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# Forces produced by conduction electrons in metals located in external fields

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The forces produced by conduction electrons in metals located in external fields are considered by a unified approach. The body forces which the electron exert on the lattice as a whole, and the electron "wind" forces acting on the defects, are found. Criteria are obtained which can be used to assess the relative magnitude of the forces created by electrons in metals. The causes of the discrepancies of the results of previous researches are found.

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If a metal is located in external field—electric or magnetic—under the action of mechanical stresses, then various types of forces arise in it, due to the fact that the conduction electrons transfer to the lattice the action of the external fields and strains that they experience. These forces can be divided into two essentially different groups; body forces, which act on the lattice as a whole, and forces that act on the lattice defects — the "electron wind" forces. The forces of the first group are important in the phenomena of interaction of a current with elastic and plastic deformations. The forces of the second group produce motion of the defects in the lattice: electron transfer, attraction of ions by electrons, acceleration of dislocations by electrons, and so on.

A significant number of works have been devoted to the analysis of body forces[1-9] and electron wind forces[10-17]; however, the situation at the present time is unsatisfactory in two respects. First, the expressions for the body forces, obtained in previous researches,[1-7] differ significantly among themselves (a critical analysis of some of these researches is contained in Ref. 8), but even the expressions for the body forces obtained in the latest, most complete researches[8,9] do not reduce to one another. Second, there is an essential difference in the methods of calculation of body forces and electron wind forces. The methods used for the calculation of the forces in the volume[5,7,8] cannot be used for obtaining the forces acting on the defects. Thus there is no single approach to the force problem. The aim of the present work is to consider the forces created by electrons in metals within the framework of common approach. The derivation of the body forces and the electron wind forces based on the use of quantum equations of motion of the electrons, written down in the form of Newton's equations (the quantum theorems of Ehrenfest for motion of electrons in a periodic field of the lattice and for the electron-quasiparticle in field external relative to the periodic

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potential, i.e., in the fields of the defects and external forces). This approach is based on Refs. 14 and 18. Such an analysis enables us to establish the reasons for the divergence of the previous papers[8,9] on body forces.

We first consider the body forces. As has been pointed out, the results of the last two researches devoted to body forces[8,9] have an essential difference. According to these works, the body forces exerted by the electrons on the metallic lattice can be written down in the following form:

$$F^{(i)} = -\frac{m_0}{e}\frac{\partial j^{(i)}}{\partial t} + \frac{1}{c}[\mathbf{j}\times\mathbf{H}]_i + \frac{\partial \psi_{ik}}{\partial x_k}. \tag{1}$$

Here, according to Kontorovich, [9]

$$\frac{\partial \psi_{ik}^{(1)}}{\partial x_k} = \frac{\partial}{\partial x_k}\int \Lambda_{ik} f(\mathbf{k})\, d\tau_{\mathbf{k}}, \tag{2}$$

whereas Pekar and Tsekvava,[8]

$$\frac{\partial \psi_{ik}^{(2)}}{\partial x_k} = -\frac{\partial}{\partial x_k}\int m_0 v_i v_k f(\mathbf{k})\, d\tau_{\mathbf{k}}. \tag{3}$$

Here $m_0$ and $e$ are the actual mass and charge of the electron, j is the current density, H is the intensity of the magnetic field, $f(\mathbf{k})$ is the nonequilibrium distribution function of the electrons, $\Lambda_{ik}$ is the Akhiezer tensor.[10]

It has been shown in Ref. 9 that, in the free electron approximation, $\Lambda_{ik} = -m_0 v_i v_k$, i.e.,

$$\partial\psi_{ik}^{(1)}/\partial x_k = \partial\psi_{ik}^{(2)}/\partial x_k,$$

but for arbitrary dispersion law of the electrons, (2) and (3) do not agree with one another, since $\Lambda_{ik} \neq m_0 v_i v_k$ in the general case. Since a very special dispersion law was chosen in Ref. 8 (the approximation of a scalar effective mass), we can then assume that the difference in the results of this research and that of Kontorovich[9] is associated with the approximate character of the dispersion law in Ref. 8. Therefore, in considering the forces acting on the lattice in what follows, we reject the limitation on the dependence of the energy of the electron on the quasimomentum.

## 1. LATTICE DRAG BY THE CONDUCTION ELECTRONS

1. The motion of the electron in an ideal lattice in the presence of external fields can, as is well known, be described by the Ehrenfest equation:

$$\langle \dot{\mathbf{p}}\rangle = \langle \mathbf{F}\rangle + \langle \mathbf{F}_{pe}\rangle, \tag{4}$$

$\hat{p} = m_0\hat{v}$ is the electron momentum operator, $m_0$ is the actual mass of the electron, v is the electron velocity operator, $\langle \mathbf{F}_{pe}\rangle$ is the force acting on the electron from the periodic potential of the lattice - $V_p$:

$$\langle \mathbf{F}_{pe}\rangle = -\langle \partial V_p/\partial \mathbf{r}\rangle, \tag{5}$$

$\langle \mathbf{F}\rangle$ are the external forces. The brackets mean averaging over the exact wave functions of the electron, which are determined by the solution of the time dependent Schrödinger equation for the electron in a periodic potential of the lattice in the presence of external fields.

In addition, the motion of the electron is determined by the Ehrenfest equation for the electron-quasiparticle:

$$\langle \hbar\dot{\mathbf{k}}\rangle = \langle \mathbf{F}\rangle. \tag{6}$$

k is the wave vector of the electron, and $\langle \mathbf{F}\rangle$ are forces external relative to the periodic potential of the lattice. The external fields are, as a rule, quasiclassical and change slowly over distances of the order of the electron wavelength. It is impossible to say this for fields produced by lattice defects, but Eq. (6) is valid also for motion of the electron in the fields of the impurities.[18]

From Eqs. (4) and (6), we find the force acting from the lattice on the electron:

$$\langle \mathbf{F}_{pe}\rangle = \langle \dot{\mathbf{p}}\rangle - \langle \hbar\dot{\mathbf{k}}\rangle. \tag{7}$$

Thus, since in the general case $\mathbf{p} \neq \hbar\mathbf{k}$, the forces of interaction of the electrons with an ideal lattice exist in the presence of external fields. The need for accounting for these forces in the kinetic analysis was first shown in Ref. 8, where these forces were obtained in the scalar effective mass approximation.

The physical nature of these forces is connected with the difference between the conduction electrons (quasiparticles) and free electrons. In the presence of external forces, the electron does not interact on the average with the ideal lattice ($\langle \dot{\mathbf{p}}\rangle = 0$ and $\langle \mathbf{F}_{pe}\rangle = 0$). The electron described by Bloch wave function is, on the average, not accelerated by the periodic field of the lattice. In external fields, the electron no longer has a Bloch wave function, becomes coupled with the lattice, and forces appear which are exerted by the lattice on the electron and by the electron on the lattice. In the quasiclassical approximation, it is not difficult to find these forces for electrons with an arbitrary dispersion law. In this approximation, Eq. (4) is of the form

$$m_0 d\mathbf{v}/dt = \mathbf{F}_{ep} + \mathbf{F}, \tag{8}$$

$$\mathbf{v} = \hbar^{-1}\nabla\varepsilon(\mathbf{k}); \tag{9}$$

$\varepsilon$ is the energy of the electron as a function of k. It follows from (8), with account of (9) that ($i = x, y, z$)

$$m_0\frac{dv^{(i)}}{dt} = F_{pe}^{(i)} + F^{(i)} = \frac{m_0}{\hbar^2}\frac{\partial^2\varepsilon}{\partial k_i \partial k_s}F^{(s)}. \tag{10}$$

We get from (10)

$$F_{pe}^{(i)} = \frac{m_0}{\hbar^2}\frac{\partial^2\varepsilon}{\partial k_i \partial k_s}F^{(s)} - F^{(i)}. \tag{11}$$

The force acting from the electron on the lattice, $F_{ep}^{(i)} = -F_{pe}^{(i)}$. Summing over all the conduction electrons, we find the total force

$$F_{ep}^{(i)} = \sum_{\mathbf{k}} F^{(i)} = \int_{\mathbf{k}} f(\mathbf{k})\left\{F^{(i)} - \frac{m_0}{\hbar^2}\frac{\partial^2\varepsilon}{\partial k_i \partial k_s}F^{(s)}\right\} d\tau_{\mathbf{k}}; \tag{12}$$

$f(\mathbf{k})$ is the distribution of the electrons over the external fields.

The force $F_{ep}^{(i)}$ is a "collisionfree" force, acting on an ideal lattice, regardless of whether electron scattering takes place in the lattice. In the effective-mass approximation, it follows from (12) that

$$F_{ep}^{(i)}=-(m_0/m^*-1)F^{(i)}. \tag{13}$$

2. The electrons accelerated by the fields are scattered in the lattice. The momenta transferred to the lattice by the electrons in the scattering processes create the "collision" force. An electron that goes over in the scattering process from the state $|\mathbf{k}\rangle$ to $|\mathbf{k}'\rangle$ transfers to the lattice as a whole, a momentum $\Delta\mathbf{p}_{\mathbf{kk}'}$ equal to the difference of the average momenta in the initial and final states of the electron:[18]

$$\Delta\bar{\mathbf{p}}_{\mathbf{kk}'}=m_0\hbar^{-1}(\nabla\varepsilon(\mathbf{k})-\nabla\varepsilon(\mathbf{k}')).$$

The resulting momentum transferred to the lattice from the entire electron subsystem per unit time is equal to the force $F_{col}$[1]:

$$\mathbf{F}_{\text{col}}=-\int_{\mathbf{k}} m_0\mathbf{v}\left(\frac{\partial f}{\partial t}\right)_{\text{col}}d\tau_{\mathbf{k}}; \tag{14}$$

$(\partial f/\partial t)_{\text{col}}$ is the total collision integral from all the electron scattering processes in the lattice. The collision integral is determined by the kinetic equation

$$\left(\frac{\partial f}{\partial t}\right)_{\text{col}}=\frac{\partial f}{\partial t}+\frac{\mathbf{F}}{\hbar}\nabla_{\mathbf{k}}f+\mathbf{v}\nabla_{\mathbf{r}}f+\frac{\partial f}{\partial\varepsilon}\Lambda_{ik}\dot{u}_{ik}; \tag{15}$$

$f(\varepsilon, \mathbf{r}, t)$ is the nonequilibrium electron distribution function, which depends on $\epsilon$, r, $t$; F is the external force acting on the electron, $u_{ik}$ is the deformation tensor.

If the metal is located in electric and magnetic fields, the external force acting on the electron is equal to

$$\mathbf{F}=e\mathbf{E}+c^{-1}[\mathbf{v}\times\mathbf{H}]; \tag{16}$$

E and H are the electric and magnetic field intensities.

Substituting (15) in (14) and (16) in (15), we find

$$F_{\text{col}}^{(i)}=-\frac{m_0}{e}\frac{\partial j^{(i)}}{\partial t}-\int_{\mathbf{k}} m_0v_i\left(\frac{\mathbf{F}}{\hbar}\nabla_{\mathbf{k}}f\right)d\tau_{\mathbf{k}}-\frac{\partial}{\partial x_k}\int_{\mathbf{k}} m_0v_iv_kfd\tau_{\mathbf{k}}, \tag{17}$$

where $\mathbf{j}$ is the current density; the term

$$\frac{\partial f}{\partial\varepsilon}\Lambda_{ik}\dot{u}_{ik}$$

does not make a contribution to the force, since the integral of $v(\partial f_0/\partial\varepsilon)\,\Lambda_{ik}$ is equal to zero. Integrating by parts in the second term, and taking it into account that

$$\sum_s\frac{\partial}{\partial k_s}F^{(s)}=\operatorname{div}_{\mathbf{k}}\mathbf{F}=0, \tag{18}$$

we write down (17) in the following form:

$$F_{\text{col}}^{(i)}=-\frac{m_0}{e}\frac{\partial j^{(i)}}{\partial t}+\int_{\mathbf{k}} f(\mathbf{k})\sum_s\frac{m_0}{m_{is}^*}F^{(s)}d\tau_{\mathbf{k}}-\int m_0v_iv_k\frac{\partial f}{\partial x_k}d\tau_{\mathbf{k}}; \tag{19}$$

here

$$\frac{1}{m_{is}^*}=\frac{1}{\hbar^2}\frac{\partial^2\varepsilon}{\partial k_i\partial k_s}$$

is the reciprocal-effective-mass tensor.

Summing (12) and (19), we obtain

$$F^{(i)}=F_{ep}^{(i)}+F_{\text{col}}^{(i)}=-\frac{m_0}{e}\frac{\partial j^{(i)}}{\partial t}+\int_{\mathbf{k}} f(\mathbf{k})F^{(i)}d\tau_{\mathbf{k}}-\frac{\partial}{\partial x_k}\int_{\mathbf{k}} m_0v_iv_kf(\mathbf{k})d\tau_{\mathbf{k}}. \tag{20}$$

Since

$$\int f(\mathbf{k})F^{(i)}d\tau_{\mathbf{k}}=enE^{(i)}+c^{-1}[\mathbf{j}\times\mathbf{H}]_i \tag{21}$$

($n$ is the electron density in the conduction band of the metal), we have

$$F_i^{(i)}=-\frac{m_0}{e}\frac{\partial j^{(i)}}{\partial t}+enE^{(i)}+\frac{1}{c}[\mathbf{j}\mathbf{H}]_i-\frac{\partial}{\partial x_k}\int m_0v_iv_kf(\mathbf{k})d\tau_{\mathbf{k}}. \tag{22}$$

At the same time, a force $Z_ieNE^{(i)}$ is exerted by the external field on the ion core of the lattice, where $Z_ieN$ is the ionic charge density of the lattice. The condition of electric neutrality

$$en+Z_ieN=0 \tag{23}$$

is satisfied in the metal with high accuracy. The total force acting on the lattice is

$$F^{(i)}=-\frac{m_0}{e}\frac{\partial j^{(i)}}{\partial t}+\frac{1}{c}[\mathbf{j}\times\mathbf{H}]_i-\frac{\partial}{\partial x_k}\int m_0v_iv_kf(k)d\tau_{\mathbf{k}}. \tag{24}$$

This expression is in complete accord with Eq. (3).

The expression (19) does not contain forces due to the inertia of the electrons in the lattice experiencing acceleration. The acceleration of the lattice $\ddot{u}_i$ makes a contribution to the force equal to $m_0nu_i$. This is equivalentto replacement in the equation of motion $F_i=\rho\ddot{u}_i$ of the density of the lattice $\rho_L$ by $\rho=\rho_m$, where $\rho_m$ is the density of the metal. The corresponding correction is $\lesssim 10^{-4}$.

Thus the difference in the results of Pekar and Tsekvava[8] and Kontorovich[9] is not connected with the scalar effective mass approximation in Ref. 8, but it holds true also for an arbitrary dispersion law, i.e., it has a fundamental character. We shall show that the difference is due to the fact that the forces of dragging of the lattice by the electrons given in Ref. 8 do not include the interactions of the electrons with the lattice deformations. When the lattice is deformed, the electron energy in the lattice changes and becomes a function of the lattice deformation $\varepsilon\equiv\varepsilon(\mathbf{k}, \mathbf{r}, u_{ik})$, where $u_{ik}$ is the deformation tensor. The dependence of the energy of the electrons on the deformation is the reason for the appearance of the deformation force.[3, 5, 7, 12]

We now consider the change in the energy of the electron upon homogeneous (quasi-homogeneous) deformation of the lattice, due to the change in the selfconsistent potential of the lattice $V_{\text{lat}}$ by an amount $\delta V_{\text{lat}}=L_{ik}u_{ik}$. Here the energy of the electron changes by an amount[20]

$$\delta\varepsilon=L_{ik}u_{ik}, \tag{25}$$

where $L_{ik}(\mathbf{k})$ is a symmetric tensor of second rank, dependent on the quasi-momentum k; $L_{ik}=L_{ki}$.

The microscopic theory of the tensor $L_{ik}$ is contained in Ref. 19. Since the tensor $L_{ik}$ determines the change in the self-consistent potential $V_{\text{lat}}$, it differs from the tensor $\Lambda_{ik}$, and in the free-electron approximation it is of course equal to zero. If the change in the energy

of the electron, due to the deformations, is of the form (25), then, according to Skobov and Kaner[7] the force $F_{def}$ corresponds to such an energy change:

$$F_{\text{def}} = \frac{\partial}{\partial x_k} \int L_{ik} f(\mathbf{k}) d\tau_{\mathbf{k}}. \tag{26}$$

We note that the connection between the electron deformation force $F_{def}$ and the mechanical stress in the lattice can be found in the following way. The elastic energy of the lattice, without account of the nonequilibrium electron subsystem, is equal to

$$\mathcal{F}_{\text{el}} = \int dv \frac{1}{2} (\rho_L \dot{u}^2 + \sigma_{ik}^{(0)} u_{ik}); \tag{27}$$

u is the displacement vector, $\sigma_{ik}$ is the tensor of the external mechanical stresses. The conduction electrons change the density of the elastic energy by an amount

$$\delta \mathcal{F}_{\text{el}}^{(e)} = u_{ik} \int L_{ik} f(k) d\tau_k. \tag{28}$$

The integral $\int L_{ik} f d\tau_k$ is equivalent to the additional electromechanical stress of the lattice $\sigma_{ik}^{(e)}$:

$$\sigma_{ik}^{(e)} = \frac{\delta \mathcal{F}_{\text{el}}^{(e)}}{\delta u_{ik}} = \int L_{ik} f(\mathbf{k}) d\tau_{\mathbf{k}}. \tag{29}$$

The body force due to the stress $\sigma_{ik}$ is equal to

$$F_{\text{def}} = \frac{\partial \sigma_{ik}}{\partial x_k} = \frac{\partial \sigma_{ik}^{(0)}}{\partial x_k} + \frac{\partial}{\partial x_k} \int L_{ik} f(\mathbf{k}) d\tau_{\mathbf{k}}. \tag{30}$$

Taking into account the force $F_{def}$, we write down the total force acting on the lattice in the form

$$F^{(i)} = -\frac{m_0}{e} \frac{\partial j^{(i)}}{\partial t} + \frac{1}{c} [\mathbf{jH}]_i + \frac{\partial}{\partial x_k} \int (L_{ik} - m_0 v_i v_k) f(\mathbf{k}) d\tau_{\mathbf{k}} + \frac{\partial \sigma_{ik}^{(0)}}{\partial x_k}. \tag{31}$$

This expression agrees with the result of Kontorvich[9] if

$$\Lambda_{ik} = L_{ik} - m_0 v_i v_k. \tag{32}$$

According to Ref. 20, the relation (32) is satisfied; thus the results of the given research are in agreement with the results of Kontorovich, [9] and the reason for the difference in his results from the results of Pekar and Tsekvava[8] is the absence in the latter of the deformation force (26). Thus, the result of Ref. 8 is shown to be incomplete, since it does not contain the force of coupling of the electrons with the lattice upon deformation of the periodic potential. Along with this, the author uses the same kinetic approach to the calculation of the forces, as in Ref. 8, assuming it to be more general, and agrees with the fact that the force should be calculated before the thermodynamic function (see Ref. 8, footnote 2). The derivation of Eq. (31) was connected with the detailed account of the forces acting on the electrons and the lattice, in particular with explicit account of the internal forces (12) acting between the electrons and the periodic potential of the lattice. We shall show that the final result can be obtained in another way, without detailed account of all the forces.

We introduce the mean momentum[2)] of the conduction electrons per unit volume, $P_e$:

$$\mathbf{P}_e = \int m_0 \mathbf{v} f(\mathbf{k}) d\tau_{\mathbf{k}} = \frac{m_e}{e} \mathbf{j}. \tag{33}$$

The momentum density of the lattice $P_{lat}$ is equal to

$$\mathbf{P}_{\text{lat}} = \rho_p \dot{\mathbf{u}}; \tag{34}$$

u is the displacement vector. We consider the physically small volume $V$ and write down the equation of motion of this volume:

$$\int dV \left\{ \frac{\partial P_e^{(i)}}{\partial t} + \frac{\partial P_p^{(i)}}{\partial t} \right\} + \oint_{S(V)} m_0 v_i v_k f dS_k = \sum F_V^{(i)}; \tag{35}$$

$S(V)$ is the surface bounding the volume $V$. The integral over the surface $S(V)$ is equal to the change in the mean momentum in the volume due to the flux of electrons across the surface $S(V)$; $\Sigma F_v$ is the sum of the external forces acting on the volume $V$.

Since the metal is electrically neutral, the sum of the electromagnetic forces is equal to $c^{-1}\,\mathbf{j} \times \mathbf{H}$. To these forces we must add the mechanical forces

$$\oint_{S(V)} \sigma_{ik} dS_k.$$

Thus,

$$\sum F_V^{(i)} = \frac{1}{c} \int [\mathbf{jH}]_i dV + \oint_{S(V)} \sigma_{ik} dS_k. \tag{36}$$

Transforming the surface integrals to volume integrals and taking (33) and (36) into account, we obtain the equation of motion of the lattice in the form

$$\rho \ddot{u}_i = \frac{\partial \sigma_{ik}}{\partial x_k} - \frac{m_0}{e} \frac{\partial j^{(i)}}{\partial t} + \frac{1}{c} [\mathbf{j} \times \mathbf{H}]_i - \frac{\partial}{\partial x_k} \int m_0 v_i v_k f d\tau_{\mathbf{k}}. \tag{37}$$

By considering (30), we obtain

$$\rho \ddot{u}_i = \frac{\partial \sigma_{ik}^{(0)}}{\partial x_k} - \frac{m_0}{e} \frac{\partial j^{(i)}}{\partial t} + \frac{1}{c} [\mathbf{j} \times \mathbf{H}]_i + \frac{\partial}{\partial x_k} \int (L_{ik} - m_0 v_i v_k) f(\mathbf{k}) d\tau_{\mathbf{k}}, \tag{38}$$

i.e., Eq. (31).

The tensor $L_{ik}$ for the free electrons is equal to zero, i.e., in this approximation, the deformation force (26) is equal to zero and the expressions (2) and (3) are identical. This is natural, since the interaction between the electrons and the field of the lattice disappears in this approximation. We note that although the integrals (3) and (26) have the same structure and can be combined into one, as is seen from the consideration of the undeformed lattice, they correspond to forces which have a different physical nature. The integral (3) corresponds to a force connected with the transfer of a mean momentum $m_0\mathbf{v}$, while the force (26) is connected only with the deformation of the periodic potential of the lattice.

The total force exerted by the conduction electrons on the lattice consists of three basic terms, each having a different physical character. We denote them by $\mathbf{F}_j$, $\mathbf{F}_H$, and $\mathbf{F}_L$ and estimate the relation of these forces, setting $\mathbf{j} = \mathbf{j}_0 e^{i\omega t}$, where $\omega$ is the frequency of the external field:

$$|F_j / F_H| = \omega / \omega_c, \tag{39}$$

where $\omega_c = eH/m_0 c$ is the cyclotron frequency of the electrons in the metal. Sometimes the force

$$\mathbf{F}_j = -\frac{m_0}{e} \frac{\partial \mathbf{j}}{\partial t}$$

is omitted in the expressions for the total force. As follows from (39), this happens only when $\omega \ll \omega_c$.

For the estimate of the force $F_L$, it is necessary to know the gradient of the nonequilibrium distribution function. When the gradient $\partial f_1/\partial x_k$ is determined by the diffuse scattering of the electrons at the surface of the metal,[14] then $\partial f_1/\partial x_x \sim f_1/l$ ($l$ is the free path length of the electrons in the metal). In this case

$$F_l \sim \frac{em_0}{e\tau}(j_s - j_0),$$

where $\tau$ is the relaxation time of the electrons in the metal, $j_s$ is the current at the surface of the metal, $j_0$ is the current in the interior, $\varepsilon$ is the coefficient of specular reflection of electrons from the surface. Then

$$F_j/F_l \sim \omega\tau\varepsilon. \tag{40}$$

If the distribution function is deformed by the sound wave, then $\partial f_1/\partial x \sim f_1/\lambda$ and

$$\frac{F_j}{F_l} \sim \omega\varepsilon\frac{\lambda}{v_F}, \quad \frac{F_H}{F_l} \sim \omega_c\tau\varepsilon^{-1}, \tag{41}$$

where $\lambda$ is the wavelength of the sound, $V_F$ is the Fermi velocity of the electron.

## 2. ELECTRON WIND FORCES ACTING ON THE LATTICE DEFECTS

The scattering of the conduction electrons by the lattice defects—impurities or diffusing atoms (ions, dislocations and so on—produces the electron wind forces, which generate motion of the defects. These forces can also be found from the equations of motion of the electrons. The motion of the electron-quasiparticle in the field of the impurity center is described by an equation similar to the Ehrenfest equation[20]:

$$\langle \dot{\hbar}\mathbf{k}\rangle = \langle \mathbf{F}_{ie}\rangle = -\left\langle \frac{\partial V_i(\mathbf{r}-\mathbf{R}_i)}{\partial \mathbf{r}}\right\rangle = -\langle \mathbf{F}_{ei}\rangle = \left\langle \frac{\partial V_i}{\partial \mathbf{R}_i}\right\rangle; \tag{42}$$

$V_i(\mathbf{r}-\mathbf{R}_i)$ is the potential of interaction of the electron with the defect, $\mathbf{r}$ and $\mathbf{R}_i$ are the coordinates of the electron and the defect. Here the potential of the lattice is absent, but the mean momentum $m_0 v$ is replaced by the quasimomentum $\hbar\mathbf{k}$. The Eq. (42) enables us to separate the interaction of the electron with the impurity center from its interaction with the periodic potential of the lattice. The electron-quasiparticle in Eq. (42) is "free" from interaction with the lattice. By averaging the value of the force (42) over all the free electrons we can find the total force acting on the defect. Direct calculation of the average value $\langle \partial V_i/\partial R_i\rangle$ turns out to be complicated. It is simpler to compute the change in the quasimomentum $\hbar\mathbf{k}$. In the transition of the electron from the state $|\mathbf{k}\rangle$ to $|\mathbf{k}'\rangle$, the momentum transferred by the electron to the scattering center is equal to (with reverse sign) the change in the quasimomentum of the electron[13,20]

$$\Delta\mathbf{p}_{\mathbf{kk}'}^{\mathbf{b}_g} = \hbar(\mathbf{k}-\mathbf{k}'-2\pi\mathbf{b}_g); \tag{43}$$

$\mathbf{b}_g$ is the reciprocal lattice vector. We note that the change in the average momentum of the electron in the scattering, $m_0(\mathbf{v}_k - \mathbf{v}_{k'})_{b_g}$ is not equal to the momentum $\Delta\mathbf{p}_{kk'}$, transferred to the defect by the electron.

The expression (43) for the transferred momentum is rigorous for the free ion, not connected with the lattice. This approximation is well satsfied for a diffusing ion, which completes the "jump" from one equilibrium position to another, i.e., in processes of electron transfer and other phenomena connected with motion of the defects in the lattice.[14] The normal ion connected with the lattice cannot always be regarded as free in the process of scattering of the electron by it. Considering the heavy ion as a classical particle, we can neglect its coupling with the lattice if the average energy transferred to the ion by the scattered electron $\delta_{ei}$ is significantly greater than the change in the potential energy of the ion $\delta u_i$ during the time of scattering $\tau_{ei} \sim 10^{-16}$ sec, i.e.,

$$\delta\varepsilon_{ei} \gg \delta u_i \sim \overline{u}_i\tau_{ei}/\tau_i; \tag{44}$$

$\tau_i$ is the period of oscillation of the ion in the lattice. This criterion is satisfied in metals as a rule.[3)]

Summing the change in the momentum transferred to the scattering center per unit time, we obtain the electron wind force

$$\mathbf{F}_{ei} = \frac{1}{N^*}\int\int_{\mathbf{kk}'}\sum_{\mathbf{b}_g}\hbar(\mathbf{k}-\mathbf{k}'-2\pi\mathbf{b}_g)\, w_{\mathbf{kk}'}^{\mathbf{b}_g} f(\mathbf{k})[1-f(\mathbf{k}')]\, d\tau_k d\tau_{k'}, \tag{45}$$

where $w_{kk'}^{b_g}$ is the probability of scattering of the electron from state $\mathbf{k}$ into $\mathbf{k}'$ in one second with transfer of momentum $\Delta\mathbf{p}_{kk'}^{b_g}$ to the defect, $f(\mathbf{k})$ is the nonequilibrium distribution function of the electrons, and $N^*$ is the concentration of defects.

Summation over the reciprocal lattice vector $\mathbf{b}_g$ is connected with the fact that from the viewpoint of momentum transfer the scattering of the electron in the transition $|k\rangle \to |k'\rangle$ is a multi-valued process, in which momenta $w\mathbf{p}_{kk'}^{b_g}$ are transferred with different probability $w_{kk'}^{b_g}$. We write

$$f(\mathbf{k}) = f_0(\mathbf{k}) + f_1(\mathbf{k}), \tag{46}$$

where $f_1(\mathbf{k})$ is the nonequilibrium addition to the equilibrium distribution function $f_0(\mathbf{k})$.

In the linear approximation of $f_1(\mathbf{k})$, the expression for $\mathbf{F}_{ei}$ can be transformed into the following form:

$$\mathbf{F}_{ei} = \frac{1}{N^*}\int\int_{\mathbf{kk}'}\sum_{\mathbf{b}_g} f_1(\mathbf{k})\,\hbar(\mathbf{k}-\mathbf{k}'-2\pi\mathbf{b}_g)\, w_{\mathbf{kk}'}^{\mathbf{b}_g} d\tau_k d\tau_{k'}. \tag{47}$$

If we neglect the umklapp processes, i.e., if we assume that $w_{kk'}^{b_g} = 0$ if $\mathbf{b}_g \neq 0$, then it is not difficult to transform (45) to the form

$$\mathbf{F}_{ei} = -\frac{1}{N^*}\int_{\mathbf{k}}\hbar\mathbf{k}\left(\frac{\partial f}{\partial t}\right)_{\text{col}}^{*} d\tau_k, \tag{48}$$

where $(\partial f/\partial t)_{\text{col}}^{*}$ is the collision integral, which is connected with the scattering of the electrons by defects:

$$\left(\frac{\partial f}{\partial t}\right)_{\text{col}}^{*} = \int_{\mathbf{k}'}\{w_{\mathbf{kk}'}^{*} f(\mathbf{k}')[1-f(\mathbf{k})] - w_{\mathbf{k}'\mathbf{k}}^{*} f(\mathbf{k})[1-f(\mathbf{k}')]\}\, d\tau_{k'}. \tag{49}$$

For specific Fermi surfaces (electron and hole) in the relaxation time approximation, the well-known expression for the electron (hole) wind force acting on the impurity center is obtained from (48) (Ref.14):

$$F_{ei}=-|e|nl\sigma_{ei}, \quad (50)$$
$$F_{hi}=|e|n_h l_h \sigma_{hi}; \quad (51)$$

$n_e(n_h)$ is the concentration of electrons (holes), $l$ ($l_h$) and $\delta_{ei}(\delta_{hi})$ are the free path lengths and the scattering cross sections of the electrons (holes) by the impurity center.

The dependence of the electron wind force on the geometry of the Fermi surface can be represented graphically if we limit ourselves to weak scattering of electrons at small angles. Then, in the quasiclassical approximation, the momentum transferred by the electron to the defect can be written down in the following form:

$$\Delta p_{kk'}^{(s)}=\hbar(\mathbf{k}_s-\mathbf{k}_s')=\hbar^2\left(\frac{\partial^2\varepsilon}{\partial k_s\partial k_l}\right)^{-1}(v_l-v_l')=m_{sl}^*(v_l-v_l'), \quad (52)$$

where

$$m_{sl}^*=\frac{1}{\hbar^2}\left(\frac{\partial^2\varepsilon}{\partial k_s\partial k_l}\right)^{-1}$$

is the effective mass tensor. Using (52), we write out the expression for the electron wind force in the following form

$$\mathbf{F}_{ei}^{(s)}=\frac{1}{N^*}\int m_{sl}^* v_l\left(\frac{\partial f}{\partial t}\right)_{\text{col}}^{*} d\tau_k. \quad (53)$$

This expression graphically illustrates the dependence of the force $F_{ei}$ on the curvature of the Fermi surface: the portions of the Fermi surface with positive curvature (electron) and the portions with negative curvature (hole) make contributions of opposing sign to the electron wind force. Using the effective mass approximation, we establish the connection between the electron wind forces and the forces acting on the lattice. We note that the electrons-quasiparticles, in processes of collision with defects, do not interact with the lattice, which follows directly from (42); therefore, using the relation (43) and summing the transferred momentum from all the electrons, we obtain the total electron wind force $\tilde{\mathbf{F}}_{ei}$ acting on all the defects and equal to the "collision" force acting on the lattice.

In the effective mass approximation, this force is equal to

$$\mathbf{F}_{\text{col}}=\tilde{\mathbf{F}}_{ei}=-\int m^*\mathbf{v}\left(\frac{\partial f}{\partial t}\right)_{\text{col}} d\tau_k. \quad (54)$$

Substituting (15) in (54), we write down

$$F_{\text{col}}^{(i)}=-\frac{m^*}{e}\frac{\partial j^{(i)}}{\partial t}+enE^{(i)}+\frac{1}{c}[\mathbf{j}\times\mathbf{H}]_i-\frac{\partial}{\partial x_k}\int m^* v_i v_k f_i(k)\,d\tau_k. \quad (55)$$

We now find the "collisionless" force of interaction of the electrons with the lattice. It follows from (4) in the effective mass approximation that

$$m_0\frac{d\mathbf{v}}{dt}=m^*\frac{d\mathbf{v}}{dt}+\mathbf{F}_{pe}, \quad (56)$$

$\mathbf{F}_{pe}$ is the force acting from the lattice on the electron. Using (56), we write down the force acting from the electron on the lattice in the following form:

$$\mathbf{F}_{ep}=-\mathbf{F}_{pe}=-\frac{(m_0-m^*)}{e}\frac{d}{dt}(e\mathbf{v})=-\frac{(m_0-m^*)}{e}\frac{\partial}{\partial t}\mathbf{j}(\mathbf{k}); \quad (57)$$

$\mathbf{j}(\mathbf{k})$ is the current generated by the electron located in the state $\mathbf{k}$.

Summing over all the electrons, we write the total expression for the "collisionless" force in the form

$$\mathbf{F}_{\text{no col}}=-\frac{(m_0-m^*)}{e}\frac{\partial\mathbf{j}}{\partial t}. \quad (58)$$

Summing (55) and (58), we obtain the total force acting from the electrons on the lattice:

$$F_{ep}^{(i)}=-\frac{m_0}{e}\frac{\partial j^{(i)}}{\partial t}+enE^{(i)}+\frac{1}{c}[\mathbf{j}\times\mathbf{H}]_i-\frac{\partial}{\partial x_k}\int m^* v_i v_k f(\mathbf{k})\,d\tau_k. \quad (59)$$

Summing (59) and the force acting on the ion "frame" of the lattice $Z_i eN\mathbf{E}$ and taking into account the condition of electrical neutrality, we find the total force in the form

$$F^{(i)}=-\frac{m_0}{e}\frac{\partial j^{(i)}}{\partial t}+\frac{1}{c}[\mathbf{j}\times\mathbf{H}]_i-\frac{\partial}{\partial x_k}\int m^* v_i v_k f(\mathbf{k})\,d\tau_k. \quad (60)$$

This expression differs from (3) by the substitution of $m^*$ for $m_0$ and is in agreement with (2) if $\Lambda_{ik}=m^* v_i v_k$.

We now show that this relation for $\Lambda_{ik}$ is satisfied in the effective mass approximation. The lattice deformation leads to the result that the electron goes from the state with wave vector $k$ to the state $k'$ with a different energy $\varepsilon(k')$. The change in energy brought about by the deformation can be written in the form

$$\delta\varepsilon(u_{ik})=\frac{\partial\varepsilon}{\partial\mathbf{p}_i}\delta p_i(u_{ik}); \quad (61)$$

p is the quasimomentum, $\delta p$ is the change in the quasimomentum due to the deformation and is equal to[21]

$$p_i'=p_i-u_{ik}p_k \quad (62)$$

or

$$\delta p_i=-u_{ik}p_k=-u_{ik}m^* v_k. \quad (63)$$

Substituting (63) in (61), we write

$$\delta\varepsilon=\Lambda_{ik}u_{ik}=-m^* v_i v_k u_{ik} \quad (64)$$

or

$$\Lambda_{ik}=-m^* v_i v_k. \quad (65)$$

We note that when the "collision" force (54) is calculated from Eq. (42), then we do not have to introduce the deformation force (26), since the interaction with the lattice is already taken into account in Eq. (54) by the replacement of the mean momentum by the quasimomentum. The term

$$\int m^* v_i v_k\frac{\partial f}{\partial x_k}d\tau_k$$

has the physical meaning of the diffusion of the quasimomentum and, in accord with (65) and (32), also contains the interaction of the electrons with the lattice and the diffusion transfer of the mean momentum.

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[1)] We have omitted the force connected with external mechanical deformations, $-u_{ik}$.

[2)] We recall that an electron in the periodic field of the lattice does not have a definite value of the real momentum, but its average momentum is a definite quantity.

[3)] The author thanks I. M. Lifshitz who called his attention to the criterion of the "quasi-free" ion in the lattice.

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# Phonon-mediated exchange interaction of impurity centers in crystals

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The interaction of impurity centers via the phonon field in ionic and atomic crystals is calculated with account taken of the permutation symmetry. The latter leads to the appearance of exchange terms in the effective-interaction operator. Estimates show that the proposed interaction is comparable in order of magnitude with the Coulomb exchange.

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1. Consider exchange interaction of two impurity centers via the crystal-lattice oscillations. The coupling of the centers with the lattice is effected by the usual electron-phonon interaction.[1)] The dependence of the energy of the indirect interaction on the spin operator is the result of allowance for the permutation symmetry. It is assumed for simplicity that the impurity centers have spin-$\frac{1}{2}$.

The initial Hamiltonian is of the form

$$\hat{H}=\hat{H}_0+\hat{H}_1, \tag{1}$$

where $\hat{H}_0$ includes the Hamiltonian of the individual centers and of the phonon system, while $\hat{H}_1$ is the operator of the interaction of the first and second centers with the lattice vibration—the perturbation operator. The orthonormalized zeroth-approximation wave functions are chosen in the form

$$[2(1\pm I_1^2)]^{-1/2}(|i\rangle\pm|j\rangle), \quad |i\rangle=a(1)b(2)|0\rangle, \quad |j\rangle=a(2)b(1)|0\rangle,$$

where a(1) and b(2) are the wave functions of the impurity centers, $|0\rangle$ is the wave function of the ground state of the phonon system, and $I_1$ is the overlap integral.

The second-order perturbation-theory correction to the system energy can be represented in the form

$$\Delta\varepsilon^{\pm}=(1\pm I_1^2)^{-2}(D_{ii}\pm D_{ij}), \tag{2}$$

where

$$D_{ij}=\sum_l{}' (E_0-E_l)^{-1}\langle i|\hat{H}_1|l\rangle\langle l|\hat{H}_1|j\rangle. \tag{3}$$

The upper sign in (2) pertains to the singlet state, and the lower to the triplet state.

Denoting the difference $\Delta\varepsilon_+ - \Delta\varepsilon_-$ by $2J_{\text{phon}}$, we can write, accurate to terms $\propto I_1^2$ (see, e.g., Ref. 2) that part of (2) which depends on the total spin of the system, in the form

$$\hat{H}_{\text{phon}}=-2J_{\text{phon}}\hat{S}_1\hat{S}_2, \quad J_{\text{phon}}=D_{ij}-2I_1^2D_{ii}. \tag{4}$$

Here $\hat{S}_1$ and $\hat{S}_2$ are respectively the operators of the electron spins of the first and second centers. The indirect-exchange operator (4) is outwardly similar to the Heisenberg Coulomb-exchange operator. Of course, these interactions are quite different in character. Since the electron-phonon interactions with the acoustic and optical lattice vibrations are different,

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