QUANTUM THEORY OF THE TRANSVERSE CONDUCTIVITY AND HALL EFFECT OF POLARONS IN CERTAIN DISORDERED STRUCTURES\

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Abstract

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M. I. KLINGER

QUANTUM THEORY OF THE TRANSVERSE CONDUCTIVITY AND HALL EFFECT OF POLARONS IN CERTAIN DISORDERED STRUCTURES*

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1. In the present communication a theory is set forth for the transverse polaron conductivity
$\sigma_t(\omega) = \sigma_t'(\omega) + i\sigma_t''(\omega)$ and for the Hall angle in a three-dimensional, generally speaking disordered, system with n (per 1 cm^3) localization centers of polarons (in local states $|i\rangle$), in which the static conductivity, $\sigma \equiv \sigma_{xx}(\omega = 0)$ and $\sigma_t \equiv \sigma_t(0) = \sigma_t'(0)$, is determined by nonadiabatic hops. The external homogeneous crossed electric and magnetic fields are denoted by $E \equiv E_x \propto e^{i\omega t}$ and $H \equiv H_z$, with $H \ll H_0 \equiv \hbar c/|e|r^2$, $r \equiv \left(\frac{3}{4\pi}N\right)^{1/3}$. Polarons (in the generalized sense of the term ([3])) are considered both in weak ($\Phi_0 \ll 1$) and in strong ($\Phi_0 \gg 1$) coupling, including small polarons; $\Phi_0 \equiv \Phi(T=0)$ is the parameter of the electron-phonon coupling; $\Phi \equiv \Phi(T) \geq \Phi_0$. Concrete examples are: the conductivity of polarons (including small ones) on impurities (ic); hopping conductivity of small polarons over sites of the host lattice (sp). The model of such systems is described in ([1]) (see below, item 2).** As for $\sigma(\omega) \equiv \mathrm{Re}\,\sigma_{xx}(\omega)$, in ([1,8]) the theory also describes the case of degenerate polarons, but at not too high concentrations N_c of current carriers, $N_c < N(1-K_0)$, with $K_0 \sim \exp(-I/2T) \ll 1$ and $I \gg T$, when the Hubbard inter-polaron repulsion is not yet the dominant factor and its characteristic energy $I > 2\zeta$; ζ is the chemical potential of the polarons, measured (as are their energy levels) from the ground level on an isolated center. In essence, a strong-coupling Bloch model with a "small" electronic resonance integral $\Delta_e(R)$ is used.

The theory is based on the approach and considerations of ([1−3]): $\sigma_t'(\omega)$ (in cases that were not discussed in ([2])) and $\sigma_t''(\omega)$ are calculated by means of an adequate deciphering of the Kubo formulas for $\sigma_t(\omega)$ (and $\sigma_{xx}(\omega)$), which contain, generally speaking, also averaging $\langle ... \rangle_{\mathrm{Av}}$ over fluctuations of local levels $\{\varepsilon_i\}$ in a band (D) of width D and over configurations $\{R_i\}$ and $\{R_{ij} \equiv |R_i - R_j|\}$. As with $\sigma_{xx}(\omega)$,

$\sigma_t(\omega) = \Sigma_t(\omega) + S_t(\omega)$: $\Sigma_t(\omega)$ and $S_t(\omega)$ are determined, respectively, by the "antisymmetric"$(x \leftrightarrow y)$ correlators $K^{(a)}_{\hat{v}_x\hat{v}_y}(t)$ of velocities $\hat{v}_x$ and by $(\omega^2 K^{(a)}_{\hat{p}_x\hat{p}_y}(t))$ of dipoles $(\hat{p}_x)$; $S_t(0) = 0$. The deciphering of the Kubo formulas for $\sigma_t(\omega)$ has been carried out by the methods of ([1]) with averaging $\langle ... \rangle_{\mathrm{Av}}$. For (sp), $\sigma_t(\omega) = \Sigma_t(\omega)$ and $S_t(\omega) = 0$.

2. The averaging $\langle ... \rangle_{\mathrm{Av}}$ as a whole is one of the basic and most difficult problems in the theory of transport under consideration in disordered systems

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* Some of the main results were briefly reported by the author in September 1969 in a survey lecture at the International Conference on Amorphous and Liquid Semiconductors (Cambridge).

** The notation and the model of the system used here are the same as in ([1],[3]). In particular, $\mathcal{E}$ is the polaron activation energy of hopping drift mobility, $\mathcal{E} \approx \frac{1}{2}\omega_{ph}\Phi_0$ for $\Phi_0 \gg 1$. Here ω_{ph} is the characteristic frequency of the essential phonons. Below, $\hbar = 1$ and $k_B = 1$, $T_{ph} = \omega_{ph}/2$.

(special discussion of it is beyond the scope of the article, cf. (5)) and as yet has no general rigorous solution for 3-dimensional systems (for the 1-dimensional case see, for example, (9)). Therefore, also bearing in mind estimates of the ω- and T-dependences and of the order of magnitude of $\sigma_t(\omega)$, an approximate averaging model is used, which in fact takes into account the "random" character of ε_i and the distribution $g_q(\varepsilon_1 \dots \varepsilon_q)$ of the polaron levels ε_i $(q \geqslant 1)$. For disordered systems of type (ic) this model in fact includes the following assumptions: 1) the overwhelming majority of possible configurations $\{R_i\}$ correspond to "conducting chains" for $R_{ij} \sim r$; 2) the "smooth" impurity potentials $|v(r)| \gg |\Delta_e(r)|$ (the band (D) is a band of "classical" concentration broadening), so that the distributions $g_q(\varepsilon_1\varepsilon_2 \dots \varepsilon_q)$ are practically not connected with fluctuations $\Delta_e(R)$: averaging over $\{\varepsilon_i\}$ (for $R_{ij} = \lambda_0 r$) and over $\{R_i\}$ are statistically independent; 3) for estimating mean quantities of the type $\chi_q \equiv \langle \Delta_e(R_{12}) \cdots \Delta_e(R_{q,1}) \rangle_{\{R_i\}}$, describing terms of q-th order (in $\Delta_e(R)$) in the expansions defining $\sigma_{\mu\nu}(\omega)$, an approximation is introduced for the higher correlation functions of the "gas" of centers (in "conducting chains")

$$P_q(R_{12} \dots R_{q,1}) \approx P_2(R_{12}) \dots P_2(R_{q-1,q}) P_2(R_{q1}),$$

used in the theory of rarefied gases (here, since $r \gg r_B$), so that $\chi_q \approx \Delta^q_{AV}$, where $\Delta_{AV} = \langle \Delta_e(R_{i2}) \rangle_{AV} \equiv \Delta_{AV}(r) = \Delta_e(R_0)$ and $R_0 = \lambda_0 r$, $\lambda_0 \sim 1$ (in any case, $\Delta^q_{AV} \equiv (\chi_q)^{1/q}$ is no greater than Δ_{AV}). Since $P_2(R)$ has evidently not been found (and a direct calculation of Δ_{AV} and λ_0 has not yet been carried out), Δ_{AV} (and λ_0) is taken to be a parameter of the theory, whose dependence on r is found from comparison of $d\sigma_{xx}/dr$ $(\propto d\Delta_{AV}/dr)$ with the corresponding experimental data, which in principle closes the calculation scheme. (From comparison of $d\sigma_{xx}/dr$ and $d\sigma_t/dr$ with experimental data one can also check the validity of the assumptions that $\Delta_{AV}^{(3)} \approx \Delta_{AV}$ and that $\Delta_{AV} = \Delta_e(\lambda_0 r)$ for $\lambda_0 \sim 1$.)

Now the adopted model is analogous to the Anderson model from (6), if it is extended to the calculation of $\sigma_{\mu\nu}(\omega)$ (for $\omega \geqslant 0$ and finite electron-phonon coupling). This analogy makes it possible to apply the results of the analysis (6) to the estimate of the averaged terms of the expansion of $\Sigma_{\mu\nu}(\omega)$ and of the principal, hopping, term $\Sigma^h_{\mu\nu}(\omega)$. The criteria (small parameters) of the theory which follow from such estimates are as follows; for small polarons (both for (ic) and for (sp)) they are given in §§ 3, 10 (1). For other polarons of weak or strong coupling in the case (ic) (and analogous cases) the main criterion has the form $\Delta_{AV} \ll \eta_0 D$, $\eta_0 \sim 1$ (cf. § 10 (1)). For $\omega \gg D$, this criterion may be $\Delta_{AV} \ll \omega$, so that the critical concentration N_{cr} would increase with increasing ω, see (1).*

2. The component $\Sigma_t(\omega)$ is determined by phase-correlated hops over 3 $(\Sigma_t(3;\omega))$ or 4 $(\Sigma_t(4;\omega))$ centers (see (1-3)). Here it is sufficient to discuss $\Sigma_t(3;\omega)$ in somewhat more detail for the following reasons: 1) according to approximate estimates (for Δ_{AV}, $\mathcal{E}$, and D of the same order of magnitude)

$$\left|\Sigma_{t'}^{(\prime\prime)}(4;\omega)\right|_{\max}\left|\Sigma_{t'}^{(\prime\prime)}(3;\omega)\right|^{-1} \lessgtr \Delta_{AV}[\max\{D;\mathcal{E}\}]^{-1}\exp(-\beta\Delta W'^{(\prime)})$$

(see (1, 2) and below), where $\Delta W'^{(\prime\prime)} < W'^{(\prime\prime)}$, see (2) (for (sp), under reasonable assumptions regarding the coefficients V_f of the electron-phonon interaction (1), it can in fact be assumed that $\beta\Delta W'^{(\prime\prime)} \ll 1$ for $T \gg \Delta_{AV}^{(p)} = \Delta_{AV}\exp(-\Phi)$, which is used in (1, 2)); in any case, the ω- and T-dependences for $\Sigma_{t'}^{(\prime\prime)}(4;\omega)$ and $\Sigma_{t'}^{(\prime\prime)}(3;\omega)$ here have an analogous character (quantitatively, formulas (2) refer to the case $\beta\Delta W'^{(\prime\prime)} < 1$ and $\beta W_D'^{(\prime)} < 1$, see (1), (2)); 2) $\Sigma_t(\omega) \simeq \Sigma_t(3;\omega)$ not only for (sp) in suitable (for example, hexagonal) lattices, but, as may be expected,

* For (ic), in the adopted model it also follows that, at least in some interval, $K' < K < 1-K''$ ($K' \ll 1$ and $K'' \ll 1$), ζ contains a term $\zeta_0 = \zeta_0(K;T)$, constant (or weakly decreasing) with T^{-1}; ζ_0 determines the corresponding activation energy W_D for $\sigma_{xx}(\omega)$; for example, $K' \approx K'' \approx \exp(-D/T)$ for $D \gg T$ in (5) (as $K \to 1$, apparently, $\zeta_0 \to 0$, i.e. $\beta\zeta \approx$ const in T). For estimates one may use approximations of the type $g_2(\varepsilon_1,\varepsilon_2) \approx g_1(\varepsilon_1)g_1(\varepsilon_2)$ (for $R_{12} \sim r \gg r_B$).

and for (ic) (and analogous cases), when there exist "conduction chains"(through the entire system of centers) over triples of centers with $R_{ij} \sim r$. In the subsequent estimates it is assumed that $\Delta_{AV}^{(p)} < T$ and $\{D,\mathcal{E}\} \gg T$. The structure of the general expressions obtained for $\Sigma_t(3;\omega)$ is rather simple. In particular, for $\omega/2T \ll 1$, $\Sigma_t'(3;\omega) \simeq \Sigma_t(3) \equiv \Sigma_t(3;0)$, and $\Sigma_t''(3;\omega)/\beta\omega$ are determined by expressions of the type

$$\beta N_c \frac{H}{H_0} \left\langle \sum_{23} \Delta_e^0(R_{12})\Delta_e^0(R_{23})\Delta_e^0(R_{31}) \sum_{\varepsilon_1\varepsilon_2\varepsilon_3} \varphi(\xi-\varepsilon_1)\varphi(\xi-\varepsilon_2)\times \right.$$

$$\left. \times \left\{ J_1(\omega_{12};\omega_{13})(1-f_\infty(\varepsilon_3)) - \frac{1}{2} J_2(\omega_{12};\omega_{13}) f_\infty(\varepsilon_3) \right\} \right\rangle_{AV},$$

where $\Delta_e^0(R_{12}) \equiv [\Delta_e(R_{12})]_{H=0}$; $\varphi(x) \equiv [2e^{\beta x/2} + e^{-\beta x/2}]^{-1}$; $f_\infty(\varepsilon) = [1 + \frac{1}{2}e^{\beta(\varepsilon-\xi)}]^{-1}$; $\beta = 1/T$ (for simplicity, the case considered is that of nondegenerate $|i\rangle$ states), $J_\alpha(x,y)$ is the contribution of the "excluded" (by summation) phonon variables of the type typical for the characteristics of such multiphonon processes, for example, the integral ($\equiv J(i\omega)$) in $\sigma \equiv \sigma_{xx}(0)$ from (79) ([1])*. In particular, for $\Phi_0 \gg 1$, $J_1''(\omega_{12};\omega_{13}) \simeq J_2''(\omega_{12};\omega_{13}) \sim |2\mathcal{E} + \omega_{13}|^{-1} J(\omega_{12})$ in $\Sigma_t''(3;\omega)$. For brevity, the estimates and the main dependences for $\beta\omega/2 \ll 1$ are given for $u_t \equiv \Sigma_t(3)/|e|N_c$ and $\Delta_t \equiv \Sigma_t''(3;\omega)/|e|\omega N_c$. (Estimates of $\Sigma_t'(3;\omega)$ in ([2]) for $\Phi_0 \gg 1$ and high T are given for the case $T > D$, when $\exp(-\beta W_D') \simeq 1$.) Both u_t and Δ_t exhibit activation-type T-dependences, similar to those for $u \equiv \sigma/|e|N_c$ [in ([1],[2],[8]) these are given for the case $T > D$, when $\exp(-\beta W_D) \simeq 1$, taking into account that in any case here $u \propto \exp(-\beta W_D)$, $W_D \lesssim D$]. The activation energies for u_t (W') and for Δ_t (W'') are different in different intervals of T and Φ_0. Generally speaking (including the case of degenerate $|i\rangle$ states),**

$$u_t \propto f'(T)\exp(-\beta W'); \qquad u_t \propto c_1' f_1'(T) e^{-\beta W_1'} + c_1'' f_2'(T) e^{-\beta W_2'}$$
$$\text{for } \Phi_0 \gg 1, \quad T > T_0, \tag{1}$$

where $W_1' = W_D' = \frac{4}{3}\mathcal{E}$ and $f_1'(T) = T^{-2}$; $W_2' = W_D' + \mathcal{E}$ and $f_2'(T) = T^{-1}$; for $\Phi_0 \gg 1$ and $T < T_1$, $W' = W'_{(\mathrm{opt})} = W_D' + \omega_{\mathrm{opt}}$ and $f'(T) = T^{-1}$ for (opt) (dominant coupling of the polaron to optical phonons), or $W' = W'_{\mathrm{ac}} = W_D'$ and $f'(T) = \mathrm{const}$ for (ac) (acoustic phonons dominate the coupling); for $\Phi_0 \ll 1$ and $T < T_{ph}$, $W' = W'_{(\mathrm{opt})} = W_D' + \omega_{\mathrm{opt}}$, but $W' = W'_{(\mathrm{ac})}$ and $f'_{(\mathrm{ac})}(T) = \mathrm{const}$. In particular, in u_t, $c_1'/c_1'' = 0$ for s-type states and nondegenerate polarons. Formulas (1), for $\Phi_0 \gg 1$ and $T > T_0$, generalize those for (sp) in an ideal lattice to the case of arbitrary strong-coupling polarons in a disordered lattice, with allowance for the additional activation factor $\exp(-\beta W_D')$. (Apparently, the situation is analogous for all $T \gg T_1$.) For Δ_t we have

$$\Delta_t \propto f''(T)\exp(-\beta W''), \tag{2}$$

where: for $\Phi_0 \gg 1$ and $T > T_0$ (apparently, analogously for all $T \gg T_1$), $W'' = W_D'' + \mathcal{E}$ and $f''(T) = T^{-5/2}$; for $\Phi_0 \gg 1$ and $T < \{T_1; T_{ph}\}$, $W'' = W''_{(\mathrm{opt})} \equiv W_D'' + \omega_{\mathrm{opt}}$ or $W'' = W''_{(\mathrm{ac})} \equiv W_D''$ and $f''_{(\mathrm{ac})}(T) = T^0$; for $\Phi_0 \ll 1$ and $T < T_{ph}$, $W'' = W''_{(\mathrm{opt})}$ or $W'' = W''_{(\mathrm{ac})}$ with $f''_{(\mathrm{ac})}(T) = T^{-1}$. The activation energies

* For (ic) (when $|\omega_{ij}| \equiv |\varepsilon_i - \varepsilon_j| \gg |\Delta_e(R_{ij})|$ for most transitions), the "subtraction" of the contribution of nondissipative transitions ([1]), contained in $J_\alpha(x, y)$, in fact reduces to that in the matrix of the polaron-phonon interaction (perturbation) $\mathcal{H}_1$; in this case, transfer of the "tunnel-band" type also has features of hopping diffusion.

In ([2]), in the case (ic), a "subtraction" adequate for the case (sp) was used; this does not change the estimates for $\Phi_0 \gg 1$ in (16), (17), but gives an inaccurate estimate for U_h at $\Phi_0 \ll 1$ in (18): the use of the "subtraction" adequate for (ic) leads, in U_h, to the replacement $\beta \to \omega_{ph}^{-1}$ for $D \ll T$ or $\beta \to D^{-1}$ for $D \gg T$ (cf. ([1])).

** The ratio of the two terms (i.e., $\sim c_1'$ and $\sim c_1''$) for $\Sigma_t(4; \omega = 0) \equiv \Sigma_t(4)$ may differ from that for $\Sigma_t(3)$.

activation energies W_D, W_D' and W_D'' are caused by fluctuations of the levels ε_i and are substantially determined by terms of the type ξ_0 in ξ: $W_D \equiv W_D[\xi_0] \lesssim D$, and similarly for W_D' and W_D'', with $\Delta' \equiv W_D' - W_D \geq 0$ and $\Delta'' \equiv W_D'' - W_D \geq 0$. Apparently, $\beta\Delta^{('')} \ll 1$ (for $T \gg \Delta_{AV}^{(p)}$) for (ic) (at least for nondegenerate $|i\rangle$-states). Defining the Hall angle $\theta(\omega) \equiv \theta(3; \omega) \equiv \Sigma_t(3; \omega)/\Sigma_{xx}(0) \equiv \theta'(\omega) + i\theta''(\omega)$, we have the following (approximate) estimates: for $\Phi_0 \ll 1$ and $T \ll T_0$ (and one-phonon processes),

$$|\theta'(0)|_{(\mathrm{ac})} \lesssim \frac{H}{H_0} \frac{\Delta_{AV}}{T} \left(\frac{\omega_{ph}}{D}\right)^2 e^{-\beta\Delta'} q_1 \quad \text{for } q_1 < 1,$$

$$|\theta''(\omega)|_{(\mathrm{ac})} \lesssim \pi\beta\omega \frac{H}{H_0} \frac{\Delta_{AV}}{T} e^{-\beta\Delta''}; \tag{3}$$

$$|\theta'(0)| \lesssim \frac{H}{H_0} \frac{\Delta_{AV}}{\mathcal{E}} e^{-\beta\Delta'} \chi, \qquad |\theta''(\omega)| \lesssim \beta\omega \frac{H}{H_0} \frac{\Delta_{AV}}{\max\{\mathcal{E}; D\}} e^{-\beta\Delta''} \quad \text{for } \Phi_0 \gg 1,$$

where

$$\chi = \left\{ c_1' \exp\left(-\frac{\beta\mathcal{E}}{3}\right) \sqrt{\frac{\mathcal{E}}{T}} + c_1'' \sqrt{\frac{T}{\mathcal{E}}} \quad \text{for } T > T_0;\ \chi_0 \text{ for } T \leq T_1 \right\},$$

$\chi_0^{(\mathrm{ac})} \sim \beta\omega_{ph}$, with, for $\Phi_0 \gg 1$, $\operatorname{sgn}\theta(\omega) = \operatorname{sgn} e$, at least for s-type states and not too strong a Fermi degeneracy (for $\theta(4; \omega)$, or for $\Phi_0 \ll 1$, the situation is more complicated). For actual parameters, for example $H \cdot H_0^{-1} = 10^{-2}$, $\omega = 10^6$ Hz; $T = 10^\circ$K, $\omega_{ph} = 10^{-3}$ eV, $\Delta_{AV}/T = 10^{-2}$ and $\omega_{ph}/D = 10^{-1}$ for $\Phi_0 \ll 1$ (ic), θ' and $\theta''(\omega)$ are very small (much smaller than in (7)), $\theta' < 10^{-6}$

and $|\theta''(\omega)| < 10^{-10}$. If the Hall angle is defined as $\nu(\omega) \equiv \Sigma_t(3;\omega)/\sigma(\omega)$, then $|\nu(\omega)|$ can only be smaller, since $\sigma(\omega) \gg \Sigma(\omega)$ ([3]).

3. Preliminary estimates give no grounds to assume that $|S_t(\omega)|$ can predominate over $|\Sigma_t(\omega)|$ and determine $\sigma_t(\omega)$ (in contrast to the situation for $\sigma(\omega)$ in ([3])). Since this is so (i.e., there is no contribution of "large" polaron dipoles ($\sim er$) to the odd conductivity $\sigma_t(\omega)$), one may consider that the estimates (1)–(3) determine $\sigma_t(\omega)$ and the properly defined Hall angle, and that the present theory apparently does not lead to a justification of the formula for the contribution $\sigma_t^H(\omega)$ (to $\sigma_t''(\omega)$) obtained in (7) for the particular case (ic) with $\Phi_0 \ll 1$ and $\omega \ll T$, within a semiquantitative theoretical-diffusion approach. In the latter it is assumed that $\sigma_t^H(\omega)$ is due to three-center hops, although in fact $\sigma_t^H(\omega)$ is rather of the "polarization" type and, for $\Phi_0 \ll 1$, has a nonactivated tunneling (nonhopping) character (see ([3])). This may be the explanation why in (7) large values were obtained for $\sigma_H(\omega)$, inconsistent with the present theory (see above) and with the corresponding experiments (see ([10])).

Institute of Semiconductors
Academy of Sciences of the USSR
Leningrad

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REFERENCES

1. M. Klinger, Reports Progr. Phys., **31**, 225 (1968).
2. M. Klinger, Phys. Stat. Solid., **31**, 515 (1969).
3. M. Klinger, DAN, **193**, No. 2 (1970).
4. I. Lifshits, UFN, **84**, 617 (1964).
5. A. Miller, E. Abrahams, Phys. Rev., **120**, 745 (1960).
6. P. W. Anderson, Phys. Rev., **109**, 1492 (1958).
7. T. Holstein, Phys. Rev., **124**, 1329 (1961).
8. M. Klinger, DAN, **183**, 311 (1968).
9. Yu. Bychkov, A. Dykhne, ZhETF, **51**, 1914 (1966).
10. M. Amitay, M. Pollak, J. Phys. Soc., Japan, Suppl., **21**, 549 (1966).

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