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Variable-range hopping: Role of Coulomb interactions

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The effect of Coulomb interactions on hopping conduction in the variable-range hopping regime is analyzed within a linear-response formalism. Here the conductivity and the dielectric function are related to the density-density response function for which a generalized master equation (GME) can be derived using the Mori-Zwanzig projector formalism. The GME can be thought of as a random resistor network with frequency-dependent internode conductances, whose values can be determined from a function related to the current-current correlator at the two nodes. We evaluate the internode conductances using a diagrammatic perturbation formalism. For a single electron hop with all the other charges frozen, we obtain hop rates correct to all orders in Coulomb interaction. This gives us a finite temperature generalization of existing results for the interacting system. We then incorporate relaxation effects that accompany electron hops, using a dynamical model of the Coulomb gap. We argue that the parameter that governs the local relaxation is related to the conductivity itself. These internode conductances are then used to calculate the dc conductivity of the network by effective-medium approximation. We show that a crossover from Efros-Shklovskii's $T^{1/2}$ behavior to Mott's $T^{1/4}$ behavior occurs due to the relaxation effects, as the temperature is increased. At low temperatures the relaxation is slow so that electrons hop in a frozen charge background and thereby sense the Coulomb gap. This gives the $T^{1/2}$ behavior. At higher temperatures the relaxation gets faster and the Coulomb gap is alleviated leading to Mott's behavior. [S0163-1829(99)05207-8]

I. INTRODUCTION

In this paper we shall be concerned with the role of Coulomb interactions in the hopping conduction of localized electrons. We shall consider situations where the Fermi level lies in the region of strongly localized states and at temperatures where variable-range hopping (VRH) dominates. It has long been realized that Coulomb interactions play a crucial role in the hopping conduction of electrons, since the localized states are not very effective in screening the long-range part of the Coulomb interaction. Since Mott's remarkable arguments, which predicted that as temperature is lowered the activated dependance of dc conductivity [$\sigma(T) \propto \sigma_0(T) \exp(-\epsilon_3/k_BT)$] should go over to the form $\sigma(T) \propto \sigma_0(T) \exp[(-T_M/T)^{1/4}]$,[1] there has been a tremendous amount of theoretical and experimental work aimed at understanding various aspects of VRH. Mott's formula was based on rather simple considerations of the hopping rate between two sites, which has the generic form,

$$\Gamma(R,E) = \Gamma_0 \exp[-2\alpha R - \Delta E/k_BT], \tag{1}$$

where R is the distance between two sites and $\Delta E > 0$ is the energy difference between the sites. In the higher-temperature range, the first term in the exponential restricts the hopping to the smallest values of R, leading to nearest-neighbor hopping. But as the temperature is lowered, the most efficient rates are obtained by hopping to longer distances, which allows for decreased activation energy. Following Mott's arguments there have been numerous efforts to put Mott's results on firmer theoretical foundations. They have largely been based on the rate equation approach of Miller and Abrahams.[2] The linearized rate equation is equivalent to a random-resistor network, which in this situation is amenable to a percolation analysis.[3] This analysis and various improved treatments of random-resistor networks yield results qualitatively identical to Mott at low temperatures.[4–14] However, all these calculations ignore Coulomb interactions.

Coulomb interactions influence the situation in several ways. One very significant effect first pointed out by Pollak[15] and Srinivasan[16] is the existence of the Coulomb gap, i.e., the vanishing of the density of states (DOS) of the Hartree energies of the localized levels precisely at the Fermi level. Subsequently, Efros and Shklovskii (ES) argued it to be a soft Coulomb gap with the DOS vanishing quadratically with energy around the Fermi level.[17] The Coulomb gap basically reflects the difference between the minimum energies of adding an electron and subtracting one from the system, without disturbing the other charges. Knotek and Pollak[18] have viewed it as the amount of lowering of the Hartree energy, which occurs due to the relaxation of the surrounding charge, when an electron is added to a site at the Fermi level. ES have extended Mott's reasoning to argue that due to the soft Coulomb gap, Mott's $T^{1/4}$ behavior should be changed to the following temperature dependence,

$$\sigma(T) = \sigma_0(T) \exp[(-T_{ES}/T)^{1/2}]. \tag{2}$$

However, ES's derivation has been questioned on the following points. The excitation energy ΔE_{ij} that enters Eq. (1) when an electron hops from site i to site j separated by a distance R_{ij} can be written in terms of the site Hartree energies $\{E_i\}$ as

$$\Delta E_{ij} = E_j - E_i - K_{ij}, \tag{3}$$

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where K_{ij} denotes the Coulomb energy $e^2/\kappa R_{ij}, \kappa$ is the background dielectric constant, and the energies E_i are given in terms of the one-electron site energies $\{\epsilon_i\}$ as

$$E_i=\epsilon_i+\sum_j K_{ij}f_j, \tag{4}$$

where f_j denotes the electron occupation number of the state at site j. ES's derivation of the soft Coulomb gap for the DOS of E_i (Ref. 17) comes from the requirement that the occupation numbers f_j in the ground state must be such that all one-electron excitation energies defined in Eq. (3) are positive definite. The soft gap predicted by ES has been confirmed in many numerical simulations. However, it should be noted that a gap in the DOS of the Hartree energies does not imply a similar form of the gap for the excitation energies ΔE_{ij}, which is what is relevant for Mott's argument, in which the DOS for ΔE was assumed to be a constant.

Further due to interactions, the hopping of an electron is accompanied by local relaxation of charge around the sites involved in the hop.[3,18,19] Around the site the electron jumps from, the electrons on surrounding sites move in, raising the Hartree energy of this site from the value it had when the electron was present on it. While around the site the electron hops to, there is an outward movement of charge and a consequent reduction of the Hartree energy from the value it had when the site was unoccupied.

Such relaxations and shifts of local energies cannot be considered systematically in the rate-equation model, which ignores interactions apart from the constraints of double occupancy of a site. The role of interactions in hopping transport has received considerable attention. Possibility of multielectron transport was first considered by Knotek and Pollak,[18] who argued that below a certain temperature correlated electron motion dominates over the independent electron-hopping process. They also argued that in the lowest range of temperatures, the conductivity must again be due to activation across the Coulomb gap. Mott introduced the notion of "charge polaron" to describe the quasiparticle that hops along with its charge cloud, which process consists of other electron hops constituting the relaxation process described above.[20] Arguing that for the hops of such quasiparticles there is no Coulomb gap, Mott found the $T^{1/4}$ law to be again valid even in the presence of interactions. This whole subject has been recently reviewed in two exhaustive papers by Ortuno and Pollak,[21] and Efros and Shklovsii.[19]

This problem has also been extensively studied experimentally for a large variety of systems. Early work provided some confirmation to Mott's $T^{1/4}$ law but was questioned due to the limited temperature range of fits. Many critical analyses have since appeared that show data can be fitted with temperature exponents that cluster around the values of 1/4 and 1/2.[19,22–26] Castner[23] has observed that for systems that are close to metal-insulator transitions (MIT), the data fits quite well to Mott's law, while for those far away from MIT, the exponent 1/2 is more appropriate. More recently, several studies have appeared that show both behaviors, with $T^{1/4}$ behavior crossing over to $T^{1/2}$ behavior as the temperature is lowered.[27–32] From further analysis of some data, it has been argued that in terms of some properly scaled variables, the crossover behavior is universal.[33,34]

The purpose of this paper is to present a calculation of the dc conductivity of the hopping electron system, which takes into account the effect of Coulomb interactions on electron transport in a systematic manner. For this purpose, we use the linear response formalism as first developed for this problem by Brenig *et al.*[35] These authors showed that the conductivity of the system is related to the density-density response function. Using Mori-Zwanzig projector formalism it is possible to recast the equations of motion of the density-density response function χ as a generalized master equation (GME).[35,36] A Markovian approximation of the GME yields the rate equation, which has formed the basis of conductivity calculations of the earlier papers. The GME can be viewed as a resistor network equation with frequency-dependant conductances between nodes, which can be calculated from a correlation function of time derivatives of electron numbers at the nodes. This formalism allows us to consider the problem of transport of interacting electrons in two parts. First, one calculates the internode conductances using a formal expression through which interactions can be incorporated by a standard diagrammatic perturbation formalism. Second, one solves the resistor network problem, which brings in the considerations of disorder and percolation in the calculation. For the latter problem, several procedures have been developed,[6,8–14] one of which we adapt for our present analysis.[12–14]

The paper is organized as follows. In Sec. II we present the basic Hamiltonian and write out the equations of the linear response formalism for the hopping conduction problem. In Sec. III we set up the formalism for the calculation of the internode conductances, and include Coulomb interactions at the lowest order in electron-hop amplitude. This calculation is to all orders in Coulomb interaction. Sec. IV is an attempt to build in the relaxation effects that accompany electron hops. The diagrammatic analysis enables us to select the processes that represent the relaxation effects. Though we can write formal expressions for these processes in a self-consistent manner, it is very difficult to compute physical quantities from them. However, guided by these expressions, we incorporate relaxation effects by a physical model, which allows us to write a certain spectral density needed for the response function directly. Section V is devoted to solving the resistor network of the above conductances for obtaining dc conductivity. We end the paper with a summary and some discussion in Sec. VI.

II. LINEAR-RESPONSE FORMALISM FOR CONDUCTIVITY

A. Hamiltonian

The relevant Hamiltonian for the system of localized electrons in interaction with phonons can be written as

$$H=\sum_i \epsilon_i n_i+\sum_{i\neq j} J_{ij}c_i^\dagger c_j+\sum_q \hbar\nu_q a_q^\dagger a_q$$
$$+\sum_{q,i}[A_i^\dagger(q)a_q^\dagger+A_i(q)a_q]n_i+\frac{1}{2}\sum_{i\neq j} K_{ij}n_in_j. \tag{5}$$

The first term is a summation over the random-site energies ϵ_i associated with the localized state at site i, J_{ij} (in the second term) is the amplitude for electron transfer between sites i and j, and the third term is the Hamiltonian for free phonons. The fourth term represents the electron-phonon interaction, and the last term represents the intersite Coulomb interaction between electrons at sites i and j, K_{ij} being defined after Eq. (3). It is assumed that the one-electron eigenstates resulting from the first and second terms of the Hamiltonian are localized. Further, we take the intrasite Coulomb interaction to be so large that the sites are at most singly occupied. We also ignore the off-diagonal part of the Coulomb interaction, which is a reasonable assumption for deeply localized states.

For subsequent analysis it is useful to apply the "polaron" canonical transformation[37,38] to the Hamiltonian, as follows:

$$\tilde{H}=e^{S}He^{-S}, \tag{6}$$

with

$$S=\sum_i S_i n_i \tag{7}$$

and

$$S_i=\sum_q \frac{1}{\hbar\nu_q}[A_i^\dagger(q)a_q^\dagger-A_i(q)a_q]n_i. \tag{8}$$

After this the Hamiltonian (apart from a negligible term proportional to n_in_j) is

$$\tilde{H}=\sum_i \tilde{\epsilon}_i n_i+\sum_{i\neq j} J_{ij}e^{(S_i-S_j)}c_i^\dagger c_j +\sum_q \hbar\nu_q a_q^\dagger a_q+\frac{1}{2}\sum_{i\neq j} K_{ij}n_in_j, \tag{9}$$

where the new site energy is

$$\tilde{\epsilon}_i=\epsilon_i-\sum_q \frac{|A_i(q)|^2}{\hbar\nu_q}. \tag{10}$$

The site energies are shifted on account of the polarization displacement of the surrounding atoms. For notational simplicity we use $\{\epsilon\}$ to refer to the energy $\{\tilde{\epsilon}\}$ given in Eq. (10).

B. Linear response theory for conductivity

The calculation of the conductivity[36,39] requires evaluation of the response of the system to a perturbation of the form $-\Sigma_j V_j(t)n_j$, where for an electric field E in the x direction $V_j(t)=eEx_je^{i\omega t}$. The deviation $\delta n_i(t)$ of the occupation number at a site i, from its equilibrium value f_i, in response to the potential switched on at $t=0$, can be written to the first order in V as

$$\delta n_i(t)=2i\sum_j \int_0^t dt' \chi''_{ij}(t-t')V_j(t'), \tag{11}$$

where the dynamic susceptibility χ'' is

$$\chi''_{ij}(t-t')=\frac{1}{2\hbar}\langle[n_i(t),n_j(t')]\rangle. \tag{12}$$

It is convenient to work with the Laplace transform of these relations, in terms of which Eq. (11) has the form

$$\delta n_i(z)=\chi_{ij}(z)V_j(z), \tag{13}$$

where $\chi_{ij}(z)$ is given by

$$\chi_{ij}(z)=2i\int_0^\infty d\tau e^{iz\tau}\chi''_{ij}(\tau)=\int_{-\infty}^\infty \frac{d\omega}{\pi}\frac{\chi''_{ij}(\omega)}{(\omega-z)}, \tag{14}$$

and $\chi''_{ij}(\omega)$ is the Fourier transform of $\chi''_{ij}(t)$. The conductivity of the system $\sigma(\omega)$ can be obtained from the dynamic susceptibility by the relation

$$\sigma(\omega)=\frac{i\omega e^2}{\Omega}\sum_{ij} x_i\chi_{ij}(\omega+i\eta)x_j. \tag{15}$$

Similarly, the dielectric-constant matrix $\kappa_{ij}(\omega)$ can be expressed in matrix notation as

$$\underline{\kappa}^{-1}=\underline{1}+\underline{\chi}(\omega)\underline{K}, \tag{16}$$

where K denotes the interaction matrix K_{ij}. The next step of the formalism is to write the equation of motion of the density-response function in a way that it resembles the rate equation. For this one defines a Kubo relaxation function $\Phi_{ij}(t)$, which is,

$$\Phi_{ij}(t)=\frac{1}{\beta}\int_0^\beta d\lambda[\langle n_i^\dagger(t)n_j(i\hbar\lambda)\rangle-\langle n_i^\dagger(t)\rangle\langle n_j(i\hbar\lambda)\rangle] \tag{17}$$

$$=\langle n_i(t)|n_j(0)\rangle, \tag{18}$$

where the angular brackets $\langle\,\rangle$ denote a thermal equilibrium average such as $\langle n_i(t)\rangle=\mathrm{Tr}\,\rho n_i(t)$, where $\rho=e^{-\beta H}/\mathrm{Tr}\,e^{-\beta H}$ is the density matrix. Eq. (18) is a shorthand notation for the right-hand side of Eq. (17). The relation between the relaxation function and the susceptibility is given by

$$i\beta[z\Phi_{ij}(z)-i\Phi_{ij}(t=0)]=\chi_{ij}(z). \tag{19}$$

Further note that the static susceptibility $\chi_{ij}=\chi_{ij}(z=0)$ is given by $\beta\Phi_{ij}(t=0)$. For noninteracting electrons, the static susceptibility is

$$\chi_{ij}=\delta_{ij}\beta f_i^0(1-f_i^0). \tag{20}$$

One now writes down in a formal manner the Laplace transform of the equation of motion of the relaxation function in terms of the quantum Liouvillian operator L,[39] as

$$\Phi_{ij}(z)=\langle n_i|\frac{i}{z-L}|n_j\rangle. \tag{21}$$

Using the Mori-Zwanzig projector formalism,[36,39] one writes the above equation as

$$z\Phi_{ij}(z)=i\beta^{-1}\chi_{ij}+\sum_m M_{im}(z)\Phi_{mj}(z), \tag{22}$$

where the matrix $\underline{M}(z)$ is

$$M_{lm}(z)=\sum_{l}\,[\omega_{il}+i\beta C_{il}(z)]\chi_{lm}^{-1}, \tag{23}$$

with

$$\omega_{il}=i\beta(\dot{n}_i|n_l)=0 \tag{24}$$

and

$$C_{il}(z)=\left(\dot{n}_i\left|Q\frac{i}{z-LQ}\right|\dot{n}_l\right) \tag{25}$$

where Q is the projection operator defined as

$$Q=1-P=1-\beta\sum_{i,j}\,|n_i)\chi_{ij}^{-1}(n_j|. \tag{26}$$

Using Eqs. (21), (22), and (23), we can write the equation for the dynamic susceptibility as

$$\chi(z)=-i\beta[z+i\beta C(z)\chi^{-1}(0)]^{-1}C(z). \tag{27}$$

This allows us to write the equation for the deviation in the occupation numbers to be

$$iz\delta n(z)=-C(z)\chi^{-1}(0)\delta n(z)-C(z)V(z). \tag{28}$$

If one uses the Markovian approximation in Eq. (28), that is, replace $C(z)$ by $C(0)$, and identifies the $C(0)$ matrix as

$$C_{ij}(z=0)=-\Gamma_{ij}+\delta_{ij}\sum_{k}\,\Gamma_{ik}, \tag{29}$$

where Γ_{ij} is the hopping rate between sites i and j, one obtains the linearized version of the standard rate equation for electron occupation numbers

$$\frac{d}{dt}n_i(t)=-\sum\,n_i(1-n_j)\Gamma_{ij}+\sum_{j}\,n_j(1-n_i)\Gamma_{ji}. \tag{30}$$

This identification of the equation of motion with a linearized rate equation, which in turn is identical to a random resistor network is of great conceptual value. The effective conductance between nodes can now be obtained from the rigorous formula for C given in Eq. (25). In its evaluation one can incorporate, in principle, all the effects of interaction. Having obtained these, one can tackle the next part of the problem, which is obtaining the conductivity of the system from the network equations. Here, disorder plays the crucial role. For simple resistances many effective methods have been developed. In a later section we shall discuss the method we have adapted for our network analysis, but first we describe the evaluation of the matrix $C(z)$.

III. EVALUATION OF THE CONDUCTANCE MATRIX

Dersch *et al.*[36] have evaluated the matrix $C(z)$ to order (J^2) at zero temperature. To this order multielectron transport and relaxation effects cannot be incorporated. So here we introduce a systematic approach based on diagrammatic perturbation theory. For this purpose we calculate the thermal-causal Green's function $\tilde{S}_{ij}(\tau)$ defined as

$$\tilde{S}_{ij}(\tau)=\langle T_\tau[\dot{n}_i(\tau)\dot{n}_j(0)]\rangle, \tag{31}$$

where τ is the complex time in the domain $[-\beta,\beta]$ and T_τ represents ordering in τ. We shall refer to $\tilde{S}_{ij}$ as the current-current Green's function, even though $\dot{n}_i$ are not quite the current operators. We can establish the relation between the matrix $C(z)$ of Eq. (25) and $\tilde{S}_{ij}(\tau)$ through its spectral function $A_{ij}(\omega)$ obtained from the relation

$$A_{ij}(\omega)=\operatorname{Im}\tilde{S}_{ij}(i\omega_k\rightarrow\hbar\omega+i\eta), \tag{32}$$

where

$$\tilde{S}_{ij}(\omega_k)=\frac{1}{2}\int_{-\beta}^{\beta}e^{i\omega_k\tau}\tilde{S}_{ij}(\tau)d\tau, \tag{33}$$

and $\omega_k=2\pi n/\beta$. Now the standard fluctuation-dissipation theorem allows us to write

$$C_{ij}(z)=\frac{1}{\beta\hbar}\int\frac{d\omega}{2\pi i}\,\frac{A_{ij}(\omega)}{\omega(\omega-z)}. \tag{34}$$

For evaluating $S_{ij}(\tau)$ we split the Hamiltonian H of Eq. (9) as $H=H_0+V$, where

$$H_0=\sum_{i}\,\epsilon_i n_i+\sum_{q}\,\hbar\nu_q a_q^\dagger a_q \tag{35}$$

and

$$V=\sum_{i\neq j}\,J_{ij}e^{S_i-S_j}c_i^\dagger c_j+\sum_{i\neq j}\,K_{ij}n_i n_j. \tag{36}$$

We now employ the formalism of finite-temperature perturbation theory. In this scheme, within interaction representation the time development of the electron and phonon operators is given by

$$a_q(\tau)=e^{-\nu_q\tau}a_q(0),\quad a_q^\dagger(\tau)=e^{\nu_q\tau}a_q^\dagger(0),$$
$$c_i(\tau)=e^{-\epsilon_i\tau}c_i(0),\quad c_i^\dagger(\tau)=e^{\epsilon_i\tau}c_i^\dagger(0). \tag{37}$$

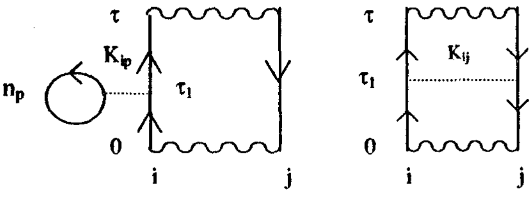
The perturbation expansion for the current-current Green's function $\tilde{S}_{ij}(\tau)$, in the interaction representation is

$$\tilde{S}_{ij}(\tau)=\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int d\tau_n\cdots\int d\tau_1 \times\langle T_\tau[\dot{n}_i(\tau)\dot{n}_j(0)V(\tau_n)\cdots V(\tau_1)]\rangle_{connected}. \tag{38}$$

All averages are now with the density matrix corresponding to H_0. The expression for the current $\dot{n}_i(\tau)$ is

$$\dot{n}_i(\tau)=\frac{1}{i\hbar}[n_i,H_0] =\frac{1}{i\hbar}\sum_{k}\,J_{ik}e^{S_i(\tau)-S_k(\tau)}[c_i^\dagger(\tau)c_k(\tau)-c_k^\dagger(\tau)c_i(\tau)]. \tag{39}$$

The perturbation Hamiltonian V in Eq. (36) includes the hopping term J_{ij} and the Coulomb-interaction term K_{ij}. So the



(a) (b)

FIG. 2. First-order terms in interaction K for $\gamma_{ij}(\tau)$, (a) Hartree term, and (b) electron-hole interaction term.

$$
\begin{aligned}
G_{ij}^{(1)}= & -1/2\sum_{n\neq m} K_{pq}\int d\tau_1\langle T_\tau[n_p(\tau_1)n_q(\tau_1)] \\
& \times[c_i^\dagger(\tau)c_j(\tau)c_j^\dagger(0)c_i(0)+i\leftrightarrow j]\rangle \\
= & \int d\tau_1\Bigg[\sum_p K_{ip}f_p^0 g_i(\tau_1)g_i(\tau-\tau_1)g_j(-\tau) \\
& +\sum_p K_{jp}f_p^0 g_i(\tau)g_j(\tau_1-\tau)g_j(-\tau_1) \\
& +K_{ij}g_i(\tau_1)g_i(\tau-\tau_1)g_j(\tau_1-\tau)g_j(-\tau_1)+i\leftrightarrow j\Bigg].
\end{aligned}
\tag{53}
$$

These are represented in Figs. 2(a) and 2(b). Figure 2(a) is just the Hartree term representing the interaction of the charge at site i (or j) with the other charges in the system. Figure 2(b) represents the electron-hole interaction between sites i and j, respectively. One can easily convince oneself that at all higher orders in K, only these two kinds of terms arise due to the diagonal nature of the Coulomb interaction retained in the Hamiltonian. This means that to include interaction to all orders, we need to sum over the bubble diagrams and the electron-hole interaction ladders. The sum-over bubble diagrams in frequency space can be written as

$$
\begin{aligned}
& \sum_k \frac{1}{\beta}g_j(\omega_k)-\sum_k \frac{1}{\beta}g_j(\omega_k)^2K_{jp}f_p \\
& +\sum_k \frac{1}{\beta}g_j(\omega_k)^3(K_{jp}f_p)^2-\cdots=\sum_k \frac{1}{\beta}\tilde{g}_j(\omega_k),
\end{aligned}
\tag{54}
$$

where

$$
\tilde{g}_j(\omega_m)=-\frac{1}{i\omega_k-E_j},
\tag{55}
$$

with E_j as defined in Eq. (3). Note that we also replace f_p^0 by f_p, where f_p is the Fermi function corresponding to the self-consistent Hartree energy E_i. For the rest of the calculations we use the $\tilde{g}_i$ in place of the bare propagator g_i.

The frequency representation of the electron-hole interaction term of Fig. 2(b) is

$$
\sum_{k,l}\frac{1}{\beta^2}K_{ij}\tilde{g}_i(\omega_m+\omega_l)\tilde{g}_j(\omega_l)\tilde{g}_i(\omega_m+\omega_k)\tilde{g}_j(\omega_k).
\tag{56}
$$

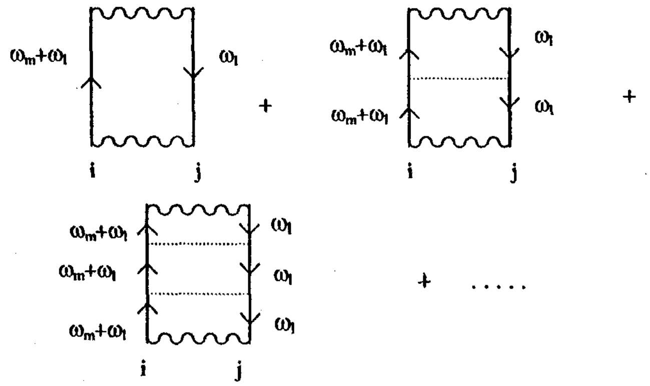


FIG. 3. Ladder summation over electron-hole interaction terms.

The next step of the calculation would be to sum over the higher-order terms of the series of the same kind implying repeated electron-hole interactions as shown in Fig. 3. This means a summation of the following series:

$$
\begin{aligned}
& \left(\sum_l \frac{1}{\beta}\tilde{g}_i(\omega_m+\omega_l)\tilde{g}_j(\omega_l)\right) \\
& \quad -K_{ij}\left(\sum_l \frac{1}{\beta^2}\tilde{g}_i(\omega_m+\omega_l)\tilde{g}_j(\omega_l)\right)^2 \\
& \quad +K_{ij}^2\left(\sum_l \frac{1}{\beta^3}\tilde{g}_i(\omega_m+\omega_l)\tilde{g}_j(\omega_l)\right)^3-\cdots \\
& =\frac{f_i-f_j}{i\omega_m-E_{ji}}\left(1-K_{ij}\frac{f_i-f_j}{i\omega_m-E_{ji}}+K_{ij}^2\left(\frac{f_i-f_j}{i\omega_m-E_{ji}}\right)^2-\cdots\right) \\
& =\frac{f_i-f_j}{i\omega_m-\Delta_{ji}},
\end{aligned}
\tag{57}
$$

where

$$
\Delta_{ji}=E_j-E_i-K_{ij}(f_i-f_j),
\tag{58}
$$

which is the energy required to transfer an electron from site i to j. In the expression for Δ_{ji} if we set the temperature to zero, the net energy required for an electron transition from a site j to an empty site i, is same as in Eq. (3), which is the excitation energy for a single-particle excitation used by Efros and Shklovskii.[17] Thus, our results are a finite temperature generalization of the earlier result, which formed the basis for the Coulomb gap for the Hartree energies in the ground state. The final form for γ_{ij} is, therefore, given by

$$
\gamma_{ij}=\sum_m F_{ij}(\omega_l-\omega_m)\left\{\left[\frac{f_i-f_j}{i\omega_m-\Delta_{ji}}\right]+i\leftrightarrow j\right\}.
\tag{59}
$$

We now need to evaluate the phonon propagation factor $F_{ij}(\omega_l)$. This has been done earlier,[38] and we express it in terms of the phonon propagator $D_q(\tau)$ defined as

$$
\begin{aligned}
D_q(\tau)&=\langle T_\tau a_q(\tau)a_q^\dagger(0)\rangle_0 \\
&=[\Theta(\tau)(1+n_q)e^{-\nu_q\tau}+\Theta(-\tau)e^{-\nu_q\tau}],
\end{aligned}
\tag{60}
$$

where n_q is the thermal number of phonons with energy $\hbar\nu_q$. The expression for $F_{ij}(\tau)$ is found to be perturbation expansion [in Eq. (38)] will contain higher orders of both. But at first we study the perturbation expansion up to order J^2 in the hopping term and to all orders in the Coulomb interaction K. This means that we wish to restrict our study at this stage to processes that involve the transfer of a single electron between sites, and the effect of Coulomb interactions on the physics of single-electron transfer. Terms of higher order in J involve transfer of more than one electron, and we shall look into such terms in the next section, when we study the physics of charge-relaxation processes.

The perturbation expansion to order J^2 can be written as

$$\begin{aligned}\tilde{S}_{ij}(\tau)=\sum_{k,l}&\langle T_\tau[W_{ik}(\tau)W_{jl}(0)]\rangle\\ &\times\Bigg\langle T_\tau\Bigg\{\exp-\tfrac{1}{2}\int d\tau'\sum_{n,m}K_{nm}n_m(\tau')n_n(\tau')\\ &\times[c_i^\dagger(\tau)c_k(\tau)-c_k^\dagger(\tau)c_i(\tau)]\\ &\times[c_j^\dagger(0)c_l(0)-c_l^\dagger(0)c_i(0)]\Bigg\}\Bigg\rangle,\end{aligned}\tag{40}$$

where

$$W_{ij}(\tau)=\frac{J_{ij}}{i\hbar}e^{S_i(\tau)-S_j(\tau)}.\tag{41}$$

The structure of Eq. (40) allows us to write

$$\tilde{S}_{ij}(\tau)=-\gamma_{ij}(\tau)+\delta_{ij}\sum_k\gamma_{ik}(\tau),\tag{42}$$

where

$$\gamma_{ij}(\tau)=F_{ij}(\tau)G_{ij}(\tau),\tag{43}$$

where $F_{ij}(\tau)$ is the phonon factor given by

$$F_{ij}(\tau)=\langle T_\tau[W_{ij}(\tau)W_{ij}(0)]\rangle,\tag{44}$$

and $G_{ij}(\tau)$ is

$$\begin{aligned}G_{ij}(\tau)&=\sum_n G_{ij}^{(n)}(\tau)\\ &=\Bigg\{\int\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int d\tau_n\cdots\int d\tau_1\\ &\quad\times\langle T_\tau[K(\tau_n)\cdots K(\tau_1)]\\ &\quad\times[c_i^\dagger(\tau)c_j(\tau)c_j^\dagger(0)c_i(0)+i\leftrightarrow j]\rangle\Bigg\}.\end{aligned}\tag{45}$$

This factorization is possible because the phononic contribution F_{ij} is not affected by the Coulomb-interaction term. The form Eq. (42) completes the analogy with the generalized resistor network. This form implies current conservation, which is merely a consequence of electron number conservation. In frequency space Eq. (43) is rewritten as

$$\gamma_{ij}(\omega_l)=\sum_m F_{ij}(\omega_l-\omega_m)\left[\sum_n G_{ij}^{(n)}(\omega_m)\right].\tag{46}$$

The first term in the series for G_{ij} [Eq. 43)] is then

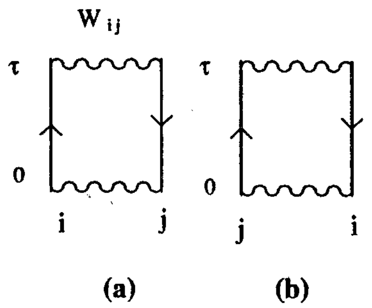


FIG. 1. Zero order diagrams for $\gamma_{ij}(\tau)$.

$$G_{ij}^{(0)}(\tau)=\langle T_\tau[c_i^\dagger(\tau)c_j(\tau)c_j^\dagger(0)c_i(0)+i\leftrightarrow j]\rangle.\tag{47}$$

At this stage we define the thermal-electron propagator $g_i(\tau)$ as

$$g_i(\tau)=\langle T_\tau[c_i(\tau)c_j^\dagger(0)]\rangle.\tag{48}$$

The Fourier transform of $g_i(\tau)$ is

$$g_i(\omega_k)=\frac{1}{2}\int_{-\beta}^{\beta}d\tau e^{i\omega_k\tau}g_i(\tau)=-\frac{1}{i\omega_k-\epsilon_i},\tag{49}$$

where $\omega_k=(2k+1)\pi/\beta$ are the fermionic Matsubara frequencies. We shall represent $g_i(\tau)$ and $g_i(\omega_k)$ by vertical lines labelled by either τ variables or frequencies. On applying Wicks theorem to Eq. (47) the zeroth-order term is

$$\begin{aligned}\gamma_{ij}^{(0)}(\tau)=&\langle T_\tau[W_{ij}(\tau)W_{ij}(0)]\rangle\\ &\times[g_j(\tau)g_i(-\tau)+g_i(\tau)g_j(-\tau)].\end{aligned}\tag{50}$$

A diagrammatic representation of $\gamma_{ij}^{(0)}(\tau)$ is shown in Figs. 1 (a) and 1(b). The W_{ij}'s are represented by the curly lines. Each of these diagrams represent the phonon-assisted hopping of a single electron from a site i to a site j. The frequency transform $G_{ij}^{(0)}(\tau)$ is

$$G_{ij}^{(0)}(\omega_m)=\sum_k[g_i(\omega_m+\omega_k)g_j(\omega_k)+i\leftrightarrow j],\tag{51}$$

which, on summing over frequencies ω_k yields

$$G_{ij}^{(0)}(\omega_k)=\frac{1}{\beta}(f_i^0-f_j^0)\left[\frac{1}{i\omega_k-\epsilon_{ji}}-\frac{1}{i\omega_k+\epsilon_{ji}}\right],\tag{52}$$

where $\epsilon_{ji}=\epsilon_j-\epsilon_i$, which in the absence of interactions represents the energy required to transfer the electron from site i to the site j, and f_i^0 is the Fermi function corresponding to the energy ϵ_i. The next term of the series for G_{ij}, which is first order in K, can be written as

$$\Gamma_{ij}(\omega)=\Gamma_{ij}(0)\left[1+\frac{\hbar\omega}{k_BT}\right]. \tag{74}$$

The result for γ_{ij} in the interacting case is expressed in Eq. (59). The effect of Coulomb interactions is to replace the site energies ϵ by the Hartree energies E and the excitation energy between sites i and j is Δ_{ji} in place of ϵ_{ji}, defined in Eq. (58). Following the same procedure as for the noninteracting case we find that the spectral function for the interacting case within this approximation is

$$\begin{aligned}A_{ij}(\omega)=\pi\left(\frac{J_0}{i\hbar}\right)^2(1-e^{-\beta\omega})e^{-D_{ij}}\\ \times\sum_q|B_{ij}(q)|^2[(f_i-f_j)\{1+n_B(\Delta_{ji})\}n(\Delta_{ji}-\omega)\\ \times\{\delta(\omega-\Delta_{ji}-\nu_q)-\delta(\omega-\Delta_{ji}+\nu_q)\}+i\leftrightarrow j].\end{aligned} \tag{75}$$

This leads to the following hop rates:

$$\begin{aligned}\Gamma_{ij}(z)=-\frac{1}{2i}\left(\frac{J_{ij}}{\hbar}\right)^2e^{-D_{ij}}\\ \times\sum_q|B_{ij}(q)|^2\Bigg[(f_i-f_j)\{1+n_B(\Delta_{ji})\}\\ \times\left\{\frac{1+n_B(\nu_q)}{\Delta_{ji}+\nu_q-z}+\frac{n_B(\nu_q)}{\Delta_{ji}-\nu_q-z}\right\}+i\leftrightarrow j\Bigg].\end{aligned} \tag{76}$$

We shall now extend the calculation of the intersite hopping rates to incorporate charge-relaxation effects. For this one has to go beyond the approximation of this section. Here we have assumed that when one electron makes a jump, the remaining electrons remain fixed in their positions. Any realistic picture of the conduction mechanism cannot choose to ignore the effect of a hopping electron on its immediate neighborhood.

IV. RELAXATION EFFECTS

The charge-relaxation effects are contained in the self-energy of the electron propagators or equivalently in the frequency-dependant dielectric constant of the system. For reasons that become evident in the following discussion, we shall focus on a certain class of processes in the self-energy. Note that for site-diagonal interactions and localized electrons, the only self-energy contribution is the Hartree term represented by the bubble diagram of Fig 2(a). Further corrections arise only when we include terms of higher orders in J, as these terms represent processes that allow for the movement of the charge in response to the potential of the electron under consideration. The two representative diagrams are shown in Figs. 4(a) and 4(b). We shall be interested in those self-energy corrections that involve the polarizability of the medium. Such diagrams can be schematically represented by Fig. 4(c), where the loop shown represents the susceptibility χ. The contribution of these diagrams can be written as

$$\Sigma_i(\omega_l)=\frac{1}{\beta}\sum_{\omega_m}g_i(\omega_l-\omega_m)\sum_{j,k}K_{ij}\chi_{jk}(\omega_m)K_{ki}. \tag{77}$$

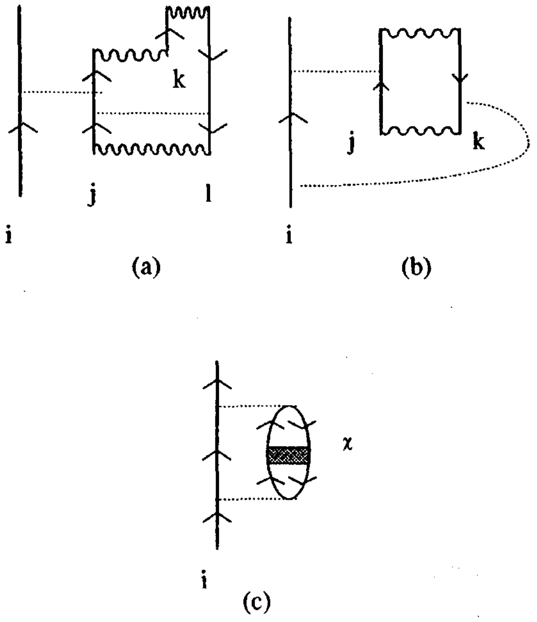


FIG. 4. Typical higher-order terms in the self-energy.

To get a further physical feeling for this set of processes, consider the situation in which one electron is added to the system at a site i at time $t=0$. This means a perturbation $V_j(t)=K_{ji}\theta(t)$. In response to this perturbation the occupation numbers at the site k changes according to Eq. (11) as

$$\delta n_k(t)=2i\sum_j\int_0^t\chi''_{kj}(t-t')K_{ji}dt'. \tag{78}$$

This means that the Hartree energy at the site i changes according to the equation

$$\delta E_i(t)=E_i(0)+2i\sum_{k,j}K_{ij}\int_0^t\chi_{jk}(t-t')K_{ki}dt'. \tag{79}$$

Taking the Laplace transform yields

$$E_i(z)=-\frac{1}{iz}\left[E_i+\sum_{kj}K_{ij}\chi_{jk}(z)K_{ki}\right]. \tag{80}$$

The second term in the right-hand side is just the counterpart of Eq. (77), when the electron at the site i is taken to be static. This, in principle, allows for a self-consistent calculation of the conductivity and the polarizability. However, the solution of such self-consistent equations for random systems is one of formidable difficulty. Here we adopt a simpler physical approach which this formal reasoning suggests. To make the ideas explicit, we first describe them in time domain, but actual calculations are done in the frequency domain and require a little different modeling.

We assume that the Hartree energies of the sites involved in the electron hop relax by a simple exponential law. Further, the relaxation is of the order of the Coulomb-gap energy Δ_C, which is given by $E_C(E_C/W)^{1/2}$, where E_C is the average Coulomb energy between neighboring sites, i.e., $E_C\propto e^2/\kappa d$ where d is the mean distance between the sites and W is the width of the band of the localized states. Thus, if the electron jumps from an occupied site i to an unoccu-

$$F_{ij}(\tau)=\frac{J_{ij}^2}{(i\hbar)^2}\exp\left(-\sum_q |B_{ij}(q)|^2 \times\{(2n_q+1)D_q(\tau)-D_q(-\tau)\}\right), \tag{61}$$

where

$$B_{ij}(q)=\frac{A_i(q)-A_j(q)}{\hbar\nu_q}. \tag{62}$$

For explicit calculations we shall expand the exponential and retain terms up to the first order in D_q, i.e,

$$F_{ij}(\tau)\simeq\frac{J_{ij}^2}{(i\hbar^2)}\exp-\sum_q |B_{ij}(q)|^2(2n_q+1) \times\{1+|B_{ij}(q)|^2[D_q(\tau)+D_q(-\tau)]\}. \tag{63}$$

Inasmuch as we are looking at the polarization effects in the system, which is brought about by phonon-assisted charge transport, we shall not detract from the physics of the problem by assuming that at most a single phonon is being exchanged in these transitions at low enough temperatures.

The exact form of the propagator is decided by the choice of $A_i(q)$. In these systems it is customary to use the deformation potential approximation,[40] where the electron phonon coupling is written as

$$A_i(q)=D(2\rho_0 Vs)^{-1/2}q^{1/2}e^{i\mathbf{q}\cdot\mathbf{R}_i}. \tag{64}$$

Here D is deformation potential constant and ρ_0, V, and s are, respectively, the density, volume, and the velocity of sound. Using the linear dispersion relation for the phonons, i.e., $\nu_q=sq$, the prefactor in the expressions for the phonon propagator can be obtained to be

$$\exp\left\{-\sum_q [|B_{ij}(q)|^2(2n_q+1)]\right\} = \exp\left[-8D^2\rho_0 Vs\sum_q \coth\left(\frac{\beta\nu_q}{2}\right) \times q\sin^2\left(\frac{qR_m}{2}\right)\Big/(\hbar\omega_q)^2\right]. \tag{65}$$

Further, if J_{ij} is taken to be of the form

$$J_{ij}=J_0 e^{-\alpha|R_i-R_j|}, \tag{66}$$

the entire prefactor can be expressed as an exponential $e^{-D_{ij}}$ and the single-phonon contribution to F_{ij} takes the form,

$$F_{ij}(\tau)=J_0^2 e^{-D_{ij}}\sum_q |B_{ij}|^2[D_q(\tau)+D_q(-\tau)]. \tag{67}$$

The hopping rates between two sites, which are correct to order J^2 but include Coulomb interactions to all orders can now be explicitly calculated. First we record the expressions for $\gamma_{ij}(\omega_l)$ for the noninteracting case. These expressions include only one phonon part of F_{ij}. Then we find,

$$\gamma_{ij}(\omega_l)=\left(\frac{J_0}{i\hbar}\right)^2 e^{-D_{ij}}\sum_q |B_{ij}(q)|^2 \times\left[\frac{n_q f_j^0(1-f_i^0)-(1+n_q)f_i^0(1-f_j^0)}{i\omega_l-\epsilon_{ji}-\nu_q} - \frac{(1+n_q)f_j^0(1-f_i^0)-n_q f_i^0(1-f_j^0)}{i\omega_l-\epsilon_{ji}+\nu_q}+i\leftrightarrow j\right]. \tag{68}$$

The spectral function $A_{ij}(\omega)$ can be evaluated as

$$\begin{aligned}A_{ij}(\omega)&=\mathrm{Im}\,\gamma_{ij}^{(0)}(i\omega_l\rightarrow\omega+i\eta)\\&=\left(\frac{J_0}{i\hbar}\right)^2 e^{-D_{ij}}(1-e^{-\beta\omega})\sum_q |B_{ij}(q)|^2\\&\quad\times[f_i^0(1-f_j^0)\{n_q\delta(\omega-\epsilon_{ji}+\nu_q)\\&\quad+(1+n_q)\delta(\omega-\epsilon_{ji}-\nu_q)\}+i\leftrightarrow j].\end{aligned} \tag{69}$$

From $A_{ij}(\omega)$ we derive the frequency-dependant transition rate $\Gamma_{ij}(z)$ as follows:

$$\begin{aligned}\Gamma_{ij}(z)&=\frac{1}{2\beta\hbar}\int\frac{d\omega}{i\pi}\frac{A_{ij}(\omega)}{\omega(\omega-z)}\\&=\left(\frac{J_0}{i\hbar}\right)^2 e^{-D_{ij}}\sum_q |B_{ij}(q)|^2\\&\quad\times\left[f_i^0(1-f_j^0)\left\{\frac{n_q}{\epsilon_{ji}-\nu_q-z}+\frac{1+n_q}{\epsilon_{ji}+\nu_q+z}\right\}+i\leftrightarrow j\right].\end{aligned} \tag{70}$$

These equations in the low-temperature limit lead to the standard expressions often used in literature for $\Gamma_{ij}(0)=\lim_{\eta\rightarrow 0}\Gamma_{ij}(i\eta)$,[3]

$$\Gamma_{ij}(0)=T_{ij}\rho(\epsilon_{ji})\exp[-\beta/2\{|\epsilon_i-\mu|+|\epsilon_j-\mu|+|\epsilon_i-\epsilon_j|\}], \tag{71}$$

where

$$T_{ij}=\left(\frac{J_0}{i\hbar}\right)^2 e^{-D_{ij}}|B_{ij}|^2$$

$$\rho(\epsilon_{ji})=\sum_q \delta(\nu_q-\epsilon_{ji}). \tag{72}$$

Here we have also assumed $B_{ij}(q)$ to be q independent. We refer to these rates as AHL rates, as they were first used by Ambegaokar, Halperin, and Langer.[3] At finite frequencies the expression for the transition rates are

$$\begin{aligned}\Gamma_{ij}(\omega)&=\Gamma_{ij}(z=\omega+i\eta)\\&=\frac{T_{ij}}{2}[f_i^0(1-f_j^0)\{[1+n(\epsilon_{ji}+\omega)]\rho(\epsilon_{ji}+\omega)\\&\quad+n(\epsilon_{ji}-\omega)\rho(\epsilon_{ji}-\omega)\}+i\leftrightarrow j],\end{aligned} \tag{73}$$

which at low temperatures is just

pied site j, in the vicinity of the Fermi level the Hartree energies at these two sites are assumed to relax in the following way:

$$E_i(t)=E_i+\frac{1}{2}\Delta_C(1-e^{-\gamma t}),$$

$$E_j(t)=E_j-\frac{1}{2}\Delta_C(1-e^{-\gamma t}). \tag{81}$$

These equations admittedly simplify grossly the complicated relaxation process, which also differs from site to site. However, the advantage is that the self-consistency problem becomes tractable if we assume γ to be related to a parameter of the density-density response function as Eq. (80) suggests. To make the connection plausible we calculate the self-energy correction given in Eq. (80) under the following simplified conditions. We assume (a) the system to be uniform and (b) the conductance matrix to be Markovian. Then Eq. (27) allows us to write

$$\chi(q,z)=-\frac{\beta C(\vec{q})}{iz-\beta C(\vec{q})\chi^{-1}(q,0)}, \tag{82}$$

where $\chi(\vec{q},0)$ and $C(\vec{q})$ are the spatial Fourier transforms of χ_{ij} and C_{ij}, respectively. Further substituting Eq. (82) in Eq. (80) one obtains

$$\delta E_i(z)=\frac{-1}{iz}\sum_q K^2(q)\chi(q,0)\frac{\beta C(q)/\chi(q,0)}{iz-\beta C(q)/\chi(q,0)}. \tag{83}$$

Defining

$$\beta C(q)/\chi(q,0)=\frac{\beta[\Gamma(0)-\Gamma(q)]}{\chi(q,0)}=q^2D_q, \tag{84}$$

one obtains

$$\delta E_i(z)=\sum_q K^2(q)\chi(q,0)\left[\frac{1}{iz}-\frac{1}{iz-q^2D(q,z)}\right]. \tag{85}$$

For the time dependence, Eq. (85) yields

$$\delta E_i(t)=\mp 2\sum_q K^2(q)\chi(q,0)[1-e^{-q^2D_q t}]. \tag{86}$$

Now the conductivity of the uniform system in Markovian approximation is simply related to D_q by the relation

$$\sigma(q,\omega)=\frac{i\omega e^2}{q^2}\chi(q,\omega)=i\omega e^2\frac{\chi(q,0)D_q}{i\omega-q^2D_q}, \tag{87}$$

which for the dc conductivity yields the well-known Einstein relation

$$\sigma_{dc}=\lim_{\omega\to 0}\lim_{q\to 0}\sigma(q,\omega)=e^2\chi(0,0)D_0. \tag{88}$$

For disordered systems Eqs. (82) and (86) are much more complicated. Our assumptions in Eq. (81) imply that the relaxation is dominated by just one rate. Comparing Eq. (86) with Eq. (81) we infer that

$$\gamma\simeq\langle q^2D_q\rangle\simeq D/\bar{R}^2, \tag{89}$$

where $\bar{R}$ is just the average-hopping distance. Then, using Eq. (88), one sees the plausible connection between γ and σ_{dc} to be

$$\gamma=\frac{1}{\bar{R}^2}\frac{\sigma_{dc}}{e^2\chi(0,0)}. \tag{90}$$

This leads to a reasonable physical picture that the local charge-relaxation rate is related to the dc conductivity itself.

With this background we return to the procedure of incorporating these relaxation and dielectric effects in the formal calculation. In principle, these self-energy calculations must now be included in the calculation of $\gamma_{ij}(\omega_l)$, which determine the internode hopping rates. Our earlier calculation without relaxation effects leads to Eqs. (75) and (76) for the spectral functions $A_{ij}(\omega_l)$ and the hop rates $\Gamma_{ij}(z)$, respectively. Due to the sharpness of the Hartree levels, we find that the spectral function consists of delta functions at the precise excitation energies associated with the hop. The relaxation effects due to the motion of other electrons cause the Hartree levels to broaden, i.e., fluctuate in time as well as shift on average by amounts of order Δ_C, the Coulomb gap. We model this directly in the spectral function by replacing the δ functions by the following expressions, which incorporates both the above effects

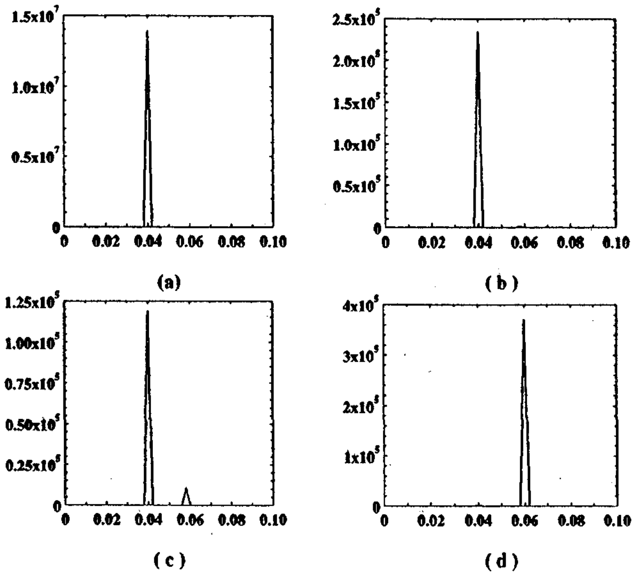
$$\delta(\omega-\Delta_{ij}\pm\nu_q)\to\frac{1}{\pi}\frac{\eta_1 a(\gamma)}{(\omega-\Delta_{ij}\pm\nu_q)^2+\eta_1^2}+\frac{1}{\pi}\frac{\eta_2[1-a(\gamma)]}{[\omega-\Delta_{ij}\pm\nu_q+\Delta_C f(\omega/\gamma)]^2+\eta_2^2}, \tag{91}$$

where the parameters a,η_1,η_2, and f are all dependent on the relaxation parameter γ alone. They are chosen as follows: $a(\gamma)=e^{-\gamma^2}$, $\eta_1=\gamma$, and $\eta_2\propto 1/\gamma^2$. Finally, the function $f(\omega/\gamma)$ is taken to be

$$f(\omega/\gamma)=\frac{1}{1+(\omega/\gamma)^2}. \tag{92}$$

This model basically reflects the time-dependant effects described qualitatively earlier. We replace the single peak at the excitation $\Delta_{ij}\pm\nu_q$ by two Lorentzians having weights $a(\gamma)$ and $[1-a(\gamma)]$. The first peak is at the original excitation energy, which is there in the absence of relaxation effects, and its weight is also unity if $\gamma=0$. The width of the peak is also taken to be γ, so as $\gamma\to 0$ we get the original δ function. The second term of Eq. (91) represents the shift in excitation energy due to relaxation effects. This shift, which is approximately given by $\Delta_C f(\omega/\gamma)$, depends on the external frequency and the relaxation rate γ through their ratio. The slow processes ($\omega\to 0$) allow the neighboring charge to relax and so the relaxation shift is large and tends to Δ_C, while the fast processes are not expected to be affected by relaxation, so the shift goes like Δ_c/ω^2. As for the broadening of this level, we expect this level to get sharper if the background relaxes fast, so we have taken the width of the level to go like γ^{-2}. Finally, the weight of the peak increases with the relaxation rate, becoming unity as $\gamma \rightarrow \infty$. There is obviously some arbitrariness in our choice, and any other function with this qualitative behavior should serve the purpose. We believe our main results are not much sensitive to the precise choice of the functions.

In Fig. 5 we plot this function as the function of phonon frequency ν for the following parameters: $\Delta_{ij}=0.04$ units, $\Delta_C=0.02$, and for four different values of the relaxation parameter γ. In Fig. 5(a) the peak occurs at $\nu=\Delta_{ij}$, while in Fig. 5(b), which has a larger value of γ, along with a peak at $\nu=\Delta_{ij}$ there is also a small peak at $\nu=0.054$. In Fig. 5(c) for a still larger γ the second peak has shifted to $\nu=0.059$ with a slightly larger weight than in Fig. 5(b). In Fig. 5(d), which is for a much larger value of γ, the peak at $\nu=\Delta_{ij}$ has shifted to $\nu=\Delta_{ij}+\Delta_C=0.06$. So with an increasing relaxation parameter the gap seen by the electron gradually becomes smaller. With this form for the spectral function the transition rates for the numerical calculation are calculated by the method detailed in the next section.



(a) (b)

(c) (d)

FIG. 5. The spectral function as modeled in Eq. (91).

V. CALCULATION OF dc CONDUCTIVITY

For the calculation of the conductivity we use the method of Movaghar and Schirmacher (MS). In their approach the rate equation is solved using a self-consistent effective medium approximation.[12,13] Using the tight-binding analogy they handle the path summation problem by a renormalized perturbation expansion. Exact solutions are possible only for Bethe lattices. For finding the conductivity they make approximations in the nature of extending results of the Bethe lattices to real systems. This method gives a good account of dc conductivity in the VRH regime.[14] The conductivity is evaluated from the following set of equations:

$$\sigma(\omega)=N_d\frac{e^2}{k_BT}\frac{n^2}{6}\int\int\int\frac{g_c(R)g(E)g(E')R^2}{[\Gamma(E,E',R,\omega)]^{-1}+[i\omega F(E')+\sigma_1(E',\omega)]^{-1}}d^3R\,dE\,dE', \tag{93}$$

where n is the number of electrons per site, N_d is the number of sites, $g(E)$ is the density of states of electrons per site, $g_C(R)$ is the radial distribution function for the position of the sites, Γ's are the hopping rates between two sites, and $F(E)$ is given by $f(E)[1-f(E)]$ and comes from the static susceptibility factor that occurs in Eq. (28). Finally, $\sigma_1(E,\omega)$ is an auxiliary energy and frequency-dependent parameter to be determined from the following self-consistent equation.

$$\sigma_1(E',\omega)=na_p\int\int\frac{g(E'')g_C(R)}{[\Gamma(E',E'',R,\omega)]^{-1}+[i\omega F(E'')+\sigma_1(E'',\omega)]^{-1}}d^3R\,dE'', \tag{94}$$

where a_p is a factor that takes into account the overcounting of paths with respect to the Bethe lattice and has been estimated to be e^{-1}. MS calculate the dc conductivity using the AHL transition rates [Eq. (71), with $T_{ij} \propto e^{-2\alpha R_{ij}}$], a constant $\rho(E)$ and taking $g_C(R)$ to be unity in Eqs. (93) and (94), which is appropriate for the noninteracting situation. The calculated conductivity shows Mott's $T^{1/4}$ behavior at low temperatures.[14] The estimated values of T_M found by them matches very well with the value suggested by Mott.[1]

The above procedure has been developed for systems in which the internode conductances are independent random variables, having the same probability distribution. This is not the case for our calculation, as the Hartree energies are obviously correlated and the conductance formula also involves the static susceptibility matrix. To tackle such correlated disorder one has to go beyond single-bond effective-medium approximation. We are not aware of any qualitatively new effects that arise in such calculations. So, as a first step, we neglect the correlations between the internode conductances calculated by us. Then these equations can be used by inserting the hop-rates Γ we have obtained and making one further approximation of taking for static susceptibility matrix, the noninteracting value given in Eq. (20). At this point we have also not invested effort in obtaining the static susceptibility for the interacting case. For dc conductivity we believe that this may not affect things qualitatively.

Before we describe the full calculation done by us, we present some exploratory calculations with these Eqs. (93) and (94). These studies also yield some insights into the connection between temperature-behaviors of conductivity and effective density of states for the excitation energies. First we study the conductivity with the AHL transition

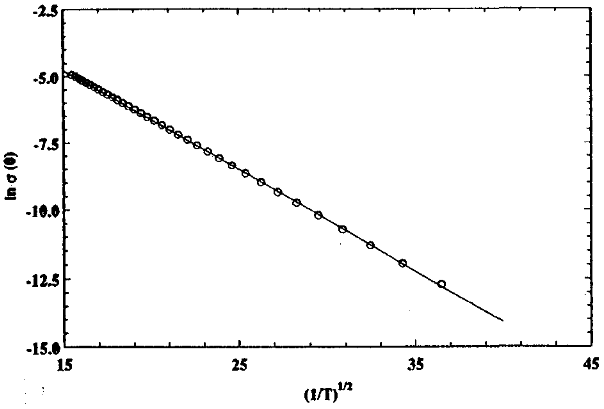


FIG. 6. $\ln \sigma(0)$ plotted with $(1/T)^{1/2}$ for a temperature range of 0.000 75–0.0042 eV, using the AHL transition rates and a DOS with a Coulomb gap.

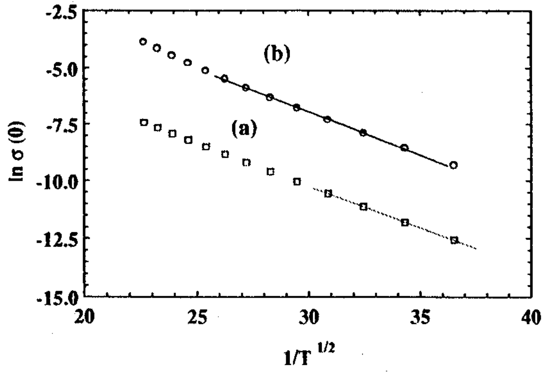


FIG. 7. $\ln \sigma(0)$ plotted with $T^{-1/2}$ for a temperature dependent DOS (Eq. 95) over a temperature range of 0.000 75 to 0.004 eV, using the AHL hop rates for (a) $T_{gc}=0.01$ eV and (b) $T_{gc}=0.002$ eV.

rates, but with an energy-dependent DOS, which has now a Coulomb gap of the following form

$$g(E)=\begin{cases}\alpha_3 E^2 & \text{for } -\Delta_C/2<E<\Delta_C/2\\ 1/W & \text{for} \Delta_C/2\leqslant|E|\leqslant W/2.\end{cases} \tag{95}$$

We work with the following set of parameters for the numerical calculation. The density of charge carriers $nN_d=6\times 10^{16}$ cm^{-3}, $W=0.1$ eV, $\alpha^{-1}=30$ Å, and $\Delta_C=0.02$ eV. The constant α_3 in Eq. (95) is decided by the condition that at $E=\pm\Delta_C/2$, $g(E)=1/W$. The range of temperature for the calculation is 0.000 75 to 0.004 eV, which implies a temperature range of 8–50 K. In Fig. 6 we plot $\ln \sigma(0)$ with $T^{-1/2}$ for this calculation. We see a very good fit to a straight line in Fig. 6 at the low-temperature end. This puts the two-site argument of Efros and Shklovskii on a firmer foundation.

Finite temperature Monte Carlo simulations for the DOS of the Hartree energies in the lattice model show that the Coulomb gap fills in with temperature. More quantitatively it seems that $g(\mu)\propto T^2$.[19] In our next set of calculations we introduce a temperature dependent DOS given by

$$g(E)=\begin{cases}aT^2+(b-cT^2)E^2 & \text{for } -\Delta_C/2<E<\Delta_C/2\\ 1/W & \text{for } \Delta_C/2\leqslant|E|\leqslant W/2,\end{cases} \tag{96}$$

where values of a,b,c are decided by a temperature T_{gc} at which the gap Δ_C disappears. We perform calculations for dc conductivity for two values of T_{gc} keeping other parameters the same as in the previous calculation. In Fig. 7 we plot these results for $\ln \sigma(0)$ against $T^{-1/2}$. As one might expect, we find that the $T^{1/2}$ behavior is seen only over the lower temperature range, the extent of the range increasing with T_{gc}.

Next we present results of a calculation with hop rates given by Eq. (76), which incorporates self-consistent Hartree correction and electron-hole interaction to all orders. At low temperatures these transition rates can be simplified to

$$\Gamma(E_i,E_j,R_{ij})=\begin{cases}e^{-2\alpha R_{ij}}e^{-\beta(|E_i-E_j|-e^2/R_{ij})} & \text{for } E_i>0,E_j<0 \text{ or } E_i<0,E_j>0\\ e^{-2\alpha R_{ij}}e^{-\beta/2(|E_i|+|E_j|+|E_i-E_j|)} & \text{for } E_i,E_j<0 \text{ or } E_i,E_j>0\ .\end{cases} \tag{97}$$

For these calculations the energy unit is taken to be $e^2\alpha^{-1}/\kappa$ and the length unit is α^{-1}. In these units the bandwidth is chosen as $W=8$, and the range of temperatures studied is $-0.06<T<0.66$. We use the DOS of Eq. (95), with $\Delta_C=0.1$ and $\alpha_3=0.5$. We present results for $n=3/4\pi$. Fig. 8 shows the plot of $\ln \sigma(0)$ with $T^{-1/2}$, in this case again the fit is good at very low temperatures over a temperature range of 0.06 to 0.26 units.

What these calculations show is that it is possible to reproduce the desired temperature variation of conductivity in the VRH regime, by incorporating interaction effects through the density of states in the conductivity formula derived from essentially independent electron approximation. For example, though our results of Fig. 7 do give a crossover from $T^{1/2}$ behavior to $T^{1/4}$ behavior, the form for the DOS given in Eq. (96) does not follow from any theory. The more significant point is that the true effect of interactions comes via the conductance matrix $C_{ij}(z)$ as in Eq. (27), and incorporation of these effects through DOS is a nice intuitive procedure that needs to be justified.

Our final set of calculations are based on zero-frequency hopping rates of Eq. (76) in which we have further incorporated the relaxation effects by replacing the δ functions as in Eq. (91). These rates are dependant on a relaxation parameter γ, which we have argued to be proportional to the conductivity $\sigma(0)$ through Eq. (90). In principle, a self-consistent calculation of the conductivity is possible from Eq. (90). However, for the disordered system the relationship between $\sigma(0)$ and γ is not quantitative. So we work with the following form for γ:

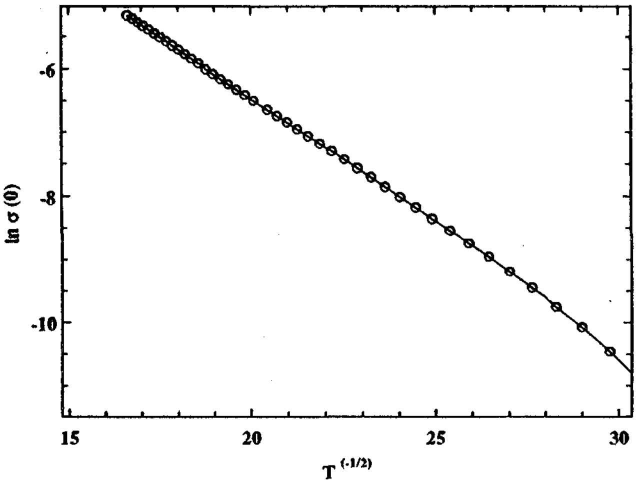


FIG. 8. ln $\sigma(0)$ plotted with $T^{-1/2}$, calculated using the transition rates for interacting electrons and a DOS with a Coulomb gap.

$$\gamma=\gamma_0 \exp\left[-\left(\frac{T_0}{T}\right)^{\nu}\right], \tag{98}$$

where the constant γ_0 is defined through a suitably chosen value that gives the right order of magnitude for the conductivity at the lowest temperature at which the calculation is performed. Further, on the basis of the numerical experience obtained from results given in Fig. 8, we can simplify the calculation by dropping the R dependence of the transfer energy Δ_{ji}, which means replacing it by just $E_{ji}=E_i-E_j$. Our earlier calculations indicated that the results are not qualitatively changed by the addition of the $e^2/\kappa R$ term, once the effect of Coulomb interaction is incorporated through the Coulomb gap in the DOS. The transition rates Γ in this case are numerically calculated from the spectral function using Eq. (91), which is then used to calculate the conductivity using Eqs. (93) and (94). We start with a value of $\gamma=10^{-5}$ at $k_BT=7.5\times10^{-4}$ eV. We present results for the DOS with the Coulomb gap, specified through Eq. (95). The parameters W, n, and Δ_C are the same as in the earlier calculation, and the temperature range covered is $0.00075<k_BT<0.00425$, i.e., from 9 to 50 K. The self-consistency in selecting γ at each temperature is achieved by doing each calculation for a range of γ values, and picking the value that is consistent with the original choice of the prefactor γ_0. In Fig. 9, we show two typical variations of conductivity with γ. One finds a regime in which conductivity varies linearly with γ followed by saturation. The saturation indicates that once the value of γ is large enough, the conductivity is not affected by the relaxation. The results of the calculation are plotted in two ways in Fig. 10. We plot ln $\sigma(0)$ with $T^{-1/2}$ and ln $\sigma(0)$ with $T^{-1/4}$. From these two curves it is clear that over a range of $0.0012<T<0.00225$ eV the conductivity shows the $T^{1/2}$ behavior and over $0.0031<T<0.00415$ eV the conductivity exhibits the $T^{1/4}$ behavior.

Further convincing evidence of crossover in the numerical calculations can be provided by obtaining the exponent as a function of temperature using the formula

$$\nu=-\frac{d^2\ln\sigma/d(\ln T)^2}{d\ln\sigma/d(\ln T)}. \tag{99}$$

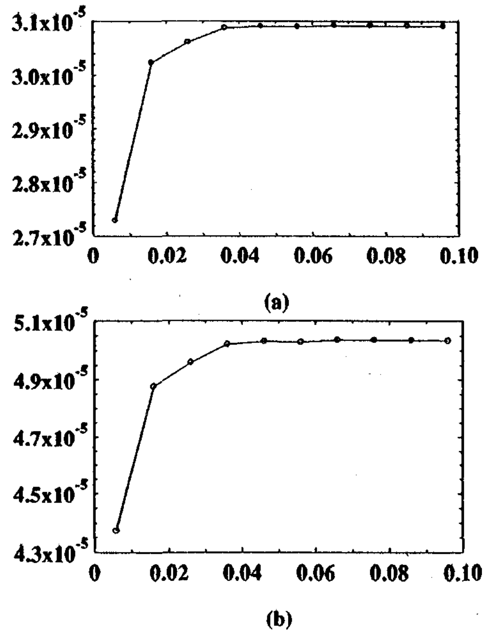


FIG. 9. Variation of conductivity with γ at two different temperatures.

A plot of ν with temperature is shown in Fig. 11. It is seen that the $\nu-T$ curve has constant values of 0.5 in the temperature range of $0.00084<T<0.0019$ and of 0.25 in the temperature range $0.0031<T<0.0046$. So the effect of relaxation is to induce a crossover in the conductivity behavior from $T^{1/2}$ at lower temperatures to $T^{1/4}$ at high temperatures.

This suggests the following physical mechanism for the two behaviors of conductivity and the crossover between them. In the lower-temperature regime when the conductivity is low, the electron hops in the background of frozen charge as the surrounding charge cannot relax sufficiently. Under these conditions the electron senses the Coulomb gap and exhibits the $T^{1/2}$-type behavior. On the other hand, in the

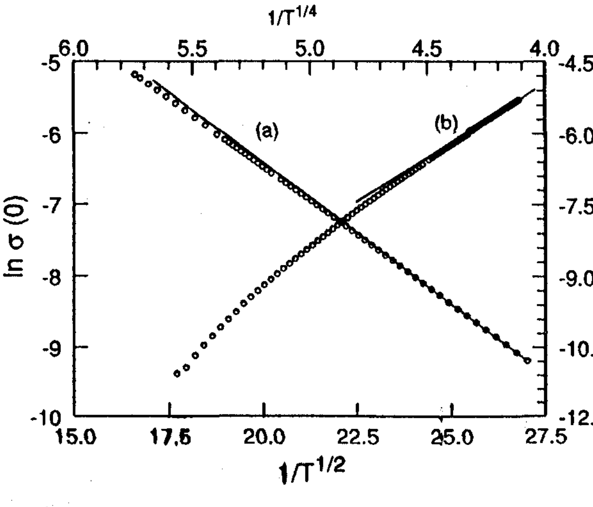


FIG. 10. (a) ln $\sigma(0)$ plotted with $T^{-1/2}$ and (b) ln $\sigma(0)$ plotted with $T^{-1/4}$ for conductivity with relaxation.

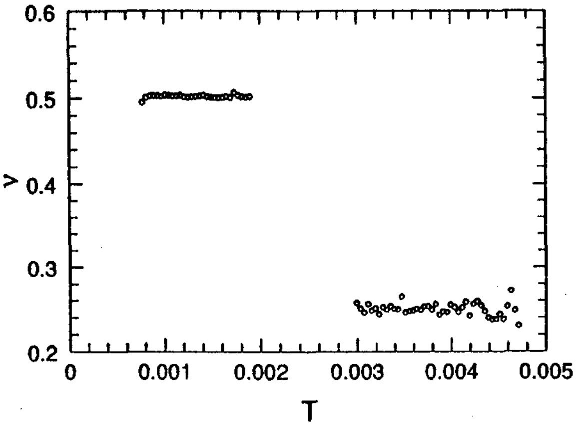


FIG. 11. Variation of the conductivity exponent with temperature.

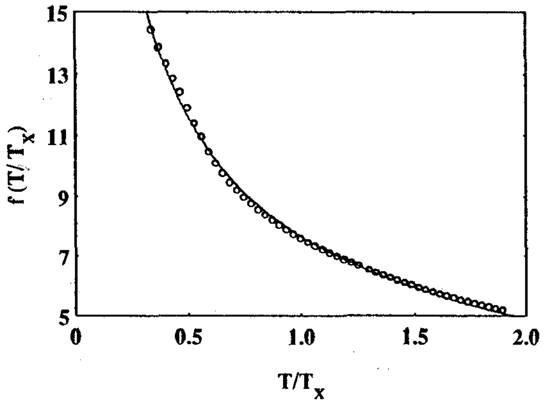


FIG. 12. The circles are the plot of $\ln \rho(0)$ with T/T_X, the full line shows the fit to the crossover function $f(T/T_X)$.

higher-temperature range of VRH, due to higher conductivity the charge around the hopping sites can relax, which in our modeling leads to a larger density of states for small excitation energies. Thus, the Coulomb gap, which is a multielectron effect gets obviated and one finds Mott-type $T^{1/4}$ behavior. This is much along the lines Mott envisaged for the behavior of the "charge polaron."[20]

We now compare our results to a detailed study of the crossover behavior in hopping conduction by Zhang *et al.*[32] This data was analyzed by Aharoni *et al.*,[34] who observed that data on different samples can be put in the following scaling form:

$$\ln \rho(0)/\rho_0 = Af(T/T_X),$$

$$f(x) = \frac{1+[(1+x)^{1/2}-1]/x}{[(1+x)^{1/2}-1]^{1/2}}, \tag{100}$$

where $\rho(0)=\sigma(0)^{-1}$, and the scale factors T_X and A depend on the individual samples but the function $f(x)$ is universal. In Fig. 12 we have fitted the conductivity choosing a crossover temperature of $T_X = 0.00191$ eV, which is in very good agreement with the crossover temperature of Massey and Lee,[41] which is $T_X = \Delta_C^{4/3}/T_M^{1/3}$. Though we have not tested the universal scaling in full detail, it is quite satisfying to find this agreement.

VI. SUMMARY

In this paper we have presented a detailed calculation of the dc conductivity of localized electrons in the variable-range hopping regime. This transport problem has two aspects, disorder and the long-range Coulomb interactions. Since it is a long calculation, we feel it would be useful to summarize the main sequence of steps and results. The starting point of the calculation is the expression of conduction and dielectric properties of the localized electrons in terms of a density-density response function of the system. Through the use of Mori-Zwanzig projector formalism, the equation of motion of the density-density response function is cast as a generalized master equation. This can be thought of as a generalized frequency-dependent random-resistor network in which the memory-function matrix plays the role of internode conductances. This identification allows us to tackle the problem in two parts. One, the evaluation of internode conductances, which can now be obtained from a rigorous formula, which basically involves computation of correlators of the time derivatives of densities at the two nodes. This correlator is evaluated using the full Hamiltonian of the problem, which includes electron-phonon interaction as well as the Coulomb interaction.

We have done a detailed analysis of this correlator using diagrammatic perturbation theory. This enables us to identify the physically more important processes through which interactions affect the conduction process. The earlier zero-temperature results are generalized to finite temperatures, and more importantly, built into the calculation in a systematic manner. We have paid particular attention to the relaxation effects that accompany electron hops. While the importance of these effects is well recognized, as far as we know, the earlier calculations that were largely based on the Markovian rate equation have not included these effects. Our modeling is basically related to a dynamical view of the Coulomb gap, which implies that due to relaxation, the energy of a site is lowered on occupation, by an amount of the order of Δ_C, while the energy of an emptied site rises by a similar amount. Further, we argue that the rate of the local relaxation is proportional to the conductivity of the sample. We show how such effects can be formally built into the conductivity calculation, and find that a good account of the crossover can be given by these ideas.

These calculations can be extended to obtain ac conductivity. Such calculations would provide further and possibly more stringent tests of these ideas. We have initiated work on these calculations. It is also of interest to examine the frequency-dependent behavior of dielectric function. These calculations are being reported in a separate paper.

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Correlated hopping in Coulomb glass

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Abstract

We have studied one aspect of the effect of Coulomb interactions on the hopping conductivity of a band of localized electrons in a disordered system, that is correlations in successive hops due to the Coulomb gap. At low temperatures, the correlation holes around sites involved in the hop do not relax, and there is an enhanced probability for backward hops. We calculate both dc and ac conductivities by considering correlated random walks in the disordered medium.

1. Introduction

In this paper we shall be concerned with the role of Coulomb interactions on the hopping conduction of localized electrons at low temperatures. In a classic paper, Mott [1] showed that as the temperature is lowered, the conductivity changes from its usual activated form $\sigma_{dc} \propto \exp(-E_3/k_B T)$ to a form $\sigma_{dc} \propto \exp[-(T_M/T)^{1/4}]$. This has been termed 'variable range hopping' (VRH), as the carrier tends to optimize between the distance of the hop and the energy barrier of the hop. Mott's formula has been used quite successfully to analyse a large number of experiments of hopping transport in impurity bands and amorphous semiconductors [2]. However, it was realized early by Efros and Shklovskii [3] that this picture ignores Coulomb interactions between the carriers. Coulomb interactions change the temperature dependence derived by Mott in a qualitative manner, i.e. to [3] $\sigma_{dc} \propto \exp[-(T_{ES}/T)^{1/2}]$. This is understood in terms of the Coulomb gap, whose existence had been shown earlier by Pollak [4] and Srinivasan [5]. They argued that in a system of localized electrons, the ground state configuration of electron occupation is such that there would be a soft gap in its excitation energy. This has been termed the 'Coulomb gap', and means that the single-particle density of states (DOS) of excitation energy has the form $\rho(\epsilon) \propto (\epsilon - \epsilon_F)^2$ around the Fermi energy ϵ_F. There have been numerous studies [6], in which the $T^{1/2}$ behaviour has been observed. Also in several studies [7, 8] one sees a crossover from $T^{1/4}$ behaviour (Mott's regime) to $T^{1/2}$ behaviour (Coulomb gap regime) as temperature is lowered.

See endnote 1

Mott's VRH arguments have been formalized using the rate equation approach of Miller and Abrahams [9]. The linearized rate equation can be solved using standard Green function

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techniques as applied to disordered systems. Physically, this amounts to calculating the conductivity of a random resistor network which is also equivalent to the calculation of diffusion of a single particle executing a random walk in a disordered medium. The main problem with such approaches lies in incorporating the effects of Coulomb interactions, as these are basically single-particle approximations of transport. The analysis of Efros and Shklovskii [3] takes into account the Coulomb interactions by incorporating their effect only through the Coulomb gap in the DOS, which again allows the use of the single-particle picture.

There have been several efforts [10–13] to incorporate the effect of Coulomb interactions on hopping conduction. Building on the work of Dersch *et al* [13], Lamba and Kumar [14] have given a detailed many-body treatment to describe the crossover from Mott's to the Coulomb gap regime. This crossover has also been well described by some empirical approaches [7, 15]. In order to consider other aspects of correlations, it is important to keep in mind the physical nature of the Coulomb gap. The Coulomb gap is basically the difference between the energy of an occupied site and a unoccupied site around the Fermi level. This happens due to correlations in the occupation of sites of the following kind. In the neighbourhood of an occupied site, the occupation of other electrons is less than average, which in turn reduces the Hartree energy associated with the occupied sites near the Fermi level. Similarly the neighbourhoods of unoccupied sites have larger than average occupation of electrons (negative holes), thereby raising their Hartree energy.

Thus when an electron jumps from an occupied site to an unoccupied site, it has to overcome an energy barrier of the order of the Coulomb gap. However, this assumes that the electron hops with the other electrons frozen at their sites. If one allows for the relaxation of correlation clouds around the two sites between which the electron hops, then the energy barrier also relaxes. The electron hopping which occurs concomitant with the charge relaxation was termed 'polaron' hopping by Mott [16]. He further argued that under these conditions the $T^{1/4}$ law should apply. Using an explicit model, Lamba and Kumar [14] argued that the relaxation of charge clouds responsible for the Coulomb gap is related to the conductivity itself. So at low temperatures when the relaxation is low due to small conductivity, the charge hopping is occurring in the frozen background of charge, and the Coulomb gap effects the conduction process. With increasing temperature, the Coulomb gap relaxes [14], leading to a crossover from the $T^{1/2}$ to the $T^{1/4}$ law.

The purpose of the present paper is to deal with one other aspect of correlated motion of carriers in the calculation of the dc and ac conductivities in the Coulomb gap regime. In particular, we wish to take into account backward correlations in hopping, which have been observed in numerical simulations of conductivities. In particular, in the simulations of Maass *et al* [17], it is seen that when disorder and Coulomb interactions are of comparable strength, the successive carrier hops are strongly correlated. A carrier is likely to jump back to the site from which it came with greater probability than in uncorrelated diffusion. This can be physically understood in the terms discussed above. At low temperatures in the $T^{1/2}$ regime, the relaxation of holes as the carrier jumps is slow, so there should be a tendency for the electron to go back to the hole it left behind in the previous jump, as the other unoccupied sites have energies higher by the order of the Coulomb gap.

See endnote 2

In this paper, we consider the effect of this correlation using a random walk model and relate the enhanced backward hopping rate to the Coulomb gap by a simple consideration. Correlated random walks [18, 19] are a class of random walks in which, unlike Markovian walks, the memory is not lost after each step. Correlated random walks have various physical applications. The two most important are conformation of polymers and tracer diffusion in metals. Most of the theoretical work has concentrated on correlated random walks on ordered lattices. Hilfer and Orbach [20] and Hilfer [21] have introduced disorder into this formalism by considering walks on a bond percolation model. We extend their treatment to a more general class of disordered systems. Our treatment is restricted to the memory of one last step only.

2. Correlated random walk

Consider the hopping of a single particle in a disordered medium. For a Markovian random walk, we start with writing a master equation for $P(i,t)$, which is the conditional probability to find a particle at site i at time t if it started from the origin at time $t = 0$. The effect of correlation is to retain the memory of the last step. So one defines the probability $P(i,j,t)$ to find a walker at site i at time t given that it arrived at i via a direct transition from site j. The probability density $P(i,t)$ is obtained by summation over all possible histories in $P(i,j,t)$ as

$$P(i,t) = \sum_j P(i,j,t), \tag{1}$$

where the sum is over all sites of the system excluding i. The initial condition that the walker is at the origin (o) at time $t = 0$ is $P(i,0) = \delta_{i,0}$. A transition rate W^{b}_{ij} is assigned to a jump from site j to site i if the previous jump was from site i to site j. A transition rate W_{ij} is assigned to a jump from site j to i if the particle had jumped to j from any site except i. The conditional probability $P(i,j,t)$ obeys the following master equation [19, 20]

See endnote 3

$$\dot{P}(i,j,t) = \sum_{k\neq i} W_{ij} P(j,k,t) + W^{\mathrm{b}}_{ij} P(j,i,t) - \left[\sum_{k\neq j} W_{ki} + W^{\mathrm{b}}_{ji}\right] P(i,j,t), \tag{2}$$

where $\dot{P}$ implies a time derivative of P. If we define $\delta W_{ij} = W^{\mathrm{b}}_{ij} - W_{ij}$, equation (2) can be rewritten as

$$\dot{P}(i,j,t) = W_{ij} P(j,t) + \delta W_{ij} P(j,i,t) - \left[\sum_k W_{ki} + \delta W_{ji}\right] P(i,j,t). \tag{3}$$

Summing over j in equation (3) we get an equation for $P(i,t)$

$$\dot{P}(i,t) = \sum_j W_{ij}[P(j,t) - P(i,t)] + \sum_j \delta W_{ji} A(j,i,t), \tag{4}$$

where we have defined

$$A(i,j,t) = P(j,i,t) - P(i,j,t). \tag{5}$$

Using equation (3) we can write an equation for $P(j,i,t)$ and thereby obtain an equation for $A(i,j,t)$. One can get a closed set of equations, by replacing $\sum_k W_{ki}$ by W_{t} which is its average over sites, $W_{\mathrm{t}} = \langle \sum_k W_{ki} \rangle$. This yields the equation

$$\dot{A}(i,j,t) = W_{ij}[P(i,t) - P(j,t)] - [W_{\mathrm{t}} + 2\delta W_{ij}] A(j,i,t). \tag{6}$$

The approximation made here seems physically reasonable for the two-site probabilities and avoids introduction of higher-order multi-site probabilities. Using initial conditions $P(i,0) = \delta_{i,0}$ and $A(j,i,0) = 0$ and taking Laplace transform of equations (4) and (6), we obtain

$$s\bar{P}(i,s) - P(i,0) = \sum_j [\bar{P}(j,s) - \bar{P}(i,s)] \left[W_{ij} - \frac{\delta W_{ij} W_{ij}}{s + W_{\mathrm{t}} + 2\delta W_{ij}} \right], \tag{7}$$

where $\bar{P}(i,s)$ denotes the Laplace transform of $P(i,t)$. We now make a further assumption by taking δW_{ij} to be site-independent, as we later relate it to the Coulomb gap. Replacing δW_{ij}

by its average value δW_b, we get an equation equivalent to the Markovian rate equation, but with a scaled frequency $\tilde{s} = sh(s)$ where

$$h(s) = \left[1 + \frac{\delta W_b}{s + W_t + \delta W_b}\right]. \tag{8}$$

Equation (7) is solved in terms of the Green function $G_{ij}(s)$

$$P(i,s) = h(s) \sum_j G_{ij}(\tilde{s}) P(j,0), \tag{9}$$

where in the matrix notation $\hat{G}$ obeys the equation

$$\hat{G}(\tilde{s} - \hat{W}) = I, \tag{10}$$

with

$$\hat{W}_{ij} = W_{ij} - \delta_{ij} \sum_k W_{ki}. \tag{11}$$

3. Model

We consider a system of randomly placed sites with a density n. Each site has an energy ϕ_i, where ϕ_i are randomly drawn from a rectangular distribution taken to be

$$P(\phi) = \frac{1}{2W} \qquad |\phi| \leqslant W, \tag{12}$$

$$P(\phi) = 0 \qquad |\phi| > W. \tag{13}$$

The DOS for the site energies has the form

$$g(\phi) = g_o = \frac{n}{2W} \qquad |\phi| \leqslant W. \tag{14}$$

In the presence of Coulomb interactions, the single site energies are modified by Hartree terms and take the form

$$\epsilon_i = \phi_i + \sum_j K_{ij} n_j, \tag{15}$$

where $K_{ij} = e^2/\kappa R_{ij}$ denotes the Coulomb interaction between electrons at the sites i and j, n_j are the site occupation numbers and κ is the dielectric constant of the medium. As shown by Efros and Shklovskii [3], the stability of the ground state requires that the DOS $g(\epsilon)$ for the Hartree energies has a gap around the Fermi level ϵ_F, and is given by

$$g(\epsilon) = \frac{C(\epsilon - \epsilon_F)^2 \kappa^3}{e^6} \qquad |\epsilon - \epsilon_F| \leqslant \Delta, \tag{16}$$

$$g(\epsilon) = g_o \qquad \Delta < |\epsilon - \epsilon_F| < W, \tag{17}$$

where C is a dimensionless constant of order unity and Δ is the width of the Coulomb gap, which is obtained by continuity to be See endnote 4

$$\Delta = \frac{e^3 g_o^{1/2}}{\kappa^{3/2}}. \tag{18}$$

Next we model δW_b. It is the difference between the probability of a jump between sites around the Fermi level and the probability of the backward hop. For temperatures $k_B T \ll \Delta$, we assume that most of the unoccupied sites available to the electron have energies higher by order Δ and the backward hop is a downward jump in energy of this order, so we take

$$\delta W_b = W_t \tanh\left(\frac{\Delta}{k_B T}\right). \tag{19}$$

For temperatures, $k_\mathrm{B}T \ll \Delta$, $\delta W_\mathrm{b} \approx W_\mathrm{t}$, which makes backward hops as probable as the jump probability to all other sites. As the temperature increases, this quantity decreases as expected. In this paper we have focused on the low-temperature regime.

The general transition rates in the Coulomb glass problem are the asymmetric rates given by, $T_{ij} = \nu_0 \exp[-(\frac{R_{ij}}{a} + \frac{|\epsilon_{ij}|+|\epsilon_i|+|\epsilon_j|}{k_\mathrm{B}T})]$ where ϵ_i, ϵ_j are Hartree energies of the sites i and j defined in equation (15), $\epsilon_{ij} = \epsilon_i - \epsilon_j - K_{ij}$ and ν_0 is taken to be the phonon Debye frequency. At low frequencies where $\sigma(\omega) = \sigma(0)$ (see the results section), the VRH and percolation pictures tell us that the critical hop is a long hop. As the frequency increases and dispersion in conductivity sets in, the hop distance decreases and is approximately proportional to $\ln(\omega)$. So at high frequencies the K_{ij} factor becomes important. We have neglected the K_{ij} factor in our calculation, so our results are not valid at high frequencies. In earlier calculations on dc conductivity, we have numerically checked [14] that the conductivity results do not change qualitatively if we replace the asymmetric transition rates by the symmetric transition rates, $W(R,\epsilon) = \nu_0 \exp[-(\frac{R}{a} + \frac{\epsilon}{k_\mathrm{B}T})]$. From this, for $k_\mathrm{B}T \ll \Delta$, we obtain

$$W_\mathrm{t} = 16\pi (k_\mathrm{B}T)^3 a^3 n \kappa^3 / e^6. \tag{20}$$

We work in the frequency units of ν_0.

4. Calculation of conductivity

For the calculation of conductivity in a disordered system, several effective medium approximations have been proposed [22]. All of them require a self-consistent calculation. In the present calculation, we adopt the procedure of Movaghar and Schirmacher [23]. In this approach one makes an effective medium approximation using the renormalized perturbation expansion. This procedure has given fairly good results for conductivity in disordered systems [24, 25], however, it is difficult to implement this method in the presence of energy disorder and asymmetric transition rates. So in this paper we use the symmetric transition rates mentioned above. The expression for frequency-dependent conductivity can be written as

$$\sigma(\omega) = \frac{(\mathrm{i}\omega)^2 e^2 h(\omega)}{6Vk_\mathrm{B}T} \sum_{ij} \langle F(\epsilon_i) R_{ij}^2 \overset{G}{\cancel{g}}_{ij}(\tilde{\omega})\rangle, \tag{21}$$

where the angular bracket denotes the configurational average, $\mathrm{i}\tilde{\omega} = \tilde{s}$ is the scaled frequency defined by equation (8), and $F(\epsilon_i) = f(\epsilon_i)(1 - f(\epsilon_i))$, where $f(\epsilon_i)$ is the Fermi function. Since our transition rates are symmetric, we take $F_i = F = q(1-q)$ for all i, where q is the number of electrons per site. Using a two-site approximation, an effective transition rate $g_{ij}(\omega)$ has been derived in [23], which obeys the equation

$$g_{ij} = \left[\frac{1}{W_{ij}} + \frac{1}{\mathrm{i}\tilde{\omega} + \sum_l g_{jl}}\right]^{-1}. \tag{22}$$

The self-consistent equation for the average value $\sigma_1(\omega)$ of $\sum_j g_{ij}$ can be recast into the form

$$\sigma_1(\tilde{\omega}) = (\sigma_1(\tilde{\omega}) + \mathrm{i}\tilde{\omega}) \int \frac{g(\epsilon) W(R,\epsilon)\, \mathrm{d}^3R\, \mathrm{d}\epsilon}{(\sigma_1(\tilde{\omega}) + \mathrm{i}\tilde{\omega}) W(R,\epsilon) + 1}, \tag{23}$$

and the conductivity is given as

$$\sigma(\omega) = \frac{Fe^2}{6Vk_\mathrm{B}Th(\omega)} \langle R^2(\tilde{\omega})\rangle \sigma_1(\tilde{\omega}), \tag{24}$$

with

$$\langle R^2(\tilde{\omega})\rangle = \left\langle \frac{R^2 W(R,\epsilon)}{\sigma_1(\tilde{\omega}) + \mathrm{i}\tilde{\omega} + W(R,\epsilon)} \right\rangle \Bigg/ \left\langle \frac{W(R,\epsilon)}{\sigma_1(\tilde{\omega}) + \mathrm{i}\tilde{\omega} + W(R,\epsilon)} \right\rangle. \tag{25}$$

Using transition rates defined in section 3 and the condition $\Delta \gg k_\mathrm{B}T$, equation (23) can be written in terms of dimensionless variables as

$$\sigma_\mathrm{l}(\tilde{\omega}) = (\sigma_\mathrm{l}(\tilde{\omega}) + \mathrm{i}\tilde{\omega})p \int\int \frac{\epsilon^2 r^2\,\mathrm{d}r\,\mathrm{d}\epsilon}{(\sigma_\mathrm{l}(\tilde{\omega}) + \mathrm{i}\tilde{\omega})W(r,\epsilon)^{-1} + 1} \tag{26}$$

where $p = 4\pi n a^3 (k_\mathrm{B}T)^3 \kappa^3/e^6 = W_\mathrm{t}/4$. Equations (24) and (26) differ from the earlier work in two respects. First, the frequency ω is replaced by the scaled frequency $\tilde{\omega}$, given by equation (8). Secondly, there is a prefactor of $h(\omega)$ in the expression of conductivity.

5. Results

We first look at the calculation of conductivity for the uncorrelated system. The previous analysis [24, 25] was done by neglecting the frequency dependence of mean square displacement, which is rather weak. Thus the frequency dependence of conductivity is largely determined by $\sigma_\mathrm{l}(\omega)$. Analysis of equation (28) shows that the significant dispersion in $\sigma_\mathrm{l}(\omega)$ sets in only when frequency becomes greater than $\sigma_\mathrm{l}(0)$. The equation for $\sigma_\mathrm{l}(0)$ is equivalent to the percolation criterion employed by Ambegaokar *et al* [26]. Solving equation (28) for $\omega = 0$ one gets

$$\sigma_\mathrm{l}(0) = \exp(-u) = \exp\left[-\left(\frac{180}{p}\right)^{1/6}\right] = \exp\left[-\left(\frac{T_{es}}{T}\right)^{\frac{1}{2}}\right]. \tag{27}$$

In the infinite frequency limit, $\sigma_\mathrm{l}(\omega)$ is proportional to the total transition rate W_t. In the intermediate frequency range the conductivity obeys a power law in frequency, $\sigma_\mathrm{l}(\omega) \propto \omega^s$. The slope is crudely given by $s = (u + \ln W_\mathrm{t})/u$. The slope increases as the temperature p decreases.

For the correlated walk, the conductivity becomes a function of a scaled frequency $\tilde{\omega}$ instead of ω. The behaviour of σ_l as a function of ω and $\tilde{\omega}$ is shown in figures 1 and 2 for two different temperatures. The curve for $\sigma_\mathrm{l}(\tilde{\omega})$ shifts to the left with respect to $\sigma_\mathrm{l}(\omega)$ on the frequency scale. The shift depends upon the frequency-dependent correlation factor $h(\omega)$. As seen from figures 1 and 2, the shift is apparent for the frequency range $\sigma_\mathrm{l}(0) < \omega < W_\mathrm{t}$. At high frequencies, $\omega \gg W_\mathrm{t}$, $h(\omega) \approx 1$ so the correlation effect is negligible. Since there is no dispersion in the low-frequency range $\omega < \sigma_\mathrm{l}(0)$, the curves again coincide. The crossover frequency W_t is temperature-dependent and does not scale with $\sigma_\mathrm{l}(0)$. Comparison of figures 1 and 2 shows that the crossover from correlated to uncorrelated hopping occurs at different frequencies for different temperatures.

The calculation of conductivity with correlated hopping requires computation of the factor $\langle R^2(\tilde{\omega})\rangle$. This leads to the reduction of the conductivity by a factor of $1/h(\omega)$. The results for conductivity for two values of p are shown in figures 3 and 4. At temperatures reported here, $h(0)$ is weakly dependent on temperature, so the change in dc conductivity is also weakly dependent on p, as seen in these figures. At higher frequencies $\omega > W_\mathrm{t}$, $h(\omega) \approx 1$, so no correlation effects are present and the curves coincide. Enhanced backward correlations increase the slope of conductivity by $\ln[h(0)]/u$. This is significant at high temperatures (small u). The increase in slope due to backward correlations decreases as temperature decreases (u increases), as seen in figures 3 and 4.

We next discuss the scaling of the ac conductivity, which has been seen in numerous studies [27, 28]. The experimental studies show that over a considerable range of temperatures scaling of the form

$$\sigma(\omega)/\sigma_\mathrm{dc} = \Psi(\omega/T\sigma_\mathrm{dc}), \tag{28}$$

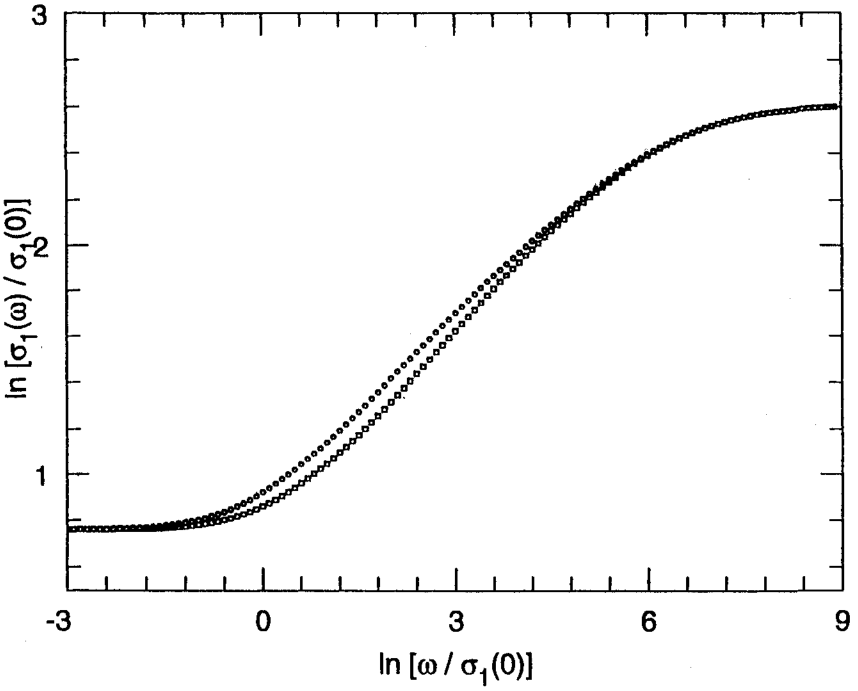

Figure 1. Plots of $\ln[\sigma_1(\omega)/\sigma_1(0)]$ with $\ln[\omega/\sigma_1(0)]$ for (○) correlated and (☐) uncorrelated hopping for $p = 0.0002$.

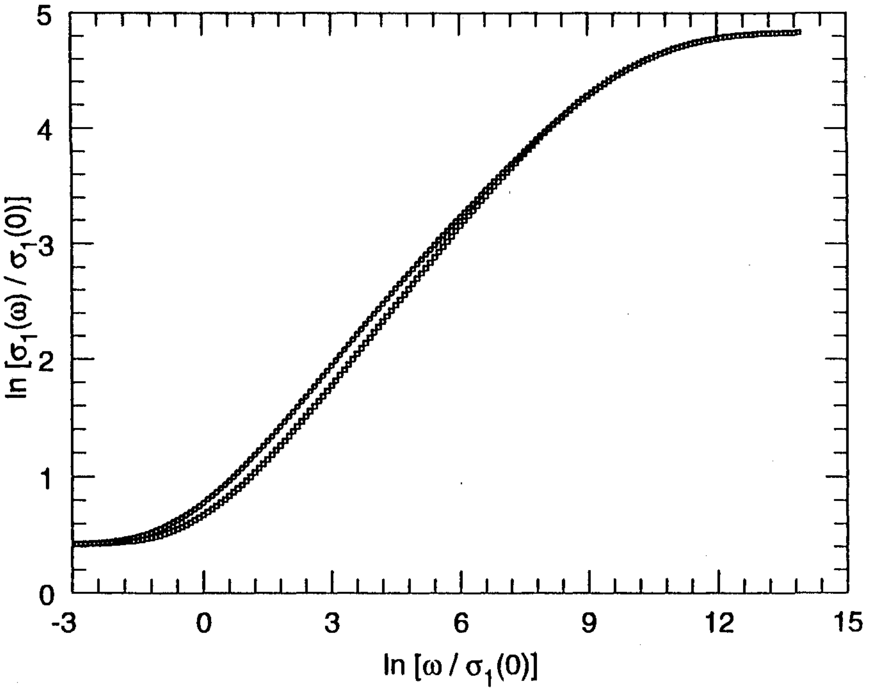

Figure 2. Plots of $\ln[\sigma_1(\omega)/\sigma_1(0)]$ with $\ln[\omega/\sigma_1(0)]$ for (○) correlated and (☐) uncorrelated hopping for $p = 0.000\,02$.

holds for a wide range of materials, including ionic conductors. In the present calculation we have already seen that the frequency dispersion of conductivity sets in only when

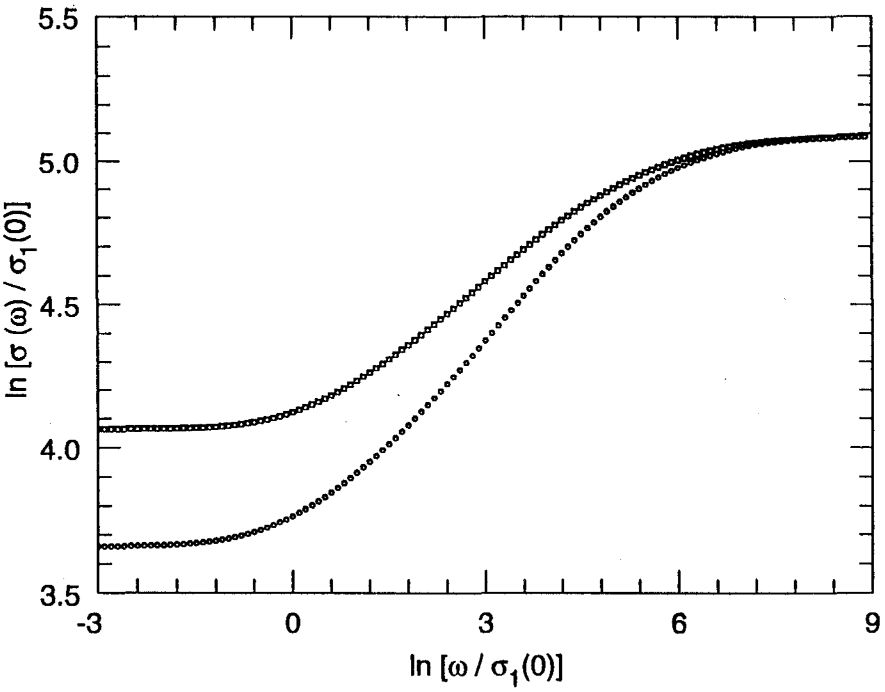

Figure 3. Logarithmic plots of scaled conductivity $\ln[\sigma(\omega)/\sigma_1(0)]$ against scaled frequency $\ln[\omega/\sigma_1(0)]$ for (○) correlated and (□) uncorrelated hopping for $p = 0.0002$.

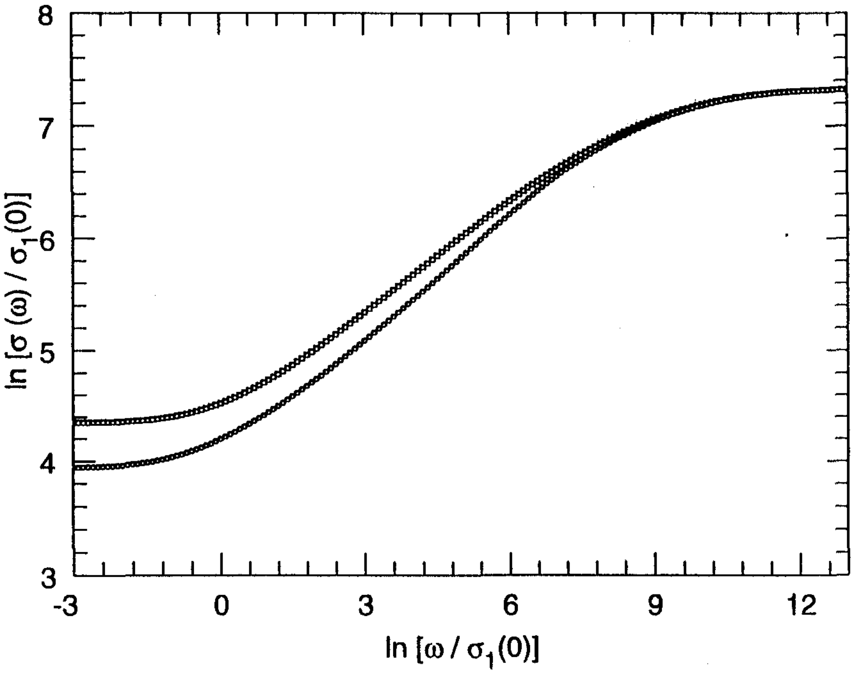

Figure 4. Logarithmic plots of scaled conductivity $\ln[\sigma(\omega)/\sigma_1(0)]$ against scaled frequency $\ln[\omega/\sigma_1(0)]$ for (○) correlated and (□) uncorrelated hopping for $p = 0.000\,02$.

$\omega > \sigma_1(0) \propto T\sigma_{dc}$. The reason for this is quite apparent in equation (23). However, the scaling of equation (28) requires that $\sigma(\omega)/\sigma_{dc}$ will not have any temperature dependence apart from that contained in $\sigma_1(0)$. This, as in earlier studies [27], is true when the temperatures are low and a Sommerfeld approximation can be made to evaluate the integrals in equations (23) and (25). Since $\tilde{\omega} = 0$ for $\omega = 0$ the equation for $\sigma_1(0)$ is the same for both correlated as well as Markovian hopping. However, for the correlated hopping the difference comes in the evaluation of the dc conductivity in which there is an additional factor of $h(o)$. Thus we can write

$$\sigma(\omega)/\sigma_{\mathrm{dc}} = \Psi\left(\frac{\tilde{\omega}}{\sigma_1(0)}\right) = \Psi\left(\frac{\omega h(\sigma_1(0))}{\sigma_{\mathrm{dc}} T h(0)}\right). \tag{29}$$

This shows that the scaling frequency changes due to correlated diffusion by the factor $h(\sigma_1(0)/h(0))$, which has been termed as the Haven ratio [28]. This factor has been introduced in an earlier work on ionic conduction on an empirical basis. Our work provides a quantitative estimate of the Haven ratio in the Coulomb gap regime.

6. Concluding remarks

In this paper, we have treated the effect of Coulomb interactions on hopping transport from two aspects. These are:

(a) depletion of single-particle DOS, which has a dominant effect on the temperature dependence of dc conductivity,
(b) the enhanced backward hopping, which is a consequence of an unrelaxed Coulomb hole (anti-hole) around an occupied (unoccupied) site.

The latter aspect has a considerable influence on the ac conductivity in the dispersive regime. We show that the scaling property of conductivity with frequency is still obeyed approximately. We also provide a quantitative estimate of Haven's ratio in the Coulomb gap regime of conduction.

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