# PHYSICS

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## Abstract

## Full Text

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# ON THE SCATTERING OF CURRENT CARRIERS BY OPTICAL VIBRATIONS

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**1.** In many cases the interaction of current carriers with optical vibrations of the crystal lattice plays an important, and often the principal, role. As was noted already by Fröhlich ([1,2]), the dominant role of the scattering of current carriers by optical phonons is an essential feature of the electrical conductivity of polar semiconductors. It is precisely this scattering that determines the kinetics of the electron gas in an external electric field. Up to now, however, allowance for this scattering at low temperatures has been connected either with assumptions whose validity is not obvious a priori ([1–4]), or with numerical methods for solving the kinetic equation ([5,6]).

Below we propose a regular method for calculating the electrical conductivity and thermopower in the case of low temperatures for scattering of electrons by optical vibrations, free of any special assumptions, in which certain elementary techniques for solving a finite-difference equation are used.

**2.** Towart and Sondheimer ([4]) showed that the kinetic equation in the case of electron scattering by optical vibrations reduces to an equation of the 11th order in finite differences. The same equation in finite differences can be obtained from the method of Fujita and Abe ([7]), which does not assume a priori the validity of the kinetic equation.

Fujita and Abe ([7]) showed that the nonequilibrium addition to the electron distribution function $\varphi_z(\mathbf{p})$ satisfies the integral equation

$$\varphi_z(\mathbf{p}) = -\frac{p_z}{2M\Gamma(\mathbf{p})} + \left(\frac{g}{2\pi}\right)^2 \frac{1}{\hbar^5} \int \frac{W(\mathbf{p},\mathbf{q})}{\Gamma(\mathbf{p})} \varphi_z(\mathbf{p}-\mathbf{q})\, d\mathbf{q}, \tag{1}$$

where $\mathbf{p}, \mathbf{q}$ are the momenta of the electron and phonon, respectively; $M$ is the effective mass of the electron; $g^2$ is a dimensionless coupling parameter, which in the case of inelastic scattering by optical phonons is equal to ([8])

$$g^2 = \frac{e^2}{2\hbar\varepsilon^*}\sqrt{\frac{2M}{\hbar\omega_0}};$$

$\varepsilon^*$ is the dielectric constant; $\omega_0$ is the limiting frequency of the optical phonons (we neglect their dispersion);

$$\Gamma(\mathbf{p}) = \left(\frac{g}{2\pi}\right)^2 \frac{1}{\hbar^5} \int W(\mathbf{p}, \mathbf{q})\, d\mathbf{q};$$

$$W(\mathbf{p}, \mathbf{q}) = 2M\hbar\gamma_q \left\{(N+1)\delta\left[p^2 - (\mathbf{p}-\mathbf{q})^2 - 2M\hbar\omega_0\right] + N\delta\left[p^2 - (\mathbf{p}-\mathbf{q})^2 + 2M\hbar\omega_0\right]\right\}$$

is the transition probability with absorption of a phonon and emission of a phonon; $\gamma_q$ in the case of scattering by optical vibrations is equal to

$$\gamma_q = \frac{4\pi\hbar^3(\hbar\omega_0)^{3/2}}{\sqrt{2M}\, q^2};$$

$$N = \left[\exp(\hbar\omega_0\beta) - 1\right]^{-1}$$

is the Planck distribution function of phonons;

$$\beta = 1/kT.$$

If one seeks the solution of (1) in the form of an expansion in spherical functions

$$\varphi_z(p) = \sum_{l,m} X_{lm}(p) Y_{lm}(\vartheta, \varphi) \tag{2}$$

and takes into account that, when calculating currents with the aid of $\varphi_z(p)$, only the harmonic $Y_{10}$ contributes to the current by virtue of the orthogonality of the spherical functions (under the integral sign in the current there will always enter the component of the momentum or velocity

$$p_z = p\cos\vartheta = \sqrt{\frac{4\pi}{3}}\, pY_{10}(\vartheta, \varphi),$$

then for the function

$$\Phi_I(\varepsilon) = \frac{\sqrt{2M\hbar\omega_0}}{\hbar} X_{10}(p)$$

we obtain the equation

$$\Phi_I(\varepsilon) = K_I(\varepsilon) + L(\varepsilon)\Phi_I(\varepsilon - 1)u(\varepsilon - 1) + M(\varepsilon)\Phi_I(\varepsilon + 1), \tag{3}$$

where $\varepsilon = p^2/2M\hbar\omega_0$; $\vartheta = \widehat{(z, \mathbf{p})}$; $\varphi$ is the azimuthal angle; $u(x)$ is the Heaviside unit function;

$$K_I(\varepsilon) = \frac{1}{g^2}\sqrt{\frac{\pi}{3}}\,\frac{\varepsilon}{(N+1)\ln(\sqrt{\varepsilon}+\sqrt{\varepsilon-1})u(\varepsilon-1) + N\ln(\sqrt{\varepsilon}+\sqrt{\varepsilon+1})},$$

$$L(\varepsilon) = \frac{1}{2}(N+1)\,\frac{\dfrac{2\varepsilon-1}{\sqrt{\varepsilon(\varepsilon-1)}}\ln(\sqrt{\varepsilon}+\sqrt{\varepsilon-1}) - 1}{(N+1)\ln(\sqrt{\varepsilon}+\sqrt{\varepsilon-1})u(\varepsilon-1) + N\ln(\sqrt{\varepsilon}+\sqrt{\varepsilon+1})}, \quad (4)$$

$$M(\varepsilon) = \frac{1}{2}N\,\frac{\dfrac{2\varepsilon+1}{\sqrt{\varepsilon(\varepsilon+1)}}\ln(\sqrt{\varepsilon}+\sqrt{\varepsilon+1}) - 1}{(N+1)\ln(\sqrt{\varepsilon}+\sqrt{\varepsilon-1})u(\varepsilon-1) + N\ln(\sqrt{\varepsilon}+\sqrt{\varepsilon+1})}.$$

The electrical conductivity and the thermoelectric emf may be written in the form

$$\sigma = e^2 I_1, \qquad \alpha = -\frac{k}{e}\left(\beta\frac{I_2}{I_1} - \mu^*\right), \quad (5)$$

where $\mu^* = \beta\mu$ is the reduced chemical potential,

$$I_1 = \beta\sqrt{\frac{2M\omega_0^3}{3\hbar\pi^5}}\,\exp\mu^*\int_0^\infty \Phi_I(\varepsilon)\,\varepsilon\exp(-\hbar\omega_0\beta\varepsilon)\,d\varepsilon,$$

$$I_2 = \beta\sqrt{\frac{2M\hbar\omega_0^5}{3\pi^5}}\,\exp\mu^*\int_0^\infty \Phi_{\mathrm{II}}(\varepsilon)\,\varepsilon\exp(-\hbar\omega_0\beta\varepsilon)\,d\varepsilon, \quad (6)$$

where $\Phi_{\mathrm{II}}(\varepsilon)$ satisfies the finite-difference equation, which can be obtained analogously to (3):

$$\Phi_{\mathrm{II}}(\varepsilon) = K_{\mathrm{II}}(\varepsilon) + L(\varepsilon)\Phi_{\mathrm{II}}(\varepsilon-1)u(\varepsilon-1) + M(\varepsilon)\Phi_{\mathrm{II}}(\varepsilon+1), \quad (3a)$$

$$K_{\mathrm{II}}(\varepsilon) = \varepsilon K_I(\varepsilon).$$

Here we assume that the electron gas is nondegenerate, its isoenergetic surfaces are spheres, and the dispersion law is parabolic.

3. To investigate the case of low temperatures ($\hbar\omega_0\beta \gg 1$), we shall use the following device (the solution of equations (3) and (3a) in the general case entails known difficulties). We divide the range of variation of $\varepsilon$ into intervals $(0,1)$, $(1,2)$, $(2,3)$, etc., and, considering $\varepsilon$ always less than unity, shall denote for the $n$-th interval

$$\Phi_I(n-1+\varepsilon) = \psi_{I,n}(\varepsilon), \qquad \Phi_{\mathrm{II}}(n-1+\varepsilon) = \psi_{\mathrm{II},n}(\varepsilon). \tag{7}$$

In each interval we expand the functions $\Phi_I$ and $\Phi_{\mathrm{II}}$ in a series in powers of $N$ ($N \ll 1$)

$$\Phi_I(n-1+\varepsilon) = \psi_{I,n}(\varepsilon) = N^{-1}\psi_{I,n}^{(-1)}(\varepsilon) + \psi_{I,n}^{(0)}(\varepsilon) + N\psi_{I,n}^{(1)}(\varepsilon) + \ldots \tag{8}$$

For $\Phi_{\mathrm{II}}$ there will be an analogous equality (in what follows we shall write all equalities for $\Phi_{\mathrm{I}}$, assuming that for $\Phi_{\mathrm{II}}$ they are analogous). Naturally, the series begins with a term proportional to $N^{-1}$, since the free term of equation (3), or (3a), written for the first interval, contains precisely $N^{-1}$.

The coefficients $K_{\mathrm{I}}(\varepsilon)$, $K_{\mathrm{II}}(\varepsilon)$, $L(\varepsilon)$, $M(\varepsilon)$ will also be expanded in a series in powers of $N$ in each interval. Now writing equations (3), (3a) for each interval, substituting for $\Phi_{\mathrm{I}}$, $\Phi_{\mathrm{II}}$, $K_{\mathrm{I}}$, $K_{\mathrm{II}}$, $L$, $M$ the corresponding expansions, and equating terms with the same powers of $N$ on the left- and right-hand sides, we obtain a chain of algebraic equations for $\psi_{\mathrm{I},n}^{(i)}(\varepsilon)$—the coefficients of expansion (8). For the first terms of expansion (8) this chain closes rapidly; therefore in principle we can find $\Phi_{\mathrm{I}}$ and $\Phi_{\mathrm{II}}$ in any interval with any degree of accuracy in $N$.

For example, if we denote

$$\begin{aligned}
K_{\mathrm{I},0}(\varepsilon) &= \frac{1}{g^2}\sqrt{\frac{\pi}{3}}\,\frac{\varepsilon}{\ln\left(\sqrt{\varepsilon}+\sqrt{\varepsilon+1}\right)}, \qquad K^*_{\mathrm{II},0}(\varepsilon) = \varepsilon K_{\mathrm{I},0}(\varepsilon),\\
B_{\mathrm{I},n}(\varepsilon) &= \frac{1}{g^2}\sqrt{\frac{\pi}{3}}\,\frac{n+1+\varepsilon}{\ln\left(\sqrt{n+\varepsilon}+\sqrt{n+1+\varepsilon}\right)},\\
B_{\mathrm{II},n}(\varepsilon) &= \frac{1}{g^2}\sqrt{\frac{\pi}{3}}\,\frac{(n+1+\varepsilon)^2}{\ln\left(\sqrt{n+\varepsilon}+\sqrt{n+1+\varepsilon}\right)},\\
D_n(\varepsilon) &= \frac{2n+1+2\varepsilon}{2\sqrt{(n+1)(n+1+\varepsilon)}} - \frac{1}{2\ln\left(\sqrt{n+\varepsilon}+\sqrt{n+1+\varepsilon}\right)},\\
C_n(\varepsilon) &= 1 + \frac{\ln\left(\sqrt{n+1+\varepsilon}+\sqrt{n+2+\varepsilon}\right)}{\ln\left(\sqrt{n+\varepsilon}+\sqrt{n+1+\varepsilon}\right)},
\end{aligned} \tag{9}$$

then we obtain:

$$\psi_{\mathrm{I},n}^{(-1)} = \frac{K_{\mathrm{I},0}}{1-D_0^2}\prod_{i=0}^{n-2} D_i,$$

$$\psi_{\mathrm{I},n}^{(0)} = B_{\mathrm{I},n-2}+D_{n-2}\psi_{\mathrm{I},n-1}^{(0)}-D_{n-2}(C_{n-2}-1)\psi_{\mathrm{I},n-1}^{(-1)}+D_{n-1}(C_{n-2}-1)\psi_{\mathrm{I},n+1}^{(-1)}, \quad n \geq 2,$$

$$\psi_{\mathrm{I},1}^{(0)} = \frac{D_0}{1-D_0^2}\left[B_{\mathrm{I},0} - \frac{K_{\mathrm{I},0}}{1-D_0^2}D_0(C_0-1)(1-D_1^2)\right] \quad \text{and so on.}$$

4. The integrals $I_1$ and $I_2$ can be written in the form:

$$I_1 = N^{-1}I_1^{(-1)} + I_1^{(0)} + NI_1^{(1)} + N^2 I_1^{(2)} + \cdots, \tag{10}$$

where

$$I_1^{(i)} = \beta\sqrt{\frac{2M\omega_0^3}{3\hbar\pi^5}}\,\exp\mu^* \sum_{n=1}^{\infty}\exp[-\hbar\omega_0\beta(n-1)]\int_0^1 \psi_{\mathrm{I},n}^{(i)}(\varepsilon)(n-1+\varepsilon)\,\exp(-\hbar\omega_0\beta\varepsilon)\,d\varepsilon \quad (i=-1,0,1,2,...).$$

Each of the integrals $I_1^{(i)}$, in turn, is a series in $\exp(-\hbar\omega_0\beta) \simeq N$; therefore in the complete $I_1$ one can collect terms with any power of $N$.

At low temperatures ($\hbar\omega_0\beta \gg 1$) the maximum of the weight of the integrand of the integral

$$\int_0^1 \psi_{\mathrm{I},n}^{(i)}(n-1+\varepsilon)e^{-\hbar\omega_0\beta\varepsilon}\,d\varepsilon$$

lies near zero, and the principal contribution to the integral is given by small values of $\varepsilon$ (most conduction electrons have small energies); therefore this integral can be replaced by an integral from zero to infinity, while thereby introducing corrections in terms of higher order in $N$. Thus, for example, $I_1$ can ⋯

is found from the formula:

$$
\begin{aligned}
I_1 = N^{-1} &\left[\beta\sqrt{\frac{2M\omega_0^3}{3\hbar\pi^5}}\exp\mu^*\int_0^1 \psi_{I,1}^{(0)}(\varepsilon)\,\varepsilon\exp(-\hbar\omega_0\beta\varepsilon)\,d\varepsilon\right]+\\
&+N^0\left[\beta\sqrt{\frac{2M\omega_0^3}{3\hbar\pi^5}}\exp\mu^*\left(\int_0^1 \psi_{I,1}^{(0)}(\varepsilon)\,\varepsilon\exp(-\hbar\omega_0\beta\varepsilon)\,d\varepsilon+\right.\right.\\
&\qquad\left.\left.+\int_0^1 \psi_{I,2}^{(-1)}(\varepsilon)(1+\varepsilon)\exp(-\hbar\omega_0\beta\varepsilon)\,d\varepsilon\right)\right]+\ldots=\\
&=N^{-1}\left[\beta\sqrt{\frac{2M\omega_0^3}{3\hbar\pi^5}}\exp\mu^*\int_0^\infty \psi_{I,1}^{(-1)}(\varepsilon)\,\varepsilon\exp(-\hbar\omega_0\beta\varepsilon)\,d\varepsilon\right]+\\
&+N^0\left[\beta\sqrt{\frac{3M\omega_0^3}{3\hbar\pi^5}}\exp\mu^*\int_0^\infty \left\{\varepsilon\psi_{I,1}^{(0)}(\varepsilon)+(1+\varepsilon)\psi_{I,2}^{(-1)}(\varepsilon)\right.\right.\\
&\qquad\left.\left.-(1+\varepsilon)\psi_{I,1}^{(-1)}\times(1+\varepsilon)\right\}\exp(-\hbar\omega_0\beta\varepsilon)\,d\varepsilon\right]+\ldots
\end{aligned}
\tag{11}
$$

The integrals from zero to infinity entering into (11) can be evaluated approximately by means of the quadrature formulas of V. I. Krylov [9]. If, in (11), one restricts oneself to the term proportional to $N^{-1}$ and approximates $\psi_{I,1}^{(-1)}$ and $\psi_{II,1}^{(-1)}$ (for small $\varepsilon$!) by the expressions $\frac{1}{g^2}\sqrt{\frac{\pi}{3}}\,\varepsilon^{1/2}$ and $\frac{1}{g^2}\sqrt{\frac{\pi}{3}}\,\varepsilon^{3/2}$, respectively, then we obtain the well-known ([3–6]) formulas for the electrical conductivity and thermoelectric power at low temperatures, which correspond to the choice of a relaxation time equal to $\tau = (2g^2\omega_0 N)^{-1}$:

$$
\sigma = \frac{e^2\sqrt{2M}\exp\mu^*}{4g^2N\,(\pi\beta)^{3/2}\omega_0\cdot\hbar^3}, \qquad \alpha = -\frac{k}{e}\left({}^5/_2-\mu^*\right). \tag{12}
$$

The proposed method makes it possible to broaden the limits of the temperature interval in which the electrical conductivity and thermoelectric power can be calculated, and it can be generalized to the case of an arbitrary dispersion law.

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