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Abstract

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THEORY OF NONSTATIONARY CONDUCTIVITY OF SEMICONDUCTORS WITH LOW MOBILITY*

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1. In the present communication, within the framework of the theory developed in ([1–3, 6]), the tensor of nonstationary conductivity $\sigma_{\mu\nu}(\omega)$ and of mobility $u_{\mu\nu}(\omega) = |eN_c|^{-1}\,\mathrm{Re}\,\sigma_{\mu\nu}(\omega)$ is calculated for a semiconductor with low mobility, in which a current carrier of the small-polaron type is described mainly by local-type functions $|sn\rangle = |s\rangle|n^{(s)}\rangle$ (a polaron packet at the s-th site ([1])) of the electron–phonon system with energy $\varepsilon_n = \sum_{fj}\hbar\omega_{fj}N_{fj}$, where $n \equiv (\ldots N_{fj}\ldots)$; the binding energy of the small polaron $\delta\varepsilon \gtrsim \hbar\omega_p\Phi_0 \gg \Delta_e(\sim \Delta_{ss'})$ (Δ_e is the width of the band of the Bloch electron); ω_p (and $\Delta\omega_p$) is the frequency (and branch width) of essential phonons; $\Phi_0 \equiv \Phi(T=0)$, see (6). In the notation of ([1–3]), in the absence of a magnetic field H ($E_\beta(\omega) = \frac{\hbar\omega}{2}\,\mathrm{cth}\,\frac{\beta\hbar\omega}{2}$; $\beta \equiv (kT)^{-1}$)

$$u_{\mu\nu}(\omega) = \frac{|e|}{E_\beta(\omega)}\lim_{\varepsilon\to+0}\int_0^\infty dt\, e^{-\varepsilon t}\cos\omega t\;\mathrm{Re}\langle v_\nu v_\mu(t)\rangle \tag{1}$$

(in the absence of degeneracy $N_c \approx N_0\exp\left[\frac{e\alpha}{k} - \beta\delta\varepsilon\right]$, where α is the thermo-e.m.f.; N_0 is the number of cells per 1 cm^3). The criteria of the theory are:

$$\Delta_e \ll \hbar\omega_p\Phi_0; \qquad \Delta_e < \left\{\Delta_e^0 \equiv (\hbar\omega_p\Phi_0 kT_1)^{1/2};\ (\hbar\omega_p\Phi_0 kT_0)^{1/2}\ \text{for}\ T > T_1\right\}\ ([1,8]),$$

$$\Delta \equiv \Delta_e\exp[-\Phi(T)] \ll \hbar\Gamma_0; \qquad \omega < \omega_p\Phi_0. \tag{2}$$

In the general case $\Gamma_0 \approx \Gamma_h + \Gamma'$ (Γ_h see in (5)), and for $kT \ll \hbar\omega_p\Phi_0$

$$\Gamma' \sim (\Delta_e/\hbar\omega_p\Phi_0)^4\,\omega_p^2(\Delta\omega_p)^{-1}\,\mathrm{sh}^{-1}(\beta\hbar\omega_p/2);$$

if $\Delta(T_0') = \hbar\Gamma_0(T_0')$, then $\Delta \ll \hbar\Gamma_0$ for $T > T_0'$, with

$$T_0' = T_0 = \gamma \left.\frac{\hbar\omega_p}{2k}\right|_{\gamma\sim 1}$$

for $\Gamma_0 \approx \Gamma_h$, and $T_0' < T_0$ for $\Gamma_0 \gg \Gamma_h$; in (2)

$$T_1 = \gamma' \left.\frac{\hbar\omega_p}{2k}(\operatorname{Ar}\operatorname{sh}\Phi_0)^{-1}\right|_{\gamma'\sim 1},$$

(see ([1,7,8]))**.

2. For $\omega \geq 0$, in the basic approximation the Ohmic mobility has the form (see (1) and ([1,3,6]))

$$u^0_{\mu\nu}(\omega) \equiv u^h_{\mu\nu}(\omega) + u^d_{\mu\nu}(\omega) = \frac{|e|}{E_\beta(\omega)} \sum_{(s',0)} \{v^{0s'}_\nu, v^{s'0}_\mu\} \times$$

$$\times \lim_{\varepsilon\to+0} \operatorname{Re} \int_0^\infty dt\, \cos\omega t \sum_{nn'} \exp(\beta F_0 - \beta\varepsilon_n)\, |\langle n^{(0)}|n'^{(s')}\rangle|^2 \times$$

$$\times \exp\left[\frac{it}{\hbar}(\varepsilon_n - \varepsilon_{n'})\right] \varphi_{nn'}(\varepsilon, t; \omega), \tag{3}$$

where $\varphi_{nn'} = \varphi^h_{nn'} + \varphi^d_{nn'}$ (or $\approx \exp(-|t|\tilde{\Gamma}_{0s'}(\omega))$,

$$\varphi^h_{nn'} = (1 - \delta_{nn'})e^{-\xi t};$$

$$\varphi^d_{nn'} = \delta_{nn'} \exp(-t\tilde{\Gamma}_{0s'}(\omega)), \qquad \delta_{nn'} \equiv \prod_{fj} \delta_{N_{fj}N'_{fj}}.$$

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** The criterion $\Delta \ll \hbar\Gamma_h$ is sufficient ([1]), but for $\Gamma_0 \gg \Gamma_h$ it is not necessary (also not necessary is the criterion $\Delta_e^2 < \mathcal{G}^2 \exp(-\varkappa\beta\mathcal{G})_{\varkappa<1}$ from ([6,8]), i.e., in ([6,8]) here one should put $\varkappa = 0$).

In (3), in the nearest-neighbor approximation, $\tilde{\Gamma}_{0s'} = \Gamma_0 - W_0(s')$, where $\Gamma_0 \approx \nu_c\Gamma_{(0)s'}$ (ν_c is the number of nearest neighbors) and $W_0(s')$ is the mean Fourier component of the probability of "scattering"$\mathbf{k} \to \mathbf{k}'$ (in the main approximation), and usually $W_0(s') \sim \Gamma_0 \sim \Gamma_{0s'}$;

$$v^{ss'}_\nu \approx \frac{i}{\hbar}\Delta_{ss'}(s'_\nu - s_\nu); \qquad \{v^{0s'}_\nu, v^{s'0}_\mu\} = \frac{|\Delta_{0s'}|^2}{\hbar^2} s'_\mu s'_\nu \sim \frac{\Delta^2_\varepsilon}{\hbar^2} a^2,$$

(see (1)) and substituting (13) into (6). Calculating multiple sums over n, n' (1–3, [5,6]), we obtain, for $\omega < \omega_p \Phi_0$, $T > T_1$,

$$u^h_{\mu\nu}(\omega) = u^h_{\mu\nu}(0)\frac{\operatorname{sh}\beta\hbar\omega/2}{\beta\hbar\omega/2}\exp\left(-\frac{\omega^2\tau_l^2}{4}\right); \tag{4}$$

$$u^h_{\mu\nu}(0) = |e|\beta\sum_{(s'|0)} s'_\mu s'_\nu \Gamma_{h;s'}; \tag{5}$$

$$\Gamma_{h;s'} = \frac{|\Delta_{0s'}|^2}{\hbar^2}\int_0^\infty dt\,\cos\omega t\left\{\exp\left[\Psi\left(t - i\frac{\hbar\beta}{2}\right)\right] - 1\right\}\exp(-2\Phi(T));$$

$$\Phi(T) = \sum_{fj}\frac{1}{2}\lambda^{0s'}_{fj}\operatorname{cth}\frac{\beta\hbar\omega_{fj}}{2}; \qquad \Psi(t) = \sum_{fj}\lambda^{0s'}_{fj}\cos\omega_{fj}t/\operatorname{sh}\frac{\beta\hbar\omega_{fj}}{2}, \tag{6}$$

$$\lambda^{0s'}_{fj} \equiv \frac{\omega_{fj}}{2\hbar}(q^{s'}_{fj} - q^0_{fj})^2; \qquad \tau_l^2 \equiv -\left(\frac{d^2\Psi(t)}{dt^2}\right)^{-1}_{t=0};$$

$$u^d_{\mu\nu}(\omega) = \frac{|e|}{E_\beta(\omega)}\frac{1}{2}\sum_{\pm}\sum_{s'}\tilde{\Gamma}_{0s'}(\pm\omega)\left(\tilde{\Gamma}^2_{0s'}(\pm\omega) + \omega^2\right)^{-1}\Delta^2_{0s'}e^{-2\Phi(T)} * . \tag{7}$$

For $T > T_1$, when $\exp[\Psi(i\hbar/2kT)] > \exp[\Psi(i\hbar/2kT_1)] = 1$,

$$\Gamma_{h;s'} \sim \Gamma_h \approx \frac{\sqrt{\pi}}{\hbar^2}\Delta^2_{0s'}\tau_l\exp[-\beta\mathcal{E}(T)],$$

where

$$\mathcal{E}(T) = \beta^{-1}\sum_{fj}\lambda^{0s'}_{fj}\operatorname{th}\frac{\beta\hbar\omega_{fj}}{4};$$

for $T < T_1$

$$\Gamma_{h;s'} \approx \frac{2\pi}{\hbar^2}\Delta^2_{0s'}\sum_{f_1 f_2}\prod_{r=1,2}\lambda^{0s'}_{f_r}\operatorname{sh}^{-1}\left(\frac{\beta\hbar\omega_{f_r}}{2}\right)\delta(\omega_{f_1} - \omega_{f_2}).$$

In (4)–(7), $u^h_{\mu\nu}$ and $u^d_{\mu\nu}$ are contributions to $u^0_{\mu\nu}$ from "jumps" of the polaron packet and its "spreading" –the analogue of band transport. For $T = T_q$, $T'_0 \lesssim T_q \leq T_0$,

* More precisely, from (1) we have:

$$u^d_{\mu\nu}(\omega) = E^{-1}_\beta(\omega)\frac{1}{N_0}\sum_{s,s';\,n}(sn|v_\mu|s'n)\,\psi^0_{n\nu}(s-s') = \sum_{kn} v_\mu(kn)\psi^0_\nu(kn),$$

where

$$\psi^0_\mu(kn) = |e|\ \mathrm{Re}\ \frac{1}{N_0}\sum_{ss'} e^{i\mathbf{k}(s-s')}\int_0^\infty dt\, e^{-\varepsilon t}\cos\omega t\,(s'n|v_\mu(t)|sn)_{\varepsilon\to+0}$$

can be obtained by the method of (8), which for equilibrium phonons also gives (7).

$u^0_{\mu\mu}(0)$ has a minimum. For $T < \mathcal{E}/2k$ and $\hbar\omega < \mathcal{E}$, $u^n_{\mu\mu}(\omega) \geq u^h_{\mu\mu}(0)$, and $u^h_{\mu\mu}(\omega)$ increases with ω*; for $T \ll \mathcal{E}/k$ the "hops" of a carrier are activated by the fluctuational deformation of the lattice the more effectively, the closer the energy $\hbar\omega$ of the photons dissipated in multiphonon processes is to the carrier binding energy $\sim\mathcal{E}$.

Practically, for $T > \{T_1, T'_0\}$ (and certainly for not too small ω) $u^0_{\mu\mu}(\omega) \approx u^h_{\mu\mu}(\omega)$, while for $\omega \gg \mathcal{E}/\hbar$, apparently, $u^0_{\mu\mu}(\omega)$ decreases with ω, so that the mobility $u^0_{\mu\mu}(\omega)$ at $\omega \sim \mathcal{E}/\hbar$ probably has a noticeable maximum (with width $\Delta\omega < \mathcal{E}/\hbar$).

3. In an analogous way one can estimate the Faraday angle θ_F and $u^{(a)}_{\mu\nu}(\omega) \equiv \frac{1}{2}(u_{\mu\nu}(\omega) - u_{\nu\mu}(\omega))$ for $H \neq 0$. For $H \parallel OZ$, in the simplest case and for not too small ω ($\ll \mathcal{E}/\hbar$), for crystals (I), in which three appropriate sites s_1, s_2, s_3 can be mutual nearest neighbors ([6]), the formula for $\theta^I_F(\omega) \equiv \theta^I_F(u^{(a)}_{xy}; u_{\mu\mu}; \omega)$ can be represented in the form (for the most essential $T < \mathcal{E}/k$)

$$\theta^I_F(\omega) \approx \frac{eN_c}{2cv_0(\omega)}\,u^I_{xy}(\omega) \approx$$

$$\approx \frac{eN_c}{2cv_0(\omega)}\left\{u^{0\mathrm{I}}_{xy}\,\frac{1-(\hbar\omega/4\mathcal{E})^2}{\beta E_\beta(\omega)} + O\left(\delta_2 u^I_{xy}\,\frac{\mathrm{ch}\,\beta\hbar\omega/2}{\beta E_\beta(\omega)}\right)\right\}, \tag{8}$$

where $v_0(\omega)$ is the refractive index at $H = 0$. In (8), $u^{0\mathrm{I}}_{xy}$ and $\delta_i u^I_{xy}$ are determined for $T > T'_0$ by the general expression (6) (in (6) $\tau_0(\beta) \approx \hbar\beta$; see also $\Psi_i(t)$):

$$u^I_{xy} \equiv u^I_{xy}(0) = \frac{|e|\beta}{2\hbar^3}\,\frac{1}{N_0}\sum_{s_1s_2s_3}(Q^0 + \delta_1 Q + \delta_2 Q)\times$$

$$\times\left\{\frac{\partial}{i\,\partial H}\left[\Delta_{s_1s_2}\Delta_{s_2s_3}\Delta_{s_3s_1}\right]\right\}_{H=0} \equiv u^{0\mathrm{I}}_{xy} + \delta_1 u^I_{xy} + \delta_2 u^I_{xy};$$

$$Q^0 = \exp\left[-\sum_{p,r=1}^{3} \Phi_{s_p s_r}(T)\right] \int_0^{\beta\hbar/2} d\tau' \left\{ 2\,\mathrm{Im} \int_0^{\infty} dt\, e^{-\Gamma_0|t|} \times \right.$$

$$\times \exp\left[\Psi_1(t) + \Psi_2\left(i\tau' + i\frac{\beta\hbar}{2}\right) + \Psi_3\left(t - i\tau' + i\frac{\beta\hbar}{2}\right)\right] -$$

$$\left. - \int_0^{\beta\hbar/2} d\tau\, \exp\left[\Psi_1\left(i\tau + i\frac{\beta\hbar}{2}\right) + \Psi_2\left(i\tau' + i\frac{\beta\hbar}{2}\right) + \Psi_3(i\tau - i\tau')\right] \right\}; \quad (9)$$

$$\delta_1 Q = \exp\left[-\sum_{p,r=1}^{3} \Phi_{s_p s_r}(T)\right] \mathrm{Re} \int_0^{\infty} dt\, e^{-\Gamma_0|t|} \int_0^{t} dt' \times$$

$$\times \left\{ \exp\left[\Psi_1(t) + \Psi_2\left(t' + i\frac{\beta\hbar}{2}\right) + \Psi_3\left(t - t' + i\frac{\beta\hbar}{2}\right)\right] + \right.$$

$$\left. + \exp\left[\Psi_1\left(t + i\frac{\beta\hbar}{2}\right) + \Psi_2\left(t' + i\frac{\beta\hbar}{2}\right) + \Psi_3(t - t')\right] \right\}; \quad (10)$$

* For $T < T_0'$ the mobility $u_{\mu\mu}(\omega)$, as ω increases, generally speaking decreases at small ω (as also for $T < T_q$), has a minimum at $\omega = \omega_q$ ($u^h_{\mu\mu}(\omega_q) = u^d_{\mu\mu}(\omega_q)$), and increases for $\omega > \omega_q$ up to $\omega \sim \mathcal{E}/\hbar$ (decreasing after the maximum). On p. 287 in (8), instead of $T < T_0' \equiv \omega_p/\Phi_0 < T_0$ one should read $T < T_0'(\ll T_0)$, $T < \dfrac{\hbar\omega_p}{2k}(\mathrm{Arsh}\,\Phi_0)^{-1}$; the contribution of acoustic phonons to $\Omega_b \equiv \Omega_0(\sim \Gamma)$, in addition to the contribution of the form (22) from (8), may contain a contribution of the form $AT^{l>0}$.

$$\delta_2 Q = -\exp\left[-\sum_{p,r=1}^{3} \Phi_{s_p s_r}(T)\right] \mathrm{Im} \int_0^{\beta\hbar/2} d\tau' \int_0^{\infty} dt \times$$

$$\times e^{-\Gamma_0|t|} \exp\left[\Psi_1\left(t + i\frac{\beta\hbar}{2}\right) + \Psi_2\left(i\tau' + i\frac{\beta\hbar}{2}\right) + \Psi_3(t + i\tau')\right]. \quad (11)$$

In particular, for $T < \mathcal{E}/k$,

$$|\overset{0}{u}{}^I_{xy}| \sim u_0 \frac{H}{H_0} \frac{\beta\Delta_e^3}{\mathcal{E}^2}; \qquad \delta_2 u^I_{xy} \sim u_0 \frac{H}{H_0} \Delta_e^3 \beta^2 \mathcal{E}^{-1} e^{-\beta\tilde{\mathcal{E}}(T)};$$

$$|\delta_1 u^I_{xy}| \sim u_0 \frac{H}{H_0} \beta^2 \mathcal{E}^{-1} \Delta_e^3 e^{-\beta\tilde{\mathcal{E}}(T)} + \Delta u^d_{xy}; \qquad \Delta u^d_{xy} \sim u_0 \frac{H}{H_0} \beta\Delta^3 (\hbar\Gamma_0)^{-2},$$

where

$$\tilde{\mathcal{E}}(T) = \mathcal{E}(T) + U(T); \quad U(T) \leqslant \mathcal{E}/3; \qquad \text{for } T > T_0 \quad \tilde{\mathcal{E}} \simeq \frac{4}{3}\mathcal{E};$$

$u_0 = |e|a^2/\hbar$; $H_0 = \hbar c/|e|a^2$. The expression Δu^d_{xy} in u^I_{xy} is the analog of u^d_{xx} in u^0_{xx}, and

$$|\Delta u^d_{xy}|\,|u^I_{xy}|^{-1} \sim (\Delta/\hbar\Gamma_0)^2(\mathcal{E}/\Delta_e)^2 e^{-2\Phi(T)} \leqslant 1$$

for $T \geqslant T_c$, and usually $T_c \leqslant T_0'$. The Hall mobility $u_H = cH^{-1}|u_{xy}|u^{-1}_{xx}$ decreases with increasing T for $T > T_q$ and for $T < T_c (< T_0')$, see ([6],[8]) (but, apparently, it may increase for $T_c < T < T_q < T_0$, if $\nu \equiv u_H(T_q)u^{-1}_H(T_c) > 1$, or decrease at all T, if $\nu < 1$).

The expression for u^I_{xy} is due to the contribution of phase-correlated transitions of the carrier over three sites s_1, s_2, s_3; $\delta_1 u^I_{xy}$ corresponds to the contribution of real correlated transitions; the leading term at $T < \mathcal{E}/k$, $\overset{0}{u}{}^I_{xy}$, is rather the contribution of (two out of three) such virtual multiphonon transitions and, unlike $\delta_1 u^I_{xy}$, contains no activation temperature dependence, describing an essentially quantum and non-Markovian transport process (with nonactivation redeformation of the lattice). For crystals (II), which do not belong to class (I), the effects odd in H (Hall, Faraday, etc.) may be due mainly to the contribution of four-site correlated transitions, and then (the formula for $u^{\text{II}}_{xy}(\omega)$ is derived analogously)*

$$|u^{\text{II}}_{xy}| \sim |u^I_{xy}|\Delta_e\mathcal{E}^{-1} \ll |u^I_{xy}| \quad \text{and} \quad |\theta^{\text{II}}_F| \sim |\theta^I_F|\frac{\Delta_e}{\mathcal{E}}.$$

The sign of $u^I_{xy}(\omega)$ and $\theta^I_F(\omega)$ is usually ([6]) determined by the sign of the carrier charge e**. As is seen from (8)–(12), usually, for $T < \mathcal{E}/k$ and $\hbar\omega \ll \mathcal{E}$, $\theta^I_F(\omega)$ decreases with increasing ω and with T (for asymptotically large ω, $\theta^I_F(\omega) \propto u^I_{xy}(\omega) \propto \omega^{-2}$).

Note added in proof. In a recent article ([10]) it is assumed that u^I_{xy} is determined by the probability of three-site hops, the result of whose estimate makes a contribution analogous to the term $\delta_1 u^I_{xy}$ from (12) (see ([6])).

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* The expression for the contribution of four-site transitions for crystals (I) determines the first correction $|\Delta$

** In (7), within the formulation of the problem and of the general approach used in (1, 3), the static ($\omega = 0$) mobility of a semiconductor with low mobility was calculated in a basis of polaron-band "waves" and in the technique ([9]), and for the principal contribution formulas were obtained analogous to the relations from ([1],[6],[8]). In view of the special features of the problem, one may think that for $T > \hbar\omega_p/2k$, when the "mean free path" of such "waves" $l \ll a$, their use as a basis is artificial.

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