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LONG-WAVE PHONONS IN METALS

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The role of many-particle interaction between ions in a metal through the conduction electrons is analyzed. It is shown that in the solution of the dynamical problem, particularly in the determination of the phonon spectrum with accuracy up to $(V_K/\epsilon_F)^2$ (V_K is the Fourier component of the pseudopotential at a reciprocal lattice point), it is necessary to take into account three- and four-particle interactions. General expressions are found for the elastic moduli or the sound velocities in non-transition metals. By means of certain general relations derived for a charged Fermi liquid, it is possible to obtain the microscopic value of the elastic modulus, which depends only on the pseudopotential of the electron-ion interaction (or on the corresponding scattering amplitude) and on the polarization operator of the interacting electron gas.

1. INTRODUCTION

UNTIL recently, the theory of metals has been developed chiefly as a one-electron theory. The electron-electron interaction has been taken into account by the introduction of the screening of the ionic potential, and in problems related to the total energy, only the energy of the interacting electron gas has been added. This has resulted in simply an effective pair potential for the interaction between ions, corresponding to indirect interaction through the conduction electrons.

Here, simply speaking, it remains an open question as to why metals exist with a complicated crystalline structure. Usually, the existence of additional forces has been implicitly assumed for the establishment of stability of the lattice; these are due to the interaction of the interior electrons of the ion shells. However, it has been found recently that these forces in metals are very weak and cannot preserve the lattice in equilibrium.

The progress made recently in the theory of metals, which is associated with the introduction of the concept of the pseudopotential, also made no change in this system of representations, since the pseudopotential is considered most frequently simply as a method of convenient description of the electron-ion interaction in the band theory. As a result, although this method systematically demonstrates the possibility of reducing the strong electron-ion interaction to an effective weak pseudopotential, and thus forms a basis of a model of quasi-free electrons (see, for example,[1]), the entire consideration is practically a one-electron one, as before. Therefore there remained the essential question of a systematic many-electron consideration of metals, which would make it possible to find both the electron and the phonon spectra within the framework of the same initial representations, and also all the physical quantities that depend on these spectra.

Such a consideration was undertaken in the researches of the authors,[2,3] in connection with the analysis of the problem of the formation of the phonon spectrum of metals. Here two circumstances were made use of. The first is the small dimensions of the ions of the non-transition metals, which remains after the separation of all valence electrons. (The ions occupy about 5–10% of the atomic volume.) As a result, the interaction between the ions is composed of the direct Coulomb interaction and the indirect interaction through the conduction electrons. This makes it possible to introduce a Hamiltonian for the description of the electron-ion system of the metal, which in turn allows us to solve the problem to any approximation.

The second important circumstance is that the scattering amplitude of the electron by the separate field in the metal, at a momentum transfer on the order of the reciprocal lattice vector **K**, is a small quantity. In the language of the pseudopotential, this means that there is a small parameter V_K/ϵ_F (V_K is the Fourier component of the pseudopotential) which, by the way, predetermines the success of the quasi-free electron model. In the band theory, this circumstance has in fact no application. In the theory developed by us, it allows us to look for the physical quantities in the form of a series expansion in powers of the pseudopotential.[2,3] Here the perturbation theory in the electron-electron interaction is not used, so that the whole consideration is to a certain degree the reverse of what is done in standard one-electron theory.

The various powers of the pseudopotential in the total energy describe the contribution from the effective two-, three-, four-ion indirect interaction through the conduction electrons, and so forth. The appearance of many-particle (unpaired) interionic forces in the metal has quite a fundamental character even in the case in which their contribution is comparatively small. In particular, the aforementioned problem of instability of metals[2,3] is involved here.

Up to the present time, in the analysis of the phonon spectra of specific metals,[2-4] we have parameterized the many-particle interactions using the general properties of the metals, particularly the fact that they possess symmetrical lattices. This approach has been very successful and allows us to explain the phonon spectra of a number of complicated metals throughout all phase space. In the present work, we carry out a microscopic analysis of the role of many-particle forces, and the dipole part of the phonon spectrum is most completely studied.

It turns out that the unpaired interaction is especially important in the dynamical problem of oscillations. Thus, whereas for the determination of the static energy with accuracy $(V_K/\epsilon_F)^2$ it is sufficient to consider only pair interactions, for the determination of the longitudinal sound velocity with the same accuracy it is necessary to include three-particle and even four-particle interactions. In other words, in the consideration of the dynamics of oscillations in many-particle interactions, terms of the same order as in the pair interaction are kept. This indicates, in particular, the incorrectness of the usual notions concerning the dynamics of metals, which take only pair forces into account (for example, see[1]).

It is essential that by using a number of exact relations for a charged Fermi liquid introduced in the present work, we can obtain a closed expression for the elastic moduli only in terms of the polarizability of the electron gas and the pseudo-potential of the electron-ion interaction.

2. LONG-WAVE PHONONS IN A METAL. THE ELASTIC MODULI

In accord with the results of[2], the energy of the electron system in a field of fixed ions with coordinates $\mathbf{R}_m$ can be represented in the form of a power series in the pseudopotential:

$$E_e = E^{(0)} + E^{(1)} + E^{(2)} + \dots \qquad (2.1)$$

Here the expression for $E^{(n)}$ has the form

$$E^{(n)} = \Omega \sum_{\mathbf{q}_1\ldots\mathbf{q}_n} \Gamma^{(n)}(\mathbf{q}_1, \ldots, \mathbf{q}_n) U_{\mathbf{q}_1} \ldots U_{\mathbf{q}_n} \Delta(\mathbf{q}_1 + \ldots + \mathbf{q}_n), \qquad (2.2)$$

where

$$U_{\mathbf{q}} = V_{\mathbf{q}} \frac{1}{N} \sum_m e^{i\mathbf{q}\mathbf{R}_m}, \qquad (2.3)$$

V_q is the Fourier component of the effective pseudopotential for the separate ion, which will be assumed to be local, Ω is the total volume, N the number of atoms in the volume of the crystal and Δ a delta function describing the law of momentum conservation.

It is clear from the definition (2.2) that the multipole $\Gamma^{(n)}(q_1, \ldots, q_n)$, which depends only on the electron-electron interaction, can be regarded as symmetrized over all its arguments without any loss of generality. On the other hand, by assuming spherical symmetry of the electron-ion interaction, we have

$$\Gamma^{(n)}(\mathbf{q}_1, \ldots, \mathbf{q}_n) = \Gamma^{(n)}(-\mathbf{q}_1, \ldots, -\mathbf{q}_n). \qquad (2.4)$$

If the ions are located at equilibrium positions, then all the $\mathbf{q}_i$ in (2.2) for $n \geq 2$ are equal to the reciprocal lattice vectors $\mathbf{K}_i$. By virtue of this fact, each successive term in the expression for the electron energy of the static lattice will contain the additional small parameter V_K/ϵ_F.

In this connection, if we consider the static energy with accuracy to within $(V_K/\epsilon_F)^2$, then it suffices in (2.1) to keep only terms up to $E^{(2)}$ inclusively. The need to account for many-particle terms arises only when we want to determine the energy with greater accuracy. In the case of an oscillatory problem, the situation is quite different. Actually, the position of the ions in (2.3) does not now coincide with equilibrium. By expanding (2.2) in terms of the displacements of the ions and extracting the part of the electron energy which plays the role of the potential energy of the oscillation problem in the daiabatic approximation, we find that the corresponding expression will contain the Fourier components of the potential even for arbitrary q. Therefore the character of the expansion in the parameter V_K/ϵ_F changes significantly and, as we shall see below, for the determination of the sound or, more generally, the phonon spectrum with accuracy up to $(V_K/\epsilon_F)^2$, with which the entire analysis is performed, it is necessary to take into account the contribution from the many-particle interactions with just this accuracy.

We write out the general expression for the dynamical matrix of a metal with one atom in the elementary cell (here we use a somewhat different notation than in[2,3]):

$$D^{\alpha\beta}(\mathbf{q}) = D_i^{\alpha\beta}(\mathbf{q}) + \sum_{n\geqslant 2} D_{(n)}^{\alpha\beta}(\mathbf{q}) \equiv D_i^{\alpha\beta}(\mathbf{q}) + D_e^{\alpha\beta}(\mathbf{q}). \qquad (2.5)$$

Here the first and second terms describe the dynamical matrix arising from the direct Coulomb interaction between ions and from the indirect interaction through the conduction electrons, respectively. Here we have for $D_{(n)}^{\alpha\beta}(\mathbf{q})$, taking into consideration (2.2), (2.3),

$$\begin{aligned} D_{(n)}^{\alpha\beta}(\mathbf{q}) = \Omega_0 \frac{n(n-1)}{M} \sum_{\mathbf{K}_1\ldots\mathbf{K}_n} \{ [(q+K_1)^\alpha (q+K_2)^\beta V_{\mathbf{q}+\mathbf{K}_1} V_{\mathbf{q}+\mathbf{K}_2} V_{\mathbf{K}_3} \ldots V_{\mathbf{K}_n} \\ \times \Gamma^{(n)}(\mathbf{q}+\mathbf{K}_1, -\mathbf{q}-\mathbf{K}_2, \mathbf{K}_3, \ldots, \mathbf{K}_n) \Delta(\mathbf{K}_1 - \mathbf{K}_2 + \mathbf{K}_3 + \ldots + \mathbf{K}_n)] \\ - [\mathbf{q} = 0] \} \end{aligned} \qquad (2.6)$$

(Ω_0 is the volume of the elementary cell). It is stipulated that here and below the terms $V_{K=0}$ are assumed to be equal to zero because of electrical neutrality.

It follows at once from (2.6) that for $n \geq 5$ the corresponding terms in the dynamical matrix have an order of smallness not less than $(V_K/\epsilon_F)^3$. As to terms with n = 3 and 4, although they contain the pseudopotential in third and fourth powers, the corresponding order of smallness does not appear through all of phase space. Actually, we note that

$$\frac{1}{\varepsilon_F} \frac{V_{\mathbf{q}}}{\varepsilon(\mathbf{q})} \bigg|_{\mathbf{q}\to 0} \sim 1$$

(we have introduced the dielectric constant $\epsilon(q)$ here in explicit form, recognizing that it always appears in the description of $\Gamma^{(n)}(q_1, \ldots, q_n)$—see[2] and the section below). Then it becomes clear that if we set $\mathbf{K}_1$ or $\mathbf{K}_2$ in the term n = 3 equal to zero (for $\mathbf{K}_1 = \mathbf{K}_2 = 0$, this term vanishes), then the separated part will be of the order $(V_K/\epsilon_F)^2$ for small $\mathbf{q}$, i.e., of the same order as the terms with $\mathbf{K} \neq 0$ in $D_{(2)}(\mathbf{q})$. A similar situation exists for n = 4, if we consider the region of small q and set $K_1 = K_2 = 0$.

Thus, for the long-wave part of the phonon spectrum, the dynamical matrix is not reduced only to $D_{(2)}^{\alpha\beta}(\mathbf{q})$, and has the following form in the approximation considered:

$$\begin{aligned} D^{\alpha\beta}(\mathbf{q}) = \frac{2\Omega_0}{M} \sum_{\mathbf{K}} \{ [(q+K)^\alpha (q+K)^\beta |V_{\mathbf{q}+\mathbf{K}}|^2 \Gamma^{(2)}(\mathbf{q}+\mathbf{K}, -\mathbf{q}-\mathbf{K}) \\ + 3(2q^\alpha q^\beta + q^\alpha K^\beta + q^\beta K^\alpha) V_{\mathbf{q}} V_{\mathbf{q}+\mathbf{K}} V_{\mathbf{K}} \Gamma^{(3)}(\mathbf{q}, -\mathbf{q}-\mathbf{K}, \mathbf{K}) \\ + 6 q^\alpha q^\beta |V_{\mathbf{q}}|^2 |V_{\mathbf{K}}|^2 \Gamma^{(4)}(\mathbf{q}, -\mathbf{q}, \mathbf{K}, -\mathbf{K})] - [\mathbf{q} = 0] \}. \end{aligned} \qquad (2.7)$$

(We have used here the symmetry of $\Gamma^{(n)}(q_1, \ldots, q_n)$ with respect to all its arguments, and the relation (2.4).)

We now consider the region of limitingly long waves and find an explicit expression for the elastic moduli from (2.7). Here we expand (2.7) in a series in q and introduce the notation

$$D^{\alpha\beta}(\mathbf{q})=\frac{\Omega_0}{M}[\alpha\beta,\gamma\delta]q^\gamma q^\delta. \tag{2.8}$$

The square brackets in (2.8) are identical with the well-known notation of Born and Huang[5] and are convenient for the direct transition to the elastic moduli[5]

$$C_{\alpha\beta\gamma\delta}=[\alpha\gamma,\ \beta\delta]+[\gamma\beta,\ \alpha\delta]-[\gamma\delta,\ \alpha\beta]. \tag{2.9}$$

We further introduce the following notation:

$$F^\alpha(\mathbf{K})\equiv\left\{\frac{\partial}{\partial q^\alpha}V_\mathbf{q}\Gamma^{(3)}(\mathbf{q},\,-\mathbf{q}-\mathbf{K},\,\mathbf{K})\right\}_{\mathbf{q}\to0},$$

$$V^\alpha(\mathbf{K})\equiv\left\{\frac{\partial}{\partial q^\alpha}V_{\mathbf{q}+\mathbf{K}}\right\}_{\mathbf{q}\to0}=\frac{\partial}{\partial K^\alpha}V_\mathbf{K}. \tag{2.10}$$

Then, comparing the expansion (2.7) with (2.8), we have for the contribution of three-particle interaction

$$\begin{aligned}[\alpha\beta,\gamma\delta]_{(3)}&=3\sum_{\mathbf{K}\neq0}V_0\Gamma^{(3)}(0,\mathbf{K},-\mathbf{K})\{2|V_\mathbf{K}|^2(\delta^{\alpha\gamma}\delta^{\beta\delta}+\delta^{\alpha\delta}\delta^{\beta\gamma})\\&+V_\mathbf{K}[K^\alpha\delta^{\beta\delta}V^\gamma(\mathbf{K})+K^\alpha\delta^{\beta\gamma}V^\delta(\mathbf{K})+K^\beta\delta^{\alpha\delta}V^\gamma(\mathbf{K})+K^\beta\delta^{\alpha\gamma}V^\delta(\mathbf{K})]\}\\&+|V_\mathbf{K}|^2[K^\alpha\delta^{\beta\delta}F^\gamma(\mathbf{K})+K^\alpha\delta^{\beta\gamma}F^\delta(\mathbf{K})+K^\beta\delta^{\alpha\delta}F^\gamma(\mathbf{K})+K^\beta\delta^{\alpha\gamma}F^\delta(\mathbf{K})].\end{aligned} \tag{2.11}$$

Correspondingly, for the contribution of the four-particle interaction we have

$$\begin{aligned}[\alpha\beta,\gamma\delta]_{(4)}&=6|V_0|^2\sum_{\mathbf{K}\neq0}|V_\mathbf{K}|^2\Gamma^{(4)}\\&\times(0,0,\mathbf{K},-\mathbf{K})(\delta^{\alpha\gamma}\delta^{\beta\delta}+\delta^{\alpha\delta}\delta^{\beta\gamma}).\end{aligned} \tag{2.12}$$

In (2.11) and (2.12), and also everywhere below, expressions with zero argument should be understood in the sense q → 0.

In the determination of the contribution of the two-particle interaction, it is appropriate to unite the indirect interaction through the electrons (the first term in (2.7)) with the direct Coulomb interaction (the first term in (2.5)), which is paired in nature. We separate here the terms with **K** = 0 and **K** ≠ 0, which we denote by $[\alpha\beta,\gamma\delta]_{(0)}$ and $[\alpha\beta,\gamma\delta]_{(p)}$, respectively.

We shall make use of the fact that, in accord with the results of previous researches,[2,3]

$$\Gamma^{(2)}(\mathbf{q},-\mathbf{q})=-{}^1\!/_2\Pi(\mathbf{q})/\varepsilon(\mathbf{q}), \tag{2.13}$$

where

$$\varepsilon(\mathbf{q})=1+4\pi e^2q^{-2}\Pi(\mathbf{q}) \tag{2.14}$$

is the statistical dielectric constant. Then, after simple transformations, we get

$$[\alpha\beta,\gamma\delta]_{(0)}=\frac{1}{2}\left(\frac{Z^2}{\Pi(0)\Omega_0^2}+\frac{2bZ}{\Omega_0^2}\right)(\delta^{\alpha\gamma}\delta^{\beta\delta}+\delta^{\alpha\delta}\delta^{\beta\gamma}), \tag{2.15}$$

$$\begin{aligned}[\alpha\beta,\gamma\delta]_{(p)}&=\frac{1}{2\Omega_0}\sum_{\mathbf{K}\neq0}\{\varphi(\mathbf{K})(\delta^{\alpha\gamma}\delta^{\beta\delta}+\delta^{\alpha\delta}\delta^{\beta\gamma})+[\delta^{\alpha\delta}K^\beta\varphi^\gamma(\mathbf{K})\\&+\delta^{\beta\delta}K^\alpha\varphi^\gamma(\mathbf{K})+\delta^{\alpha\gamma}K^\beta\varphi^\delta(\mathbf{K})+\delta^{\beta\gamma}K^\alpha\varphi^\delta(\mathbf{K})]+K^\alpha K^\beta\varphi^{\gamma\delta}(\mathbf{K})\};\end{aligned} \tag{2.16}$$

Here

$$\varphi(\mathbf{q})=\frac{4\pi Z^2e^2}{q^2\Omega_0}-\frac{|V_\mathbf{q}|^2\Pi(\mathbf{q})}{\varepsilon(\mathbf{q})}\Omega_0,$$

$$\varphi^\alpha(\mathbf{q})=\frac{\partial\varphi}{\partial q^\alpha},\qquad\varphi^{\alpha\beta}=\frac{\partial^2\varphi}{\partial q^\alpha\partial q^\beta}. \tag{2.17}$$

The value of b is determined from the limiting value of the pseudopotential

$$V_{\mathbf{q}\to0}\to-\frac{4\pi Ze^2}{q^2\Omega_0}+\frac{b}{\Omega_0}. \tag{2.18}$$

By knowing (2.11), (2.12), (2.15), and (2.16), we can find the elastic moduli for any symmetry crystal directly. We shall limit ourselves for simplicity to the case of a lattice of cubic symmetry. By using (2.9), we have for the determination of the elastic modulus $C_{11}=C_{xxxx}$, corresponding to longitudinal sound velocity in the direction of the wave vector along the cubic axis,

$$\begin{aligned}C_{11}&=\frac{Z^2}{\Omega_0^2\Pi(0)}+\frac{2bZ}{\Omega_0^2}+\frac{1}{\Omega_0}\sum_{\mathbf{K}\neq0}\Big[\varphi(\mathbf{K})+\frac{2}{3}K^\alpha\varphi^\alpha(\mathbf{K})\\&+\frac{1}{2}(K^x)^2\varphi^{xx}(\mathbf{K})\Big]+4\sum_{\mathbf{K}\neq0}\Big\{3V_0\Gamma^{(3)}(0,\mathbf{K},-\mathbf{K})\Big[|V_\mathbf{K}|^2\\&+\frac{1}{3}V_\mathbf{K}K^\alpha V^\alpha(\mathbf{K})\Big]+V_0|V_\mathbf{K}|^2K^\alpha F^\alpha(\mathbf{K})\\&+3|V_0|^2|V_\mathbf{K}|^2\Gamma^{(4)}(0,0,\mathbf{K},-\mathbf{K})\Big\}.\end{aligned} \tag{2.19}$$

In similar fashion, we can find the expression for the shear modulus:

$$C_{44}=C_{xxyy}=\frac{1}{2\Omega_0}\sum_{\mathbf{K}\neq0}(K^x)^2\varphi^{yy}(\mathbf{K}),$$

$$\begin{aligned}C'\equiv\frac{C_{11}-C_{12}}{2}=\frac{C_{xxxx}-C_{xyxy}}{2}&=\frac{1}{4}\sum_{\mathbf{K}\neq0}[(K^x)^2\varphi^{xx}(\mathbf{K})+(K^x)^2\varphi^{yy}(\mathbf{K})\\&-2K^xK^y\varphi^{xy}(\mathbf{K})].\end{aligned} \tag{2.20}$$

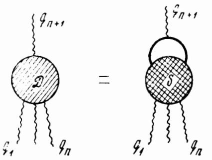
From these expressions, we can draw the conclusion that in the considered approximation, when all terms of order $(V_K/\epsilon_F)^2$ are kept, the many-particle interaction through the ions changes significantly the longitudinal velocity of sound or the modulus C_{11}, and leaves the shear modulus unchanged. Therefore the contribution of the many-particle forces to the shear modulus (2.20) begins with terms of order $(V_K/\epsilon_F)^3$. So far as the modulus C_{11} is concerned, it is necessary in its determination to know the value of the multipoles for a very specific value of the arguments: $\Gamma^{(3)}(0,\mathbf{K},-\mathbf{K})$, $\Gamma^{(4)}(0,0,\mathbf{K},-\mathbf{K})$ and $F^\alpha(\mathbf{K})$. It is shown that one can obtain general relations that are valid for a charged Fermi liquid, which allows us to connect these quantities with the simplest multipole $\Gamma^{(2)}(\mathbf{K},-\mathbf{K})$ (2.13).

3. SOME EXACT RELATIONS FOR THE CHARGED FERMI LIQUID

In this section, we shall obtain a series of exact relations that are correct for a charged Fermi liquid and connect the different multipoles $\Gamma^{(n)}(\mathbf{q}_1,\ldots,\mathbf{q}_n)$ (see (2.2)). For the derivation of these relations, we find it convenient to use the diagram representation of the multipoles, which is obtained from the corresponding energy representation (2.2). As was noted in[2], the electron energy in the field of static ions can be set in correspondence with the set of coupled vacuum diagrams in which the role of excitations in the S matrix is played by $H_{\text{int}}=H_{ei}+H_{ee}$. Then each term of (2.2) corresponds to the set of all diagrams of a definite order in H_{ei} and of arbitrary order in H_{ee}. It is known that the coefficients in the vacuum diagrams, which are obtained by use of the Wick theorem, in contrast with the diagrams for the G functions, depend on the symmetry of the diagram and on the order of the perturbation. This greatly complicates the calculations. Therefore, we shall apply the following method.

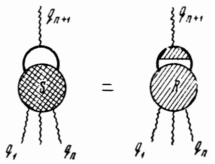
We introduce the quantities $\mathscr{D}^{(n)}(\mathbf{q}_1,\ldots,\mathbf{q}_n)$, which correspond to the vacuum diagrams. However, all the external momenta we shall consider fixed (we shall not carry out the integration over them as in (2.2)), and the coefficient in all diagrams of similar type we shall take to be equal to unity. This allows us to carry out partial summation without difficulty (to introduce the "heavy" lines exactly as was done for the Green's functions; see, for example,[6]).

Therefore, we can write down directly the following graphical equality for the complete block $\mathscr{D}^{(n+1)}$, similar to the usual equation for the vertex:



(3.1)

(The heavy lines correspond to the complete G-function.) In the mixed multipole $S^{(n)}_{(2)}$ (n entering lines of the external field and two electron lines), which is actually determined by this equality, one can separate the irreducible block in the following way:



(3.1a)

On the right hand side of this equality we have introduced the vertex T, which represents the complete block, as usual, converting particle into particle. It is not difficult to see that the mixed multipole $R^{(n)}_{(2)}$ possesses two essential properties: it is irreducible over the two electron lines and over the line of electron-electron interaction, since the corresponding parts are transferred to the complete vertex T.

The resultant equality can be represented in analytic form in the following way:

$$\mathscr{D}^{(n+1)}(\mathbf{q}_1,\ldots,\mathbf{q}_n,\mathbf{q}_{n+1}) = \int \frac{d^4p}{(2\pi)^4} T(\mathbf{q}_{n+1},\mathbf{p},-\mathbf{p}-\mathbf{q}_{n+1})$$
$$\times G(p)G(p+q_{n+1})R^{(n)}_{(2)}(\mathbf{p},-\mathbf{p}-\mathbf{q}_{n+1},\mathbf{q}_1,\ldots,\mathbf{q}_n). \qquad (3.2)$$

We now introduce the complete symmetrization of the left and right sides of (3.2) over the momenta of the external field q_1, ..., q_n. Denoting the multipole thus symmetrized as $\tilde{\mathscr{D}}^{(n+1)}$ and $\tilde{R}^{(n)}_{(2)}$, we rewrite (3.2) in the form

$$\tilde{\mathscr{D}}^{(n+1)}(\mathbf{q}_1,\ldots,\mathbf{q}_n,\mathbf{q}_{n+1}) = \int \frac{d^4p}{(2\pi)^4} T(\mathbf{q}_{n+1},\mathbf{p},-\mathbf{p}-\mathbf{q}_{n+1})$$
$$\times G(p)G(p+q_{n+1})\tilde{R}^{(n)}_{(2)}(\mathbf{p},-\mathbf{p}-\mathbf{q}_{n+1},\mathbf{q}_1,\ldots,\mathbf{q}_n). \qquad (3.2a)$$

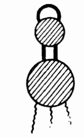
We now introduce another relation, using the technique of skeleton diagrams, developed for Fermi systems in the work of Luttinger and Ward[7] (see also[8]). By a skeleton diagram, we mean, as usual, a diagram which does not have self-energy parts, so that the replacement in it of a G line by a heavy line corresponds to summation of a whole class of diagrams. We note that the very possibility of a distinct introduction of skeleton diagrams arises after fixing of the external momenta, i.e., after transition to diagrams of the type $\mathscr{D}$.

We represent the complete multipole $\mathscr{D}^{(n)}(q_1, \ldots, q_n)$ in the form of a sum over skeleton diagrams of arbitrary order in the interelectronic interaction, in which all the fine lines are replaced by heavy lines. This multipole can be regarded as a functional of the exact G functions. Then variation of this functional can itself be represented as the variation of the separate G functions in each skeleton diagram. For the variation of the symmetrized multipole, we obtain

$$\delta\tilde{\mathscr{D}}^{(n)}(\mathbf{q}_1,\ldots,\mathbf{q}_n) = n\int \frac{d^4p}{(2\pi)^4}\delta G(p)\tilde{Q}^{(n)}_{(2)}(\mathbf{p},-\mathbf{p},\mathbf{q}_1,\ldots,\mathbf{q}_n). \qquad (3.3)$$

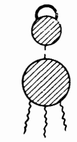
In the variation of the complete set of multipoles over all the Green's functions, n identical expressions appear each time, thanks to the symmetrization of these multipoles; these lead to the appearance of the coefficient n in (3.3).

The multipole $\tilde{Q}^{(n)}_{(2)}$ appearing upon variation has two initial electron lines and n lines of the external field. This pole is irreducible in the two electron lines. Actually, in the opposite case, in the closing of the electron ends of this multipole, we would obtain a diagram with a self-energy part:



(3.4a)

which contradicts the initial assumption that only the skeleton diagrams were varied. Similarly, we can establish the fact that the multipole $\tilde{Q}^{(n)}_{(2)}$ is also irreducible over the lines of the interelectron interaction:



(3.4b)

Thus the multipole $\tilde{Q}^{(n)}_{(2)}$ has the same properties as $R^{(n)}_{(2)}$ in (3.2a). If we go to the limit $q_{n+1} \to 0$ in $\tilde{R}^{(n)}_{(2)}$, then both multipoles become identical:

$$\tilde{R}^{(n)}_{(2)}(\mathbf{p},-\mathbf{p},\mathbf{q}_1,\ldots,\mathbf{q}_n) = \tilde{Q}^{(n)}_{(2)}(\mathbf{p},-\mathbf{p},\mathbf{q}_1,\ldots,\mathbf{q}_n).$$

The advantage of Eq. (3.3) lies in the fact that it allows us to find the derivatives in the external arguments without difficulty. For our purposes, it is necessary to find the derivative with respect to the chemical potential of the interacting electron gas:

$$\frac{d\tilde{\mathscr{D}}^{(n)}(\mathbf{q}_1,\ldots,\mathbf{q}_n)}{d\mu} = n\int \frac{d^4p}{(2\pi)^4}\frac{dG(p)}{d\mu}\tilde{Q}^{(n)}_{(2)}(\mathbf{p},-\mathbf{p},\mathbf{q}_1,\ldots,\mathbf{q}_n). \qquad (3.5)$$

(The line of electron-electron interaction does not contain μ.) It is not difficult to see that

$$\frac{dG}{d\mu} = \frac{G(\mathbf{p},\mu+d\mu)-G(\mathbf{p},\mu)}{d\mu}$$
$$= -G(\mathbf{p},\mu+d\mu)G(\mathbf{p},\mu)\left(1-\frac{d\Sigma(\mathbf{p},\mu)}{d\mu}\right)\Big|_{d\mu\to 0}. \qquad (3.6)$$

It can be shown (see[8]) that the quantity $G(p, \mu + d\mu)G(\rho, \mu)|_{d\mu \to 0}$ acts as the "static" limit of the theory of a Fermi liquid[6] ($\omega/k \to 0$):

$$G(\mathbf{p},\mu+d\mu)G(\mathbf{p},\mu)\,|_{d\mu\to 0} = \{G^2(p)\}_k. \qquad (3.7)$$

We use the Ward identity for the vertex[8]

$$1 - d\Sigma(\mathbf{p},\mu)\,/\,d\mu = T_1(\mathbf{p},-\mathbf{p},0). \qquad (3.8)$$

We emphasize that, as can be shown directly, the vertex T_1, which is unresolved in the electron-electron interaction because of electrical neutrality, stands on the right side of (3.8). Substituting (3.6)—(3.8) in (3.5), we finally get

$$\frac{d\tilde{\mathscr{D}}^{(n)}(\mathbf{q}_1,\dots,\mathbf{q}_n)}{d\mu}=-n\int\frac{d^4p}{(2\pi)^4}\times\{G^2(p)\}_k T_1(\mathbf{p},-\mathbf{p},0)\tilde{R}_{(2)}^{(n)}(\mathbf{p},-\mathbf{p},\mathbf{q}_1,\dots,\mathbf{q}_n). \tag{3.9}$$

We now consider (3.2a) in the limit $q_{n+1} \to 0$ (the static limit for the square of the Green's function is obtained automatically, inasmuch as the external field is static, i.e., $\omega = 0$). We provisionally separate the part from the total vertex T which is unresolved in the electron-electron interaction. This corresponds simply to the separation in explicit form of the dielectric constant corresponding to screening of the lines of the external field:

$$T(\mathbf{q},\mathbf{p},-\mathbf{p}-\mathbf{q}) = T_1(\mathbf{q},\mathbf{p},-\mathbf{p}-\mathbf{q})\,/\,\varepsilon(\mathbf{q}). \tag{3.10}$$

Then, substituting (3.10) in (3.2), setting $q_{n+1} = 0$, and comparing this limit with (3.9), we obtain the identity

$$\tilde{\mathscr{D}}^{(n+1)}(\mathbf{q}_1,\dots,\mathbf{q}_n,0)=-\frac{1}{n\varepsilon(0)}\frac{d\tilde{\mathscr{D}}^{(n)}(\mathbf{q}_1,\dots,\mathbf{q}_n)}{d\mu}. \tag{3.11}$$

Here, as everywhere, we mean by zero $\mathbf{q}$ the limiting value as $q \to 0$. The relation (3.9) can be obtained as any of the momenta q_i tend to zero in the initial multipole $\mathscr{D}^{(n+1)}(q_1, \dots, q_{n+1})$. Therefore, without loss of generality, we can consider $\tilde{\mathscr{D}}^{(n+1)}$ on the left side of (3.11) as a completely symmetrized multipole in all its arguments.

Carrying out the entire derivation for the diagrams of $\mathscr{D}^{(n)}$ having coefficients in all diagrams equal to unity, we transform to the multipoles $\Gamma^{(n)}$, which are determined by the expansion of the energy and have coefficients connected with the Wick expansion. It is not difficult to see that, inasmuch as we mean by $\tilde{\mathscr{D}}^{(n)}$ the entire set of symmetrized diagrams of n-th order in the electron interaction, the following equality is valid:

$$\Gamma^{(n)}(\mathbf{q}_1,\dots,\mathbf{q}_n)=\frac{1}{n}\tilde{\mathscr{D}}^{(n)}(\mathbf{q}_1,\dots,\mathbf{q}_n).$$

Using this, we obtain finally

$$\Gamma^{(n+1)}(\mathbf{q}_1,\dots,\mathbf{q}_n,0)=-\frac{1}{\varepsilon(0)}\frac{1}{n+1}\frac{d\Gamma^{(n)}(\mathbf{q}_1,\dots,\mathbf{q}_n)}{d\mu}. \tag{3.12}$$

The identities (3.12), as is seen from the derivation above, follow from the very structure of the theory of a Fermi liquid and are exact.

We now write out several simple relations that follow from (3.12) for the case of multipoles with small numbers of vertices.

First of all we find the connection between $\Gamma^{(1)}$ and $\Gamma^{(2)}$. It is not difficult to see that the quantity $\Gamma^{(1)}(0)$ can be computed exactly. Actually, it is described by the single diagram

(3.13)

since all the complications are already included in the heavy G line. Therefore,

$$\Gamma^{(1)}(0)=-2i\int\frac{d^4p}{(2\pi)^4}G(p)=n_0, \tag{3.13a}$$

where n_0 is the density of the electron gas. On the other hand, $\Gamma^{(2)}(q, -q)$ can also be found exactly.[2] This multipole has the form of (2.13). Then, using (3.12) for this case, we obtain directly

$$\Pi(0) = dn_0\,/\,d\mu. \tag{3.14}$$

Or, using the expression for the compressibility,

$$1\,/\,\varkappa = n_0^2 d\mu\,/\,dn_0,$$

we find

$$\Pi(0) = n_0^2\varkappa. \tag{3.15}$$

Thus, in this special case, we obtain the well-known relation between the compressibility and the polarization operator for $\mathbf{q} = 0$, which is usually obtained by an entirely different method.[9]

For the case of interest to us in the problem of the sound of the multipole $\Gamma^{(3)}(\mathbf{K}, -\mathbf{K}, 0)$, we have

$$\Gamma^{(3)}(\mathbf{K},-\mathbf{K},0)=\frac{1}{6}\frac{1}{\varepsilon(0)}\frac{d}{d\mu}\frac{\Pi(\mathbf{K})}{\varepsilon(\mathbf{K})}. \tag{3.16}$$

Using (3.12) twice in succession, we find another multipole

$$\Gamma^{(4)}(\mathbf{K},-\mathbf{K},0,0)=-\frac{1}{24}\frac{1}{\varepsilon(0)}\frac{d}{d\mu}\left[\frac{1}{\varepsilon(0)}\frac{d}{d\mu}\frac{\Pi(\mathbf{K})}{\varepsilon(\mathbf{K})}\right]. \tag{3.17}$$

Putting $\mathbf{K} = 0$ in these expressions, we obtain multipoles which are important for the anharmonic problem in a metal (for anharmonism of third and fourth orders, respectively),

$$\Gamma^{(3)}(0,0,0)=\frac{1}{6}\frac{1}{(\varepsilon(0))^3}\frac{d\Pi(0)}{d\mu}=\frac{1}{6}\frac{1}{(\varepsilon(0))^3}\frac{d^2n_0}{d\mu^2} \tag{3.18}$$

and

$$\Gamma^{(4)}(0,0,0,0)=\frac{1}{8}\frac{1}{(\varepsilon(0))^4}\left[\frac{1}{\Pi(0)}\left(\frac{d\Pi(0)}{d\mu}\right)^2-\frac{1}{3}\frac{d^2\Pi(0)}{d\mu^2}\right], \tag{3.19}$$

Thus, in all cases of interest to us, the multipoles can be expressed only in terms of the polarization operator and its derivatives with respect to the chemical potential. The expression for the elastic moduli contains the vector derivative of the multipole $F^\alpha(\mathbf{K})$ (2.10). We shall show that this quantity can also be reduced to the derivative of the polarization operator.

For the transformation of (2.10), we first make use of the fact that for any multipole one can carry out partial summation, making all the lines of the external field heavy:[2]

$$\Gamma^{(n)}(\mathbf{q}_1,\dots,\mathbf{q}_n)=\frac{\Lambda^{(n)}(\mathbf{q}_1,\dots,\mathbf{q}_n)}{\varepsilon(\mathbf{q}_1)\dots\varepsilon(\mathbf{q}_n)}. \tag{3.20}$$

Here $\Lambda^{(n)}$ is a multipole which no longer has blocks (polarization parts), which could refer to lines of the external field. If we transform Eq. (2.10) with the aid of (3.20), then it is easy to see that the differentiation of $V_q/\epsilon(q)$ gives a zero contribution to $F^\alpha(\mathbf{K})$ as $\mathbf{q} \to 0$, and consequently,

$$F^\alpha(\mathbf{K})=\left(\frac{V_\mathbf{q}}{\varepsilon(\mathbf{q})}\right)_{\mathbf{q}\to0}\left\{\frac{\partial}{\partial q^\alpha}\frac{\Lambda^{(3)}(\mathbf{K},-\mathbf{K}-\mathbf{q},\mathbf{q})}{\varepsilon(\mathbf{K})\varepsilon(\mathbf{K}+q)}\right\}_{\mathbf{q}\to0}. \tag{3.21}$$

For the multipole $\Lambda^{(3)}$, the following relation can be established:

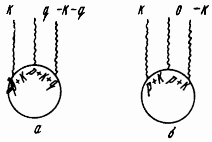
$$\left\{\frac{\partial}{\partial q^\alpha}\Lambda^{(3)}(\mathbf{K},-\mathbf{K}-\mathbf{q},\mathbf{q})\right\}_{\mathbf{q}\to0}=\frac{1}{2}\frac{\partial}{\partial K^\alpha}\Lambda^{(3)}(\mathbf{K},-\mathbf{K},0). \tag{3.22}$$

This solves our problem, inasmuch as we have, by using (3.16), (3.21), (3.22):

$$F^\alpha(\mathbf{K})=\frac{1}{12}\frac{1}{\Pi(0)}\frac{\partial}{\partial K^\alpha}\frac{d}{d\mu}\frac{\Pi(\mathbf{K})}{\varepsilon(\mathbf{K})}. \tag{3.23}$$

(We have substituted the limiting values for V_q and $\epsilon(q)$ in (3.21)). The result for (3.22) can be obtained by analyzing the set of diagrams corresponding to the left and right sides of this relation.

As an example, we consider the simplest diagrams:



(3.24)

To these diagrams correspond the analytic expressions

$$\int \frac{d^4p}{(2\pi)^4} G(p)G(p+K)G(p+K+q), \tag{3.25a}$$

$$\int \frac{d^4p}{(2\pi)^4} G(p)G(p+K)G(p+K). \tag{3.25b}$$

Carrying out differentiation in (3.25a) with respect to q, and in (3.25b) with respect to **K**, and transforming to the limit q → 0, we immediately establish the validity of (3.22). In a similar way, we can consider also diagrams of more complicated form.

4. LONGITUDINAL SOUND IN METALS

The relations obtained in the previous paragraph permit us to represent the expression for the elastic modulus C_{11} (or the longitudinal sound velocity associated with it) in closed form. For this purpose, we first note that inasmuch as $dn_0/d\mu = \Pi(0)$ (see (3.14)), the identities (3.16), (3.17) and (3.23) can conveniently be written with the help of the derivatives with respect to the electron density. We obtain

$$\Gamma^{(3)}(\mathbf{K}, -\mathbf{K}, 0) = \frac{1}{6}\frac{\Pi(0)}{\varepsilon(0)}\frac{\partial}{\partial n_0}\frac{\Pi(\mathbf{K})}{\varepsilon(\mathbf{K})}, \tag{4.1}$$

$$\Gamma^{(4)}(\mathbf{K}, -\mathbf{K}, 0, 0) = -\frac{1}{24}\left(\frac{\Pi(0)}{\varepsilon(0)}\right)^2 \frac{\partial^2}{\partial n_0^2}\frac{\Pi(\mathbf{K})}{\varepsilon(\mathbf{K})}, \tag{4.2}$$

$$F^{\alpha}(\mathbf{K}) = \frac{1}{12}\frac{\partial}{\partial K^{\alpha}}\frac{\partial}{\partial n_0}\frac{\Pi(\mathbf{K})}{\varepsilon(\mathbf{K})}. \tag{4.3}$$

Here we have taken it into account that the quantity $\Pi(0)/\epsilon(0)$ does not depend on n_0. Everywhere, expressions for the zero wave vector are understood in the limiting sense q → 0 (see Sec. 3).

Substituting (4.1)–(4.3) in (2.19) we get

$$C_{11} = \frac{n_0^2}{\Pi(0)} + \frac{2bn_0}{\Omega_0} + \frac{1}{\Omega_0}\sum_{\mathbf{K}\neq 0}\Big[\varphi(\mathbf{K}) + \frac{2}{3}K^{\alpha}\varphi^{\alpha}(\mathbf{K}) + \frac{1}{2}(K^x)^2\varphi^{xx}(\mathbf{K})\Big] - \sum_{\mathbf{K}\neq 0}\Big[2n_0|V_{\mathbf{K}}|^2\frac{\partial}{\partial n_0}\frac{\Pi(\mathbf{K})}{\varepsilon(\mathbf{K})} + \frac{1}{3}n_0K^{\alpha}\frac{\partial}{\partial K^{\alpha}}\Big(|V_{\mathbf{K}}|^2\frac{\partial}{\partial n_0}\frac{\Pi(\mathbf{K})}{\varepsilon(\mathbf{K})}\Big) + \frac{1}{2}n_0^2|V_{\mathbf{K}}|^2\frac{\partial^2}{\partial n_0^2}\frac{\Pi(\mathbf{K})}{\varepsilon(\mathbf{K})}\Big]. \tag{4.4}$$

Expression (4.4) gives the final result for the longitudinal sound velocity in metals with account of the many-particle interaction with accuracy to $(V_K/\epsilon_F)^2$ inclusively.

The first term in (4.4) describes the contribution from a continuous medium (**K** = 0). In this case, if we take the simplest approximation of the self-consistent field or the random phase method,[9] then this term leads to the well-known Bohm-Staver result[10] for the longitudinal speed of sound. This expression is also obtained in the popular "jelly" model, in which both the electrons and the ions are regarded as spread out with uniform density. However, in actuality, even very simple metals give results for the longitudinal sound velocity that differ greatly from those of the "jelly" model. Even the second term, which is associated with the nonpointlike nature of the ion, gives a much larger contribution to the sound (for more details see[11]). The same applies also to the contribution due to the discrete ion lattice (the first term in $\varphi(\mathbf{K})$ and its derivatives, see (2.17)). The role of indirect interaction between ions through the conduction electrons, described by the third and fourth terms of (4.4), changes greatly from metal to metal. However, it is important that in all cases the contribution from both terms is of the same order. This means that the terms arising from the non-pair interaction play as important a role as the terms arising from pair interaction $E^{(2)}$. Therefore, in particular, any representation operating on purely pair interaction inherently contains an incorrect description of the acoustic region and, along with this, of the phonon spectrum for the entire phase volume.

Equation (4.4) depends only on the Fourier component of the pseudopotential and the polarization operator $\Pi(q)$ of the electron gas. Here it is necessary to know the value of these quantities only at the discrete points of the sites of the reciprocal lattice. The values of V_K, at any rate for the most important first coordination spheres of the reciprocal lattice, can be determined with sufficient reliability for most of the nontransition elements, especially for extracting independent information, particularly on the measurement of the electron spectrum. The electron-ion interaction also enters into (4.4) through the quantity b, which is the mean value of the non-Coulomb part of the pseudopotential (see (2.18)). This quantity can be found with comparatively high accuracy from any form of the model of the pseudopotential verified experimentally. In particular, we can use the pseudopotential model of Henie and Abarenkov.[12,1]

For the determination of the polarization operator, we can use the usual approximation for $\Pi(q)$ (see, for example,[9,3]), but with the inapplicable condition that $\Pi(0)$ ought to satisfy the relation (3.15). It is natural that this also refers to the $\Pi(0)$, which enters in explicit form in (4.4). We note that the compressibility of the electron gas is computed with sufficient accuracy, as direct analysis shows.

Thus, there is every reason for assuming that by using (4.4) one can determine the velocity of longitudinal sound quite reliably for most nontransition metals.

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