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Abstract

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CALCULATION OF THE ELECTRICAL CONDUCTIVITY OF A SEMICONDUCTOR WITH A HIGH IMPURITY CONCENTRATION

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It is known (1) that the method of the kinetic equation is applicable only in the case when the relaxation time of the system satisfies the inequality

$$\tau \gg h/\chi T. \tag{1}$$

Condition (1) greatly narrows the range of applicability of the indicated method; for example, in the case of scattering of current carriers by charged impurities (the Conwell–Weisskopf formula (2)) this restriction excludes the region of low temperatures and high impurity concentrations (at concentrations of the order of 10^{18} cm^{-3}, condition (1) is not fulfilled even at room temperatures!). In this connection it is expedient to use a new method for calculating the electrical conductivity (3–5), not connected with the application of the kinetic equation.

As is easily shown, the electrical conductivity of an isotropic system in a constant field is equal to

$$\sigma = \int_0^\infty \varphi(\tau)\, d\tau, \qquad \varphi(\tau) = \beta \operatorname{Re} \operatorname{Sp}[\rho j j(\tau)], \tag{2}$$

where $\varphi(\tau)$ is the relaxation function of the system,

$$\rho = \exp(-\beta H)/\operatorname{Sp}(\exp(-\beta H)), \qquad j(\tau) = \exp(i\tau H/\hbar)\, j\, \exp(-i\tau H/\hbar). \tag{3}$$

Here H is the Hamiltonian of the system in the absence of the field; j is the current operator; $\beta = 1/\chi T$. The volume of the system is taken to be unity.

However, in works (3,4), in carrying out the concrete calculation, restrictions equivalent to (1) are imposed. In the present article the method (3–5) is used to study scattering of current carriers by charged impurities. It is important that in doing so it is possible to dispense with restrictions of the type (1).

§ 1. **General formulas.** Suppose that there are only current carriers of one type, which for definiteness we shall call electrons. The Hamiltonian of such a system has the form

$$H = H_0 + H', \qquad H_0 = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a^+_{\mathbf{k}} a_{\mathbf{k}}, \qquad H' = \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} a^+_{\mathbf{k}} a_{\mathbf{k}'}. \tag{4}$$

H' characterizes the interaction of the electrons with charged impurity centers; $\mathbf{k}$ is the quasimomentum of an electron in the conduction band; $a^+_{\mathbf{k}}$ and $a_{\mathbf{k}}$ are Fermi operators.

The current operator is (the field is directed along the Ox axis)

$$j = -\frac{e}{\hbar} \sum_{\mathbf{k}} \frac{d\varepsilon}{dk_x} a^+_{\mathbf{k}} a_{\mathbf{k}}. \tag{5}$$

Let us assume that H' is small compared with H_0, and apply perturbation theory (we emphasize that in doing so we neglect the bound states of the electrons; apparently this is possible for almost complete ionization of the impurity).

Expanding the exponents in (3) in powers of H' and substituting them into (2), we obtain

$$\varphi(\tau) = \beta \langle j^2 \rangle \exp[B - \mu(\tau)], \tag{6}$$

where

$$B = \langle j^2 \rangle^{-1} \int_0^\beta d\lambda \, (\beta - \lambda) \{ \langle j^2 H'_\lambda H' \rangle - \langle j^2 \rangle \langle H'_\lambda H' \rangle \},$$

$$\mu(\tau) = \hbar^{-2} \langle j^2 \rangle^{-1} \left\{ \operatorname{Im} \hbar \int_0^\tau d\theta \int_0^\beta d\lambda \, \langle H'_\lambda j[[j, H'(\theta)]] \rangle + \int_0^\tau d\theta \, (\tau - \theta) \langle j[[j, H'(\theta)], H'] \rangle \right\}. \tag{7}$$

Here

$$\langle A \rangle = \operatorname{Sp}(e^{-\beta H_0} A) / \operatorname{Sp}(e^{-\beta H_0}), \qquad H'_\lambda = e^{\lambda H_0} H' e^{-\lambda H_0}, \qquad H'(\theta) = e^{\frac{i}{\hbar} H_0 \theta} H' e^{-\frac{i}{\hbar} H_0 \theta}.$$

The first-order terms in H' vanish because $V_{\mathbf{k}\mathbf{k}} = 0$ (see (13)). All averages are easily evaluated if (4) and (5) are substituted into (7) and one passes to the H_0 representation. As a result we obtain:

$$\mu(\tau) = \frac{e^2}{\hbar^4\langle j^2\rangle}\sum_{\mathbf{k},\mathbf{k}'}\left(\frac{d\varepsilon}{dk_x} - \frac{d\varepsilon}{dk'_x}\right)^2 |V_{\mathbf{k}\mathbf{k}'}|^2 f_{\mathbf{k}}(1 - f_{\mathbf{k}'})\frac{2\sin^2(\omega_{\mathbf{k}\mathbf{k}'}\tau/2)}{\omega^2_{\mathbf{k}\mathbf{k}'}}. \quad (8)$$

Here $f_{\mathbf{k}} = \langle a^+_{\mathbf{k}} a_{\mathbf{k}}\rangle$ is the Fermi distribution function, $\omega_{\mathbf{k}\mathbf{k}'} = (\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'})/\hbar$.

In what follows we shall confine ourselves to the study of nondegenerate semiconductors, for which $f_{\mathbf{k}} = \exp[\beta(\zeta - \varepsilon_{\mathbf{k}})] \ll 1$ (ζ is the Fermi level).

§ 2. Approximation by the δ-function.

Let us consider the case in which, in the integral (2), only large values of τ* play an appreciable role. In this case

$$2\sin^2(\omega\tau/2)/\omega^2 \simeq \pi\tau\delta(\omega) \quad (9)$$

and, consequently, in $\mu(\tau)$ only the terms corresponding to transitions between states of equal energy remain. (Recall that (1) is obtained precisely from the requirement of energy conservation in transitions.)

Taking (9) into account, we find

$$\sigma = \beta\langle j^2\rangle \exp(B)/\nu, \quad (10)$$

where

$$\nu = \frac{\pi e^2}{\hbar^4\langle j^2\rangle}\sum_{\mathbf{k},\mathbf{k}'}|V_{\mathbf{k}\mathbf{k}'}|^2\left(\frac{d\varepsilon}{dk_x} - \frac{d\varepsilon}{dk'_x}\right)^2 f_{\mathbf{k}}\delta\left(\frac{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}}{\hbar}\right). \quad (11)$$

Under the assumptions (2), this gives an expression differing from the Conwell-Weisskopf formula ([2]) by a numerical coefficient of order 3. This difference is apparently connected with the greater consistency of the Kubo-Tomita-Nakano method compared with the kinetic-equation method.

The advantage of the method used is especially evident when the form of the interaction of electrons with impurity centers is refined. The potential field of an impurity center, when plasma screening is taken into account, has the form ([6])

$$V(r) = -\frac{Ze^2}{\varepsilon r}\frac{2}{\pi}\int_{k_0 r}^{\infty}\frac{\sin u}{u}\,du \quad (12)$$

* As will be shown below, this assumption is equivalent to condition (1).

and, consequently, the matrix elements

$$|V_{\mathbf{k}\mathbf{k}'}|^2 = \begin{cases} \dfrac{16\pi^2 Z^2 e^4}{\varepsilon^2(\mathbf{k}-\mathbf{k}')^4}\left\{N + 2\sum_{l<i=1}^{N}\cos(\mathbf{k}'-\mathbf{k},\, \mathbf{R}_l - \mathbf{R}_i)\right\}, & \text{if } (\mathbf{k}-\mathbf{k}')^2 > k_0^2, \\ 0, & \text{if } (\mathbf{k}-\mathbf{k}')^2 < k_0^2. \end{cases} \tag{13}$$

Here N is the concentration of impurity centers; $\mathbf{R}_i$ and eZ are, respectively, their coordinates and charge; ε is the dielectric constant of the semiconductor. The condition (7) is imposed on k_0,

$$n^{1/3} \ll k_0^4 \ll \lambda^{-4} = (2m\varkappa T/h^2)^2$$

(n, λ, and m are, respectively, the concentration, the mean de Broglie wavelength, and the effective mass of the electrons in the conduction band).

If in (13) the interference of different impurity centers is neglected, then

$$\sigma_0 = \frac{3}{2\sqrt{2\pi}}\,\frac{\varepsilon^2 n}{Z^2 e^2\sqrt{m}\,N}\,\frac{(\varkappa T)^{3/2}}{[-\operatorname{Ei}(-\alpha)]}, \tag{14}$$

where

$$\operatorname{Ei}(-x) = -\int_x^{\infty}\exp\left[\frac{-t}{t}\right]dt, \qquad \alpha = \frac{\hbar^2 k_0^2}{8m\varkappa T}. \tag{14a}$$

In (14) the factor $\exp(B)$, which gives only higher-order corrections, is absent. In the same approximation, the condition of smallness of H' used by us takes the form

$$n^{1/3} \ll \varepsilon\varkappa T/Ze^2. \tag{15}$$

Expression (14) should be compared with the analogous formula obtained in ([6]) by the method of the kinetic equation. Whereas the method of the kinetic equation (if the scattering probability is calculated in the Born approximation) requires, in order to obtain a finite conductivity, the parallel inclusion of a second mechanism of current scattering, the method used in the present work does not lead to such difficulties.

Taking into account in (13) the interference terms, one can investigate the influence of the configuration of impurity centers on the electrical conductivity of a semiconductor. We obtain:

$$\sigma = \sigma_0 \left\{ 1 + \frac{12}{N[-\operatorname{Ei}(-\alpha)]} \sum_{l<i=1}^{N} \int_{k_0 R_{li}}^{\infty} e^{-\alpha_{li} y^2} \left[(\cos^2\theta_{li} - 1) \left(\frac{\cos y}{y} - \frac{\sin y}{y^2} \right) + \cos^2\theta_{li} \sin y \right] \frac{dy}{y^2} \right\}^{-1}. \tag{16}$$

Here $R_{li} = |\mathbf{R}_l - \mathbf{R}_i|$, θ_{li} is the angle between $(\mathbf{R}_l - \mathbf{R}_i)$ and the direction of the electric field; $\alpha_{li} = \hbar^2\beta/8mR_{li}^2$.

Unfortunately, experimental data do not yet provide sufficient information about the distribution of impurity in a semiconductor. In the simplest case of a chaotic distribution (if the minimum distance between two centers is equal to the lattice constant d) we obtain

$$\sigma = \sigma_0 (1 - N/N_a)^{-1}, \tag{17}$$

where N_a is the number of atoms of the basic substance per unit volume. It follows from (17) that, for the above-mentioned distribution of impurity centers in practically interesting cases, the interference of waves scattered by different centers plays an insignificant role. Therefore we shall not take it into account below.*

* Interference may prove to be substantial for another character of impurity distribution.

§ 3. The region of low temperatures and high impurity concentration. Let us compute σ without the restrictive assumption (9). To terms of third order in H',

$$\int_0^{\infty} e^{-\mu(\tau)}\, d\tau = \frac{2}{\nu} - \int_0^{\infty} e^{-\nu\tau} \mu(\tau)\, d\tau, \tag{18}$$

where ν and $\mu(\tau)$ are defined respectively by (11) and (8). Using (2), (6), (8), (13), (14), and (18), we find:

$$\sigma = \sigma_0 e^B \left\{ 2 - \frac{b}{[-\operatorname{Ei}(-\alpha)]\sqrt{\alpha}} \int_0^{\infty} \frac{\Phi\sqrt{gx(1+x)}}{\sqrt{gx(1+x)}} \cos bx\, dx \right\}, \tag{19}$$

where

$$b = \frac{2\sqrt{2\pi}}{3} \frac{Z^2 e^4 \hbar}{\varepsilon^2 \sqrt{m}} \frac{N}{(\varkappa T)^{5/2}} [-\operatorname{Ei}(-\alpha)], \qquad g = \frac{b^2}{4\alpha}, \qquad \Phi(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-x^2}\, dx,$$

$$B = \frac{b}{2\sqrt{\alpha}[-\operatorname{Ei}(-\alpha)]}\left\{e^{-\alpha}\Phi(\sqrt{\alpha}) + \frac{1}{\sqrt{\pi}}(2e^{-\alpha}-1) - 2\sqrt{2\alpha}(1-\Phi(\sqrt{2\alpha})) - \sqrt{\alpha}\int_{\sqrt{\alpha}}^{\infty} e^{-y^2}\Phi(y)\frac{dy}{y}\right\}. \tag{20}$$

If $\alpha \ll 1^*$, then

$$B \approx (4Z^2e^4/3\varepsilon^2)(N/k_0\varkappa^2T^2). \tag{21}$$

For

$$g \ll 1, \qquad b \ll 1, \tag{22}$$

i.e., for low impurity concentrations and high temperatures, (19) reduces to (14). Consequently, (22) is the condition for applicability of the kinetic-equation method. We note that the second inequality (22) coincides with (1).

In the opposite asymptotic case of large N and small T,

$$g \gg 1, \tag{23}$$

and for σ we obtain an expression substantially different from the Conwell-Weisskopf formula:

$$\sigma = \sigma_0 e^B\left\{2 - \frac{\pi}{[-\operatorname{Ei}(-\alpha)]}\left[\sin\frac{b}{2}J_0\left(\frac{b}{2}\right) - \cos\frac{b}{2}N_0\left(\frac{b}{2}\right) - \frac{8\sqrt{\alpha}}{\pi^{1/2}b}\right]\right\}, \tag{24}$$

where J_0 and N_0 are, respectively, the Bessel and Neumann functions of zeroth order. With a reasonable choice of parameters ($\varepsilon = 20$, $m = 10^{-28}$ g), for $N = 10^{18}$ cm^{-3} condition (23) is satisfied for $T < 100$°K; for $N = 10^{16}$ cm^{-3}, for $T < 70$°K.

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* With a reasonable choice of the parameters of the problem in the region defined by (15), this condition is always satisfied.

Note: Figure translations are in progress. See original paper for figures.