FREQUENCY DEPENDENCE OF THE ELECTRIC CONDUCTIVITY OF METALS WITH IMPURITIES

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An expression for the electric conductivity of a metal with nonmagnetic impurities is obtained on the basis of the Kubo method in which two-time Green functions are employed. The expression is valid in a broad range of external field frequencies ω and temperatures T. It is shown that at high temperatures $T \gg \Theta$ the effective electron collision frequency does not depend on the frequency ω and is proportional to T. At low temperatures $T \ll \Theta$ and frequencies $T \ll \omega \lesssim \Theta$ ($\hbar$ = k = 1) it depends significantly on ω and tends to a fixed limit when $\omega \gg \Theta$. In the case of quasilocal or local oscillations of the impurity atoms it possesses some singularities from which the frequencies on the oscillations can be determined.

1. INTRODUCTION. FORMULATION OF PROBLEM.

1. As shown by Kaganov and Zhernov[1], a consistent account of the oscillations of impurity atoms in metals leads to a number of singularities in the temperature dependence of the static electric conductivity. It turns out that the Matthiessen rule is not satisfied and the impurity part of the resistance depends significantly on the temperature.

The character of this dependence yields definite information concerning the phonon spectrum of a metal with impurities and concerning the magnitude of the amplitude of electron scattering by the impurity atoms. It is obvious that similar information can be obtained by investigating the frequency dependence of the electric conductivity of a metal with impurities, and in some cases a study of the frequency dependence may turn out to be experimentally simpler than a study of the temperature dependence.

In this paper we obtain an expression for the electric conductivity of a metal with nonmagnetic impurities; this expression is valid in a wide range of frequencies and temperatures, in which such an investigation can be performed. Using the Kubo method which was employed by us earlier[2] to study the frequency dependence of the conductivity of a metal, we generalize the result of[1] to the case of an alternating electric field.

2. Let us formulate the problem briefly. We consider a simple model of a metal, which can be described by a Hamiltonian[3]:

$$H = \sum_{n} \frac{P_n^2}{2M} + \frac{1}{2} \sum_{n,m} \Phi_{nm}^{\alpha\beta} u_n^\alpha u_m^\beta + \sum_{p} \varepsilon_p a_p^+ a_p + \sum_{n,q} A_n(q) e^{-iq u_n} \rho_{-q},$$

$$(1.1)$$

where P_n and u_n are the operators of the momentum and of the displacement of the atom with mass M_n at site n, the equilibrium position of which will be denoted by R_n^0. Here $\Phi_{nm}^{\alpha\beta} = \Phi_{mn}^{\beta\alpha}$ is the dynamic matrix of the interaction of the atoms of the alloy.

We shall retain the coordinate representation for the lattice Hamiltonian, since it is particularly convenient for the analysis of the dynamics of a lattice with impurities (see[1,4]). In the derivation of the general formulas of Sec. 2 we shall not need the assumption of invariance of the force constants $\Phi_{nm}^{\alpha\beta}$ upon penetration of the impurity atoms, or any other properties of the alloy which are not reflected explicitly in the Hamiltonian (1.1). We shall assume, however, that the scattering of the conduction electrons is weak, so that we can introduce well defined single-electron states $p = (\mathbf{p}, \sigma)$ with energy ε_p, and use the representation of second quantization with respect to these states (a_p^+ and a_p—operators of creation and annihilation of the electron in a state p; $\rho_q = \sum_p a_p^+ a_{p+q}$).

The last term in (1.1) describes electron scattering;

$$A_n(q) = (1/V) v_n(q) \exp(-i q R_n^0),$$

$v_n(q)$ is the Fourier component of the pseudopotential of the scattering of an electron by an atom in the site n, and $V = V_0 N$ is the volume of the system. The usual expansion of the function $\exp(-i q \cdot u_n)$ in the small displacement u_n will be carried out later in the equations themselves, which will enable us to obtain the Debye-Waller factors of the elastic-scattering amplitudes. The latter play an important role in the character of the temperature dependence of the impurity resistance[1]. For simplicity we shall assume that the lattice of the metal is monotonic and cubic, since a generalization to more complicated cases is of no principal difficulty. We shall assume also the frequency of the external field to be not too large, so that the interband transitions and electron-electron scattering can be neglected.

3. Inasmuch as the quantum-kinetic equation for the conduction electrons in a high-frequency field has a rather complicated form (see[5]), we shall use the Kubo method, which enables us to express the kinetic coefficients of the electric-conductivity type in terms of time-dependent correlation functions or Green's functions calculated for the equilibrium system (see[8]). The longitudinal conductivity $\sigma(\mathbf{k}, \omega)$ of interest to us, which depends on the frequency ω and on the wave vector $\mathbf{k}$ of the electric field, can be written in the form[6,2]:

$$\sigma(\mathbf{k}, \omega) = \frac{ie^2}{mk^2} \sum_p \left(\mathbf{p} + \frac{\mathbf{k}}{2}\right) \mathbf{k} G_p(\mathbf{k}, \omega), \qquad (1.2)$$

where e and m are the charge and mass of the electron and $G_p(\mathbf{k}, \omega)$ is the Fourier component of the two-particle retarded Green's function (see[6]):

$$\langle\langle a_{\mathrm{p}}^{+}(t)a_{\mathrm{p+k}}(t);\rho_{-\mathrm{k}}(t')\rangle\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} G_{\mathrm{p}}(\mathbf{k},\omega)e^{-i\omega(t-t')}d\omega. \quad (1.3)$$

Thus, the problem of calculating the electric conductivity reduces to the problem of finding the Green's function (1.3) for an equilibrium system with Hamiltonian (1.1).

In Sec. 2 we obtain an equation for the Green's function (1.3) and calculate the electric conductivity in the general case for an arbitrary frequency and temperature. In Sec. 3 we consider certain particular cases which make it possible to carry out comparison with experiment. The results of this work were briefly formulated in[7]. The solutions for single-particle Green's functions for a system with Hamiltonian (1.1) are discussed in[8].

2. CALCULATION OF ELECTRIC CONDUCTIVITY IN THE GENERAL CASE

1. Let us obtain first an equation for the two-particle retarded Green's function (1.3). As usual, using the equations of motion for the operators in the Heisenberg representation with Hamiltonian (1.1), we differentiate the Green's function (1.3) with respect to time t, as a result of which we obtain a chain of equations for the Green's functions, with increasing complexity (see[8]). By assumption, the scattering of the electrons is weak, so that we can confine ourselves to the first Born approximation, just as in[1]. This makes it possible to express approximately the more complicated Green's functions which enter into the equation for the initial function (1.3) at the square of the scattering potential in terms of two-particle functions of the type (1.3). Without taking into account electron-phonon dragging processes, this splitting takes the form (see[2])

$$\langle\langle a_{\mathrm{p}}^{+}a_{\mathrm{p+k-(q+q')}}e^{-iq'u_{m}}e^{-iqu_{n}}\cdot\rho_{-\mathrm{k}}(t')\rangle\rangle \approx \langle e^{iq(u_{n}-u_{n})}\rangle\delta_{-\mathrm{q},\mathrm{q}}G_{\mathrm{p}}(\mathbf{k},t-t'),$$
$$(2.1)$$

$$\langle\langle a_{\mathrm{p}}^{+}a_{\mathrm{p+k-q}}\rho_{-\mathrm{q}'}e^{i(q+q')u_{n}};\rho_{-\mathrm{k}}(t')\rangle\rangle$$
$$\approx \langle e^{i(q+q')u_{n}}\rangle\delta_{-\mathrm{q},\mathrm{q}}\langle\langle a_{\mathrm{p}}^{+}a_{\mathrm{p+k-q}}\rho_{-\mathrm{q}'};\rho_{-\mathrm{k}}(t')\rangle\rangle$$
$$\approx \delta_{-\mathrm{q},\mathrm{q}'}[(1-n_{\mathrm{p+k-q}})G_{\mathrm{p}}(\mathbf{k},t-t') - n_{\mathrm{p}}G_{\mathrm{p}}(\mathbf{k},t-t')], \quad (2.2)$$

where $n_{\mathrm{p}} = \langle a_{\mathrm{p}}^{+}a_{\mathrm{p}}\rangle$ is the average number of electrons in the state $\mathbf{p}$. This approximation, however, still does not lead to a close system of equations as in[2], since factors of the type $\exp(-i\mathbf{q}\cdot\mathbf{u}_{n})$, describing multiphonon processes of scattering in the Hamiltonian (1.1), appear in the equations. Taking into account only single-phonon inelastic scattering processes, we expand in the resultant equations in powers of the displacement $\mathbf{u}_{n}$, retaining in the terms with the inelastic scattering only the lowest order, for example:

$$\langle\exp[-i\mathbf{q}(\mathbf{u}_{n}-\mathbf{u}_{m})]\rangle$$
$$= \exp(-W_{n}/2)\exp(-W_{m}/2)\exp\langle(\mathbf{q}\mathbf{u}_{n})(\mathbf{q}\mathbf{u}_{m})\rangle$$
$$\approx \exp(-W_{n}/2)\exp(-W_{m}/2) + \langle(\mathbf{q}\mathbf{u}_{n})(\mathbf{q}\mathbf{u}_{m})\rangle, \quad (2.3)$$

where the first term corresponds to elastic scattering with allowance for the Debye-Waller factors $W_{n}(\mathbf{q})$ = $\langle(\mathbf{q}\cdot\mathbf{u}_{n})^{2}\rangle$, the second term describing single-phonon scattering.

By performing such an expansion in the equations themselves, and not in the initial Hamiltonian (1.1), we are able to take into account that aggregate of multiphonon processes, which determines the Debye-Waller fac-

tors. Indeed, the splitting (2.1) and (2.2) corresponds to independent averaging over the states of the lattice and of the electron system, the first denoting precisely averaging over the positions of the atoms, i.e., introduction of the Debye-Waller factor into the scattering amplitude. We emphasize here that the Debye-Waller factors are exactly equal to zero for the second function (2.2), which describes the effective electron-electron scattering induced by phonons, since by virtue of momentum conservation we have in this exchange scattering $\mathbf{q}' = -\mathbf{q}$ and the displacement $\mathbf{u}_{n}$ is multiplied by a zero momentum.

As a result of the foregoing approximations we obtain the following system of equations for the Fourier components of the Green's functions (1.3):

$$(\omega + \omega_{\mathrm{pk}})G_{\mathrm{p}}(\mathbf{k},\omega) = (n_{\mathrm{p}} - n_{\mathrm{p+k}})$$
$$+ \sum_{nq}A_{n}(\mathbf{q})\langle\langle(a_{\mathrm{p}}^{+}a_{\mathrm{p+k-q}} - a_{\mathrm{p+q}}^{+}a_{\mathrm{p+k}})(1-iqu_{n})|\rho_{-\mathrm{k}}\rangle\rangle_{\omega}, \quad (2.4)$$

$$(\omega + \omega_{\mathrm{p k-p}})\langle\langle a_{\mathrm{p}}^{+}a_{\mathrm{p+k-q}}|\rho_{-\mathrm{k}}\rangle\rangle_{\omega} = \langle(a_{\mathrm{p}}^{+}a_{\mathrm{p-q}} - a_{\mathrm{p+k}}^{+}a_{\mathrm{p+k-q}})\rangle$$
$$+ \sum_{m}A_{m}(-\mathbf{q})e^{-W_{n}/2}e^{-W_{m}/2}\{G_{\mathrm{p}}(\mathbf{k},\omega) - G_{\mathrm{p-q}}(\mathbf{k},\omega)\}, \quad (2.5)$$

$$M_{n}(\omega + \omega_{\mathrm{p k-q}})^{2}\langle\langle a_{\mathrm{p}}^{+}a_{\mathrm{p+k-q}}u_{n}^{\alpha}|\rho_{-\mathrm{k}}\rangle\rangle_{\omega}$$
$$= B_{\mathrm{p k-q}\,n}^{\alpha}(\omega) + \sum_{m}\Phi_{nm}^{\alpha\gamma}\langle\langle a_{\mathrm{p}}^{+}a_{\mathrm{p+k-q}}u_{m}^{\gamma}|\rho_{-\mathrm{k}}\rangle\rangle_{\omega_{1}} \quad (2.6)$$

where

$$\omega_{\mathrm{pk}} = \varepsilon_{\mathrm{p}} - \varepsilon_{\mathrm{p+k}},$$
$$B_{\mathrm{p k-q}\,n}^{\alpha}(\omega) = M_{n}\left\langle(a_{\mathrm{p}}^{+}a_{\mathrm{p-q}} - a_{\mathrm{p+k}}^{+}a_{\mathrm{p+k-q}})\right.$$
$$\times\left\{(\omega + \omega_{\mathrm{p k-q}})u_{n}^{\alpha} + \frac{i}{M_{n}}P_{n}^{\alpha}\right\}\rangle + iq^{\alpha}A_{n}(-\mathbf{q})\{(1-n_{\mathrm{p+k-q}})G_{\mathrm{p}}(\mathbf{k},\omega)$$
$$- n_{\mathrm{p}}G_{\mathrm{p-q}}(\mathbf{k},\omega)\} + \{G_{\mathrm{p}}(\mathbf{k},\omega) - G_{\mathrm{p-q}}(\mathbf{k},\omega)\}$$
$$\times\sum_{m}A_{m}(-\mathbf{q})M_{n}\left\langle i(\mathbf{q}u_{m})\left\{(\omega + \omega_{\mathrm{p k-q}})u_{n}^{\alpha} + \frac{i}{M_{n}}P_{n}^{\alpha}\right\}\right\rangle. \quad (2.7)$$

In order to solve the integral equation (2.6) for the Green's function describing the inelastic scattering processes, we shall use the equation for the phonon Green's function in the coordinate representation

$$D_{nn'}^{\alpha\beta}(E) \equiv \langle\langle u_{n}^{\alpha}|u_{n'}^{\beta}\rangle\rangle_{E}:$$
$$M_{n}E^{2}D_{nn'}^{\alpha\beta}(E) = \delta_{nn'}^{\alpha\beta} + \sum_{m}\Phi_{nm}^{\alpha\gamma}D_{mn'}^{\gamma\beta}(E), \quad (2.8)$$

in which we can neglect the interaction of the phonons with the electrons (see[8]). Multiplying (2.6) by $D_{nn'}^{\alpha}(\omega + \omega_{\mathrm{p,k-q}})$ and summing over n and α, we obtain

$$\langle\langle a_{\mathrm{p}}^{+}a_{\mathrm{p+k-q}}u_{n}^{\alpha}|\rho_{-\mathrm{k}}\rangle\rangle_{\omega} = \sum_{n'}D_{nn'}^{\alpha\beta}(\omega + \omega_{\mathrm{p,k-q}})B_{\mathrm{p k-q}n'}^{\beta}(\omega). \quad (2.9)$$

To calculate $\langle a_{\mathrm{p}}^{+}a_{\mathrm{p-q}}\rangle$, $\langle a_{\mathrm{p}}^{+}a_{\mathrm{p-q}}u_{n}^{\alpha}\rangle$ $(\mathbf{q}\neq 0)$, and other mean values on the right side of (2.5) and (2.6) we use the equation

$$i\frac{d}{dt}\langle a_{\mathrm{p}}^{+}a_{\mathrm{p-q}}\exp(-i\mathbf{q}\mathbf{u}_{n})\rangle = 0,$$

which we solve in the same approximation as the equation for the Green's functions (2.5) and (2.6).

Substituting (2.5) and (2.9) in (2.4), we obtain a closed equation for the two-particle Green's function (see[2]):

$$(\omega + \omega_{\mathrm{pk}})G_{\mathrm{p}}(\mathbf{k},\omega) = (n_{\mathrm{p}} - n_{\mathrm{p+k}}) +$$
$$+ \sum_{nmq}A_{n}(\mathbf{q})A_{m}(-\mathbf{q})\exp(-W_{n}/2)\exp(-W_{m}/2)$$
$$\times\left\{[f_{\mathrm{p,p+q}} - f_{\mathrm{p+k,p+k+q}}]\left(\frac{1}{\omega + \omega_{\mathrm{p,k+q}}} - \frac{1}{\omega + \omega_{\mathrm{p+q,k-q}}}\right)\right.$$

$$+ [G_p(k, \omega) - G_{p+q}(k, \omega)] \left(\frac{1}{\omega + \omega_{p, k+q}} + \frac{1}{\omega + \omega_{p+q, k-q}} \right) \Big\}$$

$$+ \sum_{nmq} A_n(q) A_m(-q) \frac{1}{\pi} \int_{-\infty}^{\infty} dE \left[-\operatorname{Im} \langle\!\langle qu_n) | (qu_m) \rangle\!\rangle_{E+i\delta} \right]$$

$$\times \Big\{ \Big[\frac{f_{p,\, p-q}(E) - f_{p+k,\, p+k-q}(E)}{\omega + \omega_{p, k-q} - E} - \frac{f_{p+q,\, p}(E) - f_{p+k+q,\, p+k}(E)}{\omega + \omega_{p+q, k-q} - E} \Big]$$

$$+ \Big[\Big(\frac{1 - n_{p+k-q} + N(E)}{\omega + \omega_{p, k-q} - E} + \frac{n_{p+q} + N(E)}{\omega + \omega_{p+q, k-q} - E} \Big) G_p(k, \omega)$$

$$- \Big(\frac{1 - n_{p+} + N(E)}{\omega + \omega_{p+q, k-q} - E} G_{p+q}(k, \omega) + \frac{n_p + N(E)}{\omega + \omega_{p, k-q} - E} G_{p-q}(k, \omega) \Big) \Big] \Big\},$$

$$(2.10)$$

where

$$f_{p,\, p+q} = (n_p - n_{p+q})(\omega_{p, q})^{-1},$$

$$f_{p,\, p+q}(E) = [n_p(1 - n_{p+q}) + N(E)(n_p - n_{p+q})](\omega_{p, q} - E)^{-1},$$

$N(E) = e^{E/T} - 1)^{-1}$, and T is the temperature in energy units. To simplify the notation in the second sum of (2.10), we used the relation

$$\sum_{n'} D_{nn'}^{\alpha\beta}(\omega) M_{n'} \Big\{ \langle u_m{}^\gamma u_{n'}{}^\beta \rangle \omega + \Big\langle u_m{}^\gamma \frac{i}{M_{n'}} P_{n'}{}^\beta \Big\rangle \Big\}$$

$$= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dE}{\omega - E} N(E)[-\operatorname{Im} D_{nm}^{\alpha\gamma}(E + i\delta)], \quad \delta = 0^+,$$

which can be readily obtained by introducing spectral expansions for the correlation functions and by using Eq. (2.8) (see[8]).

Thus, taking into account the scattering of the electrons in the Born approximation and considering only single-photon inelastic processes, we obtained a closed integral equation for the Green's function, similar to the quantum kinetic equation for the nonequilibrium distribution function in an approximation linear in the external field[5]. The first sum in the right side of (2.10) describes the elastic processes of scattering with allowance for the Debye-Waller factor. The second sum, which contains the integral with respect to the frequencies of the imaginary part of the phonon Green's function, describes inelastic scattering processes of electrons both by the oscillations of the atoms of the main lattice, and by the impurities, as well as their interference.

We note one characteristic feature of this equation. The right side of (2.10) contains, besides the "collision term" which contains the Green's function, also an inhomogeneous term of second order in the scattering potential (the first square brackets in both sums). It describes the electron scattering induced by the external electric field[9]. In the case of low frequencies ($\omega\tau \ll 1$, τ—characteristic relaxation time of the system) this term is small and the principal role is played by the "collision term"[2,9]. On the other hand, in the case of high frequencies ($\omega\tau \gg 1$) it plays a principal role, whereas the collision term can be treated by perturbation theory. Therefore, going over to the solution of (2.10), let us consider the two indicated frequency regions separately.

2. Low-frequency conductivity ($\omega\tau \ll 1$). We consider the case of a weak spatial inhomogeneity, when the electric field changes little over the characteristic length of the system $1/k \gg a \sim 1/p_F$ (p_F— Fermi momentum). We can then expand in (2.10) with respect to k, retaining only the linear terms. Assuming further that in the reg-

ion of low frequencies the behavior of the electrons in the electric field is characterized by an effective collision frequency $\gamma_p(\omega)$ that depends on the frequency ω, we seek the Green's function in the form[2]

$$G_p(k, \omega) = -\frac{\partial n_p}{\partial \varepsilon_p} \frac{kp}{m} \frac{1}{\omega + i\gamma_p(\omega)}. \quad (2.11)$$

Neglecting in (2.10) the inhomogeneous terms of second order in the scattering potential, in view of their smallness, and taking into account only the imaginary part of the "collision term," a part determining the relaxation processes in the system, we obtain for the effective damping of the Green's function $\gamma_p(\omega)$ the equation

$$\gamma_p(\omega) \frac{\partial n_p}{\partial \varepsilon_p} = \sum_{qnm} A_n(q) A_m(-q) \Big\{ \exp(-W_n/2) \exp(-W_m/2)$$

$$\times \Big[\frac{\partial n_p}{\partial \varepsilon_p} - \frac{k(p+q)}{kp} \frac{\partial n_{p+q}}{\partial \varepsilon_{p+q}} \Big] \pi [\delta(\omega + \omega_{p,q}) + \delta(\omega - \omega_{p,q})]$$

$$+ \int_{-\infty}^{\infty} dE \left[-\operatorname{Im} \langle\!\langle qu_n) | (qu_m) \rangle\!\rangle_{E+i\delta} \right] \cdot$$

$$\times \Big[\Big\{ (n_{p+q} + N(E)) \frac{\partial n_p}{\partial \varepsilon_p} - (1 - n_p + N(E)) \frac{k(p+q)}{kp} \frac{\partial n_{p+q}}{\partial \varepsilon_{p+q}} \Big\} \cdot$$

$$\delta(\omega - \omega_{p,q} - E) + \Big\{ (1 - n_{p-q} + N(E)) \frac{\partial n_p}{\partial \varepsilon_p} +$$

$$- (n_p + N(E)) \frac{k(p-q)}{kp} \frac{\partial n_{p-q}}{\partial \varepsilon_{p-q}} \Big\} \delta(\omega - \omega_{p, -q} - E) \Big] \Big\}. \quad (2.12)$$

Since the Green's function (2.11) for electrons in a metal differs from zero only in a narrow layer $T \ll \mu_0$ (μ_0— Fermi energy), it follows that to calculate the conductivity (1.2) it is sufficient to determine the function $\gamma_p(\omega)$ only at $p \sim p_F$. The value of this function, averaged over the Fermi surface, is obtained by integrating with respect to ϵ_p the equation (2.12) from which we omit, by virtue of the indicated singularity, the terms

$$|(\omega + i\gamma_p)/(\omega + i\gamma_{p'})| \approx |(\omega + i\gamma_{p_F})/(\omega + i\gamma_{p_F})| = 1$$

of the functions $\partial n_{p\pm q}/\partial \epsilon_{p\pm q}$ in the right side. In the integration we take account of the fact that $\omega \ll \mu_0$ and $E_0 \ll \mu_0$, where E_0 is the maximum lattice-vibration oscillation frequency, so that $\operatorname{Im} D_{nn'}^\alpha(E) = 0$ when $E > E_0$. Since for a cubic crystal we have

$$\sum_{nm} v_n(q) v_m(-q) \exp \{-iq(R_n^0 - R_m^0)\} \operatorname{Im} \langle\!\langle qu_n) | (qu_m) \rangle\!\rangle_E = J(q^2, E)$$

It is easy to perform the integration with respect to the direction of the vector q, as a result of which we obtain for the mean value of the damping

$$\bar\gamma(\omega, T) = \frac{\pi N_F}{2 p_F^4} \int_{\omega/v_F}^{q_0} q^3 dq \frac{1}{V} \sum_{nm} v_n(q) v_m(-q)$$

$$\times \exp\{-iq(R_n^0 - R_m^0)\} \Big\{ \exp(-W_n/2) \exp(-W_m/2)$$

$$+ \frac{1}{\pi} \int_0^\infty dE \left[-\operatorname{Im} \langle\!\langle qu_n) | (qu_m) \rangle\!\rangle_{E+i\delta} \right] F\Big(\frac{E}{T}, \frac{\omega}{T} \Big) \Big\}, \quad (2.13)$$

where N_F is the electron-state density on the Fermi surface, q_0 is the maximum phonon momentum ($q_0 \leq 2p_F$) and the function $F(E/T, \omega/T)$ is equal to the function

$$F_1\Big(\frac{E}{T}, \frac{\omega}{T} \Big) = \frac{E - \omega}{T} N(E - \omega)(1 + N(E - \omega))$$

$$+ \frac{E + \omega}{T} N(E + \omega)(1 + N(E + \omega)) + 2N(E) - N(E - \omega) - N(E + \omega),$$

$$(2.14)$$

where we took account of the fact that

$$\operatorname{Im} D_{nm}^{\alpha\beta}(E + i\delta) = -\operatorname{Im} D_{nm}^{\alpha\beta}(-E + i\delta).$$

(The integration method is described in greater detail in[2].)

Expression (2.13) determines the effective frequency of the collisions between the electrons and the lattice for a specified impurity configuration. Inasmuch as the samples investigated in experiments are always of macroscopic dimensions, in which averaging actually takes place over different impurity configurations, the expression (2.13) must also be averaged over the impurity arrangements. We shall not designate this averaging specially by the symbol $\langle\ldots\rangle_c$, implying this averaging in all the concrete calculations.

Now substituting (2.13) in the expression (2.11) for the Green's function we obtain from (1.2) the conductivity of the system in the case of low frequencies. When $k \to 0$ it takes the form

$$\sigma(\omega) = ne^2 m^{-1}(\overline{\gamma}(\omega, T) - i\omega)^{-1}, \quad (2.15)$$

where n is the density of the conduction electrons. When $\omega = 0$ we get from (2.13)–(2.15) the expression for the resistance in the static case:

$$\rho(T) = \frac{1}{\sigma(0)} = \frac{m}{ne^2}\overline{\gamma}(0, T). \quad (2.15a)$$

We see that it coincides with the expression obtained in[1], apart from the Debye-Waller factors in inelastic scattering, which we have left out in some of the terms because of their smallness (see (2.13)) and which vanish in other terms (see (2.2)). As follows from[1], the resultant difference is insignificant, and two-phonon transitions must be considered for its evaluation.

3. High-frequency conductivity ($\omega\tau \gg 1$). In this case we solve (2.10) by an iteration procedure, substituting in the "collision term" the Green's function of the free electrons. In this case the term is canceled by the inhomogeneous terms that are of second order in the scattering potential (see[9,2]), as a result of which we get for the imaginary part of the Green's function of second order as $k \to 0$

$$\operatorname{Im} G_p^{(2)}(k, \omega + i\delta) = -\frac{\pi}{\omega^3}\sum_{nmq}A_n(q)A_m(-q)\frac{qk}{m}$$

$$\times \Big\{ e^{-W_n/2}e^{-W_m/2}(n_p - n_{p+q})[\delta(\omega + \omega_{p,q}) - \delta(\omega - \omega_{p,q})]$$

$$+ \frac{1}{\pi}\int_{-\infty}^{\infty}dE[-\operatorname{Im}\langle\!\langle(qu_n)|(qu_m)\rangle\!\rangle_{E+i\delta}][\{n_p(1 - n_{p-q}) \quad (2.16)$$

$$+ N(E)(n_p - n_{p-q})\}\delta(\omega + \omega_{p,q} - E) - \{n_{p+q}(1 - n_p)$$

$$+ N(E)(n_{p+q} - n_p)\}\delta(\omega - \omega_{p,q} - E)]\Big\}$$

Substituting (2.16) in (1.2) we obtain after integration with respect to p and q an expression for the real part of the second-order conductivity, which determines when $k \to 0$ the volume absorption of the high-frequency field,

$$\operatorname{Re}\sigma^{(2)}(\omega) = \frac{ne^2}{m\omega^2}\gamma(\omega, T), \quad (2.17)$$

where the effective collision frequency $\gamma(\omega, T)$ is determined by the same expression (2.13), in which the function $F(E/T, \omega/T)$, which determines the temperature dependence of the inelastic scattering, takes the form[5,2]

$$F_2\left(\frac{E}{T}, \frac{\omega}{T}\right) = 2N(E) - \left(1 - \frac{E}{\omega}\right)N(E - \omega) - \left(1 + \frac{E}{\omega}\right)N(E + \omega). \quad (2.18)$$

The obtained results (2.15) and (2.17) allow us to investigate the conductivity of a metal with impurities in a wide interval of frequencies and temperatures. The general form of these equations imposes no limitations whatever on the character of the lattice effect. It is only necessary that the electron scattering be sufficiently weak, to be able to introduce single-electron states with definite energy ϵ_p and to use the Born approximation of the scattering, when simple decoupling of (2.1) and (2.2) is possible. Within the framework of this method, it is easy also to take into account the multiphonon transitions in scattering. In the next section we shall consider certain particular cases of these formulas.

3. FREQUENCY DEPENDENCE OF ELECTRIC CONDUCTIVITY OF A METAL WITH IMPURITIES

Let us consider the temperature and frequency dependences of the effective collision frequency or damping (2.13) in different limiting cases. As shown in[2a], the frequency dependence of the elastic part of the impurity scattering turns out to be appreciable at frequencies $\omega \sim \mu_0$. In our case $\omega \ll \mu_0$, so that the lower limit of integration in (2.13) is $\omega/v_F \approx 0$, and therefore the elastic part of the damping does not depend on the frequency ω. At low impurity concentration ($c \ll 1$) it can be represented in the form (see[1])

$$\gamma_1(T) = c\eta M \int_0^{q_0} q^3 dq|\Delta b(q)|^2, \quad (3.1)$$

where we introduced the notation

$$\eta = \frac{\pi N_F}{2p_F^4}\frac{1}{MV_0}, \quad \Delta b = b_1 - b_0, \quad b_{1,0} = v_{1,0}\exp\left(-\frac{W_{1,0}}{2}\right). \quad (3.2)$$

The inelastic part of the damping is written in the form

$$\gamma'(\omega, T) = \gamma_0(\omega, T) + \Delta\gamma(\omega, T), \quad (3.3)$$

where

$$\gamma_0(\omega, T) = \gamma_0\left(\frac{T}{\Theta}\right)^5 2\int_0^{\Theta/T}x^4 dx F(x, \alpha) \quad (3.4)$$

is the damping for a pure metal without impurities (see[10,5,2b]); Θ is the Debye temperature. For the integration in (3.4) we use the explicit expression for the phonon Green's function of an ideal crystal (see, e.g.,[1]) and take into account scattering by longitudinal oscillations only, putting approximately $|v_0(q)|^2 \approx |v_0(0)|^2$, $\omega_q = sq$ (s—speed of sound), and also introducing the dimensionless variables

$$x = \frac{\omega_q}{T}, \quad \alpha = \frac{\omega}{T}, \quad \gamma_0 = \Theta\eta\frac{|v_0(0)|^2 q_0^6}{4s^6}, \quad \Theta = sq_0 \quad (3.5)$$

The frequency-temperature dependence of the damping in a pure metal (3.4) was investigated in[2b] and is therefore not considered here.

Going over to a discussion of the inelastic part of the impurity damping, we note that its temperature-frequency dependence is expressed in explicit form by the functions F_1 (2.14) or F_2 (2.18), so that we can draw certain general conclusions without using concrete representations for the phonon Green's function.

1. We consider first the simpler case of high temperatures, when $T \gg E_0$ (E_0—maximum frequency of the lattice vibrations). In this case the lattice vibrations can be treated classically, and the results of the ordinary kinetic equation should be valid. Indeed, the limiting value of the function (2.14) for low frequencies at $\omega \ll \gamma \sim T$ coincides with the value of the function F_2 (2.18) for high frequencies: when $\omega \gg \gamma \gtrsim E_0$ we have

$$F_1(x \ll 1, a \ll 1) \approx 2T/E, \quad F_2(x, a \gg x) \approx \operatorname{cth}(E/2T) \approx 2T/E.$$

Thus, in the case of high temperatures the collision frequency (2.13) does not depend on the frequency of the external field ω and turns out to be equal to the classical high-temperature value

$$\gamma^{\text{cl}}(T) = \gamma_1(T) + T\frac{\eta M}{\pi N}\int_0^\infty \frac{dE^2}{E^2}\sum_{nmq} v_n(\mathbf{q})v_m(-\mathbf{q})$$
$$\times \exp\{-i\mathbf{q}(\mathbf{R}_n{}^0 - \mathbf{R}_m{}^0)\}[-\operatorname{Im}\langle\!\langle(\mathbf{q}u_n)|(\mathbf{q}u_m)\rangle\!\rangle_{E+i\delta}]. \tag{3.6}$$

The obtained expression makes it possible to draw a general conclusion concerning the proportionality of the total resistance (2.15a), including its impurity part, to the temperature T in the case of high temperatures. A more detailed analysis of expression (3.6) with a concrete choice of the phonon Green's functions is given in[1].

2. In the case of low temperatures $T \ll \Theta$, and at frequencies $\omega \gg T$ the quantum character of the external field appears: the electrons, acquiring an energy quantum ω ($\hbar = 1$) from the high-frequency field, are scattered by the lattice vibrations, exciting phonons with frequencies $E \ll \omega$. Indeed, the function (2.18) for $\omega \gg T$ is of the form

$$F_2\left(\frac{E}{T}, \frac{\omega}{T} \gg 1\right) \approx 2N(E) - \left(1 - \frac{E}{\omega}\right)N(E - \omega),$$

where the first term describes scattering by thermal vibrations and can be neglected because of its smallness, $\sim (T/\Theta)^5 \ll 1$; the second term describes the scattering of electrons with energy ω by photons with energies $E \le \omega$. Substituting F_2 in (2.13), we obtain an expression for the damping in the quantum limit ($T \ll \omega$, $T \ll \Theta$):

$$\gamma_{\text{qu}}(\omega) = \gamma_1(T) + \frac{\eta M}{\pi N}\int_0^\omega dE\left(1 - \frac{E}{\omega}\right)\sum_{nmq} v_n(\mathbf{q})v_m(-\mathbf{q})$$
$$\times \exp\{-i\mathbf{q}(\mathbf{R}_n{}^0 - \mathbf{R}_m{}^0)\}[-\operatorname{Im}\langle\!\langle(\mathbf{q}u_n)|(\mathbf{q}u_m)\rangle\!\rangle_{E+i\delta}]. \tag{3.7}$$

Let us consider first the case of low frequencies $\omega \ll \Theta$, when it is possible to use the high-frequency representation for the phonon Green's functions, and let us assume the model proposed in[1] for a crystal with impurities. Then, using the explicit form of the Green's functions obtained in[1] in an approximation that is linear in the impurity concentration, we obtain

$$\gamma(\omega) = \gamma_0(\omega) + \gamma_1(T) + \gamma_2(\omega) + \gamma_3(\omega) + \gamma_4(\omega), \tag{3.8}$$

where

$$\gamma_0(\omega) = 0{,}4\gamma_0\left(\frac{\omega_1}{\Theta}\right)^5\left(1 - \frac{5}{6}\frac{\omega_1}{\omega}\right); \tag{3.4a}$$

$$\gamma_2(\omega) = 0{,}4\gamma_0 c(-2\varepsilon)\left(\frac{\omega_1}{\Theta}\right)^5\left(1 - \frac{5}{6}\frac{\omega_1}{\omega}\right),$$

$$\gamma_3(\omega) = 2\gamma_0 cg_1 d\left(\frac{\omega_1}{\Theta}\right)^2\left\{1 - \frac{2}{3}\frac{\omega_1}{\omega} - \varepsilon\left\langle\frac{1}{E^2}\right\rangle\Theta^2\left(\frac{\omega_1}{\Theta}\right)^2\right\},$$

$$\gamma_4(\omega) = 2\gamma_0 cg_3 d(-\varepsilon)\left(\frac{\omega_1}{\Theta}\right)^4\left(1 - \frac{4}{5}\frac{\omega_1}{\omega}\right)$$
$$+ 0{.}8\gamma_0 cg_2\left(\frac{\omega_1}{\Theta}\right)^5\left(1 - \frac{5}{6}\frac{\omega_1}{\omega}\right). \tag{3.9}$$

Here $\epsilon = 1 - M_1/M$, d is a numerical coefficient in the low-frequency representation for the distribution function of the squares of the frequencies of the phonon spectrum of the matrix $g(E^2) \approx Ed/\Theta^3$. The quantity $\langle 1/E^2\rangle$ is the value of $1/E^2$ averaged over the phonon spectrum of the matrix. For the sake of generality, we introduce the maximum frequency of the phonons taking part in the scattering, $\omega_1 = \min\{\omega, \Theta\}$. However, formulas (3.9) were obtained under the assumption $\omega \ll \Theta$, i.e., $\omega_1 = \omega$, and then the coefficients g_1, g_2, and g_3 take the simple form (see[1]):

$$g_1 = \frac{1}{q_0{}^6|v_0(0)|^2}\int_0^{q_0} q^5 dq|\Delta v(\mathbf{q})|^2, \quad g_2 = \frac{\Delta v(0)}{v_0(0)},$$

$$g_3 = \frac{\Theta^2}{q_0|v_0(0)|^2}\int_0^{q_0} q^5 dq\frac{\Delta v(\mathbf{q})v_0(\mathbf{q})}{\omega_{\mathbf{q}}{}^2}. \tag{3.10}$$

We see that the obtained expressions have the same form as formulas (3.9) of[1] for the low temperature resistance, except that in our case the role of the temperature T, which determines there the maximum energy of the phonons taking part in the scattering, is played by the frequency of the external field ω. An essential difference arises, however, when the frequency of the external field ω becomes larger than the frequency of the continuous spectrum Θ, and the damping (3.7) ceases to increase so rapidly with frequency ($\omega_1 = \Theta$). When $\omega \gg E_0$ it tends to a constant limit, for in this case it is possible to leave out from (3.7) the term with $E/\omega \ll 1$, and the limit of integration with respect to E can be replaced by E_0. For rough estimates it is possible to use in the transition frequency region $\omega < \Theta$ the formulas (3.9), but the coefficients g_1, g_2, and g_3 will not be determined by the expression (3.10). (The singularities of the behavior of the damping (3.9) near quasilocal or local frequencies will be considered below.)

We thus arrive at the conclusion that the impurity part of the damping at frequencies $\omega \lesssim \Theta$ depends significantly on the frequency of the external field ω, as a result of which the conductivity (2.17) can have a very complicated frequency dependence. Unfortunately, this region of frequencies $\omega \lesssim \Theta$ is very difficult to investigate experimentally, and we shall therefore not stop for a more detailed analysis, which is quite similar to the analysis given in[1]. We note only two features of greatest interest.

A. In the case of a sufficiently heavy impurity ($|\epsilon| \gg 1$), a quasilocal level with frequency $E_* = (|\epsilon|\langle 1/E^2\rangle)^{-1/2}$ can appear (see[1]). In this case formulas (3.9) are valid only at frequencies $\omega \ll E_*$. In the vicinity of the quasilocal frequency there is observed a fast growth of the attenuation, connected with the "inclusion" in the scattering process of quasilocal oscillations with large density near the frequency E_* itself. The main increment is produced by the function $\gamma_2(\omega)$:

$$\Delta\gamma_2(\omega \gtrsim E_\bullet) \approx c\gamma_0\left(\frac{E_\bullet}{\Theta}\right)\left(1 - \frac{E_\bullet}{\omega}\right), \tag{3.11}$$

where we used the resonant behavior of the Green's function near $E \approx E_*$ (see[1]). This maximum can be

noted on the $\sigma^{(2)}(\omega)$ plot by choosing the parameters such that

$$\frac{\Delta\gamma_2(\omega \gtrsim E_\bullet)}{\gamma_0(\omega \sim E_\bullet)} \approx c\left(\frac{\Theta}{E_\bullet}\right)^4 \approx c|\varepsilon|^2 \sim 1.$$

Analyzing the form of the $\sigma^{(2)}(\omega)$ plot, we can determine the quasilocal frequency—it will lie at the start of the rapid growth of $\sigma^2(\omega)$.

B. In the opposite case of very light impurity $(1 - \epsilon \ll 1)$ there can appear a local level with frequency $E_0 \approx (\langle E^2\rangle/(1 - \epsilon))^{1/2}$. If $E_0 \gg \Theta$, then all the Green's functions have the same form at $E \approx E_0$, accurate to terms $(\omega_q/E_0) \ll 1$:

$$\left\langle \frac{1}{N}\sum_{nm} \exp\left\{-iq(R_n^0 - R_m^0)\right\}\mathrm{Im}\langle\!\langle(qu_n)|(qu_m)\rangle\!\rangle_{E+i\delta}\right\rangle_c$$

$$\approx -\frac{c}{1-\varepsilon}q^2\frac{\pi}{M}\mathrm{sign}\,E\delta(E^2 - E_0^2). \quad (3.12)$$

Substituting in (2.13) and integrating with respect to $E > \Theta$, we obtain for the damping due to the scattering by the local oscillations

$$\Delta\gamma_{\mathrm{loc}}(\omega, T) = 2\gamma_0\frac{c}{1-\varepsilon}\frac{\Theta}{E_0}\bar{g}_1 F\left(\frac{E_0}{T}, \frac{\omega}{T}\right) \quad (3.13)$$

where

$$\bar{g}_1 = \frac{1}{q_0^6|v_0(0)|^2}\int_0^{q_0} q^5 dq|v_1(q)|^2,$$

i.e., only impurity atoms take part in the scattering. In the frequency region of interest to us $\omega \gg T$, $\omega \geq E_0 \gg \Theta$, we get

$$\Delta\gamma_{\mathrm{loc}}(\omega) = 2\gamma_0\frac{c}{1-\varepsilon}\frac{\Theta}{E_0}\bar{g}_1\left(1 - \frac{E_0}{\omega}\right), \quad (3.13a)$$

i.e., it can have an appreciable value at $(1 - \epsilon) \ll 1$ and $\bar{g}_1 \sim 1$. Therefore the increase of the absorption $\sigma^{(2)}(\omega)$ in the region of frequencies lying above the continuous spectrum of the lattice vibrations can offer evidence of the presence of local oscillations, the frequency of which can be determined from relations (3.13) and (3.13a). We note that when $E_0 \gg \Theta$ the local frequencies lie in a region accessible to experimental observation, requiring radiation with wavelengths in the far infrared region, $\lambda \gtrsim 10~\mu$.

In concluding this section we note that in the case of low temperatures and high frequencies, a noticeable contribution to the collision frequency is made by electron-electron scattering[11]. However, in the region of frequencies of interest to us $\omega \sim \Theta$, it still has little effect, since it contains the small parameter $(\omega/\mu_0)^2 \sim (\Theta/\mu_0)^2 \ll 1$, and does not change in as significant a manner as the damping (3.7) at frequencies $\omega \approx \Theta$.

Thus, the results obtained in this investigation make it possible to investigate the frequency dependence of the conductivity of metals with impurities and to obtain definite information concerning the microscopic parameters of the alloy. Of greatest interest, from our point of view, is observation of quasi-local and local oscillations of the impurity atoms, which greatly influence the behavior of the frequency of the collisions $\gamma(\omega)$ (see (3.11) and (3.13)). Also worthy of interest is observation of the very complicated character of the frequency dependence of the impurity damping at low frequencies and temperatures $T \ll \omega \ll \Theta$ (see (3.9)). We note also that the general expressions (2.15) and (2.17) obtained for the conductivity, which make no use of any concrete model for the calculation of the phonon Green's function in the expression for the collision frequency (2.13), make it possible to carry out investigations in more complicated cases. These results could be obtained in the general case because of the use of the coordinate representation for the lattice Hamiltonian (1.1), which may turn out to be convenient also in the solution of other problems in the theory of crystals with defects.

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