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

Yigal Meir

Physics Department, Ben Gurion University, Beer Sheva 84105, ISRAEL

and

Institute of Theoretical Physics, University of California at Santa Barbara,
Santa Barbara, CA 93106

Abstract

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 is agrees very well with experimental data. Quantitative comparison with experiment allows for the possible determination of the role played by polarons in the transport.

72.20.-i, 71.55.Jw, 05.60+w, 71.38+i
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 $\epsilon$ 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. Moreover, it modifies the Mott variable-range hopping law, $\log R \sim 1/T^x$, from $x = d + 1$ to $x = 1/2$. The modified exponent has been observed in many experiments [6].

The Efros-Shklovskii hopping law is expected to be relevant at low temperatures (compared to the size of the gap) [2,7], 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 [8]. A significant step was taken more recently, when Aharony and coworkers [9,10] have 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 the “microscopic” percolation picture [11], describing the transport in the strongly localized regime, indeed leads to such a universal crossover function, and to derive an equation for this function. The results agree excellently with existing experimental data [11], and allow 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 [11] of an equivalent random resistor network [12], consisting of randomly placed sites. Without interactions, the activation energy from site $i$ to site $j$ is given by $\epsilon_j - \epsilon_i$, where $\epsilon_i$ are the energy of site $i$, which in this case is distributed uniformly. The resistance between each pair of sites is given by [12] $R_{ij} = \exp \{(|\epsilon_i| + |\epsilon_j| + |\epsilon_i - \epsilon_j|)/2T + 2r_{ij}/\xi\}$, 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 $R > \exp(|\epsilon_i|/2T)$. Following [14], the percolation criterion employed here is the following [13] — 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,

$$Z_c = \frac{1}{2} \int_{-T \log R}^{T \log R} \int_{-2T \log R}^{2T \log R} \rho_0 d\epsilon_1 \int \rho_0 d\epsilon_2 \int d^d r_{12} \, \Theta(R - e^{(|\epsilon_1|+|\epsilon_2|+|\epsilon_1-\epsilon_2|)/2T+2r_{12}/\xi})$$

$$= \frac{3T}{2^{d+1} \Gamma(d/2) d(d+1)(d+2)} \xi^d \rho_0 \pi^{d/2} (\log R)^{d+1}$$

$$\equiv Z_c T (\log R)^{d+1}/T_0,$$

leading directly to the Mott hopping low, $\log R = (T_0/T)^{1/(d+1)}$ (where the last equality defines $T_0$). In the above $\rho_0$ is the uniform density of states, and $\xi$ the localization length.

In the presence of interactions, the activation energy from site $i$ to site $j$ is given by $\epsilon_j - \epsilon_i - e^2/\epsilon_{ij}$, 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 $\epsilon_i$, and to the soft gap in the Fermi surface [2]. In fact, given that constraint, Efros [14,15] has been able to derive a self-consistent equation for the density of states,

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

where $\alpha$ 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 $\epsilon_0 \simeq 0.46e^3 \sqrt{\rho_0}$.

Knotek and Pollak [16] and Mott [17] have pointed out that the resistance is not determined by the single-electron density of states, but should involve many electron excitations (polarons). Efros [14] indeed demonstrated that taking into account multi-particle excitations (i.e. not assuming that all other particles remain fixed, when electron is activated from site $i$ to site $j$), leads to an even stronger (exponential) gap in the density of states
The long-range interactions between the polarons, which are indeed the relevant excitations for the resistance, lead to a density of states which satisfies \( (2) \), and consequently the resistance should be of the Efros-Shklovskii type, \( \log R = (T_{ES}/T)^{1/2} \).

Taking these considerations into account, the percolation condition (Eq. (1)) is now modified in two ways. The probability of finding two sites, of energies \( \epsilon_i \) and \( \epsilon_j \) 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,

\[
Z_c = \frac{1}{\int 0^T \log R \rho(\epsilon) d\epsilon} \int 0^T \rho(\epsilon_1) d\epsilon_1 \int 0^T \rho(\epsilon_2) d\epsilon_2 \int d^d r_{12} \Theta(\epsilon_2 - \epsilon_1 - e^2/r_{12}) \Theta(R - e^{(\epsilon_2-\epsilon_1-e^2/r_{12})/T+2r_{12}/\xi})
\]

Using the one-parameter scaling form of \( \rho(\epsilon) \), and defining the dimensionless parameters \( x \) and \( y \) by \( 1/T = \alpha_2(e^2/\xi)x/\epsilon_0^2 \) and \( \log R = \alpha_1(e^2/\xi)y/\epsilon_0 \), where \( \alpha_i \) are numerical amplitudes, this equation can be recast in the form

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

with \( x' = \alpha_2 x \), \( y' = \alpha_1 y \), \( s_1 = \sqrt{y'^2 - 16x'} \), and \( s_2 = y' - (\epsilon_2 - \epsilon_1)x \). Eq.(1) which is an implicit equation for \( y \) in terms of \( x \), or \( \log R \) in terms of \( T \), indeed demonstrates that the resistance can be written in a scaling form

\[
\log R = Af(T/T_x), \tag{5}
\]

in agreement with Aharony et al. \[15\], with \( A \equiv (T_0/\epsilon_0)^{1/d} \), and \( T_x \equiv (\epsilon_0^{d+1}/T_0)^{1/d} \) (the numbers \( \alpha_i \) were chosen such that the amplitudes of \( 1/T^x \) in the two asymptotic regimes of \( f(x) \) will agree with the amplitudes chosen by Aharony et al.). In addition to relating the nonuniversal amplitudes \( T_x \) and \( A \) to \( \epsilon_0 \), namely to properties of the density of states, which can be independently measured, Eq.(1) gives a prescription to calculating the full scaling function from “first principles”.

\[\text{[14] [15]}\]
We have calculated the crossover function in three dimensions, using Eq. (4) and a density of states of the quasi-particles 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. [5]. Two points are noteworthy - the experimental data exhibits a rather fast crossover from the Mott regime \( (\log R \sim 1/T^{1/4}) \) to the Efros-Shklovskii regime \( (\log R \sim 1/T^{1/2}) \). 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 [10], 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.

There are two physical parameters which can be extracted from the fit — \( T_0 \) and \( \epsilon_0 \). The value of \( T_0 \) was found to be 1500 Kelvins, exactly as deduced in the experimental paper from the high temperature data. More interestingly, the best fitting value of \( \epsilon_0 \) was 0.04 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 seems to be the first verification of 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, the polarons, which has a gap which is much smaller, due to the finite size of the polaronic cloud. The comparison between the present calculation and the experiment allows for the determination of the average cloud size, which is a few atomic lengths.

To conclude, we have used the percolation picture to derive the crossover function from the Mott to the Efros-Shklovskii hopping regime. This function shows an excellent agreement with experimental data. Quantitative 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].

Acknowledgments: I thank Ora Entin-Wohlman for motivating me to work on this subject, to Y. Gefen and L. Levitov for fruitful discussions and to Mark Lee for making the experimental data of Ref. [4] available. Work at Santa Barbara was supported in part by the National Science Foundation under Grant No. PHY94-07194.

Figure Caption

Comparison of the experimental data (diamonds) to the derivative of the scaling function derived in this work (continuous line), and that of Ref. [4] (broken line). The data shows a fast crossover, and is fitted very well by the function derived here. The inset shows a comparison with the previously derived functions [Ref. [9] (broken line), and Ref. [10] (dotted line)], both showing too smooth a crossover, compared to the data.
REFERENCES

[1] M. Pollak, *Discuss. Faraday Soc.* **50**, 13 (1970).

[2] A. L. Efros and B. I. Shklovskii, *J. Phys.* **C 8**, L49 (1975).

[3] W. L. McMillan and J. Mochel, *Phys. Rev. Lett.* **46**, 556 (1981); G. Hertel et al., *Phys. Rev. Lett.* **50**, 743 (1983); R. Ashoori et al., *Phys. Rev.* **B 48**, 4616 (1993); H. Srikanth and A. K. Raychaudhuri, *J. Phys. (Condensed Matter)* **5**, L551 (1993).

[4] J. G. Massey and M. Lee, *Phys. Rev. Lett.* **75**, 4266 (1995).

[5] M. D. Hill and R. G. Egdell, *J. Phys.* **C 16**, 6205 (1983); G. Hollinger et al., *Phys. Rev.* **B 32**, 1987 (1985).

[6] See, e.g., B. I. Shklovskii and A. L. Efros, *Electronic Properties of Doped Semiconductors* (Springer-Verlag, Berlin, 1984).

[7] O. Entin-Wohlman, Y. Gefen and Y. Shapira, *J. Phys.* **C 16**, 1161 (1983).

[8] See, e.g., A. Glukhov, N. Fogel and A. Shablo, *Sov. Phys. Solid State* **28**, 583 (1986); N. V. Agrinskaya and A. N. Aleshin, *Sov. Phys. Solid State* **31**, 1996 (1989); Y. Zhang et al., *Phys. Rev. Lett.* **64**, 2687 (1990); R. Rozenbaum, *Phys. Rev.* **B 44**, 3599 (1991); S. J. Lee, J. B. Ketterson and N. Trivedi, *Phys. Rev.* **B 46**, 12695 (1992); U. Kabasawa, *Phys. Rev. Lett.* **70**, 1700 (1993);

[9] A. Aharony, Y. Zhang and M. P. Sarachik, *Phys. Rev. Lett.* **68**, 3900 (1992).

[10] See also N. V. Lien, *Phys. Lett.* **A 207**, 379 (1995).

[11] V. Ambegaokar, B. I. Halperin and and J. S. Langer, *Phys. Rev.* **B 4**, 2612 (1971); See also M. Pollak, *J. Non-Crystal. Solids* **11**, 1 (1972); B. I. Shklovskii, *Sov. Phys. JETP* **34**, 1084 (1972).

[12] A. Miller and E. Abrahams, *Phys. Rev.* **120**, 745 (1960).
[13] Y. Meir, *Europhys. Lett.* **33**, 471 (1996).

[14] A. L. Efros, *J. Phys.* **C 9**, 2021 (1976).

[15] See also A. A. Mogilyanskii and M. E. Raikh, *Sov. Phys. JETP* **68**, 1081 (1989); T. Vojta, W. John and M. Schreiber, *J. Phys. C* **5**, 4989 (1993).

[16] M.L. Knotek and M. Pollak, *Phys. Rev.* **B 9**, 664 (1974).

[17] N. F. Mott, *J. Phys.* **C 8**, L239 (1975).

[18] It should be noted, though, that most experiments [3,4] and many numerical simulations [See, e.g., M. Sarvestani, M. Schreiber and T. Vojta, *Phys. Rev.* **B 52**, R3820 (1995), and references therein], observe a gap in the single-particle density of states, which is close to parabolic.
\[ \log \left( \frac{d \log(R)}{d \log(T)} \right) \]

This calculation
Aharony et al. (Ref. 9)
Data (Ref. 4)

Slope = 1/2
Slope = 1/4