Influence of Electron-Phonon Coupling on Transport near a Mobility Edge

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The authors treat electronic transport in disordered systems, including the electron-phonon interaction, on both sides of a mobility edge ϵ_c on the same footing. By application of a mode-coupling approximation self-consistent equations are derived from which one gets the matrices describing density relaxation due to both coherent tunneling processes and hopping processes. The resulting conductivity interpolates between a metallic behavior well above and a hopping behavior well below ϵ_c.

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Transport in disordered systems showing a mobility edge ϵ_c at $T=0$ is usually described (i) in terms of hopping, if transport is well below ϵ_c, or (ii) in terms of transport in extended states above ϵ_c.[1] In particular, transport in amorphous semiconductors at sufficiently high temperatures is thought to be due to carriers thermally activated to energies just above ϵ_c; a hopping contribution is then neglected. On the other hand, if one allows for finite temperature and finite electron-phonon coupling, a mobility edge is not defined. Consequently the distinction of hopping transport versus extended-state transport becomes meaningless. A more complete theory of transport, covering both sides of ϵ_c, is needed to study the transition from metalliclike conduction well above ϵ_c to hopping conduction well below ϵ_c.[2]

Previously the influence of the dynamical electron-phonon interaction on transport in strongly disordered systems has been studied in order to explain the negative temperature coefficient of dirty metallic conductors.[3-6] In this Letter we shall essentially follow the approach of Belitz and Schirmacher[6] which is based on the mode-coupling theory of Götze[7] and Belitz and Götze.[8] However, in contrast to these authors, we shall treat a tight-binding model in *site* representation, leading quite naturally to a hopping description in the limit of small electron transfer t.[9] Our model Hamiltonian reads

$$H=\sum_i(\epsilon_i-\epsilon)n_i+t\sum_{ij}\exp(s_{ij})c_i^{\dagger}c_j+H_p, \quad (1)$$

where ϵ_i are the (renormalized) site energies, t the nearest-neighbor transfer, H_p the conventional phonon Hamiltonian, and

$$s_{ij}=\sum_q[A_{ij}(q)a_q^{\dagger}-A_{ij}(-q)a_q]/\omega_q \quad (2)$$

contains the electron-phonon coupling functions $A_{ij}(q)$ and the phonon energies ω_q. We have employed the polaron transformation,[10] although we do not study polaron effects here. The phonons then couple to the electron transfer, leading to a phonon contribution to the current. Such a contribution is essential for a description of hopping processes.[6] The site energies are distributed according to a given distribution function; the variance of the site energy differences of nearest neighbors is taken as a measure of disorder: $E^2=\langle(\epsilon_i-\epsilon_j)^2\rangle$.

The configurational averaged conductivity can be written[9]

$$\langle\sigma(z)\rangle=\frac{e^2\beta}{\sigma\Omega}\sum_{ij}R_{ij}^2\{z^2\varphi_{ij}(z)-izg_{0ij}^{-1}\}, \quad (3)$$

where $\beta=(k_BT)^{-1}$, Ω is the volume, e the electronic charge, and R_{ij} the distance between two sites i,j. The Kubo-type density correlation function[11]

$$\varphi_{ij}(z)=\left(n_i\left|\frac{i}{z-L}\right|n_j\right), \quad (4)$$

$$g_{0ij}^{-1}=(n_i|n_j), \quad LA=[H,A],$$

is expressed in terms of the density relaxation matrix

$$\Sigma_{0ij}(z)=\left(\dot{n}_i\left|\frac{i}{z-L_1}\right|\dot{n}_j\right), \quad L_1=Q_0LQ_0, \quad (5)$$

using the Zwanzig-Mori formalism by (in matrix notation)

$$\varphi(z)=i[z+i\Sigma_0(z)g_0]^{-1}g_0^{-1}. \quad (6)$$

The projector Q_0 projects outside the space $\{n_i\}$ spanned by the density. [Without inclusion of the configurational average into the Kubo brackets and with Σ_0 calculated to lowest order in t, Eq. (3) expresses the conductivity in terms of the formal solution of the linearized rate equation.[9] In this limit Σ_0 is called the frequency-dependent collision matrix, which in the Markov limit $z=0$ is given by the conventional equilibrium hopping rates.[12]]

In terms of the translationally invariant config-

uration-averaged Σ_0 the conductivity may be written as

$$\langle\sigma(z)\rangle = \frac{e^2\beta}{\sigma\Omega}\sum_{ij} R_{ij}{}^{e}\,\Sigma_{0ij}(z). \tag{7}$$

We now split $\dot{n}_i$ into a coherent and a hopping part[13]:

$$\dot{n}_i = \dot{n}_i{}^{c} + \dot{n}_i{}^{h} = (it_T\textstyle\sum_j c_j{}^{\dagger}c_i + \text{H.c.}) + [it_T\sum_j\{\exp(s_{ij}+\theta)-1\}c_j{}^{\dagger}c_i + \text{H.c.}], \tag{8}$$

where

$$t_T = te^{-\theta/2}, \quad e^{-\theta/2} = \langle\exp(s_{ij})\rangle_{\text{phonons}}, \quad \theta = \textstyle\sum_q |A_q/\omega_q|^2\coth(\beta\omega_q/2).$$

We have neglected the dependence of the coupling functions on the particular site indices i and j (denoting nearest-neighbor sites).

In contrast to Σ_0, the Van Hove correlation function

$$S_{ij}(\tau) = \langle\dot{n}_i\exp(-iL_1\tau)\dot{n}_j\rangle \tag{9}$$

decouples into a phonon part and an electron part in lowest order in t.[9] As our first major approximation we apply this decoupling to all orders in t, leading to

$$S_{ij}(\tau) = S_{ij}{}^{c} + S_{ij}{}^{h} = \langle\dot{n}_i{}^{c}\exp(-iL_1\tau)\dot{n}_j{}^{c}\rangle + (e^{F(\tau+i\beta/2)}-1)S_{ij}{}^{c}(\tau) \tag{10}$$

with

$$F(\tau) = \textstyle\sum_q |A_q/\omega_q|^2\,\text{cosech}(\beta\omega_q/2)\cos(\omega_q\tau). \tag{11}$$

Thus with

$$\Sigma_{0ij}{}^{c}(z) = \left(\dot{n}_i{}^{c}\left|\frac{i}{z-L_1}\right|\dot{n}_j{}^{c}\right), \tag{12}$$

we have

$$\Sigma_{0ij}{}^{h}(z) = \frac{1}{2\pi i}\int d\omega\,d\omega'\frac{1-e^{-\beta\omega}}{\omega(\omega-z)}\,\frac{\omega'}{1-e^{-\beta\omega'}}\,e^{-\beta(\omega'-\omega)/2}\,G(\omega'-\omega)\Sigma_{0ij}{}^{c\prime\prime}(\omega'). \tag{13}$$

We make the model assumption[5]

$$G(\omega) = \frac{1}{2\pi}\int d\tau\,e^{i\omega\tau}(e^{F(\tau)}-1) \approx \frac{\bar{G}}{\pi}\,\frac{\omega_0}{\omega^2+\omega_0{}^2} \tag{14}$$

for the phonon propagator, and consider high temperatures, $\beta\omega_0 < 2$. Then the integration in Eq. (13) can be done analytically, yielding

$$\Sigma_{0ij}{}^{h}(z=0) = \theta\Sigma_{0ij}{}^{c}(z=i\omega_0). \tag{15}$$

Here, to lowest order in the electron-phonon coupling,

$$\bar{G} = \int d\omega\,G(\omega) \approx \theta \approx 2\textstyle\sum_q |A_q/\omega_q|^2/\beta\omega_q$$

is an effective dimensionless temperature. It will be assumed to satisfy $\theta \ll 1$. Equation (15) implies that the hopping contribution to the conductivity is given by a frequency integral over the phonon propagator and the real part of the frequency-dependent coherent conductivity, which in turn depends on the hopping processes.

Here we introduce our second major approximation: We calculate $\Sigma_0{}^{c}(i\omega_0)$ for a system without dynamical electron-phonon coupling, i.e., we replace the transfer term in Eq. (1) by $t_T\sum_{ij}c_j{}^{\dagger}c_i$. In doing this we neglect the influence of the dynamical electron-phonon coupling on the frequency spectrum of the density relaxation matrix. Since only the frequency integral enters the theory, this approximation may be justified. It underestimates the contribution $\Sigma_0{}^{h}$ in the regime where dynamical electron-phonon processes become important, since these increase the density relaxation, especially at low frequencies.

$\Sigma_0{}^{c}(z)$ is expressed in terms of a current relaxation matrix

$$\Sigma_{1ij}(z) = \left(\dot{n}_i{}^{c}\left|LQ_1\frac{i}{z-Q_1LQ_1}Q_1L\right|\dot{n}_j{}^{c}\right) \tag{16}$$

using once more the Zwanzig-Mori procedure:

$$\Sigma_0{}^{c}(z) = i[z-\Omega_1g_1+i\Sigma_1(z)g_1]^{-1}g_1{}^{-1}. \tag{17}$$

Here and below, following Götze,[7] we replace all static correlation functions $(\Omega_1, g_1, \ldots)$ by their counterparts valid for an ordered system. If we neglect band-structure effects this is represented by free electrons having a temperature-dependent effective mass $m_T^* = m^* e^{\theta/2}$. In particular, to lowest order in t,

$$g_{1\,ij}{}^{-1} = (\dot{n}_i{}^c | \dot{n}_j{}^c) = 2t_T \nu/\beta, \tag{18}$$

where $\nu = n_e/n_s$ is the number of electrons per site. Q_1 now projects outside $\{n_i\}$ and $\{\dot{n}_i{}^c\}$. We treat the scattering (i.e., the current relaxation) by phonons in the adiabatic approximation, since here we are mainly interested in transport below ϵ_c, where the hopping processes are dominant. We find by a successive application of the Zwanzig-Mori procedure, replacing all higher-order relaxation kernels by $m(z)$,[7]

$$(\Sigma_1 g_1)_{ij} = m(z)\delta_{ij} + [\Sigma_1{}^{(0)}(z + im(z))g_1]_{ij}. \tag{19}$$

Thus

$$\Sigma_0{}^c(z) = \Sigma_0{}^{(0)}(z + im(z)), \tag{20}$$

where $\Sigma^{(0)}$ are the relaxation matrices of the ordered system. Using a mode-coupling approximation,[7] we write

$$m(z) = \alpha\beta\left(c_i{}^\dagger c_j + c_j{}^\dagger c_i \left| \frac{i}{z - L} \right| c_i{}^\dagger c_j + c_j{}^\dagger c_i\right)/2, \qquad \alpha = |t_T|E^2\nu. \tag{21}$$

The bond energy $\mathrm{tr} c_i{}^\dagger c_j + \mathrm{H.c.}$ is perpendicular to the space $\{\dot{n}_i{}^c\}$ for a homogeneous equilibrium system, but it has a component in the space of the particle density $\{n_i\}$. To simplify the calculation we do not calculate this component, but rather replace the correlation function in Eq. (21) by $(\varphi_{ii} + \varphi_{ij})/2$. The mode-coupling approximation constitutes our third major approximation. Using Eqs. (6), (15), and (20) we finally obtain two self-consistency equations, one for $m_1 = m(z=0)$:

$$m_1 = \alpha\beta \int_0^{q_0} k^2 dk f(k)[g_0(k)\{\Sigma_0{}^{(0)}(k_1 i m_1) + \theta\Sigma_0{}^{(0)}(k_1 i m_2 + i\omega_0)\}g_0(k)]^{-1}, \tag{22}$$

and one for $m_2 = m(z = i\omega_0)$:

$$m_2 = \alpha\beta \int_0^{q_0} k^2 dk f(k)[g_0(k)\Sigma_0{}^{(0)}(k_1 i m_2 + i\omega_0)g_0(k)]^{-1}, \tag{23}$$

$$f(k) = 4\pi a^3\{1 + \sin(ka)/ka\}/(2\pi)^3.$$

The Fourier transform of $\Sigma_0{}^{(0)}$ is then expressed by the density correlation function $\varphi^{(0)}(k_1 z)$ of the ordered system with the help of Eq. (6). The prefactor β cancels, so that we can take the limit $T = 0$ for the electron system, where $\varphi^{(0)}$ and g_0 are given by the Lindhard function, if we neglect band-structure effects. The integration extends over the Brillouin zone with $q_0 = \pi/a$. In terms of m_1 and m_2 the dc conductivity reads

$$\langle\sigma(z=0)\rangle = \sigma^c + \sigma^h = \frac{n_e e^2}{m_T^*}\left(\frac{1}{m_1} + \theta\frac{1}{m_2 + \omega_0}\right). \tag{24}$$

For $\theta = 0$ this result agrees essentially with that of Götze[7] (see also Götze, Prelovsek, and Wölfle[14]).

Figure 1 presents numerical results from Eqs. (22) and (23) for the parameters indicated. In the metallic regime well above ϵ_c the denominator of the integrand of Eq. (22) is governed by the first term describing density relaxation by coherent tunneling processes. m_1 is then small and the coherent contribution to the conductivity dominates. Its temperature coefficient is small and upon approaching ϵ_c it changes sign. On the other hand, well below ϵ_c the density relaxation due to coherent tunneling processes becomes ineffective, m_1 tends to diverge, and the hopping contribution proportional to θ dominates the conductivity. In addition the integrand of Eq. (22) is now governed by the hopping processes and m_1 will be roughly proportional to θ, too.

The peculiar temperature dependence of the dc conductivity and the thermopower found in doped and undoped amorphous semiconductors is usually interpreted in terms of bandlike transport above a mobility edge, sometimes including a second path due to hopping in localized band tail states (for a recent review see, e.g., Beyer and and Overhof[15]). The present theory, however, shows that the character of transport is neither pure coherent (bandlike) nor pure hopping, if the electron-phonon interaction is considered to be strong enough to influence the transport processes. The conductivity $\sigma(\epsilon)$ as a function of energy turns out to be a smooth function increasing gradually from low hoppinglike values to high bandlike values. To get the conductivity for the semiconducting system one has to integrate $\sigma(\epsilon)$ together with a Boltzmann distribution. Transport will

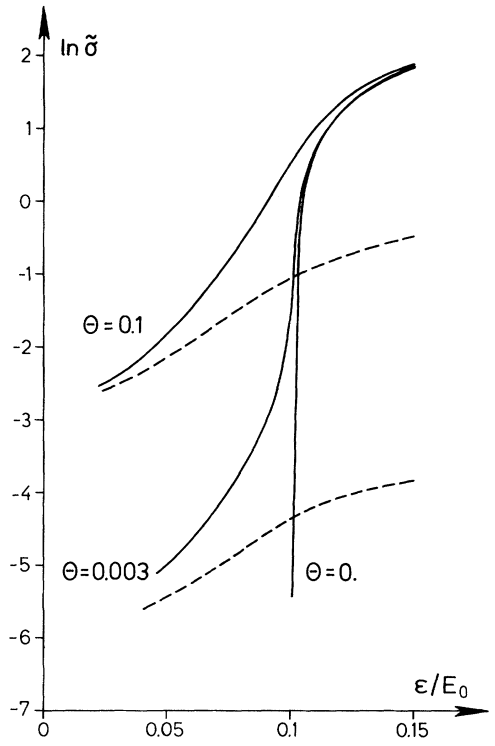

FIG. 1. The conductivity $\sigma = \tilde{\sigma} n e^2/m^* E_0$ as a function of the Fermi energy ϵ. The mobility edge for $\theta = 0$ is situated at $\epsilon = 0.25E_0$. The parameters are $\omega_0 = 0.01E_0$, $E = 0.25E_0$. Dashed lines represent $\sigma^h(\epsilon)$.

then be more or less close to ϵ_c, depending on details of the density of states and on the magnitude of the electron-phonon coupling. The energetic position of the dominant transport channel becomes a function of temperature. This effect should be considered as an additional source for the observed structure in the temperature dependence of the transport data. On the other hand, if experimental results *unambiguously* suggest an edgelike behavior of transport, one has to conclude that there are very steep tails and a mobility edge rather close to the band edge, or that the electron-phonon coupling is so weak that it may be neglected altogether.

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