

$$\begin{aligned}
t_m^n &= \frac{16\pi}{V\omega} \frac{1}{\Gamma_n^* |\mu^*|} \left( \frac{2}{3} \frac{|\mu^*| \varphi_s^2 r_c^3}{T} \right)^{1/2} \left( \frac{2}{3} \frac{|\mu^*| \varphi_s}{|h|} \right)^2 \\
&\times \exp \left[ \frac{128\pi}{9} \frac{|\mu^*| \varphi_s^2 r_c^3}{T} \left( \frac{2}{3} \frac{|\mu^*| \varphi_s}{|h|} \right)^2 \right], \\
t_m^c &= \frac{32\pi}{V\omega} \frac{c^*}{\Gamma_c^* |\mu^*|^2} \left( 2 \frac{|\mu^*| \varphi_s^2 r_c^3}{T} \right)^{1/2} \left( \frac{2}{3} \frac{|\mu^*| \varphi_s}{|h|} \right)^3 \\
&\times \exp \left[ \frac{128\pi}{9} \frac{|\mu^*| \varphi_s^2 r_c^3}{T} \left( \frac{2}{3} \frac{|\mu^*| \varphi_s}{|h|} \right)^2 \right].
\end{aligned} \tag{60}$$

When moving along the line  $s = \text{const}$ , the scale-invariant argument of the exponential remains unchanged. The change of  $t_m$  is determined by the scale non-invariant factor in the preexponential multiplier. In the case of a system with nonconserving parameter, this is the factor  $\Gamma_n^* |\mu^*| (|\mu^*| \sim |\tau| \gamma)$ , the renormalized kinetic coefficient is  $\Gamma_n^* \sim |\tau| \gamma$ , and then

$$\begin{aligned}
t_m^n &= \text{const} \cdot |\tau|^{-(\gamma+\Delta_r)} p^{1/2}(s) \left( \frac{R_c}{r_c} \right)^2 \exp \left[ \frac{128\pi}{9} p(s) \left( \frac{R_c}{r_c} \right)^2 \right], \\
\Delta_r &= \frac{6\eta \ln^{1/2}}{\nu}.
\end{aligned} \tag{61}$$

In the case of a conserved transition parameter the kinetic coefficient  $\Gamma_c^*$  is not renormalized, and  $c^* \sim |\tau| \gamma^{-2\nu}$ ; this yields

$$t_m^c = \text{const} \cdot |\tau|^{-(\gamma+2\nu)} p^{1/2}(s) \left( \frac{R_c}{r_c} \right)^3 \exp \left[ \frac{128\pi}{9} p(s) \left( \frac{R_c}{r_c} \right)^2 \right]. \tag{62}$$

In the strong-fluctuation region, the average lifetime of the metastable state has a definite scale dimensionality that depends on the conservation properties of the relaxing system, and the critical exponent  $t_m$  is determined by formulas (61) and (62).

A variant of nucleation theory, based on the ZV ideas, was developed by Langer,<sup>10</sup> who made concrete assumptions concerning the form of the coefficients in expressions of the type (47). These assumptions, which do not influence the form of the universal exponential factor, yield for the pre-exponential factor expressions that differ from those obtained in the present paper.

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## Microscopic-theory equations of the dynamics of an electron-ion system of a metal

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The equations of the dynamics of an electron-ion system in a nontransition metal with a simple anisotropic lattice are derived on the basis of the electron and ion Hamiltonian and with account taken of the scattering of the electrons by the impurities. In the quasiclassical long-wave approximation the equations reduce to the elasticity equations for the lattice and to the kinetic equation for the electrons. Microscopic expressions are derived in terms of the pseudopotential of the deformation-potential tensor and the bare elastic moduli of the lattice. It is shown that under adiabatic and neutrality conditions the long-wave oscillations in the metal can be described by the Fröhlich Hamiltonian.

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### 1. INTRODUCTION

Two essentially different approaches are presently used for the theoretical description of those electronic properties of metals which are connected with deformations of the crystal lattice. One of them, most widely used in the theory of metals, is in essence phenomenological. It is based, on the one hand, on the notion that electrons are quasiparticles with a complicated dispersion law<sup>1-3</sup> that applies to the particular crystal lattice.

On the other hand, this approach postulates the existence in the metal of "bare" phonons that do not interact with the electrons, and of corresponding "bare" elastic moduli of the metal  $\lambda_{ikim}$ . The interaction of the electrons with the phonons is the result of the change of the electron energy under the influence of the lattice deformation. This interaction is described with the aid of a deformation potential first introduced by Akhiezer.<sup>4</sup> In a strong magnetic field, an induction interaction exists besides the deformation interaction.<sup>5,6</sup> The the-

ory of the joint motion of the conduction electrons in the crystal lattice, obtained from these concepts, was developed in the absence and in the presence of a magnetic field by many workers.<sup>7-20</sup> The system of equations that describe the motion, in the lattice, of electrons that interact with one another was first written out by Silin,<sup>11</sup> and the theory was subsequently developed in the papers of Kontorovich<sup>12</sup> and Skobov and Kaner.<sup>14</sup> The use of these equations for the investigation of quantum and spin waves in metals and in a magnetic field is contained in the papers of Zyryanov, Okulov, and Silin.<sup>17-19</sup> The very length of the list of references indicates that over more than 20 years the phenomenological theory served as the basic tool for the investigation of a great variety of properties of metals.

It should be noted, however, that the equations of this theory were never derived "from first principles." Within the framework of the phenomenological theory it is impossible to explain the microscopic nature of the concepts of bare elastic moduli and a bare deformation potential. For this reason, such a theory does not permit a theoretical calculation of these quantities and does not make it possible to establish their dependence on external conditions, particularly on the magnetic field. In addition, the region of applicability of the phenomenological equations is limited to large wavelengths.

The second, microscopic approach known in metal theory starts from the concept of the metal as an aggregate of ions, located at the sites of a crystal lattice, and mobile electrons. The electrons interact with the ions both via electromagnetic forces and via scattering from the ion shells. This method dates back historically to the first papers of Bloch<sup>21</sup> and Sommerfeld and Bethe.<sup>22</sup> The electron-ion model of a metal proposed by them was subsequently actively investigated.<sup>23-31</sup> The interest in the electron-ion model was subsequently decreased because of the appearance of the phenomenological theory.

The research within the framework of the electron-ion theory was continued by Brovman and Kagan<sup>32,33</sup> in connection with the problem of the microscopic calculation of the singularities of the phonon spectrum of metals. A consistent study of this question on the basis of the phenomenological theory is impossible. The main reason is that it is impossible to separate consistently in the metal the noninteracting phonons and electrons. The point is that it is automatically implied that electrons take part in the formation of all bare phonons.<sup>33</sup> The artificial introduction of bare phonons makes the phenomenological theory (more accurately, the Fröhlich model) inapplicable in a number of cases, particularly in a quantizing magnetic field.<sup>34</sup> Difficulties arise when this theory is used to describe the properties of conductors with less than three dimensions.

Besides the study of singularities of the phonon spectrum of metals, the microscopic theory was used to investigate the thermal and electric resistances of metals.<sup>35</sup> The theory was also successfully used in the problem of lattice stability.<sup>36,37</sup> These investigations cover in the main, for the time being, the region of ap-

plication of the microscopic approach in the theory of normal metals. With one exception,<sup>34</sup> this method has not been used so far to investigate the properties of metals in a magnetic field.

Thus, use is made at present of two actually unrelated approaches that stem from substantially different ideas concerning the electron-ion system of the metal. The phenomenological approach is widely used by meets in a number of aspects with objections, due to the lack of a rigorous foundation for the procedure for separating the bare phonons and electrons. On the other hand, the existing microscopic theory, owing to its relative complexity, has apparently not yet been sufficiently well developed to permit its application to as large a group of problems as the phenomenological theory.

The purpose of the present paper is to overcome the disparity between these two approaches. To compare them it is necessary to derive for the electrons and ions of the metal equations of motion of the same type as the equations of the phenomenological theory, by starting from the Hamiltonian of the microscopic theory. In this way it would become possible to determine the microscopic gist and obtain constructive expressions for the bare elastic moduli of the metal and for the deformation potential.

In Sec. 2 is derived the Hamiltonian of the electron-ion system of the metal. The quantization is over the Bloch states of the electrons in the periodic field of the crystal. In Sec. 3 we introduce a dissipative mechanism, which we choose to be the collisions of the electrons with the impurities; Heisenberg equations of motion averaged over the positions of the impurities are derived for an arbitrary operator. In Sec. 4, in the gas approximation, the equations of the dynamics of the metal are obtained for an arbitrary wavelength of frequency. It is important that for the Bloch electrons even the gas approximation makes it possible to take into account a short-range interaction of the Fermi-liquid type between the electrons. Finally, in the last section, a limiting transition is made to the quasiclassical situation, and long-wave approximations are obtained of the same type as the known equations of the phenomenological theory; the relation of the obtained results to the standard theory is discussed.

## 2. HAMILTONIAN OF THE ELECTRONS AND IONS IN THE CRYSTAL

In accordance with the principal premises of the microscopic theory, we assume that the considered transition metal consists of lattice ions and mobile electrons. Vortical electromagnetic motion will be disregarded for only one reason, to shorten the discussion. We assume that in the ground state of the metal the ions are located at the sites of an anisotropic Bravais lattice containing one ion per unit cell. Let there be in a volume  $V$ , a total of  $N$  ions with charge  $-Z$ , with  $e < 0$  and  $Z$  an integer. The total number of electrons is  $ZN$ , and the charge of one electron is  $e$ .

The Hamiltonian  $H$  of such a system is of the form

$$H = \frac{1}{2m_0} \sum_{\alpha} p_{\alpha}^2 + \frac{1}{2M} \sum_i P_i^2 + \sum_{i,\alpha} \Phi(r_{\alpha} - R_i) + \frac{1}{2} \sum_{\alpha \neq \beta} \frac{e^2}{|r_{\alpha} - r_{\beta}|} + \frac{1}{2} \sum_{i \neq j} \frac{Z^2 e^2}{|R_i - R_j|} + \frac{1}{2} \sum_{i \neq j} g(R_i - R_j). \quad (2.1)$$

Here  $r_{\alpha}$  and  $p_{\alpha}$  are the radius vector and the momentum of the mobile electron numbered  $\alpha$ , with mass  $m_0$  and charge  $e$ ;  $R_i$  and  $P_i$  are the coordinates and momentum of the ion numbered  $i$ , with mass  $M$  and charge  $-Ze$ ;  $g(R_i - R_j)$  is the part of the energy of the direct interaction of the ions, connected with the repulsion of the ion shells;  $\Phi(r_{\alpha} - R_i)$  is the energy of the interaction of the electron with the ion (pseudopotential). Planck's constant is assumed equal to unity throughout.

We are interested next only in small oscillations of the ions about the stable equilibrium position. Connected with these small oscillations are small changes of the electron density. The constant external magnetic field is assumed in the derivation to be zero; it will be taken into account in the final equations.

The purpose being to derive linearized equations of motion, we expand the Hamiltonian (2.1) in a series in the small displacements  $\delta R_i = R_i - R_{i0}$  of the ions from the equilibrium positions  $R_{i0}$ , and write, accurate to terms quadratic in  $\delta R$ :

$$H = \frac{1}{2m_0} \sum_{\alpha} p_{\alpha}^2 + \sum_{i,\alpha} \Phi(r_{\alpha} - R_{i0}) + \frac{1}{2M} \sum_i P_i^2 + \frac{1}{2} \sum_{i,j} \delta R_i \hat{\alpha}_{ij} \delta R_j - \sum_{i,\alpha} (\delta R_i \nabla) \Phi(r_{\alpha} - R_{i0}) + \frac{1}{2} \sum_{\alpha \neq \beta} \frac{e^2}{|r_{\alpha} - r_{\beta}|} + \frac{1}{2} \sum_{i,\alpha} (\delta R_i \nabla) (\delta R_i \nabla) \Phi(r_{\alpha} - R_{i0}), \quad (2.2)$$

where the force matrix  $\hat{\alpha}_{ij}$  is due to the expansion of the energy of the direct ion-ion interaction; the linear term of this expansion is equal to zero because of the symmetry of the lattice.<sup>33</sup> The employed expansion is based on an analysis, carried out by Brovman and Kagan<sup>33</sup> of the ground state of the metal.

We express the obtained equation (2.2) in terms of elementary excitations that exist in the metal-conduction electrons and lattice vibrators. Accurate to terms quadratic in the amplitude of the vibrations we have

$$H = \sum_{sp} \varepsilon_{sp} a_{sp}^{\dagger} a_{sp} + \sum_{q\sigma} \omega_{q\sigma} b_{q\sigma}^{\dagger} b_{q\sigma} + \sum_{s',spq\sigma} V_{q\sigma}^{s's}(p) (2MN\omega_{q\sigma})^{-1/2} (b_{q\sigma} + b_{-q\sigma}^{\dagger}) a_{s',p+\mathbf{q}}^{\dagger} a_{sp} + \frac{1}{2V} \sum_{\substack{s',s'',s',s'' \\ p',p''\mathbf{q}}} u_{s',s'',s',s''}(p',p,\mathbf{q}) a_{s',p'+\mathbf{q}}^{\dagger} a_{s'',p-\mathbf{q}}^{\dagger} a_{s',p} a_{s'',p} + \frac{1}{2} \sum_{p\mathbf{q}\sigma,\sigma'} u_{q\sigma, \mu - q\sigma} e_{\sigma'}^{\dagger}(\mathbf{q}) e_{\sigma'}(-\mathbf{q}) a_{sp}^{\dagger} a_{sp} \left\langle sp \left| \frac{\partial^2 U}{\partial x_i \partial x_j} \right| sp \right\rangle. \quad (2.3)$$

The first line of this formula contains the energies of the Bloch electrons and of the lattice vibrations of the ion lattice. Here  $a_{sp}^{\dagger}$  and  $a_{sp}$  are the Fermi creation and annihilation operators for an electron with quasimomentum  $p$  and energy  $\varepsilon_{sp}$  in the band with number  $s$ , in a state a Bloch wave function  $V^{-1/2} \psi_{sp}(\mathbf{r})$ . The energy  $\varepsilon_{sp}$  and the function  $\psi_{sp}(\mathbf{r})$  are connected by the eigenvalue

equation

$$\left\{ \frac{1}{2m_0} p^2 + U(\mathbf{r}) \right\} \psi_{sp}(\mathbf{r}) = \varepsilon_{sp} \psi_{sp}(\mathbf{r}), \quad U(\mathbf{r}) = \sum_i \Phi(\mathbf{r} - R_{i0}), \quad (2.4)$$

with  $\psi_{sp}(\mathbf{r})$  normalized by the condition

$$\int d\mathbf{r} \psi_{s',p'}^{\dagger}(\mathbf{r}) \psi_{sp}(\mathbf{r}) = V \delta_{s',s} \delta_{p',p}. \quad (2.5)$$

We do not take into account here the electron spin. We denote next by  $b_{q\sigma}^{\dagger}$  and  $b_{q\sigma}$  the Bose creation and annihilation operators of a lattice vibration with quasiwave vector  $q$ , frequency  $\omega_{q\sigma}$ , and polarization vector  $e_{\sigma}(\mathbf{q})$  in the branch with number  $\sigma = 1, 2, \text{ or } 3$ . The frequency and the wave vector satisfy the equation<sup>38</sup>

$$\omega_{q\sigma}^2 e_{\sigma'}(\mathbf{q}) = \omega_{ip}^2 \frac{q_i q_k}{q^2} e_{\sigma'}^k(\mathbf{q}) + \alpha_{ik}(\mathbf{q}) e_{\sigma'}^k(\mathbf{q}), \quad (2.6)$$

where

$$\alpha_{ik}(\mathbf{q}) = \frac{n}{M} \sum_{B \neq 0} \{ A(\mathbf{q} + \mathbf{B}) (q_i + B_i) (q_k + B_k) - A(\mathbf{B}) B_i B_k \} + \frac{n}{M} g(\mathbf{q}) q_i q_k, \quad n = \frac{N}{V}. \quad (2.7)$$

Summation over the dummy indices is implied in these relations.  $\mathbf{B}$  is the reciprocal-lattice vector,  $\omega_{ip}$  is the plasma frequency of the ions,  $A(\mathbf{k})$  is the Fourier component of the direct ion-ion interaction:

$$A(\mathbf{k}) = \frac{4\pi Z^2 e^2}{k^2} + g(\mathbf{k}). \quad (2.8)$$

By  $u_{q\sigma}$  we denote in (2.3) the amplitude of the Fourier displacement of the ions:

$$\delta R_i = \sum_{q\sigma} u_{q\sigma} e_{\sigma}(\mathbf{q}) \exp(i\mathbf{q}R_{i0}), \quad u_{q\sigma} = (2MN\omega_{q\sigma})^{-1/2} (b_{q\sigma} + b_{-q\sigma}^{\dagger}). \quad (2.9)$$

The second line of (2.3) contains the energy of the electron-lattice interaction. The matrix element  $V_{q\sigma}^{s's}(\mathbf{p})$  is defined by the formulas

$$V_{q\sigma}^{s's}(\mathbf{p}) = e_{\sigma'}^k(\mathbf{q}) V_{q\sigma}^{s's}(p), \quad V_{q\sigma}^{s's}(p) = -n \int d\mathbf{r} \psi_{s',p+\mathbf{q}}^{\dagger}(\mathbf{r}) \frac{\partial \Phi(\mathbf{r})}{\partial x_i} \psi_{sp}(\mathbf{r}) \quad (2.10)$$

and can be represented in the form

$$V_{q\sigma}^{s's}(p) = iq_n \frac{4\pi e^2 Z}{q^2} M_p^{s's}(\mathbf{q}) + \xi_{q\sigma}^{s's}(p), \quad (2.11)$$

where

$$\xi_{q\sigma}^{s's}(p) = i(e_{\sigma',p+\mathbf{q}} - e_{\sigma,p}) n \int d\rho w_{s',p+\mathbf{q}}(\rho) (-i\nabla_i) w_{s,p}(\rho) + \zeta_{q\sigma}^{s's}(p). \quad (2.12)$$

In turn

$$\zeta_{q\sigma}^{s's}(p) = \frac{iq_k}{m_0} n \int d\rho w_{s',p+\mathbf{q}} \frac{\partial^2 w_{sp}}{\partial \rho_i \partial \rho_k} - \frac{iq_k}{m_0} \left( p_k + \frac{q_k}{2} \right) n \int d\rho w_{s',p+\mathbf{q}} (-i\nabla_i) w_{s,p} - iq_n \left( \Phi(\mathbf{q}) + \frac{4\pi e^2 Z}{q^2} \right) M_p^{s's}(\mathbf{q}) - in \sum_{B \neq 0} M_p^{s's}(\mathbf{q} + \mathbf{B}) \{ (q_i + B_i) \Phi(\mathbf{q} + \mathbf{B}) - B_i \Phi(\mathbf{B}) \}, \quad (2.13)$$

where  $\Phi(\mathbf{k})$  is the Fourier component of the pseudopotential, and we have introduced the amplitude  $w_{sp} = \exp(-i\mathbf{p}\mathbf{r}) \psi_{sp}$  of the Bloch wave function, normalized by the condition

$$n \int d\rho w_{s',p'} w_{sp} = \delta_{s',s}. \quad (2.14)$$

the vector  $\rho$  varies within the limits of one unit cell of the crystal lattice.

The quantity  $M_p^{s's}(\mathbf{q})$  in (2.11) is the matrix element of

a plane wave in the Bloch functions:

$$M_p^{s's}(\mathbf{k}) = n \int d\rho \psi_{p+\mathbf{k}}^*(\rho) e^{-i\mathbf{k}\rho} \psi_p(\rho); \quad (2.15)$$

the quantity  $M_p^{s's}(\mathbf{k})$  is used to express the fluctuations of the electron density  $\rho_k$ :

$$\rho_k = \frac{1}{V} \sum_{\alpha} \exp(-i\mathbf{k}\alpha) = \frac{1}{V} \sum_{s',s} M_p^{s's}(-\mathbf{k}) a_{s',p-\mathbf{k}}^+ a_{s,p}. \quad (2.16)$$

We note that  $V_{qs}^{s's}(\mathbf{p})$  is a periodic function, with the period of the reciprocal lattice, of the variables  $\mathbf{p}$  and  $\mathbf{q}$ , whereas  $M_p^{s's}(\mathbf{k})$  is periodic in  $\mathbf{p}$  but has a nonperiodic dependence on  $\mathbf{k}$ .

The quantity  $\xi_{ps}^{s's}(\mathbf{p})$  describes the influence of the microscopic fields produced by the lattice deformation on the electron-ion interaction. At  $s = s'$  the roles of the first and second terms in (2.12) are the same. On the other hand, if  $s \neq s'$ , then the first term describes that part of the microscopic field in the metal which is responsible for the effects of electron dragging by the lattice.

The third line of (2.3) contains the energy of the direct interelectron interaction. The matrix element  $\nu_{s'ss_1s_1}(\mathbf{p}', \mathbf{p}, \mathbf{q})$  is equal to

$$\nu_{s'ss_1s_1}(\mathbf{p}', \mathbf{p}, \mathbf{q}) = \frac{4\pi e^2}{q^2} M_p^{s's}(\mathbf{q}) M_p^{s_1s_1}(-\mathbf{q}) + K_{pp}^{s'ss_1s_1}(\mathbf{q}), \quad (2.17)$$

where

$$K_{pp}^{s'ss_1s_1}(\mathbf{q}) = 4\pi e^2 \sum_{\mathbf{B} \neq 0} (\mathbf{q} + \mathbf{B})^{-2} M_p^{s's}(\mathbf{q} + \mathbf{B}) M_p^{s_1s_1}(-\mathbf{q} - \mathbf{B}). \quad (2.18)$$

The last term in the Hamiltonian (2.3) describes the contribution of the pseudopotential to the direct interaction between the ions; this term in (2.3) stems from the last term in (2.2). The angle brackets denote the matrix element in the Bloch wave functions.

The Hamiltonian (2.3) takes complete account of all the umklapp processes. The summations over all the momentum variables are carried out independently, within the limits of the first Brillouin zone, and each term of the sum is a periodic function of these variables with the period of the reciprocal lattice.

### 3. INTRODUCTION OF THE DISSIPATIVE MECHANISM

Our purpose is to obtain for the system with the Hamiltonian (2.3) dynamic equations that constitute the analog of the equations of the phenomenological theory. These include the equations of the theory of elasticity of the lattice with allowance for the electromagnetic forces and for the electrons contained in the lattice, the kinetic equation for the electrons, and the equations of the electromagnetic field. The following circumstances must be borne in mind in the derivation.

At metallic densities, the interaction between the conduction electrons is not weak. Therefore, as is well known, an important role is played in the metal by Fermi-liquid effects. A consistent derivation of all the required equations with account taken of the Fermi-liquid interaction is possible only by using a diagram technique. This, however, would lead to unjustifiably

cumbersome derivations without contributing anything essential to the understanding of the processes that occur. In fact, the connection between the kinetic equation for the electrons, written in the gas approximation, with the similar equation with account taken of the Fermi-liquid interaction is well known.<sup>1-3</sup> Equally well known, from the Landau theory,<sup>39</sup> is the influence of the Fermi liquid on the propagation of elastic oscillations in it. Therefore, to avoid unnecessary complications, we confine ourselves to a derivation of the equations of the dynamics of the metal in the gas approximation. It is important that, for Bloch electrons, even this approximation makes it possible to take into account the short-range interaction of the electrons and to obtain the Landau correlation function in the Born approximation.

The second remark is connected with the fact that a complete comparison with the results of the phenomenological theory is possible only when account is taken of the dissipative collisional mechanisms. No such mechanisms are contained as yet in the Hamiltonian (2.3) in the form needed by us, although of course Eq. (2.3) does take into account the collisions of the electrons with the phonons, etc. The point is that the system with the Hamiltonian (2.3) is regarded as closed, and dynamic equations containing no collision terms will be written for it. To take these terms explicitly into account in the equations, we introduce, by way of the dissipative mechanism, the collisions of the electrons with the impurities.

Assume that the metal contains only substitutional impurities, randomly located on some of the lattice sites, which we shall designate by  $\mathbf{R}_{10}$ . The concentration  $c$  of the impurities will be assumed to be small enough to be able to use an approximation linear in the concentration. The energy of the interaction of the electron with the impurities will be designated by  $\mathcal{U}(\mathbf{r} - \mathbf{R}_i)$ . We assume this interaction to be sufficiently weak and carry out the calculations in the Born approximation. It can be shown that in the general case of  $\mathcal{U}$  that are not small the final formulas will contain in place of the Born scattering amplitude the true amplitude, and the result expressed in terms of the collision integral will turn out to be valid also in the general case. We shall also neglect in the derivation the interband transition of the electrons colliding with the impurities. Finally, we shall not stop to take into account here the contribution of the local oscillations to the scattering of the electrons by the impurities,<sup>40</sup> assuming that the impurities are such that no local and quasilocal oscillations occur. Thus, we assume that at each instant of time the impurity occupies the same position as the basic lattice ion would occupy at the site in which the impurity is located.

The Hamiltonian  $\mathcal{V}$  of the interaction of the electrons with the impurities

$$\mathcal{V} = \sum_{\alpha, i} \mathcal{U}(\mathbf{r}_{\alpha} - \mathbf{R}_i), \quad (3.1)$$

taken accurate to terms quadratic in the amplitude of the oscillations, will be written, omitting the index that labels the conduction band, in the form

$$\mathcal{Y} = \sum_{\alpha, l} \mathcal{U}(\mathbf{r}_\alpha - \mathbf{R}_{l0}) - \sum_{\alpha, l} (\delta \mathbf{R}, \nabla) \mathcal{U}(\mathbf{r}_\alpha - \mathbf{R}_{l0}) = \sum_{\mathbf{k}} Q_{\mathbf{k}} S(\mathbf{k}), \quad (3.2)$$

where  $Q_{\mathbf{k}} = Q_{\mathbf{k}}^{(1)} + Q_{\mathbf{k}}^{(2)}$  and

$$Q_{\mathbf{k}}^{(1)} = \sum_{\mathbf{p}} \mathcal{U}_{\mathbf{p}}(\mathbf{k}) a_{\mathbf{p}+\mathbf{k}}^+ a_{\mathbf{p}}, \quad Q_{\mathbf{k}}^{(2)} = - \sum_{\mathbf{p}, \mathbf{k}'} \mathcal{U}_{\mathbf{p}\sigma}(\mathbf{k}+\mathbf{k}') u_{\mathbf{k}'\sigma} a_{\mathbf{p}+\mathbf{k}+\mathbf{k}'}^+ a_{\mathbf{p}}. \quad (3.3)$$

Here

$$\mathcal{U}_{\mathbf{p}}(\mathbf{k}) = \sum_{\mathbf{B}} \mathcal{U}(\mathbf{k}+\mathbf{B}) M_{\mathbf{p}}(\mathbf{k}+\mathbf{B}), \quad (3.4)$$

$$\mathcal{U}_{\mathbf{p}\sigma}(\mathbf{k}) = \int d\mathbf{r} \psi_{\mathbf{p}+\mathbf{k}}^*(\mathbf{r}) (\nabla \mathcal{U}) \psi_{\mathbf{p}}(\mathbf{r}) e_{\sigma}(\mathbf{k}),$$

$\mathcal{U}(\mathbf{k})$  is the Fourier component of the potential of the interaction of the electron with the impurity, and we have introduced the structure factor of the impurities

$$S(\mathbf{k}) = \frac{1}{V} \sum_{\mathbf{I}} \exp(-i\mathbf{k}\mathbf{R}_{\mathbf{I}0}), \quad (3.5)$$

which is a function of the random configuration of the impurities.

The term with  $Q_{\mathbf{k}}^{(1)}$  in (3.2) describes the elastic scattering of the electrons by impurities, while the term with  $Q_{\mathbf{k}}^{(2)}$  describes the inelastic scattering of the electrons by the impurities with emission or absorption of phonons. Just as before, the summations in (3.3) are carried out within the limits of the first Brillouin zone. Thus, the total Hamiltonian of the system is represented by the sum  $H + \mathcal{Y}$  of expressions and (3.2) and is a function of the random parameters  $\mathbf{R}_{\mathbf{I}0}$ .

All the equations of the dynamics of the electron-ion systems of the metal can be obtained now in a unified manner as the Heisenberg equations of motion for the corresponding operators, averaged over the positions of the impurities. Averaging over the positions of the impurities will be designated by a superior bar:

$$\overline{(\dots)} = \frac{1}{N} \sum_{\{\mathbf{R}_{\mathbf{I}0}\}} (\dots), \quad (3.6)$$

where each variable  $\mathbf{R}_{\mathbf{I}0}$  runs through all the lattice sites in each sum.

We take an arbitrary operator  $F$ , pertaining to the system, and average the Heisenberg equation over the impurity positions

$$dF/dt = i[H + \mathcal{Y}, F]. \quad (3.7)$$

We represent the operator  $F$  in the form  $F = \bar{F} + \Delta F$ , where  $\Delta F$  is a random increment to the mean value  $\bar{F}$ . We change over in (3.7) to the interaction representation, choosing as the "unperturbed" Hamiltonian the operator  $H$ :

$$\mathcal{Y}(t) = e^{iHt} \mathcal{Y} e^{-iHt}, \quad Y(t) = e^{-iHt} F e^{iHt}, \quad Y(t) = \bar{Y}(t) + y(t), \quad (3.8)$$

and average the equation for  $Y(t)$

$$\frac{d\bar{Y}(t)}{dt} = i[\bar{\mathcal{Y}}(-t), \bar{Y}(t)] + i[\overline{\Delta \mathcal{Y}(-t)}, y(t)]. \quad (3.9)$$

It suffices to write down the equation  $y(t)$  accurate to terms linear in  $\Delta \mathcal{Y}$ :

$$\frac{dy(t)}{dt} = i[\Delta \mathcal{Y}(-t), \bar{Y}(t)]. \quad (3.10)$$

We substitute the solution of this equation, with the ini-

tial condition  $y(-\infty) = 0$ , in (3.9) and then return to the initial operator  $F$ . This yields an equation for the averaged operator  $\bar{F}$  (we shall now omit the superior bar):

$$\frac{d\bar{F}}{dt} = i[H + \bar{\mathcal{Y}}, \bar{F}] - \left( \frac{\partial \bar{F}}{\partial t} \right)_{\text{col}}, \quad (3.11)$$

where the collision term  $(\partial \bar{F} / \partial t)_{\text{col}}$  is

$$\left( \frac{\partial \bar{F}}{\partial t} \right)_{\text{col}} = \int_{-\infty}^t dt' \exp[-\varepsilon(t-t')] [\overline{\Delta \mathcal{Y}[\Delta \mathcal{Y}(t-t'), \bar{F}]}, \quad \varepsilon \rightarrow +0. \quad (3.12)$$

The operator  $\bar{\mathcal{Y}}$  in (3.11) leads to additive renormalization of the pseudopotential, which we shall disregard from now on.

Substituting in (3.11) the expression (3.2) for  $\mathcal{Y}$ , we calculate the correlator

$$\overline{s(\mathbf{k}_1) s(\mathbf{k}_2)} = \frac{c}{V} \delta_{\mathbf{k}_1, -\mathbf{k}_2}, \quad s(\mathbf{k}) = S(\mathbf{k}) - \bar{S}(\mathbf{k}), \quad \bar{S}(\mathbf{k}) = c \delta_{\mathbf{k}, 0}, \quad (3.13)$$

and write down the final expression for the collision term:

$$\left( \frac{\partial \bar{F}}{\partial t} \right)_{\text{col}} = \frac{c}{V} \sum_{\mathbf{k}} \int_0^{\infty} d\tau e^{-\varepsilon\tau} [Q_{-\mathbf{k}}[Q_{\mathbf{k}}(\tau), \bar{F}]], \quad \varepsilon \rightarrow +0. \quad (3.14)$$

Choosing  $F$  to be the operators contained in the Hamiltonian (2.3), we construct in the next section, with the aid of (3.11) and (3.14), all the necessary equations of the dynamics of the metal.

#### 4. EQUATIONS OF THE DYNAMICS OF THE ELECTRON-ION SYSTEM OF A METAL

Setting up the equations of motion entails the calculation of the collision terms in accordance with the rule (3.14). The corresponding operations are cumbersome and will not be described here. We present the results of the calculation of the linearized collision terms, neglecting in the kernel of the collision integral the influence of the inelasticity of the collisions, which leads to corrections of the order of  $(m_0/M)^{1/2} \ll 1$ .

Differentiating the displacement operator  $u_{\mathbf{q}\sigma}$  in accord with (3.11), we get

$$\frac{\partial u_{\mathbf{q}\sigma}}{\partial t} = \dot{u}_{\mathbf{q}\sigma} - \left( \frac{\partial u_{\mathbf{q}\sigma}}{\partial t} \right)_{\text{col}}. \quad (4.1)$$

We have denoted by  $\dot{u}_{\mathbf{q}\sigma}$  the operator

$$\dot{u}_{\mathbf{q}\sigma} = -i\omega_{\mathbf{q}\sigma} (2MN\omega_{\mathbf{q}\sigma})^{-1/2} (b_{\mathbf{q}\sigma} - b_{-\mathbf{q}\sigma}^{\dagger}) \quad (4.2)$$

of the velocity of the free ion lattice, which we distinguish from the derivative  $\partial u_{\mathbf{q}\sigma} / \partial t$ . The calculation of the collision term by formula (3.14) yields (we leave out the index of the band in the collision integral)

$$\left( \frac{\partial u_{\mathbf{q}\sigma}}{\partial t} \right)_{\text{col}} = - \frac{m_0^2}{MN} \sum_{\mathbf{p}} (v_{\mathbf{u}\mathbf{q}}) \frac{f(\varepsilon_{\mathbf{p}+\omega_{\mathbf{q}\sigma}}) - f(\varepsilon_{\mathbf{p}})}{\omega_{\mathbf{q}\sigma}} I_{\mathbf{p}}[\mathbf{v}] e_{\sigma}(-\mathbf{q}), \quad (4.3)$$

$$\mathbf{v} = \partial \varepsilon_{\mathbf{p}} / \partial \mathbf{p}.$$

Here  $f(\varepsilon_{\mathbf{p}}) \equiv f_{\mathbf{p}}$  is the equilibrium Fermi distribution function of the electrons with energy  $\varepsilon_{\mathbf{p}}$ , which is determined from the relation

$$e^{i\varepsilon_{\mathbf{p}}} a_{\mathbf{p}}^+ e^{-i\varepsilon_{\mathbf{p}}} = \exp(i\varepsilon_{\mathbf{p}} t) \bar{a}_{\mathbf{p}}^+ \quad (4.4)$$

and corresponds to the pole of the single-electron

Green's function for a system with Hamiltonian (2.3). In the quasiclassical situation  $\bar{\epsilon}_p$  can be obtained directly from the equations of motion. By  $I_p[\varphi_p]$  we denote the collision integral of the electrons with impurities, acting on any function  $\varphi_p$  in accordance with the rule

$$I_p[\varphi_p] = \frac{2\pi c}{V} \sum_k |\mathcal{U}_{p'}(k)|^2 \delta(\bar{\epsilon}_{p'} - \bar{\epsilon}_{p-k}) (\varphi_p - \varphi_{p-k}). \quad (4.5)$$

Differentiating (4.1) once more with respect to time, we obtain the analog of the equation of the lattice elasticity theory

$$\frac{\partial^2 u_{q\sigma}}{\partial t^2} = -\omega_{q\sigma}^2 u_{q\sigma} - \frac{1}{MN} \sum_{s s'} V_{-q\sigma}^{s's}(\mathbf{p}) a_{s'p-q}^+ a_{s\mathbf{p}} \quad (4.6)$$

$$- \frac{\partial}{\partial t} \left( \frac{\partial u_{q\sigma}}{\partial t} \right)_{\text{col}} - \left( \frac{\partial \dot{u}_{q\sigma}}{\partial t} \right)_{\text{col}} - \sum_{s p_0} u_{q\sigma} e_{\sigma i}(\mathbf{q}) e_{\sigma j}(-\mathbf{q}) f_{s\mathbf{p}} \left\langle s\mathbf{p} \left| \frac{\partial^2 U}{\partial x_i \partial x_j} \right| s\mathbf{p} \right\rangle.$$

In the calculation of the first term of the second line of (4.6) it suffices to differentiate the vector  $u_{q\sigma}$  in (4.3) in accordance with (4.1), discarding in the latter the collision term, which contains the large ion mass in the denominator. For the next-to-last term in the right-hand side of (4.6), calculation by formula (3.14) yields

$$\left( \frac{\partial \dot{u}_{q\sigma}}{\partial t} \right)_{\text{col}} = -\frac{m_0}{2MN} \sum_p \{ \widetilde{v_p I_p [a_{p-q}^+ a_p]} + \widetilde{v_{p-q} I_{p-q} [a_{p-q}^+ a_p]} \} e_{\sigma}(-\mathbf{q}), \quad (4.7)$$

where

$$\widetilde{a_{p-q}^+ a_p} = a_{p-q}^+ a_p - \frac{\partial f_p}{\partial \epsilon_p} (\bar{\epsilon}_p - \epsilon_p).$$

Equation (4.6) contains the electron operator  $a_{s'p-q}^+ a_{s\mathbf{p}}$ , which is the quantum analog of the Fourier component of the classical distribution function of the electrons over the momenta and coordinates. The deviation of the linearized equation of motion for the operator  $a_{s'p-q}^+ a_{s\mathbf{p}}$  is carried out by means of the same formulas (3.11) and (3.14). At  $s = s'$  we obtain the analog of the kinetic equation for the electrons

$$\begin{aligned} & \frac{\partial}{\partial t} a_{s'p-q}^+ a_{s\mathbf{p}} - i(\epsilon_{s'p-q} - \epsilon_{s\mathbf{p}}) a_{s'p-q}^+ a_{s\mathbf{p}} - i \sum_{\sigma} V_{-q\sigma}^{s's}(\mathbf{p}) u_{q\sigma} (f_{s\mathbf{p}} - f_{s'p-q}) \\ & - i(f_{s\mathbf{p}} - f_{s'p-q}) \frac{1}{V} \sum_{s_1 s_1'} v_{s s_1 s_1'}(\mathbf{p} - \mathbf{q}, \mathbf{p}_1, \mathbf{q}) a_{s_1'p_1-q}^+ a_{s_1 \mathbf{p}_1}, \\ & = -\frac{1}{2} I_{s\mathbf{p}} [\widetilde{a_{p-q}^+ a_p}] - \frac{1}{2} I_{s'p-q} [\widetilde{a_{p-q}^+ a_p}] - \frac{1}{2} m_0 \sum_{\sigma} \dot{u}_{q\sigma} e_{\sigma}(\mathbf{q}) \\ & \times \left\{ I_{s\mathbf{p}} [v_{s\mathbf{p}}] \frac{f(\bar{\epsilon}_{s\mathbf{p}} + \omega_{q\sigma}) - f(\bar{\epsilon}_{s\mathbf{p}})}{\omega_{q\sigma}} + I_{s'p-q} [v_{s'p-q}] \frac{f(\bar{\epsilon}_{s'p-q} + \omega_{q\sigma}) - f(\bar{\epsilon}_{s'p-q})}{\omega_{q\sigma}} \right\} \end{aligned} \quad (4.8)$$

Putting  $s' \neq s$ , we obtain the equation of the interband transitions:

$$\begin{aligned} & \frac{\partial}{\partial t} a_{s'p-q}^+ a_{s\mathbf{p}} - i(\epsilon_{s'p-q} - \epsilon_{s\mathbf{p}}) a_{s'p-q}^+ a_{s\mathbf{p}} \\ & = i(f_{s\mathbf{p}} - f_{s'p-q}) M_{s's}^{*s}(-\mathbf{q}) e_{\varphi} + i(f_{s\mathbf{p}} - f_{s'p-q}) \xi_{-qk}^{*s's}(\mathbf{p}) u_{qk} \\ & + i(f_{s\mathbf{p}} - f_{s'p-q}) \frac{1}{V} \sum_{s_1 s_1'} K_{p-q, p_1}^{s's_1 s_1'}(\mathbf{q}) a_{s_1'p_1-q}^+ a_{s_1 \mathbf{p}_1}. \end{aligned} \quad (4.9)$$

Thus, the complete system of equations of dynamics of the metal includes the equation of motion of the lattice (4.6), the kinetic equation for the electrons (4.8),

and the equation of the interband transitions (4.9). The total current  $\mathbf{j}$  in the metal is determined by the sum  $\mathbf{j} = \mathbf{j}^{(e)} + \mathbf{j}^{(i)}$ , where

$$\mathbf{j}^{(i)} = -eZn\mathbf{u},$$

$$\mathbf{j}^{(e)} = \frac{e}{2V} \sum_{p s'} \langle s'p - \mathbf{q} | \frac{1}{im_c} \nabla e^{-i\mathbf{q}\mathbf{r}} + e^{-i\mathbf{q}\mathbf{r}} \frac{1}{im_0} \nabla | s\mathbf{p} \rangle a_{s'p-q}^+ a_{s\mathbf{p}}. \quad (4.10)$$

In the employed formalism the operator  $a_{s'p-q}^+ a_{s\mathbf{p}}$  with  $\mathbf{q} \neq 0$  corresponds to the complete increment  $f_1$  to the unperturbed distribution function  $f(\epsilon_p, \mu)$  (with unperturbed energy, chemical potential, etc.).

## 5. QUASICLASSICAL EQUATIONS OF LONG-WAVE OSCILLATIONS IN A METAL. COMPARISON WITH THE PHENOMENOLOGICAL THEORY

The long-wave approximation equations can be obtained from the general equations (4.6), (4.8), and (4.9) by expanding the coefficients of these equations in a series in the small  $q$  accurate to terms of second order inclusive. In addition, we go in all the equations to the quasiclassical limit, letting the Planck constant go to zero. To this end we introduce the "Wigner function"  $\chi_s(\mathbf{p}, \mathbf{r})$  for the conduction electrons:

$$\chi_s(\mathbf{p}, \mathbf{r}) = \frac{1}{V} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}} \chi_s(\mathbf{p}, \mathbf{q}), \quad \chi_s(\mathbf{p}, \mathbf{q}) = \langle a_{s'p-q}^+ a_{s\mathbf{p}+\mathbf{q}/2} \rangle, \quad (5.1)$$

where the angle brackets denote averaging over the state of the statistical equilibrium of the system with the Hamiltonian (2.3). The equation for  $\chi_s(\mathbf{p}, \mathbf{q})$  is obtained from (4.8) with the aid of the shift  $\mathbf{p} - \mathbf{p} + \mathbf{q}/2$ , followed by averaging of this equation. The classical distribution function of the electrons is the quasiclassical limit of the "Wigner function" (for Bloch electrons,  $\chi_s(\mathbf{p}, \mathbf{r})$  does not have the properties of a Wigner function, although it coincides outwardly with this function for free electrons).

For the transition to the long-wave approximation in (4.6), (4.8), and (4.9) it is necessary to calculate, at small values of  $q$ , each of the quantities that enter in these equations. From (2.6) and (2.7) we obtain as  $q \rightarrow 0$

$$\omega_{q\sigma}^2 e_{\sigma i}(\mathbf{q}) = \omega_{i\mathbf{p}}^2 \frac{q_i q_k}{q^2} e_{\sigma k}(\mathbf{q}) + \frac{1}{Mn} \gamma_{ilm}^{(0)} e_{\sigma k}(\mathbf{q}) q_i q_m, \quad (5.2)$$

$$\gamma_{ilm}^{(0)} = n^2 \sum_{B_m=0} \frac{\partial^2}{\partial B_l \partial B_m} [A(B) B_l B_k] + n^2 g(0) \delta_{il} \delta_{km}. \quad (5.3)$$

From the definition (2.15) we obtain directly

$$M_{s's}^{*s}(\mathbf{q}) = \delta_{ss'} + iq_k \langle s'p | \Omega_k | s\mathbf{p} \rangle - \frac{1}{2} q_k q_l \langle s'p | \Omega_k \Omega_l | s\mathbf{p} \rangle + \dots, \quad (5.4)$$

where  $\Omega$  is an operator defined by the equation<sup>1,2</sup>

$$\mathbf{r} = i \frac{\partial}{\partial \mathbf{p}} + \Omega.$$

The matrix elements of the electron-ion interaction  $V_{q_i}^{s's}(\mathbf{p})$  is determined as  $q \rightarrow 0$  by Eq. (2.11), in which we now have at  $s = s'$

$$\xi_{q_i}^{*s's}(\mathbf{p}) = iq_k L_{ik}^s(\mathbf{p}). \quad (5.5)$$

The symmetrical tensor  $L_{ik}^s(\mathbf{p})$  is given by

$$L_{ik}^s(\mathbf{p}) = m_0 v_i v_k + \frac{1}{m_0} \left\langle s\mathbf{p} \left| \frac{\partial^2}{\partial x_i \partial x_k} \right| s\mathbf{p} \right\rangle - b \delta_{ik} \quad (5.6)$$

$$- n \sum_{\mathbf{B} \neq 0} M_{\mathbf{p}''}^{s''}(\mathbf{B}) \frac{\partial}{\partial B_k} [B_i \Phi(\mathbf{B})];$$

the quantity  $b = \eta \Phi(0)$  has the meaning of the energy of electron repulsion by the ion shell ( $b > 0$ ). In order of magnitude,  $b$  is equal to the Fermi energy of the electrons in the metal.

On the other hand if  $s' \neq s$ , then as  $q \rightarrow 0$  we have

$$\xi_{\mathbf{q}'}^{s''}(\mathbf{p}) = i(e_{s'p} - e_{s''p}) \langle s'\mathbf{p} | (-i\nabla_i) | s\mathbf{p} \rangle + i q_k b_{ik}^{s''}(\mathbf{p}), \quad (5.7)$$

where

$$b_{ik}^{s''}(\mathbf{p}) = \frac{p_i}{m_0} \langle s'\mathbf{p} | (-i\nabla_k) | s\mathbf{p} \rangle + \frac{1}{m_0} \left\langle s'\mathbf{p} \left| \frac{\partial^2}{\partial x_i \partial x_k} \right| s\mathbf{p} \right\rangle \quad (5.8)$$

$$- n \sum_{\mathbf{B} \neq 0} M_{\mathbf{p}''}^{s''}(\mathbf{B}) \frac{\partial}{\partial B_k} [B_i \Phi(\mathbf{B})].$$

To obtain the equation of motion of the lattice, we eliminate from (4.6) the variables connected with the interband transitions of the electrons. To this end it is necessary to solve the equation of the interband transitions (4.9), substitute the solution in Eq. (4.6), and calculate the resultant sums over the band indices. It is useful in this case to employ the sum rule obtained by Luttinger and Kohn,<sup>41</sup> which we write in the form

$$\sum_{i'} \langle s\mathbf{p} | (-i\nabla_i) | s'\mathbf{p} \rangle \langle s'\mathbf{p} | \Omega_k | s\mathbf{p} \rangle = \frac{1}{2i} \left( \delta_{ik} - m_0 \frac{\partial^2 \epsilon_{sp}}{\partial p_i \partial p_k} \right). \quad (5.9)$$

With the aid of this rule we obtain (neglecting the influence of the Fermi liquid interaction on the interband transitions):

$$Mn \frac{\partial^2 u_i}{\partial t^2} = -\gamma_{iklm} q_l q_m u_k + \left( -Mn \omega_{sp}^2 u_k + \frac{q_i q_k}{q^2} \right) \quad (5.10)$$

$$+ i q_i \frac{4\pi e^2 Z n}{q^2} \rho_q + e E_k \frac{1}{V} \sum_{\mathbf{p}} f_{sp} \left( \delta_{ik} - m_0 \frac{\partial^2 \epsilon_{sp}}{\partial p_i \partial p_k} \right)$$

$$- m_0 \frac{\partial^2 u_k}{\partial t^2} \frac{1}{V} \sum_{\mathbf{p}} f_{sp} \left( \delta_{ik} - m_0 \frac{\partial^2 \epsilon_{sp}}{\partial p_i \partial p_k} \right) + i q_k \frac{1}{V} \sum_{\mathbf{p}} L_{ik}^s(\mathbf{p}) \chi_s(\mathbf{p}, q)$$

$$+ \frac{1}{V} \sum_{\mathbf{p}} m_0 v_i I_{sp} \left[ \tilde{\chi}_s(\mathbf{p}, q) + m_0 v_k \dot{u}_k \frac{\partial f_{sp}}{\partial \epsilon} \right],$$

where

$$\gamma_{iklm} = \gamma_{iklm}^{(0)} + \frac{2}{V} \sum_{\mathbf{p}} f_{sp} (\delta \epsilon_{sp})_{iklm}. \quad (5.11)$$

The quantity  $(\delta \epsilon_{sp})_{iklm}$  describes the contribution of the electrons to the elasticity of the metal, due to the change of the electron energy on account of the interband transitions induced by the lattice deformation. In the approximation assumed here, this quantity is obtained in second order perturbation theory:

$$(\delta \epsilon_{sp})_{iklm} = \text{Re} \sum_{i'} \frac{b_{ik}^{s''}(\mathbf{p}) b_{ml}^{s''}(\mathbf{p})}{\epsilon_{s''p} - \epsilon_{s'p}}. \quad (5.12)$$

The fourth and fifth terms in the right-hand side of (5.10) describe the forces exerted on the lattice by the electrons dragged by the lattice. The first of them is due to the presence in the deformed lattice of the electric field

$$E_i = -i q_i \frac{4\pi e}{q^2} (\rho_q + Z n i q_i u_i), \quad (5.13)$$

while the second is the inertia force exerted by the accelerated dragged electrons.

In the calculations here and below we assume that the energy spectrum of the electrons does not have degeneracy points, i.e., the difference  $\epsilon_{s'p} - \epsilon_{s''p}$ ,  $s \neq s''$ , is not anomalously small at any value of  $p$ , and we are dealing with frequencies that are low compared with the characteristic value of this difference (this assumption does not exclude the possibility of overlap of the energy bands). Under these conditions the motion of the conduction electrons, in that part which is connected with the interband transitions, will follow adiabatically the motion of the lattice.

Next, using (4.8) and going in the limit to small  $q$ , we obtain the kinetic equation for the electrons:

$$\frac{\partial}{\partial t} \chi_s(\mathbf{p}, q) + i q v_s \chi_s(\mathbf{p}, q) - i \frac{\partial f_{sp}}{\partial p} q \left( \frac{4\pi e^2}{q^2} \rho_q + i q_k u_k \frac{4\pi e^2 Z n}{q^2} \right) \quad (5.14)$$

$$- i q \frac{\partial f_{sp}}{\partial p} (i L_{ik}^s(\mathbf{p}) q_k u_i) - i \frac{\partial f_{sp}}{\partial p} q \frac{1}{V} \sum_{\mathbf{p}'} K_s(\mathbf{p}, \mathbf{p}') \chi_s(\mathbf{p}', q)$$

$$+ I_{sp} \left[ \tilde{\chi}_s(\mathbf{p}, q) + m_0 v_k \dot{u}_k \frac{\partial f_{sp}}{\partial \epsilon} \right] = 0.$$

The function

$$\tilde{\chi}_s(\mathbf{p}, q) = \sum_{\mathbf{B} \neq 0} \frac{4\pi e^2}{B^2} M_{\mathbf{p}''}^{s''}(\mathbf{B}) M_{\mathbf{p}'}^{s''}(-\mathbf{B}) \quad (5.15)$$

in (5.14) describes a short-range interaction of Bloch electrons of the Fermi-liquid type. Its appearance even in the Born approximation is due to the fact that the direct Coulomb interelectron repulsion leads to a nonzero Born scattering amplitude of the Bloch electrons through zero angle.

For comparison with the phenomenological theory it is necessary to separate in explicit form, from Eqs. (5.10) and (5.14), the longitudinal electric field and to change over to the coordinate form of these equations. In addition, we introduce in (5.10) in place of the quantities  $\gamma_{iklm}$  the symmetrized coefficients<sup>42</sup>

$$\lambda_{iklm} = \gamma_{iklm} + \gamma_{kml} - \gamma_{imlk}. \quad (5.16)$$

The tensor  $\lambda_{iklm}$  corresponds to the bare elastic moduli of the phenomenological theory. We write down the obtained system of equations. The equation of motion of the lattice:

$$(M + Zm) n \frac{\partial^2 u_i}{\partial t^2} = \lambda_{iklm} \frac{\partial^2 u_m}{\partial x_k \partial x_l} \quad (5.17)$$

$$- \left( e E_k + m_0 \frac{\partial^2 u_k}{\partial t^2} \right) \frac{1}{V} \sum_{\mathbf{p}} m_0 v_i v_k \left( - \frac{\partial f_{sp}}{\partial \epsilon} \right)$$

$$+ \frac{1}{V} \frac{\partial}{\partial x_k} \sum_{\mathbf{p}} L_{ik}^s(\mathbf{p}) \chi_s(\mathbf{p}, \mathbf{r}) + \frac{1}{V} \sum_{\mathbf{p}} m_0 v_i I_{sp} \left[ \tilde{\chi}_s(\mathbf{p}, \mathbf{r}) + m_0 v_k \dot{u}_k \frac{\partial f_{sp}}{\partial \epsilon} \right].$$

The kinetic equation for the electrons:

$$\frac{\partial}{\partial t} \chi_s(\mathbf{p}, \mathbf{r}) + (v_s \nabla) \chi_s(\mathbf{p}, \mathbf{r}) + e E \frac{\partial f_{sp}}{\partial p} \quad (5.18)$$

$$- \frac{\partial f_{sp}}{\partial p} \nabla \left\{ L_{ik}^s(\mathbf{p}) \frac{\partial u_i}{\partial x_k} + \frac{1}{V} \sum_{\mathbf{p}'} K_s(\mathbf{p}, \mathbf{p}') \chi_s(\mathbf{p}, \mathbf{r}) \right\}$$

$$+ I_{sp} \left[ \tilde{\chi}_s(\mathbf{p}, \mathbf{r}) + m_0 v_k \dot{u}_k \frac{\partial f_{sp}}{\partial \epsilon} \right] = 0.$$

In the collision integral we introduce the notation

$$\tilde{\chi}_s(\mathbf{p}, \mathbf{r}) = \chi_s(\mathbf{p}, \mathbf{r}) - (\varepsilon_{sp} - e_{sp}) \frac{\partial f_{sp}}{\partial \varepsilon}, \quad (5.19)$$

and the longitudinal electric field in the metal is determined from the relations

$$\mathbf{E} = -\nabla\varphi, \quad \text{div } \mathbf{E} = 4\pi e\rho(\mathbf{r}) + 4\pi eZn \text{ div } \mathbf{u}.$$

The observed electron and ion densities are respectively

$$\rho(\mathbf{r}) = \frac{1}{V} \sum_{sp} \chi_s(\mathbf{p}, \mathbf{r}) - \frac{1}{V} \sum_{sp} f_{sp} \left( \delta_{ik} - m_0 \frac{\partial^2 \varepsilon_{sp}}{\partial p_i \partial p_k} \right) \frac{\partial u_i}{\partial x_k}, \quad (5.20)$$

$$\rho^{(i)}(\mathbf{r}) = -n \text{ div } \mathbf{u}.$$

We note that in (5.17)–(5.20) the summation over  $s$  is carried out in fact only over those energy bands through which the Fermi level passes.

The kinetic equation (5.18) has a known structure. The appearance of its third and fourth terms can be interpreted as the fact that in a deformed lattice the electron energy changes and becomes equal to

$$\varepsilon_{sp}(\mathbf{r}, t) = \varepsilon_{sp} + L_{ik}^s(\mathbf{p}) \frac{\partial u_i}{\partial x_k} + e\varphi + \frac{1}{V} \sum_{p'} K_s(\mathbf{p}, \mathbf{p}') \chi_s(\mathbf{p}', \mathbf{r}). \quad (5.21)$$

It is this quantity that should be taken as  $\tilde{\varepsilon}_{sp}$  in the collision integral. The second term in the right-hand side of (5.21) gives the known change of the electron energy under the influence of the lattice deformation. The tensor  $L_{ik}^s(\mathbf{p})$  corresponds to the quantity  $L_{ik}(\mathbf{p})$  introduced by Lang and Pavlov,<sup>43</sup> and the tensor which was designated by them as  $\langle \mathbf{p} | V_{ik}^s | \mathbf{p} \rangle$  turns out to equal

$$\langle \mathbf{p} | V_{ik}^s | \mathbf{p} \rangle = -b\delta_{ik} - n \sum_{B \neq 0} M_p^{sB}(\mathbf{B}) \frac{\partial}{\partial B_k} [B_i \Phi(\mathbf{B})]. \quad (5.22)$$

It was shown in the same paper<sup>43</sup> that the customarily assumed expression for the deformation potential  $\lambda_{ik}^s(\mathbf{p})$  is connected with the tensor  $L_{ik}^s(\mathbf{p})$  by the relation

$$\lambda_{ik}^s(\mathbf{p}) = L_{ik}^s(\mathbf{p}) - m_0 v_i^s v_k^s. \quad (5.23)$$

The last term in (5.21) describes the change of the electron energy on account of the Fermi-liquid interaction.<sup>39</sup> We shall not take into account terms of this kind and omit terms containing  $K_s(\mathbf{p}, \mathbf{p}')$ .

The elasticity-theory equation (5.17) can be rewritten in an equivalent form that does not contain explicitly the collision terms and the electric field. To reduce (5.17) to such a form, we exclude from it the collision integral with the aid of the kinetic equation (5.18):

$$(M+Zm)n \frac{\partial^2 u_i}{\partial t^2} = \left\{ \lambda_{ikim} + \frac{1}{V} \sum_{sp} m_0 v_i^s v_k^s L_{im}^s(\mathbf{p}) \left( -\frac{\partial f_{sp}}{\partial \varepsilon} \right) \right\} \frac{\partial^2 u_m}{\partial x_k \partial x_i} + \frac{\partial}{\partial x_k} \frac{1}{V} \sum_{sp} \lambda_{ik}^s(\mathbf{p}) \chi_s(\mathbf{p}, \mathbf{r}) - \frac{m_0}{e} \frac{\partial j_i}{\partial t}. \quad (5.24)$$

The total current  $\mathbf{j}$  in the metal is equal in the quasi-classical case to  $\mathbf{j}^{(i)} + \mathbf{j}^{(e)}$ , where

$$\mathbf{j}^{(i)} = -eZn\mathbf{u},$$

$$\mathbf{j}_i^{(e)} = \frac{e}{V} \sum_{sp} v_i^s \chi_s(\mathbf{p}, \mathbf{r}) + \frac{e}{V} \sum_{sp} f_{sp} \left( \delta_{ik} - m_0 \frac{\partial^2 \varepsilon_{sp}}{\partial p_i \partial p_k} \right) \dot{u}_k. \quad (5.25)$$

The last term in (5.25) is the current due to dragging of the electrons by the lattice.<sup>7,43</sup> To calculate this current we used the interband transition equation (4.9) and the expression (5.7) for the matrix elements  $\xi_{q_i}^{s's}(\mathbf{p})$

which are off-diagonal in the band index.

If a constant and homogeneous magnetic field is present in the metal, it is necessary to add to the left-hand side of the kinetic equation (5.18) the term  $\frac{e}{c} [\mathbf{v} \times \mathbf{H}] \frac{\partial}{\partial \mathbf{p}} \chi_s(\mathbf{p}, \mathbf{r}) + \frac{e}{c} \left[ \frac{\partial}{\partial \mathbf{p}} \left\{ L_{ik}^s(\mathbf{p}) \frac{\partial u_i}{\partial x_k} + (\mathbf{p} - m_0 \mathbf{v}^s) \dot{\mathbf{u}} \right\} \times \mathbf{H} \right] \frac{\partial f_{sp}}{\partial \mathbf{p}}$  (5.26)

and now take  $\mathbf{E}$  to mean the total electric field, including its solenoidal part. The connection between the current  $\mathbf{j}$  and the field  $\mathbf{E}$  is determined by Maxwell's equations. In the equation of motion of the lattice (5.24) it is necessary to add to the right-hand side the force  $\mathbf{j} \times \mathbf{H}/c$  that acts on a unit volume of the metal in the magnetic field.<sup>14,20</sup>

We consider now the low-frequency oscillations in a situation wherein the adiabaticity conditions are satisfied, and calculate the adiabatic elastic moduli of the metal under the assumption that the conduction electrons are situated in one energy band. To this end we solve the dispersion equation that follows from relations (5.17) and (5.18), neglecting the collisions and the solenoidal fields ( $\mathbf{H} = 0$ ). The solution can be represented in the form of the equation of elasticity theory, from which the electronic variables have been excluded:

$$Mn \frac{\partial^2 u_i}{\partial t^2} = \{ \nu(\varepsilon_p) [ \langle m_0 v_i^s v_k^s \rangle \langle m_0 v_l^s v_m^s \rangle - \langle m_0 v_i^s v_k^s \rangle \langle L_{lm}^s(\mathbf{p}) \rangle - \langle L_{ik}^s(\mathbf{p}) \rangle \langle m_0 v_l^s v_m^s \rangle ] - \nu(\varepsilon_p) [ \langle L_{ik}^s(\mathbf{p}) L_{lm}^s(\mathbf{p}) \rangle - \langle L_{ik}^s(\mathbf{p}) \rangle \langle L_{lm}^s(\mathbf{p}) \rangle ] + \lambda_{ikim} \} \frac{\partial^2 u_m}{\partial x_k \partial x_i}. \quad (5.27)$$

Here  $\nu(\varepsilon_p)$  is the state density of the Bloch electrons on the Fermi surface, and the angle brackets denote averaging over the Fermi surface:

$$\langle \dots \rangle = \frac{1}{\nu(\varepsilon_p)} \frac{1}{V} \sum_{sp} (\dots) \delta(\varepsilon_p - \varepsilon_{sp}). \quad (5.28)$$

The first three terms in the right-hand side of (5.27) give the electronic renormalization of the adiabatic elastic moduli, corresponding to the results of Brovman and Kagan.<sup>33</sup> For the isotropic situation, these terms were obtained by Kaner and the author.<sup>34</sup> The second line contains a renormalization of the type usually obtained in the phenomenological theory.

The first two terms in the first line of (5.27) describe the contribution made to the elastic moduli by the longitudinal electric field in the metal; this field can be obtained from the kinetic equation (5.17) and turns out to be

$$\mathbf{E} = -\nabla\varphi, \quad e\varphi = -\langle \lambda_{ik}^s(\mathbf{p}) \rangle \frac{\partial u_i}{\partial x_k}. \quad (5.29)$$

The quantity  $e\varphi$  corresponds to the renormalization used in phenomenological theory for the chemical potential and taken with a minus sign. Relation (5.29) can be therefore regarded as an expression for the electroneutrality condition  $\delta\rho = 0$ , where  $\delta\rho$  is the uncompensated charge density in the metal.

The electroneutrality condition for low-frequency adiabatic oscillations in a metal can be taken into account directly in the Hamiltonian (2.3). To this end we take the long-wave part of the operator (2.3), expanding the



coefficients in the sums in small  $q$  and retaining terms of order not higher than second. Next, using (4.9), we eliminate the variables connected with the interband transitions. Finally, using the Bogolyubov canonical transformation from the operators  $b_{q\sigma}$  and  $b_{q\sigma}^+$  to the new Bose operators  $\tilde{b}_{q\sigma}$  and  $\tilde{b}_{q\sigma}^+$ , we reduce the long-wave part of the operator (2.3) to the form

$$H = \sum_p \epsilon_p a_p^+ a_p + \sum_{q\sigma} \tilde{\omega}_{q\sigma} \tilde{b}_{q\sigma}^+ \tilde{b}_{q\sigma} + \sum_{pq} iL_{ik}(p) q_k \tilde{u}_{qi} a_{p+q}^+ a_p + \frac{1}{2V} \sum_{pp'} K(p, p') a_{p-q}^+ a_p a_{p'+q} + \frac{1}{2} V \sum_q \left( \frac{4\pi e Z n}{q^2} i q_i \tilde{u}_{qi} + \frac{4\pi e}{q^2} \rho_q \right) (-e Z n i q_i \tilde{u}_{-qi} + e_{p-q}) + A(u), \quad (5.30)$$

where  $A\{u\}$  is connected with the work done by the dragging forces on the electrons when the lattice is deformed. Here

$$\tilde{u}_{qi} = \sum_{\sigma} \tilde{\epsilon}_{\sigma}^i(q) (2MN\tilde{\omega}_{q\sigma})^{-1/2} (\tilde{b}_{q\sigma} + \tilde{b}_{-q\sigma}^+),$$

and the frequency  $\tilde{\omega}_{q\sigma}$  and the polarization vector  $\tilde{\epsilon}_{\sigma}(q)$  are determined from the equation (5.2), in which we must set the plasma ion frequency  $\omega_{ip}$  equal to zero, and replace the coefficients  $\gamma_{iklm}^{(0)}$  by  $\lambda_{iklm}$ . Imposition of the electroneutrality condition in the form  $\delta\rho=0$  causes the term in the third line of (5.30), which represents the electrostatic energy of the uncompensated charge of the metal, in the form  $\frac{1}{2} \int \rho\phi dV$ , to vanish, as well as the term  $A\{u\}$ . The remaining terms in the first two lines of (5.30) yield the Fröhlich Hamiltonian supplemented by a short-range Fermi-liquid-type interaction of the Bloch electrons.

Thus, the Fröhlich Hamiltonian was obtained as the long-wave part of the exact operator (2.3) assuming adiabaticity of the electron motion and by imposing the neutrality condition in the form  $\delta\rho=0$ . The fact that it is precisely on these assumptions that the Fröhlich model is based was noted by Kaner and the author.<sup>34</sup>

As for the relation of Eqs. (5.17) and (5.18) to the phenomenological theory, this question was analyzed by Gurevich, Lang, and Pavlov.<sup>9,43</sup> We shall therefore not dwell on this question here.

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*Note added in proof (10 September 1979).* It must be emphasized that all the obtained equations and the quantities in them pertain to the laboratory reference frame; this is indicated by the very method of their derivation. A characteristic feature of these equations is the explicit presence of terms that describe the dragging of the electrons by the lattice. I. M. Lifshitz has called the author's attention to the fact that for a correct interpretation of the obtained relations it is necessary to take into account the "non-freedom" of the electrons in the metal, which manifests itself in the fact that the conduction electron retains for a finite time interval the memory of the concrete ion of the lattice, and then moves to the next ion. The lack of freedom of the electrons in the metal is a direct consequence of the band

structure of their energy spectrum and is the main cause of the dragging of the electrons by the lattice. In particular, on account of the dragging effect there arises an additional contribution from the motion of the lattice to the electron velocity, equal to

$$\Delta v_i^* = (\delta_{ik} - m_0 \partial^2 \epsilon_{ij} / \partial p_i \partial p_k) \dot{u}_k.$$

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## Capture of photoexcited carriers by shallow impurity centers in germanium

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Measurements were made of the lifetimes  $\tau_f$  of free carriers and the relaxation time  $\tau_r$  of the submillimeter impurity photoconductivity when carriers are captured by attracting shallow donors and acceptors in Ge. It is noted that in samples with capture-center concentration  $N_{rec} \gtrsim 10^{11} \text{cm}^{-3}$  the relaxation time  $\tau_r$  greatly exceeds  $\tau_f$  in the temperature range 4.2-12 K. The measured values of  $\tau_f$  are compared with the calculation of cascade recombination by the classical model. To evaluate the data on  $\tau_r$ , the distinguishing features of this model are considered for the nonstationary case. The substantial difference between the values of  $\tau_f$  and  $\tau_r$  is attributed to re-emission of the carriers from the excited states of the shallow impurities.

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### 1. INTRODUCTION

One of the important mechanisms of recombination of free carriers by attracting Coulomb centers in semiconductors is cascade capture with participation of the excited impurity states; the theory of this mechanism was developed by a number of workers.<sup>1-4</sup> The calculations were made only for the stationary case, and the possible differences between the characteristic times in stationary and nonstationary conditions were not discussed. Generally speaking, however, such differences can exist. In fact, according to Abakumov *et al.*<sup>4</sup> the recombination of the carriers proceeds via their diffusion in energy space over highly excited states of the impurity centers in the region of negative energies up to a binding level with energy  $|\varepsilon| \approx kT$ , and the probability of the thermal ejection from highly excited states  $|\varepsilon| < kT$  into the free band is large compared with the probability that the carriers will drop down via cascade of excited states to the ground state. Thus, high excited states of the impurities exchange carriers in practice only with the free band, and consequently, can play the role of sticking levels. The number of such states under definite conditions can be quite large.

Usually the sticking centers and recombination centers are separated in space, and direct exchange of carriers between them does not take place. In the case of cascade recombination on shallow impurity centers

this is not so, so that the sticking levels discussed by us belong to the recombination centers themselves. The presence of sticking levels should manifest itself primarily in the values of the characteristic times measured by stationary and nonstationary methods. In an experimental verification of the calculations performed in Refs. 1-4, the lifetimes were determined by different methods. The published experimental data on carrier recombination on impurity centers in semiconductors are on the whole in agreement with the calculations of Abakumov *et al.*<sup>4</sup> Attention is called, however, to the large scatter of the data obtained by different authors.<sup>5-8</sup> The measured lifetimes differ both in the values and in the temperature dependence.

On the one hand this is partially due to the inadequacy of the procedures in a number of cases when the relaxation time  $\tau_r$  of the excess carrier density is identified with the stationary lifetime of the carriers without valid grounds, or when the measured  $\tau_r$  is in fact determined not from the carrier recombination but, for example, from the dielectric relaxation of the space charge in the semiconductor. On the other hand, the mechanism of cascade recombination is not always decisive in the capture, even in the case of Coulomb attracting centers. For deep impurities, a large role can be played by recombination with participation of optical phonons.<sup>9</sup> At high concentrations of the centers, this mechanism can be substantial also for shallow impuri-