

Universal Crossover between Efros-Shklovskii and Mott Variable-Range-Hopping Regimes

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A universal scaling function, describing the crossover between the Mott and the Efros-Shklovskii hopping regimes, is derived using the percolation picture of transport in strongly localized systems. This function agrees very well with experimental data. Quantitative comparison with experiment allows for the possible determination of the role played by quasiparticles in transport. [S0031-9007(96)01894-7]

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Electronic interactions are known to play an important role in the strongly localized regime. More than two decades ago, Pollak [1], and Efros and Shklovskii [2] pointed out that the long-range nature of the interactions leads to a dip in the single-particle density of states, $\rho(\epsilon)$, at the Fermi energy. Using a constraint on the single-particle excitations, Efros and Shklovskii [2] argued that this soft gap is of the form $\rho(\epsilon) \sim \epsilon^{d-1}$, where ϵ is the energy measured from the Fermi energy and d the space dimension. The gap in the density of states was indeed observed by tunneling [3,4] and photoemission [5] measurements [6]. Assuming that single-electron hopping dominates the transport, Efros and Shklovskii demonstrated that the change in the form of the density of states modifies the Mott variable-range-hopping law, $\ln R \sim 1/T^x$, from $x = d + 1$ to $x = 1/2$. While later it was argued [7] that the optimal transport is by partially formed quasiparticles (where the degree of formation depends on temperature), the modified exponent has been observed in many experiments [8].

The Efros-Shklovskii hopping law is expected to be relevant at low temperatures (compared to the size of the gap) [2,9], and in the last few years there have been a multitude of experiments aimed at exploring the crossover between the Mott to the Efros-Shklovskii hopping regimes as a function of temperature [10]. A significant step was taken more recently, when Aharony and co-workers [11,12] argued that this crossover is described by a universal scaling function, and obtained this scaling function phenomenologically using energy additivity. It is the aim of this paper to demonstrate that, with the assumption of quasiparticle transport, the “microscopic” percolation picture [13], describing the transport in the strongly localized regime, indeed leads to such a universal crossover function. The derived crossover function agrees excellently with existing experimental data [4], and allows quantitative comparison between features in the density of the states and the transport data, taken on the same physical system.

The starting point of this calculation is the mapping of the resistance problem into a percolation criterion [13] of an equivalent random resistor network [14] consisting of randomly placed sites. Without interactions, the activation energy from site i to site j is given by $\epsilon_j - \epsilon_i$,

where ϵ_i are the energy of site i , which in this case is distributed uniformly. The resistance between each pair of sites is given by [14] $R_{ij} = \exp\{(|\epsilon_i| + |\epsilon_j| + |\epsilon_i - \epsilon_j|)/2T + 2r_{ij}/\xi\}$, where all resistances are measured in some unit of resistance. Since the resistances vary exponentially, the overall resistance will be determined by the weakest link, which is the largest resistance, R , such that the cluster formed by all resistances (bonds), satisfying $R > R_{ij}$, percolates. Clearly, all states participating in the percolating network (defined as occupied sites) must satisfy $R > \exp(|\epsilon_i|/2T)$. (Note the distinction between occupied sites, namely, sites that participate in the transport, and occupied impurities.) Following [13], the percolation criterion employed here is the following [15]—given such an occupied site, the number of bonds attached to it has to be higher than a critical threshold, Z_c , for the system to percolate,

$$\begin{aligned} Z_c &= \frac{1}{2 \int_{-T \ln R}^{T \ln R} \rho_0 d\epsilon} \int_{-2T \ln R}^{2T \ln R} \rho_0 d\epsilon_1 \int \rho_0 d\epsilon_2 \\ &\times \int d^d r_{12} \Theta(R - e^{(|\epsilon_1| + |\epsilon_2| + |\epsilon_1 - \epsilon_2|)/2T + 2r_{12}/\xi}) \\ &= 3T \frac{\xi^d \rho_0 \pi^{d/2} (\ln R)^{d+1}}{2^{d+1} \Gamma(d/2) d(d+1)(d+2)}, \\ &\equiv Z_c T (\ln R)^{d+1} / T_0, \end{aligned} \quad (1)$$

leading directly to the Mott hopping law, $\ln R = (T_0/T)^{1/(d+1)}$ [where the last equality in (1) defines T_0]. In the above, ρ_0 is the uniform density of states and ξ the localization length.

In the presence of interactions, the activation energy from site i to site j is given by [2] $\epsilon_j - \epsilon_i - e^2/r_{ij}$, where r_{ij} is the distance between the sites (where all other particles are assumed to remain fixed). Since an activation from the ground state has to be positive, this leads to a constraint on the distribution of ϵ_i and to the soft gap in the Fermi surface [2]. In fact, given that constraint, Efros [16,17] has been able to derive a self-consistent equation for the density of states, $\rho(\epsilon)$,

$$\rho(\epsilon)/\rho_0 = \exp\left\{\alpha \int_0^\infty d\epsilon_1 \frac{\rho(\epsilon_1)}{(\epsilon + \epsilon_1)^d}\right\}. \quad (2)$$

where α is some numerical constant, and an infinite band was assumed. The resulting density of states is clearly of the form $\rho_0 f(\epsilon/\epsilon_0)$, with $\epsilon_0 \sim (e^{2d}\rho_0)^{1/(d-1)}$, and it can be very well approximated in three dimensions by $f(x) = x^2/(1+x^2)$, with $\epsilon_0 \approx 0.46e^3\sqrt{\rho_0}$.

Knotek and Pollak [18] and Mott [19] have pointed out that the resistance is not determined by the single-electron density of states, but should involve many-electron excitations. Efros [16] indeed demonstrated that taking into account multiparticle excitations (i.e., not assuming that all other particles remain fixed, when the electron is activated from site i to site j) leads to an even stronger (exponential) gap in the density of states [16,20]. He went on to suggest that the relevant excitations for the resistance are polarons and to show that the long-range interactions between the polarons lead to a density of states which satisfies (2). Consequently, the resistance should be of the Efros-Shklovskii type, $\ln R = (T_{ES}/T)^{1/2}$. These arguments, however, were later challenged [21,22] on symmetry grounds.

While, unlike the noninteracting case, no exact mapping of the transport problem into a percolation picture exists, the effects of electron-electron interactions can

be taken into account in this picture in a mean-field-like manner. Assuming transport by (possibly partially formed) quasiparticles, with long-range Coulombic interactions [23], and hopping length larger than the typical quasiparticle size, the percolation condition [Eq. (1) is now modified in two ways. The probability of finding two sites, of energies ϵ_i and ϵ_j and distance r_{ij} apart is proportional to $\rho(\epsilon_1)\rho(\epsilon_2)\Theta(\epsilon_2 - \epsilon_1 - e^2/r_{12})$, where $\rho(\epsilon)$ satisfies (2), and the activation energy from site i to site j is given by $\epsilon_j - \epsilon_i - e^2/r_{ij}$. The resulting percolation condition can now be written in the form

$$Z_c = \frac{1}{\int_{-T \ln R}^0 \rho(\epsilon) d\epsilon} \int_{-2T \ln R}^0 \rho(\epsilon_1) d\epsilon_1 \times \int_0^{2T \ln R} \rho(\epsilon_2) d\epsilon_2 \int d^d r_{12} \Theta(\epsilon_2 - \epsilon_1 - \epsilon^2/r_{12}) \times \Theta(R - e^{(\epsilon_2 - \epsilon_1 - \epsilon^2/r_{12})/T + 2r_{12}/\xi}). \quad (3)$$

Using the one-parameter scaling form of $\rho(\epsilon)$, and defining the dimensionless parameters x and y by $1/T = (e^2/\xi)x/\epsilon_0^2$ and $\ln R = (e^2/\xi)y/\epsilon_0$, this equation can be recast in the form

$$1 = \int_{-(y+s_1)/2x}^0 f(\epsilon_1) d\epsilon_1 \int_{\max\{\epsilon_1+(y+s_1)/2x, 0\}}^{\epsilon_1+(y+s_1)/2x} f(\epsilon_2) d\epsilon_2 \left\{ (s_2 + \sqrt{s_2^2 + 8x})^{d/4} - 1/(\epsilon_2 - \epsilon_1)^d \right\} / \int_{-(s_1+y)/2x}^0 f(\epsilon_1) d\epsilon_1, \quad (4)$$

with $s_1 = \sqrt{y^2 - 16x}$, and $s_2 = y - (\epsilon_2 - \epsilon_1)x$. Equation (4), which is an implicit equation for y in terms of x , or $\ln R$ in terms of T , indeed demonstrates that the resistance can be written in a scaling form

$$\ln R = AF(T/T_x), \quad (5)$$

in agreement with Aharony *et al.* [11], with $A \equiv (T_0/\epsilon_0)^{1/d}$, and $T_x \equiv (\epsilon_0^{d+1}/T_0)^{1/d}$. In addition to relating the nonuniversal amplitudes T_x and A to ϵ_0 , namely, to properties of the density of states which can be independently measured, Eq. (4) gives a prescription to calculating the full scaling function.

We have calculated the crossover function in three dimensions using Eq. (4) and a density of states of the quasiparticles of the form $\rho(\epsilon) = \rho_0 \epsilon^2/(\epsilon^2 + \epsilon_0^2)$. In Fig. 1 we compare the derivative of the scaling function to the data published in Ref. [4]. In comparison we also plot the phenomenological function derived by Aharony *et al.* [11]. Two points are noteworthy—the experimental data exhibits a rather fast crossover from the Mott regime ($\ln R \sim 1/T^{1/4}$) to the Efros-Shklovskii regime ($\ln R \sim 1/T^{1/2}$). The presently derived scaling function shows an excellent agreement with the data. The phenomenological scaling function, and also the scaling function derived from the procedure suggested by Lien [12], show a rather smooth crossover, which has a poorer agreement with the data (see inset). Moreover, as one

crosses over to the Efros-Shklovskii regime, the scaling function [4] predicts that, instead of a monotonic increase in the exponent from 1/4 to 1/2, there is an overshoot in the slope, a feature which is clearly seen in the experimental data.

Two fitting parameters were used in the fit— T_0 and ϵ_0 [or, alternatively, T_0 and $T_{ES} \approx 3.546(\epsilon_0^2 T_0)^{1/3}$]. The value of T_0 was found to be 1220 K, close to the value of 1500 K deduced in the experimental paper from the high temperature data. More interestingly, the best fitting value of ϵ_0 was 0.03 meV, an order of magnitude smaller than what one would deduce from the single-electron density of states, measured *on the same sample*, by tunneling spectroscopy. This verifies the fact that it is not the single-electron density of states that determines the resistivity, but rather the density of states of the dressed particles, which has a much smaller gap. Similar narrowing of the Coulomb gap has been observed in experiments [24] and numerical simulations [7,25], which also take into account multielectron hopping. More detailed comparison between the present calculation and future experiments should yield more information on the nature of the elementary excitations participating in the transport.

In conclusion, we have used the percolation picture to derive the crossover function from the Mott to the Efros-Shklovskii hopping regime. This function shows an

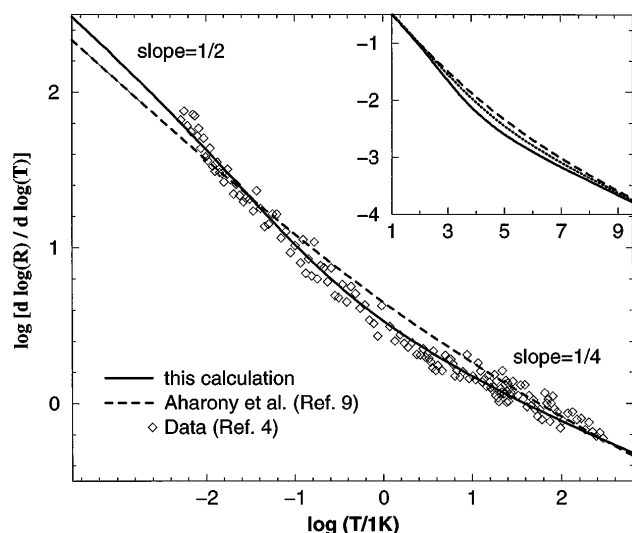


FIG. 1. Comparison of the experimental data (diamonds) to the derivative of the scaling function derived in this work (continuous line), and that of Ref. [11] (broken line). The data show a fast crossover and are fitted very well by the function derived here. The inset shows a comparison with the previously derived functions [Ref. [11] (broken line), and Ref. [12] (dotted line)], both showing too smooth a crossover, compared to the data.

excellent agreement with experimental data. Comparison with the experiment allows a quantitative analysis of the effect played by the many-particle excitations in the system. We hope that this work will stimulate more work in this direction, especially experimental investigations of the resistivity and the density of states in the same samples such as those pioneered by Massey and Lee [4].

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