development of just a few years' standing. The author tries to introduce thermodynamics (more precisely thermostatics) and the mechanics of fluids (including elasticity and plasticity of solids) coherently. First the Newtonian mechanics of rigid bodies and the elements of continuum mechanics are summarized, then the concept of temperature is introduced via the zero'th law of thermodynamics. The simultaneous treatment mentioned above starts with the characterization of solids, liquids and gases in terms of continuum mechanics and with the definition of states and properties of changes in terms of thermodynamics. Then, the first law of thermodynamics, the manner of heat processes and the applications of the first law to solids are discussed. In the following paragraphs the state of motionless fluids, the mixtures of phases, the characteristics of fluid motion, the conservation of mass in a fluid flow, the equations relating process phenomena, the momentum equations for fluid in motion, the applications of the first law of thermodynamics to fluid in motion and the properties of adiabatic flow are treated.

This book meets the immediate requirements of the mechanical engineering student in an undergraduate course, and of other engineering students taking courses in thermodynamics and fluid mechanics.

J. I. HORVÁTH

Printed in Hungary

A kiadásért felel az Akadémiai Kiadó igazgatója — Műszaki szerkesztő: Várhelyi Tamás

A kézirat nyomdába érkezett: 1971. IV. 21. — Terjedelem: 11 (A/5) ív, 14 ábra

71.71638 Akadémiai Nyomda, Budapest — Felelős vezető: Bernát György

L. Jánossy

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Budapest, August 25th—September 4th, 1969
(Supplement to Acta Physica Academiae Scientiarum Hungaricae)

edited by A. Somogyi

The International Conference on Cosmic Rays is held biennially. At the 11th Conference in Budapest, 485 so far unpublished scientific papers were presented. As the studies published in four volumes show, research into cosmic rays, especially problems closely connected with space research, has developed at a great pace since the last conference in 1967 (Calgary, Canada).

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S. DEME

SEMICONDUCTOR DETECTORS FOR NUCLEAR RADIATION MEASUREMENT

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edited by I. DÉZSI

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Acta Physica Academiae Scientiarum Hungaricae, Tomus 30 (3), pp. 231—240 (1971)

PHONON FREQUENCY DISTRIBUTION FUNCTIONS OF COPPER, NICKEL AND VANADIUM

By

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(Received 28. IX. 1970)

The frequency distribution functions of phonons in copper, nickel and vanadium have been determined by root sampling technique using BHATIA and HORTON's model of electron-ion interaction. The results are compared with curves obtained from inelastic neutron scattering experiments and other theoretical calculations. The calculated distribution for copper agrees in its broad features with the experimental spectrum of SVENSON et al. obtained by neutron scattering method. In the case of nickel, a reasonably satisfactory agreement is obtained with the frequency distribution measured by MOZER et al. in incoherent neutron scattering experiments. For vanadium, the present as well as other theoretical calculations show considerable discrepancies with experiment. The lattice specific heats and the equivalent Debye temperatures obtained from the calculated frequency distributions agree reasonably well with the experimental data for copper and nickel, but not in the case of vanadium.

I. Introduction

The frequency distribution function $G(\omega)$ of the normal modes of vibration of crystals is a quantity of considerable importance in the study of their many thermal and transport properties. During the last few years there has been considerable interest in the experimental study of lattice vibrations in metals through the measurement of frequency — wave vector dispersion relations with the help of inelastic neutron scattering technique [1]. Analyses of these dispersion relations by means of the Born—von Kármán model have provided information about interatomic force constants which in turn has been used to obtain the frequency distribution functions. For certain metals like nickel and vanadium, which scatter neutrons primarily incoherently, $G(\omega)$ has been directly measured by incoherent inelastic neutron scattering experiments. It would be interesting to consider the theoretical side of the problem in the light of a suitable lattice dynamical model.

It is now well established that conduction electrons in metals considerably modify their vibration frequencies and these are responsible for the failure of the Cauchy relation. BHATIA [2] and BHATIA and HORTON [3] have propounded an elastic force model for studying the phonon frequencies of cubic metals by considering the ion—electron interaction through the screening of the long-range Coulomb forces between the ions. The ion—ion interaction is described by the first two terms in a Taylor expansion of the potential energy. The model has provided a plausible description of vibration spectra

and heat capacities of alkali metals [2, 4] (Li, Na, K) and noble metals [3, 5] (Ag, Au). It has also been used to explain the temperature variation of thermal expansion [6], electrical and thermal resistivities [7], and the x-ray Debye—Waller factor [8] of a number of cubic metals. Recently SANGAL and SHARMA [9] have studied the lattice vibrations in transition metals of body-centred cubic structure on the basis of this model by considering the second-neighbour interionic interactions.

In the present paper we report a computation of the phonon frequency distribution functions of copper, nickel and vanadium on the basis of the BHATIA and HORTON [2, 3] model and compare the results with measured distributions and with those obtained by other models. Earlier work [10—12] on the frequency distribution of vanadium using force models does not show satisfactory agreement with experiment. It was thought worth while to examine this metal in the light of BHATIA's model. From the computed distributions, the lattice specific heats of these metals are evaluated and compared with available calorimetric data.

II. Secular determinant

The secular equation for the determination of angular frequencies ω of the normal modes of vibration in a cubic metal can be written as

$$|D(q) - M\omega^2 I| = 0, \tag{1}$$

where M is the mass of the atom and I is the unit matrix of order three. In BHATIA and HORTON's model [2, 3], the elements of the dynamical matrix $D(\mathbf{q})$ are given by

$$\begin{aligned} D_{ii}(\mathbf{q}) &= 4\alpha_1(3 - C_1 C_2 - C_2 C_3 - C_3 C_1) + \\ &\quad + 4\alpha_2(2 - C_i C_j - C_i C_k) + \\ &\quad + 2K_e f^{-1} a^3 q_i^2, \\ D_{ij}(\mathbf{q}) &= 4\alpha_2 S_i S_j + 2K_e f^{-1} a^3 q_i q_j, \\ &\qquad (fcc) \end{aligned} \tag{2a}$$

and

$$\begin{aligned} D_{ii}(\mathbf{q}) &= 8(\alpha_1 + \alpha_2)(1 - C_1 C_2 C_3) + \\ &\quad + 4K_e f^{-1} a^3 q_i^2, \\ D_{ij}(\mathbf{q}) &= 8\alpha_2 S_i S_j C_K + 4K_e f^{-1} a^3 q_i q_j, \\ &\qquad (bcc) \end{aligned} \tag{2b}$$

where

$$f = 1 + \frac{K_e q^2}{4\pi e^2 n^2}. \tag{3}$$

Here q_i is the i^{th} Cartesian component of the phonon wave vector $\mathbf{q}$; n is the number of electrons per unit volume; a is the semi-lattice parameter; α_1 and α_2 are the force constants for the first-neighbour ion—ion interaction; and the parameter K_e arises from electron—ion interaction. A comparison of the long-

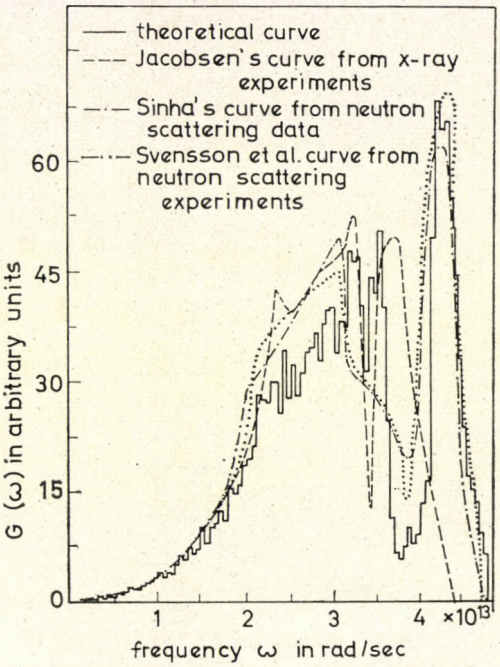

Fig. 1. The phonon frequency distribution function of copper

wave limit of Eqs. (2) with the elastic matrix for a cubic crystal yields the following relations between elastic constants and force constants:

$$\begin{aligned} \alpha_1 &= (a/2)(C_{11} - C_{12} - C_{44}), \\ \alpha_2 &= -a(C_{11} - C_{12} - 2C_{44}), \\ K_e &= (2C_{11} - C_{12} - 3C_{44}), \quad (fcc) \end{aligned} \tag{4a}$$

and

$$\begin{aligned} \alpha_1 &= (a/2)(C_{11} - C_{12}), \\ \alpha_2 &= -(a/2)(C_{11} - C_{12} - 2C_{44}), \\ K_e &= C_{11} - C_{44}. \qquad (bcc) \end{aligned} \tag{4b}$$

III. Numerical computation

The computation of the phonon frequency distribution functions for copper, nickel, and vanadium has been made by root sampling technique for a discrete subdivision of wave vector space [13]. In order to get a fairly reasonable survey of frequencies, the reciprocal space was divided into miniature cells with axes one-fortieth of the length of the reciprocal lattice cell. Using

Table I

Values of constants used in the calculation

Metal	Elastic constants (10^{11} dynes/cm^2)			Lattice parameter (Å)	Density (gm/cm^3)
	C_{11}	C_{12}	C_{44}		
Copper	17.620	12.494	8.177	3.603	9.018
Nickel	24.60	15.00	12.38	3.524	8.91
Vanadium	22.795	11.870	4.255	3.028	6.022

symmetry considerations, vibration frequencies were determined from the roots of secular Eq. (1) at nonequivalent points (1686 points for copper and nickel, and 1661 points for vanadium) lying within the 1/48th irreducible part of the first Brillouin zone. Each frequency was weighted according to the symmetrically equivalent points, which gave 192,000 frequencies in the whole Brillouin zone. The number of frequencies falling into intervals $\Delta\omega = 0.05 \times 10^{13}$ rad/sec were counted and from these the histogram giving the frequency distribution was constructed. The calculated frequency distributions are displayed in Figs. 1—3 along with experimental curves and other theoretical calculations. The curves are drawn with arbitrary units for $G(\omega)$, but are normalized to the same area. The numerical values of the elastic constants and other parameters used in the calculations are given in Table I. The elastic constants of copper refer to 0°K and are values extrapolated from the measurements of OVERTON and GAFFNEY [14] at 4.2 °K. For nickel and vanadium the elastic constants refer to room temperature and are taken from the measurements of DE KLERK [15] and ALERS [16], respectively.

Using the computed frequency distributions, the constant volume specific heat C_v per gram atom was calculated in the usual manner by numerical integration. In Fig. 4 the calculated C_v are compared with experimental values. A more sensitive comparison with calorimetric data is made in terms of the Debye temperature Θ. The Θ versus T curves for copper and nickel are displayed in Figs. 5 and 6 along with empirical data.

IV. Discussion

A. Frequency distribution

For convenience we discuss separately the results for the three metals.

(1) Copper. The frequency distribution of the normal modes of vibration in copper has been experimentally obtained both through diffuse scatter-

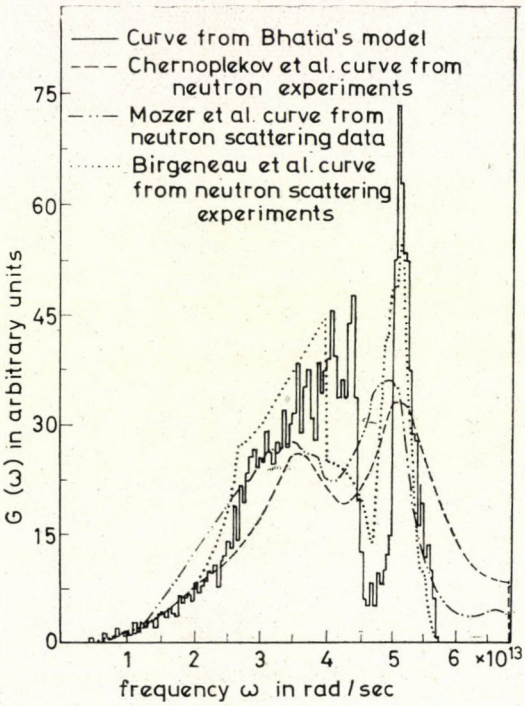

Fig. 2. The phonon frequency distribution function of nickel

ing of x-rays and slow neutron spectroscopy. JACOBSEN [17] has determined the frequency distribution of copper by fitting the third-neighbour Born — von Kármán force constant model to the frequency versus wave vector dispersion relation obtained from his diffuse x-ray scattering measurements at room temperature. Too much reliance cannot be bestowed on his result, however, because of the inherent uncertainty in diffuse x-ray experiments. SINHA [18] and SVENSSON et al. [19] have carried out reliable calculations of the frequency distribution of copper using sixth-neighbour general force constant models determined from the analysis of phonon dispersion relations measured at room temperature by neutron spectrometry. These distributions are shown in Fig. 1. The neutron scattering results agree broadly in the location and intensity of major peaks, but differ appreciably from those obtained by JACOBSEN on the high frequency side. A perusal of Fig. 1 shows that our calculated spectrum

is in satisfactory agreement with that of SVENSSON et al. The major peaks and the high frequency end appear at the same position in both the spectra.

(2) Nickel. Information about the frequency distribution of lattice vibrations in nickel has been obtained directly by CHERNOPLEKOV et al. [20] and MOZER et al. [21] using incoherent inelastic neutron scattering techniques. These data are plotted in Fig. 2 together with the distribution calculated by BIRGENEAU et al. [22] from the fourth-neighbour Born — von Kármán model fitted to their frequency versus wave factor dispersion relations measured by neutron spectroscopic method. For normalization, the cut-off frequency of the experimental curves is taken as 6.84×10^{13} rad/sec. It will be seen that our spectrum qualitatively resembles the experimental curve of MOZER et al. The major peaks in the calculated and experimental curves are found to be at nearly the same positions. The heights of the calculated peaks are greater than the experimental values, but their form is similar to that of the experimental curve. Our calculated spectrum shows striking similarity with that of BIRGENEAU et al. with regard to the location and the intensity of peaks.

(3) Vanadium. EISENHAUER et al. [23] and MOZER et al. [21] have obtained the frequency distributions of vanadium from incoherent inelastic neutron scattering experiments. These distributions are shown in Fig. 3 along with the curves calculated by HENDRICKS et al. [24] using a noncentral three-force-constant model, and by CLARK et al. [25] using a noncentral four-constant model. Because of uncertainty in the upper end of the experimental curves, we have arbitrarily cut them off at 5.65×10^{13} rad/sec for normalization.

A perusal of the various frequency distributions plotted in Fig. 3 reveals several striking features. The calculated and the experimental distributions differ with regard to the position and intensity of peaks. The calculated curves show two distinct widely spread maxima with a sharp dip between them, the higher frequency peak having less intensity than the low frequency one, while the experimental curves have flat maxima with a small dip between them and the high frequency peak is more intense than the low frequency peak. The maximum frequency of our calculated distribution is in fair agreement with experiment though the experimental value is not well defined. An overall comparison of the various computed frequency distributions reveals that they all resemble each other in their broad features, but none of them agree with the experimental curves. Our calculated curve is, however, somewhat nearer to the experimental curve with regard to the location of the dip and the high frequency peak. It appears from the present study that none of the models is a satisfactory description of vanadium.

B. Specific heat

The experimental data for the specific heat of copper below 20 °K have been taken from the work of KOK and KEESOM [26] while those for above

20 °K from papers by GIAUQUE and MEADS [27] and MARTIN [28]. The latter two measurements are inconsistent and vary within wide limits. In the case of nickel, the experimental heat capacities have been obtained from the measurements of EUCKEN and WERTH [29] and BUSEY and GIAUQUE [30], those for vanadium from the measurements of CLUSIUS et al. [31]. The specific heats of nickel reported by the different workers are fairly consistent in the

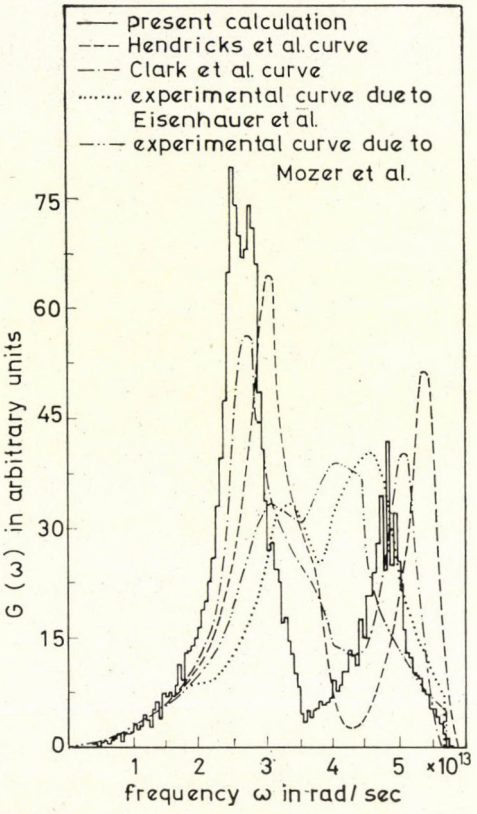

Fig. 3. The phonon frequency distribution function of vanadium

temperature range studied. The experimental specific heats have been plotted after correction for the electronic contribution. The values of the coefficient of the electronic specific heat, γ, used for this purpose, are given in Table II.

It will be seen from Fig. 5 that the theoretical and experimental $\Theta - T$ curves for copper are similar in shape, although the theoretical values are systematically higher. However, the discrepancy between them is nowhere greater than 3%. Between 70 and 130 °K, the theoretical Θ values lie very close to the measurements of MARTIN. It is a particularly striking feature of

Table II

Electronic specific heat coefficients for copper, nickel and vanadium

Metal	γ (μcal/mole deg^2)	Source
Copper	172	RAYNE[a]
Nickel	1740	CLUSIUS and SCHACHINGER[b]
Vanadium	1550	CLUSIUS et al.[c]

a) J. RAYNE, Phys. Rev., **95,** 1428, 1954.
b) K. CLUSIUS and L. SCHACHINGER, Z. Naturforsch., **7a**, 185, 1952.
c) K. CLUSIUS, P. FRANZOSINI and U. PIESBERGEN, Z. Naturforsch., **15a,** 728, 1960.

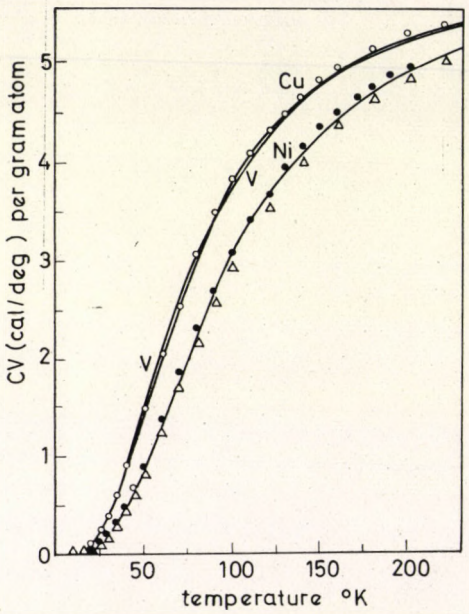

Fig. 4. Comparison of the calculated and observed lattice specific heats of copper, nickel and vanadium. Experimental data: ○ copper; ● nickel; △ vanadium

the theoretical curve that the minimum appears to have about the right depth and position.

As is seen in Fig. 6, the experimental Θ values for nickel lie very close to the experimental values. The difference between the observed and theoretical values nowhere exceeds 4%. For vanadium, the theoretical and experimental Θ values reveal considerable discrepancies: the experimental values being 30% higher than theoretical ones. These discrepancies may be attributed to the neglect of the temperature dependence of elastic constants and other anharmonic effects, due in part to the assumption of short-range interionic interactions in the theory. Using neutron scattering experiments, TURBERFIELD and

EGELSTAFF [32] have observed that the frequency spectrum of vanadium contains a tail at higher frequency. They have also found that the spectrum does not obey the usual Debye ω^2 law in the lower frequency region. These abnormal behaviours indicate that there is something special about the lattice dynamics

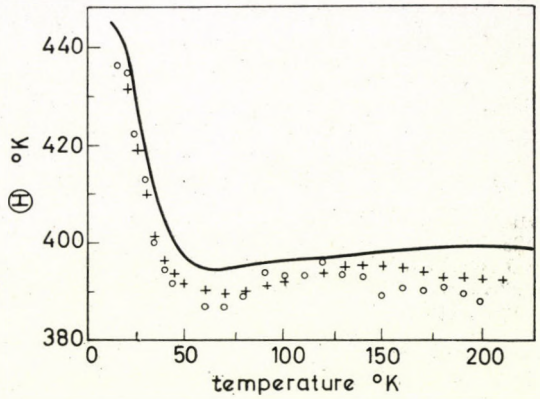

Fig. 5. The Debye temperature of copper as a function of temperature. Solid line shows the present calculation. Experimental points: ○ KOK and KEESOM, × GIAUQUE and MEADS, + MARTIN

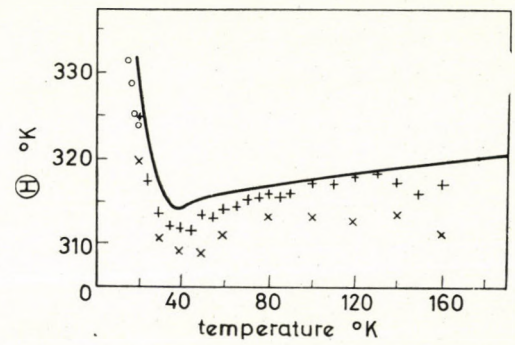

Fig. 6. The Debye temperature versus temperature curve for nickel. Solid line represents the present calculation. Experimental points: ○ EUCKEN and WERTH, + BUSEY and GIAUQUE

of vanadium. It emerges from the present study that BHATIA and HORTON's electron gas model gives a reasonable representation of thermal properties of copper and nickel, but not those of vanadium.

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ФУНКЦИИ РАСПРЕДЕЛЕНИЯ ЧАСТОТЫ ФОНОНОВ В МЕДИ, НИКЕЛЕ И ВАНАДИИ

ЯЙ ПРАКАШ, Б. С. СЕМУЭЛ и П. К. ШАРМА

Резюме

Определены функции распределения частот фононов в меди, никеле и ванадии методом отбора корней, используя модель Батиа и Гортона для электронно — ионного взаимодействия. Результаты сравнены с кривыми, полученными из опытов по неупругому рассеянию нейтронов а также и другими теоретическими расчётами. Расчётная кривая в случае меди в общих чертах согласуется с экспериментальной кривой, полученной Свессоном и др. из измерения рассеяния нейтронов. В случае никеля также имеется приемлемое совпадение с экспериментальным распределением частоты, полученным Мозерем и др. из опытов по некогерентному рассеянию нейтронов. В случае ванадия, настоящие, также, как и другие теоретические расчёты значительно расходятся с экспериментальными результатами. Удельные теплоёмкости решёток и эквивалентные температуры Дебая, полученные из рассчитанных распределений частот достаточно хорошо совпадают с ксэпериментальными данными для меди и никеля, а в случае ванадия имеется значительное расхождение.

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ANGULAR MOMENTUM AND UNITARY SPINOR BASES OF THE LORENTZ GROUP*

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The matrix of the boost operator has a rather complicated form in angular momentum basis while it reduces to a diagonal form $e^{i\alpha\nu}$ in the unitary spinor basis. The overlap coefficients between the two bases turn out to be complex Wigner coefficients of the rotation group. With the aid of these coefficients an expression for the boost function is derived in terms of a power series in $e^{-2\alpha}$.

It has been shown in [1] and in the revised versions [2, 3] that if the notion of spinor is generalized to the unitary case, the unitary representations of the Lorentz group can be expressed in a simpler form than those in O(3), O(2, I), E(2) bases. In the spinor basis the Lorentz group figures as an SO(3, C) group (the group of three-dimensional complex rotations) isomorphic with the proper Lorentz group. Such an interpretation is possible since there exists a combination of the generators satisfying the commutators of two independent angular momenta. A similar decomposition holds for the O(4) group. Though in the above spinor basis Lie Algebras of the O(3, I) and the O(4) groups coincide, for unitary representations all generators of the latter group are Hermitean, whereas in the Lorentz group the generators of the two complex angular momenta are pairwise adjoint to each other. In the spinor basis the unitary representations of the O(4) group are simply a product of two D-functions and the transition to the angular momentum basis can be accomplished by means of the Wigner coefficients of the real rotation group. Hence it seems natural that the overlap coefficients between O(3) and O(2, C) (spinor) bases of the Lorentz group can be interpreted as an analytic continuation of the familiar Wigner coefficients [2]. The overlap coefficients have been derived earlier for a special case by KUZNETSOV et al. [4].

The expression for the boost function $d^{j\sigma\sigma}_{ll'\mu}(\alpha)$ in the angular momentum basis is rather complicated. On the other hand, in the spinor basis the matrix of the boost operator along the z-axis is diagonal and has the form $e^{i\alpha\nu}$. The purpose of this paper is to show that complicated formulas containing multiple sums for the function $d^{j\sigma\sigma}_{ll'\mu}(\alpha)$ can be reduced to the product of two overlap coefficients

* This work has been completed at JINR, Dubna, USSR.

which accomplish the transition between O(3) and O(2, C) bases. These coefficients are essentially complex Wigner coefficients and can be treated easily since they possess a number of properties well-known from the rotation group.

In Section 1 the eigenfunctions of the O(3) and O(2, C) bases are constructed. In Section 2 the overlap coefficients between the two bases are calculated and in Section 3 it is shown that they are essentially complexified Wigner coefficients of the real rotation group. In Section 4 an explicit form for the boost function is presented in terms of a power series of the form $\Sigma_k a_k e^{-2k\alpha}$.

1. The basis functions

Denoting the infinitesimal generators of spatial rotations and boosts along the k-axis ($k = 1, 2, 3$) by M_k and N_k, respectively, the combinations

$$\frac{1}{2}(M_k + iN_k) = J_k \quad \text{and} \quad \frac{1}{2}(M_k - iN_k) = K_k$$

satisfy

$$[J_k, J_l] = i\varepsilon_{klm} J_m, \quad [K_k, K_l] = i\varepsilon_{klm} K_m, \quad [J_k, K_l] = 0.$$

For unitary representations $J_k = K_k^+$ holds. The Casimir operators $\vec{J}^2$, $\vec{K}^2$ of the two complex angular momenta $\vec{J}$, $\vec{K}$ are the Casimir operators of the Lorentz group:

$$\vec{J}^2 | > = j(j+1)| >, \quad \vec{K}^2 | > = j^*(j^*+1) | >, \tag{1.1}$$

where

$$j = \frac{1}{2}(j_0 - 1 + i\sigma), \tag{1.2}$$

($j_0 = 0, \pm\frac{1}{2}, \pm 1, \ldots, 0 \leq \sigma < \infty$ for the principal series). Irreducible unitary representations can be characterized by (j_0, σ) or by (j, j^*).

In unitary spinor basis the generators M_3 and N_3 are diagonal:

$$\begin{aligned} M_3 | jj^*;\ \mu\nu > &= \mu | jj^*;\ \mu\nu >, \\ N_3 | jj^*;\ \mu\nu > &= \nu | jj^*;\ \mu\nu >, \end{aligned} \tag{1.3}$$

where μ takes integer (half-integer) values for single-(double-) valued represent-

ations, while ν is continuous and real within the range $-\infty < \nu < \infty$. In terms of J_3 and K_3 Eq. (1.3) reads:

$$\begin{aligned} J_3|jj^*;\ mm^*> &= m\ |jj^*;\ mm^*>, \\ K_3|jj\ ;\ mm^*> &= m^*|jj^*;\ mm^*>, \end{aligned} \tag{1.4}$$

with

$$m = \frac{1}{2}(\mu + i\nu), \qquad m^* = \frac{1}{2}(\mu + i\nu). \tag{1.5}$$

Since m plays a part in the complex rotation group analogous to that of the third component of the usual angular momentum, we reserve the notation m for the eigenvalue of the complex angular momentum J_3, and the eigenvalue of the real angular momentum will be denoted by μ.

In addition to satisfying Eq. (1.1) eigenfunctions in the O(3) basis satisfy:

$$\begin{aligned} \vec{M}^2|jj^*;\ l\mu> &= l(l+1)|jj^*;\ l\mu>, \\ M_3|jj^*;\ l\mu> &= \mu|jj^*;\ l\mu>. \end{aligned} \tag{1.6}$$

In order to evaluate the overlap coefficients between the two bases it is convenient to choose a representation of the basis vectors which makes the calculation simple. The hyperboloid and the cone $p^2 = 0$ are two possible choices. Whichever of them is considered for the generators $M_{\mu\nu} = i(p_\mu \partial_\nu - p_\mu \partial_\nu)$, $Imj(j+1) = 1/2\, j_0 \sigma$ is automatically equal to zero, so we are restricted to the special case $j_0 = 0$, or $\sigma = 0$. However, it was pointed out by LOMONT and MOSES [4] that on the cone there exists a canonical transformation which yields generators realizing arbitrary values of j_0 and σ, characteristic for the principal series. This is due to the fact that on the cone the helicity $\lambda = \vec{M}\,\vec{p}/|\vec{p}|$ is a Poincaré- and Lorentz-invariant quantity. The generators given in [5] are:

$$\vec{M} = \vec{M}^{(0)} + \vec{M}^{(1)}, \quad \vec{N} = \vec{N}^{(0)} + \vec{N}^{(1)}, \tag{1.7}$$

where

$$\begin{aligned} \vec{M}^{(0)} &= \frac{1}{i}(\vec{p} \times \nabla_{\vec{p}}), \quad \vec{N}^{(0)} = \frac{1}{i} p \nabla_{\vec{p}} \quad (p \equiv |\vec{p}| = p^0), \\ \vec{M}^{(1)} &= \left(\lambda \frac{p^1}{p + p^3}, \ \lambda \frac{p^2}{p + p^3}, \lambda\right), \\ \vec{N}^{(1)} &= \left(-\lambda \frac{p^2}{p + p^3}, \ \lambda \frac{p^1}{p + p^3}, 0\right). \end{aligned} \tag{1.8}$$

Choose two coordinate systems on the cone:

S system:

$$p^0 = e^a,\ p^1 = e^a \sin\vartheta\cos\varphi,\ p^2 = e^a \sin\vartheta\sin\varphi, p^3 = e^a\cos\vartheta, \tag{1.9}$$

C system:

$$p^0 = e^{a'}\, ch\,\beta, p^1 = e^{a'}\cos\varphi, p^2 = e^{a'}\sin\varphi, p^3 = -\,e^{a'}\, sh\,\beta\,.$$

In terms of these parameters the Casimir operators for the S system are

$$\begin{aligned}\vec{J}^2 &= \frac{1}{4}\left(\frac{\partial^2}{\partial a^2} + 2(1-\lambda)\frac{\partial}{\partial a} + \lambda^2 - 2\lambda\right),\\ \vec{K}^2 &= \frac{1}{4}\left(\frac{\partial^2}{\partial a^2} + 2(1+\lambda)\frac{\partial}{\partial a} + \lambda^2 + 2\lambda\right).\end{aligned} \tag{1.10}$$

(The same expressions are valid for the C system with the substitution $a \to a'$.)

The eigenfunction is $e^{-(1+i\sigma)a}$, provided $\lambda = j_0$. (The other solution is connected with the equivalent representation $(-j_0, -\sigma)$.] The remaining operators we need are:

$$\vec{M}^2 = \vec{M}^{(0)2} + \frac{2\lambda\mu}{1+\cos\vartheta}, \tag{1.11}$$

$$M_3 = \frac{1}{i}\,\frac{\partial}{\partial\varphi} + \lambda\,, \tag{1.12}$$

$$N_3 = -\,\frac{1}{i}\,\frac{\partial}{\partial\beta}\,. \tag{1.13}$$

Using (1.6), (1.11) and (1.12), we find the normalized eigenfunctions in O(3) basis to be:[1]

$$\begin{aligned}\langle a\vartheta\varphi|l\mu\rangle &= \sqrt{2\pi(2l+1)}\, e^{-(1+i\sigma)a}\, e^{i\varphi(\mu-\lambda)}\, d^l_{\lambda\mu}(\vartheta) =\\ &= \sqrt{2\pi(2l+1)}\, e^{-(1+i\sigma)a}\, D^l_{\lambda\mu}(\varphi,\vartheta,-\varphi) \qquad (\lambda \equiv j_0)\,.\end{aligned} \tag{1.14}$$

In a similar way we get the spinor basis in the form

$$\langle a'\beta\varphi|\mu\nu\rangle = \eta\sqrt{2}\, e^{-(1+i\sigma)a'}\, e^{i(\mu-\lambda)\varphi}\, e^{-i\nu\beta}, \qquad (\lambda \equiv j_0) \tag{1.15}$$

Here η is a phase factor:

$$\eta = \begin{cases} 2^{i\sigma}\eta_0 & \text{if } j_0 = \lambda \geq \mu;\ \lambda+\mu \geq 0 \text{ or } \lambda+\mu < 0;\\ 2^{i\sigma}\eta_0\,\dfrac{\sin\pi(j-m)}{\sin\pi(j^*-m^*)} & \text{if } \mu \geq \lambda = j_0,\ \lambda+\mu \geq 0 \text{ or } \lambda+\mu < 0\end{cases} \tag{1.16}$$

[1] The scalar product is defined by $\langle f|g\rangle = \dfrac{1}{(2\pi)^3}\int \dfrac{d^3p}{2p^0}\langle p|f\rangle^*\langle p|g\rangle$.

with[2]

$$\eta_0 = \Gamma\begin{bmatrix} -j+j^*+l+1,\ j\ -m\ +1,\ j\ +m\ +1 \\ j-j^*+l+1,\ j^*-m^*+1,\ j^*+m^*+1 \end{bmatrix}^{1/2}.$$

[j and m are defined by (1.2) and (1.5).] In what follows we shall consider 4 cases according to the signs of $\lambda+\mu$ and $\lambda-\mu$. The inequalities $\lambda+\mu \geq 0$ and $\lambda+\mu < 0$ in Eq. (1.16) merely indicate that the phase factors in these cases coincide.

2. The overlap coefficients

After performing an integration on the hyperboloid we obtain the overlap coefficients in the form[3]

$$\langle \mu\nu|l\mu\rangle = \eta^*\, 2^{i\sigma}\sqrt{\frac{2l+1}{4\pi}}\,\Gamma\begin{bmatrix} l+\lambda'+1, l-\mu'+1 \\ l-\lambda'+1, l+\mu'+1 \end{bmatrix}^{1/2} \cdot$$
$$\cdot\,\Gamma\begin{bmatrix} j'-m'+1, j'+m'+1 \\ \lambda'-\mu'+1, \lambda'+i\sigma+1 \end{bmatrix} {}_3F_2\left[\begin{matrix} -l+\lambda', l+\lambda'+1, j'-m'+1 \\ \lambda'-\mu'+1, \lambda'+i\sigma+1 \end{matrix}\right], \tag{2.1}$$

where

$$\lambda' = \frac{1}{2}(|\lambda+\mu|+|\lambda-\mu|),\quad \mu' = \frac{1}{2}(|\lambda+\mu|-|\lambda-\mu|),$$
$$j' = \frac{1}{2}(\lambda'-1+i\sigma),\quad m' = \frac{1}{2}(\mu'+i\nu) \tag{2.2}$$

and ${}_3F_2$ is the generalized hypergeometric function of unit argument. No problem of convergence arises since the ${}_3F_2$ function entering Eq. (2.1) is a terminating series.

According to Eq. (2.2) we have 4 cases, namely:

1) $j_0 = \lambda \geq \mu$, $\lambda+\mu \geq 0$, for which Eq. (2.1) takes the form

$$\langle \mu\nu|l\mu\rangle_1 = \eta^*\, 2^{i\sigma}\sqrt{\frac{2l+1}{4\pi}}\,\Gamma\begin{bmatrix} j+j^*+l+2, l-\mu+1 \\ l-j\ -j^*, \quad l+\mu+1 \end{bmatrix}^{1/2} \cdot$$
$$\cdot\,\Gamma\begin{bmatrix} j-m+1,\ j+m+1 \\ j+j^*-\mu+2,\ 2j+2 \end{bmatrix} {}_3F_2\left[\begin{matrix} j+j^*-l+1, j+j^*+l+2,\ j-m+1 \\ j+j^*-\mu+2, 2j+2 \end{matrix}\right]. \tag{2.3}$$

[2] The shorthand notation $\Gamma\begin{bmatrix} a,\ b,\ \ldots\ x \\ u,\ v,\ \ldots\ z \end{bmatrix} \equiv \frac{\Gamma(a)\Gamma(b)\ldots\Gamma(x)}{\Gamma(u)\Gamma(v)\ldots\Gamma(z)}$ is used.

[3] The trivial factor $\delta_{j_0' j_0}\delta(\sigma'-\sigma)$ is omitted in the following.

2) $\mu \geq \lambda = j_0$, $\lambda + \mu \geq 0$ for which

$$\langle \mu\nu|l\mu\rangle_2 = \eta^* 2^{i\sigma} \sqrt{\frac{2l+1}{4\pi}} \Gamma\begin{bmatrix} -j-j^*+l,\ l+\mu+1 \\ j+j^*+l+2,\ l-\mu+1 \end{bmatrix}^{1/2} \cdot$$
$$\cdot \Gamma\begin{bmatrix} -j^*+m^*,\ j+m+1 \\ -j-j^*+\mu,\ j-j^*+\mu+1 \end{bmatrix} {}_3F_2\begin{bmatrix} -l+\mu, l+\mu+1, -j^*+m^* \\ -j-j^*+\mu, j-j^*+\mu+1 \end{bmatrix}. \tag{2.4}$$

3) $\lambda = j_0 > \mu$, $\lambda + \mu < 0$, for which

$$\langle \mu\nu|l\mu\rangle_3 = \eta^* 2^{i\sigma} \sqrt{\frac{2l+1}{4\pi}} \Gamma\begin{bmatrix} j+j^*+l+2,\ l-\mu+1 \\ -j-j^*+l,\ l+\mu+1 \end{bmatrix}^{1/2} \cdot$$
$$\Gamma \cdot \begin{bmatrix} j-m+1, -j^*-m^* \\ j+j^*-\mu+2, j-j^*-\mu+1 \end{bmatrix} {}_3F_2\begin{bmatrix} -l-\mu,\ l-\mu+1, j-m+1 \\ j+j^*-\mu+2, j-j^*-\mu+1 \end{bmatrix}. \tag{2.5}$$

4) $j_0 = \lambda < \mu$, $\lambda + \mu < 0$, for which

$$\langle \mu\nu|l\mu\rangle_4 = \eta^* 2^{i\sigma} \sqrt{\frac{2l+1}{4\pi}} \Gamma\begin{bmatrix} -j-j^*+l,\ l+\mu+1 \\ j+j^*+l+2, l-\mu+1 \end{bmatrix}^{1/2} \cdot$$
$$\cdot \Gamma\begin{bmatrix} -j^*+m^*, -j^*-m^* \\ -j-j^*+\mu,\ -2j^* \end{bmatrix} {}_3F_2\begin{bmatrix} -j-j^*-l-1, -j-j^*+l, -j^*+m^* \\ -j-j^*+\mu, -2j^* \end{bmatrix}. \tag{2.6}$$

There exist two fundamental relations between the ${}_3F_2$ hypergeometric functions of unit argument [6]. From the three-term relation (see Appendix)

$$\frac{\sin \pi\beta_{45}\, Fp(0;45)}{\Gamma(\alpha_{012}, \alpha_{013}, \alpha_{023})} + \frac{\sin \pi\beta_{50}\, Fp(4;05)}{\Gamma(\alpha_{124}, \alpha_{134}, \alpha_{234})} + \frac{\sin \pi\beta_{04} Fp(5)}{\Gamma(\alpha_{125}, \alpha_{135}, \alpha_{235})} = 0 \tag{2.7}$$

we obtain

$$\langle \mu\nu|l\mu\rangle_1 = \langle \mu\nu|l\mu\rangle_2.$$

In a similar way the two-term relation

$$Fp(0;45) = Fp(0;14)$$

yields

$$\langle \mu\nu|l\mu\rangle_1 = \langle \mu\nu|l\mu\rangle_3, \quad \langle \mu\nu|l\mu\rangle_2 = \langle \mu\nu|l\mu\rangle_4$$

and thus the overlap coefficients (2.3), (2.4), (2.5), (2.6) are all equal. In order to make clear the meaning of these equalities let us consider the first overlap coefficient $\langle \mu\nu \mid l\mu\rangle_1$ in the range of the second one, i.e. in the quadrant

$\mu - \lambda > 0, \mu + \lambda > 0$. Due to the parameter $j + j^* - \mu + 2 = \lambda - \mu + 1$ in the denominator of the ${}_3F_2$ function and to the factor $1/\Gamma(j + j^* - \mu + 2)$, the coefficient $\langle \mu\nu \mid l\mu \rangle_1$ is an undetermined quantity of $0.\infty$ type. Taking the limit we arrive at the coefficient $\langle \mu\nu \, l \, l\mu \rangle_2$ as it is given by equation (2.4). The above transformations of the Thomae-Wipple functions produce this limit automatically. In the case of the remaining coefficients we face a similar situation.

It is worth mentioning that for an arbitrary choice of the phase η the overlap coefficients in the four quadrants differ by a phase factor. We have chosen the value of η [see Eq. (1.16)] in such a way that the equality of the $\langle \mu\nu \mid l\mu \rangle_{1,2,3,4}$ should hold.

3. Relation to the Wigner coefficients

One of the possible forms of the Wigner coefficients for the three-dimensional real rotation group is [7]:

$$C(j_1 j_2 j_3; m_1 m_2) = \sqrt{2j_3+1} \times$$

$$\times \Gamma\begin{bmatrix} j_1+m_1+1, j_2-m_2+1, j_3-m_3+1, j_3+m_3+1 \\ j_1-m_1+1, j_2+m_2+1, j_1+j_2-j_3+1, j_1+j_2+j_3+2 \end{bmatrix}^{1/2} \cdot$$

$$\Gamma(j_1-j_2+j_3+1,-j_1+j_2+j_3+1)^{1/2} \cdot \frac{1}{\Gamma(j_3-j_2+m_1+1, j_3-j_1-m_2+1)} \cdot$$

$$\cdot {}_3F_2\begin{bmatrix} -j_1-j_2+j_3, -j_1+m_1, -j_2-m_2 \\ -j_1+j_3-m_2+1, -j_2+j_3+m_1+1 \end{bmatrix}. \tag{3.1}$$

Using the relation [6]

$$\frac{\sin \pi\beta_{23}}{\pi\Gamma(\alpha_{023})} Fp(0; 45) = \frac{Fn(2)}{\Gamma(\alpha_{134}, \alpha_{135}, \alpha_{345})} - \frac{Fn(3;24)}{\Gamma(\alpha_{124}, \alpha_{125}, \alpha_{245})} .$$

(3.1) can be written in the form

$$C(j_1 j_2 j_3; m_1 m_2) = e^{\mp i\pi(j_3+m_3)} \Gamma\begin{bmatrix} j_1+m_1+1, j_1-m_1+1, j_3-m_3+1 \\ j_2+m_2+1, j_2-m_2+1, j_3+m_3+1 \end{bmatrix}^{1/2} \cdot$$

$$\cdot \Gamma\begin{bmatrix} j_1+j_2-j_3+1, j_1-j_2+j_3+1, j_1+j_2+j_3+2 \\ -j_1+j_2+j_3+1 \end{bmatrix}^{1/2} \frac{1}{\Gamma(j_1-j_2-m_3+1, 2j_1+2} \Bigg] \cdot$$

$$\cdot {}_3F_2\begin{bmatrix} j_1-j_2-j_3, j_1-j_2+j_3+1, j_1-m_1+1 \\ j_1-j_2-m_3+_1, 2j_1+2 \end{bmatrix}. \tag{3.2}$$

This form of the Wigner coefficients will be complexified with the prescription $\mp$ for $Im(j_2 + m_2) \gtrless 0$. Namely, let us introduce the notations:

$$\begin{aligned} j_1 &\equiv j = \frac{1}{2}(j_0 - 1 + i\sigma), & m_1 &\equiv m = \frac{1}{2}(\mu + i\nu), \\ j_2 &\equiv -j^* - 1 = \frac{1}{2}(-j_0 - 1 + i\sigma), & m_2 &\equiv m^* = \frac{1}{2}(\mu - i\nu), \\ j_3 &\equiv l, & m_3 &\equiv \mu. \end{aligned} \tag{3.3}$$

Then, comparing (3.2) with the overlap coefficients (2.3), we find:

$$\langle \mu\nu | l\mu \rangle = e^{\pm i\pi(j_2+m_2)} \frac{1}{2} \left[\frac{\sin \pi(-j_1 - j_2 + j_3)}{\sin \pi(j_2 + m_2) \sin \pi (j_2 - m_2)} \right]^{1/2} C(j_1 j_2 j_3; m_1 m_2)$$
$$\left(Im\,(j_2 + m_2) \gtrless 0\right).$$

Thus the overlap coefficient is proportional to the complexified Wigner coefficients defined in (3.2). This result is quite clear, since the spinor basis is the eigenstate of $\vec{J}^2, J_3; \vec{K}^2, K_3$ and we want to obtain the angular momentum basis which is the eigenstate of $(\vec{J} + \vec{K})^2 = \vec{M}^2$ and $J_3 + K_3 = M_3$.

It must be emphasized that Eq. (3.2) cannot be considered as defining the Wigner coefficients for arbitrary complex values of the parameters, since this would require further considerations. Eq. (3.2) has the sense discussed above and it is defined for the values of parameters given by Eq. (3.3).

In view of the relations between the functions the overlap coefficients possess a number of symmetry properties which are the complex counterparts of those of the real Wigner coefficients. Here we mention that as a consequence of $|j_0| \leq l$ we have a triangle inequality for the complex angular momenta: $|j_1 - j_2| \leq j_3$. Permutation of 1, 2 and 3 of course, is not allowed now.

4. Matrix elements of the boost operator in angular momentum basis

The overlap coefficients make it possible to obtain an expression for the boost function $d^{j_0\sigma}_{ll'\mu}(\alpha)$ defined by

$$d^{j_0\sigma}_{ll'\mu}(\alpha) = \langle l\mu | e^{i\alpha N_3} | l'\mu \rangle .$$

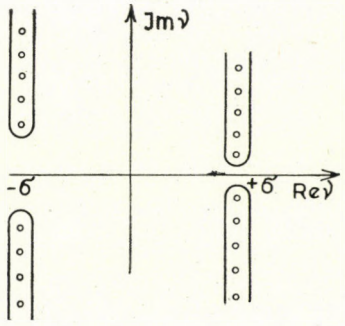
Since the spinor basis is an eigenstate of N_3, we get the integral representation

$$d^{j_0\sigma}_{ll'\mu}(\alpha) = \int_{-\infty}^{\infty} d\nu\, e^{i\alpha\nu} \langle \mu\nu | l\mu \rangle^* \langle \mu\nu | l'\mu \rangle . \tag{4.1}$$

The relation of Eq. (4.1) to the O(4) group is treated in [8]. As is seen from (2.1), the integrand of (4.1) has four types of poles on the *complex* ν plane, namely

$$\text{a)}\ \nu = i(\lambda' + 1 + \mu' + 2k) - \sigma,$$
$$\text{b)}\ \nu = i(-\lambda' - 1 + \mu' - 2k) + \sigma,$$
$$\text{c)}\ \nu = i(-\lambda' - 1 - \mu' - 2k) - \sigma,$$
$$\text{d)}\ \nu = i(\lambda' + 1 - \mu' + 2k) + \sigma, \qquad (k = 0, 1, 2, \ldots)$$

where λ' and μ' are defined by Eq. (2.2). The position of the poles in the case $j_0 \geqq \mu \geqq 0$ is shown in the Figure. Before closing the contour of integration



the asymptotic behaviour of the integrand for large ν is required. We find for the overlap coefficients the following asymptotic formula:

$$\langle \mu\nu|l\mu\rangle = \sqrt{(2l+1)\pi}\,\frac{1}{\Gamma(2j+2, j+j^*-\mu+2)}\,\Gamma\begin{bmatrix} j+j^*+l+2,\ l-\mu+1 \\ -j-j^*+l,\ l+\mu+1 \end{bmatrix} \cdot$$
$$\cdot\, {}_2F_2\left[\begin{matrix} j+j^*-l+1, j+j^*+l+2 \\ 2j+2, j+j^*-\mu+2 \end{matrix}; 1\right]\left(\frac{i\nu}{2}\right)^{2j+1+l-j_0} e^{\mp \pi\nu/2}\,(1+o(1)) \qquad (\mathrm{Re}\,\nu \gtrless 0).$$

(We have here omitted an irrelevant phase factor.) The leading term of the integrand is $e^{-\pi|\mathrm{Re}\nu|-\alpha\,\mathrm{Im}\nu}$ so for $\alpha > 0$ the contour can be closed on the upper half plane. Thus, only the poles of the a) and d) types make a contribution. The final result is:

$$\frac{1}{2\pi i}\,d^{j_0\sigma}_{ll'\mu}(\alpha) = \sum_{k=0}^{\infty}(-1)^k\frac{(\lambda'+\mu'+k)!}{k!}\,\frac{\langle\mu\nu|l'\mu\rangle\langle\mu\nu|l\mu\rangle^*}{\Gamma(j'+m'+1, j'^*+m'^*+1)}\bigg|_{\nu=\nu_k} e^{i\alpha\nu_k} +$$
$$+\sum_{k=0}^{\infty}(-1)^k\frac{(\lambda'-\mu'+k)!}{k!}\,\frac{\langle\mu\nu|l'\mu\rangle\langle\mu\nu|l\mu\rangle^*}{\Gamma(j'-m'+1, j'^*-m'^*+1)}\bigg|_{\nu=\nu'_k} e^{i\alpha\nu'_k}, \qquad (4.2)$$

where

$$\nu_k = i(\lambda'+1+\mu'+2k) - \sigma,\ \nu'_k = i(\lambda'+1-\mu'+2k) + \sigma$$

and λ', μ', j', m' are defined by Eq. (2.2). For $\alpha < 0$ we can obtain an analogous formula by closing the contour on the lower half-plane. However, it is easier to use the unitarity in the form $d^{j_0\sigma}_{ll'\mu}(\alpha) = d^{j_0\sigma}_{l'l\mu}(-\alpha)^*$, in which case we have to change the sign on the left hand side of (4.2) and to substitute $\nu_k \to \nu_k^*$, $\nu_k \to \nu_k'^*$.

Acknowledgements

I would thank Professor J. SMORODINSKY for helpful discussions and comments.

Appendix

For the readers' convenience we cite the definition of the *Fp* and *Fn* functions [6]. Consider 6 quantities r_i ,for which

$$\sum_{i=0}^{5} r_i = 0$$

holds and define

$$\alpha_{lmn} = \frac{1}{2} + r_l + r_m + r_n\,,\ \beta_{mn} = 1 + r_m - r_n\,.$$

Then the Thomae—Wipple functions are defined by

$$Fp(l;\, mn) = \frac{1}{\Gamma(\alpha_{ghj}, \beta_{ml}, \beta_{nl})}\, {}_3F_2\left[\begin{matrix}\alpha_{gmn}, \alpha_{hmn}, \alpha_{jmn} \\ \beta_{ml}, \beta_{nl}\end{matrix};\ 1\right]$$

$$Fn(l;\, mn) = \frac{1}{\Gamma(\alpha_{lmn}, \beta_{lm}, \beta_{ln})}\, {}_3F_2\left[\begin{matrix}\alpha_{lhj}, \alpha_{lgj}, \alpha_{lgh} \\ \beta_{lm}, \beta_{ln}\end{matrix};\ 1\right],$$

where g, h, j represent those 3 numbers out of the six integers 0, 1, . . ., 5 not already represented by l, m and n.

For these functions two fundamental relations hold. According to the first one, $Fp(l;\, mn)$ functions with fix l and with different m, n are all equal. The second fundamental theorem is a three-term relation. One of its possible forms is given by Eq. (2.7). In our case the last term in Eq. (2.7) becomes zero in view of the Γ-function in the denominator.

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БАЗИСЫ УГЛОВОГО МОМЕНТА И УНИТАРНЫХ СПИНОРОВ ГРУППЫ ЛОРЕНЦА

М. ХУСАР

Резюме

Матрица оператора «буста» имеет сложный вид в базисе углового момента, в то же время она сводится к диагональной форме $e^{ia\nu}$ в базисе унитарных спиноров. Коэффициентами переразложения между двумя базисами являются комплексные коэффициенты Вигнера группы вращений. С домощью этих коэффициентов задается выражение для функции «буста» $d^{j}_{\mu'\mu}(\alpha)$ в виде степенного ряда.

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SUR LA VITESSE DE PROPAGATION DES ULTRASONS DANS LES SOLUTIONS AQUEUSES DE QUELQUES HALOGÈNES IV.

CHLORURES DES MÉTAUX ALCALINO-TERREUX

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(Reçu 10. XII. 1970)

Utilisant une méthode de diffraction, les auteurs déterminent la vitesse de propagation des ultrasons dans les solutions aqueuses des chlorures des métaux alcalino-terreux, dans un domaine de température et de concentration. On présente les variations des vitesses en fonction des paramètres considérés, en comparaison avec les vitesses correspondantes de l'eau; les modifications que l'on constate sont attribuées aux changements structuraux causés par la variation des valeurs de la température et de la concentration, aussi bien qu'aux interactions électriques.

Les recherches concernant certaines propriétés des solutions aqueuses des halogènes des métaux alcalins et alcalino-terreux, effectuées par l'intermédiaire des mesurages acoustiques, sont continuées dans le présent travail pour les sels suivants: $MgCl_2$, $CaCl_2$, $SrCl_2$ et $BaCl_2$.

Procédé expérimental

La vitesse de propagation des ultrasons a été mésurée par la méthode de la diffraction de la lumière monochromatique sur un faisceau ultrasonique obtenu d'un générateur piézo-électrique pourvu d'un stabilisateur de fréquence et d'un fréquencemètre [1].

Les caractéristiques de l'installation sont les suivantes:

Fréquence: $\nu = 2$ MHz $\pm$ 2 kHz

Longueur d'onde de la lumière: $\lambda = 5460{,}74$ Å

Distance focale de l'installation: F = 171,9 cm.

Les mesurages ont porté sur un domaine de concentration entre 0,2 M et 3 M et un intervalle de température de 15 °C jusqu'à 50 °C, étant étendus aussi sur l'eau distillée; les résultats sont affectés d'erreurs jusqu'à 3‰.

Résultats expérimentaux

La vitesse des ultrasons subit des modifications le long d'une courbe analogue à la croissance de la température dans les quatre solutions étudiées. On peut remarquer les mêmes modifications sur les formes paraboliques des courbes, semblables à celles obtenues pour l'eau distillée pour le même domaine

de température. Dans les figures 1, 2, 3 et 4 sont présentées les variations des vitesses par rapport à la température pour les solutions aqueuses des chlorures de magnésium, calcium, strontium et baryum, à des concentrations différentes. Dans la grande majorité des cas n'ont été mises en évidence que les branches ascendantes des paraboles, marquant la tendance de diminution des pentes concomitamment avec la croissance de la température. En général, dans l'intervalle recherché n'ont pas été atteintes les températures auxquelles les vitesses deviennent maximales pour les concentrations données. L'allure des courbes nous permet de déduire le déplacement vers des températures plus basses de la vitesse maximale avec l'accroissement de la concentration; ces courbes ont été mises en évidence aux solutions de $MgCl_2$ pour les concentrations de 2 M et 2,5 M et de $SrCl_2$ pour la concentration de 1,5 M.

Les vitesses se situent à des valeurs supérieures à celles de l'eau aux mêmes températures, dans tous les cas étudiés et l'on constate leur augmentation dans le même sens que la concentration.

La formule de Willard ne peut pas être appliquée à la dépendance de la vitesse de la température, les déviations cependant semblent être inférieures à celles correspondantes aux solutions de chlorures alcalines.

Dans les conditions de l'accroissement de la concentration à des températures constantes, les vitesses se placent sur des courbes avec coefficients angulaires positifs.

L'on constate que dans tous les cas les modifications ont lieu en deux étapes: dans la première, dans le domaine des solutions diluées, d'après certaines courbes, dans la seconde étape le long d'une droite. Les intervalles dans lesquels les vitesses présentent des variations en ligne courbe à gradients de concentrations croissantes, diffèrent selon la solution et la température; ainsi, dans le cas de la chlorure de magnésium cet intervalle s'étend jusqu'à la concentration de 0,2 M, comme il s'ensuit de la figure 5, et pour les solutions des chlorures de: Ca, Sr et Ba, présentées sur les figures 6, 7 et 8 jusqu'à 0,5 M environ. Avec l'élévation de la température les valeurs $\Delta v/\Delta c$ diminuent, la variation de la vitesse avec la concentration marquant une tendance prononcée à devenir linéaire. En ce qui concerne les domaines des pentes constantes, on remarque la même mise en ordre avec les températures pour toutes les solutions, à l'exception des intersections causées par le dépassement des vitesses maximales. L'élévation de la température diminue systématiquement les valeurs: $\Delta v/\Delta c$, de même que dans les parties précédentes des courbes, de la région à une faible concentration. Un comportement différent a été mis en évidence dans le cas de la solution aqueuse de $CaCl_2$, qui présente des déviations de la linéaire à toutes les températures et concentrations étudiées. Avec la croissance de ces paramètres apparaît une tendance d'atténuation des déviations sans atteindre cependant aux droites caractéristiques des autres électrolytes, au moins dans les intervalles expérimentaux respectifs.

La dépendance de la vitesse de propagation des ultrasons de la concentration pour: t = const. montre des différenciations entre les quatre solutions,

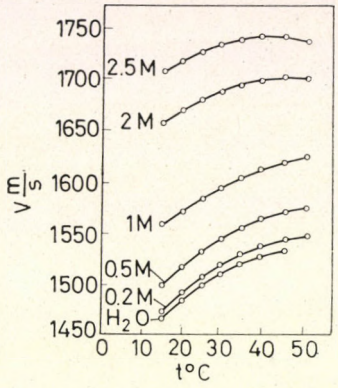

Fig. 1. Variation de la vitesse de propagation des ultrasons dans la solution aqueuse de $MgCl_2$ en fonction de la température

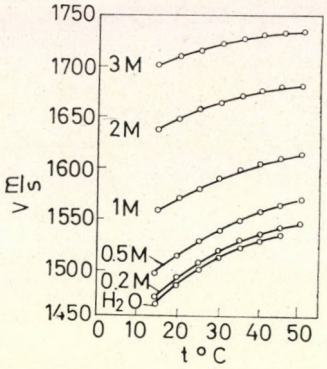

Fig. 2. Variation de la vitesse de propagation des ultrasons dans la solution aqueuse de $CaCl_2$ en fonction de la température

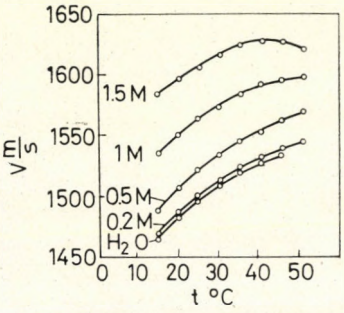

Fig. 3. Variation de la vitesse de propagation des ultrasons dans la solution aqueuse de $SrCl_2$ en fonction de la température

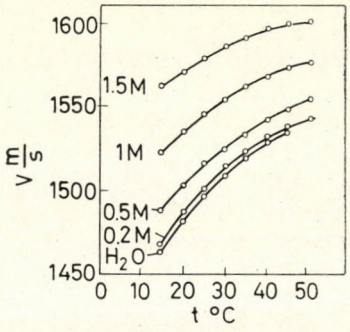

Fig. 4. Variation de la vitesse de propagation des ultrasons dans la solution aqueuse de $BaCl_2$ en fonction de la température

illustrées sur la fig. 9 à 30 °C. Par analogie aux autres températures, les vitesses ont des valeurs croissantes avec la diminution du poids moléculaire des sels pour les mêmes concentrations.

A des concentrations inférieures à 1,5 M, les différences de vitesse correspondantes aux différentes substances augmentent avec l'accroissement de la concentration. La déviation constatée antérieurement dans le cas de la solution de $CaCl_2$ est aussi mise en évidence, de même que les autres observations faites en ce qui concerne les deux étapes de la variation de vitesse en fonction de la concentration.

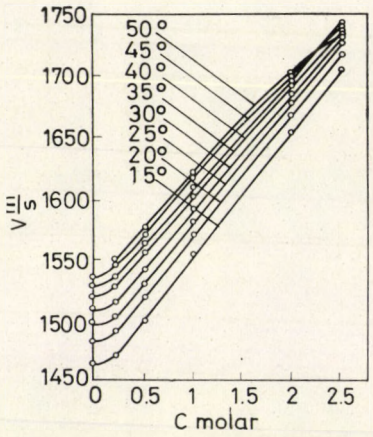

Fig. 5. Variation de la vitesse de propagation des ultrasons dans la solution aqueuse de $MgCl_2$ en fonction de la concentration

Interprétation des résultats

La valeur de la vitesse de propagation des ultrasons est déterminée par les propriétés élastiques du milieu parcouru, donc implicitement par ses caractéristiques structurelles dans les états d'équilibre correspondants aux mesurages [2, 3].

Aux systèmes étudiés, formés d'éléments structurels complexes, soumis aux interactions des différents champs de force, correspondent les états d'équilibre imposés par les paramètres pris en considération dans le présent travail: la température et la concentration. Les déplacements d'états imposés par les modifications des variables mentionnés sont reflétés par les variations de vitesse mises en évidence [4].

Le comportement anormal de l'eau qui se manifeste par l'augmentation de la vitesse avec la température jusqu'à une valeur maximale, suivie par sa diminution, est dû aux deux actions d'effet opposé de l'agitation thermique: la dilatation et le déplacement de l'équilibre entre les deux structures présentes dans l'eau.

L'effet de la dissolution des sels se manifeste par l'augmentation de la vitesse, analogue à celui produit par l'agitation thermique, à la suite de la destruction progressive des structures tridymitiques. La superposition des deux causes, actionnant dans le même sens, a pour conséquence d'installer plus rapidement l'effet, d'inverser la dépendance de la vitesse de la température, effet mis en évidence par le déplacement des maxima vers des températures plus réduites.

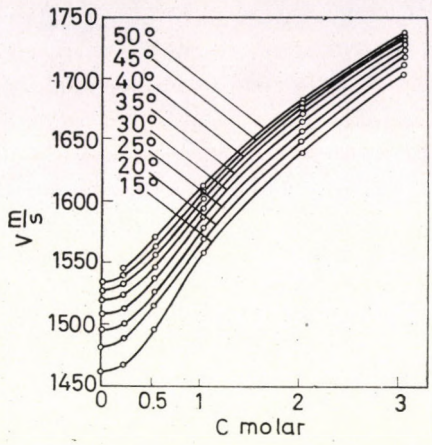

Fig. 6. Variation de la vitesse de propagation des ultrasons dans la solution aqueuse de $CaCl_2$ en fonction de la concentration

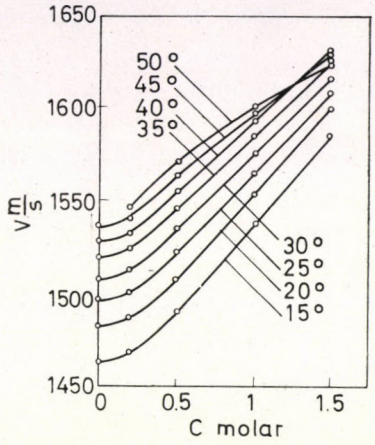

Fig. 7. Variation de la vitesse de propagation des ultrasons dans la solution aqueuse de $SrCl_2$ en fonction de la concentration

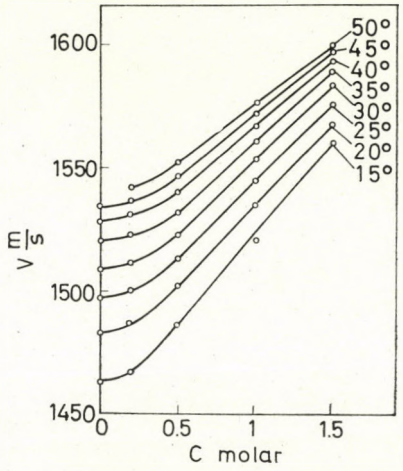

Fig. 8. Variation de la vitesse de propagation des ultrasons dans la solution aqueuse de $BaCl_2$ en fonction de la concentration

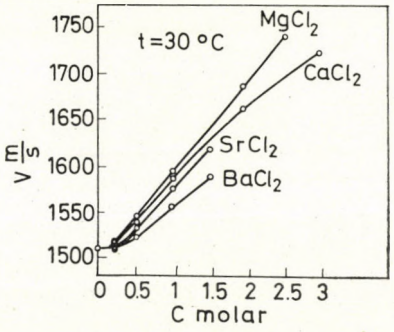

Fig. 9. Variation comparative des vitesses de propagation des ultrasons en fonction de la concentration, dans les solutions aqueuses de: $MgCl_2$, $CaCl_2$, $SrCl_2$ et $BaCl_2$

L'accroissement de la concentration des solutions est suivi par l'augmentation de la vitesse, étant donné la réalisation des structures plus compactes à densité plus grande. Concomitamment les effets de l'agitation thermique sont limités par les champs électriques des ions, fait reflété par la réduction des gradients de température de la vitesse avec l'accroissement de la concentration [5, 6, 7].

La disposition des courbes: $v = f(c)$ dans le sens de la diminution des poids des cations à une température constante s'explique probablement par l'augmentation du degré d'hydratation avec la diminution des dimensions des cations pour les électrolytes étudiés. Les valeurs des rayons des ions sont les suivantes: Mg^{++}: 0,65 Å, Ca^{++}: 0,99 Å, Sr^{++}: 1,13 Å et Ba^{++}: 1,35 Å. L'augmentation de la densité dans le sens de l'accroissement des poids moléculaires pour un nombre identique d'ions dans la solution semble avoir une moindre contribution à la modification de la vitesse des ultrasons que l'effet de compression des sphères d'hydratation.

Conclusions

1. La vitesse des ultrasons dans les solutions aqueuses des chlorures des métaux alcalino-terreux varie avec la température, la concentration et les proprietés du cation.

2. La variation de la vitesse avec la température ne peut pas être décrite par une fonction du type Willard.

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О СВЕРХЗВУКОВЫХ СКОРОСТЯХ В ВОДНЫХ РАСТВОРАХ НЕКОТОРЫХ ГАЛОГЕННЫХ СОЛЕЙ IV.

Хлориды щёлочно-земельных металлов

Д. АУСЛЭНДЕР и ЛИА ОНИЦИУ

Резюме

В статье описаны явления, наблюдаемые при сверхзвуковых скоростях в водных растворах хлоридов щёлочно-земельных металлов в некотором диапазоне температуры и концентрации. Наблюдения проводились дифракционным методом.

Значения изменения скорости приведены в зависимости от изученных параметров и сравниваются с соответствующими изменениями, которые были наблюдены в воде. Полученные отклонения могут быть объяснены структурными изменениями, вызванными изменением концентрации и температуры, а также электрическими взаимодействиями.

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ON THE STABILITY OF AN ANHARMONIC CRYSTAL

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The properties of an f.c.c. lattice displaying central nearest-neighbour interaction are considered on the basis of PLAKIDA and SIKLÓS's self-consistent method for investigating anharmonic crystals in an approximation of the lowest-order (the third and fourth inclusively) anharmonic terms. The cases of fixed crystal volume and constant external pressure are investigated and the results obtained with the help of the Lennard-Jones (12-6) interatomic potential are discussed.

1. Introduction. Basic equations

In a previous paper [1] we have used a recently developed general method for investigating the properties of highly anharmonic crystals [2, 3] as the basis of a pseudoharmonic approximation for determining the conditions for stability of an anharmonic crystal by taking account of the third and fourth order anharmonic terms.

This restriction has proved to be expedient, since the ratio $\sqrt{\overline{u}^2}/l$ of the mean square relative displacement $\sqrt{\overline{u}^2}$ of nearest-neighbour atoms and the mean distance l between them is small enough up to the instability point and by permitting one to diminish to some extent the undesirable effect of distortion due to the omission of all the odd terms of anharmonicity it improves the results of the pseudoharmonic theory. Although the calculations were considerably simplified, the results approached those obtained when the effect of damping of phonons was taken into account [4].

In the present paper the properties of a face-centred cubic lattice displaying central nearest-neighbour interaction are investigated in the same lowest-order anharmonic terms approximation as in [1] but with allowance for phonon damping. The Lennard-Jones (12-6) interatomic potential is used. The properties of the crystal at fixed volume (Section 2) and fixed external pressure (Section 3) are considered, and the results obtained for the case of small anharmonicity are compared with those given by conventional perturbation theory.

The investigation is based on a self-consistent system of equations for a f.c.c. lattice consisting of N identical atoms of mass M whose Hamiltonian in the central pair force approximation is of the form (see [4])

$$H = \sum_l \frac{P_l^2}{2M} + \frac{1}{2} \sum_{l \neq m} \Phi(|R_l - R_m|) , \tag{1}$$

where P_l and R_l are the momentum and position operators for the l-th atom. The summation is performed only over the z nearest neighbours (in this case $z = 12$).

The self-consistent system of equations for determination of the lattice constant d as well as expressions for the phonon frequency spectra ϵ_{kj}, the phonon damping Γ_{kj} and the internal energy E of the anharmonic crystal can be obtained by using double-time Green functions [2, 3]. Here we shall simply write down the expressions for these quantities without deriving them (see [3, 4]):

The equation of state from which the equilibrium lattice constant $d = l\sqrt{2}$ is obtained is

$$P = -\frac{1}{3V}\sum_{l,\alpha} l_\alpha \left\langle \frac{\partial U}{\partial R_l^\alpha} \right\rangle = -\frac{zl}{6v}\tilde{\Phi}^{(1)}(l)\,, \tag{2}$$

where P is the external pressure, $v = V/N = l^3/\sqrt{2}$ and $\tilde{\Phi}(l)$ is the self-consistent potential, defined here in the approximation

$$\begin{aligned}\tilde{\Phi}(l) = \langle \Phi(|\mathbf{R}_l - \mathbf{R}_0|)\rangle \approx \exp\left\{\frac{1}{2}\sum_{\alpha,\beta}\langle (u_l^\alpha - u_0^\alpha)(u_0^\beta - u_0^\beta)\rangle \nabla_\alpha \nabla_\beta\right\}\Phi(l) \approx \\ \approx \Phi(l) + \frac{1}{2}\sum_{\alpha,\beta}\langle (u_l^\alpha - u_0^\alpha)(u_l^\beta - u_0^\beta)\rangle \frac{\partial^2 \Phi(l)}{\partial l_\alpha \partial l_\beta}\,.\end{aligned} \tag{3}$$

The renormalized phonon frequencies ϵ_{kj} and phonon widths Γ_{kj} are

$$\epsilon_{kj} = \omega_{kj} + Re\, M_{kj}(\epsilon_{kj}) \approx \tilde{\alpha}\omega_{0kj}\left[1 - \frac{Re\, M_{kj}(\epsilon_{kj})}{\omega_{kj}}\right] \tag{4}$$

and

$$\Gamma_{kj} = -\,Im\, M_{kj}(\epsilon_{kj} + i\varepsilon) \approx -\,Im\, M_{kj}(u_{kj} + i\varepsilon)\,, \tag{5}$$

where ω_{0k_j} are the phonon frequencies in the harmonic approximation and ω_{k_j} those in the pseudoharmonic approximation;

$$\tilde{\alpha}^2 = \left\{\tilde{\Phi}^{(2)}(l) + \frac{c}{l}\tilde{\Phi}^{(1)}(l)\right\}\Big/ f_0$$

is the renormalization coefficient

$$(f_0 = \Phi^{(2)}(r_0),\quad c = 3\delta - 1,\quad \delta = \omega_k^2/\omega_{kj}^2 = \sum_j \omega_{kj}^2/3\omega_{kj}^2 \approx 1{,}40\ \ [1]);$$

and M_{kj} is the self-energy operator [4].

The internal energy of the system can be written in the form

$$E = \langle H \rangle = \frac{N}{2} \{ z\tilde{\Phi}(l) + \varepsilon(\theta) \} + 5\tilde{F}_3(\theta), \tag{6}$$

where

$$\varepsilon(\theta) = -\frac{z}{2} \tilde{\alpha}^2 f_0 \bar{u}_l^2 = \frac{1}{N} \sum_k \frac{1}{2\pi\omega_k} \int_0^\infty \frac{d\omega^2}{2\omega} \omega_k^2 \coth \frac{\omega}{2\theta} \{ -Im\, G_k(\omega + i\varepsilon) \} \tag{7}$$

and $\tilde{F}_3(\theta)$ is the anharmonic contribution of odd-derivative terms to the free energy

$$\tilde{F}_3(\theta) = \frac{1}{12\pi} \int_0^\infty d\omega \coth \frac{\omega}{2\theta} \sum_k \frac{\omega^2 - \omega_k^2}{\omega_k} \{ -Im\, G_k(\omega + i\varepsilon) \}. \tag{8}$$

$\bar{u}_l^2$ in formula (7) is the mean square relative longitudinal displacement of neighbouring atoms.

In the high- and low-temperature limits the quantities M_k ($k \equiv \{ kj \}$), $\tilde{F}_3(\theta)$ and $\varepsilon(\theta)$ can be written explicitly. For high temperatures, i.e. $\theta \gg \omega_D$, where $\omega_D \approx 1.05\, \omega_L$ is the Debye energy in the pseudoharmonic approximation, we have (see [4]):

$$M_k(\omega) = -\theta \frac{g^2(\theta, l)}{f^3(\theta, l)} \omega_k S_k(\nu), \tag{9}$$

where

$$g(\theta, l) = \tilde{\Phi}^{(3)}(l), \; f(\theta, l) = \tilde{\Phi}^{(2)}(l),$$

$$S_k(\nu) = \frac{1}{32\, N} \sum_{p,p'} \frac{\Delta(p + p' - k)}{\lambda_k^2 \lambda_p^2 \lambda_{p'}^2} F^{(2)}(-k, p, p') \times$$

$$\times \left\{ \frac{(\lambda_p + \lambda_{p'})^2}{(\lambda_p + \lambda_{p'})^2 - \nu^2} + \frac{(\lambda_p - \lambda_{p'})^2}{(\lambda_p - \lambda_{p'})^2 - \nu^2} \right\},$$

$$\nu = \frac{\omega}{\omega_L/2}, \quad \omega_L = \omega_{0L} \sqrt{\frac{f(\theta, l)}{f_0}}, \quad \omega_{0L} = \sqrt{\frac{8 f_0}{M}}.$$

ω_{0L} is the maximum frequency in the harmonic approximation; the dimensionless sum $S_k(\nu)$ has been calculated for some values of $\{ kj \}$ by MARADUDIN et al. [5]. Hence

$$\tilde{F}_3(\theta) \approx -N\theta^2 A \cdot \frac{g^2(\theta), l)}{f^3(\theta, l)}, \quad (A \approx 5{,}6 \cdot 10^{-2}), \tag{10}$$

$$\varepsilon(\theta) \approx 3\theta \left\{ \frac{1}{1 - \mu\theta \dfrac{g^2(\theta, l)}{f^3(\theta, l)}} + \frac{\omega_L^2}{24\, \theta^2} \right\} \Bigg\}. \tag{11}$$

$$(\mu = 2A \approx 0{,}11).$$

In the low-temperature limit ($\theta \ll \omega_D$) the corresponding quantities are:

$$M_k(\omega) = -\omega_k \frac{g^2(\theta, l)}{f^3(\theta, l)} \left\{ \varepsilon_0 S_{0k}(\nu) + \frac{3\pi^4}{5} \frac{\theta^4}{\omega_D^3} S_{1k}(\nu) \right\}, \tag{12}$$

where

$$S_{0k}(\nu) = \frac{1}{(1{,}02)\, 8^2 N} \sum_{p,p'} \frac{\Delta(p+p'-k)}{\lambda_k^2 \lambda_p \lambda_{p'}} F^2(-k, p, p') \frac{(\lambda_p + \lambda_{p'})}{(\lambda_p + \lambda_{p'})^2 - \nu^2}$$

and

$$S_{1k}(\nu) = \frac{1}{(120{,}8) 8^2} \sum_{j_1 j_2} \int_{-1}^{1} d\cos\Theta \int_0^{2\pi} d\Phi \frac{G^2(kj; \Phi, \Theta, j_1; kj_2)}{\lambda_{kj}^2 \lambda_{kj_2}^2 d_{j_1}^5 (\Theta\Phi)} \cdot \frac{2\lambda_{kj_2}}{\lambda_{kj_2}^2 - \nu^2}.$$

The notations in S_{0k} and S_{1k} are the same as in [4];

$$\varepsilon_0 = \varepsilon_0^0 \sqrt{\frac{f(\theta, l)}{f_0}} \approx 1{,}02\, \omega_L$$

(ε_0^0 is the zero point energy per atom in the harmonic approximation.)
In this case

$$\left.\begin{aligned} \tilde{F}_3(\theta) &\approx -N\varepsilon_0 \frac{g^2(\theta, l)}{f^3(\theta, l)} \left\{ \varepsilon_0 B + \frac{3\pi^4}{5} \frac{\theta^4}{\omega_D^3} C \right\}, \\ B &\approx 1.85 \cdot 10^{-3}, \quad C \approx 1.25 \cdot 10^{-2}, \end{aligned}\right\} \tag{13}$$

$$\left.\begin{aligned} \varepsilon(\theta) &\approx \frac{\varepsilon_0}{1 - \nu_0 \varepsilon_0 \dfrac{g^2(\theta, l)}{f^3(\theta, l)}} + \frac{3\pi^4}{5} \frac{\theta^4}{\omega_D^3} \left\{ 1 + \nu_1 \varepsilon_0 \frac{g^2(\theta, l)}{f^3(\theta, l)} \right\}, \\ \nu_0 &= 4B \approx 7.3 \cdot 10^{-3}, \qquad \nu_1 = 8C \approx 0.10. \end{aligned}\right\} \tag{14}$$

2. Lattice at fixed volume

In investigating the self-consistent system of equations for the crystal lattice we shall use the Lennard-Jones (12-6) model potential

$$\Phi_{L-J}(l) = D \left\{ \left(\frac{r_0}{l} \right)^{12} - 2 \left(\frac{r_0}{l} \right)^6 \right\}. \tag{15}$$

Substituting (15) into (3) and performing the summation for all the terms in

the derivatives of the pair potential, we easily get

$$\tilde{\Phi}(l) = D\left\{\xi^{12} - 2\xi^6 + \frac{1}{6}y\left[(13-c)\xi^{14} - (7-c)\xi^8\right]\right\}, \tag{16}$$

where the notation $\xi \equiv r_0/l$ and the dimensionless variable $y = (6/r_0)^2 \bar{u}_l^2$ have been introduced.

In this section the properties of the f.c.c. lattice at fixed volume, with $l = r_0 = \text{const.}$, are considered. Determining the force constants and the renormalization coefficient $\tilde{\alpha}$ with the help of (16) and substituting them into Eq. (7), we obtain the equation for y as a function of temperature and external pressure. Below, this equation is analyzed in the high- and low-temperature limits.

2a. *High temperatures* ($\theta \gg \omega_D$)

In the case of high temperatures Eqs. (7) and (11) give the following equation for y:

$$\left\{\lambda_1 y\left[1 + \frac{D(H_1 - H_2)}{f_0^2}y\right] - \beta\right\}\left(1 + \frac{DH_2}{f_0^2}y\right)\left\{1 - \frac{zA}{6}\theta\frac{g_0^2}{f_0^3}\times\right.$$
$$\left.\times\left[1 + \frac{D}{f_0}\left(\frac{2H_3}{g_0} - \frac{3H_2}{f_0}\right)y\right]\right\} = 1, \tag{17}$$

where

$$\lambda_1 = \frac{zD}{3\theta} = \frac{4D}{\theta} = \frac{M\omega_{0L}^2 r_0^2}{144\,\theta}, \quad \beta = \frac{\omega_{0L}^2}{24\,\theta^2} \ll 1,$$

$$H_1 = h_0 + \frac{c}{r_0}\left(2g_0 + \frac{(c-2)f_0}{r_0}\right), \quad H_2 = h_0 + \frac{c}{r_0}\left(g_0 - \frac{2f_0}{r_0}\right),$$

$$H_3 = \Phi^{(5)}(r_0) + \frac{c}{r_0}\left(h_0 - \frac{3g_0}{r_0} + \frac{6f_0}{r_0}\right)$$

$$h_0 = \Phi^{(4)}(r_0), \quad g_0 = \Phi^{(3)}(r_0).$$

Eq. (17) shows that in the constant volume case the lattice is stable in the whole region of temperatures, i.e. the solution of (17) is real for $y > 0$ in the whole region of the parameter λ_1. However, it is necessary to note that in the present case the problem of the dynamical stability of the lattice can be solved consistently only if the short-range correlations due to the hard-core part of the interatomic potential are carefully taken into account.

If there is a small of anharmonicity ($\theta \ll D$, $y \ll 1$) the solution of Eq.

(17) can be written in the form

$$y=\frac{\theta}{4D}\left\{1+\theta\left[2A\frac{g_0^2}{f_0^3}-\frac{1}{4}\frac{H_1}{f_0^2}\right]+\beta\left[1-\frac{\theta}{4}\frac{(2H_1-H_2)}{f_0^2}\right]\right\}. \tag{18}$$

This leads to expressions for the physical quantities coinciding with the results of the conventional perturbation theory if $c = 0$, i.e. in the approximation in which only the leading highest-order derivatives of the interatomic potential figure (see [6, 7]).

From (18) we obtain the following expressions for the physical characteristics of the crystal:

renormalized frequencies:

$$\epsilon_{kj}\approx\omega_{0kj}\left\{1+\frac{\theta}{8}\frac{H_1}{f_0^2}(1+\beta)-\theta\frac{g_0^2}{f_0^3}Re\,S_{kj}\right\}, \tag{19}$$

phonon widths:

$$\Gamma_{kj}\approx\theta\frac{g_0^2}{f_0^3}\omega_{0kj}\,Im\,S_{kj}, \tag{20}$$

where

$$Re\,S_{kj}\equiv Re\,S_{kj}(\lambda_{kj}),\ Im\,S_{kj}\equiv Im\,S_{kj}(\lambda_{kj}+i\varepsilon);$$

internal energy:

$$\left.\begin{aligned}\frac{1}{N}E\approx-\frac{zD}{2}+3\theta\left\{1+\beta-\theta\left[\left(\frac{1}{8}\frac{H_1}{f_0^2}-\frac{1}{16}\frac{H_4}{f_0^2}\right)-\frac{A}{3}\frac{g_0^2}{f_0^3}\right]\right\},\\ H_4=h_0+\frac{c}{r_0}\left(2g_0+\frac{cf_0}{r_0}\right);\end{aligned}\right\} \tag{21}$$

external pressure:

$$P\approx\frac{21\,l}{2vr_0}(1+a_1)\,\theta\left\{1+\beta-\theta\left[0{,}25\frac{H_1}{f_0^2}-0{,}10\frac{(1+a_2)}{(1+a_1)}\frac{h_0}{f_0^2}-2A\frac{g_0^2}{f_0^3}\right]\right\}, \tag{22}$$

where

$$a_1=\frac{c}{r_0}\frac{f_0}{g_0},\ a_2=\frac{c}{r_0}\frac{1}{\Phi^{(5)}(r_0)}\left\{2h_0+\frac{(c-2)\,g_0}{r_0}-\frac{2cf_0}{r_0^2}\right\}.$$

It should be noted here that in order to determine the internal energy and pressure with an accuracy to the terms of θ^2 inclusively it has been necessary to take into account terms of the order of y^2 in the self-consistent potential $\tilde{\Phi}(l)$.

2b. Low temperatures ($\theta \ll \omega_D$)

Eqs. (7) and (14) give the following equation for determining y:

$$\lambda y\left(1+\frac{DH_2}{f_0^2}y\right)^{-1/2}\left(1+\frac{DH_1}{f_0^2}y\right)=1+\eta\left(1+\frac{DH_2}{f_0^2}y\right)^{-2}+$$
$$+\varepsilon_0^0\frac{g_0^2}{f_0^3}\left(1+\frac{DH_2}{f_0^2}y\right)^{1/2}\left[1+\frac{D}{f_0}\left(\frac{2H_3}{g_0}-\frac{3H_2}{f_0}\right)y\right]\times \qquad (23)$$
$$\times\left[\nu_0+\nu_1\eta\left(1+\frac{DH_2}{f_0^2}y\right)^{-2}\right],$$

where $\lambda = zD/\varepsilon_0^0$ is the dimensionless coupling parameter for atoms and

$$\eta=\frac{3\pi^4}{5}\left(\frac{\theta}{\omega_{0D}}\right)^4\ll 1\,.$$

Although Eq. (23) has real solutions in the whole region of the parameter λ, with regard to the problem of the lattice stability the same remarks apply as in the case of high temperatures. For small anharmonicity ($\varepsilon_0^0 \ll zD$, $y \ll 1$) the solution of (23) takes the form

$$y=\frac{\varepsilon_0^0}{zD}=\left\{1+\varepsilon_0^0\left[\nu_0\frac{g_0^2}{f_0^3}-\frac{(2H_1-H_2)}{24f_0^2}\right]+\eta\left[1+\varepsilon_0^0\left(\nu_1\frac{g_0^2}{f_0^3}-\frac{(2H_1+H_2)}{12f_0^2}\right)\right]\right\}. \qquad (24)$$

This gives results for the physical quantities coinciding with those of conventional perturbation theory when $c = 0$, i.e. $H_1 = H_2 = h_0$.

With the help of (24) the characteristics of the system are obtained in the following form:

$$\epsilon_{kj}\approx\omega_{0kj}\left\{1+\varepsilon_0^0\left[\frac{1}{24}\frac{H_1}{f_0^2}(1+\eta)-\frac{g_0^2}{f_0^3}(Re\,S_{0kj}+\eta\,Re\,S_{1kj})\right]\right\}; \qquad (25)$$

$$\Gamma_{kj}\approx\omega_{0kj}\varepsilon_0^0\frac{g_0^2}{f_0^3}\left[Im\,S_{0kj}+\eta\,Im\,S_{1kj}\right]; \qquad (26)$$

$$\frac{1}{N}E\approx-\frac{zD}{2}+\varepsilon_0^0\left\{1+\varepsilon_0^0\left[\frac{(H_4+2H_2-2H_1)}{48f_0^2}-\frac{g_0^2}{f_0^3}(5B-\nu_0)\right]+\right.$$
$$\left.+\eta\left[1-\varepsilon_0^0\left(\frac{(2H_1+2H_2-H_4)}{24f_0^2}-\frac{g_0^2}{f_0^3}(\nu_1-5C)\right)\right]\right\}; \qquad (27)$$

$$P \approx \frac{21\,l}{6vr_0}(1+a_1)\,\varepsilon_0^0\left\{1+\varepsilon_0^0\left[\nu_0\frac{g_0^2}{f_0^3}-\frac{(2H_1+H_2)}{24f_0^2}+0{,}034\frac{(1+a_2)}{(1+a_1)}\frac{h_0}{f_0^2}\right]+\right.$$
$$\left.+\eta\left[1-\varepsilon_0^0\left(-\nu_1\frac{g_0^2}{f_0^3}+\frac{(2H_1+H_2)}{12f_0^2}-0{,}069\frac{(1+a_2)}{(1+a_1)}\frac{h_0}{f_0^2}\right)\right]\right\}. \tag{28}$$

It is clear that on account of the zero-point vibrations of atoms the pressure is different from zero even when $\theta = 0$. As in the high-temperature case, in obtaining the expressions for E and P terms of the order of y^2 have been taken into account in $\tilde{\Phi}(l)$.

3. The lattice at constant external pressure

In the case of isotropic external pressure $P = \text{const.}$ the dependence of the mean distance l between atoms on temperature can be determined from Eq. (2) after substituting into it the expression for $\tilde{\Phi}^{(1)}(l)$ defined by Eq. (16). In the approximation of small pressure considered in this work l is given by

$$l = l_0 - \frac{1}{18}r_0 p\,, \tag{29}$$

where

$$l_0 = l|_{\overline{p=0}} \quad r_0\left(1+\frac{\sigma_1}{4}y\right) \quad \text{and} \quad p = P\left(\frac{3v_0 r_0}{2zDl_0}\right) \ll 1$$

is a dimensionless small pressure ($v_0 = l_0^3/\sqrt{2}$). The renormalization coefficient $\tilde{\alpha}$ and force constants in this case read

$$\left.\begin{aligned} \tilde{\alpha}^2 &= 1-\sigma y+\sigma_1 p,\\ f &= f_0\left(1-\sigma y+\frac{7}{6}p\right),\\ g &\approx g_0(1-y+p). \end{aligned}\right\} \tag{30}$$

The following notations have been introduced in (29)—(30):

$$\sigma \equiv \frac{35+c}{36}\,, \quad \sigma_1 \equiv \frac{21-c}{18}\,.$$

Below the cases of high and low temperatures are considered separately.

3a. High temperatures ($\theta \gg \omega_D$)

Substituting the expressions given by (30) into Eq. (7) and taking into account (11), we get the equation for determining the parameter y in the form:

$$\left\{\lambda_1 y \frac{(1-\sigma y+\sigma_1 p)}{\left(1-\sigma y+\frac{7}{6}p\right)}-\beta\right\}\left(1-\sigma y+\frac{7}{6}p\right)\times \\ \times\left\{1-2A\theta\frac{g_0^2}{f_0^3}\frac{(1-y+p)^2}{\left(1-\sigma y+\frac{7}{6}p\right)^3}\right\}=1\,. \tag{31}$$

In the region $\theta \leq \theta_c$, where

$$\frac{\theta_c}{D} \approx 0{,}5\,(1+2{,}1\,p-0{,}18\,\beta_c)\,, \tag{32}$$

the solution of (31) is real and in the vicinity of the critical point ($\tau \leqq 1$) takes the form

$$y \approx 0{,}4\{1+1{,}2\,p+0{,}34\,\beta_c-1{,}9\sqrt{1-\tau}\}, \tag{33}$$

where $\tau \equiv \theta/\theta_c$. The physical quantities in this case are:

$$\epsilon_{kj} \approx 0{,}8\,\omega_{0kj}\{1+0{,}32\,p+0{,}48\sqrt{1-\tau}-2{,}86\tau\,Re\,S_{kj}\}\,, \tag{34}$$

$$\Gamma_{kj} \approx 2{,}3\,\tau\omega_{0kj}\,Im\,S_{kj}\,, \tag{35}$$

$$\frac{1}{N}E \approx -\frac{zD}{2}+3\theta_c\{2-2{,}2\,p+1{,}1\,\beta_c-2{,}3\sqrt{1-\tau}\}, \tag{36}$$

$$C_p = \frac{k}{N}\left[\frac{\partial}{\partial\theta}(E+3PV)\right]_p \approx 3k\cdot\frac{1{,}15}{\sqrt{1-\tau}}\,, \tag{37}$$

$$\alpha_p = \frac{k}{l}\left[\frac{\partial l}{\partial\theta}\right]_p \approx \frac{kr_0}{l\theta_c}\cdot\frac{0{,}10}{\sqrt{1-\tau}}\,. \tag{38}$$

It is clear from these expressions that the system is dynamically instable if $\theta > \theta_c$ (i.e. when the renormalized phonon frequency ϵ_{kj} becomes complex), as in the pseudoharmonic approximation [1]. The internal energy remains finite at $\theta \lessapprox \theta_c$, but the specific heat at constant pressure C_p and the coefficient of linear thermal expansion α_p tend to infinity as $\theta \to \theta_c$.

Far from the critical point, i.e. in the small anharmonicity limit, when $\theta \ll D$, $y \ll 1$, the solution of Eq. (31) is given by

$$y \approx \frac{1}{\lambda_1}\left\{1+\beta-\sigma_1 p+\theta\left[\frac{\sigma}{20{,}6}\frac{h_0}{f_0^2}+2A\frac{g_0^2}{f_0^3}\right]\right\}, \tag{33'}$$

and the corresponding physical quantities are

$$\epsilon_{kj} \approx \omega_{0kj}\left\{1+\frac{\sigma_1}{2}p-\theta\left[\frac{\sigma}{41{,}2}\frac{h_0}{f_0^2}(1+\beta)+\frac{g_0^2}{f_0^3}Re\,S_{kj}\right]\right\}, \tag{34'}$$

$$\Gamma_{kj} \approx \omega_{0kj}\,\theta\,\frac{g_0^2}{f_0^3}Im\,S_{kj}, \tag{35'}$$

$$\frac{1}{N}E \approx -\frac{zD}{2}+3\theta\left\{1+\beta-\frac{\sigma_1}{2}p+\theta\left[\frac{\sigma}{41{,}2}\frac{h_0}{f_0^2}+\frac{1}{16}\frac{H_4}{f_0^2}+\frac{A}{3}\frac{g_0^2}{f_0^3}\right]\right\}, \tag{36'}$$

$$C_p \approx 3k\left\{1+\beta+\theta\left[\frac{\sigma}{20{,}6}\frac{h_0}{f_0^2}+\frac{1}{8}\frac{H_4}{f_0^2}+\frac{2A}{3}\frac{g_0^2}{f_0^3}\right]\right\}, \tag{37'}$$

$$\alpha_p \approx \frac{\sigma_1 kr_0}{16\,lD}\left\{1+\beta+\theta\left[\frac{\sigma}{10{,}3}\frac{h_0}{f_0^2}+4A\frac{g_0^2}{f_0^3}\right]\right\}. \tag{38'}$$

3b. Low temperatures ($\theta \ll \omega_D$)

The equation for determining y is obtained from Eqs. (30), (7) and (14) and has the following form:

$$\lambda y\left\{1-\frac{49}{8}\frac{z}{\lambda}\nu_0\frac{(1-y)^2}{(1-\sigma y)^{5/2}}\right\}=\frac{1}{(1-\sigma y)^{1/2}}\left\{1-\lambda p y\frac{(\sigma_1-7/12)}{(1-\sigma y)^{1/2}}+\right.$$
$$\left.+\frac{\eta}{(1-\sigma y)^2}\left[1+\frac{49}{8}\frac{z}{\lambda}(\nu_1-\nu_0)\frac{(1-y)^2}{(1-\sigma y)^{5/2}}\right]\right\}. \tag{39}$$

The critical parameters λ_0 and θ_c restricting the region of existence of real solutions of equation (39) for $y>0$, $\lambda \geqslant \lambda_0$, $\theta \leqslant \theta_c$ are given by the formulas

$$\frac{\theta_c}{\omega_{0D}} \approx \frac{1}{2{,}5\pi}(\lambda-\lambda_0)^{1/4} \quad \text{and} \quad \lambda_0 \approx 3{,}5(1-p)\,. \tag{40}$$

The solution near the critical point ($\theta \leq \theta_c$) can be written in the form

$$y \approx 0{,}6\left\{1+0{,}8p-0{,}47(\lambda-\lambda_0)-0{,}52\sqrt{(\lambda-\lambda_0)(1-\tau^4)}\times\right.$$
$$\left.\times[1-0{,}47(\lambda-\lambda_0)]+0{,}6(\lambda-\lambda_0)(1-\tau^4)\right\}, \tag{41}$$

which leads to the following expressions for the physical characteristics of the lattice:

$$\epsilon_{kj} \approx 0{,}63\,\omega_{0kj}\left\{1+0{,}65\,p+0{,}35\,(\lambda-\lambda_0)+\right.$$
$$\left.+0{,}4\sqrt{(\lambda-\lambda_0)(1-\tau^4)}\ -33{,}2\,Re\,S_{0kj}-2{,}07\cdot 10^2\,\eta_c\,Re\,S_{1kj}\right\}, \tag{42}$$

$$\Gamma_{kj} \approx 21\,\omega_{0kj}\left\{Im\,S_{0kj}+6{,}25\,\eta_c\,Im\,S_{1kj}\right\}, \tag{43}$$

$$\frac{1}{N}E \approx -\frac{zD}{2}+\varepsilon_0^0\left\{0{,}96-0{,}13\,p+0{,}17(\lambda-\lambda_0)-0{,}11\times\right.$$
$$\left.\times\sqrt{(\lambda-\lambda_0)(1-\tau^4)}\,[1+2{,}2\,(\lambda-\lambda_0)]\right\}, \tag{44}$$

$$C_p \approx 3{,}7\,k\cdot\frac{12\pi^4}{5}\,\frac{\theta^3}{\omega_{0D}^3}\,\frac{[1+2{,}2\,(\lambda-\lambda_0)]}{\sqrt{(\lambda-\lambda_0)(1-\tau^4)}}, \tag{45}$$

$$\alpha_p \approx 10{,}4\,\frac{kr_0}{l}\,\frac{3\pi^4}{5}\,\frac{\theta^3}{\omega_{0D}^4}\left\{\frac{[1-0{,}5\,(\lambda-\lambda_0)]}{\sqrt{\lambda-\lambda_0)\,(1-\tau^4)}}-2{,}3\right\}. \tag{46}$$

It can be seen, as in the pseudoharmonic approximation, that the system becomes unstable when $\lambda < \lambda_0$ or $\theta > \theta_c$ (see Eq. (42)]. The internal energy is finite at $\theta \leq \theta_c$, but the specific heat and the coefficient of linear thermal expansion tend to infinity as $\theta \to \theta_c$.

Far from the critical point ($\lambda \gg 1$, $y \ll 1$) the solution of Eq. (39) is given by

$$y \approx \frac{\varepsilon_0^0}{zD}\left\{1-\left(\sigma_1-\frac{7}{12}\right)p+\varepsilon_0^0\left[\frac{\sigma}{6\cdot 20{,}6}\,\frac{h_0}{f_0^2}+\nu_0\,\frac{g_0^2}{f_0^3}\right]+\right.$$
$$\left.+\eta\left[1+\varepsilon_0^0\left(\frac{\sigma}{20{,}6}\,\frac{h_0}{f_0^2}+\nu_1\,\frac{g_0^2}{f_0^3}\right)\right]\right\} \tag{41'}$$

and leads to the following expressions for the physical quantities:

$$\epsilon_{kj} \approx \omega_{0kj}\left\{1+\frac{\sigma_1}{2}\,p-\varepsilon_0^0\left[\frac{\sigma}{6\cdot 20{,}6}\,\frac{h_0}{f_0^2}\,(1+\eta)+\frac{g_0^2}{f_0^3}\,(Re\,S_{0kj}+\eta Re\,S_{1kj})\right]\right\}. \tag{42'}$$

$$\Gamma_{kj} \approx \omega_{0kj}\varepsilon_0^0\,\frac{g_0^2}{f_0^3}\left\{Im\,S_{0kj}+\eta\,Im\,S_{1kj}\right\}, \tag{43'}$$

$$\frac{1}{N}E \approx -\frac{zD}{2}+\varepsilon_0^0\left\{1-\varepsilon_0^0\left[\frac{(\sigma_2-\sigma)}{6\cdot 20{,}6}\,\frac{h_0}{f_0^2}+\frac{g_0^2}{f_0^3}\,(5B-\nu_0)\right]\right\}+$$
$$+\eta\left[1+\varepsilon_0^0\left(\frac{(3\sigma-\sigma_2)}{3\cdot 20{,}6}\,\frac{h_0}{f_0^2}+\frac{g_0^2}{f_0^3}\,(\nu_1-5c)\right)\right], \tag{44'}$$

where

$$\sigma_2 \equiv \sigma+\frac{12-c}{4}-\frac{DH_4}{2f_0^2} \approx 1{,}5\,;$$

$$C_p \approx k \cdot \frac{12\pi^4}{5} \frac{\theta^3}{\omega_{0D}^3} \left\{1 + \varepsilon_0^0 \left[\frac{(3\sigma - \sigma_2)}{3 \cdot 20{,}6} \frac{h_0}{f_0^2} + \frac{g_0^2}{f_0^3}(\nu_1 - 5C)\right]\right\}, \tag{45'}$$

$$\alpha_p \approx \frac{\sigma_1 k r_0}{12\, lD} \cdot \frac{3\pi^4}{5} \frac{\theta^3}{\omega_{0D}^3} \left\{1 + \varepsilon_0^0 \left[\frac{\sigma}{20{,}6} \frac{h_0}{f_0^2} + \nu_1 \frac{g_0^2}{f_0^3}\right]\right\}. \tag{46'}$$

4. Discussion

Using the general method developed in [2, 3] we have considered the properties of a three-dimensional lattice in the lowest-order anharmonic approximation. If the results of the present work are compared with those of [1] in which a pseudoharmonic approximation was used for the same purpose, it will be seen that by accounting for phonon damping a lower critical temperature θ_c and a higher critical value of the dimensionless coupling parameter λ are obtained. The same result has been found for the case when the higher-order anharmonic terms are taken into account [4, 8].

The values of the critical parameters and physical quantities obtained in this paper, especially in the high-temperature limit, agree well with those arrived at earlier in [4] by a method accounting for the higher-order anharmonicities and using the Morse interatomic model potential.

Thus, it appears that because the values of the mean square relative displacements of atoms in the lattice are sufficiently small up to the critical point (the evaluation of the longitudinal displacements from the calculations of Section 3 gives

$$\frac{\sqrt{\bar{u}_{lc}^2}}{l_c} = \frac{r_0 \sqrt{y_c}}{6\, l_c} \approx \begin{cases} 0{,}10, & \theta \gg \omega_D \\ 0{,}11, & \theta \ll \omega_D \end{cases}$$

it is expedient in many cases to use the lowest-order anharmonic approximation when applying PLAKIDA and SIKLÓS' self-consistent theory for investigating the properties of anharmonic crystals in wide intervals of temperatures and external pressure. Such a procedure considerably simplifies the calculations and makes it possible to use the Lennard-Jones pair potential, which is more realistic in comparison with other model potentials. It should also be noted that more accurate results have been arrived at by taking account of all of the lower-order terms in calculating the derivatives of the pair potential, both in this work [see Eq. (16)] and in [1].

The results obtained in the case of small anharmonicity agree well with those of the ordinary perturbation theory. The critical temperature obtained in this work corresponds to the transition of the system from the crystal state to the uniform density state and is close to the melting temperature (see discussion in [4]).

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О СТАБИЛЬНОСТИ АНГАРМОНИЧЕСКИХ КРИСТАЛЛОВ

ВО ХОНГ АНЬ

Р е з ю м е

С помощью самосогласованного метода развитого в [1, 2] для исследования ангармонических кристаллов рассмотрены свойства гранецентрированных кубических решёток с центрально симметричным взаимодействием ближайших соседей в приближении наинизших ангармонических членов (третьего и четвёртого включительно). Исследованы случаи постоянного объёма и постоянного внешнего давления. Обсуждены результаты, полученные с помощью 12—6 межатомного потенциала Леннарда-Джонса.

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REARRANGEMENT CONTRIBUTION TO THE SYMMETRY ENERGY AND SINGLE PARTICLE POTENTIAL

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The G matrix elements are determined as the function of the relative momenta for the $N = Z$ nuclear matter and the $Z = 0$ neutron gas cases. From this we determine the symmetry energy and its rearrangement part and the single particle potential and its rearrangement part. The saturation condition is fulfilled and the rearrangement terms turn out to be small.

I. The symmetry energy

The total energy of the infinite nuclear matter with different neutron and proton number can be written as

$$E = -C_1 A + C_2 \left(\frac{N-Z}{A}\right)^2 A = E(\text{pot}) + E(\text{kin}), \tag{1}$$

where C_1 is the infinite nuclear matter energy and C_2 the symmetry energy. Both C_1 and C_2 have parts due to the potential and the kinetic energy. The potential energy, according to the Brueckner—Goldstone expansion, can be written as

$$E(\text{pot}) = \frac{1}{2}\sum_{m=0}^{k_N}\sum_{n=0}^{k_N}(k_m k_n|G_{NN}|k_m k_n) + \\ + \frac{1}{2}\sum_{m=0}^{k_P}\sum_{n=0}^{k_P}(k_m k_n|G_{PP}|k_m|k_n) + \sum_{m=0}^{k_N}\sum_{n=0}^{k_P}(k_m k_n|G_{NP}|k_m k_n), \tag{2}$$

where G_{NN} is the neutron—neutron, G_{NP} the neutron—proton and G_{PP} the proton—proton interaction part of the G matrix, k_N the neutron Fermi momenta and k_P the proton Fermi momenta, and the exchange terms are included in G.

$$G_{PP}(k_N k_P) = \sum_{s,m_s} G(sm_s, T=1, \quad T_3=1; \quad k_N k_P),$$

$$G_{NN}(k_N k_P) = \sum_{s,m_s} G(sm_s, T=1, \quad T_3=-1; \quad k_N k_P), \tag{3}$$

$$G_{NP}(k_N\, k_P) = \frac{1}{2} \sum_{s,m_s} [G(sm_s, T=1, \quad T_3=0; \quad k_N\, k_P) + \\ + G(sm_s, T=0, \quad T_3=0; \quad k_N\, k_P)] \,,$$

where s,m_s are the spin and its third component, T, T_3 the isotopic spin and its third component.

We can express the G matrix elements as the function of the relative momenta (the total momentum dependence is weak, so we can take an average of it) and the integrals can be written as

$$\frac{E(\text{pot})}{A} = \frac{c}{k_F^3} \int_0^{k_P} P_1(k_P, k)\, G_{PP}(k_N, k_P, k)\, dk + \\ + \frac{c}{k_F^3} \int_0^{k_N} P_1(k_N, k)\, G_{NN}(k_N, k_P, k)\, dk + \frac{2c}{k_F^3} \int_0^{\frac{k_N+k_P}{2}} P_2(k_N, k_P, k) \cdot \\ \cdot G_{NP}(k_N, k_P, k)\, dk, \tag{4}$$

where

$$P_1(K, k) = \frac{2}{3} k^2\, dk (K-k)^2 (2K+k) \,,$$

$$P_2(k_N, k_P, k) = \begin{cases} \dfrac{4}{3} k_P^3\, k^2\, dk \quad \text{if} \quad 0 < k < \dfrac{1}{2}(k_N - k_P) \\ k\, dk \left[\dfrac{2}{3} k(k_N^3 + k_P^3 + k^3) - \dfrac{1}{8}(k_N^2 - k_P^2)^2 - \right. \\ \left. - k^2(k_N^2 + k_P^2) \right] \quad \text{if} \quad \dfrac{1}{2}(k_N - k_P) < k < \dfrac{1}{2}(k_N + k_P) \,, \end{cases} \tag{5}$$

and

$$c = \frac{1}{2} \frac{1}{(2\pi)^6} (8\pi)^2 \frac{2}{3\pi^2}, \quad k_F^3 = \frac{2}{3\pi^2} \varrho \,, \tag{6}$$

where ϱ is the density of the system. The G matrix elements were calculated by SPRUNG et al. [1] for the density domain $0.4\ fm^{-1} \leq k_F \leq 1.6\ fm^{-1}$, using the reference spectrum method [2] in the same way as they had done in an earlier paper [3], only with slight modifications. An explicit calculation of DAHLBLOM [4] based on the three body cluster theory of BETHE [5] has shown that the intermediate state energy is small, so that it is justifiable to make it equal to zero in the calculations. The potentials used for the calculation are the soft core REID potentials [6]. The matrix elements were determined for the $N = Z$ (nuclear matter) and $Z = 0$ (neutron gas) cases. The comparison of them shows [7] that the assumption of BRUECKNER et al. [8], namely that

$$G_{NN}(k_N, k_P, k) \sim G_{NN}(k_N, k_N, k) \tag{7a}$$

is justified even for the two extreme cases $Z = 0$ and $Z = N$. The approximation is very good for $k_F \geq 1$ fm^{-1}, around nuclear matter density the deviation is only a few percent. It becomes worse at small densities, at $k_F = 0.4$ fm^{-1} the deviation is already 20—25%. Similar approximation is valid of course for the proton—proton interaction. The treatment of the unlike particle interaction is somewhat more doubtful but it seems reasonable to assume that

$$G_{NP}(k_N, k_P, k) \sim G_{NP}(k_A, k_A, k)\,, \tag{7b}$$

where

$$k_A^2 = \frac{k_N^2 + k_P^2}{2}\,. \tag{8}$$

With the above simplification we can expand the G matrix elements around their average density value. Going to the fourth order

$$\begin{aligned} G_{NN}(k_N, k) = G_{NN}(k_F, k) + \left.\frac{dG_{NN}}{dk_N}\right|_{k_N=k_F} (k_N - k_F) + \\ + \frac{1}{2}\left.\frac{d^2 G_{NN}}{dk_N^2}\right|_{k_N=k_F} (k_N - k_F)^2 + \frac{1}{6}\left.\frac{d^3 G_{NN}}{dk_N^3}\right|_{k_N=k_F} (k_N - k_F)^3 + \\ + \frac{1}{24}\left.\frac{d^4 G_{NN}}{dk_N^4}\right|_{k_N=k_F} (k_N - k_F)^4, \end{aligned} \tag{9a}$$

$$\begin{aligned} G_{NP}(k_A, k) = G_{NP}(k_F, k) + \left.\frac{dG_{NP}}{dk_A}\right|_{k_A=k_F} (k_A - k_F) + \\ + \frac{1}{2}\left.\frac{d^2 G_{NP}}{dk_A^2}\right|_{k_A=k_F} (k_A - k_F)^2. \end{aligned} \tag{9b}$$

Substituting (9a, b) and (5) into (4), we can expand everything as the function of $x = (N-Z)/A$, where part of C_2(pot) and C_4(pot) is a rearrangement contribution arising from the fact that G_{NN}, G_{NP} and G_{PP} are density dependent.

The symmetry energy calculations can be performed very easily owing to the fact that the G matrix elements are linear functions of

$$\begin{aligned} G_{PP} &= 4a_1 + 4b_1 k/k_F, \\ G_{NN} &= 4a_2 + 4b_2 k/k_F, \\ G_{NP} &= 2(a_3 + \alpha) + 2(b_3 + \beta) k/k_F, \end{aligned} \tag{10}$$

where $a_1 b_1$, $a_3 b_3$ and $a_2 b_2$ are the $T = 1$ contributions ($T_3 = 1, 0, -1$) to the interaction and α, β the $T = 0$ ones. In the above given density domain a, b, α, β can be represented very well with the following curves

$$a(y) = \frac{-0{,}9898}{y} - 1{,}1276 - 1{,}0658y + 0{,}2475y^2, \tag{11a}$$

$$b(y) = [1.7568 - 3.8708\,y + 3.6925y^2]\ \mathrm{k}_F/y, \tag{11b}$$

$$(y) = \frac{-8{,}2566}{y} - 0{,}5134 - 2{,}6061y + 1{,}1006y^2, \tag{11c}$$

$$(y) = [1.655 + 5.035y - 0.2669y^2]\ k_F/y, \tag{11d}$$

where

$$y = \begin{cases} k_P \\ k_A \\ k_N \end{cases} \quad \text{for} \quad T_3 = \begin{cases} 1 \\ 0 \\ -1\,. \end{cases}$$

Putting (9) (10) into (4) the potential energy turns out to be

$$\frac{E(\mathrm{pot})}{A} = \varepsilon_0\,(T=1) + \varepsilon_0(T=0) + x^2\,[\varepsilon_2(T=1) + \varepsilon_{2R}(T=1) + \tag{12}$$
$$+ \varepsilon_R(T=0) + \varepsilon_{2R}(T=0)] + x^4[\varepsilon_4(T=1) + \varepsilon_{4R}(T=1) +$$
$$+ \varepsilon_4(T=0) + \varepsilon_{4R}(T=0)]\,,$$

where ε_R means the rearrangement energy contribution. The $T = 1$ and $T = 0$ terms have the same sign in zeroth order but different signs in second order. On the other hand, the sign of the $T = 1$, $T_3 = 0$ term is the same as that of the $T = 1$, $T_3 = \pm 1$ for the zeroth order and opposite for second order. $\varepsilon_2(T = 1)$ and $\varepsilon_{2R}(T = 1)$ have opposite signs and the relative importance of ε_{2R} increases very fast with density: for the smallest k_F values $\varepsilon_2(T = 1) \sim 2\ \varepsilon_{2R}$ $(T = 1)$, but for large k_F $\varepsilon_2\,(T = 1) \sim 1/6\ \ \varepsilon_{2R}\,(T = 1)$. At nuclear matter density the factor is around 2/3. On the other hand for $T = 0$ ε_2 is always more than a magnitude higher than ε_{2R} and since $\varepsilon_2(T = 0)$ is also much higher than $\varepsilon_2(T = 1)$ (for small k_F values the factor is around 6, for high ones it is around 20) so the dominating term is always the $\varepsilon_2(T = 0)$. $\varepsilon_{2R}(T = 1)$ and $\varepsilon_{2R}(T = 0)$ have different signs and partly cancel each other. This reduces the importance of the rearrangement terms even more.

Since SPRUNG's results [1] give very small binding, we have to multiply the matrix elements (so the a, b, α, β) by a correction factor to get the correct nuclear matter volume energy. We are using here two types of correction: first we multiply all the $T = 1$ and $T = 0$ terms to get the correct binding (the correction factor is then 1.2239) and in the second case we suppose that the 3-body clusters would give a much greater contribution for tensor forces than for central ones [4], and so all the missing binding is due to the $T = 0$ terms, so we multiply only α, β (the correction factor in this case is 1.5432). The results for the energy in the two cases are shown in Figs. 1a and b, respectively. The minimizing density for the first type of correction is around

$k_F = 1.43$ fm^{-1} and for the second one around 1.38 fm^{-1}. The symmetry energy in the two cases is

$$16.35 + 14.13 = 30.48 \text{ MeV} \quad \text{and} \quad 19 + 13 = 32 \text{ MeV}. \tag{13}$$

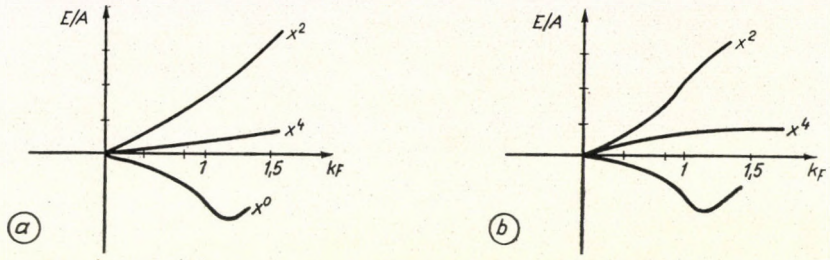

Fig. 1. Infinite nuclear system energy as the function of the Fermi momenta. The three curves represent the zeroth, second and fourth order terms in x. a) and b) are the values for the first and second type of correction

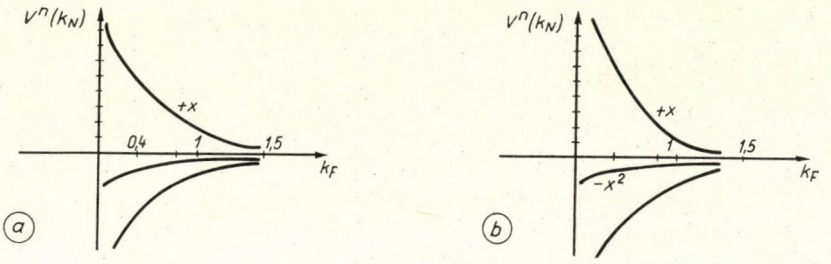

Fig. 2. $V^n(k_N)$ as the function of the Fermi momenta. The three curves represent the zeroth-first and second order terms in x. a) and b) are the values for the first and second type of correction

The first term comes in both cases from the potential energy, the second one from the kinetic energy. The experimental energy is (31 ± 1) MeV, so the agreement is very good. The rearrangement contribution in the first case is 1.3 MeV and 0.1 MeV in the second case, which shows that it is more important for relatively larger $T = 1$ forces. If we increase the values of a, b by a factor of 2 and correspondingly decrease α, β, the density increases to $k_F = 1.6$ fm^{-1}, and the symmetry energy is

$$(18 + 10 + 3) \text{ MeV},$$

where the first term is the kinetic energy, the second the potential energy without rearrangement and the third the rearrangement contribution.

One can see, that the rearrangement terms are very small in our results. BRUECKNER et al. [8] on the other hand, obtained much higher values.

They used, however, Gammel—Thaler potential, which overestimates the $T=1$ forces, and as we see, larger $T=1$ forces give larger rearrangement expressions. The use of the Gammel—Thaler potential can be the reason of their different results.

It is interesting to note that the coefficient of the x^4 term is extremely small. It shows that CAMERON probably overestimated the importance of this term [9] when he supposed that for big nuclei it can give a big contribution to the binding energy (of course for finite nuclei the surface symmetry energy can give quite large contribution to the 4^{th} order term).

The minimizing density of the infinite nuclear system changes if the number of protons and neutrons differs. The total energy of a nuclear system is:

$$\frac{E}{A} = f_1(\varrho) + f_2(\varrho)\, x^2 , \tag{14}$$

and the minimum condition

$$\frac{d(E/A)}{d\varrho} = \frac{df_1}{d\varrho} + \frac{df_2}{d\varrho}\, x^2 . \tag{15}$$

If $x = 0$, the solution of (15) is ϱ_0. For $x \neq 0$, the solution of (15) can be written as

$$\varrho = \varrho_0(1 + ax^2), \tag{16}$$

where

$$a = -\left[\frac{df_2}{d\varrho} \Big/ \frac{d^2 f_1}{d\varrho^2}\right]_{\varrho=\varrho_0} . \tag{17}$$

For the two different corrections a is ~ -1.06 and -0.96, respectively. So for large nuclei $\varrho_{\min}$ decreases slightly.

II. One particle energy at the Fermi surface

The energy of a particle at the Fermi surface can be written as

$$\epsilon(k_F) = T(k_F) + U(k_F) , \tag{18}$$

where the potential energy consist of two terms (8)

$$U(k_F) = V(k_F) + U_R(k_F) , \tag{19}$$

and for a neutron it can be written as

$$U^n(k_N) = E(k_N, k_P) - E(k_{N-1}, k_P) . \tag{20}$$

Again using the (7a,b) approximations

$$V^n(k_N) = \sum_{m=0}^{k_N} G_{NN}\left(k_N, \frac{|k_N - k_m|}{2}\right) + \sum_{m=0}^{k_P} G_{NP}\left(k_A, \frac{|k_N - k_m|}{2}\right), \qquad (21)$$

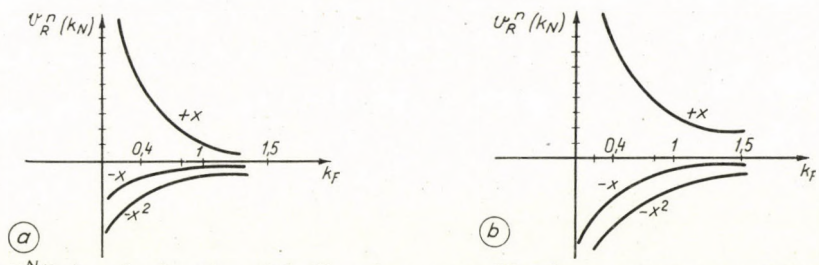

Fig. 3. $V_R^N(k_N)$ as the function of the Fermi momenta. The three curves represent the zeroth, first and second order terms in x. a) and b) are the values for the first and second type of correction

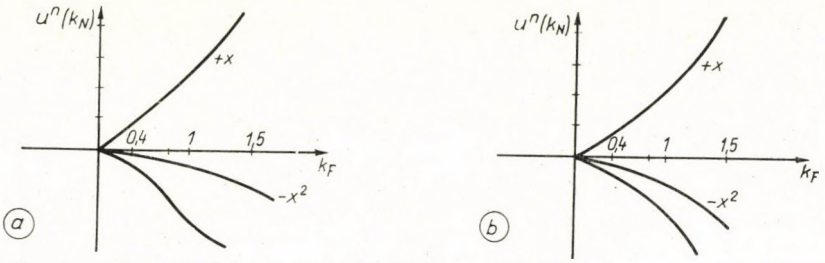

Fig. 4. One particle potential energy as the function of the Fermi momenta. The three curves represent the zeroth, first and second order terms in x. a) and b) are values for the first and second type of correction

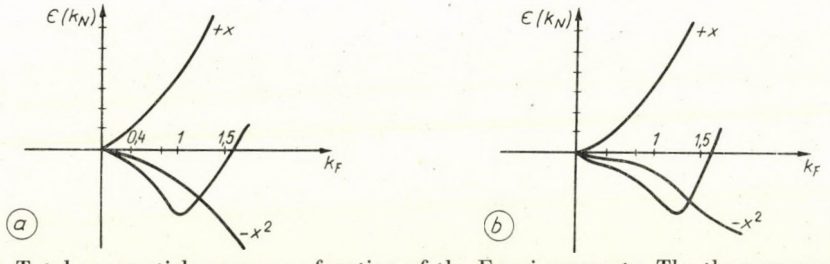

Fig. 5. Total one particle energy as function of the Fermi momenta. The three curves represent the zeroth, first and second order terms in x, a) and b) are values for the first and second type of correction

$$V_R^n(k_N) = \frac{1}{2} \sum_{m=0}^{k_N} \sum_{n=0}^{k_N} [G_{NN}(k_N, k) - G_{NN}(k_{N-1}, k)] + \\ + \sum_{m=0}^{k_N} \sum_{n=1}^{k_P} [G_{NF}(k_A, k) - G_{NF}(k_{A-1}, k)] , \tag{22}$$

$$k = \frac{k_m - k_n}{2} ,$$

where we neglected the terms proportional to A^0 compared with those proportional to A.

The calculation of (21) is straightforward. We again expand the integrals as a function of x, but keep only the linear and quadratic terms

$$V^n(k_F) = V_0^n(T=1) + V_0^n(T=0) + x\,[V_1^n(T=1) + V_{1R}^n(T=1) + \\ + V_1^n(T=0)] + x^2\,[V_2^n(T=1) + V_{2R}^n(T=1) + \\ + V_2^n(T=0) + V_{2R}^n(T=0)] , \tag{23}$$

where $V_1^n(T=0)$ is again much bigger (by a factor 10) than $V_1^n(T=1)$, (where the $T_3 = \pm 1$ and the $T_3 = 0$ terms partly cancel each other), and V_{1R}^n is again the same order of magnitude as V_1^n (at nuclear matter density slightly smaller) so it is not too important.

For the calculation of $V_R^n(k_N)$ we have to expand $G_{NN}(k_{N-1}, k)$ and $G_{NP}(k_{A-1}, k)$ around the k_N, k_A values

$$\left.\begin{aligned} G_{NN}(k_N, k) - G_{NN}(k_{N-1}, k) &= \frac{dG_{NN}(k_N, k)}{dk_N} (k_{N-1} - k_N), \\ G_{NP}(k_A, k) - G_{NP}(k_{A-1}, k) &= \frac{dG_{NP}(k_A, k)}{dk_N} (k_{A-1} - k_A), \end{aligned}\right\} \tag{24}$$

where

$$k_{N-1} - k_N = \frac{-\pi^2}{\Omega k_N}, \qquad k_{A-1} - k_A = \frac{-\pi^2}{2\Omega k_N k_A} . \tag{25}$$

Integrating and expanding as the function of x we can determine $V_R^n(k_F)$.

Figs. 2 and 3 contain the $V^n(k_N)$ and $V_R^n(k_N)$ curves, respectively, Fig. 4 the one particle potential energy and Fig. 5 the total one particle energy at the Fermi surface for the two types of correction. At nuclear matter density the energy of the last particles is $\epsilon(k_F) \sim -16$ MeV, which is as it should be. The rearrangement energy is 11.5—12 MeV, in good agreement with BRUCKNER's value [10]. On the other hand, the coefficient of the x term is higher for us ($U_1 = 35.5$ MeV or 41 MeV instead of 31.5 MeV) and the rearrangement energy contribution is very unimportant.

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ПЕРЕСТАНОВОЧНЫЙ ВКЛАД В ЭНЕРГИЮ СИММЕТРИИ И В ОДНОЧАСТИЧНЫЙ ПОТЕНЦИАЛ

Й. НЕЙМЕТ

Резюме

Определяется ядерная матрица как функция относительно импульса для случаев $N = 2$ и $Z = 0$. На основе этого определяются энергия симметрии и её перестановочная часть, и одночастичный потенциал с его перестановочной частью. Условие насыщения удовлетворяется, зависимость от импульса слаба, и так имеется возможность для усреднения, и написания интегралов.

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TRIAXIAL STATES OF LIGHT NUCLEIDES*

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The triaxial shapes of the first excited state of ^{16}O and of the ground states of ^{24}Mg and ^{32}S are studied in detail. Multipartite nucleon—nucleon interaction potentials, coupling Wigner central forces to Majorana exchange forces with both having Gaussian radial dependence, are employed in a variational calculation carried out in a Cartesian harmonic oscillator basis of states.

Among the fundamental nuclear quantities computed are binding energies, equilibrium oscillator energies, quadrupole moments Q_0 and Q_2, monopole moments, $B(E2)$ transition probabilities, and root-mean-square radii. For ^{16}O, ample comparisons are made between the ground and excited states, while for ^{24}Mg and ^{32}S, comparisons are made among the oblate, prolate, and triaxial shapes of the ground states of this pair of nucleides.

1. Introduction

In the literature [1—6], it has been asserted that the triaxial or asymmetric shape of the first excited state of ^{16}O and of the ground states of ^{24}Mg and ^{32}S lie lower in energy than corresponding oblate and prolate shapes, as determined from Hartree—Fock calculations employing effective nucleon-nucleon interaction potentials.

However, despite the fact that a Cartesian harmonic oscillator basis of states was utilized in each of the references cited above, not a single one presents the results of a full-fledged energy minimization with respect to a different oscillator energy along each of the three coordinate directions. This can probably be traced to the overriding computer costs arising from such a detailed investigation.

The goal of the paper at hand is to present the results of a complete triaxial variation involving the aforementioned nuclear states. The calculation is a variational one, performed in a rectangular basis of states. Three different effective nucleon – nucleon interaction potentials are analysed in this connexion. These are discussed in Section 2. In Section 3, the nucleon configurations under study are reviewed. Sections 4, 5, and 6 capsulise the predicted fundamental properties of $^{16}O^*$, ^{24}Mg, and ^{32}S, respectively. And, lastly, conclusions are drawn in Section 7.

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2. The effective nucleon—nucleon interaction potentials

The nucleon—nucleon interaction potentials employed in this study include the bipartite potentials of [1] and the tripartite potentials of [7]. Each part of every one of these potentials is associated with the coupling of a Wigner central force to a Majorana exchange force, where both have Gaussian radial dependence. The following formula may be used to generate these potentials

$$V(r) = \sum_{i=1}^{k} S_i \left[1 - M_i + M_i P_M\right] e^{-r^2/\mu_i^2}. \tag{1}$$

Here, the parameters S are strengths in units of MeV, the parameters μ represent ranges in units of fm, the dimensionless parameters M signify Majorana exchange coefficients, and P_M is the Majorana exchange operator.

The two-part interactions are generated by setting $K = 2$ in Eq. (1), and the three-part interactions, by letting $K = 3$. By imposing specific initial conditions on these interactions, parameter sets are evolved from which calculations of binding energies and other fundamental nuclear quantities may be carried out.

The parameter set B_1 of BRINK and BOEKER (B—B) [1] was determined by assuming a ground state binding energy (B.E.) of —28.3 MeV and an equilibrium harmonic oscillator energy $\hbar\omega$ of 21.0 MeV for ^{4}He, and a binding energy per nucleon of nuclear matter of — 15.75 MeV and an equilibrium Fermi momentum k_F of 1.45 fm^{-1}. Evolution of the B—B set C_1 involved only one differing assumption, that of an equilibrium $\hbar\omega$ for ^{4}He of 23.8 MeV.

The tripartite S—B parameter sets SB_1, SB_4, and SB_6 [7], which display significantly greater accuracy than the B—B sets in predictions of ground state binding energies for the light nucleides, assumed values of —29.1 MeV and 24.1 MeV for the ^{4}He B.E. and equilibrium $\hbar\omega$, respectively, in exact agreement with experimental results. The nuclear matter values were as for the B—B sets, both also being in accord with experiment.

And, the tripartite N—B parameter sets NB_1, NB_3, and NB_6 [7], which yielded dramatically improved equilibrium oscillator energies for the light nucleides as well as improved B.E. values in comparison to both the S—B and B—B parameter sets, imposed conditions on the B.E. and $\hbar\omega$ of the finite nucleide ^{40}Ca rather than on the nuclear matter properties. They were a B.E. of —419.6 MeV and an $\hbar\omega$ of 9.9 MeV, both in congruence with experimental results. The assumptions for ^{4}He mirrored those of the S—B sets.

A compilation of the eight parameter sets B_1, C_1, SB_1, SB_4, SB_6, NB_1, NB_3, and NB_6 is given in Table I. It should be noted that no account of the Coulomb repulsion was taken in determining them.

3. The nucleon configurations

In Table II, the nucleon configurations for the ^{16}O ground state and first excited state, and the three states of ^{24}Mg and ^{32}S, are given for a rectangular harmonic oscillator basis of states. Therein, the letter O designates an oblate shape, the letter P, a prolate shape, the letter S, a spherical shape, and the letter T, a triaxial state.

Table I

Representative B—B, S—B, and N—B parameter sets. The strengths S are in MeV and the ranges μ are in fm

Set	μ_1	S_1	M_1	μ_2	S_2	M_2	μ_3	S_3	M_3
B_1	0.7	389.5	−0.529	1.40	−140.60	0.4864	—	—	—
C_1	0.7	271.0	−1.635	1.40	−117.40	0.3815	—	—	—
SB_1	0.3	41868.0	−62.680	0.45	−10203.53	−60.4320	0.6	−1735.10	37.981
SB_4	0.5	1686.0	−8.430	1.00	−404.51	−2.1660	1.5	−1.58	60.026
SB_6	0.5	1630.0	−5.270	1.00	−392.30	−0.7870	2.0	−1.80	6.273
NB_1	0.8	415.0	−26.160	1.20	−237.93	−13.2280	1.6	−5.47	83.013
NB_3	0.5	453.0	−48.140	1.00	−132.28	−11.6560	1.5	−17.42	8.301
NB_6	0.6	477.0	−33.560	1.20	−154.94	−5.5260	2.4	−5.96	3.720

Table II

Nucleon configurations for ^{16}O, ^{24}Mg, and ^{32}S

Nucleide	Configuration Designation	Configuration
^{16}O	*O(S)*	$(000)^4(100)^4(010)^4(001)^4$
	O(T)	$(000)^4(100)^4(010)^4(200)^4$
^{24}Mg	*MG(O)*	$(000)^4(100)^4(010)^4(001)^4(200)^4(020)^4$
	MG(P)	$(000)^4(100)^4(010)^4(001)^4(110)^4(101)^4$
	MG(T)	$(000)^4(100)^4(010)^4(001)^4(200)^4(110)^4$
^{32}S	*S(O)*	$(000)^4(100)^4(010)^4(001)^4(200)^4(020)^4(002)^4(110)^4$
	S(P)	$(000)^4(100)^4(010)^4(001)^4(110)^4(101)^4(011)^4(200)^4$
	S(T)	$(000)^4(100)^4(010)^4(001)^4(200)^4(020)^4(110)^4(101)^4$

4. The $^{16}O^*$ state

The first excited state of ^{16}O is generally assumed to be a $4p - 4h$ excitation of the ground state [1, 2]. Given the spherical configuration in Table II for the ^{16}O ground state, the excitation involves raising a particle quartet

from the $(001)^4$ level to the $(200)^4$ level, yielding a triaxial configuration. Experimentally, this first excited state is a O^+ level lying 6.06 MeV above the ground state. In order to compute its excitation energy, the difference in binding energies between the ^{16}O ground state and the $4p - 4h$ excited state must be taken. The binding energy equation is expressed as follows for $^{16}O^*$

$$\begin{aligned} \text{B.E.}(^{16}O^*) &= 9.75\ \hbar\omega_x + 5.75\ \hbar\omega_y + 3.75\ \hbar\omega_z + 38.25\ V(000) \\ &+ 32.5\ V(100) + 17.5\ V(010) + 10.5\ V(200) + 3.0\ V(020) \\ &+ 6.0\ V(110) + 2.5\ V(210) + 7.5\ V(300) + 2.25\ V(400). \end{aligned} \tag{2}$$

Here, the potential energy matrix elements $V(n_x, n_y, n_z)$, expressed as functions of relative quantum numbers n_x, n_y, and n_z, are defined in [1].

Table III lists both the ^{16}O ground and excited state energy predictions of the octet of parameter sets under examination. On the average, the B—B sets achieve an average excitation energy ΔE of 24.3 MeV, the S—B sets, an average value of 40.8 MeV, and the N—B sets, an average of 41.6 MeV. All are substantially higher than the experimental value. Also, it should be noted that the B—B values of ΔE may not be any more accurate than the S—B and N—B values, for the former represent excitations from ground states which are noticeably underbound in contrast to the latter, as indicated in Table III.

Although the magnitudes of the predicted triaxial $\hbar\omega$ values are greater for the S—B sets than for the B—B and N—B sets, an objective comparison is best afforded through an analysis of various fundamental nuclear quantities. Among these are the quadrupole moments Q_0 and Q_2, the monopole moment $\langle R^2 \rangle$, the $B(E2)_{2^+ \to 0^+}$ transition probability, and the root-mean-square (r.m.s.) radius $\langle r^2 \rangle^{\frac{1}{2}}$. Table IV tabulates these quantities for the excited state $^{16}O^*$.

The intrinsic quadrupole moment Q_0, which measures the charge deformation of a nucleus, is calculated from the equation

$$Q_0 = \frac{\hbar^2}{2m}\left[\frac{2N_x}{\hbar\omega_x} - \frac{N_y}{\hbar\omega_y} - \frac{N_z}{\hbar\omega_z}\right], \tag{3}$$

where the total quantum numbers N_x, N_y, and N_z along the x-, y-, and z-directions, respectively, are given by

$$N_x = \sum_{i=1}^{A}\left(n_{x_i} + \frac{1}{2}\right), \tag{4}$$

$$N_y = \sum_{i=1}^{A}\left(n_{y_i} + \frac{1}{2}\right) \tag{5}$$

Table III

Energy results for ^{16}O, including the triaxial B. E. (TE) and three triaxial equilibrium $\hbar\omega$ values of the first excited state, and spherical B. E. (SE) and equilibrium $\hbar\omega$ of the ground state

Set	TE	$\hbar\omega_x$	$\hbar\omega_y$	$\hbar\omega_z$	SE	$\hbar\omega$	ΔE
B_1	−82.3	8.0	17.0	11.0	−106.7	13.4	24.4
C_1	−75.4	8.0	17.0	12.0	−99.6	13.7	24.2
SB_1	−99.2	10.0	21.0	15.0	−140.0	17.2	40.8
SB_4	−100.6	10.0	21.0	15.0	−141.8	17.2	41.2
SB_6	−99.7	10.0	20.0	14.0	−139.6	17.0	39.8
NB_1	−100.6	8.0	15.0	12.0	−142.3	12.8	41.7
NB_3	−100.9	8.0	15.0	12.0	−142.5	12.8	41.6
NB_6	−101.3	8.0	15.0	12.0	−142.7	12.7	41.4

Table IV

Various fundamental nuclear properties of $^{16}O^*$, as computed from the B—B, and N—B parameter sets

Set	Q_0	Q_2	$\langle R^2\rangle$	$B(E^2)$	$\langle r^2\rangle^{\frac{1}{2}}$
B_1	74.01	0.89	81.61	196.10	3.19
C_1	75.27	−1.63	80.36	202.83	3.17
SB_1	60.08	−1.58	64.42	129.21	2.84
SB_4	60.08	−1.58	64.42	129.21	2.84
SB_6	58.69	−1.19	65.81	123.33	2.87
NB_1	78.32	−5.53	82.31	192.44	3.21
NB_3	78.32	−5.53	82.31	192.44	3.21
NB_6	78.32	−5.53	82.31	192.44	3.21

and

$$N_z = \sum_{i=1}^{A} \left(n_{z_i} + \frac{1}{2} \right) , \tag{6}$$

Here, the quantity $(\hbar^2/m) = 41.5$ MeV · fm^2, and A represents the total number of nucleons in the nucleus. The magnitude of Q_0 is somewhat less for the S—B parameter sets than for the B—B and N—B sets.

Another quadrupole moment, Q_2, is defined for asymmetric nucleides by

$$Q_2 = \frac{\hbar^2}{m} \left[\frac{N_z}{\hbar\omega_z} - \frac{N_y}{\hbar\omega_y} \right]. \tag{7}$$

The values for Q_2 are of much smaller magnitude than those for Q_0, with

different values being predicted by each of the three groups of parameter sets.

In order to compute the monopole moment $\langle R^2 \rangle$, the following equation is invoked

$$\langle R^2 \rangle = \frac{\hbar^2}{2m} \left[\frac{N_x}{\hbar\omega_x} + \frac{N_y}{\hbar\omega_y} + \frac{N_z}{\hbar\omega_z} \right]. \tag{8}$$

Again, the S—B predictions for $\langle R^2 \rangle$ are lower than corresponding B—B and N—B predictions.

The $B(E2)_{2^+ \to 0^+}$ values gauge the strengths of electric quadrupole transitions between the 2^+ and 0^+ levels of a deformed nucleus. The relationship between $B(E2)$ and the intrinsic quadrupole moment Q_0 is

$$B(E2)_{2^+ \to 0^+} = \frac{5}{16\pi} e^2 Q_0^2, \tag{9}$$

where $e^2 = 0.36$, assuming an effective charge of $\frac{1}{2}e$ for protons. The $B(E2)$ results follow the trend of the Q_0 values, with the predicted S—B probabilities being the lowest.

Lastly, the r.m.s. radius is determined from the equation

$$\langle r^2 \rangle^{1/2} = \left(\frac{\hbar^2}{2mA} \left[\frac{N_x}{\hbar\omega_x} + \frac{N_y}{\hbar\omega_y} + \frac{N_z}{\hbar\omega_z} \right] \right)^{1/2}. \tag{10}$$

And, once again, the S—B values are lower than the B—B and N—B predictions, characterizing their differences in predictions of equilibrium oscillator energies.

It should be emphasized that the various equations for nuclear properties presented in this section strictly apply to $4n$ doubly even nucleides, such as ^{16}O, ^{24}Mg, and ^{32}S.

5. The triaxial state of ^{24}Mg

Energy results for the nucleide ^{24}Mg are tabulated in Table V. Included in that Table are the predicted oblate and prolate energy minimum for each parameter set as well as the difference ΔE between the better of the latter two and the triaxial energy. The configuration of the triaxial shape is given in Table II, while the corresponding equation for its ground state B.E. is

$$\begin{aligned} \text{B.E.}(^{24}\text{Mg}) = {} & 13.75\ \hbar\omega_x + 9.75\ \hbar\omega_y + 7.75\ \hbar\omega_z + 69.0\ V(000) \\ & + 56.25\ V(100) + 38.75\ V(010) + 25.0\ V(001) \\ & + 17.25\ V(200) + 7.5\ V(020) + 3.0\ V(002) + 8.25\ V(110) \\ & + 7.5\ V(101) + 4.5\ V(011) + 8.75\ V(210) + 2.5\ V(201) \\ & + 5.0\ V(120) + 2.5\ V(111) + 11.25\ V(300) + 1.5\ V(220) \\ & + 2.25\ V(400) + 2.25\ V(310). \end{aligned} \tag{11}$$

For ^{24}Mg, the triaxial state does indeed lie lowest, with ΔE averaging 9.3 MeV for the B—B sets, 17.9 MeV for the S—B sets, and 12.3 MeV for the N—B sets. This means that the theoretical ^{24}Mg B.E. is brought that much closer to the experimental B. E. of —228.3 MeV.

Table V

Energy results for ^{24}Mg, including the three triaxial equilibrium $\hbar\omega$ values, triaxial B. E. (*TE*), oblate B. E. (*OE*), prolate B. E. (*PE*), and the difference ΔE between the better of the latter two and *TE*, for the B—B, S—B, and N—B parameter sets

Set	$\hbar\omega_x$	$\hbar\omega_y$	$\hbar\omega_z$	*TE*	*OE*	*PE*	ΔE
B_1	9.0	12.0	15.0	—153.0	—143.9	—139.5	9.1
C_1	9.0	13.0	15.0	—143.1	—133.7	—130.2	9.4
SB_1	12.0	16.0	19.0	—200.9	—185.9	—178.8	15.0
SB_4	12.0	16.0	19.0	—202.3	—188.8	—182.2	20.1
SB_6	12.0	16.0	18.0	—200.0	—187.2	—181.5	18.5
NB_1	9.0	12.0	14.0	—206.8	—193.5	—193.6	13.2
NB_3	9.0	12.0	14.0	—206.4	—193.6	—193.6	12.8
NB_6	9.0	12.0	14.0	—207.1	—194.9	—196.1	11.0

Table VI

Various fundamental nuclear properties of the triaxial state of ^{24}Mg, as computed from the B—B, S—B, and N—B parameter sets

Set	Q_0	Q_2	$\langle R^2\rangle$	$B(E2)$	$\langle r^2\rangle^{\frac{1}{2}}$
B_1	72.39	—24.90	121.27	187.63	3.18
C_1	75.05	—19.58	118.61	201.57	3.14
SB_1	53.42	—16.93	91.83	102.17	2.77
SB_4	53.42	—16.93	91.83	102.17	2.77
SB_6	52.45	—14.99	92.80	98.49	2.78
NB_1	70.81	—21.74	122.85	179.52	3.20
NB_3	70.81	—21.74	122.85	179.52	3.20
NB_6	70.81	—21.74	122.85	179.52	3.20

The equilibrium triaxial $\hbar\omega$ values for the S—B parameter sets are greater than those for the B—B and N—B sets, as was the case for ^{16}O*. Table VI reflects the effect of such a difference in terms of the quadrupole and monopole moments, transition probabilities, and r.m.s. radii. It is seen that the magnitudes for all of these quantities are definitely lower for the S—B sets.

6. The triaxial state of ^{32}S

Although the enhancements of the ^{32}S ground state binding energy afforded by the triaxial state are less than those afforded to the ^{24}Mg ground state, the triaxial state still lies lower than the other possible shapes, as depicted by Table VII. The average ΔE gains are 3.6 MeV for the B—B sets, 7.5 MeV for the S—B sets, and 1.9 MeV for the N—B sets. These thus bring the calculated ^{32}S B.E. nearer its experimental value of —322.7 MeV. The triaxial ^{32}S binding energies are determined from the following equation

$$\begin{aligned}\text{B.E.}(^{32}\text{S}) &= 17.75\ \hbar\omega_x + 15.75\ \hbar\omega_y + 11.75\ \hbar\omega_z + 101.25\ V(000) \\ &+ 80.0\ V(100) + 72.5\ V(010) + 47.5\ V(001) + 24.75\ V(200) \\ &+ 18.75\ V(020) + 7.5\ V(002) + 18.0\ V(110) + 10.5\ V(101) \\ &+ 12.0\ V(011) + 13.75\ V(210) + 11.25\ V(201) + 12.5\ V(120) \\ &+ 3.75\ V(021) + 5.0\ V(102) + 15.0\ V(300) + 11.25\ V(030) \\ &+ 7.5\ V(111) + 2.25\ V(400) + 2.25\ V(040) + 2.25\ V(220) + \\ &+ 1.5\ V(202) + 1.5\ V(211) + 0.75\ V(121) + 2.25\ V(310) \\ &+ 2.25 V(130) + 2.25\ V(301). \end{aligned} \tag{12}$$

With respect to the triaxial $\hbar\omega$ values, once again the S—B predictions are greater than the B—B and N—B predictions. These, in turn, lead to lower values of the quadrupole and monopole moments, transition probabilities, and r.m.s. radii. Table VIII provides a breakdown of these quantities.

7. Summary and conclusions

A $4p - 4h$ excitation of the ^{16}O ground state to a triaxially deformed state, while theoretically feasible, yields an excitation energy far in excess of the experimentally determined value of 6.06 MeV as computed from various multipartite effective nucleon—nucleon interaction potentials. The B—B predictions for the excitation do appear to be better than the S—B and N—B predictions, yet are still much too high.

However, the assumption of a triaxial deformation for the ground states of the nucleides ^{24}Mg and ^{32}S is certainly justified, as tangible gains over the binding energies predicted by corresponding oblate and prolate shapes are realized when it is considered.

The S—B predictions for the equilibrium triaxial $\hbar\omega$ values are greater than those of the B—B and N—B parameter sets, with this resulting in S—B values for the quadrupole and monopole moments, $B(E2)_{2^+ \to 0^+}$ transition probabilities, and r.m.s. radii that are of significantly lower magnitude.

Table VII

Energy results for ^{32}S, including the three triaxial equilibrium $\hbar\omega$ values, triaxial B. E. (*TE*), oblate B. E. (*OE*), prolate B. E. (*PE*), and the difference ΔE between the better of the latter two and *TE*, for the B—B, S—B, and N—B parameter sets

Set	$\hbar\omega_x$	$\hbar\omega_y$	$\hbar\omega_z$	*TE*	*OE*	*PE*	ΔE
B_1	10.0	11.0	14.0	—220.9	—206.1	—217.6	3.3
C_1	10.0	11.0	14.0	—209.1	—193.8	—205.3	3.8
SB_1	12.0	13.0	17.0	—292.1	—266.4	—283.0	9.1
SB_4	12.0	14.0	17.0	—292.5	—270.0	—285.3	7.2
SB_6	12.0	13.0	17.0	—290.6	—269.0	—284.5	6.1
NB_1	9.0	10.0	13.0	—297.8	—277.0	—294.7	3.1
NB_3	9.0	10.0	13.0	—295.8	—277.1	—294.4	1.4
NB_6	9.0	10.0	13.0	—297.8	—278.8	—296.7	1.1

Table VIII

Various fundamental nuclear properties of the triaxial state of ^{32}S, as computed from the B—B, S—B, and N—B parameter sets

Set	Q_0	Q_2	$\langle R^2\rangle$	$B(E2)$	$\langle r^2\rangle^{\frac{1}{2}}$
B_1	53.46	—49.58	170.64	102.33	3.27
C_1	53.46	—49.58	170.64	102.33	3.27
SB_1	44.13	—43.57	142.62	69.72	2.99
SB_4	47.78	—36.27	138.97	81.72	2.95
SB_6	44.13	—43.57	142.62	69.72	2.99
NB_1	61.29	—56.18	187.71	134.49	3.42
NB_3	61.29	—56.18	187.71	134.49	3.42
NB_6	61.29	—56.18	187.71	134.49	3.42

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ТРЕХОСНЫЕ СОСТОЯНИЯ ЛЕГКИХ ЯДЕР

Ф. Р. РУЭЛ (мл.)

Резюме

Детально изучены трехосные формы первого возбужденного состояния ^{16}O и основных состояний ^{24}Mg и ^{32}S. В расчетах применялся вариационный принцип с учетом многочастичного нуклон-нуклонного потенциала в предположении, что центральносимметричные силы Вигнера и обменные силы Майорана зависят от расстояния как функция Гаусса, а в качестве базисных функций использовались волновые функции гармонического осциллятора.

Среди прочих основных ядерных характеристик рассчитаны энергии связей, равновесные осцилляторные энергии, квадрупольные моменты Q_0 и Q_2, монопольные моменты, вероятности перехода $B(E2)$ и среднеквадратичные радиусы. Для ^{16}O проведено подробное сравнение основного и возбужденного состояний, а для ^{24}M и ^{32}S сравнены сжатые, растянутые и триаксиальные формы основных состояний этих пар ядер.

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ИССЛЕДОВАНИЕ РЕАКЦИЙ РАДИАЦИОННОГО ЗАХВАТА БЫСТРЫХ НЕЙТРОНОВ, ПРИВОДЯЩИХ К СПОНТАННО-ДЕЛЯЩИМСЯ ИЗОМЕРАМ ^{242}Am и ^{244}Am

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ОБЪЕДИНЕННЫЙ ИНСТИТУТ ЯДЕРНЫХ ИССЛЕДОВАНИЙ, ЛАБОРАТОРИЯ ЯДЕРНЫХ РЕАКЦИЙ, ЛАБОРАТОРИЯ НЕЙТРОННОЙ ФИЗИКИ, ДУБНА, СССР

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Измерена зависимость отношения сечений образования спонтанно делящихся изомеров ^{242}Am и ^{244}Am и мгновенного деления в реакциях ^{241}Am + n и ^{243}Am + n от энергии нейтронов вплоть до 16 Мэв. Эти отношения оказались одного порядка для обоих изомеров и монотонно уменьшаются с ростом энергии нейтронов. Полученные результаты обсуждаются на основе модели двугорбого барьера деления.

Исследования спонтанно делящихся изомеров показали, что эти состояния характеризуются рядом необычных свойств:

1. вероятность спонтанного деления повышена до 10^{30} раз по сравнению с основным состоянием [1, 2].

2. изомерное отношение остается постоянным при изменении вносимого в ядро момента [3].

3. наблюдается корреляция между образованием спонтанно делящихся изомеров и вынужденным делением [4, 5].

Эта корреляция четко проявляется в реакциях радиационного захвата нейтронов, приводящих к спонтанно делящимся изомерам ^{242}Am и ^{244}Am [4, 6]. Измеренные функции возбуждения указывают на пороговый характер этих реакций. При этом порог реакции образования делящегося изомера оказывается близким к порогу деления (6,4 Мэв для ^{242}Am и 6,2 Мэв для ^{244}Am), хотя энергия изомерного состояния составляет около 3 Мэв [7, 8].

Такие свойства изомерных состояний, повидимому, связаны со сложной структурой барьера деления. Проведенные В. М. Струтинским расчеты оболочечных поправок к капельному барьеру деления показали, что в ряде ядер при значениях параметра деформации $\sim$0,6 реальный барьер деления имеет минимум [9] (фиг. 1). Если этот минимум достаточно глубокий, то в нем будет иметь место система уровней, нижний из которых является изомерным. Сечение реакции образования ядра в изомерном состоянии, а также ход функции возбуждения существенно зависят от параметров двугорбого барьера. Поэтому исследование таких реакций позволяет получить ряд сведений о структуре барьера деления.

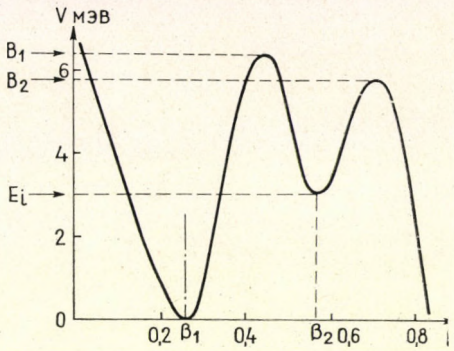
Целью данной работы являлось измерение функций возбуждения реакций образования спонтанно делящихся изомеров ^{242}Am и ^{244}Am при радиационном захвате нейтронов до энергии 16 Мэв.

Измерения были проведены на электростатическом генераторе Лаборатории нейтронной физики ОИЯИ. Схема экспериментальной установки представлена на фиг. 2. Пучок протонов или дейтонов падал на мишень, укрепленную на дне цилиндра Фарадея, который служил для измерения тока пучка. Модуляция пучка производилась при помощи прямоугольных импульсов напряжения с амплитудой до 4 кв, которые подавались на плоскопараллельные пластины. Для регистрации осколков деления использовался многонитевой искровой счетчик [10], наполненный смесью N_2 (10 торр), и He (750 торр). Облучаемые мишени из ^{241}Am и ^{243}Am весом 0,4 $\frac{\text{мг}}{\text{см}^2}$ и площадью 12 см^2 находились внутри счетчика. При надлежащем выборе рабочего напряжения счетчик был практически нечувствителен к интенсивному потоку α-частиц из мишени (фон счетчика не превышал 1—2 импульсов в час). Импульсы со счетчика, вызываемые осколками деления, подавались на временной анализатор, работа которого была синхронизована с модуляцией пучка ускоренных частиц. Измерялось число импульсов во время облучения мишени (это число определяло выход осколков мгновенного деления), а также временное распределение импульсов, когда пучок не попадал на мишень. В этом случае выход осколков связан с распадом спонтанно делящихся изомеров, образующихся в реакциях радиационного захвата нейтронов. Идентификация спонтанно делящихся изомеров производилась по их периодам полураспада (14 мсек для ^{242}Am и 1,1 мсек для ^{244}Am [11]). Изомеры, которые могли бы получаться в реакциях (n, n′) и (n, 2n) имели заметно меньшие периоды полураспада, и их выход не мог исказить полученные результаты.

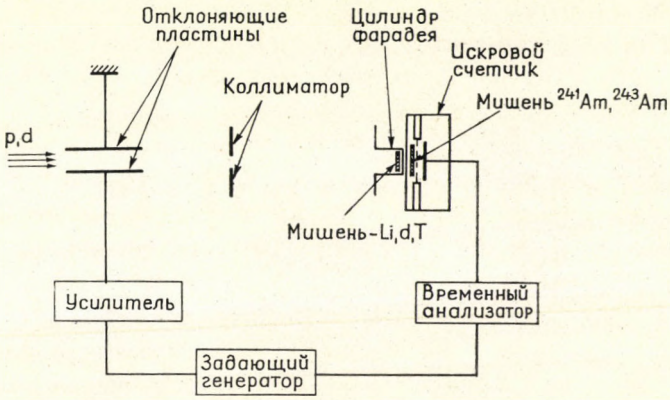
Источником нейтронов служили реакции ^{7}Li(p,n)^{7}Be, ^{3}T(p,n)^{3}He, ^{2}D(d,n)^{3}He, ^{3}T(d,n)^{4}He. Толщина мишени дейтерия или трития соответствовала потери энергии дейтонов $\sim$1 Мэв. Спектр нейтронов из такой мишени в реакции D + d при энергии дейтонов 3,5 Мэв представлен на фиг. 3. Этот спектр рассчитан из известного сечения реакции и углового распределения нейтронов для телесного угла, определяемого геометрией опыта. Для получения нейтронов с энергией до 2,3 Мэв использовалась толстая литиевая мишень. Спектры нейтронов из этой мишени при различных энергиях протонов, рассчитанные аналогичным способом, также представлены на фиг. 3. В этом случае измеренный выход осколков мгновенного и запаздывающего деления относится к широкому диапазону энергий нейтронов (от порога реакции до максимальной энергии, определяемой энергией протонов). Выход осколков, относящийся к более узкому интервалу энергий, равен, очевидно, разности выходов при двух соседних энергиях. Энергия протонов менялась

от 2,75 Мэв до 4,0 Мэв с интервалом 0,25 Мэв, что соответствовало диапазону энергий нейтронов от 0,8 до 2,0 Мэв.

Из измеренного на опыте отношения выходов осколков запаздывающего и мгновенного деления после введения поправок на распад изомера можно



Фиг. 1. Двугорбый барьер деления. V — энергия деформации; β — параметр деформации; E_i — энергия изомерного уровня; B_1, B_2 — высоты первого и второго барьеров; β_1, β_2 — параметры деформации основного и изомерного состояний



Фиг. 2. Схема экспериментальной установки

получить отношение сечений этих процессов. Зависимость этих отношений от энергии нейтронов представлена на фиг. 4. В случае реакции ^{241}Am + n приведено также отношение сечений для тепловых нейтронов, измеренное с использованием той же методики и мишени [5]. Из фиг. 4 видно, что отношение сечений образования изомера и мгновенного деления в реакциях ^{241}Am + n и ^{243}Am + n близки по порядку величины и монотонно убывают с ростом энергии нейтронов. Для энергии нейтронов 16 Мэв спонтанно делящийся изомер ^{242}Am уже не наблюдался, поэтому для отношения сечений приведена верхняя граница. Выход изомера ^{244}Am при этой энергии нейтронов невозможно увидеть

на фоне изомера ^{242}Am, который образуется со значительно большим сечением в реакции ^{243}Am (n, 2n). Сечения деления ^{241}Am и ^{243}Am нейтронами известны [12, 13], поэтому из измеренных отношений сечений запаздывающего и мгновенного деления можно получить функции возбуждения реакций образования спонтанно делящихся изомеров ^{242}Am и ^{244}Am. Эти функции возбуждения для реакции ^{241}Am + n представлены на фиг. 5. Для реакции ^{243}Am + n функции возбуждения имеют аналогичный вид. Чтобы показать, как меняются с ростом энергии нейтронов сечения реакций, приводящих к основным состояниям ^{242}Am и ^{244}Am, на фиг. 5 представлена функция возбуждения реакции ^{238}U (n, γ)^{239}U [17] (для ^{241}Am и ^{243}Am подобные измерения еще не проведены).

Из фиг. 5 видно, что функции возбуждения реакций, приводящих к основному и изомерному состояниям, подобны лишь при энергиях нейтронов выше 1,5 Мэв. При уменьшении энергии нейтронов ниже 1,5 Мэв сечение реакции для изомера не растет, как для основного состояния, а падает, обнаруживая такой же пороговый вид, как сечение мгновенного деления ^{241}Am нейтронами. Более подробно вид функции возбуждения реакций образования ^{242}Am и ^{244}Am вблизи порога исследован в работах [4, 6].

Как уже отмечалось [4—6], пороговый ход функции возбуждения реакций образования спонтанно делящихся изомеров трудно объяснить на основе прежних представлений об изомерных состояниях, но он получает естественное объяснение в модели двугорбого барьера. В этой модели для заселения изомерного состояния необходимо преодолеть барьер, разделяющий первый и второй минимум, и этот же барьер в ряде случаев определяет порог деления.

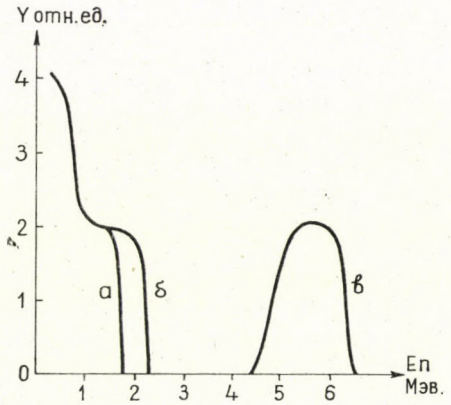
Анализ функции возбуждения реакции образования изомерного состояния на основе модели двугорбого барьера позволяет получить ряд сведений о параметрах этого барьера. При этом предполагается, что процессы деления и образования изомера можно рассматривать как двухступенчатые. После захвата нейтрона образуется составное ядро, в котором устанавливается тепловое равновесие (энергия возбуждения сосредоточена на одночастичных степенях свободы). Когда энергия возбуждения переходит на колебательные степени свободы, то ядро может преодолеть первый барьер и оказаться во второй потенциальной яме. Если эта яма достаточно глубока, то в ней будет иметь место сильное взаимодействие между колебательными и одночастичными степенями свободы. В результате этого во второй яме может снова наступить тепловое равновесие, и образуется такое же составное ядро, как и после захвата нейтрона, характеризующееся, однако, большей деформацией и меньшей тепловой энергией. Испускание γ-квантов из такого ядра приводит к образованию спонтанно делящихся изомеров, а переход через второй барьер — к делению. Отношение сечений этих процессов имеет вид [14, 16]:

$$\frac{\sigma_i}{\sigma_f} = \frac{\Gamma_{\gamma 2}}{\Gamma_{f2}}, \qquad (1)$$

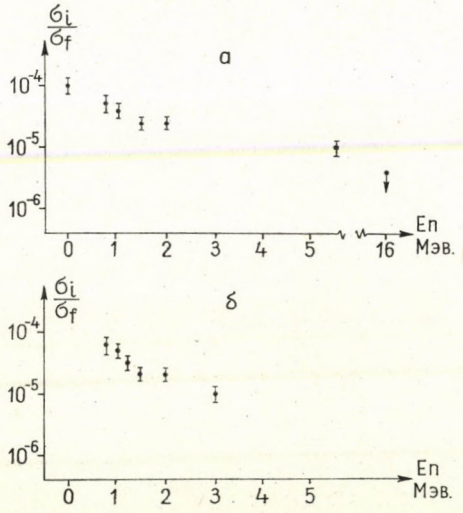
где $\Gamma_{\gamma 2}$ и Γ_{f2} — радиационная и делительная ширина уровней во второй яме.

$$\Gamma_{f2} = \frac{N_2}{2\pi\varrho(E^* - E_i)}, \tag{2}$$

$$\Gamma_{\gamma 2} \sim \frac{1}{\varrho(E^* - E_i)} \int_0^{E^* - E_i} (E^* - E_i - E)^3 \, \varrho(E)\, dE, \tag{3}$$



Фиг. 3. Спектры нейтронов в реакциях. а) ^{7}Li + p ($E_p = 3{,}5$ Мэв); б) ^{7}Li + p ($E_p = 4{,}0$ Мэв); в) ^{2}D + d ($E_d = 3{,}5$ Мэв)



Фиг. 4. Зависимость отношения сечений образования спонтанно делящегося изомера и деления (σ_i/σ_f) от энергии нейтронов (E_n). а) в реакции ^{241}Am + n; б) в реакции ^{243}Am + n

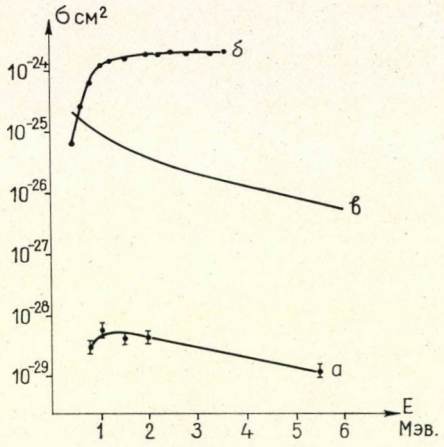
где $\varrho(E)$ — плотность уровней во второй яме при энергии возбуждения E; N_2 — число открытых каналов для перехода через второй барьер; E^* — энергия возбуждения составного ядра, равная сумме энергии связи нейтрона и его кинетической энергии; E_i — энергия изомерного уровня. Для ядра ^{242}Am значение E_i принималось равным 3,2 Мэв [8]. При расчетах плотности уровней во второй яме и числе открытых каналов на втором барьере значение параметра плотности уровней a принималось равным 28,6 [18] (как и для первой ямы). При энергии возбуждения ниже вершины второго барьера число открытых каналов заменялось проницаемостью для перехода через этот барьер. При этом параметр $\hbar\omega$, характеризующий кривизну второго барьера выбирался равным 600 кэв. В расчетах радиационной ширины принималось, что $\Gamma_{\gamma 2} = 0{,}03$ эв при $E^* = 5{,}5$ Мэв (энергия связи нейтрона в ядре ^{242}Am). Кроме того, в расчетах отношений $\Gamma_{\gamma 2}/\Gamma_{f2}$ предполагалось, что к изомерному состоянию приводит лишь испускание таких γ-квантов, после которых ядро остается с энергией возбуждения ниже вершины второго барьера; в противном случае произойдет деление после испускания γ-кванта. Распределение γ-квантов по энергиям определяется выражением (3).

Из выражений (2), (3) можно видеть, что радиационная ширина сравнительно мало меняется с ростом энергии возбуждения, в то время как делительная ширина при этом быстро растет, пока энергия возбуждения не достигает вершины барьера деления; после этого рост сильно замедляется. Поэтому рассчитанные по формулам (2), (3) зависимости отношений $\Gamma_{\gamma 2}/\Gamma_{f2}$ от энергии возбуждения для различных значений высоты второго барьера (фиг. 6) обнаруживают излом при энергии возбуждения, близкой к энергии второго барьера. При других значениях параметров a, $\hbar\omega$ и $\Gamma_{\gamma 2}$ при $E^* = 5{,}5$ Мэв форма рассчитанных кривых остается практически такой же, меняются лишь абсолютные значения отношений $\Gamma_{\gamma 2}/\Gamma_{f2}$. Поэтому по излому кривой, описывающей зависимость отношения сечений образования изомера и деления от энергии возбуждения, можно определить высоту второго барьера, оставаясь, естественно, в рамках рассмотренного выше двухступенчатого хода реакции.

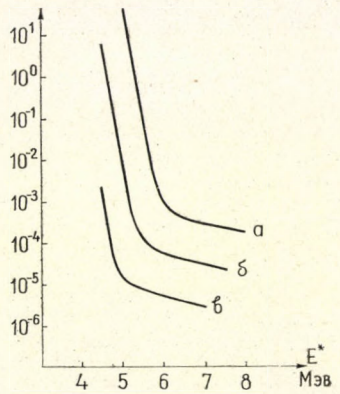
Из фиг. 4 видно, что измеренные отношения σ_i/σ_f мало меняются во всем используемом на опыте диапазоне энергий нейтронов (0—2 Мэв для ^{242}Am и 0,8—3,0 Мэв для ^{244}Am). Отсюда можно заключить, что, повидимому, высоты вторых барьеров у обоих ядер не превышают минимальных полученных на опыте энергий возбуждения (5,55 Мэв для ^{242}Am и 6,0 Мэв для ^{244}Am). Из сравнения измеренных значений σ_i/σ_f и рассчитанных отношений $\Gamma_{\gamma 2}/\Gamma_{f2}$ можно предполагать, что высоты вторых барьеров для обоих ядер близки к 5,5 Мэв.

Из приведенных выше оценок следует, что высота второго барьера относительно дна второй ямы (энергии изомерного уровня) не превышает 2,5 Мэв. Такой малой высоте второго барьера при параметре $\hbar\omega = 600$ кэв соответствуют времена жизни по отношению к делению порядка 10^{-9} сек.

Чтобы объяснить наблюдаемые времена жизни изомеров ^{242}Am и ^{244}Am, которые на 6—7 порядков выше, необходимо предположить, что либо второй барьер аномально широкий (параметр $\hbar\omega$ не более 300 кэв), либо канал деления со спином, соответствующим спину изомерного состояния, лежит по крайней мере на 1 Мэв выше вершины второго барьера.



Фиг. 5. Функции возбуждения реакций:
а) ^{241}Am(n, γ)^{242m}Am;
б) ^{241}Am (n, f)
в) ^{238}U (n, γ)^{239}U



Фиг. 6. Рассчитанные зависимости отношений $\Gamma_{\gamma 2}/\Gamma_{f2}$ от энергии возбуждения составного ядра (E^*) для различных значений высоты второго барьера (B_2). а) B_2=6,0 Мэв; б) B_2=5,5 Мэв; в) B_2 = 5,0 Мэв

Если принять сечение образования основного состояния ^{242}Am при радиационном захвате нейтронов с энергией 1 Мэв того же порядка, что и для ^{239}U (фиг. 5), то изомерное отношение оказывается $\sim 5.10^4$, т. е. практически то же, что и для реакций с заряженными частицами [3]. В то же время для тепловых нейтронов изомерное отношение составляет 3.10^{-7} или в 1000 раз меньше. Такую большую разницу изомерных отношений можно объяснить тем, что барьер, разделяющий первую и вторую ямы выше энергии связи нейтрона и поэтому препятствует заселению изомерного состояния. Из корреляции процессов образования изомера и деления следует, что этот барьер определяет порог деления и составляет 6,4 Мэв для ^{242}Am и 6,1 Мэв для ^{244}Am.

В работе [15] отмечалось, что функции возбуждения реакций образования спонтанно делящихся изомеров при радиационном захвате нейтронов должны характеризоваться двумя максимумами, которые связаны с дипольными колебаниями ядра. Расстояние между максимумами зависит от деформации ядра в изомерном состоянии. В случае ^{242}Am один из максимумов должен лежать при энергии 1—2 Мэв, а другой — при энергии 7—10 Мэв. Из

фиг. 5 видно, что наблюдается максимум при малых энергиях, однако в области больших энергий ошибки измерений и малое число экспериментальных точек не позволяют сделать окончательно вывода.

*

В заключение авторы выражают благодарность Г. Н. Флерову, И. М. Франку и Ф. Л. Шапиро за постоянный интерес к работе. Авторы благодарят также эксплуатационную группу во главе с И. А. Чепурченко за бесперебойную работу электростатического генератора.

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INVESTIGATION OF THE RADIATIVE CAPTURE OF FAST NEUTRONS PRODUCING THE SPONTANEOUSLY DECAYING ISOMERS ^{242}Am AND ^{244}Am

T. NAGY, A. G. BELOV, YU. P. GANGRSKY, B. N. MARKOV, I. V. SIZOV and I. F. HARISOV

Abstract

The ratios of the production cross-sections of the spontaneously decaying isomers ^{242}Am and ^{244}Am and of the prompt fissions taking place during the reactions ^{241}Am + n and ^{243}Am + n have been measured as functions of the energy of neutrons up to 16 MeV. Our measurements show that these ratios are of the same order of magnitude for both isomers and decrease monotonously with the increase of the energy of neutrons. The results obtained can be interpreted on the basis of the double-peak potential barrier model.

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THEORY OF ANHARMONIC CRYSTALS IN PSEUDOHARMONIC APPROXIMATION

III. CRYSTAL WITH WEAK COUPLING

By

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The dependence of the instability temperature on the arbitrary external pressure is investigated for a crystal with weak coupling.

In a previous paper [1] the properties of an anharmonic linear chain under arbitrary external tension were considered in a pseudoharmonic approximation. In this paper I present an additional investigation of the properties of a chain in which the coupling of atoms is weak [$\lambda = (\pi D/\omega_{0L}) \leq 2$]. As I established in the earlier paper it is necessary in this case to investigate the properties of the chain in the low temperature limit.

It was shown in [1] that the self-consistent equation which determines the properties of the chain can be written

$$\lambda\alpha\, y(\alpha) = \int_0^{\pi/2} d\varphi \sin\varphi \coth \frac{\alpha \sin\varphi}{2\tau}, \tag{1}$$

where the notations are the same as in [1] and

$$y(\alpha) = \ln \frac{\alpha^2 - \dfrac{P^*}{6}}{\left(\alpha^2 - \dfrac{P^*}{3}\right)^2}. \tag{2}$$

In the low temperature limit the self-consistent equation (1) can be rewritten in the form

$$\lambda\alpha\, y(\alpha) = 1 + \frac{\pi^2}{3}\left(\frac{\tau}{\alpha}\right)^2. \tag{3}$$

The instability temperature can be obtained as a simultaneous solution of Eq. (3) and its derivative [1]:

$$\lambda\{y(\alpha) + \alpha y'(\alpha)\} = -\frac{2\pi^2}{3}\frac{\tau^2}{\alpha^3}. \tag{4}$$

The critical temperature can be obtained as a simultaneous solution of Eqs. (3) and (4) and the second derivative of (3):

$$\lambda\{2y'(\alpha)+\alpha y''(\alpha)\} = 2\pi^2 \frac{\tau^2}{\alpha^4} . \tag{5}$$

It is convenient to rewrite Eqs. (3)–(5) in the following form:

$$\lambda = \frac{1+\frac{\pi^2}{3}\left(\frac{\tau}{\alpha}\right)^2}{\alpha y(\alpha)} , \tag{6}$$

$$\lambda = -\frac{1+\pi^2\left(\frac{\tau}{\alpha}\right)^2}{\alpha^2 y'(\alpha)} , \tag{7}$$

$$\lambda = 2\frac{1+2\pi^2\left(\frac{\tau}{\alpha}\right)^2}{\alpha^3 y''(\alpha)} . \tag{8}$$

It is easy to see that if $P^* = 0$ Eqs. (7) and (8) are incompatible and consequently there can be no critical temperature. The analytical solution of the

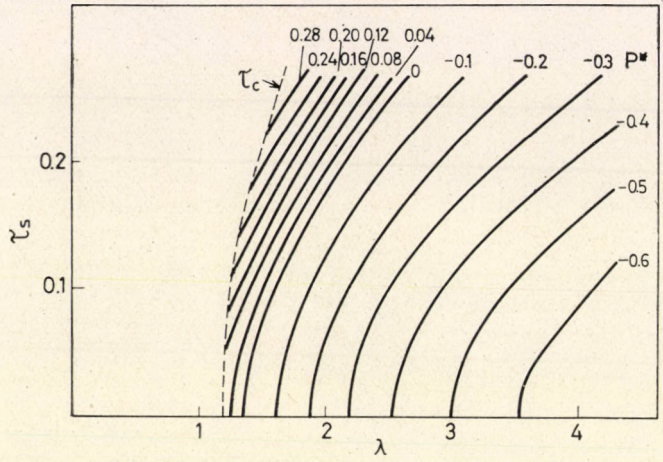

Fig. 1. The dependence of the instability temperature $\tau_s = \Theta_s/\omega_{0L}$ on the dimensionless coupling constant λ of the atoms

system of equations (6)—(8) in the case of $\tau = 0$ gives a value for the critical tension of $P_c^* = 0.055$, with $\alpha_c \sim 0.266$, and $\lambda_0^c \approx 1.21$.

The results of numerical solutions of these systems of equations are given in Figs. 1 and 2. In Fig. 1 the dependence of the instability temperature

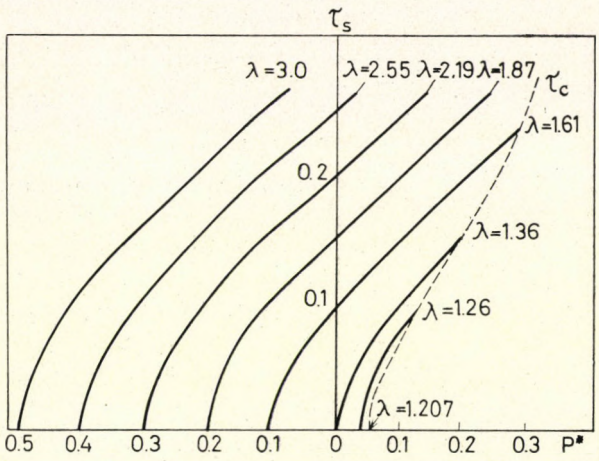

Fig. 2. The dependence of the instability temperature τ_s on the reduced tension P_1^*

$\tau_s = (\theta_s/\omega_{0L})$ on the dimensionless coupling constant $\lambda = (\pi D/\omega_{0L})$ is given for some values of P^*. In Fig. 2 the instability temperature is presented as a function of reduced tension P^* for some values of λ. In both figures the critical curves are denoted by the dotted line.

The results at the temperature $\tau = 0.1 - 0.2$ agree quite well with the results of [1] for the same temperature and with the asymptotic expressions of [2] for $P^* \ll 1$.

It is interesting to point out that the critical temperature is equal to zero at the finite pressure $P_c^* = 0.055$. As was shown in [3], the behaviour of a three-dimensional lattice does not differ qualitatively from that of the one-dimensional lattice discussed in [1] and consequently an analogous situation should hold in the three-dimensional case. For the f.c.c. lattice in the case of $\tau = 0$ numerical solution gives a value for the critical pressure of $P_c^* \sim 0.052$, with $\lambda_0^{(c)} \sim 1.27$.

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ТЕОРИЯ АНГАРМОНИЧЕСКИХ КРИСТАЛЛОВ В ПСЕВДОГАРМОНИЧЕСКОМ ПРИБЛИЖЕНИИ

III. Кристаллы со слабой связью

Т. ШИКЛОШ

Р е з ю м е

Исследуется зависимость температуры неустойчивости от натяжения в случа кристалла со слабой связью атомов.

Acta Physica Academiae Scientiarum Hungaricae, Tomus 30 (3), pp. 305—320 (1971)

ON THE GEODESICS OF CERTAIN SYMMETRIC SPACES

By

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Geodesics of Riemannian spaces admitting certain types of Killing's motions are considered. It is shown that corresponding to the geodesics there are curves in a lower-dimensional space which reveal a striking resemblance to the force laws of general relativity. The forces which emerge are of the electromagnetic and of the potential type. Some connections with KALUZA's five-dimensional theory are discussed. The so-called totally covariant calculus for such spaces is also developed.

Introduction

It was shown by KALUZA soon after the discovery of general relativity that one can retain the general features of an electrovac theory from a five-dimensional formalism [1]. It was essentially this work which stimulated the numerous unified theories in the twenties and the early thirties. The five-dimensional Riemannian spaces involved in these theories generally possess some symmetry properties; in KALUZA's theory, for example, this symmetry is a Killing motion, and it is shown that the equation

$$R_{\alpha\beta} = 0,$$

$R_{\alpha\beta}$ being the five-dimensional Ricci tensor, can be split into two equations

$$\bar{R}_{ik} = T_{ik} - \frac{1}{2} q_{ik} T^r_r,$$

$$F^r_{i;r} = 0 .$$

Here F_{ik} is the electromagnetic tensor, T_{ik} is its energy-momentum tensor, $\bar{R}_{ik}$ is the Ricci tensor in four dimensions, and F_{ik} is related to the Killing vector of the five-dimensional space.

Attention has been mainly directed to such field equations, while the features of the geodesics of these varieties have not been investigated in detail. However, it can be shown that to the five-dimensional geodesics there correspond curves in four dimensions and that the first curvature of these curves is equal to an electromagnetic force.

The aim of this paper is to extend this result and show that in a Riemannian space of arbitrary dimensions admitting several Killing motions, geodesics can be projected onto a variety of lower dimensions and that the first curvature of the curves obtained in this manner is an electromagnetic force. An additional term which may be present in the curvature is a force of the potential type (i.e. a gradient of a scalar), although this term can always be removed by means of a conform transformation of the metric of the lower-dimensional space. The variety obtained is generally not a subspace of the original one, though it is a Riemannian space whose metric is fixed by that of the larger space. This structure of the geodesics is easily revealed if the Killing motions of the embedding space form an Abelian group.

The first Section of the paper recalls the proof of a theorem which states that to require a Riemannian space to admit several Killing motions forming an Abelian group is nothing else but to require the existence of a special coordinate system in which the metric tensor is independent of some variables.

A general covariant treatment of such Riemannian spaces is developed in the second Section and the concept of a parameter space corresponding to the motions is introduced. In order to handle both the parameter and the covariant indices in a uniformly covariant way, para-covariant and totally covariant differentiation are also defined. This formalism is then applied to the special coordinate system of Section I.

The third Section is devoted to the decomposition of the equations of geodesics. The special coordinate system is used here to show that curves corresponding to geodesics are actually force laws in a lower dimensional variety.

I

We first recall and give the proof of a theorem arising in the theories of Riemannian spaces and partial differential equations. In a form adapted to our problem, this states that:

The necessary and sufficient conditions of the existence of a coordinate system (C.S.) in which the metric tensor $g_{\alpha\beta}$ of an n-dimensional Riemannian space V_n is independent of the coordinates $x^1, \ldots, x^r$ $(r<n)$ are that there exist r linearly independent Killing vectors, $K_{A|}{}^{\alpha}$*, and that these vectors form an Abelian group of motions, i.e. the generators

$$G_{A|} = K_{A|}{}^{\alpha}\partial_{\alpha} \quad ** \tag{1}$$

* The stroke in $K_{A|}{}^{\alpha}$ means that the preceding subscript or supercript is not a covariant index but is simply the name of the quantity. Such indices will also apper in bold face type.

** Greek indices will always run from 1 to n, while capital Latin ones from 1 to r. For any types of index we adopt the usual summation convention.

fulfil the relations

$$G_{A|}\,G_{B|} - G_{B|}\,G_{A|} = 0\,. \tag{2}$$

By linear independence of the vectors $K_{A|}{}^{\alpha}$ we mean that the relation

$$\lambda^{R|}\,K_{R|}{}^{\alpha} = 0$$

in any point of the space can only be satisfied by the trivial set of the scalars

$$\lambda^{A} = 0\,.$$

This guarantees, for instance, that none of the vectors $K_{A|}{}^{\alpha}$ can vanish at any particular point.

Before proving the theorem we recall that by definition a Killing vector $K_{A|\alpha}$ satisfies Killing's equation

$$K_{A|\alpha;\beta} + K_{A|\beta;\alpha} = 0\,^{*}. \tag{3}$$

Expressing the Christoffel symbols by $g^{\alpha\beta}$ and the derivatives of $g_{\alpha\beta}$, (3) can be cast in the form

$$K_{A|}{}^{\varrho}{}_{,\beta}\,g_{\varrho\alpha} + K_{A|}{}^{\varrho}{}_{,\alpha}\,g_{\varrho\beta} + K_{A|}{}^{\varrho}\,g_{\alpha\beta,\varrho} = 0\,. \tag{4}$$

It should also be remarked that in consequence of the symmetry of the Christoffel symbols $\left\{{}_{\beta}{}^{\alpha}{}_{\gamma}\right\}$ in the two subscripts, (2) can be written in the following way:

$$G_{A|}\,G_{B|} - G_{B|}\,G_{A|} = K_{A|}{}^{\varrho}\,K_{B|}{}^{\sigma}{}_{;\varrho}\,\partial_{\sigma} - K_{B|}{}^{\varrho}\,K_{A|}{}^{\sigma}{}_{;\varrho}\,\partial_{\sigma} = 0\,.$$

This operator equation still does not seem to be covariant, because the operator $K_{A|}{}^{\varrho}{}_{;\alpha}\,\partial_{\varrho}$ is not a covariant vector. However, if we demand (2) to be valid for any function in a particular C.S., then, applying it to the function $f = x^{\alpha}$, we get

$$(G_{A|}\,G_{B|} - G_{B|}\,G_{A|})\,x^{\alpha} = K_{A|}{}^{\varrho}\,K_{B|}{}^{\alpha}{}_{;\varrho} - K_{B|}{}^{\varrho}\,K_{A|}{}^{\alpha}{}_{;\varrho} = 0,$$

which is covariant and will guarantee that (2) is fulfilled in any C.S.

The proof of the theorem goes as follows. Assume first that there exists

* The semicolon denotes covariant differentiation with respect to a variable indicated by a subscript, providing the subscript does not precede a stroke or is not a bold face index; the sign ∂_{α} or a comma instead of the semicolon denote the ordinary partial derivative.

a C.S. in which $g_{\alpha\beta}$ depends only on $x^{r+1}, \ldots, x^n$, and define r linearly independent vectors* by

$$K_{A|}{}^{\alpha} = \delta_A^{\alpha} . \tag{5}$$

These will satisfy (4) according to the assumption

$$g_{\alpha\beta\,.A} = 0 .$$

Using (1) and (5) one can readily verify that (2) is also satisfied.

The proof of the reversed statement is a bit more involved. Assume that there exist r linearly independent vectors $K_{A|}{}^{\alpha}$ satisfying (2) and (3). First we will show that one can choose a C.S. in which

$$K_{A|}{}^{\alpha} = \delta_A^{\alpha} .$$

There exists a C.S. in which the non-vanishing vector $K_{1|}{}^{\alpha}$ has the form [4]

$$K_{1|}{}^{\alpha} = \delta_1^{\alpha} . \tag{6}$$

Using (6), we utilize (2) for the case $A = 1$, $B = 2$ by applying it to the function x^{α}, which gives

$$K_{2|}{}^{\alpha}{}_{,1} = 0 .$$

Thus the equation

$$\sum_{\varrho=2}^{n} K_{2|}{}^{\varrho}\, \psi_{,\varrho} = 0$$

has $n - 2$ independent solutions $\psi^k(x^2, \ldots, x^n)$, $(k = 3, \ldots, n)$, all independent of x^1. Performing a coordinate transformation

$$\begin{aligned} x'^1 &= x^1 . \\ x'^2 &= h(x^2, \ldots, x^n), \\ x'^{k'} &= \psi^k(x^2, \ldots, x^n); \qquad (k = 3, \ldots, n). \end{aligned}$$

where h is chosen so as to avoid the vanishing of the Jacobian, we have

$$K_{1|}{}'^{\alpha} = \delta_1^{\alpha} \qquad \text{[i.e. (6) is unchanged]}$$

and

$$K_{2|}{}'^{k} = \sum_{\varrho=2}^{n} K_{2|}{}^{\varrho}\, \psi^{k}{}_{,\varrho} = 0 ; \qquad (k = 3, \ldots, n).$$

* By vectors we naturally mean vector fields having continuous derivatives of at least the first order.

$K_{2l}{}'^2$ cannot be zero as it would not then be linearly independent of $K_{1l}{}'^{\alpha}$. A transformation of the kind

$$x''^1 = x'^1 - \int_0^{x'^2} \frac{K_{2l}{}'^1}{K_{2l}{}'^2}\, dx'^2\,,$$

$$x''^2 = \int_0^{x'^2} \frac{1}{K_{2l}{}'^2}\, dx'^2\,,$$

$$x''^k = x'^k\,; \qquad (k = 3, \ldots, n)$$

eaves (6) unchanged and leads to the desi red form of $K_{2l}{}''^{\alpha}$:

$$K_{2l}{}''^{\alpha} = \delta_2^{\alpha}.$$

By repeating this procedure we finally end up with a C.S. where

$$K_{Al}{}^{\alpha} = \delta_A^{\alpha}. \tag{7}$$

We still have to show that if (7) is valid $g_{\alpha\beta}$ is independent of x^A. By assumption $K_{Al}{}^{\alpha}$ is a Killing vector; thus it fulfils (4), which, using (7), will give

$$g_{\alpha\beta,A} = 0\,,$$

which was to be proved.

The C.S. in which (7) is valid is called a special coordinate system (S.C.S.). Similar systems play an essential role in the group theoretical classification of the space-times of general relativity [3].

The most general transformations leaving (7) unchanged have the form

$$x'^A = x^A + f^A(x^{r+1}, \ldots, x^n)\,,$$

$$x'^j = f^j(x^{r+1}, \ldots, x^n)\,; \qquad (j = r+1, \ldots, n).$$

We call such a transformation a special coordinate transformation (S.C.T.). The subgroup

$$x'^A = x^A + f^A(x^{r+1}, \ldots, x^n),$$

$$x'^j = x^j; \qquad (j = r+1, \ldots, n)$$

of the S.C.T.-s is called the group of gauge transformations (see the end of Section II), while a transformation of the form

$$x'^A = x^A,$$

$$x'^j = f^j(x^{r+1}, \ldots, x^n); \qquad (j = r+1, \ldots, n)$$

is a restricted coordinate transformation.

A Riemannian space admitting r linearly independent Killing vectors forming an Abelian group of motions will be denoted by V_n^r.

II

In this Section we examine the structure of a V_n^r in detail. We shall assume that the matrix $\| k_{AB} \|$ of the scalar products

$$k_{AB|} = K_{A|\varrho} K_{B|}{}^{\varrho}$$

of the Killing vectors is not singular. The inverse $\| k^{AB} \|$ of $\| k_{AB} \|$ can be used to raise the capital Latin subscript of a $K_{A|\alpha}$:

$$K^{A|}{}_{\alpha} = k^{AR|} K_{R|\alpha}.$$

Note that $K^{A}{}_{|\varrho}$ is generally not a Killing vector.

In a V_n^r there exists a set of $n - r$ independent scalar functions $\varphi^{\mathbf{k}}(x^1, \ldots, x^n)$ satisfying

$$K_{A|}{}^{\varrho} \varphi^{\mathbf{k}}{}_{,\varrho} = 0 \,^{*}. \tag{8}$$

In fact, the requirement (8) is fulfilled by the functions $\varphi^{\mathbf{k}} = x^k$ in the S.C.S. of a V_n^r. Obviously, given such a set any function $F(\varphi^{\mathbf{r+1}}, \ldots, \varphi^{\mathbf{n}})$ will also satisfy (8). Introducing the notation

$$\gamma_{\varrho}^{\mathbf{k}} = \varphi^{\mathbf{k}}{}_{|\varrho}, \tag{9}$$

we have

$$K_{A|}{}^{\varrho} \gamma_{\varrho}^{\mathbf{k}} = K^{A|\varrho} \gamma_{\varrho}^{\mathbf{k}} = 0. \tag{10}$$

Owing to the independence of the functions $\varphi^{\mathbf{k}}$ the vectors $\gamma_{\varrho}^{\mathbf{k}}$ are linearly independent. Thus, according to (10) the vectors

$$K_{A|\varrho}, \ \gamma_{\varrho}^{\mathbf{k}} \tag{11}$$

form a set of n linearly independent vectors in a V_n^r. We may then introduce the "inverse" γ-s:

$$\begin{aligned} K_{A|\varrho} \gamma_{\mathbf{k}}^{\varrho} &= 0 \,, \\ \gamma_{\varrho} \gamma_{\mathbf{k}}^{\varrho} &= \delta_k^i \,; \end{aligned} \tag{12}$$

these $n(n - r)$ equations uniquely define the $n(n - r)$ quantities $\gamma_{\mathbf{a}}^{\alpha}$.

* From now on small Latin indices (except r and n) will run from $r + 1$ to n.

To characterize unambiguously a vector U^α we can use any one of the following four sets of scalars:

$$\begin{aligned} U^{\mathbf{a}} &= \gamma^{\mathbf{a}}_{\varrho}\, U^{\varrho}, & U^{\mathbf{a}} &= \gamma^{\mathbf{a}}_{\varrho}\, U^{\varrho}, \\ U^{A|} &= K^{A|}{}_{\varrho}\, U^{\varrho}; & U_{A|} &= K_{A|\varrho}\, U^{\varrho}; \\ U_{\mathbf{a}} &= \gamma^{\varrho}_{\mathbf{a}}\, U_{\varrho}, & U_{\mathbf{a}} &= \gamma^{\varrho}_{\mathbf{a}}\, U_{\varrho}, \\ U^{A|} &= K^{A|\varrho}\, U_{\varrho}, & U_{A|} &= K_{A|}{}^{\varrho}\, U_{\varrho}\,. \end{aligned} \tag{13}$$

Similar quantities for tensors of higher order can also be formed, e.g.

$$T^{A|\alpha\beta}{}_{\mathbf{a}} = K^{A|}{}_{\varrho}\, \gamma^{\sigma}_{\mathbf{a}}\, T^{\varrho\alpha\beta}{}_{\sigma}\,.$$

The tensor

$$\varepsilon^{\alpha}_{\beta} = \gamma^{\alpha}_{\mathbf{r}}\, \gamma^{\mathbf{r}}_{\beta} \tag{14}$$

is a projector, i.e.

$$\varepsilon^{\alpha}_{\varrho}\, \varepsilon^{\varrho}_{\beta} = \varepsilon^{\alpha}_{\beta}\,,$$

in accordance with (12). Equations (10) and (12) give

$$\varepsilon^{\alpha}_{\varrho}\, K_{A|}{}^{\varrho} = \varepsilon^{\varrho}_{\alpha}\, K_{A|\varrho} = 0$$

and

$$\varepsilon^{\alpha}_{\varrho}\, \gamma^{\varrho} = \gamma^{\alpha};\;\; \varepsilon^{\varrho}_{\alpha} \cdot \gamma^{\mathbf{k}}_{\varrho} = \gamma^{\mathbf{k}}_{\alpha}\,. \tag{15}$$

We can express $\varepsilon^{\alpha}_{\beta}$ by means of the vectors $K_{A|\alpha}$ in the following way:

$$\varepsilon^{\alpha}_{\beta} = \delta^{\alpha}_{\beta} - K^{R|\alpha}\, K_{R|\beta} = \delta^{\alpha}_{\beta} - K_{R|}{}^{\alpha}\, K^{R|}{}_{\beta}. \tag{16}$$

This relation is proved by multiplying it by and then contracting it with the n linearly independent vectors (11) and finally taking (15) into account.

By means of (16) one can decompose the fundamental form of a V_n^r:

$$\begin{aligned} g_{\alpha\beta}\, dx^{\alpha}\, dx^{\beta} &= g_{\alpha\varrho}\, (\varepsilon^{\varrho}_{\beta} + K^{R|\varrho}\, K_{R|\beta})\, dx^{\alpha}\, dx^{\beta} = \\ &= g_{\varrho\sigma}\, (\varepsilon^{\sigma}_{\alpha} + K^{T|\sigma}\, K_{T|\alpha})\, \varepsilon^{\varrho}_{\beta}\, dx^{\alpha}\, dx^{\beta} + K^{R|}{}_{\alpha}\, K_{R|\beta}\, dx^{\alpha}\, dx^{\beta} = \\ &= g_{\varrho\sigma}\, \varepsilon^{\varrho}_{\alpha}\, \varepsilon^{\sigma}_{\beta}\, dx^{\alpha}\, dx^{\beta} + K^{R|}{}_{\alpha}\, K_{R|\beta}\, dx^{\alpha}\, dx^{\beta}, \end{aligned} \tag{17}$$

where in the last step (16) has been used. Introducing

$$g_{\mathbf{ik}} = \gamma^{\varrho}_{\mathbf{i}}\, \gamma^{\sigma}_{\mathbf{k}}\, g_{\varrho\sigma}\,, \tag{18}$$

(17) can be rewritten

$$g_{\alpha\beta}\, dx^{\alpha}\, dx^{\beta} = g_{\mathbf{rs}}\, \gamma^{\mathbf{r}}_{\alpha}\, \gamma^{\mathbf{s}}_{\beta}\, dx^{\alpha}\, dx^{\beta} + K^{R|}{}_{\alpha}\, K_{R|\beta}\, dx^{\alpha}\, dx^{\beta}\,.$$

The quantities g_{ik} form a nonsingular matrix; one can readily show that in consequence of (10) and (12) we have

$$g_{ir}\, g^{ik} = \delta_r^k$$

if

$$g^{k} = \gamma_\varrho\, \gamma_\sigma^{k}\, g^{\varrho\sigma}.$$

The g_{ik}-s are the components of a metric tensor of a V_{n-r} and play an important part in the derivation of force laws in Section III.

We turn now to questions of tensor analysis. From the partial derivatives of a quantity B one can form the expressions

$$B_{,A|} = K_{A|}{}^{\varrho}\, B_{,\varrho};\quad B_{,a} = \gamma_a^{\varrho}\, B_{,\varrho}. \tag{19}$$

The first is called the inner derivative of B in the direction of $K_{A|}$, while the second is the p-derivative of B with respect to φ^{a}. B is said to be A-cyclic if $B_{,A|} = 0$.

We will show that g_{ik} is A-cyclic for any A. To do this we calculate

$$\begin{aligned} g_{ik,A|} = (g_{\mu\nu}\, \gamma^{\mu}\, \gamma^{\nu}_{k})_{,\varrho}\, K_{A|}{}^{\varrho} = \left([\mu\varrho, \nu] + [\nu\varrho, \mu]\right) \cdot \gamma^{\mu}\, \gamma^{\nu}_{k}\, K_{A|}{}^{\varrho} + \\ + g_{\mu\nu}\, \gamma^{\mu}_{i}\, \gamma^{\nu}_{k,\varrho} \cdot K_{A|}{}^{\varrho} + g_{\mu\nu}\, \gamma^{\mu}_{k}\, \gamma^{\nu}_{i,\varrho}\, K_{A|}{}^{\varrho}, \end{aligned} \tag{20}$$

where $[\alpha\beta, \gamma]$ is the Christoffel symbol of the first kind. In order to evaluate $g_{\mu\nu}\gamma^{\mu}\gamma^{\nu}_{k,\varrho}\, K_{A|}^{\varrho}$ we differentiate the second relation of (12) and use (14) to get

$$\varepsilon^{\nu}_{\tau}\, \gamma^{\tau}_{k,\varrho} = -\, \gamma^{\tau}_{k}\, \gamma^{r}_{\tau,\varrho}\, \gamma^{\nu}_{r},$$

which together with (16) gives

$$\gamma^{\nu}_{k\,\varrho} = K^{R|\nu}\, K_{R|\tau} \cdot \gamma^{\tau}_{k,\varrho} - \gamma^{\tau}_{k}\, \gamma^{r}_{\tau,\varrho}\, \gamma^{\nu}_{r}.$$

This, multiplied by $g_{\mu\nu}\gamma^{\mu}\, K_{A|}^{\varrho}$ and contracted for ϱ and ν, yields

$$\gamma^{\nu}_{k,}\, \gamma^{\mu}\, g_{\mu\varrho}\, K_{A|}{}^{\varrho}. \tag{21}$$

Since by definition (9) $\gamma^{r}_{\tau,\varrho} = \gamma^{r}_{\varrho,\tau}$, and as a consequence of (10)

$$K_{A|}{}^{\varrho}\, \gamma^{r}_{\varrho,\tau} = -\, K_{A|}{}^{\varrho}{}_{,\tau}\, \gamma^{r}_{\varrho},$$

we may write (21) in the form

$$\gamma^{\nu}_{k,\varrho}\, \gamma^{\mu}_{i}\, g_{\mu\nu}\, K_{A|}{}^{\varrho} = \gamma^{\tau}_{k}\, \gamma^{r}_{\varrho}\, \gamma^{\nu}_{r}\, \gamma^{\mu}\, g_{\mu\nu}\, K_{A|}{}^{\varrho}{}_{,\tau} = \gamma^{\tau}_{k}\, \gamma^{\mu}_{i}\, g_{\mu\nu}\, K_{A|}{}^{\varrho}{}_{,\tau}{}^{*}$$

* In the last step we have used

$$\gamma^{r}_{\varrho}\, \gamma^{\nu}_{r}\, g_{\mu\nu}\, \gamma^{\mu}_{i} = \varepsilon^{\nu}_{\varrho}\, g_{\mu\nu}\, \gamma^{\mu} = g_{\mu\varrho}\, \gamma^{\mu}_{i},$$

which is a result of (14) and (16).

If we substitute into (19) the latter expression and the expression obtained from it by interchanging i and k, we get

$$g_{\mathbf{ik},Al} = \gamma^{\mu}_{\mathbf{i}} \gamma^{\nu}_{\mathbf{k}} (K_{Al\mu;\nu} + K_{Al\nu;\mu}) ,$$

which on the assumption that $K_{A|\alpha}$ is a Killing vector gives

$$g_{\mathbf{ik},Al} = 0 , \tag{22}$$

which was to be proved.

According to the remarks following (8) any function of the $\varphi^{\mathbf{k}}$-s will equally satisfy (8). Thus as well as the coordinates we may also transform the parameter functions $\varphi^{\mathbf{k}}$. A transformation

$$\varphi'^{\mathbf{k}} = \varphi'^{\mathbf{k}} (\varphi^{\mathbf{r}+\mathbf{1}}, \ldots, \varphi^{\mathbf{n}})$$

is called a parameter or "p-transformation" if the Jacobian

$$\left\| \frac{\partial \varphi'^{\mathbf{k}}}{\partial \varphi} \right\|$$

is of rank $n - r$. The definition of the p-tensors is straightforward: for example, we call $V_{\mathbf{k}}$ a covariant p-vector if for a p-transformation it transforms like

$$v'_{\mathbf{k}} = \frac{\partial \varphi^{\mathbf{r}}}{\partial \varphi'^{\mathbf{k}}} V_{\mathbf{r}} .$$

Note that for a p-transformation the ordinary coordinates (o-coordinates) remain unchanged, and thus the ordinary tensors (o-tensors) behave like p-scalars; likewise for an o-transformation the p-tensors are to be treated as o-scalars. From definition (9) it can be readily shown that $\gamma^{\alpha}_{\mathbf{i}}$ is a contravariant p-vector and a covariant o-vector. From (12) is follows that $\gamma^{\beta}_{\mathbf{k}}$ is a contravariant o- and covariant p-vector. It can also be verified that the inner derivation in any direction will not alter the p-behaviour of a p-tensor. The ordinary partial derivative of a p-tensor with respect to a variable x^{α}, however, is not a p-tensor, and therefore we need a p-covariant rule of differentation. Consider the o-covariant derivative of the o-vector $U^{\alpha} = \gamma^{\alpha}_{\mathbf{r}} U^{r}$, where $U^{\mathbf{a}}$ is an arbitrary p-vector

$$U^{\alpha}_{;\beta} = (\gamma^{\alpha}_{\mathbf{r},\beta} + \left\{ {}_{\beta}{}^{\alpha}{}_{\varrho} \right\} \gamma^{\varrho}_{\mathbf{r}}) U^{\mathbf{r}} + \gamma^{\alpha}_{\mathbf{r}} U^{\mathbf{r}}{}_{,\beta} .$$

Multiplying this equation by $\gamma^{\mathbf{a}}_{\varkappa}$ and summing for α, we get a p-contravariant and o-covariant vector, as U^{α}; β is a p-scalar:

$$U^{\varrho}{}_{;\beta} \gamma^{\mathbf{a}}_{\varrho} = U^{\mathbf{a}}{}_{,\beta} + (\gamma^{\mathbf{a}}_{\sigma} \gamma^{\varrho}_{\mathbf{r}} \left\{ {}_{\varrho}{}^{\sigma}{}_{\beta} \right\} - \gamma^{\sigma}_{\mathbf{r}} \gamma^{\mathbf{a}}_{\sigma,\beta}) U^{\mathbf{r}} . \tag{23}$$

We call the R.H.S. of (23) the p-covariant derivative of U^a with respect to x^β. The quantity in brackets can be regarded as the analogue of the ordinary Christoffel symbols of the second kind, and may be denoted by

$$\left\{ {\mathbf{a}\ \ \ } \atop {\mathbf{b}\ \beta} \right\} = \gamma^{\mathbf{a}}_{\sigma} \gamma^{\varrho}_{\mathbf{b}} \left\{ {\ \sigma\ \ } \atop {\beta\ \varrho} \right\} - \gamma^{\sigma}_{\mathbf{b}} \gamma^{\mathbf{a}}_{\sigma,\beta}. \tag{24}$$

By the p-covariant derivative of a p-covariant vector z_α with respect to x^β we mean

$$z_{\mathbf{a},\beta} - \left\{ {\mathbf{a}\ \ \ } \atop {\ \ \beta} \right\} z_{\mathbf{r}}.$$

This can be shown to be a p-covariant and o-covariant vector.

We can define now the totally covariant derivative of a tensor of arbitrary p- and o-covariant character with respect to x^β; this is the partial derivative of the tensor plus terms with appropriate signs containing o-Christoffel symbols for o-indices and the symbols (24) for p-indices. For example totally covariant derivative of $V^{\mathbf{a}\alpha}$ with respect to x^β is

$$V^{\mathbf{a}\alpha}_{\ \ \ \eta;\beta} = V^{\mathbf{a}\alpha}_{\ \ \ \eta,\beta} + \left\{ {\mathbf{r}\ \ \ } \atop {\ \ \beta} \right\} V^{\mathbf{r}\alpha}_{\ \ \ \eta} + \left\{ {\ \ \alpha} \atop {\varrho\ \beta} \right\} V^{\mathbf{a}\varrho}_{\ \ \ \eta} - \left\{ {\ \ \varrho} \atop {\eta\ \beta} \right\} V^{\mathbf{a}\alpha}_{\ \ \ \varrho}.$$

From now on the semicolon will always denote the totally covariant derivative.

Obviously the totally covariant derivative of a p- or an o-scalar coincides with its o- or p-covariant derivative respectively.

The totally covariant derivative of an arbitrary tensor can also be "projected" by means of the γ-s. Thus e.g.,

$$U^{\mathbf{a}}_{\ ;\mathbf{b}} = U^{\mathbf{a}}_{\ ;\varrho} \gamma^{\varrho}_{\mathbf{b}} = U^{a}_{\ ,\varrho} \cdot \gamma^{\varrho}_{\mathbf{c}} + \left\{ {\mathbf{r}\ \ \ } \atop {\ \ \varrho} \right\} \gamma^{\varrho}_{\mathbf{b}} U^{r},$$

which is called the totally covariant derivative of U^a with respect to $\gamma^{\mathbf{b}}$. The quantities

$$\left\{ {\mathbf{b}\ \ \ } \atop {\mathbf{c}\ \varrho} \right\} = \left\{ {\mathbf{c}\ \ \ } \atop {\ \ \varrho} \right\} \gamma^{\varrho}_{\mathbf{c}}$$

are called p-Christoffel symbols of the second kind. A straightforward but lengthy calculation shows that

$$\left\{ {\mathbf{b}\ \ \ } \atop {\mathbf{c}\ \ \ } \right\} = \frac{1}{2} g^{\mathbf{ar}} \left(g_{\mathbf{rb},\mathbf{c}} + g_{\mathbf{rc},\mathbf{b}} - g_{\mathbf{bc},\mathbf{r}} \right),$$

where $g_{\mathbf{ab},\mathbf{c}}$ is defined according to the second relation of (19). It can be shown that

$$g_{\mathbf{ab};\mathbf{c}} = g_{\mathbf{ab};\varrho} \gamma^{\varrho}_{\mathbf{c}} = g^{\mathbf{ab}}_{\ \ ;\mathbf{c}} = g^{\mathbf{ab}}_{\ \ ;\varrho} \gamma^{\varrho}_{\mathbf{c}} = 0,$$

which are the analogues of the corresponding o-relations.

We shall now apply the formalism developed above to a S.C.S. of a V_n^r (see Section I). Thus we are assuming (7) to hold, and therefore

$$K_{A|\alpha} = g_{\alpha\varrho} K_{A|}{}^{\varrho} = g_{\alpha A}. \tag{26}$$

and consequently,

$$k_{AB|} = K_{A|\varrho} K_{B|}{}^{\varrho} = K_{A|B} = K_{B|A} = g_{AB}. \tag{27}$$

In accordance with the remarks following (8) we may take

$$\varphi^{\mathbf{k}} = x^k. \tag{28}$$

A S.C.S. together with this choice of the functions $\varphi^{\mathbf{k}}$ is called a natural system (N.S.) of a V_n^r.

We shall work in a N.S. By definition (9) we have

$$\gamma_a^{\mathbf{k}} = \delta_a^k. \tag{29}$$

Taken with (12) this gives

$$\gamma_i^k = \delta_{\mathbf{i}}^k \quad \text{and} \quad \gamma_{\mathbf{i}}^A = -K^{A|}{}_i,$$

which make possible the calculation of g_{ik} by means of (18):

$$g_{\mathbf{ik}} = g_{ik} - K^{R|}{}_i K_{R|h}.$$

This equation and the relations (26) and (27) enable us to express $g_{\alpha\beta}$ by means of $g_{\mathbf{ik}}$, $K_{A|\alpha}$ and $k_{AB|}$:

$$\begin{aligned} g_{ab} &= g_{\mathbf{ab}} + K^{R|}{}_a K_{R|b}, \\ g_{aB} &= K_{B|a}, \\ g_{AB} &= k_{AB|}. \end{aligned} \tag{30}$$

These in turn allow us to calculate $g^{\alpha\beta}$:

$$\begin{aligned} g^{ab} &= g^{\mathbf{ab}}, \\ g^{aB} &= -g^{\mathbf{ar}} K^{B|}{}_r, \\ g^{AB|} &= (k^{AB|} + K^{A|}{}_r K^{B|}{}_s g^{\mathbf{rs}}). \end{aligned} \tag{31}$$

A N.S. is at the same time a S.C.S., so $g_{\alpha\beta}$ is independent of x^A. Thus as a consequence of (30) and (31), $k_{AB|}$, $k^{AB|}$, $k_{A|}$ and $K^{A|}{}_{\alpha}$ together with $g_{\mathbf{ab}}$ are also independent of these variables. This incidentally is in agreement with (22), which due to (7) can now be written in the form

$$g_{\mathbf{ab}\,,A|} = g_{\mathbf{ab}\,,\varrho} K_{A|}{}^{\varrho} = g_{\mathbf{ab}\,.A} = 0.$$

It will be noted that in (30) and (31) p- and o-indices are mixed up. If we perform the S.C.T.

$$\begin{aligned} x'^A &= x^A + f^A(x^{r+1}, \ldots, x^n), \\ x'^k &= x'^k(x^{r+1}, \ldots, x^n), \end{aligned} \tag{32}$$

then (7) will remain valid. On the other hand (28), and consequently the relations (29), (30) and (31), will become void, i.e. the new system will not be a N.S. However, if simultaneously with the o-transformation (32) we perform a p-transformation

$$\varphi'^{\mathbf{k}} = x'^k(\varphi^{\mathbf{r+1}}, \ldots, \varphi^{\mathbf{n}})$$

and take (28) into account, then not only (7) but also (28) will be left unchanged, and the new system will be a N.S. again.

Such a pair of simultaneously performed transformations is called a natural transformation (N.T.). Accordingly the gauge transformation

$$\begin{aligned} x'^A &= x^A + f^A(x^{r+1}, \ldots, x^n), \\ x'^k &= x^k \end{aligned}$$

is a N.T. calling forth

$$K'_{Ala} = K_{Ala} - k_{AR} f^R{}_{,a},$$

which enlightens the designation "gauge".

III

We shall now investigate the nonminimal geodesics of a V_n^r. If we choose a parameter s such that $g_{\varrho\sigma}\dot{x}^\varrho \dot{x}^\sigma = e^*$, where $e = \pm 1$, then the equations of a geodesic are

$$\ddot{x}^\alpha + \left\{ {\varrho \atop \sigma}{\alpha} \right\} \dot{x}^\varrho \dot{x}^\sigma = 0 . \tag{33}$$

According to (13) we introduce $n - r$ p-vectors

$$V^{\mathbf{a}} = \gamma^{\mathbf{a}}_\varrho \dot{x}^\varrho$$

and r scalars

$$C_{Al} = K_{Al\varrho} \dot{x}^\varrho . \tag{34}$$

We wish to show that C_{Al} is constant along the geodesic, i.e. that

$$\frac{dC_A}{ds} = 0 . \tag{35}$$

* The dot denotes the derivative with respect to s.

We have

$$\frac{dC_{A|}}{ds} = K_{A|\varrho,\sigma}\,\dot{x}^{\varrho}\,\dot{x}^{\sigma} + K_{A|\varrho}\,\ddot{x}^{\varrho} =$$
$$= K_{A|\varrho,\sigma}\,\dot{x}^{\varrho}\,\dot{x}^{\sigma} - K_{A|\varrho}\left\{{}_{\sigma}{}^{\varrho}{}_{\tau}\right\}\dot{x}^{\sigma}\,\dot{x}^{\tau} =$$
$$= K_{A|\varrho;\sigma}\,\dot{x}^{\varrho}\,\dot{x}^{\sigma}\,,$$

but in consequence of (3) $K_{A|\varrho;\sigma}$ is antisymmetric in ϱ and σ, and thus (35) is indeed satisfied.

One can invert the relations (34):

$$\dot{x}^{\alpha}\,V^{\mathbf{r}}\,\gamma_{\mathbf{r}} + K^{R|\alpha}\,C_{R|}\,. \tag{36}$$

By means of (34) and (16), the relations (36) are seen to be fulfilled identically.

We substitute $\ddot{x}^{\alpha}$, obtained by differentiating (36) into (33), and use (36) again to express every $\dot{x}^{\alpha}$ by the $V^{\mathbf{a}}$-s and $C_{A|}$-s. Finally we multiply the resulting expression by $\gamma_{\alpha}^{\mathbf{a}}$ and contract α to get

$$\dot{V}^{\mathbf{a}} + \left\{{}_{\mathbf{r}}{}^{\mathbf{a}}{}_{\mathbf{t}}\right\} V^{\mathbf{r}}\,V^{\mathbf{t}} = -\,2\,\gamma_{\varrho}^{\mathbf{a}}\,\gamma^{\sigma}\,K^{R|\varrho}{}_{;\sigma}\,C_{R|}\,V^{\tau} - \gamma_{\varrho}^{\mathbf{a}}\,K^{R|\varrho}{}_{;\sigma}\,K^{T|\sigma}\,C_{R|}\,C_{T|}\,; \tag{37}$$

where $\left\{{}_{\mathbf{r}}{}^{\mathbf{a}}{}_{\mathbf{t}}\right\}$ is the Christoffel symbol (25). The first term on the R.H.S. can be rewritten

$$-\,2\,\gamma_{\varrho}^{\mathbf{a}}\,\gamma_{\mathbf{r}}^{\sigma}\,K^{R|\varrho}{}_{;\sigma}\,C_{R|}\,V^{\mathbf{r}} = 2\,\gamma_{\varrho}^{\mathbf{a}}\,g^{\varrho\tau}\,\gamma_{\mathbf{r}}^{\sigma}\,K^{R|}{}_{\sigma;\tau}\,C_{R|}\,V^{\mathbf{r}} =$$
$$= \gamma_{\mathbf{t}}^{\tau}\,g_{\mathbf{at}}\,\gamma^{\sigma}\,(K^{R|}{}_{\sigma,\tau} - K^{R|}{}_{\tau,\sigma})\,C_{R|}\,V^{\mathbf{r}}, \tag{38}$$

where

$$\gamma_{\varrho}^{\mathbf{a}}\,g^{\varrho\tau} = \gamma^{\tau}\,g^{\mathbf{ta}} \tag{39}$$

and (3), together with the obvious relation

$$K^{R|}{}_{\alpha;\beta} - K^{R|}{}_{\beta;\alpha} = K^{R|}{}_{\alpha,\beta} - K^{K|}{}_{\alpha,\beta}\,,$$

have been used.

The second term of (37) is reformulated as follows

$$-\,\gamma_{\varrho}^{\mathbf{a}}\,K^{R|\varrho}{}_{;\sigma}\,K^{T|\sigma}\,C_{R|}\,C_{T|} = -\,\gamma_{\varrho}^{\mathbf{a}}\,g^{\varrho\tau}(k^{RQ|}\,K_{Q|\tau})_{;\sigma}\,K^{T|\varrho}\,C_{R|}\,C_{T|} =$$
$$= g^{\mathbf{ar}}\,\gamma_{\mathbf{r}}^{\varrho}\,k^{RQ|}\,k^{TV|}\,K_{Q|\sigma;\varrho}\,K_{V|}{}^{\varrho}\,C_{R|}\,C_{T|} =$$
$$= \frac{1}{2}\,g^{\mathbf{ar}}\,\gamma_{\mathbf{r}}^{\varrho}\,k^{RQ|}\,k^{TV|}\,k_{QV|,\varrho}\,C_{R|}\,C_{T|} = \tag{40}$$
$$= -\,\frac{1}{2}\,g^{\mathbf{ar}}\,\gamma_{\mathbf{r}}^{\varrho}\,k^{RT|}{}_{,\varrho}\,C_{R|}\,C_{T|}\,.$$

Here we have made use of (39) and of

$$\gamma_{\varrho}^{\mathbf{a}}\,K^{R|\varrho}{}_{;\alpha} = k^{RQ|}\,\gamma_{\varrho}^{\mathbf{a}}\,K_{Q|}{}^{\varrho}{}_{;\alpha}\,,$$

which is a consequence of (10). The equation

$$k^{AB|}{}_{,\alpha} = -k^{AR|}\,k^{BQ|}\,k_{RQ|\,\alpha}\,,$$

which is a consequence of

$$k^{AR|}\,k_{RB|} = \delta^A_B\,,$$

has also been used. Inserting (38) and (40) into (37), we get

$$\dot{V}^{\mathfrak{a}} + \left\{ {\mathfrak{r}\ \ \mathfrak{a}\atop \mathfrak{t}} \right\} V^{\mathfrak{r}}\,V^{\mathfrak{t}} = g^{\mathfrak{a}\mathfrak{t}}\,\gamma^{\varrho}_{\mathfrak{t}}\,\gamma^{\sigma}_{\mathfrak{r}}\,(C_{R|}\,K^{R|}{}_{\sigma,\varrho} - C_{R|}\,K^{R|}{}_{\varrho,\sigma})\,V - \\ - \frac{1}{2}\,g^{\mathfrak{a}\mathfrak{t}}\,\gamma^{\varrho}_{\mathfrak{t}}\,k^{RT|}{}_{,\varrho}\,C_{R|}\,C_{T|}\,. \tag{41}$$

The significance of this equation becomes especially lucid in a N.S., because as a result of (29) we then have

$$V^{\mathfrak{a}} = \dot{x}^a\,,$$

with $K^{A|}{}_{\alpha}$ and $k^{AB|}$ independent of x^A, and moreover

$$K^{A|}{}_{B} = k^{AR|}\cdot K_{R|B} = k^{AR|}\,k_{RB|} = \delta^A_B\,.$$

Thus (41) can be cast in the form

$$\ddot{x}^a + \left\{ {\mathfrak{a}\atop \mathfrak{r}\ \ \mathfrak{t}} \right\} \dot{x}^r\,\dot{x}^t = g^{\mathfrak{a}\mathfrak{t}}\,(C_{R|}\,K^{R|}{}_{r,t} - C_{R|}\,K^{R|}{}_{t,r})\,\dot{x}^r - \frac{1}{2}\,g^{\mathfrak{a}\mathfrak{t}}\,k^{RT|}{}_{,t}\,C_{R|}\,C_{T|}\,. \tag{42}$$

The first term of the R.H.S. of (42) has the form of an electromagnetic force (similar terms in classical mechanics are sometimes called gyroscopic forces). The second force is of the potential type. The "electromagnetic" field

$$F_{rt} = C_{R|}\,K^{R|}{}_{r,t} - C_{R|}\,K^{R|}{}_{t,r}$$

is a rotation of the "vector potential" $C_R K^{RI}{}_a$.

If we pass from one N.S. to another, the *o*- and *p*-indices behave equivalently. For such systems (42) is thus a covariant equation. Our result can be put in yet another way: There exists a Riemannian space V_{n-r} with the metric g_{ik} in which for a set of constants C_A a curve described by Eqs. (42) can be found that corresponds to a geodesic of the original V^r_n, the C_A-s then being given by (34).

One may ask if it is possible to find a Lagrangian which when used in a variation principle will lead to the equations (42). The answer to this question is affirmative, since the function

$$L = [(e - C_{R|}\,C_{T|}\,k^{RT|})\,g_{\ ,}\dot{x}^r\,\dot{x}^t]^{1/2} + C_{R|}\,K^{R|}{}_{t}\,\dot{x}^t \tag{43}$$

will meet this requirement. We stress, however, that the choice of the parameter s is such that

$$g_{\alpha\beta}\dot{x}^{\alpha}\dot{x}^{\beta} = e\,,$$

which in a N.S. reads

$$g_{\cdot}\,\dot{x}^{r}\dot{x}^{t} + k^{RT|}\,C_{R|}\,C_{T|} = e\,.$$

Taking this into account and using (43) in the Euler—Lagrange equations, (42) will readily be regained.

We can also define a new metric tensor

$$\bar{g}_{ab} = (e - C_{R|}\,C_{T|}\,k^{RT|})\,g_{\mathbf{ab}}\,.$$

Using a parameter s' for which

$$\bar{g}_{rt}\frac{dx^{r}}{ds'}\frac{dx^{t}}{ds'} = \text{const.}\,,$$

the Euler—Lagrange equations

$$\frac{\partial L}{\partial x^{a}} - \frac{d}{ds'}\frac{\partial L}{\partial\dfrac{dx^{a}}{ds'}} = 0\,,$$

with the L defined by (43), will lead to

$$\frac{d^{2}x^{a}}{ds'^{2}} + \left\{\overline{\begin{matrix} a \\ r\ t \end{matrix}}\right\}\frac{dx^{r}}{ds'}\frac{dx^{t}}{ds'} = \bar{g}^{at}\,(C_{R|}\,K^{R|}{}_{r,t} - C_{R|}\,K^{R|}{}_{t,r})\frac{dx^{r}}{ds'}\,,$$

where $\left\{\overline{\begin{matrix} a \\ b\ c \end{matrix}}\right\}$ is formed from $\bar{g}_{ab}$ in the usual way.

It will be apparent that the potential force can be removed by redefining the metric tensor only at the price of making the new metric dependent on the constants $C_{A|}$.

Conclusions

Looking at the reasoning of Section III from the other way round, we see that a potential-like term of the first curvature of a curve in a V_m can always be removed by redefining the metric of V_m. The new metric tensor is the product of the old one and the so-called conform factor [4].

On the other hand, an electromagnetic (or gyroscopic) force can only be removed at the expense of increasing the dimensions of the space. However, the larger space obtained this way will possess Killing symmetries constituting an Abelian group of motions.

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О ГЕОДЕЗИЧЕСКИХ НЕКОТОРЫХ СИММЕТРИЧНЫХ ПРОСТРАНСТВ

А. ШЕБЕШТЕН

Резюме

Изучены геодезические римановых прстранств, допускающих некоторые типы движения Киллинга. Показано, что в них геодезическим линиям соответствуют кривые в пространстве с меньшим числом измерений, что находится в удивительном сходстве с законом сил в общей теории относительности. Встречающиеся здесь силы имеют электромагнитный и потенциальный характер. Обсуждается связь между этими свойствами и пятимерной теорией Калуцы. Развит метод так называемого полностью ковариантного расчёта для таких пространств.

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COMMUNICATIONES BREVES

ÜBER DIE AUSBREITUNG DER COMPTON-LINIE

Von

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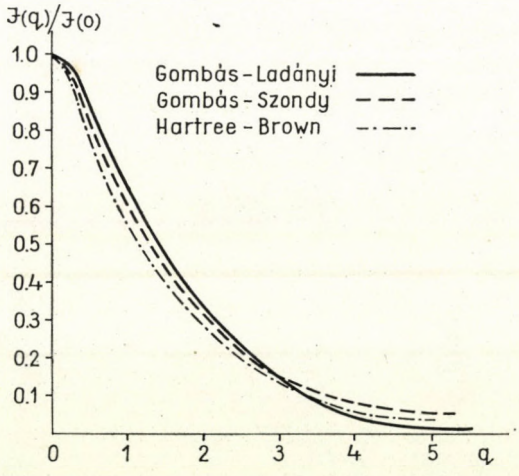
A. Kónya untersuchte in 1949 [1] ein von Burkhardt [2] begründetes, aus statistischen Überlegungen stammendes Verfahren und wandte es bei mehrerlei Elektronendichteverteilungen an. Der Verfasser benützte diese Methode für das Gombás—Ladányi Atom-Modell [3, 4]. In der vorliegenden Arbeit führt der Verfasser Berechnungen an dem in 1968 veröffentlichten Gombás—Szondy Modell [5] durch. Es ist bei diesem Modell charakteristisch, dass die Austauschenergie nicht eingebaut ist. Eben darum ist das erhaltene Ergebnis mit der von Brown berechneten [6] Hartreeschen Elektronenverteilung gewonnenen Intensitätsverteilung des Compton-Bandes zu vergleichen.

In jedem Falle wird der Streuprozess für das Ne-Atom untersucht. Der einfallende Röntgenstrahl ist die MoKα Linie und der Streuwinkel beträgt 180°. Die Intensität ist $J(q)$, wo q eine mit der Wellenlängenverschiebung l proportionale Grösse ist.



Die Abbildung zeigt $\frac{J(q)}{J(o)}$. Die Halbwertsbreite ist auf Grund $\frac{J(q)}{J(o)} = \frac{1}{2}$ durch $2l = 0{,}02066\ q$ in Å angegeben: deren Grösse sich bei dem GOMBÁS—SZONDY Modell als 0,026 Å und bei der Hartreeschen Elektronenverteilung als 0,023 Å (in genauem Einklang mit dem von KÓNYA [1] veröffentlichten Wert) ergibt.

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TIRED LIGHT AND THE "MISSING MASS" PROBLEM

By

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I. Introductory remarks

The paradox of the discrepancy between the "number mass" and "dynamical mass" for clusters of galaxies has been known since the 1930's. All attempts to resolve this paradox to date must be considered inconclusive at best. The solution proposed by AMBARTSUMIAN — that clusters are expanding and thus the Virial Theorem cannot be used to calculate the dynamical mass — is generally held to be untenable [1, 2, 3, 4]. The other, most popular, hypothetical solution to the paradox is the well known "missing", i.e. non-luminous and as yet undetected, mass. A number of searches based on the assumption that this hypothetical "hidden mass" exists in familiar forms have all yielded negative results [5, 6, 7].

The "missing mass" hypothesis is appealing for cosmological reasons as well as that it appears to be the only feasible solution that will not require changes in accepted theory. The most popular relativistic cosmology, for which the cosmological constant is zero, requires a mass density for the universe which is substantially greater than that observed. In fact, 90 to 99 percent of the matter in the universe would have to be in the form of "missing mass". The most recent speculation is that perhaps the "missing mass" is in the form of black holes. However, the presence of a black hole has, as yet, never been detected and identified. Furthermore, the mass discrepancy for clusters of galaxies places another, rather stringent requirement on the form of the "missing mass". As BURBIDGE and BURBIDGE have pointed out [1], "If this material is distributed uniformly inside and outside clusters it will not affect the arguments concerning the stability of clusters. Only if it is also clustered will the argument be changed. If it were concentrated sufficiently to stabilize loose clusters, there would have to be a much higher density of intergalactic matter inside loose clusters than inside condensed clusters. This would appear to be improbable".

All currently popular cosmologies interpret the cosmological redshift as a genuine Doppler shift. However, when the systematic redshifts of the nebulae

were first discovered it was proposed by MACMILLAN that perhaps the redshifts were due to a secular decrease in the frequency of light as it traveled through space [8] — the well known "tired light" hypothesis. When the mass discrepancy for clusters of galaxies was discovered in the thirties, and several times since then, it has been speculated in passing that the tired light hypothesis might resolve the paradox; but for various reasons it appears that this possibility has never been thoroughly investigated [2]. Since the paradox is still with us after almost forty years, perhaps a thorough, quantitative investigation of the "tired light" hypothesis is justified.

We must emphasize at this point, however, that we do not argue that the "tired light" hypothesis is the *only* acceptable solution to the mass discrepancy paradox. Our only intent is to demonstrate explicitly that it is a viable solution which is not at variance with any observational results. If one chooses to test the hypothesis, we suggest an experiment at the end of this paper which should unambiguously show whether or not the "tired light" hypothesis has any value.

II. Discussion

Unquestionably, the most popular and time-honored device used when one tinkers with a field theory is to introduce an exponential into the equation for the potential of the field. Aside from NEWTON, EULER and YUKAWA, others who have used this device are NEUMANN [9], MILNE [10], FREUND et al. [11], and GERASIM [12]. Let us assume then, as a formalism for the "tired light" hypothesis, that the frequency of light (ω) at a distance r from a source which has a frequency ω_0 is

$$\omega = \omega_0 \exp(-\alpha r),$$

where α is an attenuation coefficient. For r less than 10^3 megaparsecs (mpc) the approximation

$$\omega = \omega_0(1 - \alpha r)$$

is valid. We assume now that the cosmological redshift is entirely due to the exponential factor, i.e. that the cosmological redshift is purely a "tired light" phenomenon. This gives us

$$\omega = \omega_0(1 - Hr/c),$$

H being the Hubble constant and c the velocity of light.

The mass for a cluster of galaxies determined by the Virial Theorem (M_v) is given by the equation:

$$M_v = V^2R/G,$$

where G is the constant of gravitation, R twice the harmonic weighted (by

mass) mean distance between cluster members, and V the root-mean-square space velocity for cluster members determined from the redshift dispersion of the galaxies in the cluster. Reinterpretation of the cosmological redshift as due to a "tired light" effect will affect V in the above equation leading to a corrected Virial Theorem mass prediction (M_c) given by:

$$M_c = \frac{(V-1.73HR')^2 R}{G},$$

where R' is the dynamical radius of the cluster [13]. Naturally M_c should be equal to the number mass (M_n); thus, defining the mass discrepancy as $A = M_v/M_n$, we have for the mass discrepancy

$$A^{1/2} = \frac{V}{V-1.73HR'}.$$

As the dynamical radii of clusters, except in the case of the Coma cluster, are not well known, we shall rearrange the above equation to give R' in terms of A and V. We get:

$$R' = \frac{V}{1.73H}(1-1/A^{1/2}). \tag{1}$$

It but remains to check and see if the above equation leads to reasonable dynamical radii for clusters of galaxies.

III. Observation

As the value of A depends on M_n, which in turn depends on the mass to luminosity (M/L) ratios of the various types of galaxies, we shall briefly consider the M/L ratios deduced from observation. Perhaps the most reliable M/L ratios are those obtained by PAGE from observations of double galaxies [14]. However, two corrections must be applied to PAGE's values. As VAN DEN BERGH has pointed out [3], the values obtained by PAGE are almost certainly in error as many of the pairs used by PAGE are located in clusters where the application of the Virial Theorem is highly questionable. He recomputed the M/L ratios excluding the pairs that are cluster members. The exclusion of cluster members reduces PAGE's value for E and SO systems by about 50%. Also, as POVEDA has noted [15], the assumption of circular orbits for pairs is, by analogy with diatomic molecules, unlikely to be valid. Accordingly, VAN DEN BERGH's values of M/L (which assume circular orbits) should be reduced by about 20%. Making these modifications, one obtains 40 for the M/L ratio for E and SO galaxies and 3.5 for S or Irr systems. (M/L is in units of solar mass and luminosity.)

From the literature one may, for particular clusters, get the values of the velocity dispersion (V), the percentage of E and SO galaxies in the cluster, and the average M/L ratio computed from the Virial Theorem $(\overline{M/L})_v$. ([1, 3, 4, 16, 17 and 18].) The value of A may then be determined by dividing $(\overline{M/L})_v$ by the average M/L ratio computed from the percentage of E and SO galaxies and the values of M/L given above. Using the values of V and A so obtained (and $H = 100$ km/sec per mpc) the predicted dynamical radii (R') may be computed using Eq. (1). All of the relevant values appear in Table I for four clusters with more than fifty members.

Table I

The predicted values of the dynamical radius (R') for four clusters with more than fifty members and the quantities for each cluster necessary to obtain the predictions

Cluster	V (km/sec)	%E + SO	$\overline{M/L}$	$(\overline{M/L})_v$	A	R' (mpc)
Hercules	1093	30	15	100	6.7	3.9
Coma	1730	approx. 100	40	350	9.0	6.7
Virgo	1040	40	18	600	33	5.0
NGC 541	703	50	22	240	11	2.8

The only cluster for which R' is observationally well known is Coma where R' is about 6.3 mpc. The agreement for this cluster is quite good considering that A and H are only accurate to a factor of about 1.5. As for the other clusters, it is known that there are members, usually much fainter and less massive, outside of the central area of condensation where most of the bright, heavy galaxies are located; e.g. the "southern extension" of the Virgo cluster. Thus it would seem that the values of R' in Table I are at least not unreasonable.

One of the two serious objections that can be made against the use of the "tired light" hypothesis in the above manner is that it reinterprets most of the normal velocity dispersion (V), calculated from the redshifts, as being simply an indication of distance and not of velocity of recession. Consequently, the relaxation time for mass segregation, which is approximately proportional to the cube of the actual velocity, must in general be reduced. For instance, in the case of the Coma cluster the relaxation time must be reduced by a factor of 28. Thus one should observe extensive mass segregation if the "tired light" hypothesis is to be an acceptable explanation of the mass discrepancy paradox.

But one can claim that extensive mass segregation is observed. Let us take as an example the cluster NGC 541. ZWICKY and HUMASON report that there are three distinct levels of mass segregation present in the cluster [4]. 1) a central region with five pairs of galaxies actually in contact, 2) a region

with a radius of about 0.47 mpc where practically all the bright, massive galaxies are located, and 3) a less readily delimitable region where there are many faint galaxies of small mass associated with the cluster. In the Coma cluster virtually all of the massive galaxies are located within a radius of one mpc of the center, while small-mass cluster members are observed at distances of up to 6.3 mpc from the center.

IV. Maxwell's equations and photon rest mass

The second serious objection to the "tired light" hypothesis is that Maxwell's equations must be altered. The hypothesis, as formulated above, implies that the Poynting vector ($\vec{S}$) normally given by

$$\vec{S} \sim \vec{E} \times \vec{H} ,$$

must be changed to

$$\vec{S} \sim e^{-Hr/c}(\vec{E} \times \vec{H}) , \tag{2}$$

where $\vec{E}$ and $\vec{H}$ are the electric and magnetic field vectors for, in this case, an isotropic, spherically symmetric field. The exponential factor in Eq. (2) gives the electromagnetic field a finite range and consequently photons with finite rest mass. The modification of Maxwell's equations which includes finite rest mass photons is the Proca equation [19]:

$$\partial^{\lambda} F_{\lambda\nu} + \mu^2 A_{\nu} = (4\pi/c) J_{\nu} ,$$

which yields a Poynting vector of the form

$$\vec{S} \sim e^{-2\mu r}(\vec{E} \times \vec{H}) ,$$

μ being the photon rest mass. Thus, reinterpretation of the cosmological redshift as a "tired light" effect implies that the photon should have a rest mass:

$$\mu = H/2c.$$

It is empirically established that the value of μ in terms of the characteristic length of the field is less than 10^{-10} cm^{-1} [19]. The value of $H/2c$ is about 10^{-26} cm^{-1}; thus the above interpretation of the cosmological redshift is not at variance with any empirical observations. Looking at the other side of the coin, we may say that the cosmological redshift sets an upper limit of about 10^{-63} grams to the photon rest mass — a value 15 orders of magnitude better than that of GOLDHABER and NIETO [19].

V. A testable consequence

As we have already noted, the "tired light" hypothesis is highly speculative and the principal aim of this paper is to demonstrate that this hypothesis

can resolve the mass discrepancy paradox for clusters of galaxies, though it may very well not be the correct explanation. Astronomically there is no direct method of distinguishing between the "tired light" hypothesis and those theories which interpret the cosmological redshift as the result of a real velocity of recession. Interestingly, there is, however, a consequence of the tired light hypothesis that may be terrestrially testable.

The above interpretation of the cosmological redshift demands that the universe be static. Concomitantly, due to the energy loss of electromagnetic radiation (the tired light effect), the mass-energy density of the universe must be decreasing. This, of course, is a violation of both the perfect cosmological principle and the principle of conservation of mass-energy. There are two ways of avoiding this dilemma. One is to assume that the energy lost by radiation is replaced by the "continuous creation" of matter *ex nihilo* throughout space (a mechanism similar to that of Steady State cosmology). This we tentatively reject because of its metaphysical nature. The other is to assume that the lost energy does not cease to exist, but is reconstituted into intergalactic hydrogen [8].

The recent experiments designed to test the "continuous creation" hypothesis of Steady State cosmology suggest that an analogous experiment might be done to test this "continuous reconstitution" hypothesis. One would simply pump electromagnetic radiation into a confining cavity to see if it decays into hydrogen. The most effective way to do this would be to use radio-frequency radiation and a cavity with superconducting walls to maximize the lifetime of the photons. In a straight-forward manner it may be shown that the number of hydrogen atoms (n) produced in a spherical cavity of radius r with a skin depth δ in a time t is:

$$n \simeq \frac{HrPt}{3\delta\omega E_0},$$

where P is the power of the source of radiation, ω its frequency, H the Hubble constant, and E_0 the rest energy of the hydrogen atom. If we take $r = 3$ meters, $\omega = 10^8$ *Hz*, and $P = 10^3$ watts, this should result in a production rate of several hydrogen atoms per day. If the experiment could be done, the results would be of interest and it would either corroborate or lay to rest forever the "tired light" hypothesis.

Addendum

While this paper was in the press, the work of VIGIER [20] and DUCHESNE and VIGIER [21] has come to our attention. They furnish empirical evidence of a convincing nature which indicates that, contrary to current belief, the photon

has a finite rest-mass. Unfortunately, the experiment does not admit of a quantitative determination of the rest-mass.

However, the "tired light" interpretation of the cosmological red-shift is certainly more plausible and appealing if one can show from independent observations (as one evidently is able to do) that the photon has a finite rest-mass. In any event, as we noted in our paper, the cosmological red-shift demands a value limit of 10^{-63} grams for the photon rest-mass. Clearly, in the laboratory it will prove quite difficult to obtain an accurate value for so small a quantity. But if it turns out to be 10^{-63} grams, then the "tired light hypothesis" is in fact the correct solution to the missing mass problem.

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13. That R' must be the dynamical radius of the cluster may be demonstrated in the following manner. (The dynamical radius is defined as the distance from the center of the cluster beyond which galaxies are no longer physical members of the cluster.) Consider the ith galaxy located at a distance r_i from the near edge of the cluster with a redshift s_i. According to current theory its space velocity in one dimension with respect to the center of the cluster $(v_r)_i$ will be

$$(v_r)_i = s_i - s_0 ,$$

where s_0 is the redshift of the center of the cluster which is just the mean of the values of $(v_r)_i$. But according to the "tired light" hypothesis the true space velocity in one dimension of the ith galaxy $(u_r)_i$ will be $(v_r)_i$ minus the apparent velocity of recession due to the cosmological redshift, i.e.

$$(u_r)_i = (v_r)_i - H_i .$$

It is impossible to know r_i for any particular galaxy, but this is not important as we are only interested in the mean of all of the values of r_i. It is easy to see that the mean of the r_i's is approximately equal to the dynamical radius of the cluster (R').
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NEW MODEL FOR CRITICAL STATE OF TYPE II SUPERCONDUCTORS

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In type II superconductors a superconducting – normal lattice system is formed in the mixed state between the lower and upper critical magnetic fields (H_{c1} and H_{c2}). At normal places the value of the magnetic field will be maximal, at other places less or zero. Magnetic vortices come into being which cover the whole specimen like a network of filaments. In the presence of an external field $H_{c1} < H < H_{c2}$ the intensity of the internal field is determined by the density n of the vortex lines:

$$B(H) = n\Phi_0, \tag{1}$$

where Φ_0 denotes the elementary magnetic flux. In the equilibrium case this value is macroscopically the same throughout the specimen. If an electric current of density j is passed through the specimen in the direction x, providing H points in the direction z, a vortex density gradient will be induced in the y direction:

$$\frac{4\pi}{c} j = \frac{\partial B(H)}{\partial y} = \frac{\partial n}{\partial y} \Phi_0. \tag{2}$$

The so-called Lorentz force per unit surface of the vortices is

$$F_L = \frac{1}{c} j \times B = \frac{1}{c} j \times n\Phi_0. \tag{3}$$

The vortices are fixed by an opposing pinning force F_P arising from the presence of inhomogeneities, lattice defects and alloy grains like pinning centres in the material.

The critical state is considered to be that in which j is so big that F_L is just equal to F_P. In this case the superconducting material carries the greatest possible supercurrent and the inner field is defined by the relation

$$\frac{1}{c} j_{(c)} \times B = F_{P(c)}, \tag{4}$$

where $F_{P(c)}$ is the maximal pinning force at the given temperature [1].

If $F_L > F_P$, then the flux lines begin a convective and dissipative flow with a velocity v characterised by the viscosity coefficient η from the formula

$$F_L - F_P = \eta v. \tag{5}$$

In this "flux-flow" state the current also flows through the normal kernels of the lattice system of the material and is accompanied by a measurable electric field intensity E and by the appearance of a resistance ϱ

$$E = \frac{1}{c} nv\Phi_0 = \frac{1}{c} vB$$

and

$$\varrho = \frac{\mathrm{d}E}{\mathrm{d}j} = \frac{1}{c^2} \frac{n\Phi_0^2}{\eta} = \frac{\Phi_0}{c^2 \eta} B.$$

By means of this method the critical current can be determined in the case when all the vortices are bound in the same way with an equal pinning force.

Our experiments on In- (2–4%) Bi alloys have shown, however, that the current–voltage characteristics have two or more different curvatures, or linear parts, which points to the existence of two or more critical current values.

In the following calculations the range $B\lambda^2 \gg 1$ will be examined and it will be supposed that the specimen is macroscopically homogeneous [2].

Further, since the effective distance of the interaction between vortices is equal to the penetration depth λ, vortices lying within this distance from each other will be considered as forming a vortex band.

According to the principle of our model the different critical currents can be explained by supposing that one part of the vortices is unbound while their other part is bound. The force acting on a band of unpinned vortices is

$$F^i_{\text{unpinned}} = \sum_j^i \left(\frac{j \times \Phi_0}{c} - \sum_k F^{uj}_{uk} - \sum F^{uj}_{bk} \right), \tag{6}$$

where the first summation refers to the chosen i-th vortex band. The first term of the right side is the Lorentz force acting on the j-th vortex, the second and the third terms denote the forces arising from the unbound and bound vortices, respectively. Taking into consideration that $F^j_k = -F^k_j$ and the effects of the distant vortices compensate each other, the second term vanishes. Introducing the quantity

$$F = \frac{1}{n_u n_b} \sum_j \sum_k F^{uj}_{bk}, \tag{7}$$

which denotes the average force a bound vortex exerts on an unbound one, we can write

$$F^i_{\text{unpinned}} = n^i_u \left[\frac{j \times \Phi_0}{c} - n_b F \right]. \tag{8}$$

Similarly if all the pinning centres exert the same pinning force, then the force acting on a band of pinned vortices will be

$$F^i_{\text{pinned}} = \sum_j^i \left(\frac{j \times \Phi_0}{c} - \sum_k F^{bj}_{uk} - \sum_k F^{bj}_{bk} - F_p \right). \tag{9}$$

As $\sum_j^i \sum_k F^{bj}_{bk} = 0$ we get

$$F^i_{\text{pinned}} = n^i_k \left[\frac{j \times \Phi_0}{c} + n_u F - F_p \right]. \tag{10}$$

In a critical state the resultant of the forces acting on the vortex band is zero. This state can be realised in two ways:

1) If $F_{\text{unpinned}} = F_{\text{pinned}} = 0$, then the arising forces are determined by means of formulas (8) and (10):

$$F = \frac{1}{n_b} \frac{j_{(c)} \times \Phi_0}{c} \tag{11}$$

$$F_p = \frac{n_u + n_b}{n_b} \frac{j_{(c)} \times \Phi_0}{c}, \tag{12}$$

where

$$n_u + n_b = n.$$

In this case there is a unique relation between the critical current and field and the material characteristics:

$$\alpha = |j_{(c)} \times B| = c n_b |F_p|. \tag{13}$$

2) Since the value $0 < F < F_{\max}$ is determined by the interactions among the vortices, the case can be realised when $F_{\text{unpinned}} = 0$ and $F_{\text{pinned}} < 0$, then only the unpinned vortices begin to move. This is the first critical current, for which the relation

$$\frac{j_{(c1)} \times \Phi_0}{c} = n_b F_{\max} \tag{14}$$

is valid.

By raising further the current density j we reach a state when all the vortices just begin to flow. The critical current at which this occurs is determined by the relation

$$\frac{j_{(cII)} \times \Phi_0}{c} = F_p - n_u F_{\max} . \tag{15}$$

Consequently two critical currents exist. Corresponding to these two critical currents two characteristic α-parameters can be defined:

$$\alpha_I = j_{(cI)} B = c \frac{B}{\Phi_0} n_b F_{\max} , \tag{16}$$

$$\alpha_{II} = j_{(cII)} B = c \frac{B}{\Phi_0} (F_p - n_u F_{\max}) . \tag{17}$$

The flux-flow resistances can be calculated in a similar way as in the KIM model [3], that is

$$\varrho_I = \varrho_n \frac{B - n_b \Phi_0}{H_{c2}(T)} , \tag{18}$$

$$\varrho_{II} = \varrho_n \frac{B}{H_{c2}(T)} , \tag{19}$$

where ϱ_n is the normal resistivity and T is the absolute temperature. From these the bound vortex density n_b can also be determined:

$$n_b = \frac{1}{\varrho_n} [\varrho_{II}(B) - \varrho_I(B)] \frac{H_{c2}(T)}{\Phi_0} . \tag{20}$$

Eqs. (14), (15) and (20) also make it possible to calculate the value $F_{\max}$ and to compare it with measurable quantities:

$$F_{\max} = \frac{1}{c} \frac{\varrho_n}{\varrho_{II} - \varrho_I} \frac{j_{(cI)} \Phi_0^2}{H_{c2}(T)} . \tag{21}$$

In general, if there are N pinning forces of different intensities then there willbe a corresponding number of critical currents. Thus in the above case 1) now we similarly get

$$\alpha = j_{(c_i)} B = c \sum_i F_{pi} n_{bi} . \tag{22}$$

Since $F_{pk} > F_{pi}$ if $k > i$, possibility 2) is the one when the vortices get into a critical state in groups. According to this instead of the force F in the formula

(7) the force is exerted by the still bound k-th vortex on the unbound i-th type vortex will be

$$F^{ik} = \frac{\sum_{j}^{i} \sum_{l}^{k} F_{bl}^{uj}}{n_{bi}\, n_{bk}} . \tag{23}$$

In this model the k-th critical current will be

$$\frac{j_{(ck)} \times \Phi_0}{c} + \frac{\sum_{i<k} F^{ik}}{n_{bk}} = F_{pk} , \tag{24}$$

and the k-th flux-flow resistance

$$\varrho_k = \varrho_n \frac{B - \sum_{j=k}^{N} n_{bj}\, \Phi_0}{H_{c2}(T)} . \tag{25}$$

These equations contain the case, when there are N different pinning centres and forces, moreover according to this fact N different resistances, critical currents and fields.

The formula (20) gives a simple possibility for controlling the validity of the model, since n_b can be estimated when all the other data are known. If the number of Bi-atoms on the unit surface is computed, and supposed that one pinning centre is composed of the Bi atoms being not farther from each other than $\xi \sim \lambda \approx 1000$ Å, a new n_b value can be got by a simple calculation. Having made the computations and compared these two results we have found that they are of the same order. This result is relatively very accurate, so it verifies the model in a convincing experimental way.

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RECENSIONES

L. D. Landau, A. I. Achieser und E. M. Lifschitz:

Mechanik und Molekularphysik

(in German) Akademie-Verlag, Berlin, 1970, 309 pp.

This can be regarded as a supplement to the well known textbooks by Landau and Lifschitz. The aim of the authors has been to describe the fundamental physical phenomena and the important laws of physics. As the authors endeavoured to reduce the length of the text as much as possible, the treatment is restricted mainly to essentials and details of smaller significance have been omitted. Deductions from formulas are given only in so far as they are indispensable for the understanding of relations between phenomena. The formulas are deduced on the simplest possible examples. The elements of algebra, trigonometry, as well as vector algebra and differential calculus are assumed to be known. Likewise, a knowledge of the fundamental concepts of physics and chemistry taught at the secondary school are required for the understanding of the book. The authors intend the book for students in the physical faculties of universities and in high schools or technical universities where physics plays an important role, as well as for secondary school physics masters.

In Part I the book is concerned with point mechanics and the concept of space, the mechanics of rigid bodies and the theory of vibrations. Part II deals with applications in many fields of physics. The chapter on atoms, isotopes and molecules is short but more detailed treatments are given of the problems of the symmetry of molecules and crystals and thermodynamics; special regard is paid in the latter section to phase transitions, chemical reactions and surface phenomena, thermal conductivity and friction.

Without striving for completeness the book provides a good introduction to the study of the more important physical phenomena and laws. A special virtue is the authors' clear way of expression and concise language already well known from their other books, which bring to light relations that in other treatments usually remain concealed, owing to the variety of partial results.

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Department of Atomic Physics
Polytechnical University, Budapest

P. A. Egelstaff and M. J. Poole:

Experimental Neutron Thermalisation

with a Mathematical Appendix by P. Schofield. International Series of Monographs in Nuclear Energy, Vol. 106, Pergamon Press, Oxford—London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1970

Since it became known that a self-sustaining fission reaction can take place in natural uranium only if the neutrons generated in the fission lose their energy, slow down and come more or less into thermal equilibrium with the moderator in which they move, the investigation of the thermalisation of neutrons has become one of the most important fields of research in reactor physics. A knowledge of the thermalisation processes of neutrons is important not only from the point of view of reactor research, however, but also because these processes provide useful information on the microphysical characteristics of moderator materials.

The 13 chapters of this book by Egelstaff and Poole give an excellent and almost complete treatment of all problems of importance in the field, ranging from the elementary processes of neutron thermalisation to their macro-consequences:

Chapter 1 is a brief summary of the theory of scattering. Although the material can be found in any textbook of nuclear physics, it could have hardly been omitted here.

Chapter 2 on the other hand, containing as it does the theory of neutron scattering in condensed matter, is already devoted to problems that are an essential part of the realization

of fundamental aims. The advantages of the Van Hove correlation method are pointed out here with remarkable skill.

The conception that the scattering function describing the process of scattering underlies any thermalisation problem is formulated at the end of Chapter 3.

In Chapter 4 the authors briefly summarize the procedures of neutron energy measurement, restricting themselves to give a survey of main features only. Reference to the use of pulsed reactors should have been included in the list of pulsed neutron sources. Neutron detectors and the methods of measurement provided by up-to-date computer technique are also outlined here.

Methods of measuring the differential scattering cross-sections of neutrons are dealt with in Chapter 5 and the interpretation of the scattering law based on these measurements in the following Chapter.

As in many cases the angular dependent differential cross-section or the so-called total cross-section are required instead of the double differential cross-section, the authors very sensibly devote a separate chapter to the theoretical and experimental problems of these cross-sections. Chapter 7 contains important data on water and zirconium hydride.

Chapter 8 is of direct importance for nuclear engineers. In this Chapter a summary of measurements of neutron spectra developing in the various moderating and cooling media is given. Valuable data can be found for graphite, beryllium, beryllium oxide, zirconium hydride, light and heavy water, and even for benzene and polyethylene.

It is of great practical importance to know the equilibrium energy spectrum developing in reactors. In Chapter 9 the experimental methods applicable to the determination of this spectrum are described. The advantages of the various procedures are analysed and the errors imposed by the limits of resolution are investigated.

Chapter 10 describes the results related to the experimental determination of the kernel in the integral equation of thermalisation. For the most important moderators, a beautiful summary is given of the kernel characteristic of the energy exchange between neutrons and the moderator.

Chapter 11 deals with the time course of thermalisation and with the theoretical and experimental efforts that have been devoted to detecting the dynamics of formation of the equilibrium spectral distribution.

Chapter 12 is a theoretical and experimental investigation of the anisotropy of the kernel used to describe energy transfer and finally, Chapter 13 is devoted to the methods of measurement and theoretical problems of neutron spectra observed in particular reactors.

The Appendix by SCHOFIELD, which is a brief summary of the mathematical fundamentals required for thermalisation investigations, is also worth mentioning.

EGELSTAFF and POOLE's book is a useful monograph for all those engaged in reactor design; it is also indispensable for experimentalists using neutron beams in their work, where the shaping of neutron beams and adjustment of their energy spectrum is a very frequently occurring problem. It can be warmly recommended that EGELSTAFF and POOLE's book be consulted on these problems. Credit is due to Pergamon Press for having published a long-needed book.

L. PÁL

GY. A. NAGY and M. SZILÁGYI:

Introduction to the Theory of Space-Charge Optics

(in Hungarian) Akadémiai Kiadó, Budapest, 1967

Although the literature on general electron optics is very extensive and some works have been published on the topic even in Hungarian, no monograph summing up the whole field, including space-charge has been available until the appearance of the present book. Even at present in world literature there is only one book of similar standard and of a similar scope. The book has therefore filled a gap both in Hungarian and world literature.

The book is divided into six Chapters.

In Chapter 1 (by GY. A. NAGY) the fundamental equations of the subject, the exact and approximate methods of calculation and the methods of measurement are worked out.

For the calculation of the electric and magnetic field a method generally applicable for space-charge and current density is given.

Based on the relations obtained in the calculation of fields the part on the equations of motion describes the formulae serving as a basis for subsequent chapters.

The material of Chapter 2 (by GY. A. NAGY) which deals with the treatment of space-charge flow is a direct introduction to the design of electron guns. The general laws applicable to any space-charge flow are described. The simplified equations underlying the treatment and the most general equations are also given. The conditions of space-charge-limited flow, the scale law, the 3/2 law and several methods of calculating the flow pattern are included here.

The part presenting theorems of general validity is followed by a part on actual cases of space-charge flow, with detailed calculations including formulas for design.

The actual cases of space-charge flow have been selected with due regard to their practical importance.

Chapter 3 (by M. SZILÁGYI) is devoted to the design and calculation of the gun types called for when a high current density is required. Taking the fundamental idea suggested by J. R. PIERCE as his starting point SZILÁGYI determines the dimensions of electrodes emitting and accepting electron current, the shape and potential of electrodes replacing the omitted electrode parts and space-charge parts. The disturbing effect of openings for transmitting the electron current and the limits imposed by the calculation of the deviations due to the thermal speeds of the electron are given.

The first major part of Chapter 4 (by M. SZILÁGYI) describes the properties of the electron beam of parallel flow and introduces the necessary characteristics of the beam. It is shown that the distribution of potential, space-charge and current density in such beams can be determined in a relatively simple way and that though it can only be found as an approximation in the actual cases the effect of these beams on the environment can be still taken into account. Finally, information is provided on the highest value of current that can be transmitted in such beams.

The second part of the Chapter goes on to investigate real beams. The reasons for the changes of the shape of the beam, the value of the smallest diameter and the highest transmissible intensity of the current when it comes to considering real cases are here made both apparent and comprehensible.

Chapter 5 (by M. SZILÁGYI) is concerned with beaming, the most important field of the electron optics of space-charge. Only beaming accomplished with the aid of electric fields is treated here and the detail is such as cannot be found anywhere else in the literature. According to the importance of the subject this Chapter contains most of the new material so far unpublished. The applications of beaming, their advantages and disadvantages are treated very thoroughly in the introductory part. Using the optical analogue the most important principle of beaming, the system applying a periodical electric field is described, the characteristics necessary in any description of beaming systems are introduced and a general method for calculating the dependence of beams on the initial conditions is given.

All important cases met with in practice are commented on in a detail not encountered even in original publications. Not only trajectories near the axis, but in accessible cases, trajectories far from the axis are determined. The conditions of beaming are investigated in full and the current density distribution necessary for a good beaming is also considered.

The richess of the field is shown by the variety of beaming procedures described at length in the Chapter, considering that a good choice of the beaming procedure most suitable for a given purpose is only possible by comparing the various procedures.

Chapter 6 (by GY. A. NAGY) deals with beaming by magnetic field. The backbone of the treatment is the description of the most important beaming procedures, beaming by the Brillouin procedure, with a periodic magnetic field and with a quadrupole field. The conditions of beaming, the consequences of the general initial conditions, and the calculation of the deviations due to the inaccuracy of the realization of the magnetic field are investigated. The section on the beaming problems of tubes of partially and fully screened cathodes deserves particular emphasis.

Beaming with a magnetic quadrupole field is treated for several cases not mentioned in the literature, including the case of an electric and a magnetic field acting simultaneously.

A very important advantage of the treatment, which greatly increases the usefulness of the book is that, although the underlying fundamental principles are as general as possible, end formulas, diagrams and structural details suitable for dimensioning are provided at the end of each chapter.

Each chapter is followed by an ample, sometimes almost complete list of references. The best proof of the authors' high competency in this field is the large number of their own publications quoted.

It seems to be desirable to publish this book of high theoretical standard, at the same time suitable for direct practical use and containing several original results, in foreign languages!

K. SIMONYI

S. DEME

SEMICONDUCTOR DETECTORS FOR NUCLEAR RADIATION MEASUREMENT

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Tihany, June 17—21, 1969

edited by I. DÉZSI

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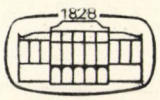

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L. Jánossy

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A MAGNETOHYDRODYNAMICAL DYNAMO MODEL

By

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(Received 10. II. 1970)

The solution of a magnetohydrodynamical system of equations for an incompressible real conducting medium is given for the instationary case. It is shown that the results of SZABÓ for ideal media are reobtained in the case when the hydrodynamical viscosity of the real medium tends to zero.

Introduction

It is known that the flow of electrically conducting media in a magnetic field may result in an increase in the magnetic field. The problem belongs to the sphere of so-called magnetohydrodynamical dynamo theory, which is at present also used to explain the origin of the magnetic field of the Earth and stars.

This paper is concerned with a dynamo model which takes as its starting point an infinite, homogeneous, incompressible, hydrodynamically real, electrically conducting medium with a velocity distribution

where

$$\left.\begin{aligned} v_x = v_0 I(z)\,,\ v_y = 0\,,\ v_z = 0\,, \\ I(z) = \begin{cases} 1 & \text{for} \quad z < 0 \\ 0 & \text{for} \quad z > 0 \end{cases} \end{aligned}\right\} \tag{1}$$

at the instant $t = 0$ in a homogeneous $\vec{H}_0 = \{0,\ 0,\ H_0\}$ magnetic field.

It will be shown that the induced magnetic and electric field intensities and the velocity distribution for $t > 0$ can be explicitly evaluated.

The solution of this model for a hydrodynamically ideal medium has been solved by SZABÓ [1]. The corresponding stationary problem was solved already in 1937 by HARTMANN [2].

The theoretical and practical importance of the problem is clear when it is remembered that the strong magnetic fields connected with sunspots can be explained, at least qualitatively as resulting from the flow of the highly conducting plasma, and that by using this effect it is possible to generate very strong magnetic fields under laboratory conditions [3].

The most essential conclusion of this paper is that an additional magnetic field is generated in the direction of flow of the medium, while an electric field is induced at right angles to the direction of flow and the direction of the magnetic field. In the asymptotic case $t \to \infty$, the absolute values of the induced magnetic and electric fields are

$$H_x = \frac{1}{2}\sqrt{\frac{\varrho}{\mu_0}}\, v_0 , \tag{2}$$

$$E_y = \frac{1}{2}\mu_0 H_0 v_0 . \tag{3}$$

The velocity distribution for $t \to \infty$ in the whole infinite medium is

$$v_x = \frac{v_0}{2} . \tag{4}$$

As can be seen from Eqs. (2)—(3) the values of the induced magnetic and electric field in the asymptotic case (when the stationary state sets in) are independent of the hydrodynamical viscosity of the medium and depend only on the values v_0 and H_0 determined by the initial conditions, the density (ϱ) of the flowing conducting medium and the magnetic permeability. This means that momentum is transferred from the half space $z < 0$ to the half space $z > 0$ until the velocity of the medium in the two half spaces is equalized. Accordingly, the velocity distribution developing in the flowing conducting medium is such that the magnetic energy density per unit volume of the medium is constant in time. Such a velocity distribution results in the constancy of the induced magnetic and electric field, as is also shown by Eqs. (2) and (3).

Instationary magnetohydrodynamical flow of incompressible real media

For our model we take an infinite, homogeneous, incompressible, hydrodynamically real, electrically conducting medium at instant $t = 0$ in a homogeneous magnetic field of intensity $\vec{H}_0$, where $\vec{H}_0$ is parallel with the positive z axis of the rectangular Cartesian coordinate system. The velocity distribution at the instant $t = 0$ is

$$v_y = 0\,;\ v_z = 0 \quad \text{and} \quad v_x = v_0 I(z)\,, \text{ where } I(z) = 1 \quad \text{if} \quad z < 0,$$
$$\text{and} \quad I(z) = 0 \text{ if } z > 0.$$

The problem is to determine the induced magnetic and electric field intensities and the velocity distribution for $t > 0$.

The initial conditions of the problem are

$$\left.\begin{array}{lll} v_x = v_0\, I(z); & v_y = 0; & v_z = 0 \\ H_x = 0; & H_y = 0; & H_z = H_0 \\ p = p_0 & & \end{array}\right\} \text{for } t = 0. \tag{5}$$

In this case the basic magnetohydrodynamical equations are [4]:

$$\varrho \frac{\partial \vec{v}}{\partial t} + \varrho(\vec{v}\,\mathrm{grad})\,\vec{v} = -\,\mathrm{grad}\,p - \mu_0 \vec{H} \times \mathrm{rot}\,\vec{H} + \eta \Delta \vec{v}\,, \tag{6}$$

$$div\ \vec{v} = 0, \tag{7}$$

$$\frac{\partial \vec{H}}{\partial t} = \mathrm{rot}\,(\vec{v} \times \vec{H}) + \nu_\mathrm{m} \Delta \vec{H}\,, \tag{8}$$

$$div\ \vec{H} = 0, \tag{9}$$

$$\mathrm{rot}\,\vec{E} = -\,\mu_0 \frac{\partial \vec{H}}{\partial t}\,. \tag{10}$$

The above equations are written in the Giorgi MKSA system of units using the standard notations, i.e. $\vec{E}$ and $\vec{H}$ are the electric and the magnetic field intensities, respectively, μ_0 is the magnetic permeability of the vacuum, p is pressure, η and $\vec{v}$ are the hydrodynamical viscosity and the velocity of the medium, respectively, $\nu_m = (\sigma\mu_0)^{-1}$ is the magnetic viscosity of the medium.

Owing to the symmetry of the problem the quantities in Eqs. (6)—(10) depend only on the coordinate z and time t and hence

$$\varrho \frac{\partial v_x}{\partial t} + \varrho v_z \frac{\partial v_x}{\partial z} = \mu_0 H_z \frac{\partial H_x}{\partial z} + \eta \frac{\partial^2 v_x}{\partial z^2}\,, \tag{11}$$

$$\varrho \frac{\partial v_z}{\partial t} = -\frac{\partial}{\partial z}\left(p + \mu_0 \frac{H_x^2}{2}\right), \tag{12}$$

$$\frac{\partial H_x}{\partial t} = H_z \frac{\partial v_x}{\partial z} + \nu_m \frac{\partial^2 H_x}{\partial z^2}\,, \tag{13}$$

$$\frac{\partial H_z}{\partial t} = \nu_m \frac{\partial^2 H_z}{\partial z^2}\,, \tag{14}$$

$$\frac{\partial E_y}{\partial z} = \mu_0 \frac{\partial H_x}{\partial t}\,, \tag{15}$$

$$\frac{\partial H_z}{\partial z} = 0\,, \tag{16}$$

$$\frac{\partial v_z}{\partial z} = 0\,. \tag{17}$$

From Eqs. (16)—(17) and the initial conditions we obtain

$$H_z = H_0 \quad \text{and} \quad v_z \equiv 0. \tag{18}$$

Taking Eq. (18) into consideration Eqs. (11)—(15) can be written

$$\varrho \frac{\partial v_x}{\partial t} = \mu_0 H_0 \frac{\partial H_x}{\partial z} + \eta \frac{\partial^2 v_x}{\partial z^2}, \tag{19}$$

$$0 = \frac{\partial}{\partial z}\left(p + \mu_0 \frac{H_x^2}{2}\right), \tag{20}$$

$$\frac{\partial H_x}{\partial t} = H_0 \frac{\partial v_x}{\partial z} + \nu_m \frac{\partial^2 H_x}{\partial z^2}, \tag{21}$$

$$\frac{\partial E_y}{\partial z} = \mu_0 \frac{\partial H_x}{\partial t}. \tag{22}$$

From Eqs. (19)—(22) the induced magnetic and electric field as well as the velocity distribution v_x for $t > 0$ can be determined.

It is useful to introduce the following new dimensionless variables and quantities:

$$\left.\begin{gathered} \xi = \mu_0 \sigma v_0 z; \quad \tau = \sigma \mu_0 v_0^2 t \\ u = \frac{v_x}{v_0}; \; h = \frac{H_x}{H_0}; \; E = \frac{E_y}{v_0 \mu_0 H_0}; \; P = \frac{2p}{\mu_0 H_0^2}; \\ \lambda^2 = \frac{\mu_0 H_0^2}{\varrho v_0^2}; \quad \vartheta = \frac{\eta}{\varrho \nu_m}. \end{gathered}\right\} \tag{23}$$

Eqs. (19)—(22) now take the form

$$\frac{\partial u}{\partial \tau} = \lambda^2 \frac{\partial h}{\partial \xi} + \vartheta \frac{\partial^2 u}{\partial \xi^2}, \tag{24}$$

$$0 = \frac{\partial}{\partial \xi}(P + h^2), \tag{25}$$

$$\frac{\partial h}{\partial \tau} = \frac{\partial u}{\partial \xi} + \frac{\partial^2 h}{\partial \xi^2}, \tag{26}$$

$$\frac{\partial E}{\partial \xi} = \frac{\partial h}{\partial \tau}. \tag{27}$$

For the new variables the initial conditions for $\tau = 0$ are the following:

$$h = 0; \; u = I(\xi); \quad \frac{\partial u}{\partial \xi} = -\delta(\xi); \quad P = \frac{2p_0}{\mu_0 H_0^2}. \tag{28}$$

Eqs. (24) and (26) are coupled differential equations for u and h, the solution of which must be sought by the Laplace transformation. For the Laplace transform we obtain the following differential equations:

$$p\bar{u} - I(\xi) = \lambda^2 \frac{\partial \bar{h}}{\partial \xi} + \vartheta \frac{\partial^2 \bar{u}}{\partial \xi^2}, \tag{29}$$

$$ph = \frac{\partial \bar{u}}{\partial \xi} + \frac{\partial^2 \bar{h}}{\partial \xi^2}. \tag{30}$$

Differentiating Eq. (29) with respect to ξ and taking into account that $I'(\xi) = -\delta(\xi)$, we get

$$p \frac{\partial \bar{u}}{\partial \xi} + \delta(\xi) = \lambda^2 \frac{\partial^2 \bar{h}}{\partial \xi^2} + \vartheta \frac{\partial^2}{\partial \xi^2} \left(\frac{\partial \bar{u}}{\partial \xi} \right). \tag{31}$$

Expressing $\bar{u}_\xi$ from Eq. (30) and substituting it into Eq. (31) we obtain the following differential equation for the Laplace transform of h:

$$\frac{\partial^4 \bar{h}}{\partial \xi^4} - \frac{p(1+\vartheta)+\lambda^2}{\vartheta} \frac{\partial^2 \bar{h}}{\partial \xi^2} + \frac{p^2}{\vartheta} \bar{h} + \frac{\delta(\xi)}{\vartheta} = 0. \tag{32}$$

Since the expression

$$F\{\varphi^{(n)}\} = (ik)^n F\{\varphi\} \tag{33}$$

is valid for the Fourier transform of a derivative [5] and the Fourier transform of the Dirac δ is equal to unity, the Fourier transform of the unknown function $\bar{h}(\xi, p)$ with respect to ξ will be

$$h(k, p) = - \frac{1}{k^2(p+\lambda^2) + p^2 + \vartheta (k^4 + k^2 p)}. \tag{34}$$

Using the following notations

$$b = \frac{p(1+\vartheta)+\lambda^2}{2\vartheta} \quad \text{and} \quad c = \frac{p^2}{\vartheta}. \tag{35}$$

Eq. (35) becomes

$$h(k, p) = - \frac{1}{\vartheta} \frac{1}{k^4 + 2bk^2 + c}. \tag{36}$$

Applying the inverse Fourier transformation, we obtain for $\bar{h}(\xi, p)$

$$\bar{h}(\xi, p) = \frac{s}{2\vartheta rs(r^2 - s^2)} \left(e^{-r|\xi|} - \frac{r}{s} e^{-s|\xi|} \right), \tag{37}$$

where

$$r = \frac{\sqrt{p(1+\vartheta)+\lambda^2 - \sqrt{[p(1+\vartheta)+\lambda^2]^2 - 4\vartheta p^2}}}{\sqrt{2\vartheta}}, \tag{38}$$

$$s = \frac{\sqrt{p(1+\vartheta)+\lambda^2 + \sqrt{[p(1+\vartheta)+\lambda^2]^2 - 4\vartheta p^2}}}{\sqrt{2\vartheta}}. \tag{39}$$

Substituting into Eq. (37) the expressions for r and s given by Eqs. (38) and (39), we get

$$\bar{h}(\xi, p) = -g_1(p, \vartheta, \lambda)\left[\exp\left(-\frac{\sqrt{p(1+\vartheta)+\lambda^2 - \sqrt{[p(1+\vartheta)+\lambda^2]^2 - 4\vartheta p^2}}}{\sqrt{2\vartheta}}|\xi|\right) - \right.$$
$$\left. -g_2(p, \vartheta, \lambda)\exp\left(-\frac{\sqrt{p(1+\vartheta)+\lambda^2 + \sqrt{[p(1+\vartheta)+\lambda^2]^2 - 4\vartheta p^2}}}{\sqrt{2\vartheta}}|\xi|\right)\right], \tag{40}$$

where

$$\left.\begin{aligned} g_1(p, \vartheta, \lambda) &= \frac{\sqrt{p(1+\vartheta)+\lambda^2 + \sqrt{[p(1+\vartheta)+\lambda^2]^2 - 4\vartheta p^2}}}{2\sqrt{2}\,p\sqrt{[p(1+\vartheta)+\lambda^2]^2 - 4\vartheta p^2}}, \\ g_2(p, \vartheta, \lambda) &= \frac{\sqrt{p(1+\vartheta)+\lambda^2 - \sqrt{[p(1+\vartheta)+\lambda^2]^2 - 4\vartheta p^2}}}{\sqrt{p(1+\vartheta)+\lambda^2 + \sqrt{[p(1+\vartheta)+\lambda^2]^2 - 4\vartheta p^2}}}. \end{aligned}\right\} \tag{41}$$

The limit $\vartheta \to 0$ corresponds to the case when the hydrodynamical viscosity is zero.

To determine the function $h(\xi, \tau)$ the inverse Laplace transform of the function $\bar{h}(\xi, p)$ given by Eq. (40) must be evaluated.

This is not possible in a direct way owing to the complicated form of the function. We may, however, determine the value of $h(\xi, \tau)$ for $\tau \to \infty$ without carrying out the inverse transformation. The following theorem [6] is valid for the behaviour of the function in infinity:

$$\lim_{\tau\to\infty} h(\xi, \tau) = \lim_{p\to 0}[p\bar{h}(\xi, p)]. \tag{42}$$

Using this theorem, Eq. (40) yields

$$\lim_{p\to 0}[p\bar{h}(\xi, p)] = -\frac{1}{2\lambda}, \tag{43}$$

thus

$$h(\xi, \infty) = -\frac{1}{2\lambda}. \tag{44}$$

The asymptotic behaviour of the function $h(\xi, \tau)$ for viscous flowing media agrees with the result ($\eta = 0$) obtained for ideal flowing media [1].

For the further behaviour of the function $h(\xi, \tau)$, however, we must consider its expansion in series.

Determination of the function $h(\xi, \tau)$ by expansion in series

Write the expression determined by Eq. (34) in the form

$$h(k, p) = -\frac{1}{k^2(p+\lambda^2)+p^2} \frac{1}{1+\dfrac{k^4+k^2 p}{k^2(p+\lambda^2)+p^2}\vartheta} . \tag{45}$$

Expanding expression (45) in series in terms of ϑ and neglecting the higher powers terms in ϑ, we obtain

$$h(k, p) = -\frac{1}{k^2(p+\lambda^2)+p^2}\left(1-\frac{k^2(k^2+p)}{k^2(p+\lambda^2)+p^2}\vartheta\right) . \tag{46}$$

The expansion is valid if

$$\left|\frac{k^2(k^2+p)}{k^2(p+\lambda^2)+p^2}\vartheta\right| < 1 . \tag{47}$$

For liquid metals the value of ϑ is of the order of magnitude 10^{-6} (for gases it is at least two orders of magnitude smaller), so the inequality (47) is fulfilled for the values of k, the order of magnitude of which is less than 10^3. The function $h(k, p)$ tends to zero as $1/k^4$, thus the absolute value of the integrand of the integral expanding the function $\bar{h}(\xi, p)$ tends to zero for large values of k. Consequently, large values of k make only a very small contribution to the function of $\bar{h}(\xi, p)$ and we do not commit any essential error — at least not as regards the shape of the function $\bar{h}(\xi, p)$ — if this contribution is taken to be zero. Thus, in the expansion in series we keep only the values of k which fulfil inequality (47); for larger k values $h(k, p)$ is taken to be zero.

The inverse Fourier transform of $h(k, p)$ is

$$\bar{h}(\xi, p) = -\frac{1}{2\pi(p+\lambda^2)}\int_{-\infty}^{\infty}\frac{e^{ik\xi}\,dk}{k^2+\dfrac{p^2}{p+\lambda^2}} + \frac{\vartheta}{2\pi}\int_{-\infty}^{\infty} e^{ik\xi}\frac{k^4+k^2 p}{[k^2(p+\lambda^2)+p^2]^2}\,dk. \tag{48}$$

We shall denote the value of the first term of the sum on the right hand side of Eq. (48) by $\bar{h}_1(\xi, p)$. After integration with respect to this term becomes

$$\bar{h}_1(\xi, p) = -\frac{1}{2p\sqrt{p+\lambda^2}}\exp\left(-\frac{p|\xi|}{\sqrt{p+\lambda^2}}\right). \tag{49}$$

The second term

$$\frac{\vartheta}{2\pi}\int_{-\infty}^{\infty} e^{ik\xi}\frac{k^4+k^2 p}{[k^2(p+\lambda^2)+p^2]^2}\,dk= \\ =\frac{\vartheta}{2\pi}\left(\frac{\partial^4}{\partial\xi^4}-p\frac{\partial^2}{\partial\xi^2}\right)\int_{-\infty}^{\infty} e^{ik\xi}\frac{dk}{[k^2(p+\lambda^2)+p^2]^2} \tag{50}$$

since

$$k^4+k^2 p=\frac{\partial^4}{\partial\xi^4}-p\frac{\partial^2}{\partial\xi^2}\,. \tag{51}$$

The integral of Eq. (50) can be evaluated by applying the convolution theorem [5]. The following result is obtained for $\bar{h}(\xi, p)$:

$$\bar{h}(\xi,p)=-\frac{\exp[-p|\xi|(p+\lambda^2)^{-1/2}]}{2p\sqrt{p+\lambda^2}}\left(1+\vartheta-\frac{5}{2}\vartheta\lambda^2\frac{1}{p+\lambda^2}+\right. \\ \left.+\frac{3}{2}\vartheta\lambda^4\frac{1}{(p+\lambda^2)^2}+\frac{\lambda^2}{2}\vartheta|\xi|\frac{p^2}{(p+\lambda^2)^{5/2}}\right)\,. \tag{52}$$

Knowing the function $\bar{h}(\xi, p)$ the asymptotic behaviour of the function $h(\xi, \tau)$ can be determined. If $\tau \to \infty$, by using (42) we obtain from (52)

$$\lim_{p\to 0}[p\bar{h}(\xi,p)]=-\frac{1}{2\lambda}\,, \tag{53}$$

i.e.

$$h(\xi,\infty)=-\frac{1}{2\lambda}\,, \tag{54}$$

which agrees with the result obtained from Eq. (40) on the basis of a similar consideration, and is therefore a direct proof of the validity of the expansion.

The function $h(\xi, \tau)$ is determined from Eq. (52) by inverse Laplace transformation term by term. The inverse Laplace transforms of the first and second term in the sum on the right-hand side of Eq. (52) are known [1], the Laplace transform of further terms can be determined on the basis of the convolution theorem [6]. Hence for the function $h(\xi, \tau)$ we obtain

$$h(\xi,\tau)=(1+\vartheta)\left(-\frac{1}{2\lambda}+|\xi|e^{-\lambda^2\tau}+\frac{1}{2\pi}\int_{\lambda^2}^{\infty}e^{-R\tau}g(R,\xi)\,dR\right)+ \\ +\frac{5}{4}\vartheta\left(\frac{1}{\lambda}-\frac{e^{-\lambda^2\tau}}{\lambda}-2\lambda^2|\xi|\tau e^{-\lambda^2\tau}\right)- \\ -\frac{3}{4}\vartheta\left(\frac{1}{\lambda}-\frac{e^{-\lambda^2\tau}}{\lambda}-\lambda\tau e^{-\lambda^2\tau}-\lambda^4\tau^2|\xi|e^{-\lambda^2\tau}\right)+$$

$$+\frac{\lambda^2}{\sqrt{\pi}}\vartheta|\xi|^2\tau^{1/2}e^{-\lambda^2\tau}\left(1-\frac{4}{3}\lambda^2\tau+\frac{4}{15}\lambda^4\tau^2\right)+$$

$$+\frac{\lambda}{\sqrt{\pi}}\vartheta|\xi|\tau^{1/2}e^{-\lambda^2\tau}\left(\frac{\lambda^2}{3}\tau-\frac{1}{2}\right)-\frac{5}{4\pi}\vartheta\lambda^2e^{-\lambda^2\tau}\int_{\lambda^2}^{\infty}\frac{g(R,\xi)}{R-\lambda^2}dR+ \tag{55}$$

$$+\frac{5}{4\pi}\vartheta\lambda^2\int_{\lambda^2}^{\infty}e^{-R\tau}\frac{g(R,\xi)}{R-\lambda^2}dR-\frac{3}{4\pi}\vartheta\lambda^4\int_{\lambda^2}^{\infty}w_1\,g(R,\xi)\,dR+$$

$$+\frac{\lambda^2}{2\sqrt{\pi}\pi}\vartheta|\xi|\int_{\lambda^2}^{\infty}w_2\,g(R,\xi)\,dR+\frac{\lambda^4}{\pi\sqrt{\pi}}\vartheta|\xi|\int_{\lambda^2}^{\infty}w_3\,g(R,\xi)\,dR+$$

$$+\frac{\lambda^6}{\pi\sqrt{\pi}}\vartheta|\xi|\int_{\lambda^2}^{\infty}w_4\,g(R,\xi)\,dR\,,$$

where

$$w_1=\frac{e^{-\lambda^2\tau}}{(R-\lambda^2)^2}-\frac{\tau e^{-\lambda^2\tau}}{R-\lambda^2}-\frac{e^{-R\tau}}{(R-\lambda^2)^2}\,,$$

$$w_2=e^{-R\tau}\int_0^{\sqrt{\tau}}e^{(R-\lambda^2)x^2}\,dx\,,$$

$$w_3=\frac{e^{-R\tau}}{R-\lambda^2}\int_0^{\sqrt{\tau}}e^{(R-\lambda^2)x^2}\,dx-\frac{\tau^{1/2}e^{-\lambda^2\tau}}{R-\lambda^2}\,, \tag{56}$$

$$w_4=\frac{\tau^{3/2}e^{-\lambda^2\tau}}{R-\lambda^2}-\frac{3}{2}\frac{\tau^{1/2}e^{-\lambda^2\tau}}{(R-\lambda^2)^2}+\frac{3}{2}\frac{e^{-R\tau}}{(R-\lambda^2)^2}\int_0^{\sqrt{\tau}}e^{(R-\lambda^2)x^2}\,dx\,,$$

$$g(R,\xi)=\frac{\cos\dfrac{R\xi}{\sqrt{R-\lambda^2}}}{R\sqrt{R-\lambda^2}}\,.$$

Knowing $\bar{h}(\xi,p)$, the function $\bar{u}(\xi,p)$ can be determined from Eq. (30)

$$\bar{u}(\xi,p)=-Ae^{-a|\xi|}\left[B\left(a-\frac{p}{a}\right)+C\left(1+\frac{p}{a^2}\right)+C\left(\frac{p}{a}-C\right)|\xi|\right], \tag{57}$$

where

$$\left.\begin{aligned}A&=\frac{1}{2p\sqrt{p+\lambda^2}}\,;\ a=\frac{p}{\sqrt{p+\lambda^2}}\,;\ C=\frac{\lambda^2\vartheta p^2}{2(p+\lambda^2)^{5/2}}\\ B&=1+\vartheta-\frac{5}{2}\vartheta\lambda^2\frac{1}{p+\lambda^2}+\frac{3}{2}\vartheta\lambda^4\frac{1}{(p+\lambda^2)^2}\,.\end{aligned}\right\} \tag{58}$$

Eq. (27) yields the differential derivate of the Laplace transform of E with respect to ξ

$$\frac{\partial\bar{E}}{\partial\xi}=p\bar{h}. \tag{59}$$

Hence

$$\bar{E}(\xi, p) = \frac{1}{2} \exp\left(-\frac{p|\xi|}{\sqrt{p+\lambda^2}}\right)\left(\frac{B}{p} - \frac{C}{p} - \frac{C^2}{p^2}\sqrt{p+\lambda^2}\right), \tag{60}$$

where B and C are the abbreviations introduced in Eq. (58). The asymptotic behaviour of the functions $u(\xi, \tau)$ and $E(\xi, \tau)$ can be determined from Eqs. (57) and (60), if $p \to 0$, (i.e. $\tau \to \infty$). In this case

$$\lim_{\tau\to\infty} u(\xi,\tau) = \lim_{p\to 0} [p\bar{u}(\xi,p)] = \frac{1}{2} \tag{61}$$

and

$$\lim_{\tau\to\infty} E(\xi,\tau) = \lim_{p\to 0} [p\bar{E}(\xi,p)] = \frac{1}{2}. \tag{62}$$

On the basis of Eqs. (54), (61) and (62) one can conclude that the asymptotic behaviour ($\tau \to \infty$) of the functions $h(\xi, \tau)$, $u(\xi, \tau)$ and $E(\xi, \tau)$ is the same for real ($\eta \neq 0$) hydrodynamical media as for ideal ($\eta = 0$) media [1].

If $\bar{u}(\xi, p)$ and $\bar{E}(\xi, p)$ are known, the functions $u(\xi, \tau)$ and $E(\xi, \tau)$ can be calculated in a similar way as $h(\xi, \tau)$ from $\bar{h}(\xi, p)$. Hence for $\tau \to \infty (t \to \infty)$ the induced magnetic and electric fields and velocity distribution are

$$H_x = \frac{1}{2}\sqrt{\frac{\varrho}{\mu_0}}\, v_0, \tag{63}$$

$$E_y = \frac{1}{2}\mu_0 v_0 H_0, \tag{64}$$

$$v_x = \frac{v_0}{2}. \tag{65}$$

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МАГНЕТОГИДРОДИНАМИЧЕСКАЯ «ДИНАМО» МОДЕЛЬ

Я. ФИРТКО

Резюме

Приведено решение системы магнетогидродинамических уравнений для нестационарного случая несжимаемых реальных проводящих сред. Показано, что в случае, когда гидродинамическая вязкость среды стремится к нулю, полученные результаты приводят к результатам Й. Сабо.

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ON THE TRACE OF THE PRODUCT OF PAULI AND DIRAC MATRICES

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Several methods for the determination of the trace of the product of an arbitrary number of Pauli matrices are established. Formulae are derived for the evaluation of various types of products of two traces when terms of the type $\sigma_{i1}\sigma_{i2}\ldots\sigma_{in}$ occur in both of them. Expressions are found for the product of two different traces and the square of the trace of an arbitrary number of Pauli matrices. Similar formulae are obtained when Dirac matrices occurring as $\sum_{i=1}^{5}\gamma_i A_i$ are considered instead of Pauli matrices. From this all previous results in which γ_5 has been considered separately are recovered. A useful identity for traces involving either Pauli or Dirac matrices is given.

Introduction

One of the purposes of this paper is to reduce the problem of the calculation of the trace of the product of any odd or even number of Pauli matrices, to one involving a smaller number — in the final stage, two or three — of Pauli matrices. First the formulae for the determination of various types of products of two traces when $\sigma_{i1}\sigma_{i2}\ldots\sigma_{in}$ occur in both traces (summation over the dummy suffixes i_r is implied) are derived and then expressions for the product of two different traces and the square of the trace of an arbitrary number of Pauli matrices. Next, the five Dirac matrices γ_1, γ_2, γ_3, γ_4 and γ_5 are considered simultaneously instead of the Pauli matrices and similar expressions are obtained. More explicitly, the Dirac matrices occur in the trace as product of an arbitrary number of elements like $\sum_{i=1}^{5} A_i\gamma_i$. From the results obtained in this second stage all the results of the author's previous paper [1], in which Dirac matrices occur in the form $\sum_{i=1}^{4} A_i\gamma_i$ and γ_5 may occur separately, can be reproduced. An identity for traces involving either Pauli or Dirac matrices has been established. This is found to be useful in the reduction of the formulae and in demonstrating the equivalence of some of the results in our deduction. In this connection it should be mentioned that CHISHOLM [2] has evaluated the sums $\sum_{r=i}^{3}\sigma_r\sigma_a\sigma_b\ldots\sigma_d\sigma_r$ and $\sum_{r=i}^{3}\ldots\sigma_r\ldots Sp(\sigma_r\sigma_a\sigma_b\ldots\sigma_d)$. CHISHOLM [2] has also solved the same problem for Dirac matrices. CAIANIELLO

and FUBINI [3] and KAHANE [4] have investigated various aspects of the problem of evaluating the trace of the product of Dirac matrices. The calculations are set out in three sections: Section I deals with the Pauli matrices whereas Sections II and III with Dirac matrices. I have generally followed the notation and method of [1].

I

All the formulae derived here are based on the following algebraic properties of Pauli matrices:

$$\sigma_i \sigma_j + \sigma_j \sigma_i = 2\,\delta_{ij}, \tag{1}$$

$$\sigma_i \sigma_j = \epsilon_{ijk}\,\sigma_k + \delta_{ij}, \tag{2}$$

where ϵ_{ijk} is the Levi Civita tensor of the third rank. Let us use the abbreviated notation

$$\text{trace} \quad (A_1 A_2 A_3 \ldots A_n) = (A_1 A_2 A_3 \ldots A_n), \tag{3}$$

$$A = A_i\,\sigma_i, \tag{4}$$

$$A \cdot B = A_i\,B_i\,. \tag{5}$$

Summation over $i = 1, 2, 3$ is to be done. (Throughout this paper summation is implied whenever repeated suffixes occur.)

Let us denote $(A_1 A_2 A_3 \ldots A_n)$ by S, i.e.

$$S = (A_1 A_2 A_3 \ldots A_n). \tag{6}$$

When n is even we already know the result

$$S = \sum_{i=2}^{n} (-1)^i\, A_1 \cdot A_i (A_2 A_3 \ldots A_{i-1} A_{i+1} \ldots A_n). \tag{7}$$

For n odd we shall develop other methods for the evaluation of S, some of which may be applicable for even n also.

We can write

$$\begin{aligned} S &= \sum_{i,j} A_{1i}\, A_{2j}\ (\sigma_i \sigma_j A_3 \ldots A_n) = \\ &= A_1 \cdot A_2 (A_3 A_4 \ldots A_n) + i\epsilon_{ijk}\, A_{1i}\, A_{2j} (\sigma_k A_3 A_4 \ldots A_n) = \\ &= A_1 \cdot A_2 (A_3 A_4 \ldots A_n) - \frac{1}{2} \sum_{r \geq 3}^{n} (-1)^r (A_1 A_2 A_r) \\ &\qquad\qquad (A_3 A_4 \ldots A_{r-1} A_{r+1} \ldots A_n). \end{aligned} \tag{8}$$

This formula is valid when n is odd.

S can also be written in the form

$$S = \sum_{i,j,k} A_{1i}\, A_{2j}\, A_{3k}\ (\sigma_i\, \sigma_j\, \sigma_k\, A_4\, A_5 \ldots A_n). \tag{9}$$

The summation here can be split up in the following manner:

$$\sum_{i,j,k} = \sum_{i\neq j\neq k} + \sum_{i=j\neq k} + \sum_{i=k\neq j} + \sum_{i\neq j=k} + \sum_{i=j=k} . \tag{10}$$

Application of Eq. (10) provides the third formula for S, which is valid for any n, even or odd:

$$\begin{aligned} S = {} & A_1 \cdot A_2 (A_3 A_4 \ldots A_n) + A_2 \cdot A_3 (A_1 A_4 \ldots A_n) - \\ & - A_1 \cdot A_3 (A_2 A_4 \ldots A_n) + \frac{1}{2} (A_1 A_2 A_3)(A_4 A_5 \ldots A_n). \end{aligned} \tag{11}$$

Let us now discuss some relations involving the product of two traces. We have

$$\begin{aligned} (\sigma_i\, A_1 A_2 \ldots A_n)(\sigma_i\, A'_1\, A'_2 \ldots A'_m) = \sum_{i=1}^{n} (-1)^{i+1} (A_1 A_2 \ldots A_{i-1} A_{i+1} \ldots A_n) \cdot \\ \cdot (A_i\, A'_1\, A'_2 \ldots A'_m). \end{aligned} \tag{12}$$

Here n is odd and m may be either even or odd. Knowing that

$$\sum_{i,j} = \sum_{i=j} + \sum_{i\neq j} . \tag{13}$$

We obtain with the help of Eqs. (1) and (2)

$$\begin{aligned} T_2 = (\sigma_i\, \sigma_j\, A_1 A_2 \ldots A_n)(\sigma_i\, \sigma_j\, A'_1\, A'_2 \ldots A'_m) = \\ = 3\,(A_1 A_2 \ldots A_n)(A'_1\, A'_2 \ldots A'_m) - 2\,(\sigma_k\, A_1 A_2 \ldots A_n)(\sigma_k\, A'_1 A'_2 \ldots A'_m). \end{aligned} \tag{14}$$

By repeated application of Eq. (14) we get

$$\begin{aligned} T_3 = (\sigma_i\, \sigma_j\, \sigma_k\, A_1 A_2 \ldots A_n)(\sigma_i\, \sigma_j\, \sigma_k\, A'_1\, A'_2 \ldots A'_n) = \\ = -6(A_1 A_2 \ldots A_n)(A'_1\, A'_2 \ldots A'_m) + 7(\sigma_i\, A_1 A_2 \ldots A_n)(\sigma_i\, A'_1\, A'_2 \ldots A'_m). \end{aligned} \tag{15}$$

In general, if we write

$$\begin{aligned} T_{m+1} = (\sigma_{i_1}\, \sigma_{i_2} \ldots \sigma_{i_{m+1}}\, A_1 A_2 \ldots A_n) \cdot (\sigma_{i_1}\, \sigma_{i_2} \ldots \sigma_{i_{m+1}}\, A'_1\, A'_2 \ldots A'_m) = \\ = \alpha_m (A_1 A_2 \ldots A_n)\,(A'_1\, A'_2 \ldots A'_m) + \beta_m (\sigma_i\, A_1 A_2 \ldots A_n)\,(\sigma_i\, A'_1\, A'_2 \ldots A'_m) \end{aligned} \tag{16}$$

then

$$\alpha_{m+1} = 3\beta_m\,, \qquad \beta_{m+1} = \alpha_m - 2\beta_m\,, \tag{17}$$

and we easily obtain

$$\beta_m = \sum_{r=0}^{m-2} (-3)^r - 2(-3)^{m-1} \tag{18}$$

and

$$\alpha_m = 1 - \beta_m\,. \tag{19}$$

In Eqs. (14), (15) and (16) both n and m can be either even or odd. With the help of Eq. (12) we obtain

$$\begin{aligned}(\sigma_i\,\sigma_j\,A_1A_2\ldots A_n)(\sigma_i\,\sigma_j\,A_1'A_2'\ldots A_m') = 3(A_1A_2\ldots)(A_1'A_2'\ldots) - \\ -2\sum_{r>s}(-1)^{r+s}(A_1A_2\ldots)''[(A_rA_sA_1'A_2'\ldots) - A_rA_s(A_1'A_2'\ldots)]\,.\end{aligned} \tag{20}$$

Here n must be even but m can be either even or odd.

In Eq. (20) the notation of double primes over the trace $(A_1A_2\ldots)''$ implies that the two unprimed Pauli matrices (in this case A_r and A_s) which are now present in the other term, are now absent from the trace $(A_1A_2\ldots)$. This notation in the general form, with any number of primes over the notation of trace, will be widely used in this paper.

Comparing Eqs. (14) and (20) we have

$$\begin{aligned}(\sigma_i\,A_1A_2\ldots A_n)(\sigma_i\,A_1'A_2'\ldots A_m') = \sum_{r>s}(-1)^{r+s}(A_1A_2\ldots)''\times \\ \times[(A_rA_sA_1'A_2'\ldots) - A_r\cdot A_s(A_1'A_2'\ldots)]\,.\end{aligned} \tag{21}$$

When n and m are both even, Eq. (12) is not applicable and must be replaced by Eq. (21).

A particular case of Eq. (21) is

$$(\sigma_i\,A_1A_2)(\sigma_i\,A_1'A_2'\ldots A_m') = 2(A_1A_2A_1'A_2'\ldots A_m') - 2A_1\cdot A_2(A_1'A_2'\ldots A_m')\,. \tag{22}$$

If we use the relation (7) in the left hand side of Eq. (22), taking m to be odd, we obtain Eq. (8) for determining S. With the help of Eq. (1) we can write

$$\begin{aligned}(A_1A_2\ldots A_n) = 2\sum_{i=2}^{n-1}(-1)^i\,A_1\cdot A_i(A_2A_3\ldots A_{i-1}A_{i+1}\ldots A_n) - \\ -(A_2A_3\ldots A_1A_n)\end{aligned} \tag{23}$$

where n is odd.

From Eq. (23) we obtain the identity

$$\sum_{i=2}^{n}(-1)^i\,A_1\cdot A_i(A_2A_3\ldots A_{i-1}A_{i+1}\ldots A_n) = 0\,. \tag{24}$$

This identity proves to be very useful in reducing the number of terms occurring in the expansion of some traces.

Through successive application of Eq. (12) we can write

$$(\sigma_i \sigma_j \sigma_k A_1 A_2 \dots A_n)(\sigma_i \sigma_j \sigma_k A_1' A_2' \dots A_m') = 7(\sigma_i A_1 A_2 \dots A_n) \tag{25}$$

$$(\sigma_i A_1' A_2' \dots A_m') + \sum_{i>j>k} (-1)^{i+j+k} (A_1 A_2 \dots A_n)''' \sum_P \delta_P P(A_i A_j A_k A_1' A_2' \dots A_m').$$

In Eq. (25) and elsewhere, P is any permutation of the suffixes (in this case i, j and k), and $\delta_p = \pm 1$ depending on whether P is an even or odd permutation. The notation $\sum_P$ denotes summation over all the possible permutations. Now it can be shown that

$$\sum_P \delta_P P(A_i A_j A_k A_1' A_2' \dots) = \tag{26}$$
$$= 6([A_i A_j A_k - A_i \cdot A_j A_k + A_i \cdot A_k A_j - A_j \cdot A_k A_i] A_1' A_2' \dots).$$

Eq. (25) combined with Eq. (15) enables us to establish that

$$(A_1 A_2 \dots A_n)(A_1' A_2' \dots A_m') = -\frac{1}{6} \sum_{i>j>k} (-1)^{i+j+k} (A_1 A_2 \dots A_n)''' \cdot \tag{27}$$
$$\cdot \sum_P \delta_P P(A_i A_j A_k A_1' A_2' \dots A_m').$$

With the help of Eqs. (27) and (26), and taking $n = 3$ and m as either even or odd, we obtain formula (11) for the determination of S.

Eq. (27) can also be rewritten in the following alternative form:

$$(A_1 A_2 \dots A_n)(A_1' A_2' \dots A_m') = \sum_{i>j>k} (-1)^{i+j+k} (A_1 A_2 \dots A_n)''' \cdot$$
$$\cdot \sum_{r>s} (-1)^{r+s} (A_i \cdot A_r' A_j \cdot A_s' - A_j \cdot A_r' A_i \cdot A_s')(A_k A_1' A_2' \dots A_m')'' \dots \tag{28}$$
$$= -\sum_{i>j>k} (-1)^{i+j+k} (A_1 A_2 \dots A_n)''' \cdot \tag{29}$$
$$\cdot \sum_{r>s>t} (-1)^{r+s+t} (A_1' A_2' \dots A_m')''' \sum_P \delta_P P[A_i \cdot A_r' A_j \cdot A_s' A_k \cdot A_t'].$$

The general relation (29) leads to the particular relations

$$(A_1 A_2 A_3)(A_1' A_2' \dots A_m') = \tag{30}$$
$$= -2 \sum_{r>s>t} (-1)^{r+s+t} \sum_P \delta_P P[A_3 \cdot A_r' A_2 \cdot A_s' A_1 \cdot A_t'](A_1' A_2' \dots A_m')''',$$

$$(A_1A_2A_3)(A_r'A_s'A_t') = -4\sum_P \delta_P P[A_3 \cdot A_t'A_2 \cdot A_s'A_1 \cdot A_r']. \tag{31}$$

$$(A_1A_2 \ldots A_n)^2 = -\sum_{i>j>k} (-1)^{i+j+k}(A_1A_2 \ldots A_n)''' \cdot \cdot \sum_{r>s>t} (-1)^{r+s+t} \sum_P \delta_P P[A_i \cdot A_rA_j \cdot A_sA_k \cdot A_t](A_1A_2 \ldots A_n)'''. \tag{32}$$

In Eqs. (29)—(32) permutation P of the suffixes r, s and t is implied.

By putting $A_1, A_2, A_3 = \sigma_1, \sigma_2, \sigma_3$ in relation (30) we get another formula for the determination of S:

$$(A_1A_2 \ldots A_n) = \frac{1}{2}\sum_{r>s>t} (-1)^{r+s+t}(A_tA_sA_r)(A_1A_2 \ldots A_n)'''. \tag{33}$$

In Eqs. (28)—(33), both n and m must be odd.

We have now established four equations (7), (8), (11) and (33) for determining $(A_1A_2 \ldots A_n)$.

For $n = 5$, using identity (24), we get according to both Eqs. (8) and (11)

$$S_5 = (A_1A_2A_3A_4A_5) = A_1 \cdot A_2(A_3A_4A_5) + A_2 \cdot A_3(A_1A_4A_5) - - A_1 \cdot A_3(A_2A_4A_5) + A_4 \cdot A_5(A_1A_2A_3)\,. \tag{34}$$

Eq. (33) gives 10 terms for S_6, which can be reduced to four terms with the help of the identity given by Eq. (24). For other odd values of n, Eqs. (8) and (33) give more terms than Eq. (11).

S_n for even values of n are found from Eqs. (7) and (11). For $n = 6$ we get from Eq. (11)

$$S_6 = (A_1A_2A_3A_4A_5A_6) = A_1 \cdot A_2(A_2A_3A_4A_5A_6) + A_2 \cdot A_3(A_1A_4A_5A_6) - - A_1 \cdot A_3(A_2A_4A_5A_6) + \frac{1}{2}(A_1A_2A_3)(A_4A_5A_6). \tag{35}$$

Eq. (11) gives as expression for S_n shorter than that of Eq. (7) and is thus most convenient for determining S_n for both odd and even values of n.

II

The notation and method of Section I are mostly followed in Sections II and III also. For Dirac matrices, the anticommutation relation (1) is replaced by

$$\gamma_i\gamma_j + \gamma_j\gamma_i = 2\,\delta_{ij}, \tag{36}$$

where the suffixes of γ matrices can be 1, 2, 3, 4 and 5. We use the abbreviated notation given by Eq. (3), except that here

$$A = A_i \gamma_i , \tag{37}$$

$$A \cdot B = A_i B_i , \tag{38}$$

$$\gamma_5 = \gamma_1 \gamma_2 \gamma_3 \gamma_4 . \tag{39}$$

Summation over $i = 1, 2, 3, 4$ and 5 is to be done.
With the help of relation (10) we can write

$$\begin{aligned} S = (A_1 A_2 \ldots A_n) &= \sum_{i,j,k} A_{1i} A_{2j} A_{3k} (\gamma_i \gamma_j \gamma_k A_4 A_5 \ldots A_n) = \\ &= A_1 \cdot A_2 (A_3 A_4 \ldots) + A_2 \cdot A_3 (A_1 A_4 \ldots) - A_1 \cdot A_3 (A_2 A_4 \ldots) - \\ &\quad - \frac{1}{2} \epsilon_{ijklm} A_{1i} A_{2j} A_{3k} (\gamma_l \gamma_m A_4 A_5 \ldots A_n) , \end{aligned} \tag{40}$$

where ϵ_{ijklm} is a Levi Civita tensor.

It can be easily shown that the last term of Eq. (40) is

$$-\frac{1}{4} \sum_{s>r} (-1)^{r+s} (A_1 A_2 A_3 A_r A_s) (A_4 A_5 \ldots A_n)'' .$$

This is the $\Sigma_{i \neq j \neq k}$ part of $\Sigma_{i,j,k}$ and can be rewritten in the form (as in [1])

$$\begin{aligned} \sum_{i \neq j \neq k} &= \sum_{i \neq j \neq k} A_{1i} A_{2j} A_{3k} A_{4l} (\gamma_i \gamma_j \gamma_k \gamma_l A_5 A_6 \ldots A_n) = \\ &= \sum_{i \neq j \neq k \neq l} + \sum_{\substack{i \neq j \neq k \\ l = i}} + \sum_{\substack{i \neq j \neq k \\ l = j}} + \sum_{\substack{i \neq j \neq k \\ l = k}} \end{aligned} \tag{41}$$

Now

$$\sum_{i \neq j \neq k \neq l} = \epsilon_{ijklm} A_{1i} A_{2j} A_{3k} A_{4l} (\gamma_m A_5 A_6 \ldots A_n) . \tag{42}$$

With the help of Eqs. (41) and (42) we obtain the second formula for S:

$$\begin{aligned} S = ([&A_1 \cdot A_2 A_3 A_4 - A_1 \cdot A_3 A_2 A_4 + A_2 \cdot A_3 A_1 A_4 + \\ &+ A_1 \cdot A_4 A_2 A_3 - A_2 \cdot A_4 A_1 A_3 + A_3 \cdot A_4 A_1 A_2] \\ &A_5 A_6 \ldots A_n) - \frac{1}{4} (A_1 A_2 A_3 A_4) \cdot (A_5 A_6 \ldots A_n) - \\ &- \frac{1}{4} \sum_{r \geq 5}^{n} (-1)^r (A_1 A_2 A_3 A_4 A_r)(A_5 A_6 \ldots A_{r-1} A_{r+1} \ldots A_n) . \end{aligned} \tag{43}$$

Proceeding in a way similar to that used in deriving Eq. (41), we obtain

$$\sum_{i \neq j \neq k \neq l} = \sum_{i \neq j \neq k \neq l \neq m} + \sum_{\substack{i \neq j \neq k \neq l \\ m = i}} + \sum_{\substack{i \neq j \neq k \neq l \\ m = j}} + \sum_{\substack{i \neq j \neq k \neq l \\ m = k}} + \sum_{\substack{i \neq j \neq k \neq l \\ m = l}} . \tag{44}$$

Applying relations (44) and (10) we have the third formula for S:

$$\begin{aligned} S = A_{1i}\,A_{2j}\,A_{3k}\,A_{4l}\,A_{5m}\,(\gamma_i\gamma_j\gamma_k\gamma_l\gamma_m\,A_6\,A_7\ldots A_n) = \\ = ([A_1\cdot A_2A_3A_4 - A_1\cdot A_3A_2A_4 + A_2\cdot A_3A_1A_4 + A_1\cdot A_4A_2A_3 - \\ - A_2\cdot A_4A_1A_3 + A_3\cdot A_4A_1A_2]\,A_5A_6\ldots) - \\ -\frac{1}{4}(A_1A_2A_3A_4)(A_5A_6\ldots) + ([-A_1\cdot A_5\{A_2A_3A_4\} + \\ + A_2\cdot A_5\{A_1A_3A_4\} - A_3\cdot A_5\{A_1A_2A_4\} + A_4\cdot A_5\{A_1A_2A_3\}]\times \\ \times A_6A_7\ldots) + \frac{1}{4}(A_1A_2A_3A_4A_5)\,(A_6A_7\ldots). \end{aligned} \tag{45}$$

In this equation terms of the type $\{A_2A_3A_4\}$ stand for

$$\{A_2A_3A_4\} = A_2A_3A_4 - A_2\cdot A_3A_4 + A_2\cdot A_4A_3 - A_3\cdot A_4A_2. \tag{46}$$

Using relation (10) we arrive at the following result for the product of two traces:

$$\begin{aligned} (\gamma_i\gamma_j\gamma_k\,A_1\,A_2\ldots A_n)\,(\gamma_i\gamma_j\gamma_k\,A_1'A_2'\ldots A_m') = \\ = 3\,(\gamma_i\gamma_j\,A_1\,A_2\ldots A_n)(\gamma_i\gamma_j\,A_1'\,A_2'\ldots A_m') + \\ + 13(\gamma_i\,A_1A_2\ldots A_n)(\gamma_i\,A_1'\,A_2'\ldots A_m') - 15\,(A_1A_2\ldots A_n)\cdot \\ \cdot\,(A_1'\,A_2'\ldots A_m'). \end{aligned} \tag{47}$$

By repeatedly applying Eq. (47) we obtain

$$\begin{aligned} (\gamma_i\gamma_j\gamma_k\gamma_l\,A_1\,A_2\ldots A_n)\,(\gamma_i\gamma_j\gamma_k\gamma_l\,A_1'\,A_2'\ldots A_m') = \\ = 22\,(\gamma_l\gamma_j\,A_1\,A_2\ldots A_n)\,(\gamma_i\gamma_j\,A_1'\,A_2'\ldots A_m') + \\ + 24\,(\gamma_i\,A_1\,A_2\ldots A_n)\,(\gamma_i\,A_1'\,A_2'\ldots A_m') - 45\,(A_1\,A_2\ldots A_n)\cdot \\ \cdot\,(A_1'\,A_2'\ldots A_m'), \end{aligned} \tag{48}$$

$$\begin{aligned} (\gamma_i\gamma_j\gamma_k\gamma_l\gamma_m\,A_1\,A_2\ldots A_n)(\gamma_i\gamma_j\gamma_k\gamma_l\gamma_m\,A_1'\,A_2'\ldots A_m') = \\ = 90\,(\gamma_i\gamma_j\,A_1\,A_2\ldots A_n)\,(\gamma_i\gamma_j\,A_1'\,A_2'\ldots A_m') + \\ + 241\,(\gamma_i\,A_1\,A_2\ldots A_n)\cdot(\gamma_i\,A_1'\,A_2'\ldots A_m') - \\ - 330\,(A_1\,A_2\ldots A_n)\,(A_1'\,A_2'\ldots A_m'). \end{aligned} \tag{49}$$

In general, proceeding in this way we can evaluate

$$(\gamma_{i1}\gamma_{i2}\ldots\gamma_{in}\,A_1\,A_2\ldots)\,(\gamma_{i1}\,\gamma_{i2}\ldots\gamma_{in}\,A_1'\,A_2'\ldots).$$

For odd values of n we have a relation similar to Eq. (12):

$$(\gamma_i A_1 A_2 \dots A_n)(\gamma_i A'_1 A'_2 \dots A'_m) = \\ = \sum_{i=1}^{n} (-1)^{i+1}(A_1 A_2 \dots A_{i-1} A_{i+1} \dots A_n)(A_i A'_1 A'_2 \dots A'_m). \tag{50}$$

Corresponding to Eqs. (20) and (25) we have the relations

$$(\gamma_i \gamma_j A_1 A_2 \dots A_n)(\gamma_i \gamma_j A'_1 A'_2 \dots A'_m) = \\ = 5(A_1 A_2 \dots A_n)(A'_1 A'_2 \dots A'_m) - 2 \sum_{i>j} (-1)^{i+j}(A_1 A_2 \dots A_n)'' \times \\ \times [(A_i A_j A'_1 A'_2 \dots A'_m) - A_i \cdot A_j (A'_1 A'_2 \dots A'_m)] \tag{51}$$

and

$$(\gamma_i \gamma_j \gamma_k A_1 A_2 \dots A_n)(\gamma_i \gamma_j \gamma_k A'_1 A'_2 \dots A'_m) = \\ = 13\,(\gamma_i A_1 A_2 \dots A_n)(\gamma_i A'_1 A'_2 \dots A'_m) + \\ + \sum_{i>j>k} (-1)^{i+j+k}(A_1 A_2 \dots A_n)''' \sum_P \delta_P P(A_i A_j A_k A'_1 A'_2 \dots A'_m). \tag{52}$$

From Eqs. (52) and (47) we have for odd values of n and m

$$(\gamma_i \gamma_j A_1 A_2 \dots A_n)(\gamma_i \gamma_j A'_1 A'_2 \dots A'_m) = \\ = \frac{1}{3} \sum_{i>j>k} (-1)^{i+j+k}(A_1 A_2 \dots A_n)''' \sum_P \delta_P P(A_i A_j A_k A'_1 A'_2 \dots A'_m) \\ + 5(A_1 A_2 \dots A_n)(A'_1 A'_2 \dots A'_m). \tag{53}$$

Relation (51) can be applied when either n or m is even. In a similar manner we obtain

$$(\gamma_i \gamma_j \gamma_k \gamma_l A_1 A_2 \dots A_n)(\gamma_i \gamma_j \gamma_k \gamma_l A'_1 A'_2 \dots A'_m) = \\ = -44 \sum_{i>j} (-1)^{i+j}(A_1 A_2 \dots A_n)''([A_i A_j - A_i \cdot A_j] A'_1 A'_2 \dots A'_m) + \\ + \sum_{i>j>k>l} (-1)^{i+j+k+l}(A_1 A_2 \dots A_n)'''' \times \\ \times \sum_P \delta_P P(A_i A_j A_k A_l A'_1 A'_2 \dots A'_m) + \\ + 65\,(A_1 A_2 \dots A_n)(A'_1 A'_2 \dots A'_m) \tag{54}$$

and

$$
\begin{aligned}
&(\gamma_i\gamma_j\gamma_k\gamma_l\gamma_m A_1 A_2 \dots A_n)(\gamma_i\gamma_j\gamma_k\gamma_l\gamma_m A_1' A_2' \dots A_m') = \\
&\quad = 24(\gamma_i\gamma_j A_1 A_2 \dots A_n)(\gamma_i\gamma_j A_1' A_2' \dots A_m') + \\
&\quad + 241(\gamma_i A_1 A_2 \dots A_n)(\gamma_i A_1' A_2' \dots A_m') - 120(A_1 A_2 \dots A_n) \times \\
&\quad \times (A_1' A_2' \dots A_m') + 22 \sum_{i>j>k} (-1)^{i+j+k} (A_1 A_2 \dots A_n)''' \times \\
&\quad \times \sum_P \delta_P P(A_i A_j A_k A_1' A_2' \dots A_m') - \\
&\quad - \sum_{i>j>k>l>m} (-1)^{i+j+k+l+m} (A_1 A_2 \dots A_n)'''' \times \\
&\quad \times \sum_P \delta_P P(A_i A_j A_k A_l A_m A_1' A_2' \dots A_m') .
\end{aligned}
\tag{55}
$$

Comparing Eqs. (48) and (54), we have for even values of n and m the result

$$
\begin{aligned}
&(\gamma_i A_1 A_2 \dots A_n)(\gamma_i A_1' A_2' \dots A_m') = \\
&\quad = \frac{1}{24} \sum_{i>j>k>l} (-1)^{i+j+k+l} (A_1 A_2 \dots A_n)'''' \times \\
&\quad \times \sum_P \delta_P P(A_i A_j A_k A_l A_1' A_2' \dots A_m') .
\end{aligned}
\tag{56}
$$

For this case where n and m are both even relation (50) is not applicable In Eqs. (52), (54) and (55) permutation P of the suffixes i, j, k, l and m is implied.

Similarly from Eqs. (49) and (55) we obtain for odd values of n and m

$$
\begin{aligned}
&(A_1 A_2 \dots A_n)(A_1' A_2' \dots A_m') = \\
&\quad = -\frac{1}{120} \sum_{i>j>k>l>m} (-1)^{i+j+k+l+m} (A_1 A_2 \dots A_n)''''' \times \\
&\quad \times \sum_P \delta_P P(A_i A_j A_k A_l A_m A_1' A_2' \dots A_m') .
\end{aligned}
\tag{57}
$$

Putting $n = m$ and $A_i' = A_i$ we can obtain from Eq. (57) a relation for $(A_1, A_2 \dots A_n)$ [2]:

Taking $A_1, A_2, A_3, A_4, A_5 = \gamma_1, \gamma_2, \gamma_3, \gamma_4, \gamma_5$ and $n = 5$, we obtain from Eq. (57)

$$
\begin{aligned}
&S = (A_1 A_2 \dots A_n) = \\
&\quad = -\frac{1}{4} \sum_{i>j>k>l>m} (-1)^{i+j+k+l+m} (A_i A_j A_k A_l A_m)(A_1 A_2 \dots A_n)''''' .
\end{aligned}
\tag{58}
$$

In a manner given in Section I, taking $n = 3$ and m even, we obtain from Eqs. (52) and (47) the first relation (40) for S. Similarly, taking $n = 4$, m odd in Eqs. (54), (48) and $n = 5$, m arbitrary in Eqs. (55) and (49) we derive the second and third relations (43) and (45), respectively, for S.

Eqs. (40) and (43) both give the same number of terms in the expansion of S for $n = 7$ and 9. On the other hand, (45) gives 11 terms for $n = 7$. But these can be reduced to 9 terms by using the identity (24), which is also valid when A stands for $\sum_{i=1}^{5} A_i\gamma_i$. For all values of $n > 13$ Eq. (45) gives the smallest number of terms.

III

From the results of Section II we shall now go on to derive similar results to those obtained in [1], in which A stands for $\sum_{i=1}^{4} A_i\gamma_i$ and the dummy suffixes in terms like

$$(\gamma_{i1}\gamma_{i2}\ldots\gamma_{in}A_1A_2\ldots)(\gamma_{i1}\gamma_{i2}\ldots\gamma_{in}A_1'A_2'\ldots)$$

are restricted to the values 1, 2, 3 and 4. To do this we split the summation over the dummy suffixes occurring in Section II in the following manner:

$$\sum_{i=1}^{5} = \sum_{i=1}^{4} + \text{terms corresponding to } i = 5 \text{ only.}$$

By following this prescription we obtain from Eq. (40), taking $A_1 = \gamma_5$

$$\begin{aligned} S' = (\gamma_5 A_2 A_3 \ldots A_n) &= A_2 \cdot A_3 (\gamma_5 A_4 A_5 \ldots A_n) - \\ &- \frac{1}{4}\sum_{s>r}(-1)^{r+s}(\gamma_5 A_2 A_3 A_r A_s)(A_4 A_5 \ldots A_n)''. \end{aligned} \tag{59}$$

Assuming that in Eq. (43) A_4 only involves γ_5 we can have the relation

$$\begin{aligned} S' = &(\gamma_5[A_1 \cdot A_2A_3 - A_1 \cdot A_3A_2 + A_2 \cdot A_3A_1]\, A_4A_5\ldots) \\ &+ \frac{1}{4}\sum_{i\geq 4}(-1)^i(\gamma_5 A_1A_2A_3A_i)(A_4A_5\ldots A_{i-1}\,A_{i+1}\ldots). \end{aligned} \tag{60}$$

Similarly, assuming that in Eqs. (43) and (45) A_5 only involves γ_5, we obtain third formula for S':

$$\begin{aligned} S' = &(\gamma_5[A_1\cdot A_2A_3A_4 - A_1\cdot A_3A_2A_4 + A_1\cdot A_4A_2A_3 + \\ &+ A_2\cdot A_3A_1A_4 - A_2\cdot A_4A_1A_3 + A_3\cdot A_4A_1A_2]\times \\ &\times A_5A_6\ldots) - \frac{1}{4}(A_1A_2A_3A_4)(\gamma_5A_5A_6\ldots) + \\ &+ \frac{1}{4}(\gamma_5A_1A_2A_3A_4)(A_5A_6\ldots). \end{aligned} \tag{61}$$

Taking n and m to be even and odd successively, we get from Eq. (47)

$$(\gamma_5\gamma_i\gamma_j A_1 A_2 \ldots A_n)(\gamma_5\gamma_i\gamma_j A_1' A_2' \ldots A_m') = \\ = 4(\gamma_5 A_1 A_2 \ldots)(\gamma_5 A_1' A_2' \ldots) - 4(A_1 A_2 \ldots)(A_1' A_2' \ldots) + \\ + (\gamma_i\gamma_j A_1 A_2 \ldots)(\gamma_i\gamma_j A_1' A_2' \ldots), \tag{62}$$

and

$$(\gamma_i\gamma_j\gamma_k A_1 A_2 \ldots A_n)(\gamma_i\gamma_j\gamma_k A_1' A_2' \ldots A_m') = \\ = 6(\gamma_5\gamma_i A_1 A_2 \ldots)(\gamma_5\gamma_i A_1' A_2' \ldots) + \\ + 10(\gamma_i A_1 A_2 \ldots)(\gamma_i A_1' A_2' \ldots). \tag{63}$$

Similarly from Eq. (48) we obtain

$$(\gamma_i\gamma_j\gamma_k\gamma_l A_1 A_2 \ldots A_n)(\gamma_i\gamma_j\gamma_k\gamma_l A_1' A_2' \ldots A_m') = \\ = 10(\gamma_i\gamma_j A_1 A_2 \ldots)(\gamma_i\gamma_j A_1' A_2' \ldots) + \\ + 6(\gamma_5\gamma_i\gamma_j A_1 A_2 \ldots)(\gamma_5\gamma_i\gamma_j A_1' A_2' \ldots) \tag{64}$$

and

$$(\gamma_5\gamma_i\gamma_j\gamma_k A_1 A_2 \ldots A_n)(\gamma_5\gamma_i\gamma_j\gamma_k A_1' A_2' \ldots A_m') = \\ = 10(\gamma_5\gamma_i A_1 A_2 \ldots)(\gamma_5\gamma_i A_2' A_1' \ldots) + \\ + 6(\gamma_i A_1 A_2 \ldots)(\gamma_i A_1' A_2' \ldots). \tag{65}$$

In an identical manner Eq. (49) yields

$$(\gamma_5\gamma_i\gamma_j\gamma_k\gamma_l A_1 A_2 \ldots A_n)(\gamma_5\gamma_i\gamma_j\gamma_k\gamma_l A_1' A_2' \ldots A_m') = \\ = 40(\gamma_5 A_1 A_2 \ldots)(\gamma_5 A_1' A_2' \ldots) - 40(A_1 A_2 \ldots)(A_1' A_2' \ldots) + \\ + 16(\gamma_i\gamma_j A_1 A_2 \ldots)(\gamma_i\gamma_j A_1' A_2' \ldots) \tag{66}$$

and,

$$(\gamma_i\gamma_j\gamma_k\gamma_l\gamma_m A_1 A_2 \ldots)(\gamma_i\gamma_j\gamma_k\gamma_l\gamma_m A_1' A_2' \ldots) = \\ = 120(\gamma_5\gamma_i A_1 A_2 \ldots)(\gamma_5\gamma_i A_1' A_2' \ldots) + \\ + 136(\gamma_i A_1 A_2 \ldots)(\gamma_i A_1' A_2' \ldots). \tag{67}$$

In general

$$(\gamma_{i_1}\gamma_{i_2} \ldots \gamma_{i_n} A_1 A_2 \ldots)(\gamma_{i_1}\gamma_{i_2} \ldots \gamma_{i_n} A_1' A_2' \ldots)$$

and

$$(\gamma_5\gamma_{i_1}\gamma_{i_2} \ldots \gamma_{i_{n-1}} A_1 A_2 \ldots)(\gamma_5\gamma_{i_1}\gamma_{i_2} \ldots \gamma_{i_{n-1}} A_1' A_2' \ldots)$$

can be easily evaluated, in a similar way, from the expression for

$$(\gamma_{i_1}\gamma_{i_2} \ldots \gamma_{i_n} A_1 A_2 \ldots)(\gamma_{i_1}\gamma_{i_2} \ldots \gamma_{i_n} A_1' A_2' \ldots)$$

in which case A's and summation over dummy suffixes are defined in the manner of Section II.

These general results an not treated in [1].

Relation (50) of Section II remains unaltered in this Section. Eq. (51) yields

$$(\gamma_i\gamma_j A_1 A_2 \ldots)(\gamma_i\gamma_j A_1' A_2' \ldots) = 4(A_1 A_2 \ldots)(A_1' A_2' \ldots) - 2\sum_{i>j}(-1)^{i+j}(A_1 A_2 \ldots)''[(A_i A_j A_1' A_2' \ldots) - A_i \cdot A_j (A_1' A_2' \ldots)]. \tag{68}$$

From Eq. (53) the following relation is obtained:

$$(\gamma_5\gamma_i A_1 A_2 \ldots)(\gamma_5\gamma_i A_1' A_2' \ldots) = \frac{1}{6}\sum_{r>s>t}(-1)^{r+s+t}(A_1 A_2 \ldots)''' \sum_P \delta_P P(A_r A_s A_t A_1' A_2' \ldots). \tag{69}$$

Eq. (56) leads to

$$(\gamma_5 A_1 A_2 \ldots A_n)(\gamma_5 A_1' A_2' \ldots) = \sum_{i>j>k>l}(-1)^{i+j+k+l}(A_1 A_2 \ldots)'''' \times \times \sum_{r>s>t>u}(-1)^{r+s+t+u}(A_1' A_2' \ldots)'''' \times \sum_P \delta_P P[A_i \cdot A_r' A_j \cdot A_s' A_k \cdot A_t' A_l \cdot A_u']. \tag{70}$$

In Eqs. (69) and (70), permutation P of the suffixes r, s, t and u is implied.

Putting $n = 4$ and $A_1, A_2, A_3, A_4 = \gamma_1, \gamma_2, \gamma_3, \gamma_4$ in Eq. (70), we obtain

$$S' = (\gamma_5 A_1 A_2 \ldots) = \frac{1}{4}\sum_{i>j>k>l}(-1)^{i+j+k+l}(\gamma_5 A_i A_j A_k A_l)(A_1 A_2 \ldots)''''. \tag{71}$$

Taking $A_i' = A_i$ and $n = m$, we can obtain from Eq. (70) an expression for the square of S'.

In identity (24), where in general $A = \sum_{i=1}^{5} A_i\gamma_i$ for Dirac matrices, if we assume that A_n only involves γ_5, then Eq. (24) reduces to the following identity:

$$\sum_{i=2}^{n}(-1)^i A_1 \cdot A_i (A_2 A_3 \ldots A_{i-1} A_{i+1} \ldots A_n \gamma_5) = 0. \tag{72}$$

In this Section all the relations except that given by Eqs. (59) and (67) rea derived in [1] in a different manner. It is found that among the various formulae for determining S', that given by Eq. (61) is the most convenient for $n > 8$.

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О СЛЕДЕ ПРОИЗВЕДЕНИЯ МАТРИЦ ПАУЛИ И ДИРАКА

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Резюме

Предложено несколько методов для определения следа произведения любого числа матриц Паули. Даны формулы для вычисления произведений двух следов различного типа в случае, когда в обоих имеются члены типа $\sigma_{i_1}\sigma_{i_2}\ldots\ldots\sigma_{in}$. Выведены выражения для произведений двух следов и квадрата следа в случае произвольного числа матриц Паули. Подобные формулы получены и для матриц Дирака, построенны как $\sum_{i=1}^{5}\gamma_i A_i$ вместо матриц Паули. Из них также можно получить все наши предыдущие результаты, когда же γ_5, были рассмотрены в отдельности.

Выведено очень полезное тождество для следов, содержащих либо матрицы Паули, либо матрицы Дирака.

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ON THE ELASTIC MODULI OF ALKALINE AND NOBLE METALS III

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A new term is given in the energy expression for the elementary cell of a monovalent metal under uniaxial tension. This term accounts for the interaction of the quadrupole moment of the deformed elementary cells. The calculated values of c_{11} and c_{12} for potassium and silver are given.

1. In the two previous papers of this series [1, 2] the author has described a method for obtaining the elastic moduli c_{11} and c_{12} of alkaline and noble metals using the theory of monovalent metals developed by GOMBÁS [3—8]. The method leads to an approximate expression for the energy of the Wigner—Seitz cell of a monovalent metal subjected to uniaxial elastic deformation, the elementary cell in this case being regarded as a rotational ellipsoid instead of a sphere. The ratio of the ellipsoidal axes is obtained at the minimum of the cell energy and this yields the Poisson ratio for the cell very near the unstrained equilibrium state, while the compressibility, the unstrained equilibrium energy and radius of the cell are known from GOMBÁS's theory. Then the elastic moduli c_{11} and c_{12} can be calculated from these quantities.

GOMBÁS's theory of monovalent metals accounts for the cohesion of the alkaline, alkaline earth and noble metals on a purely theoretical basis, without introducing any empirical or semiempirical parameter giving the energy of the elementary cell as a function of the cell radius, the Wigner—Seitz cell being approximated by a sphere of equal volume. The compressibility, energy and equilibrium lattice constants of the cell can be evaluated for the equilibrium case, when the cell energy is minimum, giving results in excellent agreement with experimental values measured at an adequately low temperature or even extrapolated to absolute zero.

The metal is treated in GOMBÁS's theory as a system composed of a positive metal ion lattice and an approximately free gas of valence electrons. The valence electrons are treated in a modified lattice potential consisting of the electrostatic potential of the ion cores and a nonclassical pseudopotential being the result of the Pauli principle. In calculating the energy of an elementary cell it is now unnecessary to orthogonalize the eigenfunctions of the valence electrons to those of the core electrons, since the pseudopotential

automatically compensates for this, and thus one obtains the deepest possible energy states for the valence electrons.

GOMBÁS's energy expression for an elementary cell can be written as follows:

$$U = U^E + U^W + H, \tag{1}$$

where U^E is the total self energy of the valence electrons, U^W the total interaction energy of the valence electrons with the ion cores and H the interaction energy of the ion cores.

U^E and U^W can be written further as

$$U^E = E_C + E_A + E_W + E_F \tag{2}$$

and

$$U^W = W_C + W_E + W_A + W_W + W_K, \tag{3}$$

where the indices are C for Coulomb-type, A for exchange, W for correlation, F for zero-point and E for non-Coulomb-type electrostatic energy, and the index K represents the energy resulting from the pseudopotential.

The interaction energy of the ion cores H is approximately zero for alkaline metals, and for noble metals can be given as an average value, so the elementary cells are to be regarded as electrically neutral in equilibrium configuration, since they can be approximated by spheres. GOMBÁS has shown that in this case the calculations can be carried out using free-electron eigenfunctions for the valence electrons (while as regards the ion cores the results for free atomic ions calculated by the self-consistent field method were used). Expression (1) was calculated by GOMBÁS for some monovalent metals at different elementary cell radii. For alkaline metals U can be given in a simple analytical form as a function of the cell radius:

$$U = -\frac{c_1}{R} + \frac{c_2}{R^3} \tag{4}$$

(for c_1 and c_2 see [3]). For noble metals the numerically computed values of U can be approximated analytically in the form:

$$U = -\frac{A}{R} + \frac{B}{R^n}, \tag{5}$$

where A, B and n are constants.

It must be stressed that the analytical forms [4], [5] are always connected with complete spherical symmetry, i.e. the shape of the Wigner—Seitz cell does not change. It follows that in calculating the energy of the elementary

cell every elementary sphere has to be taken electrically neutral from the outside, so there is no direct interaction term between different cells, as the ion core interaction occurring in the unstrained symmetry conditions has been taken into account already with the term H in (1).

Now we have the elementary cell energy as a function of the sphere radius $U(R)$, the equilibrium cell radius R_0 and minimal cell energy U_0 can be obtained form the equilibrium condition

$$\frac{dU}{dR} = 0 \,. \tag{6}$$

For spherical symmetric deformation of the elementary cell (i.e. isotropic compression or dilatation) the cell radius is

$$R = R_0(1 + \Lambda). \tag{7}$$

Near the equilibrium state Λ is a small quantity, and the cell energy can be given up to the second order as

$$U = U_0 + \frac{R_0^2}{2}\left(\frac{d^2 U}{dR^2}\right)_{R_0} \Lambda^2. \tag{8}$$

From (8) one gets for the compressibility $\varkappa$ (see [1])

$$\frac{1}{\varkappa} = \frac{1}{12\pi R_0}\left(\frac{d^2 U}{dR^2}\right)_{R_0} \tag{9}$$

or, introducing

$$V_0 = \frac{4\pi R_0^3}{3}$$

and

$$w_0 = -\frac{U_0}{V_0} \tag{10}$$

and using (5):

$$\frac{1}{\varkappa} = \frac{n w_0}{9} \,. \tag{11}$$

Thus

$$U = U_0\left(1 - \frac{9}{2 w_0 \varkappa}\Lambda^2\right). \tag{12}$$

2. If a uniaxial tension stress deforms the Wigner—Seitz cell, the spherical symmetry is lost and hence the elementary cell is more accurately represented by a rotational ellipsoid than by a sphere. Let the two main axes a and b of the rotational ellipsoid be given, by

$$\left.\begin{aligned} a &= R_0(1+\Lambda) \\ b &= R_0(1+\mu\Lambda) \end{aligned}\right\} \tag{13}$$

and let the direction of the stress be the direction of the axis a.

To a first approximation (see [1]) the cell energy can be taken as

$$U_1 = U_0(1-\varphi_\mu \Lambda^2), \tag{14}$$

where

$$\varphi_\mu = \frac{3}{10\, w_0 \varkappa}(3+4\mu+8\mu^2). \tag{15}$$

A further term has to be introduced into the energy expression (14) because of the change of the electrostatic interaction between the ion core and valence electronic charge, resulting from non symmetrical deformation of the elementary cells:

$$U_2 = U_0(1-\Phi_\mu \Lambda^2), \tag{16}$$

where

$$\Phi_\mu = \varphi_\mu + \frac{4e^2}{75\, R_0\, U_0}(1-\mu)^2. \tag{17}$$

3. In the case of uniaxial tension stress plainly the whole lattice will be deformed. Every Wigner—Seitz cell or elementary sphere will change its shape to a rotational ellipsoid of parallel rotational axis, and with this there will be a change in the interaction energy of the ionic lattice. Let us assume, however, that the ion cores themselves do not alter during the deformation of the lattice and that even the eigenfunctions of the valence electrons remain the same as in the unstrained equilibrium (this assumption is similar to that used in the usual first order perturbation). The change in the ion core interaction energy can now be calculated as an electrostatic interaction between the deformed Wigner—Seitz cells because the rotational ellipsoids are not electrically neutral i.e. the deformed elementary cells have a linear electric quadrupole moment.

It is known [9] that a rotational ellipsoid with axes a and b ($a > b$) has a linear electric quadrupole moment directed along the a axis if it has a point charge $+e$ at the origin and a uniform negative charge density of

$$\varrho_0 = -\frac{3e}{4\pi a b^2}.$$

The quadrupole moment Q_{11} is then given as

$$Q_{11} = \frac{e}{5}(a^2-b^2) \tag{18}$$

and all other Q_{ik} are zero.

Using (13)

$$Q_{11} = \frac{2}{5} eR_0^2(1-\mu)\Lambda \tag{19}$$

up to the first order in Λ.

Let $V(r)$ be the potential in the crystal due to all such quadrupole moments. Then, owing to this field, the energy of the elementary cell placed in the origin will be

$$W = \int_{(\text{cell})} \varrho V \, d\Omega = \frac{1}{2} \left(\frac{\partial^2 V}{\partial x_1^2} \right)_0 Q_{11} \tag{20}$$

up to the second order.

The electrical potential of a linear quadrupole moment Q_{11} at a point given relative to Q_{11} by (r, ϑ) is

$$V = \frac{Q_{11}}{2r^3} (3\cos^2\vartheta - 1). \tag{21}$$

Let there be a quadrupole moment Q_{11} at the point (r, ϑ) and a parallel quadrupole moment Q_{11} at the origin. The interaction energy of these two quadrupole moments together can be calculated from (20) and (21). The half of this belonging to each moment is:

$$W_{r,\vartheta} = \frac{9}{8} \frac{Q_{11}^2}{r^5} \left(1 - 10\cos^2\vartheta + \frac{35}{3}\cos^4\vartheta \right). \tag{22}$$

The interaction energy for one elementary cell is found by summing up (22) for the whole lattice and using (19):

$$W = \frac{9}{5} e^2 R_0^2 (1-\mu)^2 \Lambda^2 \sum_i \frac{1}{r_i^5} \left(1 - 10\cos^2\vartheta_i + \frac{35}{3}\cos^4\vartheta_i \right). \tag{23}$$

Let the smallest distance between two atoms in a given lattice be δ,

$$r_i = \delta\xi. \tag{24}$$

It is known that

$$\delta = \beta R_0, \tag{25}$$

where

$$\beta = (\sqrt{3}\,\pi)^{1/3} \quad \text{for s.c.c. lattices}$$

and

$$\beta = \sqrt{2} \left(\frac{2\pi}{3} \right)^{1/3} \quad \text{for f.c.c. lattices.}$$

Let us take

$$S = \sum_i \xi_i^{-5} \left(1 - 10\cos^2\vartheta_i + \frac{35}{3}\cos^4\vartheta_i\right) \tag{26}$$

and

$$\eta = -\frac{27}{8}\beta^{-5}. \tag{27}$$

The U_2 in (16) has to be corrected further by W given by (23) and so the total cell energy will be

$$U = U_0(1 + \Psi_\mu \Lambda^2), \tag{28}$$

where

$$\Psi_\mu = \varphi_\mu - h(1-\mu)^2(1+\eta S) \tag{29}$$

and

$$h = -\frac{4e^2}{75\, R_0\, U_0}.$$

The energy term (28) has its minimum if

$$\left.\begin{aligned} \left(\frac{\partial U}{\partial \mu}\right)_\Lambda &= 0 \\ \left(\frac{\partial U}{\partial \Lambda}\right)_{\Lambda\to 0} &= 0. \end{aligned}\right\} \tag{30}$$

and

From (30) we obtain the equilibrium Poisson ratio as

$$\mu_0 = -\frac{1}{4}\,\frac{1 + \frac{5}{3}\varkappa w_0 h(1+\eta S)}{1 - \frac{5}{12}\varkappa w_0 h(1+\eta S)}. \tag{31}$$

Let us finally introduce another constant g as in [2], with

$$g = \frac{5}{12} w_0 h = \frac{e^2}{60\, R_0^4}. \tag{32}$$

Then

$$\mu_0 = -\frac{1}{4}\,\frac{1 + 4g\varkappa(1+\eta S)}{1 - g\varkappa(1+\eta S)}. \tag{33}$$

The elastic moduli c_{11} and c_{12} can now be obtained in the same form as in [2], i.e.

$$c_{11} = \frac{3}{5\varkappa}[4 - 8\, g\varkappa(1+\eta S)] \tag{34}$$

and

$$c_{12} = \frac{3}{5\varkappa}[1+4g\varkappa(1+\eta)S]. \tag{35}$$

Eq. (26) was then calculated for s.c.c. and f.c.c. lattices.

The numerical results are given in Table I, where c_{11} and c_{12} were calculated from Eqs. (34) and (35) assuming s.c.c. lattice for potassium and f.c.c. lattice for silver. The results of FUCHS' calculation for potassium and the available experimental values were quoted already in [1] and [2].

Table I

All data in 10^{11} dyne/cm^2

		K	Ag
	(34)	0.479	17.87
c_{11}	FUCHS	0.440	—
	experiments	0.457*	12.4
	(35)	0.374	7.63
c_{12}	FUCHS	0.380	—
	experiments	0.374*	9.34

* Measured at 73°K

As can be seen, the results are far better for potassium than for silver. There is, however, a quite remarkable overlapping of the ion cores with silver and so some of the basic assumptions of this and of the previous articles are only rough approximations for noble metals, even when the cells are at the equilibrium state. For unstrained equilibrium or for spherically symmetric deformations these discrepancies can be corrected by using a more sophisticated pseudopotential [10], but for nonspherically symmetric deformations the present method is only adequate for alkaline metals, where such overlappings are practically negligible.

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О МОДУЛЕ УПРУГОСТИ ЩЕЛОЧНЫХ И БЛАГОРОДНЫХ МЕТАЛЛОВ III.

Й. АНТАЛ

Резюме

В данной работе, являющейся продолжением предыдущих двух статей [1, 2], выведен новый член выражения энергии элементарной ячейки одновалентных металлов в случае одноосного растяжения. Появление этого члена вызвано взаимодействием квадрупольных моментов деформированных элементарных ячеек. Рассчитаны значения c_{11} и c_{12} для калия и серебра.

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ON THE DERIVATION OF THE HARTREE–FOCK EQUATIONS

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A simple general derivation of the Hartree—Fock equations is given. The derivation is based on the Brillouin theorem which is proved in its most general form for a Slater determinant built up from not necessarily orthogonal spin orbitals. The Hartree—Fock equations can be obtained as a specific formulation of the Brillouin theorem for the case of orthogonal spin orbitals.

As the possibility of finding alternative derivations of the Hartree—Fock equations has been the subject of recent discussion in the literature [1, 2], it seems to be of interest to present the following simple and general derivation based on the Brillouin theorem. This theorem is treated not as a consequence of the Hartree—Fock equations but is first proved to be a necessary condition which should be satisfied for the Slater determinant wave function with the lowest energy value. It is then shown that the theorem is also a necessary and sufficient condition for the stationariness of the energy expectation value and that the Hartree—Fock equations can be obtained as consequences of the Brillouin theorem. This second part of the treatment has some similarities to those given by DAHL et al. [2] and LEFEBVRE [3] but is more general (and also more general than the usual derivation [4]) because no restriction is put on the variations of the one-electron orbitals. It is usual either to consider specified variations [1—3] or to introduce Lagrangian multipliers [2, 4] in order to ensure that the one-electron orbitals remain orthogonal even after variation. Since, however, any Slater determinant wave function can also be built up from orthonormalized spin orbitals, the conservation of the orthogonality of the spin orbitals puts no physically meaningful restriction on the variations of the wave function; accordingly, as will be seen, there is no need for such a condition.

The Brillouin theorem for the Slater determinant with the lowest energy value

The Brillouin theorem states that: The matrix element of the n-electron Hamiltonian vanishes between the n-electron single Slater determinant wave function giving the lowest expectation value for the energy (the "best" Slater

determinant) and any single Slater determinant wave function which can be obtained from the former by replacing one filled spin orbital with an arbitrary unfilled spin orbital orthogonal to the filled orbitals (i.e. there is no mixing between these wave functions).

If the interchanged spin orbitals have different spins the theorem is trivial, owing to the orthogonality of the spin functions; and if they have the same spins, an indirect proof can be given.

Let us assume that the "best" Slater determinant is

$$\Psi_0 = \mathcal{A}\,[\varphi_1(1)\varphi_2(2)\ldots\varphi_i(i)\ldots\varphi_n(n)], \tag{1}$$

i.e. for a given n-electron Hamiltonian $\hat{H}$ the lowest expectation value $\bar{H} = H_{00}$ belongs to Ψ_0. We denote by Ψ_1 the wave function which can be obtained from Ψ_0 by replacing the spin orbital φ_i with a spin orbital ψ_i:

$$\Psi_1 = \mathcal{A}\,[\varphi_1(1)\varphi_2(2)\ldots\psi_i(i)\ldots\varphi_n(n)]. \tag{2}$$

$\langle\varphi_k \mid \psi_i\rangle = 0$, hence $\langle\Psi_0 \mid \Psi_1\rangle = 0$. There is no need to assume that the spin orbitals φ_k are mutually orthogonal; the appropriate normalization coefficients should be included in the antisymmetrizing operator $\mathcal{A}$.

Let us assume that the theorem is not valid, i.e. that Ψ_0 is the "best" Slater determinant but $H_{01} \neq 0$.

First we form a linear combination

$$\Psi = c_1\Psi_0 + c_2\Psi_1\,, \tag{3}$$

and determine the coefficients in such a way as to obtain a minimum energy for the wave function Ψ. The lowest root of the secular equation

$$\begin{vmatrix} H_{00}-E & H_{01} \\ H_{01}^* & H_{11}-E \end{vmatrix} = 0 \tag{4}$$

is

$$E_2 = H_{00} + \frac{1}{2}(H_{00}-H_{11})\left[\sqrt{1-\frac{4|H_{01}|^2}{(H_{00}-H_{11})^2}}-1\right]. \tag{5}$$

(The notation $H_{ij} = \langle\Psi_i \mid \hat{H} \mid \Psi_j\rangle$ is used).

According to our assumption $H_{00} < H_{11}$, therefore if $H_{01} \neq 0$, then E_2 will be smaller than H_{00}. It is easy to see, however, that the wave function Ψ is the sum of two determinants differing only in one row and thus can be written as a single determinant:

$$\Psi = \mathcal{A}[\varphi_1(1)\varphi_2(2)\ldots(c_1\varphi_i + c_2\psi_i)(i)\ldots\varphi_n(n)]. \tag{6}$$

(The appropriate normalization coefficients should be included in the c_i-s and $\mathcal{A}$.)

The wave function Ψ can thus be written as a single Slater determinant. Its energy E_2 is lower than H_{00} and consequently Ψ_0 cannot be the "best" Slater determinant. This contradicts the original premise, thus the theorem is proved. (If, however, $H_{01} = 0$, the lowest root of the secular equation is $E = H_{00}$.)

The Brillouin theorem for a Slater determinant with a stationary energy value

To vary the wave function $\Psi_0 = \mathcal{A}\,[\varphi_1(1)\varphi_2(2) \ldots \varphi_n(n)]$ normalized to 1 the spin orbitals must be varied. There is no need to regard the spin orbitals as orthonormalized, accordingly there is no need to require that this property be conserved during the variation. It should be noted that the normalization of the determinant wave function can change during the most general variation.

Let

$$\delta\varphi_k = \eta \sum_{\lambda=1}^{\infty} c_{k\lambda}\, \varphi_\lambda\, \delta(\chi_k, \chi_\lambda), \tag{7}$$

$$(\chi = \alpha \text{ or } \beta)$$

where η is an arbitrary complex quantity tending to zero. This variation is the most general one, because one can construct a complete system of functions from the filled orbitals having spin χ_k and from arbitrary unfilled orbitals of the same spin which are orthogonal to the filled orbitals. The only requirement is that the function represented by the sum should be finite and regular. Evidently an arbitrary number of $c_{k\lambda}$-s can be equal to zero, which permits the realization of specific variations. The wave function obtained after the variation is a determinant for which every element is the sum of two terms $[(\varphi_k + \delta\varphi_k)(i)]$, and it can therefore be written as a sum of 2^n determinants. The majority of these, however, are proportional to the square or to higher powers of η and are therefore negligible as compared with terms of the first order in η ("independence of the variations"). Accordingly,

$$\begin{aligned} \delta\Psi &= \sum_{k}^{n} \mathcal{A}\,[\varphi_1(1)\,\varphi_2(2) \ldots \delta\varphi_k(k) \ldots \varphi_n(n)] = \\ &= \eta \sum_{k=1}^{n} \sum_{\lambda=1}^{\infty} c_{k\lambda}\, \delta(\chi_k, \chi_\lambda)\, \mathcal{A}\,[\varphi_1(1)\,\varphi_2(2) \ldots \varphi_\lambda(k) \ldots \varphi_n(n)]. \end{aligned} \tag{8}$$

Summing over λ separately up to n and from $n + 1$:

$$\delta\Psi = \eta \left\{ \sum_{k=1}^{n} c_{kk}\, \Psi_0 + \sum_{k=1}^{n} \sum_{\lambda=n+1}^{\infty} c_{k\lambda}\, \delta(\chi_k, \chi_\lambda)\, \mathcal{A}\,[\varphi_1(1)\,\varphi_2(2) \ldots \varphi_\lambda(k) \ldots \varphi_n(n)] \right\}. \tag{9}$$

In the sum corresponding to the values $\lambda \leqslant n$ we have taken into account that if $\lambda \neq k$ the determinants have two equal rows.

The norm of the wave function after variation is

$$\langle \Psi_0 + \delta\Psi \mid \Psi_0 + \delta\Psi \rangle = 1 + \langle \delta\Psi \mid \Psi_0 \rangle + \langle \Psi_0 \mid \delta\Psi \rangle + \langle \delta\Psi \mid \delta\Psi \rangle. \quad (10)$$

The last term is proportional to η^2 and can be omitted. It is easy to see that

$$\begin{aligned} \langle \delta\Psi | \Psi_0 \rangle &= \eta^* \sum_{k=1}^{n} c_{kk}^* , \\ \langle \Psi_0 | \delta\Psi \rangle &= \eta \sum_{k=1}^{n} c_{kk} \end{aligned} \quad (11)$$

because Ψ_0 is orthogonal to all terms of the second sum in the expression for $\delta\Psi$. ($\langle \varphi_k \mid \varphi_\lambda \rangle = 0$, if $k \leqslant n$, $\lambda > n$.)

Thus we obtain

$$\langle \Psi_0 + \delta\Psi | \Psi_0 + \delta\Psi \rangle = 1 + \eta^* \sum_{k=1}^{n} c_{kk}^* + \eta \sum_{k=1}^{n} c_{kk}. \quad (12)$$

The expectation value of the Hamiltonian after variation is

$$\begin{aligned} \bar{H} + \delta\bar{H} = H_{00} + \delta\bar{H} = \frac{\langle \Psi_0 + \delta\Psi | \hat{H} | \Psi_0 + \delta\Psi \rangle}{\langle \Psi_0 + \delta\Psi | \Psi_0 + \delta\Psi \rangle} = \\ = \frac{1}{1 + \eta^* \sum_{k=1}^{n} c_{kk}^* + \eta \sum_{k=1}^{n} c_{kk}} \left\{ \left\langle \Psi_0 \left(1 + \eta \sum_{k=1}^{n} c_{kk} \right) \mid \hat{H} \mid \Psi_0 \left(1 + \eta \sum_{k=1}^{n} c_{kk} \right) \right\rangle + \right. \\ + \eta^* \sum_{k=1}^{n} \sum_{\lambda=n+1}^{\infty} c_{k\lambda}^* \, \delta(\chi_k, \chi_\lambda) \langle \mathcal{A}[\varphi_1(1)\, \varphi_2(2) \ldots \varphi_\lambda(k) \ldots \varphi_n(n)] \mid \hat{H} \mid \Psi_0 \rangle + \\ \left. + \eta \sum_{k=1}^{n} \sum_{\lambda=n+1}^{\infty} c_{k\lambda} \, \delta(\chi_k, \chi_\lambda) \langle \Psi_0 | \hat{H} | \mathcal{A}[\varphi_1(1)\, \varphi_2(2) \ldots \varphi_\lambda(k) \ldots \varphi_n(n)] \rangle \right\}. \end{aligned} \quad (13)$$

We have again dropped the terms proportional to η^2. After a further term containing η^2 has been omitted and the division by the denominator standing at the beginning of the expression has been carried out, the first matrix element gives just $H_{00} = \langle \Psi_0 \mid \hat{H} \mid \Psi_0 \rangle$, and we obtain

$$\begin{aligned} \delta\bar{H} = \frac{\eta^* \sum_{k=1}^{n} \sum_{\lambda=n+1}^{\infty} c_{k\lambda}^* \, \delta(\chi_k, \chi_\lambda) \langle \mathcal{A}[\varphi_1(1)\, \varphi_2(2) \ldots \varphi_\lambda(k) \ldots \varphi_n(n)] \mid \hat{H} \mid \Psi_0 \rangle}{1 + \eta^* \sum_{k=1}^{n} c_{kk}^* + \eta \sum_{k=1}^{n} c_{kk}} + \\ + \text{ complex conjugate.} \end{aligned} \quad (14)$$

It follows that for arbitrary variations $\delta\bar{H} = 0$ if, and only if, the Brillouin theorem is satisfied, i.e. the Slater determinant Ψ_0 has a stationary value of $\bar{H}$ ($\delta\bar{H} = 0$) if, and only if, the matrix element of the Hamiltonian is zero between Ψ_0 and any Slater determinant which can be obtained from Ψ_0 by replacing one filled orbital by an unfilled orbital which is orthogonal to the filled orbitals. LEFEBVRE [3] earlier gave a derivation of the Brillouin theorem for the case of a Slater determinant with a stationary energy value, using a similar but not identical method.

It follows from the comparison of the above two theorems that if there exists a Slater determinant for which the energy reaches its exact lower limit (for the set of wave functions which can be written with a single Slater determinant), this Slater determinant will have a stationary energy value too. This is usually assumed in all approaches based on the variation principle, although it is questionable whether it may be regarded as evident *a priori* for all types of trial wave functions.

The Hartree—Fock equations as consequences of the Brillouin theorem

Using an appropriate orthogonalization procedure one can always arrange that the wave function Ψ_0 considered in the discussion of the Brillouin theorem be given as a Slater determinant built up from orthonormalized spin orbitals. In this case we can obtain the Hartree—Fock equations expressing the Brillouin theorem in terms of one-electron orbitals.

According to the Brillouin theorem

$$\langle \Psi_0 | \hat{H} | \Psi_1 \rangle = 0 , \tag{15}$$

where

$$\hat{H} = \sum_{l}^{n} H^N(l) + \sum_{l<k}^{n} \frac{1}{r_{lk}} . \tag{16}$$

H^N is the one-electron part of the Hamiltonian.

Ψ_0 and Ψ_1 differ in one spin orbital, as above: instead of φ_l in Ψ_0, there is ψ_r in Ψ_1. Since the Brillouin theorem is trivial if $\chi_l \neq \chi_r$, we assume $\chi_l = \chi_r$. All spin orbitals concerned are orthonormalized, and so, using the known formulae [4], Eq. (15) can be rewritten in terms of the integrals over the spatial parts of the orbitals:*

$$\int \varphi_l^*(1)\, H^N(1)\, \psi_r(1)\, dv_1 + \sum_{i \neq l}^{n} \left[\iint \varphi_l^*(1)\, \varphi_l^*(2)\, \frac{1}{r_{12}}\, \varphi_i(1)\, \psi_r(2)\, dv_1\, dv_2 - \right.$$
$$\left. - \delta(\chi_i, \chi_l) \iint \varphi_l^*(1)\, \varphi_l^*(2)\, \frac{1}{r_{12}}\, \psi_r(1)\, \varphi_i(2)\, dv_1\, dv_2 \right] = 0 . \tag{17}$$

* Here and further on φ and ψ denote only those parts of the orbitals which depend on the spatial coordinates.

Taking the complex conjugate of this equation, using the hermiticity of the operator H^N in the first integral and interchanging the notations of the variables of integration in the second one, we obtain

$$\int \psi_r^*(1)\, H^N(1)\, \varphi_l(1)\, dv_1 + \sum_{i \neq l}^{n} \left[\iint \psi_r^*(1)\, \varphi_l^*(2)\, \frac{1}{r_{12}}\, \varphi_i(2)\, \varphi_l(1)\, dv_1\, dv_2 - \right.$$
$$\left. - \delta(\chi_i, \chi_l) \iint \psi_r^*(1)\, \varphi_l^*(2)\, \frac{1}{r_{12}}\, \varphi_i(1)\, \varphi_l(2)\, dv_1\, dv_2 \right] = 0 \,. \tag{18}$$

Taking the integration over r_1 separately and contracting:

$$\int \psi_r^*(1) \left\{ H^N(1)\, \varphi_l(1) + \sum_{i \neq l}^{n} \left[\left(\int |\varphi_i(2)|^2 \frac{1}{r_{12}}\, dv_2 \right) \varphi_l(1) - \right. \right.$$
$$\left. \left. - \delta(\chi_i, \chi_l) \left(\int \varphi_l^*(2)\, \varphi_l(2)\, \frac{1}{r_{12}}\, dv_2 \right) \varphi_i(1) \right] \right\} dv_1 = 0 \,. \tag{19}$$

This equation shows that the function of r_1 in the brackets is orthogonal to ψ_r. According to the derivation of the Brillouin theorem ψ_r may be any function orthogonal to all orbitals in Ψ_0 which have a spin χ_l. Consequently, the function in the brackets can be expressed as a linear combination of the functions occurring in Ψ_0 and having spin χ_l.

$$H^N(1)\, \varphi_l(1) + \sum_{i \neq l}^{n} \left(\int |\varphi_i(2)|^2 \frac{1}{r_{12}} dv_2 \right) \varphi_l(1) - \sum_{i \neq l}^{n} \delta(\chi_i, \chi_l) \left(\int \varphi_l^*(2)\, \varphi_l(2) \frac{1}{r_{12}} dv_2 \right) \varphi_i(1) =$$
$$= \sum_{i}^{n} \lambda_{li}\, \delta(\chi_i, \chi_l)\, \varphi_i(1) \,. \quad (l = 1, 2 \ldots n) \tag{20}$$

These are the Hartree—Fock equations [4].

The hermiticity of the λ matrix can be easily seen if one multiplies this equation by $\varphi_k^*(1)$ and the corresponding equation for φ_k by $\varphi_l^*(1)$ and then integrates both over r_1, and makes the necessary interchanges of variables of integration.

The equation can be transformed with the aid of the usual unitary transformation [4] into a pseudo-eigenvalue equation whose solutions for different orbital energies are automatically orthogonal, while solutions with equal orbital energies can be orthogonalized in such a way that the functions obtained also satisfy the Hartree—Fock equations. On the other hand the Brillouin theorem follows from the Hartree—Fock equations, so these are fully equivalent for the case of orthonormalized spin orbitals.

In the usual derivation the Lagrangian multipliers are introduced in order to ensure the orthonormality of the orbitals. As can be shown, in the

usual derivation the fact that in the case of equal orbital energies there can be solutions which are not necessarily orthogonal (even if they may be orthogonalized) is connected with a not fully consistent application of the Lagrangian multipliers.

Except for the first theorem, the present derivation can be applied without any essential change for the case of doubly filled orbitals; one has only to take into account that the spatial parts of the orbitals and their variations and the terms in formula (14) describing the variation of the energy are equal in pairs.

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О ВЫВОДЕ УРАВНЕНИЙ ХАРТРИ–ФОКА

И. МАЙЕР

Резюме

Приводится простой и общий вывод уравнений Хартри—Фока. Вывод основан на теореме Бриллюэна, которая доказывается в наиболее общем виде для детерминантной волновой функции, построенной из не обязательно ортогональных спин-орбиталей. Система уравнений Хартри—Фока может быть получена как специальная формулировка теоремы Бриллюэна для случая ортогональных спин-орбиталей.

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NON-LOCAL REGGE POLE THEORY

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Non-local theory is applied to study the strong interaction at very high energies. The Regge poles are considered in a non-local S-matrix theory. The S-matrix satisfying unitarity on the mass shell, relativistic covariance and macrocausality is established. The form-factor characterizing the non-locality is found by using the asymptotic behaviour of scattering amplitudes for $E \to \infty$ and the requirement that the total sections of elastic scattering tend to constant limits as $E \to \infty$.

A non-local theory of scalar fields and non-local quantum electrodynamics in which the ultraviolet infinies are absent without any regularization was constructed in [1, 2]. As the non-locality is characterized by a certain constant having the sense of elementary length l in order to find the non-locality effects it is necessary to study the reactions in the region of high energies $E \geqslant 1^{-1}$. The most useful way of studying the phenomena in this high energy region seems to be the Regge pole theory, and thus the task set out in this paper will be the construction of the Regge poles in the non-local theory.

The results obtained provide a check on the non-locality at very high energies.

§ 1. The perturbation expansion of quantized field theory enables us to replace the local propagator $\Delta^c(k)$ by a certain non-local propagator $D'(k)$ as follows [1, 2]:

$$\frac{1}{k^2 - m^2} = \Delta^c(k) \to D^c(k) = V(k^2)\,\Delta^c(k) = \frac{V(k^2)}{k^2 - m^2}\,.$$

Here, the form-factor $V(k^2)$ is a certain generalized analytical function of the VEKUA type [3], decreasing in any direction of the k-plane as $k^2 \to \infty$. It is possible to choose adequate form-factors $V(k^2)$ such that the theory is freed from ultraviolet divergences and the S-matrix satisfies the unitary and macrocausality conditions [1].

In order to establish a non-local theory of strong interactions, however, the perturbation theory cannot be used [4, 5], and so it is necessary to construct a S-matrix satisfying all the fundamental physical requirements and next to study the analyticity of the matrix elements of this matrix.

The S-matrix is an operator mapping the space of in-states Φ_{in} on the space of out-states Φ_{out}:

$$\Phi_{\text{out}} = S\Phi_{\text{in}}.$$

With the help of this matrix the corresponding field operators transform as follows:

$$S\varphi_{\text{in}} S^{-1} = \varphi_{\text{out}}.$$

As in the earlier papers [1, 2], φ_{in} and φ_{out} are considered to be local, and the non-locality appears only in the interaction, i.e. only in the S-matrix.

The first physical requirement of a S-matrix is that it should be unitary on the mass shell:

$$\langle a\,|SS^{+}|\,b\rangle = \langle a|b\rangle\,, \tag{1.1}$$

where $|\,a\rangle$ and $|\,b\rangle$ are two arbitrary physical states.

The second requirement is that the relativistic covariance

$$U(\Lambda, a)SU^{-1}(\Lambda, a) = S \tag{1.2}$$

should hold.

$U(\Lambda, a)$ are the irreducible unitary representations of the Poincaré group.

Thirdly, the macrocausality principle must be formulated in agreement with the relativistic covariance:

$$\frac{\delta}{\delta\varphi(x)}\left(\frac{\delta S}{\delta\varphi(y)}\,S^{-1}\right) = 0 \tag{1.3}$$

beside the regions G and G_l, where

$$G:\ x^0 \geqslant y^0\,(x-y)^2 > 0$$

$$G_l: -l^2 \leqslant (x-y)^2 \leqslant l^2.$$

In the region G_l, (1.3) is proportional to a certain relativistic-invariant generalized function $A_l(x-y)$ having the property that, arbitrary functions $f(x)$, nonvanishing in a certain limited region G_f of space-time, transform to functions

$$F(x) = \int d^4 y\, A_l(x-y)\, f(y)$$

non-vanishing only in a limited region of space-time $G_F = G_f + \delta G_f$, where δG_f is limited and belongs entirely to the interior of region G_{fl}, so that $x \in G_{fl}$ if and only if $-l^2 \leqslant (x-y)^2 \leqslant l^2$. Here $y \in G_f$.

It is clear that the macrocausality principle (1.3) and the relativistic covariance (1.2) are compatible.

§ 2. Let us examine the scattering process

$$a + b \to c + d\,. \tag{I}$$

with matrix elements

$$\langle c(p_2)\, d(q_2)|S-1|a(p_1)b(q_1)\rangle = (2\pi)^4\, \delta^4(p_2+q_2-p_1-q_1)\, M_b^{\mathrm{I}}(p_2, q_2; p_1, q_1)\,.$$

The relativistic covariance means that M_a^{I} is a certain function of the Mandelstam variables s and t:

$$M_a^{\mathrm{I}}(p_2, q_2; p_1, q_1) = T_a^{\mathrm{I}}(s, t)\,.$$

Let $T_c^{\mathrm{I}}(s, t)$ be the scattering amplitude of the process (I) in local theory. This is related to the amplitude $T_c^{\mathrm{II}}(s, t)$ of the crossing process

$$a + \bar{d} \to c + \bar{b} \tag{II}$$

by the crossing symmetry

$$T_c^{\mathrm{I}}(n, t) = T_c^{\mathrm{II}}(s, t)^*\,. \tag{2.1}$$

In non-local theory the microcausality principle is violated in the region G_l, and therefore the analyticity of the scattering amplitudes $T(s, t)$ is probably also violated. Following [6], however, we shall assume that the microcausality is violated only *minimally*, so that:

a) $T_a^J(s, t)$ have a spectrum similar to that of $T_c^J(s, t)$ i.e. T_a^J and T_c^J have the same singular points in the finite planes of the arguments and they have the same asymptotic behaviours at infinity. Otherwise, if the complex angular momenta plane is considered, then their partial amplitudes have the same behaviour in this plane.

b) $T_a^J(s, t)$ verify the crossing symmetry (2.1).

c) $T_a^J(s, t)$ satisfy the macrocausality principle (1.3).

In the set of the analytical functions, the two analytical functions which verify condition a) are identical. Therefore, following [1, 2, 7, 8, 9, 10], we assume that $T_a^J(s, t)$ are generalized analytical functions of the VEKUA type i.e. they have the form [3]:

$$T_a^J(s, t) = e^{\omega^J(s,t)}\, T_c^J(s, t)\,, \tag{2.2}$$

where $T_c^J(s, t)$ can be the causal scattering amplitudes of the corresponding process.

By using an assumption weaker than a), BLOKHINTSEV [6] assumed in his non-local model that $T_a^J(s, t)$ are the analytical functions having the forms similar to (2.2):

$$T_a^J(s, t) = T_a^J(s, t)\, \varrho^J(s, t)\,.$$

But the form-factors $\varrho^J(s, t)$ possess poles in the finite planes of arguments.

It is possible to prove easily that $T_a^J(s, t)$ given by (2.2) are totally compatible with the non-locality introduced in [1, 2]. In effect, let us assume $T_c(s, t)$ to be the causal scattering amplitude and let us study the scattering in the t-channel by exchanging a particle with spin equal J. The polar approximation of the amplitude gives

$$T_c(s,t) \approx g^2 \frac{P_J(\cos\Theta_t)}{t-m_J^2} \to g^2 \frac{(\cos\Theta_t)^J}{t-m_J^2} \approx g^2 \frac{s^J}{t-m_J^2} .$$

The non-locality is introduced as follows:

$$\frac{1}{t-m_J^2} \to \frac{V(s,t)}{t-m_J^2},$$

where $V(s, t)$ is a certain generalized analytical function of VEKUA type. Then

$$T_c(s,t) \to T_a(s,t) \approx g^2 \frac{V(s,t)}{t-m_J^2},$$

which agrees with (2.2) in the t-channel.

Therefore, following the results obtained in [1, 2] it can be concluded that the S-matrix whose matrix elements are given by formula (2.2) satisfies all the physical requirements expressed by (1.1), (1.2) and (1.3).

In order to verify the crossing symmetry (2.1), it is necessary that

$$\omega^{\mathrm{I}}(u,t) = \omega^{\mathrm{II}}(s,t)^* \tag{2.3a}$$

and

$$T_c^{\mathrm{I}}(u,t) = T_c^{\mathrm{II}}(s,t)^* . \tag{2.3b}$$

§ 3. In the s-channel the scattering amplitude of process (I) has the form

$$A(s,t) = e^{\omega^{\mathrm{I}}(s,t)}\, \varphi(s,t).$$

Expanding this into the partial amplitudes $f_l(s)$, we obtain

$$A(s,t) = \sum_{l=0}^{\infty} (2l+1)\, e^{\omega^{\mathrm{I}}(s,\cos\Theta_s)} f_l(s)\, P_l(\cos\Theta_s). \tag{3.1}$$

By using the Watson–Sommerfield transformation, (3.1) becomes

$$A(s,t) = \frac{1}{2i} \int_\Gamma (2l+1)\, e^{\omega^{\mathrm{I}}(s,\cos\Theta_s)} \frac{P_l(-\cos\Theta_s)}{\sin\pi l} f(l,s)\, dl ,$$

where Γ is the well known contour in the l-plane.

Use of assumption a) of § 2 allows us to represent $A(s, t)$ in the form

$$A(s,t)=\frac{1}{2i}\int_{b-i\infty}^{b+i\infty}(2l+1)\,e^{\omega^{\mathrm{I}}(s,\cos\Theta_s)}\frac{P_l(-\cos\Theta_s)}{\sin\pi l}f(l,s)\,dl+$$
$$+\pi\sum_{n=0}^{k}(2\alpha_n(s)+1)\,e^{\omega^{\mathrm{I}}(s,\cos\Theta_s)}\frac{P_{\alpha_n(s)}(-\cos\Theta_s)}{\sin\pi\alpha_n(s)}\beta_n(s), \tag{3.2}$$

where $\beta_n(s)$ are the residues of $f(l, s)$ at the pole $l_n = \alpha_n(s)$.

Similarly, the amplitudes $A_{\pm}(s, t)$ of the odd and even states are given as follows:

$$A_{\pm}(s,t)=\frac{1}{2i}\int_{b-i\infty}^{b+i\infty}(2l+1)\,e^{\omega^{\mathrm{I}}(s,\cos\Theta_s)}\frac{1\pm e^{i\pi l}}{\sin\pi l}P_l(\cos\Theta_s)f(l,s)\,dl+$$
$$+\pi\sum_{k=1}^{n}(2\alpha_k(s)+1)e^{\omega^{\mathrm{I}}(s,\cos\Theta_s)}\frac{1\pm e^{i\pi\alpha_k}}{\sin\pi\alpha_k(s)}P_{\alpha_k}(\cos\Theta_s)\,\beta_k(s)\,. \tag{3.3}$$

As $(\cos\Theta_s)\gg 1$ and s is fixed, the integral can be neglected, and we obtain

$$A_{\pm}(s,t)\approx\pi\sum_{k=1}^{n}\frac{2\alpha_k(s)+1}{2\sin\pi\alpha_k(s)}(1\pm e^{i\pi\alpha_k(s)})\,e^{\omega^{\mathrm{I}}(s,\cos\Theta_s)}(\cos\Theta_s)^{\alpha_k(s)}\,\beta_k(s)\,. \tag{3.4}$$

Passing to the t-channel, (3-4) becomes

$$A_{\pm}(s,t)=\pi\sum_{k=1}^{n}\frac{2\alpha_k(t)+1}{2\sin\pi\alpha_k(t)}\beta_k(t)\,e^{\omega^{\mathrm{II}}(t,s)}(1\pm e^{i\pi\alpha_k(t)})\left(\frac{s}{2\,p(t)\,p'(t)}\right)^{\alpha_k(t)}. \tag{3.5}$$

If there is at least a leading pole $\alpha_0(t)$, then $A_{\pm}(s, t)$ are equivalent to

$$A_{\pm}(s,t)\approx\pi\frac{2\alpha_0(t)+1}{2\sin\pi\alpha_0(t)}\beta_0(t)\,e^{\omega^{\mathrm{II}}(t,s)}\,(1\pm e^{i\pi\alpha_0(t)})\left(\frac{s}{2\,p(t)\,p'(t)}\right)^{\alpha_0(t)}. \tag{3.6}$$

In order to evaluate the asymptotic form of $\omega^{\mathrm{II}}(t, s)$ for large s, let us consider the forward elastic scattering of the equal mass particles. In this case $A_{\pm}(s, t)$ are rewritten as

$$A_{\pm}(s,t)\approx\pi\frac{2\,\alpha_0(t)+1}{2\sin\pi\alpha_0(t)}\beta_0(t)\,e^{\omega^{\mathrm{II}}(t,s)}(1\pm e^{i\pi\alpha_0(t)})\left(\frac{s}{2m^2}\right)^{\alpha_0(t)}.$$

The imaginary parts are thus given by

$$Im\,A_{\pm}(s,t)\approx sB_0^{\pm}(t)\,e^{(\alpha_0(t)-1)ln s}\,e^{\omega^{\mathrm{II}}(t,s)},$$

where $B_0^{\pm}(t)$ are the functions of t.

Expanding $\omega^{II}(t, s)$ and $\alpha_0(t)$ into the power series of t and restricting in the first terms for small t, we have

$$\omega^{II}(t, s) \approx \omega_0^{II}(s) + \omega_1^{II}(s)\, t\,,$$

and

$$\alpha_0(t) \approx \beta + \gamma t\,.$$

Then

$$A_{\pm}(s, t) \approx \pi \frac{2\alpha_0(t)+1}{2 \sin \pi\alpha_0(t)} \beta_0(t)(1 \pm e^{i\pi\alpha_0(t)})\, e^{\omega_0^{II}(s)+\beta \ln s/s_0 + (\omega_1^{II}(s)+\gamma)\, t}\,.$$

The differential sections are defined by

$$\frac{d\sigma_{\pm}(s, t)}{dt} \sim |A_{\pm}(s, t)|^2$$

or

$$\frac{d\sigma_{\pm}(s, t)}{dt} \to |F(t)|^2 \exp 2\left[\omega_0^{II}(s) + (\beta - 1) \ln \frac{s}{s_0} + (\omega_1^{II}(s)+\gamma)\, t\right]. \tag{3.7}$$

The total sections are given by

$$\sigma_{\pm}(s) = \frac{\pi}{s} Im A_{\pm}(s, 0) \approx B_0^{\pm}(0)\, e^{\omega_0^{II}(s)+(\beta-1) \ln s)}\,. \tag{3.8}$$

Utilizing the experimental finding that $\sigma_{\pm}(s)$ tend to constant values as $s \to \infty$, we see that $\omega_0^{II}(s)$ behaves like

$$\omega_0^{II}(s) \approx (1 - \beta) \ln s \qquad \text{for } s \to \infty. \tag{3.9}$$

To define uniquely the form of $\omega_0(s)$ it is not sufficient to take (3.9) together with the condition expressing the principle correspondance

$$e^{\omega(s, t)} \to 1 \qquad \text{as } l \to 0. \tag{3.10}$$

However, the actual experimental data suggest that we can assume that the non-locality damps very quickly as $l \to 0$. Mathematically this means that

$$\exp\{\omega(s, t)\} - 1 \approx 0(l^n) \tag{3.11}$$

for $l \to 0$ and arbitrary positive natural n.

Eqs. (3.9), (3.10) and (3.11) allow $\omega_0^{II}(s)$ to be defined as follows:

$$\exp \omega_0^{II}(s) = \exp\left\{-(\beta - 1)\, K_0\left[\left(\frac{1}{l^2|s|}\right)^2\right]\right\}, \tag{3.12}$$

where $K_0(x)$ is the Hankel function of the imaginary argument

$$K_0(x) = \int_0 e^{-x \operatorname{ch} \varphi} d\varphi .$$

It is clear that the asymptotic region of $\omega_0^{II}(s)$ given by (3.12) is higher than that of $P_l(\cos\theta)$, hence formula (3.8) can also give the non-local effect at very high energies.

If we assume that the non-locality is universal, i.e. that all the scattering amplitudes are given by formula (2.2), then

$$T_a(s,t) = e^{\omega(s,t)} T_c(s,t)$$

with a *unique* function $\omega(s,t)$.

It is possible to write $\omega(s,t)$ in the form

$$\omega(s,t) = \omega(s) + \omega(t) . \tag{3.13}$$

Taking this and (3.7), we obtain

$$A_{\pm}(s,t) \approx F(t) \exp\left\{(1-\beta) K_0\left(\frac{1}{l^4|s|^2}\right) + (\beta-1)\ln s\right\} \times \\ \times \exp\left\{(1-\beta)\exp\left(-\frac{1}{l^4|t|^2}\right) + \gamma\right\} t . \tag{3.14}$$

and

$$\frac{d\sigma_{\pm}(s,t)}{dt} \to |F(t)|^2 \exp 2\left\{(1-\beta) K_0\left(\frac{1}{l^4|s|^2}\right) + (\beta-1)\ln s\right\} \times \\ \times \exp 2\left\{(1-\beta)\exp\left(-\frac{1}{l^4|t|^2}\right) + \gamma\right\} t . \tag{3.15}$$

§ 4. With the function $\omega(s,t)$ given by (3.13), not all the pictures of the local Regge pole theory are varied for un-large s and fixed t. For example, in the reaction

$$\pi^- + \pi^0 \to \bar{p} + n$$

the Regge pole has an isotopic spin equal to 1, and barionic charge and strangeness equal to zero, $G = +1$ and odd spin. Assuming that this Regge pole corresponds to a ϱ-meson, we find

$$A_{\varrho}(s,t) \approx -\frac{\pi}{2}[2\alpha_{\varrho}(t)+1]\beta_{\varrho}(t) \frac{1-e^{i\pi\alpha_{\varrho}(t)}}{\sin \pi\alpha_{\varrho}(t)} \times \\ \times \left(\frac{s}{2\,p(t)\,p'(t)}\right)^{\alpha_{\varrho}(t)} \exp\{\omega(s)+\omega(t)\} . \tag{4.1}$$

For $|t| \ll l^{-1}$ the differential section given by (4-1) agrees with the picture given by the experimental data [11].

It should be noted that the classification of the elementary particles with respect to the families of Regge trajectories is identical with that in local theory.

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НЕЛОКАЛЬНАЯ ТЕОРИЯ ПОЛЮСОВ РЕДЖЕ

ТРАНЬ ХУУ ФАТ

Резюме

В данной работе применена нелокальная теория к изучению сильных взаимодействий при очень высоких энергиях. Рассмотрены полюсы Редже в теории нелокальных S-матриц. Установлено существование S-матрицы, удовлетворяющей условиям унитарности на массовой оболочке, релятивистической ковариантности и макропричинности. Используя асимптотическое поведение амплитуды рассеяния при $E \to \infty$, и требование, чтобы полное сечение упругого рассеяния стремилось к постоянному пределу при $E \to \infty$, найдён формфактор, характеризирующий нелокальность.

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ENTROPIC CHANGES IN A MEASURED QUANTUM-MECHANICAL OBJECT

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The processes connected with the entropy of measured quantum mechanical objects are investigated. The entropic characteristics of the measurement process are determined by means of the so-called entropy balance. It is shown that the Shannon entropy of quantal objects described by non-commutative operators is always positive in the post-measurement state. From the entropy balance of quantum mechanical measurement also follows that the measurement of the characteristics of quantal objects provides some information on quantities not measured.

Introduction

In the last decades the conceptual and mathematical apparatus of information theory has been successfully applied in various fields of physical science [1, 2, 3]. These applications have been possible because the physical phenomena in question are to a great extent describable by means of probability or statistical formalism. The probabilistic interpretation of quantum mechanics permits a direct application of the terms of information theory also in the description of an individual particle, as to each quantal object can be attached a value of its probability uncertainty, the measure of which is called the (information-theoretical) entropy [4].

Although the entropy of a quantal object may generally change in any physical process, the change that takes place during a measurement is especially important. Before measurement (the pre-measurement state) the measured observable generally has a non-zero entropy. After the measurement (the post-measurement state) this entropy is decreased, and in the optimal case it completely vanishes. As the measured quantal object is described by a set of observables which are mutually stochastically related, the removal of the entropy of a measured observable generally affects the entropy of the non-measured observable of the object. The determination of these various entropic changes forms the subject of this paper.

The entropic changes in a measured object play an important role in the physical description of the link between the measured micro-object and measuring macrophysical instrument, since according to the entropy law the total entropy of the whole measuring complex — measuring instrument and measured

object — should increase (or at least be constant) during the measurement, so that the negative entropic change of the measured object must be compensated for by a corresponding positive entropic change of the measuring instrument. By considering the measuring instrument as a physical statistical system, it is possible to determine this necessary positive change of its physical entropy using the well known relation between the physical and information-theoretical entropy [5].

From the point of view of information theory, the measuring process may be simulated by a mathematical model, called the entropic model of quantum measurement [6]. In this model the measured object and measuring instrument are represented by two probability systems. The measured observable τ_0, a random variable, is determined on the set of the physical states of the measured object. The measuring instrument may occur in one of its pointer positions representing the basic set on which the random variable τ_m is defined through the scale values attached to the pointer positions. During the measurement a statistical linkage is established between the random variables τ_0 and τ_m, by means of which the measuring instrument obtains information about the measured object. The measure of the statistical linkage between the random variables τ_0 and τ_m is in information theory given by a quantity called the information [7].

We shall first recall some terms of information theory which will be used in the further physical considerations. The measure of the probability uncertainty of a quantal observable represents the information-theoretical entropy, which is defined as follows [8]:

A random variable (observable) $\tilde{x}$ defined on a complete set of physical states S with the probability distribution given by the scheme

S	A_1	A_2	...	A_n
P	p_1	p_2	...	p_n
$\tilde{x}$	x_1	x_2	...	x_n

$$\sum_{i=1}^{n} p_i = 1,$$

has an information-theoretical entropy (the magnitude of its probability uncertainty) of

$$H = -\sum_{i=1}^{n} p_i \log_a p_i . \tag{1}$$

If not otherwise stated, we shall take $a = e$. The entropy as a function of the variables $p_1, p_2, \ldots, p_n$ (i.e. the elements of the probability distribution of the random variable $\tilde{x}$) fulfils a system of important mathematical axioms [8].

In order to quantitatively characterize the statistical linkage between the random variables $\tilde{x}$ and $\tilde{y}$ we need the data given by the transfer matrix [9]:

$$R = \begin{pmatrix} r_1(1) & \dots & r_1(n) \\ \vdots & & \vdots \\ r_n(1) & & r_n(n) \end{pmatrix},$$

where $r_i(j)$ is the conditional probability for assuming the j-th value of the random variable $\tilde{y}$ when the random variable $\tilde{x}$ has its i-th value. The information contained in the random variable $\tilde{y}$ about the random variable $\tilde{x}$ is given [10] by the formula

$$I(\tilde{x};\tilde{y}) = \sum_{i,j} p_i r_i(j) \log \frac{r_i(j)}{\sum_k p_k r_k(j)}, \tag{2}$$

which can be rearranged in the form

$$I = -\sum_i q_i \log q_i + \sum_i p_i \sum_j r_i(j) \log r_i(j), \tag{3a}$$

where

$$q_i = \sum_k p_k r_k(i).$$

If the random variables $\tilde{x}$ and $\tilde{y}$ are continuous with the density functions $p(x)$ and $q(y)$, respectively, formula (2) takes the form

$$I = \int_Y \int_X p(x) r_x(y) \log \frac{r_x(y)}{q(y)} \, dx \, dy, \tag{3}$$

where $r_x(y)$ represents the transfer function between the random variables $\tilde{x}$ and $\tilde{y}$.

The entropy of a measured quantal object changes by various ways, depending on the measuring conditions. When only one observable is measured, not only does its probability uncertainty change but also the probability uncertainties of those observables of the measured object with which it is statistically linked. Depending on the physical situation of the measurement, one may use various entropic characteristics of the measured quantal object in its description. The most important of these are the following: The total probability uncertainties of the measured object in its pre-or post-measurement state (H_b or H_a, respectively) and their difference ($\Delta H = H_a - H_b$), the pre- and post-measurement probability uncertainties of the measured observable, the entropic change of the non-measured observables during the measurement, etc. Which of them is used depends on the character of the problem.

1. The entropic changes in a quantal measurement

The basic assumption of the theory of quantum measurements is that in measuring a quantum-mechanical object one marks a system of eigenfunctions of the measured observable [11] and the result of a measurement represents one of these eigenvalues. The general wave function of the quantal object is thus reduced to an eigenfunction. This change of wave function is accompanied by a corresponding change in the entropy of the measured object, here considered as an information source. We shall now determine this entropic change for the measured quantal object.

Consider the general quantal object Σ described by an assembly of observables $G_1, G_2, \ldots, G_s$ to which the operators $\hat{O}_1, \hat{O}_2, \ldots, \hat{O}_s$ are associated. We shall denote by symbols $\{\varphi_{i_1}\}, \{\varphi_{i_2}\}, \ldots, \{\varphi_{i_s}\}$ the sets of eigenfunctions of the operators $\hat{O}_1, \hat{O}_2, \ldots, \hat{O}_s$ satisfying the quantal eigenvalue equations

$$\hat{O}_j \varphi_{i_j} = g_{i_j} \varphi_{i_j}, \qquad j = 1, 2, \ldots, s$$

where g_{i_j} denotes the i-th eigenvalue of the operator $\hat{O}_j$. We shall further denote by $U_{j_k l_m}$ the elements of the operator of the unitary transformation between the systems of eigenfunctions $\{\varphi_{j_k}\}$ and $\{\varphi_{l_m}\}$, whence

$$\varphi_{j_k} = \sum_{l_m} U_{j_k l_m} \varphi_{l_m} .$$

Let the quantal object Σ under study be described by the wave function

$$\Psi(x) = \sum_{i_1} \mu_{i_1} \varphi_{i_1} = \sum_{i_2} \mu_{i_2} \varphi_{i_2} = \ldots = \sum_{i_s} \mu_{i_s} \varphi_{i_s} .$$

The elements of the probability distributions $P_1, P_2, \ldots, P_s$, which are given on the sets of physical states of the quantal object Σ for the observable $G_1, G_2, \ldots, G_s$ are determined by means of the well-known equation

$$p_{i_j} = \mu_{i_j} \mu_{i_j}^{+} = |\mu_{i_j}|^2 . \qquad i = 1, 2, \ldots, n. \tag{4}$$

Between the observables $G_1, G_2, \ldots, G_s$ certain statistical dependences may exist which are described by means of the assembly of transfer matrices $R(p, t)$, $p, t = 1, 2, \ldots, s$, whose elements are determined by the elements $r_{i_p}(j_t)$ of the operator of the unitary transformation $U_{i_p j_t}$ between the p-th and t-th sets of eigenfunctions:

$$r_{i_p}(j_t) = U_{i_p j_t} \cdot U_{l_p j_t}^{+} = |U_{i_p j_t}|^2 \cdot \quad p, t = 1, 2, \ldots, s. \tag{4a}$$

The total probability uncertainty $H(P^{(z)})$ of the quantal object Σ is given by the entropy of the joint probability distribution $P^{(z)}$ [12], which is de-

fined on the product set $Z = S_1 \oplus S_2 \oplus \ldots \oplus S_s$, where $S_1 = \{s_1^{(1)}, s_2^{(1)}, \ldots, s_n^{(1)}\}$, $S_2 = \{s_1^{(2)}, \ldots, s_n^{(2)}\}$, $\ldots$, $S_s = \{s_1^{(s)}, \ldots, s_n^{(s)}\}$ are the sets of quantum states of observables $G_1, G_2, \ldots, G_s$. The elements of the product set Z represent all ordered n-groups of quantum states $(s_i^{(1)}, s_j^{(2)}, \ldots, s_m^{(s)})$, on which a vector random variable $\tilde{z} = \{g_{i_1}, g_{i_2}, \ldots, g_{i_s}\}$ is determined, where g_{i_k} represents k-th eigenvalue of the observable G_l. Denoting by $P_{i_1, i_2 \ldots, i_s}$ the elements of the joint probability distribution $P^{(z)}$, the total entropy of the measured quantal object is, according to Eq. (1), given by the relation

$$H(P^{(z)}) = - \sum_{i_1, i_2, i_3, \ldots, i_s} P_{i_1 i_2 \ldots i_s} \log P_{i_1 i_2 \ldots i_s} . \tag{5}$$

The elements of the joint probability distribution $P^{(z)}$ can also be written in the form

$$P_{i_1 i_2 \ldots i_s} = p_{i_1} \cdot r_{i_1}(i_2) \cdot r_{i_2}(i_3) \ldots r_{i_{s-1}}(i_s) , \tag{6}$$

where $r_{i_k}(i_{k+1})$, $k = 1, 2, \ldots, s-1$, represents the element of the transfer matrices $R(k, k+1)$, and p_{i_1} is an element of the probability distribution of the i-th observable.

Substituting Eq. (6) into (5) we find

$$\begin{aligned} H(P^{(z)}) = & - \sum_{i_1} p_{i_1} \log p_{i_1} - \sum_{i_1} p_{i_1}^{(1)} \cdot \sum_{i_2, i_3, \ldots, i_s} r_{i_1}(i_2) \cdot \\ & \cdot r_{i_2}(i_3) \ldots . \; r_{i_{s-1}}(i_s) \cdot \log r_{i_1}(i_2) \, r_{i_2}(i_3) \ldots r_{i_{s-1}}(i_s) . \end{aligned} \tag{7}$$

Eq. (7) determines the total entropy of the measured quantal object with the joint probability $P^{(z)}$ in its pre-measurement state. Since there are generally statistical dependences between the observable describing this object, its entropy has a smaller value than the sum of the entropies of the individual observables. We have [13]

$$H(P^{(z)}) \leq H(P_1) + H(P_2) + \ldots H(P_s) , \tag{7a}$$

where $P_1, P_2, \ldots, P_s$ are the probability distributions of the observables $G_1, G_2, \ldots, G_s$. In the relation (7a) the sign $=$ is to be taken only when all the observables are stochastically independent from each other, i.e. when

$$P_{i_1 i_2 \ldots i_s}^{(z)} = \prod_{k=1}^{s} p_{i_k} ,$$

where p_{i_k} represents the element of the probability distribution of the k-th observable.

The entropy change of the measured quantal object Σ during the measurement is given by the entropy balance of measurement, i.e. by the difference

between the total entropy of the object in its pre-measurement state $H_b(P^{(z)})$ and in its post-measurement state $H_a(P^{(z)})$:

$$\Delta H_t = H_a(P^{(z)}) - H_b(P^{(z)}). \tag{8}$$

During the measurement of the observable G_1 the probability distribution of the measured object changes. Denoting by $w = \{w_{i_1}, w_{i_1}, \ldots, w_{n_1}\}$ the post-measurement probability distribution of the measured observable, we can write according to Eq. (8) the total entropy change

$$\Delta H_t = -\sum_{i_1} w_{i_1} \log w_{i_1} + \sum_{i_1} p_{i_1} \log p_{i_1} - \sum_{i_1} (w_{i_1} - p_{i_1}) \cdot \sum_{i_2, i_3, \ldots, i_s} r_{i_1}(i_2) \cdot r_{i_2}(i_3) \ldots r_{i_{s-1}}(i_s) \cdot \log r_{i_1}(i_2) \cdot r_{i_2}(i_j) \ldots r_{i_{s-1}}(i_s). \tag{8a}$$

According to the entropy law a change ΔH_t in the entropy of the measured quantal object requires a minimal change $-k\Delta H_t$ in the physical entropy of the measuring instrument, k being Boltzmann's constant.

Let us now turn to the determination of the total post-measurement entropy $H_a(P^{(z)})$ of a measured quantal object. When only one observable is measured (for example G_1), the post-measurement entropy is

$$H_a = -\sum_{i_1} w_{i_1} \log w_{i_1} - \sum_{i_1} w_{i_1} \sum_{i_2, i_3, \ldots, i_s} r_{i_1}(i_2)\, r_{i_2}(i_3)\, r_{i_3}(i_4) \ldots \cdot \cdot r_{i_{s-1}}(i_s) \cdot \log r_{i_1}(i_2)\, r_{i_2}(i_3)\, r_{i_3}(i_4) \ldots r_{i_{s-1}}(i_s).$$

If the probability uncertainty of the measured observable is totally removed, we have

$$H_a(P^{(z)}) = H_b(P^{(z)}) - H(P_1).$$

Taking into account the relations (5) and (6), as well as the equation

$$H(P_1) = -\sum_{i_1=1}^{n} p_{i_1} \cdot \log p_{i_1},$$

we find

$$H_a(P^{(z)}) = -\sum_{i_1, i_2, \ldots, i_s} p_{i_1}\, r_{i_1}(i_2)\, r_{i_2}(i_3) \ldots r_{i_{s-1}}(i_s) \cdot \log r_{i_1}(i_2)\, r_{i_2}(i_3) \cdot r_{i_3}(i_4) \ldots r_{i_{s-1}}(i_s), \tag{9}$$

i.e. the total post-measurement entropy of the measured quantal object is equal to its general conditional entropy [13].

We shall next determine the foregoing entropic characteristics for the sake of simplicity, only for two observables G_1 and G_2. In this case relation (9) turns out to be

$$H_a(P^{(z)}) = -\sum_{i_1} p_{i_1} \sum_{i_2} r_{i_1}(i_2) \log r_{i_1}(i_2). \tag{10}$$

Substituting Eqs. (4) and (4a) into Eq. (10), we have

$$H_a(P^{(z)}) = -\sum_{i_1} |\mu_{i_1}|^2 \sum_{i_2} |U_{i_1 i_2}|^2 \log |U_{i_1 i_2}|^2. \tag{10a}$$

From Eq. (10) it is easy to see that the post-measurement entropy $H_a(P^{(z)})$ vanishes when

$$|U_{i_1 i_2}|^2 = \delta_{i_1 i_2}. \tag{11}$$

Consequently, for the corresponding operators $\hat{O}_1$ and $\hat{O}_2$ it holds that

$$\hat{O}_1 \hat{O}_2 - \hat{O}_2 \hat{O}_1 = 0, \tag{12}$$

i.e. the operators $\hat{O}_1$ and $\hat{O}_2$ commute. Thus we can state that only in the case when the operators associated with the observables G_1 and G_2 commute does the total entropy of the measured object vanish through the measurement of one of the observables.

When the observables $G_1, G_2, \ldots, G_m$ possess continuous spectra, then the eigenvalue problem can be written in the form

$$\hat{O}_i \varphi(l_i, x) = \mu(l_i) \varphi(l_i, x). \tag{13}$$

Let the wave function $\Psi_c(x)$ of the considered quantum-mechanical system be

$$\Psi_c(x) = \int \mu(l_1) \cdot \varphi(l_1, x)\, dl_1 = \int \mu(l_2) \varphi(l_2, x)\, dl_2 \ldots = \int \mu(l_m) \cdot \varphi(l_m, x)\, dl_m. \tag{13a}$$

The unitary transformation of the observables in this case turns out to be the integral one:

$$\varphi(l_i, x) = \int U(l_i, l_j) \varphi(l_j, x)\, dl_j\,. \tag{14}$$

The functions $p(l_1) = |\mu(l_1)|^2, p(l_2) = |\mu(l_2)|^2, \ldots, p(l_m) = |\mu(l_m)|^2$ and $r_{l_i}(l_j) = |U(l_i, l_j)|^2$ give the probability density functions of the observables G_1, $G_2, \ldots, G_m$ and the transfer functions $r_{l_i}(l_j)$ determining the statistical dependences between them, respectively. The change of the total entropy during the measurement and the post-measurement entropy of the measured object, while the observable G_1 is being completely measured, are found in a similar way:

$$\begin{aligned} \Delta H_t = H_a(P^{(z)}) - H_b(P^{(z)}) = &- \int u(l_1) \log u(l_1)\, dl_1 + \int p(l_1) \log p(l_1)\, dl_1 - \\ &- \int\int \ldots \int\int (u(l_1) - p(l_1) - p(l_1))\, r_{l_1}(l_2)\, r_{l_2}(l_3) \ldots r_{l_{m-1}}(l_m) \\ &\log \left[r_{l_1}(l_2) \cdot r_{l_2}(l_3) \ldots r_{l_{m-1}}(l_m) \right] dl_1\, dl_2 \ldots dl_m, \\ H_a(P_c^{(z)}) = &- \int\int \ldots \int p(l_1) \cdot r_{l_1}(l_2) \cdot r_{l_2}(l_3) \ldots r_{l_{m-1}}(l_m) \cdot \log r_{l_1}(l_2) \cdot \\ &\cdot r_{l_2}(l_3) \ldots r_{l_{m-1}}(l_m)\, dl_1\, dl_2 \ldots dl_m. \end{aligned} \tag{15}$$

The foregoing quantities occurring in the entropy balance of measurement represent basic quantitative characteristics of the measuring process from the entropic point of view.

2. Information and the measurement

In the preceding Section we have dealt with the change of the probability uncertainty of a measured system when performing the measurement of one of its observables. We now turn to the problem, of how the probability uncertainty of an observable G_p changes when we measure the observable G_1, or in other words how much information about the observable G_p is contained in the observable G_1. Consider again the physical system described in the preceding Section. Determining the i-th value of the observable G_1, the entropy balance of the variable G_p is $H_p = -\sum_{i_p} p_{i_p} \log p_{i_p}$ in the pre-measurement state and $H'_i = \sum_{j_p} r_{i_1}(j_p) \log r_{i_1}(j_p)$ in the post-measurement state. Therefore, the mean change of the probability uncertainty in the observable G_p when a measurement of the observable G_1 is performed is

$$\Delta H = H_p - \sum_i p_i H'_i = I(G_1; G_p) = -\sum_{i_p} p_{i_p} \log p_{i_p} + \\ + \sum_{i_1} p_{i_1} \sum_{j_p} r_{i_1}(j_p) \ln r_{i_1}(j_p) \,. \tag{16}$$

We can see that the expression for the mean entropy change ΔH is identical with that for the information (see Eq. (2)).

The change of the total entropy of the joint probability distribution of an assembly of observables $G_2, \ldots, G_s$ during the measurement of the observable G_1 is

$$\Delta H = I(G_1; G_2, \ldots, G_s) = -\sum_{i_2, i_3, \ldots, i_s} P_{i_2 i_3 \ldots i_s} \log P_{i_2 i_3 \ldots i_s} + \\ + \sum_{i_1, i_2, \ldots, i_s} p_{i_1} \cdot r_{i_1}(i_2) \cdot r_{i_2}(i_3) \ldots r_{i_{s-1}}(i_s) \log r_{i_1}(i_2)\, r_{i_2}(i_3) \ldots r_{i_{s-1}}(i_s). \tag{17}$$

Since the elements $P_{i_2 i_3 \ldots i_s}$ and p_{i_1} of the joint probability distributions of the observables $G_2, G_3, \ldots, G_s$ and the measured observable G_1, respectively, as well as the elements of the transfer matrices $R(1, 2)$, $R(2,3)$, . . ., are linked with the physical parameters of the measured quantum-mechanical object according to the relations (4) and (4a), when we substitute these relations into Eqs. (16) and (17) we get expressions in which only the quantum-mechanical terms occur.

Where the observables have a continuous probability distribution it is possible to give the mean magnitude of the entropic change of observables G_2, $G_3, \ldots, G_s$ by measurement of the continuous observable G_1. In accordance with Eqs. (17), (13) and (13a), we find

$$I = -\int\int \ldots \int |\mu(l_2)|^2 \, |U(l_2, l_3)|^2 \cdot |U(l_3, l_4)|^2 \ldots |U(l_{s-1}, l_s)|^2 \cdot$$
$$\cdot \log [|\mu(l_2)|^2 \, |U(l_2, l_3)|^2 \cdot |U(l_3, l_4)|^2 \ldots |U(l_{s-1}, l_s)|^2] \, dl_2 \cdot$$
$$\cdot dl_3 \ldots dl_s + \int\int \ldots \int |\mu(l_1)|^2 \, |U(l_1, l_2)|^2 \cdot |U(l_2, l_3)|^2 \ldots \cdot \qquad (18)$$
$$\cdot |U(l_{s-1}, l_s)|^2 \cdot \log [|U(l_1, l_2)|^2 \cdot |U(l_2, l_3)|^2 \ldots |U(l_{s-1}, l_s)|^2] \cdot$$
$$\cdot dl_1 \, dl_2 \ldots dl_s .$$

It can be shown that the maximum entropy change during the measurement will be obtained when $|\, U_{i_1 j_p}|^2 = r_{i_1}(j_p) = \delta_{i_1 j_p}$ or when $|\, U(l_i, l_j)\,|^2 = \delta(l_i - l_j)$, i.e. when the observables G_1 and G_p are compatible. This shows that the criterion of simultaneous measurability of the physical observables can be expressed by means of their entropic characteristics. This is of importance in the mathematical analysis of the quantum-mechanical formalism [14].

Since the general aim of a measurement is to reduce the probability uncertainty of the measured system as much as possible, one may, using the relations (8a), (15) and (18), find parameters of the measured object and measuring instrument (e.g. elements of transfer matrices, etc.) for which the entropy balance of measurement becomes optimal.

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ИЗМЕНЕНИЕ ЭНТРОПИИ КВАНТОВО-МЕХАНИЧЕСКИХ ОБЪЕКТОВ ПРИ ИЗМЕРЕНИИ

В. МАЕРНИК

Резюме

Обсуждаются процессы, связанные с энтропией системы, при измерении квантово-механических объектов. Определены энтропийные характеристики процесса измерения, при измерениях проведенных в так называемом режиме баланса энтропии. Показано, что энтропия Шеннона квантованных объектов, которая описывается с помощью некоммутирующих операторов, после измерения всегда положительна. Далее, из баланса энтропии квантово-механических измерений следует, что измерение наблюдаемых характеристик квантовых объектов дает некоторые информации и о неизмеренных величинах.

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COMMUNICATIO BREVIS

VALIDITY OF KOVÁCS AND NAGY'S EQUATION AS A MEASURE OF THE TOTAL EQUIVALENT MEAN SHEAR STRAIN IN TWISTED 99.7% Al WIRES

By

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KOVÁCS and FELTHAM [1] and KOVÁCS and NAGY [2] derived an equation for the total equivalent mean shear strain $\bar{\gamma}$ of a wire plastically twisted about its axis at constant tensile load. In this equation $\bar{\gamma}$ consists of a torsional shear strain ND/L and the shear strain component equivalent to the associated tensile strain $\Delta L/L_0$, as follows:

$$\bar{\gamma} = \alpha\pi ND/L + \beta\Delta L/L_0\,, \tag{1}$$

where N is the number of turns of twist, D is the diameter of the wire, L_0 and L are the initial and instantaneous lengths of the wire, α and β are constants. KOVÁCS and FELTHAM [1] took the numerical values of α and β to be 1/3 and 2.24, respectively, but they indicated that these values were underestimated because the mean torsional strain was evaluated on the assumption that the wire was purely elastic: they pointed out that GAYDON's [3] assumption of ideal plasticity would be more appropriate. Recent work [4, 5] has indicated that the values of α and β are $2\pi/3$ and 3, respectively.

Eq. (1) can be written in the form:

$$\Delta L/L_0 = -(\alpha/\beta)ND/L + \bar{\gamma}/\beta$$

or

$$\epsilon = -(\alpha/\beta)\Theta + \bar{\gamma}/\beta, \tag{2}$$

where $\epsilon = \Delta L/L_0$ and $\Theta = ND/L$.

By partial differentiation of ϵ with respect to θ at constant $\bar{\gamma}$ we get

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$$\left(\frac{\partial \epsilon}{\partial \Theta}\right)_{\bar{\gamma}} = -(\alpha/\beta) = -2\pi/9 = -0.698 \tag{3}$$

Eq. (3) shows that the rate of change of tensile strain per unit torsional strain at constant $\bar{\gamma}$ has a constant value of -0.698 determined by the constants α and β. Since the value of $\left(\frac{\partial \epsilon}{\partial \Theta}\right)_{\bar{\gamma}}$ can be determined experimentally, this

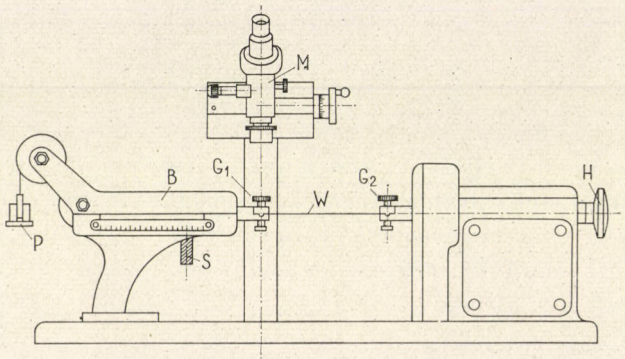

Fig. 1. Schematic diagram of twisting machine

gives a direct test of the validity of the KOVÁCS—NAGY equation [Eq. (1)]. We have used this approach in an investigation on wires made of commercial purity Al (99.7% Al + 0.25% Fe).

Annealed Al wires (0.05 cm diameter, 15 cm long) were subjected to uniform twisting at room temperature using the machine shown in Fig. 1. The associated change in sample length was measured up to fracture with an accuracy of 10^{-3} cm. The axial stresses applied on the sample undergoing torsional deformation varied from 0.75 to 2.25 kg/mm^2; such stresses did not exceed the yield stress.

Fig. 2 shows that for samples with the same thermal history, $\Delta L/L_0$ at certain ND/L increases as the magnitude of the applied stress is increased.

The values of $\left(\frac{\partial \epsilon}{\partial \Theta}\right)_{\bar{\gamma}}$ were calculated from Fig. 2 using the least squares method. These values are given in Table I and are plotted against $\bar{\gamma}$ in Fig. 3. The average value of $\left(\frac{\partial \epsilon}{\partial \Theta}\right)_{\bar{\gamma}}$ over the whole range of $\bar{\gamma}$ is approximately equal to the constant $\alpha/\beta = -0.7$. The resemblance of the experimentally determined values of α/β to that given by Eq. (3) indicates that the KOVÁCS—NAGY equation is valid.

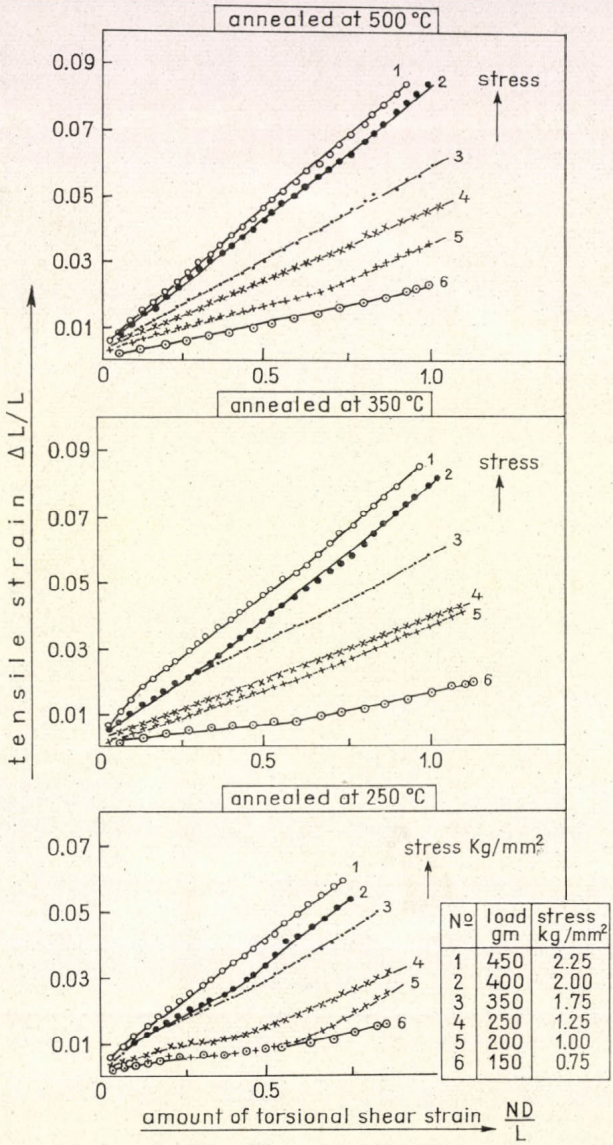

Fig. 2. Tensile strains $\Delta L/L_0$ associated with plastic twisting ND/L in pre-annealed aluminium wires under different constant loads

For specimens annealed at 500 °C before testing, scattered values of α/β are noted for $\bar{\gamma} < 100$. Under these conditions the values of α/β range between —0.6 and —0.4. This may be attributed to the effect of annealing. Annealing at 250, 350 and 500 °C for 5 hours was found to influence the values of ND/L and $\Delta L/L_0$ as well as the angle of inclination between the torsional lines

Table I

$\bar{\gamma}$	$\left(\frac{\partial \epsilon}{\partial \Theta}\right)_{\bar{\gamma}}$		
	250 °C	350 °C	500 °C
0.435		—0.65	
0.440			—0.52
0.450	—0.62		
0.480			—0.60
0.500	—0.80		
0.600			—0.60
0.620			—0.61
0.630		—0.70	
0.640	—0.82		
0.700	—0.65	—0.40	—0.40
0.800			—0.52
0.920		—0.50	
1.000	—0.70		—0.68
1.200	—0.63	—0.70	—0.70
1.400	—0.72	—0.65	
1.500			—0.70
1.600	—0.67	—0.63	
1.700	—0.82		
1.790		—0.76	
1.800	—0.80		
1.880			—0.62
2.000		—0.60	—0.70

Table II

Sample history	Φ	ND/L	$\Delta L/L_0$
As received and twisted	47°	0.198	0.0069
Annealed at 250 °C	56°	0.924	0.0289
Annealed at 350 °C	75°	1.100	0.0420
Annealed at 500 °C	66°	1.020	0.0377

and wire axis, as shown in Table II. The appearance of torsional lines, which was used for determining Φ, is shown in Fig. 4. It is apparent that annealing at 250 and 350 °C causes the values of Φ, ND/L and $\Delta L/L_0$ to increase while annealing at 500 °C causes these values to decrease. Since Φ represents the

deformability of the specimen, annealing at 500 °C makes the material less deformable. This is also indicated by the decrease of ND/L and $\Delta L/L_0$.

The changes may be attributed to the presence of Al_3Fe, which has been observed to form under similar conditions [6, 7]. This is in agreement with the observations of PETTY [8] on the relation of deformability to the shape and size distribution of precipitate particles.

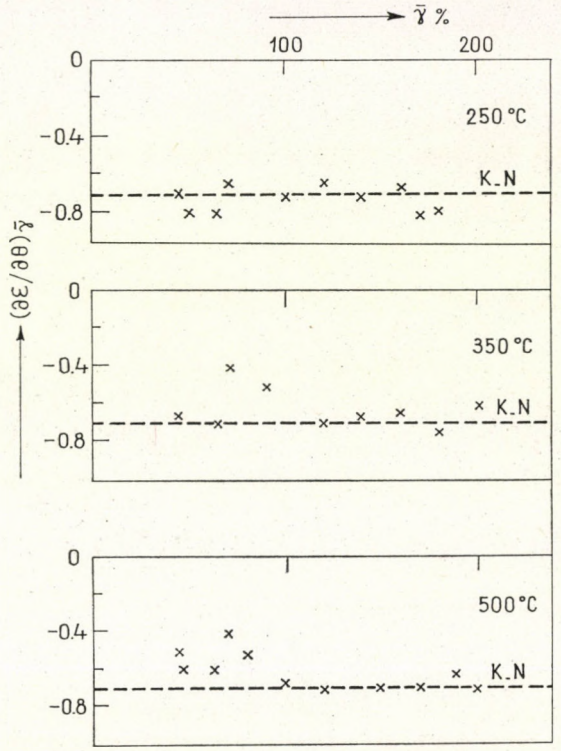

Fig. 3. Variation of the relative change of tensile strain with plastic torsion (W versus γ) from the KOVÁCS and NAGY value

Acknowledgement

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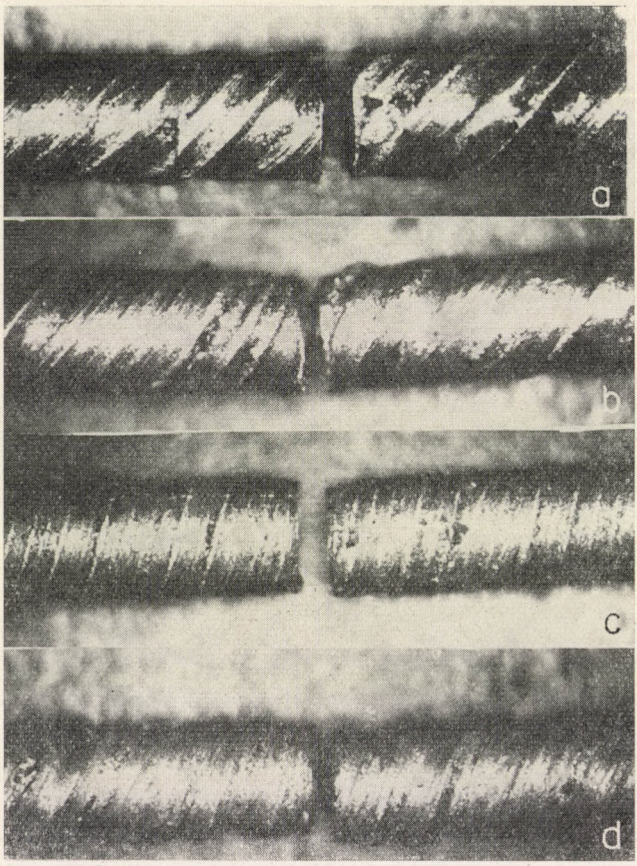

Fig. 4. Photographs of surfaces of Al samples twisted till fracture at room temperature. 50×. Initial history:
a) As received; b) Annealed at 250 C; c) Annealed at 350 C; d) Annealed at 500 C

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RECENSIONES

A. J. LYON: Dealing with Data

Pergamon Press, Oxford—New York—Toronto—Sydney—Braunschweig, 1970, XVII + 392 p.

The book is an excellent guide for graduate students and young scientists to problems arising in connection with data analysis. Almost every discipline in the natural sciences is based on experimental data and dealing with them is not always as easy as often imagined.

Chapters 1 and 2 give a review on the possible sources of experimental and computational errors. These are recommended to students who are beginning laboratory studies.

Chapters 3, 4 and 5 deal with such basic statistical problems as standard errors, propagation of errors, significance tests. Special interest is devoted to range methods; these make otherwise complicated statistical studies straightforward and rapid to apply even at the laboratory bench. Any research worker who does not have a thorough grounding in statistical studies will find interesting topics in these chapters.

Chapter 6 gives a guide to fitting a straight line in an elementary but effective manner. Some of the practical advice given on the choice of the scales of a graph and rejection of outliers is very useful. The generally more difficult problem of fitting of curves is treated in Chapter 9.

Computational errors and numerical methods such as integration and differentiation are briefly discussed in Chapters 7 and 8. The use of slide rules, logarithm tables and desk calculating machines is also described. This part can be recommended to students of non-mathematical sciences such as biology or mineralogy. Electronic computers and their related special problems, such as Monte Carlo methods and double precision variables are, however, not discussed. As these are generally applied in physics, chemistry and many other fields, it would have been useful for a young expert to find something about them in the book.

The numerous well-chosen examples and problems form an important part of the book. These examples will be helpful to tutors in setting effective teaching courses of their students and greatly facilitate self-education. Some very useful tables and summaries in the appendices complete the book and make it easy to use directly in the laboratory.

G. NÁRAY-SZABÓ

John Pecham and the Science of Optics

(Perspectiva communis) Edited with an Introduction, English translation and Critical Notes by DAVID C. LINDBERG
The University of Wisconsin Press, Madison, Milwaukee and London, 1970, 300 pages

Over the past few decades historians have considerably neglected medieval contributions to the science of optics. This has mainly been due to the fact that modern editions of basic texts have simply not been available. However, with the publication of the first English edition of JOHN PECHAM's study "Perspectiva communis" DAVID C. LINDBERG has made this most widely known and cited of all medieval works on optics available for scientists.

A lecturer of the Franciscan schools at the universities of Paris and Oxford and later Archbishop of Canterbury, JOHN PECHAM (1292) was one of the men most actively engaged in the criticism and assimilation of the science of Islam and ancient Greece newly discovered in the XIIIth century. In addition to participating in the philosophical controversies associated

with the new Aristotelianism, Pecham was interested in several technical aspects of scientific thinking. The revival in the West of the ancient traditions of optics in particular, developed to a high level by the Greeks, but enriched by the newer discoveries of Islamic scientists — especially ALHAZEN (IBN AL-HAITHAN) — was largely due to the efforts first of ROBERT GROSSETESTE and later ROGER BACON. PECHAM was heir to this tradition, and in "Perspectiva Communis" he attempted to reconcile all available authorities on optics and to express their conclusions in easily understandable terms.

In Part I PECHAM discusses the propagation of light and colour, the conditions of visual perception, the anatomy and physiology of the eye, the physiology of vision and the errors of direct vision. Part II contains a discussion of vision by reflected rays. Part III is devoted to vision by refracted rays as well as to the rainbow and the Milky Way. Thus PECHAM intended his study as introduction to the science of optics, especially to the optical theory of its original source, ALHAZEN.

LINDBERG's edition of "Perspectiva Communis" strikes a marvellous balance between a literal and interpretative translation. The Latin text, based on 11 early manuscripts, is printed with the English translation on the opposite pages. LINDBERG also provides the reader with an introduction placing PECHAM in an appropriate historical perspective and gives detailed explanations of the text and references to many other medieval works.

The book reviewed here is of value to scientists studying medieval science, particularly with regard to the development of optics in the late Middle Ages and the Renaissance. Art historians will find this book exceedingly useful, as many renaissance painters relied on PECHAM's study of the theory of perspective. The book is an excellent example of a medieval university textbook and as such will be of interest to students of the history of education.

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