Coulomb correlations in hopping through a thin layer

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A detailed microscopic investigation of the effect of Coulomb correlations on the inelastic contribution to tunneling via localized states through thin amorphous barriers is presented. The theoretical calculation together with experimental results show that Coulomb correlations play an important role and also imply that localized states whose single-particle energies lie well below the Fermi level participate in transport due to the Coulomb correlations.

I. INTRODUCTION

Theoretical and experimental interest in transport via localized states in tunnel junctions is a subject of increasing interest due to its importance in microelectronic devices.[1] At the same time, such structures constitute a model system for studying the role of electron-electron interactions and correlations in transport phenomena in general.

The presence of localized states in the barrier of a metal-insulator-metal tunnel junction leads to a wide variety of transport mechanisms. Experimental work on amorphous silicon (a-Si) tunnel junctions demonstrates a crossover from direct tunneling to resonant tunneling to inelastic hopping with increasing barrier thickness, temperature, and applied bias voltage.[2,3] At sufficiently low temperature and bias, direct tunneling from one electrode to the other dominates the conduction in thin barriers. As the barrier is made thicker, resonant tunneling[4] via individual localized states formed by defects in the barrier eventually dominates. This process is elastic and coherent. Increasing temperature and/or bias voltage quickly lead to a regime in which phonon-assisted hopping processes dominate the conduction.[5] These processes are inelastic and incoherent. The first hopping channel of this kind to contribute consists of chains of two localized states approximately aligned in the tunneling direction and dividing the barrier roughly into three equal segments. An electron tunnels elastically to the first site, hops to the second site accompanied by the absorption or emission of a phonon, and then tunnels elastically to the far electrode. Chains consisting of increasing numbers of localized states contribute to the conduction as the temperature, bias, or barrier thickness are increased further. In the thickest junctions, a crossover to Mott variable range hopping was observed.[2,3]

All of these transport processes involving localized states are expected to be highly correlated due to the presence of electron-electron interactions. Efros and Shklovskii predicted that the Coulomb interactions between electrons on different sites in a system exhibiting variable range hopping should lead to a gap in the density of states at sufficiently low temperature and to a crossover from the Mott $T^{-1/4}$ to a $T^{-1/2}$ law.[6] Such a crossover has been observed experimentally.[7] Little attention has been paid, however, to the role of the on-site Coulomb interaction in hopping transport. Glazman and Matveev predicted that the on-site Coulomb interaction U would cause resonant tunneling via localized states to become highly correlated.[8] They further predicted that, in tunnel junctions with a high density of localized states, these correlations should reveal themselves most clearly in the magnetic field dependence of the conductance. Two of us (D.E. and M.R.B) have recently demonstrated this effect experimentally, but were led to postulate correlations in the hopping transport channels incorporating two localized states in order to account fully for the data.[2]

In this paper we extend the calculation of Ref. 8 to cover the case of correlations in the hopping chains containing two localized states. We show that the magnetic field dependence of the zero bias conductance contribution of these chains can be written as $G_2(H,T) = \sigma_2 T^{4/3} f_2(\mu_B H/k_B T)$. We compute the conductance normalized to its zero field value, $f_2(x)$, exactly in the limits of zero magnetic field and very strong field, and approximately for arbitrary fields. Unlike the function $f_1(x)$, describing the correlations in the resonant tunneling channel, found in Ref. 8, $f_2(x)$ depends upon the distribution of localized states as a function of energy. Finally, we compare the theory with the experimental results and find quantitative agreement between the two. A brief discussion of the implications follows.

II. CLASSIFICATION OF THE CONDUCTION CHANNELS

Although the transport at low bias through the two-impurity conduction channels involves electrons within a narrow energy interval of order $k_B T$ around the Fermi level, the conductance depends in a crucial way upon the

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single-particle energies of the localized states that constitute each chain. The zeroth order Hamiltonian (with no tunneling term) describing the two-site chains can be written as

$$H = \sum_{i\sigma} \epsilon_{i\sigma} n_{i\sigma} + \sum_{\sigma\sigma'} U_{12} n_{1\sigma} n_{2\sigma'} + \sum_i U n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where U and U_{12} are the Coulomb interaction energies for two electrons to occupy the same site and different sites, respectively; $\epsilon_{i\sigma} = \epsilon_i + \sigma\mu_B H$ is the energy of an electron with spin $\sigma = \pm 1$ at site $i = 1, 2$, measured from the Fermi level. In the experiments on a-Si tunnel junctions,[2] the Coulomb energies U and U_{12} are estimated to be of the order of 100 meV and 10 meV, respectively, i.e., much greater than $\mu_B H$, $k_B T$, and eV. The last circumstance allows us to develop the following classification of hopping chains.

In the absence of interactions only the impurities with energy levels close to the chemical potential participate in transport. In the case of resonant tunneling through a single localized state with strong on-site interaction U there are two types of relevant impurities: the ones with $\epsilon \approx 0$ or $\epsilon \approx -U$. We will denote these impurities as types A and B, respectively. A type A impurity has an energy level close to the Fermi level (with accuracy $k_B T$) and, therefore, may accept either 0 or 1 electron, because the energy for the second electron is shifted by $U \gg k_B T$. For a type B impurity $\epsilon \approx -U$, i.e., it is always occupied by at least one electron. It may or may not accept a second electron, since its energy shifted by the Coulomb interaction is now in the vicinity of the Fermi level. The contributions to the conductance from these two types of impurities are identical due to the electron-hole symmetry.[8]

In the case of hopping through a chain of two impurities we need a more detailed classification to account for the intersite interaction U_{12}. Instead of a single type A we have to introduce three subtypes: A, A', and A'', corresponding to energy levels close to 0, $-U_{12}$, and $-2U_{12}$, respectively; type B must be split into B, B', and B'', corresponding to $\epsilon \approx -2U_{12} - U$, $-U_{12} - U$, and $-U$. There are eight types of two-impurity chains, listed in Table I using this notation, that can contribute to the conductance. For each of these eight types the processes of electron tunneling from the left lead to site 1, hopping from 1 to 2, and tunneling from site 2 to the right lead are allowed, i.e., do not require activation energy exceeding $k_B T$.

TABLE I. The eight types of chains: energies and allowed occupation numbers.

Type of chain	ϵ_1	ϵ_2	Number of electrons
AA	0	0	$0 \leftrightarrow 1$
$A'A'$	$-U_{12}$	$-U_{12}$	$1 \leftrightarrow 2$
$A'B''$	$-U_{12}$	$-U$	$1 \leftrightarrow 2$
$B''A'$	$-U$	$-U_{12}$	$1 \leftrightarrow 2$
$A''B'$	$-2U_{12}$	$-U - U_{12}$	$2 \leftrightarrow 3$
$B'A''$	$-U - U_{12}$	$-2U_{12}$	$2 \leftrightarrow 3$
$B'B'$	$-U - U_{12}$	$-U - U_{12}$	$2 \leftrightarrow 3$
BB	$-U - 2U_{12}$	$-U - 2U_{12}$	$3 \leftrightarrow 4$

To find the conductance, one has to take into account all the eight types of chains. However, some of the chains are equivalent due to electron-hole symmetry $n_{i\sigma} \to 1 - n_{i\sigma}$. Applied to the Hamiltonian (1), this transformation changes the energies of the localized states according to the rule

$$\epsilon_{i\sigma} \to -\epsilon_{i\sigma} - U - 2U_{12}. \quad (2)$$

One can easily see that under the transformation (2) the last four types of chains (see Table I) are reduced to the first four. Additionally, the $A'B''$ and $B''A'$ chains are also equivalent due to left-right symmetry. Thus in our calculations we need to consider only the AA, $A'A'$, and $A'B''$ chains.

III. CONDUCTANCE OF A SINGLE AA CHAIN

Here we consider the contribution of the first type of chain, AA. Analogous calculations for $A'A'$ and $A'B''$ chains are outlined in Appendixes A and B. For the AA configuration five different occupations of the two-impurity sites are possible: $(0,0)$, $(\uparrow,0)$, $(\downarrow,0)$, $(0,\uparrow)$, $(0,\downarrow)$. We denote the probability that the first localized site be occupied by a spin σ and the second site be empty by $P_{\sigma 0}$, the probability that the first site be empty and the second be occupied by a spin σ by $P_{0\sigma}$, and the probability that both of these sites are empty by P_{00}. These occupation probabilities are not independent, since

$$P_{00} + \sum_\sigma (P_{\sigma 0} + P_{0\sigma}) = 1. \quad (3)$$

Following Refs. 5 and 8, we solve the transport problem in the framework of the kinetic equation approach. Assuming without loss of generality $\epsilon_1 < \epsilon_2$, the four independent kinetic equations may be written as

$$\begin{aligned} \dot{P}_{\sigma 0} &= 2\Gamma_l [f_{l\sigma} P_{00} - (1 - f_{l\sigma}) P_{\sigma 0}] \\ &\quad -2\gamma [P_{\sigma 0} N - P_{0\sigma}(N+1)], \end{aligned} \quad (4)$$

$$\begin{aligned} \dot{P}_{0\sigma} &= 2\Gamma_r [f_{r\sigma} P_{00} - (1 - f_{r\sigma}) P_{0\sigma}] \\ &\quad +2\gamma [P_{\sigma 0} N - P_{0\sigma}(N+1)]. \end{aligned} \quad (5)$$

Here we have introduced the Bose function $N = [\exp\beta(\epsilon_2 - \epsilon_1) - 1]^{-1}$ for the absorbed phonons ($\beta \equiv 1/k_B T$), the fermion occupation numbers $f_{l\sigma}(\epsilon_1)$ and $f_{r\sigma}(\epsilon_2)$ in the two leads, the widths of the levels with respect to tunneling to the left and right electrodes, Γ_l and Γ_r, and a parameter γ that characterizes the phonon-assisted tunneling between the two sites,[5]

$$\Gamma_l = \pi \sum_k |T_k|^2 \delta(\epsilon_k - \epsilon_1), \quad (6)$$

$$\gamma = \pi \sum_q |T_q|^2 \delta(\Delta\epsilon - \omega_q), \quad (7)$$

$$\Gamma_r = \pi \sum_p |T_p|^2 \delta(\epsilon_p - \epsilon_2). \quad (8)$$

Here $\Delta\epsilon = |\epsilon_2 - \epsilon_1|$; ω_q is the frequency of the absorbed phonon; T_k and T_p are the matrix elements of transitions from state k in the left lead to the first impurity, and from the second impurity to state p in the right lead; and T_q is the matrix element of tunneling between the two impurity states accompanied by the absorption of phonon q (see Ref. 5).

The two terms in the right-hand side of Eq. (4) have a simple physical meaning: the occupation of site 1 can be changed by the processes of tunneling between the left lead and the first impurity, or by hopping between the two sites.[9] Correspondingly, the first term in the right-hand side of kinetic equation (4) represents the current $I_\sigma^{l\to 1}$ of electrons with spin σ from the left lead to site 1, whereas the second term gives the current $-I_\sigma^{1\to 2}$ from site 2 to site 1. A similar interpretation applies to Eq. (5).

In the stationary regime $\dot{P}_{\sigma 0} = \dot{P}_{0\sigma} = 0$. Therefore the three currents $I_\sigma^{l\to 1}$, $I_\sigma^{1\to 2}$, and $I_\sigma^{2\to r}$ are equal and may be written as

$$\begin{aligned} I_\sigma &= 2e\Gamma_l[f_{l\sigma}P_{00} - (1-f_{l\sigma})P_{\sigma 0}] \\ &= 2e\gamma[NP_{\sigma 0} - (N+1)P_{0\sigma}] \\ &= 2e\Gamma_r[(1-f_{r\sigma})P_{0\sigma} - f_{r\sigma}P_{00}]. \end{aligned} \tag{9}$$

To calculate the conductance of the chain in the linear regime $eV \ll k_BT$, we take the derivative of the current with respect to voltage, $G_\sigma = \partial I_\sigma/\partial V$. Then the partial conductance G_σ can also be written in three equivalent forms,

$$\begin{aligned} G_\sigma &= 2e\Gamma_l f_{l\sigma}P_{00}\left(\frac{1}{P_{00}}\frac{\partial P_{00}}{\partial V} - \frac{1}{P_{\sigma 0}}\frac{\partial P_{\sigma 0}}{\partial V} + \beta e\right) \\ &= 2e\gamma NP_{\sigma 0}\left(\frac{1}{P_{\sigma 0}}\frac{\partial P_{\sigma 0}}{\partial V} - \frac{1}{P_{0\sigma}}\frac{\partial P_{0\sigma}}{\partial V}\right) \\ &= 2e\Gamma_r f_{r\sigma}P_{00}\left(\frac{1}{P_{0\sigma}}\frac{\partial P_{0\sigma}}{\partial V} - \frac{1}{P_{00}}\frac{\partial P_{00}}{\partial V}\right). \end{aligned} \tag{10}$$

We reckon all the electron energies from the chemical potential of the right electrode, so that $f_{l\sigma}$ is a function of voltage while $f_{r\sigma}$ is constant. We also used the fact that in equilibrium, at $V = 0$, the current is zero, and, consequently,

$$\begin{aligned} f_{l\sigma}P_{00} &= (1-f_{l\sigma})P_{\sigma 0}, \\ NP_{\sigma 0} &= (N+1)P_{0\sigma}, \\ f_{r\sigma}P_{00} &= (1-f_{r\sigma})P_{0\sigma}. \end{aligned}$$

We do not know the derivatives of the occupation probabilities in Eq. (10). However, we can find the partial conductance G_σ,

$$G_\sigma = \frac{2\beta e^2}{(\Gamma_l f_{l\sigma}P_{00})^{-1} + (\gamma NP_{\sigma 0})^{-1} + (\Gamma_r f_{r\sigma}P_{00})^{-1}}. \tag{11}$$

To express the conductance explicitly in terms of the energies of the localized states, we use the following values of the equilibrium probabilities of occupations:

$$\begin{aligned} P_{00} &= Z^{-1}, \\ P_{\sigma 0} &= Z^{-1}\exp(-\beta\epsilon_{1\sigma}), \\ P_{0\sigma} &= Z^{-1}\exp(-\beta\epsilon_{2\sigma}), \end{aligned}$$

where the partition function Z is defined as

$$Z = 1 + \sum_\sigma \left[e^{-\beta\epsilon_{1\sigma}} + e^{-\beta\epsilon_{2\sigma}}\right]. \tag{12}$$

This gives the following result for the conductance of an AA chain:

$$G^{AA} \equiv \sum_\sigma G_\sigma = \sum_\sigma \frac{2\beta e^2}{Z}\left[\frac{(e^{\beta\epsilon_{1\sigma}}+1)}{\Gamma_l} + \left|\frac{e^{\beta\epsilon_{2\sigma}} - e^{\beta\epsilon_{1\sigma}}}{\gamma}\right| + \frac{(e^{\beta\epsilon_{2\sigma}}+1)}{\Gamma_r}\right]^{-1}. \tag{13}$$

The above calculation shows how to find the contribution to the total conductance of an AA chain. Similar calculations for the other types of chains are outlined in Appendixes A and B.

IV. AVERAGE CONDUCTANCE

Thus far we have calculated the conductance of a single two-impurity chain. In the experiments on a-Si junctions, however, many chains of each type contribute to the conductance, and the junctions are of sufficiently large area to be in the self-averaging regime.[2,3,8] In order to compare our calculation with the experimental results, we need to average over the positions and energies of the localized states. Note that the conductance of any chain strongly depends on the positions of localized sites as reflected in the parameters

$$\Gamma_l = E_\Gamma \exp(-2z_1/a), \tag{14}$$

$$\Gamma_r = E_\Gamma \exp(-2z_2/a), \tag{15}$$

$$\gamma = E_\gamma(\epsilon_1, \epsilon_2)\exp(-2r_{12}/a). \tag{16}$$

Here $z_{1,2}$ denote the distances from the localized sites to the nearest lead, r_{12} is the distance between the two sites, and a is the localization length. In the first approximation the preexponential factors E_X, which represent the energy scale of the corresponding transition rate, may be considered to be independent of the coordinates. The formulas for the partial conductances of the AA and $A'B''$ chains have the same general form

$$G_\sigma = \frac{2\beta e^2}{D}\left(\frac{A}{\Gamma_l} + \frac{B}{\gamma} + \frac{C}{\Gamma_r}\right)^{-1} \tag{17}$$

[see Eq. (13) and Appendix B]. The parameters A, B, C, and D depend on the energies of the localized states, but, to a good approximation, not on their coordinates. For $A'A'$ chains, this inverse resistance structure (17) is valid only in the limiting cases of low and high fields ($x = 0$ and $x = \infty$, see Appendix A). Let us find the maximum possible value of the conductance for fixed ϵ_1, ϵ_2. Obviously,

$$\begin{aligned} \frac{A}{\Gamma_l} + \frac{B}{\gamma} + \frac{C}{\Gamma_r} &\geq 3\left(\frac{A}{\Gamma_l}\frac{B}{\gamma}\frac{C}{\Gamma_r}\right)^{1/3} \\ &\geq 3\left(\frac{ABC}{E_\Gamma^2 E_\gamma}\right)^{1/3}\exp\left(\frac{2d}{3a}\right). \end{aligned} \tag{18}$$

Here d is the width of the barrier. Thus the maximum possible conductance of a single chain is

$$G_\sigma^{\max} = \frac{2\beta e^2}{3D}\left(\frac{E_\Gamma^2 E_\gamma}{ABC}\right)^{1/3} \exp\left(-\frac{2d}{3a}\right). \tag{19}$$

This maximum value is achieved if the impurities are in the optimal positions: they must be aligned along the tunneling direction (z axis), with the distances z_1, r_{12}, and z_2 chosen in such a way that

$$\frac{A}{\Gamma_l} = \frac{B}{\gamma} = \frac{C}{\Gamma_r}. \tag{20}$$

This optimal position corresponds to $z_1 \approx r_{12} \approx z_2 \approx d/3$. Due to the strong exponential dependence of conductance on the coordinates of the localized sites, only the chains close to the optimal configuration give a significant contribution to the conductance. Then one can write the integral over the positions of the sites in terms of their displacements from the optimal positions, and the conductance averaged over the positions and energies of impurities takes the form

$$\langle G\rangle = \frac{2\beta e^2}{3} g_1 g_2 J \exp\left(-\frac{2d}{3a}\right) \sum_\sigma \int \left(\frac{E_\Gamma^2 E_\gamma}{ABC}\right)^{1/3} \frac{d\epsilon_{1\sigma} d\epsilon_{2\sigma}}{D}, \tag{21}$$

$$J = \int \frac{d\zeta_1 d\zeta_2 d^2\rho}{\exp(2\zeta_1/a) + \exp[-2(\zeta_1+\zeta_2)/a]\exp(\rho^2/ar_{12}^0) + \exp(2\zeta_2/a)}. \tag{22}$$

Here ζ_i is the displacement of the ith impurity from its optimal position in the longitudinal (z) direction, ρ is the displacement in the transverse direction, and r_{12}^0 is the optimal value of r_{12}. We have also introduced the densities of states g_1 and g_2 appropriate for the single-particle energies of the first and second localized sites, respectively.

In the first approximation $r_{12}^0 = d/3$ and does not depend on $\epsilon_{i\sigma}$. This allows us to factorize the integral over the coordinates. Further, the dimensional estimate of (22) gives $J = \alpha a^3 d$, with α being a numerical factor, whose exact value is unimportant for our purposes.

In calculating the integral (21) we have assumed that the density of localized states is independent of energy on the scale of $\mu_B H$ around the appropriate values (Table I). In the experiment $\mu_B H$ is less than 500 μV, and this is a good approximation. However, we have so far left open the possibility that the density of localized states may vary over energies on the scale of U, which is estimated to be on the order of 100 meV in the experiments with a-Si barriers. In this case all the eight types of chains listed in Table I contribute to the tunneling current.

For the AA chain, comparing (13) with (17) we see that

$$\begin{aligned} A &= e^{\beta\epsilon_{1\sigma}} + 1, \\ B &= |e^{\beta\epsilon_{2\sigma}} - e^{\beta\epsilon_{1\sigma}}|, \\ C &= e^{\beta\epsilon_{2\sigma}} + 1, \\ D &= 1 + \sum_\sigma \left(e^{-\beta\epsilon_{1\sigma}} + e^{-\beta\epsilon_{2\sigma}}\right). \end{aligned}$$

The substitution of these formulas into Eq. (21) gives

$$\begin{aligned} \langle G^{AA}(H,T)\rangle &= \sigma_2 T^{4/3} g_A^2 J_1\left(\frac{\mu_B H}{k_B T}\right), \\ \sigma_2 &= \frac{4\alpha}{3} a^3 d e^2 (E_\Gamma^2 E_\gamma')^{1/3} \exp\left(-\frac{2d}{3a}\right), \end{aligned} \tag{23}$$

where g_A is the density of states at energy $\epsilon = 0$ corresponding to the A-type states and

$$J_1(x) = \frac{1}{2}\sum_\sigma \int \left(\frac{|x_2 - x_1|}{(e^{x_1}+1)\,|e^{x_2} - e^{x_1}|\,(e^{x_2}+1)}\right)^{1/3} \times \frac{dx_1 dx_2}{1 + (1+e^{-2\sigma x})(e^{-x_1} + e^{-x_2})}. \tag{24}$$

Here we have taken into account the fact that the preexponential factor in the phonon-mediated hopping rate γ is proportional to the energy of the phonon

$$E_\gamma = E_\gamma' |\epsilon_2 - \epsilon_1|,$$

which can easily be proven for acoustic phonons.[5]

An important property of result (23) for the average conductance due to AA chains is that the latter depends on magnetic field only through the ratio

$$x = \frac{\mu_B H}{k_B T}. \tag{25}$$

This is not surprising since the origin of the magnetoresistance is the spin polarization of electrons occupying the impurity states, and the characteristic scale for this polarization is $H \sim k_B T/\mu_B$. We therefore expect all other contributions to the average conductance to depend on magnetic field through the same variable x,

$$\langle G^{AA}(H,T)\rangle = \sigma_2 T^{4/3} g_A^2 J_1(x), \tag{26}$$

$$\langle G^{A'A'}(H,T)\rangle = \sigma_2 T^{4/3} g_{A'}^2 J_2(x), \tag{27}$$

$$\langle G^{A'B''}(H,T)\rangle = \sigma_2 T^{4/3} g_{A'} g_{B''} J_3(x), \tag{28}$$

$$\langle G^{A''B'}(H,T)\rangle = \sigma_2 T^{4/3} g_{A''} g_{B'} J_3(x), \tag{29}$$

$$\langle G^{B'B'}(H,T)\rangle = \sigma_2 T^{4/3} g_{B'}^2 J_2(x), \tag{30}$$

$$\langle G^{BB}(H,T)\rangle = \sigma_2 T^{4/3} g_B^2 J_1(x). \tag{31}$$

Above we proved the general form (26) [see Eq. (23)]; this also proves (31) due to the electron-hole symmetry. The other two relations, (27) and (28) [and therefore symmetry-related Eqs. (30) and (29)] are discussed in Appendixes A and B.

The universal dimensionless functions $J_1(x)$, $J_2(x)$, and $J_3(x)$ need to be calculated numerically. In terms

of these functions the magnetic field dependence of the total average conductance due to two-site inelastic chains can be found by summing the contributions from each type of chain,

$$\langle G_2(x)\rangle = \sigma_2 T^{4/3}\Big[(g_A^2+g_B^2)J_1(x)+(g_{A'}^2+g_{B'}^2)J_2(x) +2(g_{A'}g_{B''}+g_{A''}g_{B'})J_3(x)\Big]. \tag{32}$$

Below we concentrate on the total average conductance normalized to its value in zero field,

$$f_2(x) = \frac{\langle G_2(x)\rangle}{\langle G_2(0)\rangle}. \tag{33}$$

The function $f_2(x)$ may be compared with the experimental data for a-Si barriers (see next section). Apart from the universal functions $J_i(x)$, it contains information about the density of localized states at different energies, g_A, $g_{A'}$, ..., etc.

In the limit of high magnetic field, we can find f_2 exactly, because at $x=0$ and $x\to\infty$ the contributions of all types of chains reduce to the general form (17). The asymptotic values of the functions $J_i(x)$ are

$$J_1(0)=3.853,\quad J_1(\infty)=3.102, \tag{34}$$
$$J_2(0)=3.868,\quad J_2(\infty)=3.102, \tag{35}$$
$$J_3(0)=3.017,\quad J_3(\infty)=0, \tag{36}$$

so that

$$f_2(\infty) = \frac{3.10(g_A^2+g_B^2+g_{A'}^2+g_{B'}^2)}{3.85(g_A^2+g_B^2)+3.87(g_{A'}^2+g_{B'}^2)+6.03(g_{A'}g_{B''}+g_{A''}g_{B'})}, \tag{37}$$

where g_A is the density of type A states, etc.

V. DISCUSSION

If all of the localized sites contributing to transport were to be found in the range of energies encompassed by the A series of energies or the B series, but not both, then the calculation predicts $f_2(\infty)=0.80$. If, on the other hand, the density of localized states is taken to be the same at the six energies enumerated above, then $f_2(\infty)=0.45$, in excellent agreement with the experimental results (see Fig. 2 below). If we take the experimental value to be 0.45 ± 0.10, then we reach the interesting conclusion that the density of states at the six energies are all within a factor of 2 or 3 of one another, barring any pathological dependence of the density of localized states on energy.

For arbitrary fields the integrals $J_1(x)$ and $J_3(x)$ were calculated numerically and are shown in Fig. 1. The exact numerical evaluation of $J_2(x)$ is quite cumbersome for arbitrary x (see Appendix A). However, $J_2(0)$ is within 0.5% of $J_1(0)$ and $J_1(\infty)=J_2(\infty)$ by particle-hole symmetry. Thus we feel it is justified in this context by the requirement of monotonicity and near coincidence at the end points to take $J_1(x)\approx J_2(x)$ for arbitrary x for the purpose of comparing theory and experiment.

Note that $f_2(x)$ depends upon the relative density of states at the various single-particle energies enumerated in Table I. In contrast, the function $f_1(x)$ derived in Ref. 8 for the magnetic field dependence of the resonant contribution to the conductance is independent of the ratio $g_A/g_{B''}$ (these are the two approximate single-particle energies that yield a contribution to resonant tunneling since there is no U_{12} term in this case). $J_1(x)$, $J_2(x)$, and $J_3(x)$ all decrease monotonically with x, so the predicted magnetoresistance is always positive.

The magnetoresistance of the two-site hopping chains arises physically from two distinct mechanisms. For simplicity consider a single AA chain. Each localized site has associated with it two spin-degenerate localized states, so there are two separate channels associated with the chain: one for spin up electrons and one for spin down electrons. These two channels are highly correlated because the on-site and the intersite Coulomb interactions permit at most one electron to be anywhere on the chain. The application of a strong magnetic field ($x\gg1$) splits the spin degeneracy. When the distribution of localized states is dense, the net effect is on average to replace every pair of correlated channels with a single, uncorrelated channel capable of transporting spin down electrons only.[2] Intermediate fields have this effect only partially, of course. Similar reasoning applies to the $A'A'$, $B'B'$, and BB chains. The dashed curve marked A/B in Fig.

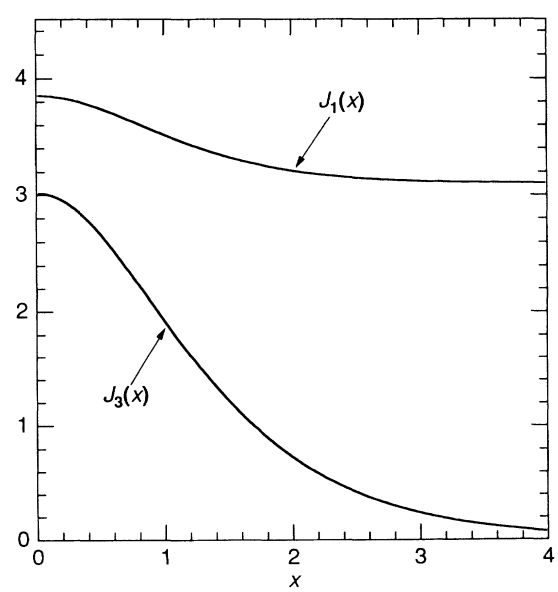

FIG. 1. Numerical calculation of the functions $J_1(x)$ and $J_3(x)$.

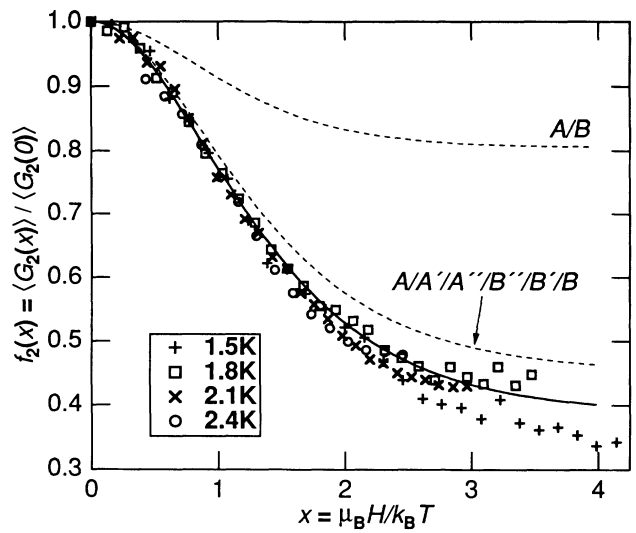

FIG. 2. Theoretical prediction for $f_2(x)$ when only A or B states are present (dashed curve A/B), and when the states at all six energies are present in equal proportions (dashed curve $A/A'/A''/B''/B'/B$). The solid line is the prediction for a particular choice of the distribution of localized states (see text). The markers are experimental data from Ref. 2.

2 shows the theoretical prediction for $f_2(x)$ if the localized states are all type A or all type B. The proximity of $f_2(x)$ to 1 for $x \gg 1$ for these two cases indicates the strong degree of correlation present in zero field, since two correlated channels (zero field) do not conduct much more than one uncorrelated channel (strong field).

A different mechanism is responsible for the suppression of the conductance of the $A'B''$, $A''B'$, $B'A''$, and $B''A'$ chains (hereafter called AB chains) in a strong magnetic field. The A series of states and the B series differ fundamentally in that in a strong field the A series transport only spin down electrons while the B series transport only spin up electrons.[10] Thus, a strong field completely breaks the AB chains and leads to a more drastic suppression of the conductance if AB chains are present (in zero field). This is reflected by the limit $J_3(\infty) = 0$. The dashed curve marked $A/A'/A''/B''/B'/B$ in Fig. 2 shows the prediction if the density of localized states is the same for all six relevant energies. The various symbols are experimental data for four different temperatures from a Mo/a-Si/Mo tunnel junction with $d = 120$ Å.[2] The data were obtained by subtracting off the resonant tunneling contribution to the conductance; this procedure amplifies the noise and the small systematic errors in the data since the resonant conductance ranges from 86% of the total conductance at 1.5 K down to 74% at 2.4 K. The solid curve shows the prediction of the theory if the ratio of the density of states g_A:$g_{A'}$:$g_{A''}$:$g_{B''}$:$g_{B'}$:g_B is taken to be 1:1.2:1.4:1.4:1.2:1, corresponding to a slight bump in the density of localized states below the Fermi level. We do not feel that the data warrant such a close comparison with the theory given the scatter in the data and the approximations in the theory. We show this curve simply to indicate that the data are consistent with the theory when the density of states at each of the six relevant single-particle energies is roughly the same within a factor of about 2.

Thus, we reach the interesting conclusion when we combine the theory with the experimental data that hopping conduction via localized states in disordered materials is in fact highly correlated by the presence of a strong on-site Coulomb interaction with additional correlations present due to intersite Coulomb interactions. Localized states whose single-particle energies lie far below the Fermi level participate in hopping transport.[11] Finally, we find that the single-particle density of localized states in unhydrogenated amorphous silicon is roughly constant from $\epsilon = 0$ down to at least $\epsilon = -U$. We point out that the theoretical methods of this paper can be combined with transport measurements in other disordered insulators to form a crude spectroscopy of the distribution of localized states.

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APPENDIX A: CONDUCTANCE OF AN $A'A'$ CHAIN

We consider the second type of chain where $\epsilon_1 \approx \epsilon_2 \approx -U_{12}$. Now we have eight possible states, $(\sigma, 0)$, $(0, \sigma)$, (σ, σ), and $(\sigma, -\sigma)$, where $\sigma = \uparrow$ for spin up and $\downarrow$ for spin down. The (0,0) state is very high in energy and consequently cannot be occupied. The associated probabilities are given by $P_{\sigma 0}$, $P_{0\sigma}$, $P_{\sigma\sigma}$, and $P_{\sigma-\sigma}$, respectively. We have four independent master equations,

$$\dot{P}_{\sigma 0} = 2\Gamma_r \sum_{\sigma'} [P_{\sigma\sigma'}(1 - f_{r\sigma'}) - P_{\sigma 0} f_{r\sigma'}] + 2\gamma [P_{0\sigma}(N+1) - N P_{\sigma 0}] , \quad \text{(A1)}$$

$$\dot{P}_{0\sigma} = 2\Gamma_l \sum_{\sigma'} [P_{\sigma'\sigma}(1 - f_{l\sigma'}) - P_{0\sigma} f_{l\sigma'}] + 2\gamma [P_{\sigma 0} N - (N+1) P_{0\sigma}] , \quad \text{(A2)}$$

$$\dot{P}_{\sigma\sigma} = 2\Gamma_l [P_{0\sigma} f_{l\sigma} - P_{\sigma\sigma}(1 - f_{l\sigma})] + 2\Gamma_r [P_{\sigma 0} f_{r\sigma} - P_{\sigma\sigma}(1 - f_{r\sigma})] , \quad \text{(A3)}$$

$$\dot{P}_{\sigma-\sigma} = 2\Gamma_l [P_{0-\sigma} f_{l\sigma} - P_{\sigma-\sigma}(1 - f_{l\sigma})] + 2\Gamma_r [P_{\sigma 0} f_{r-\sigma} - P_{\sigma-\sigma}(1 - f_{r-\sigma})] . \quad \text{(A4)}$$

Taking the derivative with respect to voltage in the limit $V \to 0$, we obtain a system of equations for the logarithmic derivatives $W_X = P'_X / P_X$. Solving these equations and substituting in the expression for the conductance

$$G = 2e\gamma N \sum_{\sigma} P_{\sigma 0} (W_{\sigma 0} - W_{0\sigma}) ,$$

we obtain

$$G(x) = \beta e^2 \sum_\sigma \left\{ \frac{e^{-\sigma x}}{a_\sigma^{-1} + R_{0\sigma}^{-1}} + \frac{R_{0\sigma}}{a_\sigma + R_{0\sigma}} \sum_{\sigma'} \frac{R_{0\sigma'}}{a_{\sigma'} + R_{0\sigma'}} \times \left[\sum_{\sigma''} e^{\sigma'' x} \left(\frac{1}{a_{-\sigma''} + R_{0\sigma''}} + a_{\sigma''}^{-1} \right) \right]^{-1} \right\}, \quad \text{(A5)}$$

where

$$a_\sigma^{-1} = R_{l\sigma}^{-1} + R_{r\sigma}^{-1},$$
$$R_{l\sigma} = \frac{2\Gamma_l}{Z} e^{-\beta\epsilon_2} f_l(\epsilon_{1\sigma} + U_{12}),$$
$$R_{r\sigma} = \frac{2\Gamma_r}{Z} e^{-\beta\epsilon_1} f_r(\epsilon_{2\sigma} + U_{12}),$$
$$R_{0\sigma} = \frac{2\gamma}{Z} e^{-\beta\epsilon_{1\sigma}} N(\Delta\epsilon),$$
$$Z = e^{-\beta(\epsilon_1+\epsilon_2+U_{12})} \times \sum_\sigma \left[1 + e^{-2\sigma x} + e^{\beta(\epsilon_{1\sigma}+U_{12})} + e^{\beta(\epsilon_{2\sigma}+U_{12})} \right],$$

and f and N are Fermi and Bose functions, respectively. The presence of $R_{0\sigma}/(R_{0\sigma} + a_\sigma)$ in the second term of (A5) spoils the usual inverse resistance structure of the conductance (17). However, the general form (27) of the average conductance due to $A'A'$ chains still holds. To prove this, one only has to show that the conductance $\langle G^{A'A'} \rangle$ scales as $T^{4/3}$ if temperature and magnetic field are changed proportionally, so that their ratio x is constant. This can be done in the same way as in Ref. 5. At fixed x one can easily see from Eq. (A5) that the optimal position of the two impurities in a chain corresponds to

$$\Gamma_l \sim \gamma \sim \Gamma_r \sim \Gamma \equiv (E_\Gamma^2 E_\gamma)^{1/3} \exp\left(-\frac{2d}{3a}\right).$$

To find the average conductance, the maximum value $G \sim \beta\Gamma$ should be multiplied by the "phase volume" of the nearly optimal chains. The latter is proportional to T^2, because only the sites with energies $\epsilon_i \sim T$ contribute to the conductance. Taking into account that $E_\gamma \sim \Delta\epsilon \sim T$, we find $\langle G^{A'A'} \rangle \sim T^{4/3}$, with the proportionality coefficient depending on x, in complete agreement with Eq. (27).

The limit $x = 0$ restores the structure (17) with the following parameters:

$$A = e^{-\beta(\epsilon_1+U)} + 1,$$
$$B = 2\left[e^{-\beta(\epsilon_1+U)} - e^{-\beta(\epsilon_2+U)} \right],$$
$$C = e^{-\beta(\epsilon_1+U)} + 1,$$
$$D = 2 + e^{\beta(\epsilon_1+U)} + 2e^{\beta(\epsilon_2+U)}.$$

Thus we arrive at the exact result $J_2(0) = 3.87$, very close to $J_1(0) = 3.85$. In addition we have $J_1(\infty) = J_2(\infty)$ as required by particle-hole symmetry.

APPENDIX B: CONDUCTANCE OF AN $A'B''$ CHAIN

We consider the third type of chain, $\epsilon_1 \simeq -U_{12}$ and $\epsilon_2 \simeq -U$. The number of unknowns amounts to seven, $P_{0\sigma}$, $P_{\sigma\sigma}$, $P_{-\sigma\sigma}$, and P_{02}, following the same notation as before. In the presence of a magnetic field there are seven master equations which can be written as

$$\dot{P}_{0\sigma} = 2\Gamma_r[(1 - f_{r\sigma})P_{02} - f_{r-\sigma}P_{0\sigma}] + 2\Gamma_l[(1 - f_{l\sigma})P_{\sigma\sigma} - f_{l\sigma}P_{0\sigma}] + 2\Gamma_l[(1 - f_{l-\sigma})P_{-\sigma\sigma} - f_{l-\sigma}P_{0\sigma}], \quad \text{(B1)}$$
$$\dot{P}_{\sigma\sigma} = 2\Gamma_l[f_{l\sigma}P_{0\sigma} - (1 - f_{l\sigma})P_{\sigma\sigma}], \quad \text{(B2)}$$
$$\dot{P}_{-\sigma\sigma} = 2\Gamma_l[f_{l-\sigma}P_{0\sigma} - (1 - f_{l-\sigma})P_{-\sigma\sigma}] + 2\gamma[(N+1)P_{02} - NP_{-\sigma\sigma}], \quad \text{(B3)}$$
$$\dot{P}_{02} = 2\gamma \sum_\sigma [NP_{-\sigma\sigma} - (N+1)P_{02}] + 2\Gamma_r \sum_\sigma [f_{r-\sigma}P_{0\sigma} - (1 - f_{r\sigma})P_{02}]. \quad \text{(B4)}$$

The above equations can be solved using the same technique as in Sec. III. As a result we find the same general form (17) of the partial conductance G_σ with the following parameters:

$$A = e^{-\beta(\epsilon_{1\sigma}+U_{12})} + 1,$$
$$B = \left| e^{-\beta(\epsilon_{2\sigma}+U)} - e^{-\beta(\epsilon_{1\sigma}+U_{12})} \right|,$$
$$C = e^{-\beta(\epsilon_{2\sigma}+U)} + 1,$$
$$D = e^{-\beta(\epsilon_{2\sigma}+U)} + (1 + e^{2\sigma x}) \times [1 + e^{-\beta(\epsilon_{1\sigma}+U_{12})} + e^{-\beta(\epsilon_{1-\sigma}+U_{12})}].$$

Using these results back in (21) and comparing with Eq. (28) we obtain

$$J_3(x) = \frac{1}{2} \sum_\sigma \int \left(\frac{|x_2 - x_1|}{(e^{x_1} + 1) \mid e^{x_2} - e^{x_1} \mid (e^{x_2} + 1)} \right)^{1/3} \times \frac{dx_1 dx_2}{e^{-x_2} + (1 + e^{-2\sigma x})[1 + e^{-x_1}(1 + e^{2\sigma x})]}. \quad \text{(B5)}$$

The result of a numerical calculation of integral (B5) is plotted in Fig. 1.

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[9] We neglect tunneling from site 1 to the right electrode in comparison with hopping to the second site, because the tunneling amplitude decays exponentially with the distance.

[10] The reason for this is simple. Consider a single type A site with $x \gg 1$. If the spin up state is within k_BT of the Fermi level, then the spin down state is approximately $2\mu_B H$ below the Fermi level and will always be occupied, thus preventing occupation of the spin up state due to the on-site Coulomb correlation. If, on the other hand, the spin down state is within k_BT of the Fermi level, then the spin up state will lie well above the Fermi level and will always be empty. Thus, type A sites transport only spin down electrons. Similar reasoning applies to type B sites under particle-hole symmetry.

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