The relation between the phonon-drag thermopower and the electroacoustic coefficient

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It is shown that the phonon-drag thermopower is determined by a certain average of the electroacoustic coefficient over the directions and polarizations of the sound.

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The thermopower Q is a kinetic coefficient that determines the electric field $\mathbf{E}$ appearing in a sample in the presence in it of a temperature gradient ∇T and in the absence of an electric current $\mathbf{j}$:

$$\mathbf{E}=Q\nabla T,\quad \mathbf{j}=0$$

(for a crystal with cubic symmetry). In a metal at low temperatures, the thermopower Q is represented in the form of a sum[1]

$$Q=Q_e+Q_{ph}=aT+bT^3, \tag{1}$$

where the first term is related to the direct action of the temperature gradient on the electron system, and the second to the dragging of the electrons by the phonon flux created by the temperature gradient.

The drag thermopower Q_{ph} is physically related to the acoustoelectric effect, which consists in the action of an electric field (or emf) on the propagation of a sound wave along a metal. An order-of-magnitude relation between the thermopower Q_{ph} and the acoustoelectric coefficient was established by Zavaritskiĭ[2]:

$$Q_{ph}\sim C_{ph}s\zeta, \tag{2}$$

where C_{ph} is the heat capacity of the lattice and s is the sound velocity. The acoustoelectric coefficient entering in (2) corresponds to the most natural setup of the experiment[2] and is defined as the coefficient of proportionality between the difference in potentials ΔV at the ends of a long sample, induced by a sound wave propagating along the sample (and completely damped in it), and its initial energy flux density W.

$$\Delta V=\zeta W. \tag{3}$$

For a metal with isotropic characteristics, the relation (2) is exact with a coefficient 1/3 on the right-hand side.

It turns out that an analog of the relation (2) can be obtained also for a real anisotropic metal. Here Q_{ph} is determined by a certain weighted average of $\zeta(\mathbf{n})$ ($\mathbf{n}$ is the direction relative to the crystallographic axes) over the directions $\mathbf{n}$. This is easily understood if we imagine that initially the temperature gradient takes the phonons out of equilibrium, and then they create the thermopower via the acoustoelectric effect. The weight with which the averaging of $\zeta(\mathbf{n})$ takes place is generally nontrivial since it depends on the character of the disequilibrium of the phonons. However, in the low-temperature limit, it can be found accurately

We write down the set of kinetic equations for the electron and phonon distribution functions in the presence of a temperature gradient. Neglecting the phonon scattering due to all but the electronic mechanism (this is justified for metals at low temperatures),[1)] we eliminate the nonequilibrium phonon distribution function from the first equation (Ref. 3, Sec. 82) and reduce it to the form

$$X_{\mathbf{k}}^T\equiv-\frac{\varepsilon_{\mathbf{k}}-\mu}{T}\frac{\partial f_{\mathbf{k}}^0}{\partial\varepsilon_{\mathbf{k}}}\mathbf{v}_{\mathbf{k}}\nabla T+\sum_{\mathbf{k}'\mathbf{q}\lambda}\Bigl[(P_{\mathbf{k}\mathbf{q}\lambda}^{\mathbf{k}'}-P_{\mathbf{k}}^{\mathbf{k}'\mathbf{q}\lambda}) \times\Bigl(2T\sum_{\mathbf{k}_1\mathbf{k}_2}P_{\mathbf{k}_1\mathbf{q}\lambda}^{\mathbf{k}_2}\Bigr)^{-1}\hbar\omega_{\mathbf{q}\lambda}\frac{\partial n_{\mathbf{q}\lambda}^0}{\partial(\hbar\omega_{\mathbf{q}\lambda})}\mathbf{v}_{\mathbf{q}\lambda}\nabla T\Bigr]=\hat{L}\varphi_{\mathbf{k}}, \tag{4}$$

where $\varepsilon_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are the energy and the group velocity of electrons with quasimomentum $\mathbf{k}$; $\omega_{\mathbf{q}\lambda}$ and $v_{\mathbf{q}\lambda}$ are the frequency and group velocity of phonons with quasimomentum $\mathbf{q}$ and polarization λ; $f_{\mathbf{k}}^0$ and $n_{\mathbf{q}\lambda}^0$ are the Fermi and Bose distribution functions, $\varphi_{\mathbf{k}}$ is introduced by the relation

$$f_{\mathbf{k}}=f_{\mathbf{k}}^0-\frac{\partial f_{\mathbf{k}}^0}{\partial\varepsilon_{\mathbf{k}}}\varphi_{\mathbf{k}}$$

($f_{\mathbf{k}}$ is the nonequilibrium electron distribution function); $\hat{L}$ is the integral collision operator (which takes into account all possible electron collisions, and also the drag of the electrons by the phonons); $P_{\mathbf{k}\mathbf{q}\lambda}^{\mathbf{k}'}$ and $P_{\mathbf{k}}^{\mathbf{k}'\mathbf{q}\lambda}$ are the probabilities of electron-phonon transitions:

$$P_{\mathbf{k}\mathbf{q}\lambda}^{\mathbf{k}'}=\sum_{\mathbf{G}}\frac{2\pi}{\hbar}|g_{\mathbf{k}'\mathbf{k}}^{\lambda}|^2f_{\mathbf{k}}^0(1-f_{\mathbf{k}'}^0)n_{\mathbf{q}\lambda}^0\delta(\varepsilon_{\mathbf{k}'}-\varepsilon_{\mathbf{k}}-\hbar\omega_{\mathbf{q}\lambda})\delta_{\mathbf{k}'-\mathbf{k}-\mathbf{q},\mathbf{G}},$$

$$P_{\mathbf{k}}^{\mathbf{k}'\mathbf{q}\lambda}=\sum_{\mathbf{G}}\frac{2\pi}{\hbar}|g_{\mathbf{k}'\mathbf{k}}^{\lambda}|^2f_{\mathbf{k}}^0(1-f_{\mathbf{k}'}^0)(1+n_{\mathbf{q}\lambda}^0)\delta(\varepsilon_{\mathbf{k}'}-\varepsilon_{\mathbf{k}}+\hbar\omega_{\mathbf{q}\lambda})\delta_{\mathbf{k}'-\mathbf{k}+\mathbf{q},\mathbf{G}},$$

where $g_{\mathbf{k}'\mathbf{k}}^{\lambda}$ is the matrix element of the electron-phonon interaction, and is connected with the corresponding component of the deformation potential $\Lambda_{\mathbf{k}}$ by the relation

$$|g_{\mathbf{k}'\mathbf{k}}^{\lambda}|^2=\hbar q^2|\Lambda_{\mathbf{k}}|^2/2\rho\omega_{\mathbf{q}\lambda}.$$

We should find $\varphi_{\mathbf{k}}$ from Eq. (4) and calculate the thermoelectric current. However, it is more convenient to use the method of Ref. 4 to express the thermoelectric current $\mathbf{j}^T$ in terms of another function $\psi_{\mathbf{k}}$, which is the solution of the kinetic equation

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$$\frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}} \mathbf{v}_{\mathbf{k}} = \hat{L}\psi_{\mathbf{k}}, \tag{5}$$

used in the theory of electric conduction. The possibility for this follows from the formal chain of equations:

$$\mathbf{j}^T = -2e \sum_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}} \varphi_{\mathbf{k}} = -2e \left(\mathbf{v}_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}}, \varphi_{\mathbf{k}} \right)$$

$$= -2e \left(\mathbf{v}_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}}, \hat{L}^{-1} X_{\mathbf{k}}^T \right)$$

$$= -2e \left(\hat{L}^{-1} \mathbf{v}_{\mathbf{k}} \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}}, X_{\mathbf{k}}^T \right) = -2e (\psi_{\mathbf{k}}, X_{\mathbf{k}}^T)$$

(use is made of the Hermitian character of the operator $\hat{L}$). Consequently, we get for the thermopower

$$Q = Q_e + Q_{ph},$$

$$Q_e = -\frac{2e}{3\sigma} \sum_{\mathbf{k}} \frac{\varepsilon_{\mathbf{k}} - \mu}{T} \frac{\partial f_{\mathbf{k}}^0}{\partial \varepsilon_{\mathbf{k}}} \psi_{\mathbf{k}} \mathbf{v}_{\mathbf{k}},$$

$$Q_{ph} = \frac{e}{3\sigma T} \sum_{\mathbf{q}\lambda} \hbar\omega_{\mathbf{q}\lambda} \frac{\partial n_{\mathbf{q}\lambda}^0}{\partial (\hbar\omega_{\mathbf{q}\lambda})} \sum_{\mathbf{k}\mathbf{k}'} (P_{\mathbf{k}\mathbf{q}\lambda}^{\mathbf{k}} - P_{\mathbf{k}}^{\mathbf{k}'\mathbf{q}\lambda}) \psi_{\mathbf{k}} \mathbf{v}_{\mathbf{q}\lambda} \Big/ \sum_{\mathbf{k}\mathbf{k}'} P_{\mathbf{k}\mathbf{q}\lambda}^{\mathbf{k}}, \tag{6}$$

where σ is the conductivity (for simplicity, we have assumed cubic symmetry of the crystal). The expression for Q_e in the case of a slow energy dependence of $\psi_{\mathbf{k}}$ reduces to the well-known Mott formula.[1] The expression for Q_{ph} is simplified in the low-temperature limit, when the momentum of the thermal phonon is less than all the characteristic dimensions of the Fermi surface:

$$Q_{ph} = \frac{\pi}{90} \frac{e}{\sigma} T^3 \sum_{\lambda} \int \frac{d\Omega_{\hat{\mathbf{q}}}}{(\hbar s_{\hat{\mathbf{q}}\lambda})^4} \mathbf{v}_{\hat{\mathbf{q}}\lambda} \int \frac{|\Lambda_{\mathbf{k}}|^2}{v_{\mathbf{k}}^2} \times \frac{\partial \psi_{\mathbf{k}}}{\partial k_q} \delta(\cos\theta)\, dS_{\mathbf{k}} \Big/ \int \frac{|\Lambda_{\mathbf{k}}|^2}{v_{\mathbf{k}}^2} \delta(\cos\theta)\, dS_{\mathbf{k}}, \tag{7}$$

where θ is the angle between $\mathbf{q}$ and $\mathbf{v}_{\mathbf{k}}$; $s_{\hat{\mathbf{q}}\lambda}$ is the phase velocity of the phonon; integration is carried out over the directions $\hat{\mathbf{q}} = \mathbf{q}/q$. The integrals over $S_{\mathbf{k}}$ in (7) turn out to be the same as in the expressions for the acoustoelectric current $\mathbf{j}^A$ (Ref. 4) and the sound absorption coefficient Γ (Ref. 5):

$$\mathbf{j}_{\mathbf{q}\lambda}^A = \frac{eqW}{(2\pi\hbar)^2 \rho v_{\hat{\mathbf{q}}\lambda} s_{\hat{\mathbf{q}}\lambda}} \int \frac{|\Lambda_{\mathbf{k}}|^2}{v_{\mathbf{k}}^2} \frac{\partial \psi_{\mathbf{k}}}{\partial k_q} \delta(\cos\theta)\, dS_{\mathbf{k}},$$

$$\Gamma_{\mathbf{q}\lambda} = \frac{q}{(2\pi)^2 \hbar \rho v_{\hat{\mathbf{q}}\lambda}} \int \frac{|\Lambda_{\mathbf{k}}|^2}{v_{\mathbf{k}}^2} \delta(\cos\theta)\, dS_{\mathbf{k}}.$$

Using these expressions, we write out (7) in the form

$$Q_{ph} = \frac{\pi}{90} \frac{T^3}{\sigma} \sum_{\lambda} \int \frac{d\Omega_{\hat{\mathbf{q}}}}{(\hbar s_{\hat{\mathbf{q}}\lambda})^3} \frac{\mathbf{j}_{\mathbf{q}\lambda}^{A(0)} v_{\hat{\mathbf{q}}\lambda}}{\Gamma_{q\lambda}}, \tag{8}$$

where $\mathbf{j}_{\mathbf{q}\lambda}^{A(0)}$ is the value of $\mathbf{j}_{\mathbf{q}\lambda}^A$ at $W = 1$. Noting that the acoustoelectric coefficient ζ, measured in the $v_{\hat{\mathbf{q}}\lambda}$ direction, is connected with $\mathbf{j}_{\mathbf{q}\lambda}^A$ in the following way:

$$\zeta^\lambda (\hat{\mathbf{v}}_{\hat{\mathbf{q}}\lambda}) = \mathbf{j}_{\hat{\mathbf{q}}\lambda}^{A(0)} \hat{\mathbf{v}}_{\hat{\mathbf{q}}\lambda} / \Gamma_{\mathbf{q}\lambda}\sigma,$$

we obtain the desired relation between Q_{ph} and $\zeta(\mathbf{n})$:

$$Q_{ph} = \frac{\pi}{90} T^3 \sum_{\lambda} \int d\Omega_{\hat{\mathbf{q}}} \frac{v_{\hat{\mathbf{q}}\lambda}}{(\hbar s_{\hat{\mathbf{q}}\lambda})^3} \zeta^\lambda (\hat{\mathbf{v}}_{\hat{\mathbf{q}}\lambda}). \tag{9}$$

Thus, although an explicit separate calculation of each of the quantities Q_{ph} and $\zeta(\mathbf{n})$ is not possible in the general case, we have succeeded in establishing quantitative relation between them.

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[1)]The final formulas (8) and (9) are preserved even in the presence of other mechanisms of phonon scattering if we can write them in the Γ approximation; in this case Γ and ζ in (8) and (9) must be determined with account taken of these additional scattering mechanisms.

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