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Abstract

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THEORY OF LOW-TEMPERATURE TRANSPORT PHENOMENA IN SEMICONDUCTORS WITH LOW MOBILITY

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1. In papers ([1], [6]) a theory was proposed for high-temperature transport phenomena in semiconductors with low mobility, i.e., in a certain approximation, a solution of the problem of non-Boltzmann transport in an electron-phonon system with strong interaction, whose parameter is $\Phi_0 \gg 1$ (see below the criterion $\hbar\Gamma \gg \Delta$). To calculate the transport coefficients σ_{MN}, their general expressions ([2]) of the type

$$D_{MN} = \int_{-\infty}^{\infty} \frac{dl}{2\pi} \operatorname{Re}\operatorname{Sp} e^{\beta F - \beta H} N(\mathcal{H} - l + i\varepsilon)^{-1} M(\mathcal{H} - l - i\varepsilon)^{-1} \bigg|_{\varepsilon\to+0}, \quad (1)$$

are used; for these, effective expansions are constructed in the basis of localized small-polaron functions $|sn\rangle$ ([4], [6b]) (s is the cell number, $n \equiv (\dots N_{fj} \dots)$, N_{fj} are phonon numbers), where $\mathcal{H}$, M, N are the Hamiltonian and the current operators for the "one-particle" system, and

$$(sn|\mathcal{H}|sn) = \varepsilon_n - \varepsilon_{\text{pol}},$$

where ([6a]), p. 1.4)

$$\varepsilon_n = \sum_{fj} \hbar\omega_{fj} N_{fj}; \qquad \varepsilon_{\text{pol}} = \varepsilon_0 + (s|\delta V|s) - \delta\varepsilon, \qquad \delta\varepsilon = \sum_{fj} |V_{fj}^{ss}|^2 \omega_{fj}^{-1}.$$

According to ([6b]), for $\operatorname{Re} D_{MN}$ the first correction δ_1 and the second correction δ_2 are smaller than the principal term $\operatorname{Re} D^0_{MN}(00;00)$ (respectively for $\operatorname{Im} D_{MN}$), if (below $\hbar = c = k = 1$)*

$$\Delta \ll \Gamma, \qquad \Gamma \ll \omega_p; \quad (2)$$

$$\Delta_e^2(\omega_p\Phi_0T)^{-1}\ll 1,\qquad \Delta_e^2(\omega_p\Phi_0)^{-2}\underset{\chi<1}{\lesssim}\exp(-\beta\hbar\mathcal{E}_0)\ll 1, \tag{3}$$

for we have**

$$|\delta_1|\cdot|\operatorname{Re}D_{MN}|^{-1}\sim\Delta_e(\omega_p\Phi_0)^{-1};\qquad |\delta_2|\cdot|\operatorname{Re}D_{MN}|^{-1}\in\left\{\Delta_e^2(\omega_p\Phi_0T)^{-1};\Delta_e^2(\omega_p\Phi_0)^{-2}\exp(\beta\hbar\mathcal{E}_0)\right\}.$$

In (2), (3):

$$\Delta=\Delta_0\exp[-\Phi(T)],$$

where usually $\Delta_0\simeq\Delta_e$, Δ_e is the width of the electronic band;

$$\Phi(T)\equiv\frac{1}{2}\sum_{fj}\lambda_{fj}^{ss'}\operatorname{cth}\left(\frac{\beta\omega_{fj}}{2}\right);$$

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* For $\Delta\ll\Gamma$, the method for estimating the corrections in ([6b]) is equivalent to taking account of the successive subtraction, at $\Delta\ll\Gamma$, of small contributions of "singular" matrix elements (in the resolvent expansion) in which sets n are repeated (the account of the operation ir is essential, and footnote ([4]) in ([6b]) refers only to the first correction).

** In paper ([6b]) it should read: in III, 11, instead of $\Delta_e(\omega_p\Phi_0)^{-1}\ll 1$, read

$$\Delta_e^2(\omega_p\Phi_0)^{-2}\lesssim\exp(-\beta\hbar\mathcal{E}_0)\ll 1;$$

in Appendix 2.v, P.2.9, instead of $\operatorname{Re}D_{MN}^0(00;10)$, read $\operatorname{Im}D_{MN}^0(00;10)$; in P.2.10, instead of $\exp(-\beta V_0)$, read $\exp(+\beta\mathcal{E}_0)$; in the last estimate, instead of

$$|\delta_2|\cdot|\operatorname{Re}D_{MN}^0(00;10)|^{-1}\lesssim(\Omega/\omega_p)^{1/2},$$

read

$$|\delta_2|\cdot|\operatorname{Re}D_{MN}|^{-1}\in\left\{\Delta_e^2(\omega_p\Phi_0T)^{-1};\Delta_e^2(\omega_p\Phi_0)^{-2}e^{\beta\hbar\mathcal{E}_0}\right\}$$

(i.e., the second condition (3) is sufficient). In P.38 ([6b]) the correction must have the form:

$$\delta_1D_{MN}=D_{MN}^1(00;00)-D_{MN}^0(00;00)\sim(\mathcal{H}')^3,$$

since

$$\delta_0 G \sim (\mathcal{H}')^3.$$

$\Phi(0) \equiv \Phi_0$; $\quad \lambda_{fj}^{ss'}$ are the lattice-deformation parameters; at $T \gg \omega_p$ and $\Phi_0 \gg 1$

$$\Gamma \simeq \Gamma_b' \equiv 2\pi \sum_{k;\, n,n'(\neq n)} \exp(\beta F_0 - \beta\varepsilon_{nk}) |(kn|\mathcal{H}'|kn')|^2 \delta(\varepsilon_{nk} - \varepsilon_{n'k}) \simeq \Gamma_0 e^{-\beta\mathcal{E}_0}, \tag{4}$$

$$\Gamma_0 \equiv \frac{\sqrt{\pi}}{2}\Delta_e^2(\mathcal{E}_0 T)^{-1/2}, \qquad \mathcal{E}_0 \equiv \sum_{fj} \frac{1}{4}\lambda_{fj}^{ss'}\omega_{fj}. \tag{5}$$

Above, ω_p is the characteristic frequency of the essential phonons. Let us note that $\Gamma \simeq \Gamma' \gg \Delta$ at $T > T_0$ and for not too small Δ_e, $T_0 \sim \omega_p$ [6] (in the general case $T_0 \gtrsim \omega_p$).

2. Let us consider here the basic relations of the theory of transport phenomena in the same semiconductors, but at low $T < T_0' \equiv \omega_p/\Phi_0 < T_0$. In this range of T, considering for simplicity the static case, we have for $\sigma_{MN}^{(s,a)} \equiv \frac{1}{2}(\sigma_{MN} \pm \sigma_{NM})$:

$$\sigma_{MN}^{(a)} = N_c \int_0^\infty dt\, e^{-\varepsilon t}(\Psi_{MN} - \Psi_{NM}) \int_0^t d\tau\, \frac{2}{\pi\hbar} \ln \operatorname{cth} \frac{\pi\tau}{2\beta\hbar},$$

$$\sigma_{MN}^{(s)} = \frac{1}{2}\beta N_c \int_0^\infty dt\, e^{-\varepsilon t}(\Psi_{MN} + \Psi_{NM}) \equiv \frac{N_c}{2}(\varphi_{MN} + \varphi_{NM}), \tag{6}$$

where

$$\Psi_{MN}(t) \equiv \operatorname{Re}\operatorname{Sp} \exp(\beta F - \beta\mathcal{H})\, N \exp(i\mathcal{H}t) M \exp(-i\mathcal{H}t). \tag{7}$$

It is convenient to compute the trace in the basis of orthonormalized functions

$$(kn) \equiv u_{nk} e^{i\mathbf{kx}} \equiv N_0^{-1} \sum_s e^{-i\mathbf{ks}} |sn\rangle = |\mathbf{k} + 2\pi\mathbf{g}, n\rangle, \tag{8}$$

describing the state of the carrier (polaron) in the band and the phonon system ($\mathbf{k}$ is the total quasimomentum of the system; $\mathbf{g}$ is a reciprocal-lattice vector). The energy of the system unperturbed in the kn-basis is $(kn|\mathcal{H}|kn) \equiv \varepsilon_{nk} = \varepsilon_n + \varepsilon_n(\mathbf{k})$, and in the nearest-neighbor approximation

$$\varepsilon_n(\mathbf{k}) = E(\mathbf{k}_n)\exp[-\Phi(n)] = \varepsilon_n(\mathbf{k}+2\pi\mathbf{g}),$$

$$\Phi(n) \equiv \frac{1}{2}\sum_{fj}\lambda_{fj}^{ss'}(1+2N_{fj}),$$

where $E(\mathbf{k})$ is the dispersion law in the corresponding electron band, $\mathbf{k}_n = \mathbf{k} - \sum fjN_{fj}$ is the carrier quasimomentum (to within $2\pi\mathbf{g}$), and the mean width of the bands $\varepsilon_n(\mathbf{k})$ is Δ; for $\Phi_0 \gg 1$, $\Delta \ll \omega_p$. The perturbation matrix is $(kn|\mathcal{H}'|k'n') \equiv (kn|\mathcal{H}'|k'n')_{n\neq n'}$. The transport under consideration is determined by scattering of band carriers between $|kn\rangle$-states by means of multiphonon processes. Since $\mathcal{H}$ is translationally invariant, in the reduced-$\mathbf{k}$ scheme

$$(kn|\mathcal{H}'|k'n') = \delta_{kk'}(kn|\mathcal{H}'|kn'). \tag{9}$$

In the principal approximation of the theory one should set:

$$(kn|\rho_0(\mathcal{H})|k'n') \equiv (kn|\exp(\beta F - \beta\mathcal{H})|k'n') \simeq f_0(kn)\delta_{kk'}\delta_{nn'}, \tag{10}$$

$$f_0(kn) = \exp(\beta F_0 - \beta\varepsilon_{nk}); \qquad \delta_{nn'} \equiv \prod_{fj}\delta_{N_{fj},N'_{fj}}, \tag{11}$$

and, at $H = 0$ (H is the external magnetic field), for $(kn|M|k'n')$

$$(kn|M|k'n') = \delta_{kk'}\left[(kn|M^0|kn)\delta_{nn'} + M_{nn'}(\mathbf{k})\right] \simeq \delta_{kk'}\delta_{nn'}M^0(kn).$$

The operator defined in (9) satisfies, as is easy to show, the basic Van Hove relation (5), and below the consequence of (9, 10) is used. We find that

$$\varphi^a_{MN} \equiv \sum_{kn} N^0(kn)\, f'_M(kn) = \sum_{kn} N^0(kn)\, f'_M(\varepsilon; kn), \tag{12}$$

$$f'_M(\varepsilon; kn) = \beta\ \mathrm{Re}\int_0^\infty dt\, e^{-\varepsilon t}(kn|\rho_0 e^{i\mathcal{H}t}Me^{-i\mathcal{H}t}|kn) = \beta\ \mathrm{Re}(kn|\rho_0 f'_M(\varepsilon)|kn). \tag{13}$$

Further (10),

$$Y f'_M(\varepsilon) = (\varepsilon - iL_0 - iYL')^{-1}\,(M' + iYL'Df'_M(\varepsilon))$$

and

$$I_\varepsilon Df'_M(\varepsilon) \equiv [\varepsilon + DL'(\varepsilon - iL_0 - iYL')^{-1}YL']Df'_M(\varepsilon) =$$

$$= Q_M(\varepsilon) \equiv D[1 + iL'(\varepsilon - iL_0 - iYL')^{-1}Y]M; \tag{14}$$

$$(\alpha|D\hat{f}|\alpha') \equiv (\alpha|\hat{f}|\alpha')\delta_{\alpha\alpha'}; \qquad (\alpha|Y\hat{f}|\alpha') \equiv (\alpha|\hat{f}|\alpha')_{\alpha\neq\alpha'}, \tag{15}$$

$$DM \equiv M^0, \qquad L_0\hat{f} \equiv [\mathcal{H}_0, \hat{f}]; \qquad L'\hat{f} \equiv [\mathcal{H}', \hat{f}], \qquad YM \equiv M'.$$

Using (10)–(15) and the expansion (in $\mathcal{H}'$) $\rho_0(\mathcal{H}_0+\mathcal{H}')$ and $(\varepsilon-iL_0-iY')^{-1} = (\varepsilon - iL_0)^{-1} + (\varepsilon - iL_0)^{-1}iYL'(\varepsilon - iL_0)^{-1} + \cdots$, one can obtain an equation for $f'(kn) \equiv \sum'_M f'_M(kn)F_M + f'_j(kn)E$. Neglecting the contribution $Q_M(\varepsilon) - M^0$ and the higher-order correction terms in $\mathcal{H}'$, indicated below, in $I_\varepsilon Df'_M(\varepsilon)|_{\varepsilon\to+0}$, we obtain, in the basic approximation so defined, the transport equation*

$$\left(\frac{\partial f}{\partial t}\right)_{\text{dyn}} + \left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = 0; \qquad \left(\frac{\partial f}{\partial t}\right)_{\text{dyn}} = -\beta f_0(kn)Q(kn),$$

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} \equiv I_0 f'(kn) = \Omega_{kn} f'(kn) - \sum_{n''} \omega_{kn;kn''}\delta(\varepsilon_{nk} - \varepsilon_{n''k})\, f'(kn''); \tag{16}$$

$$Q(kn) = \sum_M{}' M^0(kn)F_M + eEv^0(kn), \tag{17}$$

$$\Omega_{kn} \equiv \sum_{n''} \omega_{kn;kn''}\delta(\varepsilon_{kn} - \varepsilon_{kn''}); \qquad \omega_{kn;kn} = 0; \qquad \langle\Omega_{kn}\rangle_0 \equiv \Omega_b.$$

The expression for $\omega_{kn,kn''}$, including terms $\sim (\mathcal{H}')^{2+l}|_{l=1,2,\ldots}$, is analogous to the corresponding expression in § IV (9), if $l \equiv (k,n)$ and (9) is taken into account (and therefore it is not written out explicitly; item 4 in (6b) refers only to the possible case when, for $T < T'_0$, one may restrict oneself to the lowest approximation in $\mathcal{H}'$, $\omega^0_{kn;kn''} = 2\pi|(kn|\mathcal{H}'|kn'')|^2$). For

$$\frac{e\hbar}{m^*c}H \ll \Delta,$$

i.e.

$$H \ll H_0 = \hbar c/|e|a^2,$$

we again have (16), but

$$\left(\frac{\partial f}{\partial t}\right)_{\text{dyn}} = -\beta f_0(kn)Q(kn) - e(\mathbf{v}\times\mathbf{H}]\cdot\nabla_k f'(kn), \tag{18}$$

$m^* = \hbar^2(\Delta a^2)^{-1}$ is the mean effective mass, a is the lattice constant.

It is not difficult to take into account the contribution $\delta\sigma_{MN} = \sum f'_M(n,n';\mathbf{k})N'_{nn'}(\mathbf{k})$ of the nondiagonal elements $N'_{nn'}(\mathbf{k})$ in σ_{MN}, and in the lowest approximation in $\mathcal{H}'$, $\sigma^{nd}_{MN} \equiv \sigma^{(s)}_{M'N'} \sim M^e N^e \Delta_e^{-2}\beta\Gamma'_b N_c$, $M^e \equiv |(s|M|s')|$.

* F_M is the external force conjugate to the flux M; to the charge flux $M = \mathbf{j} = e\mathbf{v}$ there is conjugate the electric field $\mathbf{E}$ ($\mathbf{v}$ is the velocity operator); incidentally, $v^0(kn) = (kn|\mathbf{v}|kn) = \partial\varepsilon_n(\mathbf{k})/\partial\mathbf{k}$, $v'_{nn'}(\mathbf{k}) = (nk|\mathbf{v}|n'k)_{n\neq n'}$.

Corrections to the principal approximation (for σ_{MN}) defined by formulas (10)–(12), (16)–(18), due to the contribution of $\delta\sigma_{MN}$ and to the higher, in $\mathcal{H}'$, approximations in $Q_M(\varepsilon)$ and $I_{\varepsilon f'_M}(\varepsilon)$ not taken into account in the principal definition, are small for $\Phi_0 \gg 1$, $\beta\Delta \ll 1$, if

$$|\langle\delta v_{nk}\rangle_0| \ll \langle v_{nk}\rangle_0, \qquad \Omega_b \ll \Delta, \quad \text{i.e.} \quad \Delta_e < \Delta_e^0(\omega_p,\Phi_0) \ll \omega_p\Phi_0, \tag{19}$$

where δv_{nk} is the correction to $v_{nk} = |\mathbf{v}^0(nk)|$. Relations (10)–(12), (16)–(18) make it possible to calculate the kinetic coefficients σ_{MN} under (19) and at low $T \lesssim T'_0$.

3. Equation (16)–(18) is solved in the usual way, and for ($H \parallel OZ$)

$$f'(\mathbf{kn}) = \left\{1 - eHI_0^{-1}\left(v_y(\mathbf{kn})\frac{\partial}{\partial k_x} - v_x(\mathbf{kn})\frac{\partial}{\partial k_y}\right)\right\}^{-1} I_0^{-1}Q(\mathbf{kn}). \tag{20}$$

From (12), (20) it follows that at $H = 0$ the drift (ohmic) mobility is

$$u_{ij}^{(s)}(T) \equiv |e|\frac{\beta}{2}\left\langle v_i(\mathbf{kn})I_0^{-1}v_j(\mathbf{kn}) + v_j(\mathbf{kn})I_0^{-1}v_i(\mathbf{kn})\right\rangle_0, \tag{21}$$

$$i,j \equiv x,y,z; \qquad \langle\ldots\rangle_0 \equiv \iiint_{\text{(over the Brillouin zone)}} \frac{V(d\mathbf{k})}{(2\pi)^3}\sum_n f_0(n\mathbf{k})(\ldots),$$

and approximately (cf. ([3]))

$$u(T) \sim |e|\beta\Delta(T)\big(m^*(T)\Omega_b\big)^{-1} = \frac{|e|a^2}{\hbar}\frac{\beta\Delta^2}{\Omega_b}. \tag{22}$$

In the principal approximation $\Omega_b \sim \exp(-\beta\omega_p)$, i.e. it increases with T (two-phonon scattering of a polaron in a narrow band $\Delta \ll \omega_p$). Since $\Delta(T)$ decreases as T increases, one should expect that, in the main, $u(T)$ decreases exponentially as T increases.

From (12), (16)–(18), for $H < H_0\Omega_b\Delta^{-1} \ll H_0$ and $T < T_0'$, it follows that the Hall mobility $u_H = |R_H|\sigma$ has the form

$$u_H(T) = \frac{\left| e \left\langle v_y(\mathbf{kn}) I_0^{-1} \left(v_y(\mathbf{kn}) \frac{\partial}{\partial k_x} - v_x(\mathbf{kn}) \frac{\partial}{\partial k_y} \right) I_0^{-1} v_x(\mathbf{kn}) \right\rangle_0 \right|}{\left\langle v_y(\mathbf{kn}) I_0^{-1} v_y(\mathbf{kn}) \right\rangle_0} \sim \frac{|e|}{m^*\Omega_b}, \tag{23}$$

i.e. $u_{Hu}^{-1} \sim (\beta\Delta)^{-1} \gg 1$. For $T > T_0$ also usually $u_H \gg u$, if $\sum_{fi} \chi_{fi}^{ss'} \omega_{fi}$ are the same for all nearest s, s'; u_H contains terms of the form ([7])

$$u_H^0 = |e| a^2 \hbar^{-1} \Delta_e \xi_0^{-1} (\beta\xi_0)^{-1/2} \exp(\beta\xi_0)$$

and

$$\delta u_H \equiv |e| a^2 \hbar^{-1} \Delta_e (\xi_0 T)^{-1/2} \times \exp(-\beta U_0) \ll u_H^0,$$

i.e. $u_H \sim u_H^0$ (in the preliminary estimates ([6a]) only the part of u_H of the form δu_H, the same as in (11), was included). For $T < T_0'$ the thermopower is

$$\gamma_0 \simeq \frac{1}{eT}(\mu - \varepsilon_{\text{pol}} - \delta\varepsilon),$$

just as for $T > T_0$ ([6a]). (For $T \gg T_0$ and $N_i \ll N_0$,

$$\gamma_0 \simeq e^{-1} \left(\ln \frac{N_i}{N_0} + \frac{\delta\varepsilon}{T} \right),$$

and usually one may put $\gamma_0 \sim -e^{-1} \ln(N_i/N_0)$.)

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