Consistent hopping criterion in the Efros-Shklovskii regime

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We address the variable-range hopping regime in the domain where the measuring temperature T is of the order of the characteristic Efros-Shklovskii temperature T_{ES}. In such a range, current theories imply $r_{hop}/\xi < 1$, where r_{hop} is the hopping length and ξ is the localization length, clearly in contradiction with the standard criterion for hopping conduction. We consider impurity overlap wave functions of the form $\psi(r) \propto r^{-n} \exp(-r/\xi)$ and include the preexponential factor of the hopping probability as a logarithmic correction in the Mott optimization procedure. From the general expressions derived, the standard Efros-Shklovskii law is recovered for $T \ll T_{ES}$, whereas an extended preexponential sensitive regime, consistent with $r_{hop}/\xi > 1$, is found for $T_{ES} \gtrsim T$. We argue that the expression resulting from an interplay between preexponential and exponential factors is a consistent extension of the classical Efros-Shklovskii argument. An additional parameter in the theory is directly related to the decay of the impurity wave functions and could be seen as a probe into their behavior. A fit of reference experimental data to the proposed theory yields consistent results.

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I. INTRODUCTION

It is well known that in many Anderson insulators, resistivity obeys Mott's law[1] at sufficiently low temperatures, a regime of electron transport known as variable-range hopping (VRH). In such regime the hopping length goes beyond nearest-neighbor impurities and depends on temperature through the activation energy. Knotek and Pollak[2] and Efros and Shklovskii[3] proposed that Coulomb interactions, if relevant, cause a depression in the density of states in the vicinity of the Fermi energy, so that $g(\varepsilon)=\alpha_d \varepsilon^{d-1}$. The energy ε is measured from the Fermi energy and α_d is a dimension-dependent constant. A percolation argument, which singles out bottleneck resistors in the Miller-Abrahams network, leads to $\ln R(T) \propto \left(\frac{T_{ES}}{T}\right)^{1/2}$, with T_{ES} a characteristic temperature and the exponent 1/2 is independent of dimensionality.

Within the random resistor network model of Miller and Abrahams (MA),[4] the resistance associated with a hopping event between two localized states lying in a narrow band ε_0 about the Fermi level is given by

$$R_{ij} = R_{ij}^0(r_{ij}, \varepsilon_{ij}) \exp\left[\frac{2r_{ij}}{\xi} + \frac{\varepsilon_{ij}}{k_B T}\right]. \quad (1)$$

Here, r_{ij} is the separation between donor i and j, and ε_{ij} is the energy difference of the corresponding localized states. Both Mott and Efros-Shklovskii (ES) laws can be derived using Mott's optimization approach, whose central argument is that the resistance in Eq. (1) is dominated by the exponential factor and determined by the *optimal hop* between localized states. Full prefactor details, nonetheless, must be derived by percolation arguments. The optimization procedure also leads to the ratio $r_{hop}(T)/\xi \sim (T_M/T)^{1/4}$ in the Mott regime and

$$r_{hop}(T)/\xi \sim (T_{ES}/T)^{1/2}, \quad (2)$$

in the ES regime. For the VRH models to be valid, the optimal hopping distance r_{hop} must be greater than the localization length ξ; i.e., $r_{hop}(T)/\xi > 1$.[5–9] This *hopping criterion* implies that the characteristic temperatures T_M and T_{ES} should be higher than the measuring temperature T.

In the critical regime, the carrier concentration N is close to the critical concentration N_c and, hence, $T_{ES} \propto \left(1-\frac{N}{N_c}\right)^{\nu}$ can be very small.[10] Thus, when $T \geqslant T_{ES}$, the previous hopping criterion is violated even though the data can be well described by the ES law (stretched exponential of inverse temperature to the power 1/2). For this reason, it has been controversial as to whether the VRH is consistently the dominant conduction mechanism in samples in the critical regime.[6,7,9–12]

In a detailed study on samples of Ge:Ga, Si:As, and Si:P in the critical regime, Castner[12] addressed some of the previous inconsistencies by observing that the behavior of the dielectric-response function introduces a new length scale into the MA resonance energy. This fact is translated into a more complex form of the wave function to be considered for the elementary MA hopping probability, where the temperature-dependent preexponential factor in Eq. (1) becomes relevant. Nevertheless, the issue of the ratio $r_{hop}/\xi < 1$ persists, and it is argued that serious questions remain on the correct form of the behavior of the tails of the wave function in the critical regime.

In this paper, we address the validity of the hopping criterion when $T_{ES} \sim T$. This is the case in many reference systems where T_{ES} ranges from 0.1 to 350 K, but is typically below a few tens of degrees.[7,13–15] As noted above, the standard hopping criterion, satisfied only when $T_{ES} \gg T$, is obtained by optimizing the argument of the exponential part of the resistance. It is therefore not surprising that the criterion fails when the preexponential factor of the hopping probability becomes important. Here, we introduce corrections to Mott's optimization procedure by explicitly taking into account a family of impurity overlap wave functions of the form $\psi(r)=cr^{-n}\exp[-r/\xi]$ and by including the preexponential factor of the hopping probability as a logarithmic correction. Such a more general form of the wave functions can model a broader set of localized states near the Fermi level like short-range structural defects[16,17] $(n=1)$ or longer-ranged defects. We argue that, for the commonly not too large hopping lengths $(r_{hop}/\xi \sim 10)$, the logarithmic correction is quite relevant and cannot be neglected.

The procedure proposed here extends, depending on the decay of the wave-function overlap, the validity of the hopping criterion into the regime where T_{ES} is of the order of T. The analytical expressions derived recover the well-known expressions when $T_{ES} \gg T$. The full preexponential factor of the resistivity is determined appropriately by percolation arguments. It is important to note that we do not address the physical basis that accounts for the relative size of T_{ES}; i.e., it may be due to a large localization length or to electron-electron interactions. The proposed theory regards this parameter as intrinsic to the particular system.

II. MOTT OPTIMIZATION AND THE HOPPING CRITERION

The energy or distance dependence of the preexponential factor of the hopping probability is important when r_{ij}/ξ or ε_{ij}/k_BT is close to unity. In this limit, fluctuations in the hopping distance or energy differences do not imply a large change in the hopping probability, i.e., in the bond strength in the MA network. In order to take into account the prefactor and to cast the problem in terms of Mott style optimization,[16] one can conveniently write Eq. (1) as $R_{ij}/A = \exp[\lambda_{ij}]$. Here, $A = \pi d s^5 \hbar^4 \kappa \xi^2 / E_1^2 e^6$ (Ref. 16) is a material-dependent constant with dimensions of resistance, E_1 is the deformation potential constant, s is the sound velocity, d is the material density, κ is the dielectric constant, and e is the electron charge. The augmented exponent λ_{ij} is given by

$$\lambda_{ij} = \frac{2r_{ij}}{\xi} + \frac{\varepsilon_{ij}}{k_BT} + \ln\left[\frac{R_{ij}^0}{A}\right]. \tag{3}$$

We can generalize the usual expression for R_{ij}^0/A using an impurity wave function around site i that includes power-law prefactors,[16,18] $\psi_i^{(n)}(r) = c_n |r - r_i|^{-n} \exp[-|r - r_i|/\xi]$, so that

$$\frac{R_{ij}^0}{A} = \left(\frac{k_BT}{\varepsilon_{ij}}\right) e^{\varepsilon_{ij}/k_BT} [Q_n(\varepsilon_{ij})]^2 \left| I_n\left(\frac{r_{ij}}{\xi}\right)\right|^{-2}. \tag{4}$$

In this expression $1/Q_n(q = \varepsilon_{ij}/\hbar s) = \int [\psi^{(n)}(r)]^2 \exp[i\vec{q}\cdot\vec{r}] d^3r$, and $I_n(r_{ij}/\xi)$ is the exact coupling energy of the form

$$I_n(r_{ij}) = \int \psi_i^{(n)}(r)\psi_j^{(n)}(r)\frac{e^2}{\kappa|r - r_j|}d^3r - \int \psi_i^{(n)}(r)\psi_j^{(n)} \times (r)d^3r \int (\psi_i^{(n)})^2(r)\frac{e^2}{\kappa|r - r_j|}d^3r, \tag{5}$$

between localized states separated by r_{ij}.[16] In Ref. 18, $I_n(r_{ij})$ is evaluated for any n by making a convenient change to an elliptic coordinate system and taking the limit $r_{ij}/\xi \gg 1$ that leads to a notable simplification of the equations. The main purpose of this paper is to extend the theory in order to take into account contributions that become important at $r_{ij}/\xi \sim 1$. The integral $Q_n(\varepsilon_{ij})$ has, in general, the structure of the particular case $Q_0(\varepsilon_{ij}) = [1 + (\varepsilon_{ij}\xi/2\hbar s)^2]^2$, which is an exact result. The case for general n modifies the overall power from 2 to $2-n$ and introduces denominators consisting of a finite number of terms in powers of $q = \epsilon_{ij}/\hbar s$. Following the standard procedure,[16] one assumes that in the low-temperature limit $\varepsilon_{ij} \ll 2\hbar s/\xi$ $(q \to 0)$, so that one can approximate $Q_n(\varepsilon_{ij}) = Q_{ij} = 1$. Then one can write

$$\frac{R_{ij}^0}{A} = \left(\frac{k_BT}{\varepsilon_{ij}}\right) e^{\varepsilon_{ij}/k_BT} \left| I_n\left(\frac{r_{ij}}{\xi}\right)\right|^{-2}, \tag{6}$$

and

$$\lambda_{ij} = \frac{\varepsilon_{ij}}{k_BT} - \ln\frac{\varepsilon_{ij}}{k_BT} - 2\ln\left| I_n\left(\frac{r_{ij}}{\xi}\right)\right|. \tag{7}$$

From now on we restrict ourselves to the ES regime by taking into account the Coulomb repulsion via its effect on the density of states $g(\varepsilon)$. Following Mott's procedure, r_{ij} is replaced by the typical separation r between impurities involved in the hopping process and ε_{ij} by the optimal electrostatic energy between those impurities $e^2/\kappa r$. We then arrive at the function of hopping distance

$$\lambda(r) = \frac{e^2}{\kappa k_BTr} - \ln\frac{e^2}{\kappa k_BTr} - 2\ln\left| I_n\left(\frac{r}{\xi}\right)\right|. \tag{8}$$

The value of r for the optimal resistivity is determined by finding the roots of $d\lambda/dr = 0$.[16] It is found that, in general, I_n can be written in the form

$$I_n \propto e^{-r/\xi}\left(\frac{r}{\xi}\right)^{1-2n}\left[1 + \sum_{i=1}^{4n} A_i^{(n)}(\xi/r)^i\right], \tag{9}$$

where $A_i^{(n)}$ are constants for a particular n. Equation (9) holds true for $n \leqslant 0$; otherwise, logarithmic corrections appear. In the limit $r/\xi > 1$, we only keep the first term in the expansion as a first approximation,[18]

$$|I_n|^2 \propto \left(\frac{r}{\xi}\right)^{2-4n} e^{-2r/\xi}. \tag{10}$$

This expression lends itself to a simple analytical equation for the optimal hopping length

$$\frac{r_{hop}}{\xi} = \frac{1}{4}[(1 - 4n) + \sqrt{X + (1 - 4n)^2}], \tag{11}$$

where $X = T_{ES}/T$ and $k_BT_{ES} = 8e^2/\kappa\xi$. As expected, when $X \gg 1$ (and $n = 0$), we recover the usual ES expression [Eq. (2)]. On the other hand, in the opposite limit $X \ll (1-4n)^2$, Eq. (11) reduces to $(1/4)(1 - 4n + |1 - 4n|)$, which is finite for $n < 1/4$. In the latter limit, the hopping criterion r_{hop}/ξ is independent of temperature and depends critically on the behavior of the prefactor of the wave-function decay, being greater than 1 for the value range $n < -1/4$. That is, when $T_{ES}/T \sim 1$, the hopping criterion is satisfied for wave functions of longer range than purely exponential decay. Thus, the introduction of the prefactor of the wave function is necessary to make the system well behaved (satisfy the hopping criterion) in the region $T_{ES}/T \sim 1$.

Equation (11) is plotted in Fig. 1. For $T \ll T_{ES}$, the curves for $n = 0$, $n = -1/4$, and $n = 1/4$ converge to the regular ES dependence; thus the value of n in the impurity wave function is irrelevant in this temperature region. For $n = 1/4$, the prefactor becomes energy and/or distance independent, making no contributions to the optimal resistance. Such a special

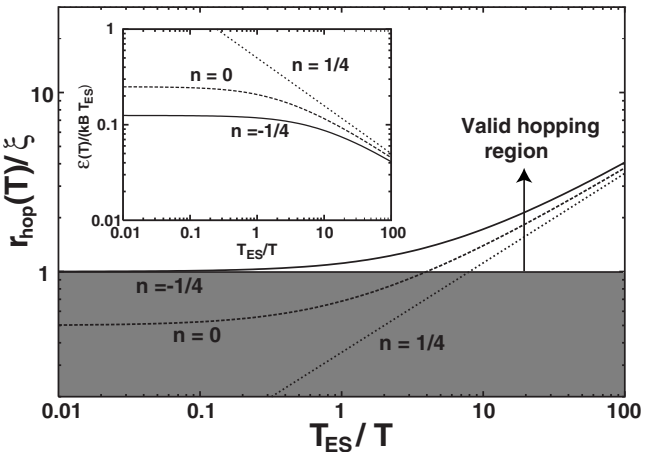

FIG. 1. Ratio of the hopping length to the localization length as a function of temperature for three different wave-function decays when preexponential logarithmic corrections are considered. The shaded region depicts the locus where the hopping criterion is violated. In the inset, the behavior of the optimal band size is shown. The case for $n=1/4$ leads to the same temperature dependence as that of the standard ES law. The dashed line ($n=0$) corresponds to hydrogenic wave functions.

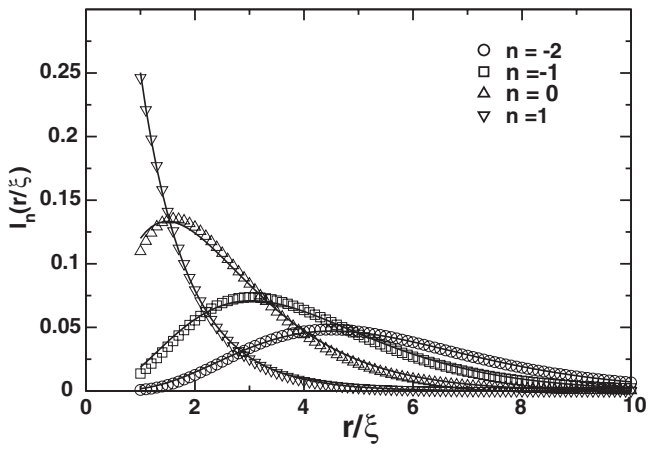

FIG. 2. Interdonor separation dependence of the coupling energy integral, derived numerically, for several wave-function forms chosen. The solid lines represent fits to the numerical estimate.

value of n serves as a reference for the relative effect of the proposed corrections. The longer the range (smaller n) of the impurity overlap with respect to the $n=1/4$ case, the larger the temperature region of validity of the hopping criterion. Note that in the current approximation, and for the case $n=-1/4$, the hopping criterion is met for all values of T_{ES}/T.

We emphasize the convenience of depicting the hopping criterion against T_{ES}/T. As mentioned before, we take T_{ES} as a material-dependent parameter, itself independent of temperature. Figure 1 can then represent, for a fixed T_{ES}, a particular temperature range when such material obeys Efros-Shklovskii physics. Systems exhibiting different values of T_{ES} will be represented by different vicinities in temperature on the same curve.

To improve on the above crude but explicitly solvable model approximation, we can use a semianalytical approach that consists in determining, first, the coupling energy integral I_n by numerical means and then using a fitting procedure to arrive at an analytical expression. Figure 2 shows several reference I_n versus r/ξ curves and their proposed fits (continuous lines). Clearly, there is a region ($r/\xi<4$) where preexponential effects are strong, while for larger values of r/ξ, I_n has a purely exponential decay.

A general simple fit for $|I_n|^2$ is given by

$$\left|I_n\left(\frac{r_{ij}}{\xi}\right)\right|^2 \propto \left(\frac{r_{ij}}{\xi}\right)^{2b_n} e^{-2r_{ij}/\xi}, \tag{12}$$

where $b_n \approx 1.42-1.56n$. As before, the solutions to $d\lambda(r)/dr=0$ give the optimal hopping length as a function of temperature

$$\frac{r_{hop}}{\xi} = \frac{1}{4}[(2b_n-1)+\sqrt{X+(2b_n-1)^2}]. \tag{13}$$

Both Eqs. (11) and (13) can be written as

$$\frac{r_{hop}}{\xi} = \frac{1}{4}(a_n+\sqrt{X+a_n^2}). \tag{14}$$

This form has been verified through extensive numerical computations of the minima of Eq. (8). Here, a_n is a linear function of n and the parameters in it depend on the approximation used; i.e., in our first analytical scheme $a_n=1-4n$, while in the semianalytical fitting model $a_n=2b_n-1$.

A final more accurate approach to the optimization procedure will be described. An appropriate numerical method must be employed in order to go beyond the previous approaches and check their accuracy, since it is difficult to find a closed analytical form for any n. The numerical solution for the roots of

$$\frac{d\lambda(r)}{dr} = \frac{1}{r} - \frac{e^2}{\kappa k_B T r^2} - 2\frac{1}{I_n(r/\xi)}\frac{dI_n(r/\xi)}{dr}, \tag{15}$$

gives the optimal values for the hopping distance as a function of temperature. As I_n has the form $\int \exp \times[-(r/\xi)x]f(x,y)dxdy$, its derivative is readily obtained for any n. In order to correctly compare the numerical results with the previous approaches, one must choose $T_{ES}=8e^2/\kappa\xi$ as the temperature scale and ξ as the natural length scale. In this way, for each T/T_{ES} chosen, we arrive at an optimal value for r/ξ.

Figure 3 depicts Eq. (14) for $n=0$, comparing the three computational schemes for the overlap integral: (i) the analytical model (open circles), (ii) the semianalytical model based on a numerical fit (open squares), and (iii) the direct numerical integration without assuming a particular analytical form for the overlap integral (dashed line) and solving directly for the optimal value of $\lambda(r)$. As T approaches T_{ES}, all cases develop a plateau value for r_{hop}/ξ. No further changes in this ratio occur in the limit $T>T_{ES}$. Cases (i) and (ii) give rather different regions of validity for the hopping criterion, where the semianalytical fit yields a larger range of consistency. The case where the optimal condition is computed numerically, using a more exact method than the previous approximations, shows that the system complies with

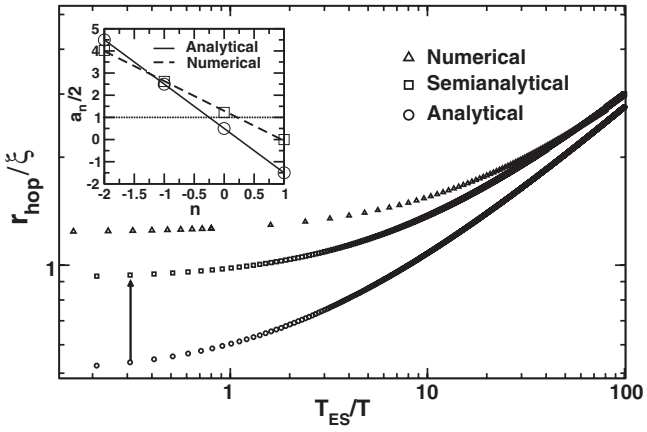

FIG. 3. The ratio of the optimal hopping length to the localization length as a function of T_{ES}/T for (i) the first analytical approximation (open circles), (ii) the semianalytical approach (open squares), and (iii) a precise numerical estimation of the overlap integral (open triangles), for the fixed value $n=0$ (hydrogenic case). Note the continuous trend toward a consistent validation of the hopping criterion as the theory is evaluated with higher precision. In the inset we show the parameter $a_n/2$ of Eq. (14) for the first analytical approximation (continuous line) and the plateau value for the precise numerical estimate (dashed line) as a function of n. All points above $a_n/2=1$ satisfy the hopping criterion.

the hopping criterion in all the temperature range for the particular case of s-type wave functions ($n=0$). This result suggests that prefactors in the wave function yield important corrections to the hopping criterion when included in the optimization scheme.

From the above results and from an operational viewpoint, one concludes that if the hopping criterion is violated when employing the standard ES law for data fitting, it may be a signal that preexponential factors should then be included in the analysis and could also be a signature of a nontrivial wave-function decay. This scenario is possible if T/T_{ES} is not too large, which is a rather common situation.[7,8,10,13]

III. RESISTIVITY

We will now derive the expressions for the resistivity corresponding to the two analytical approximations described above. By introducing Eq. (12) in Eq. (8) and using the parameters obtained by optimization, we show that the optimal value of λ_{ij} follows the general form

$$\lambda_n = (X + a_n^2)^{1/2}, \tag{16}$$

where we have neglected logarithmic corrections in $X=T_{ES}/T$. This is reasonable as long as $X>1$. In order to compute the resistivity, one still needs to resort to percolation theory to fully account for effects beyond the optimal resistor as the physics is dominated by the correlation length; i.e., $\rho(T)=L_0R_0\exp[\lambda_n]$, with $R_0(n,T)=R_{ij}^0(\lambda_n)$ and $L_0=\bar{r}\lambda_n^\nu$ the correlation radius of the critical subnetwork. Here, ν is the critical exponent of the correlation length and $\bar{r}=\xi\lambda_n/2$ is an average hopping distance.[16] In the discussion, we will explain the approximation of neglecting logarithmic terms in Eq. (16) in relation to the competing correlation lengths produced by exponential and power-law disorders.

By identifying $\rho_0(n,T)$ with $(\xi/2)R_0(n,T)$, the expression for the system resistivity is

$$\rho_n(T)/\rho_0(n,T) = \lambda_n^{(1+\nu)}e^{\lambda_n}, \tag{17}$$

with λ_n given by Eq. (16). For the case of our simplest analytical model, we have

$$\rho_n(T)/\rho_0(n,T) = [X+(1-4n)^2]^{(\nu+1)/2}\exp\{[X+(1-4n)^2]^{1/2}\}, \tag{18}$$

with

$$\rho_0 = \frac{1}{X}\{[X+(1-4n)^2]^{1/2}+(1-4n)\}^{4n-1}, \tag{19}$$

except for numerical prefactors. It is easily verified that in the limit $X \gg (1-4n)^2$, one recovers

$$\rho_n(T) = \left(\frac{T_{ES}}{T}\right)^{(4n+\nu-2)/2}\exp\left[\left(\frac{T_{ES}}{T}\right)^{1/2}\right], \tag{20}$$

which gives the correct expectations, up to numerical prefactors, for the hydrogenic case ($n=0$) and for short-range potentials ($n=1$) found in the literature. The limit $X \gg (1-4n)^2$ above is itself a different result since it had only been derived in the literature for the cases of $n=0$ and $n=1$.[16,18]

On the other hand, for the semianalytical approximation, we have

$$\rho_n(T) = X^{-1}[X+(2b_n-1)^2]^{(\nu+1)/2}\{[X+(2b_n-1)^2]^{1/2} + (2b_n-1)\}^{1-2b_n}\exp\{[X+(2b_n-1)^2]^{1/2}\}. \tag{21}$$

Taking, again, the limit $X \gg (2b_n-1)^2$,

$$\rho_n(T) \propto \left(\frac{T_{ES}}{T}\right)^{(\nu-2b_n)/2}\exp\left[\left(\frac{T_{ES}}{T}\right)^{1/2}\right]. \tag{22}$$

Supposing that $\nu \sim 1$, the $(\nu-2b_n)/2$ power can be estimated. It is close to -1 if $n=0$ and $\sim 2/3$ when $n=1$. These results differ from those of the original ES formulation. Nevertheless, the discrepancy occurs only in the power-law prefactor of the resistance in a range of temperatures where they can be disregarded.

In Fig. 4, we depict the behavior of the resistivity as a function of temperature. We have only represented results for $T_{ES}>T$ since this assumption is built into Eqs. (16) and (17) when logarithmic contributions are dropped. The resistivity decreases monotonously with T_{ES}/T until this ratio is of the order of 10. Below this ratio, there is a region where the resistivity can actually increase comparatively weakly. Curves for both $n=-1$ (slower wave-function decay) and $n=0$ are nonmonotonic, so that resistivity can both decrease and increase with temperature in a certain range. According to our results, the nonmonotonic temperature dependence can occur without breaking the hopping criterion, depending on the relative values of T and T_{ES} and the nature of the localized states in the material. An experimental observation of a decrease in resistivity as the temperature is lowered in

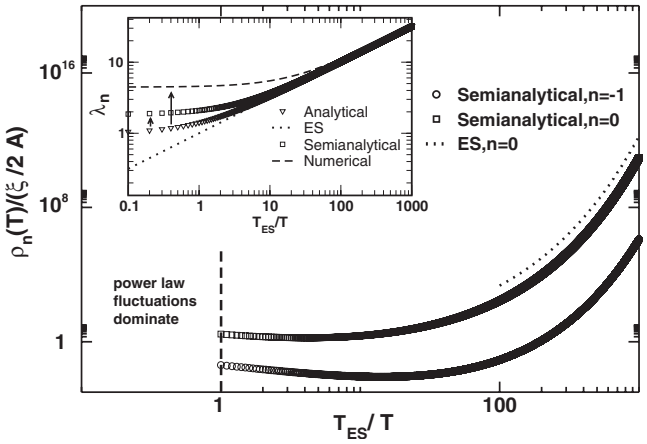

FIG. 4. Temperature dependence of the resistivity including power-law corrections. The dotted line shows the pure $\exp(T_{ES}/T)^{1/2}$ behavior, which is valid only when $T_{ES} \gg T$. Resistivities for the fitted semianalytical cases are shown for $T_{ES} > T$ (see text). In the inset, we show the optimal exponent λ_n for $n=0$. The dashed line is the ES stretched exponential. The fitted and analytical approximations are below the limit of validity of percolation theory (see text). The dashed curve is the more precise numerical approximation.

the hopping regime has been reported recently.[18,19] Other candidate systems recently reporting such nonmonotonous behavior below the Mott VRH regime include recent work by Laiho *et al.*,[20] although other possible effects could be involved.

IV. DISCUSSION

A. Consistency of the theory

The first issue we discuss concerns the validity of the optimization and/or percolation treatment considered here. We are relying on the fact that one may extend such a treatment to a situation where the fluctuations of resistors in the Miller-Abrahams network are sufficiently strong for an optimization treatment to work. When this is not the case, a mean-field treatment is the tool of choice. The argument for how strongly resistors fluctuate depends critically on the relative value of the hopping lengths and the localization length. If the two distances are very similar, i.e., $\xi \sim r$, fluctuations in the resistance are weak as compared to the situation where $\xi \ll r$. Another way to check the adequacy of the optimization treatment is to estimate the size of λ_n [see Eq. (16)] as a function of T_{ES}/T. The result is depicted in the inset of Fig. 4 for the case of $n=0$ (s-type wave function) for the analytical model (inverted triangles), the semianalytical or fitted model, and the direct numerical computation of the optimization scheme. Below $T_{ES}/T \sim 10$, the value of λ_0 ranges from 1 to 5. Numerical simulations in a cubic simple lattice have concluded that the minimum λ_n that assures a large enough spread of the resistances for the validity of percolation theory is ~4.5, although it has been judged to be smaller for bcc and fcc lattices.[16] In the region of interest, our most detailed model (dashed curve in the inset) values of λ_n are close to 5 (see inset of Fig. 4), which implies that the results are on the limit of validity of percolation theory. While this validates our treatment for a range of temperatures and wave-function decays, it is obvious that a mean-field approach to the problem could be appropriate to the limit studied here.

A related point to the previous discussion is whether power-law fluctuations can generate a percolation scenario. Here, we turn to previous work on power-law disorder compared to exponential disorder, both of which are mixed in the present context. It has been shown[21,22] that, for a network whose elementary resistors between sites i and j are of the form $R_{ij} \sim \exp(\Lambda r_{ij})$ with $r_{ij} \in [0,1]$, a single critical bond dominates only in the limit $\Lambda \to \infty$. This is the strongly disordered limit. If Λ, on the other hand, is finite, then there is a correlation length $\zeta \sim \Lambda^{\nu}$ below which we have critical properties, while above it the network is Euclidean. Interestingly, as shown in Ref. 21 and more generally in Refs. 22 and 23, the same applies to power-law resistors where $R_{ij} \sim (r_{ij}/\xi)^{\alpha}$, with α playing the same role as Λ for exponential distributions. In the context of the present paper, two competing correlation lengths arise from the exponential and power-law contributions, respectively, where the dominant one is the larger of the two. This last argument justifies the neglect of the logarithmic terms in the correlation length contribution to the resistivity in Eq. (17), as long as the correlation length due to the exponential fluctuation is the largest.

In this light, a way to estimate the effective value of Λ is by using the exponential relation of Eq. (1) and normalizing the exponent by multiplying and dividing by the typical hopping length. We then have the form discussed before with $\Lambda \sim r_{hop}/\xi$; i.e., the disorder strength is related to the ratio in our hopping criterion. This makes sense physically, because when $\Lambda \to \infty$ one has $\xi \ll r_{hop}$, which is the strongly localized regime. On the other hand, if $\Lambda \sim 1$, the exponential disorder is much weaker and the hopping criterion is appreciably affected by power-law fluctuations. In conclusion, the size of r_{hop}/ξ determines the strength of exponential fluctuations, and the proximity of this parameter to one signals important effects of power-law fluctuations.

Another consistency check regarding our approach is the comparison between the expressions for the optimal energy band ε_0 and the width of the Coulomb gap 2Δ. In order for the ES regime to be in force, one requires that $2\Delta > \varepsilon_0$. The half-width of the Coulomb gap can be obtained from the relation $\Delta/k_B T_{ES} = (C_M/C_E^3)^{1/2}(T_{ES}/T_M)^{1/2}$,[16] where C_M ad C_E are coefficients defined by the percolation procedure, for the Mott and ES regimes, respectively. Comparing such relation to our analytical expression for the optimal bandwidth (see Fig. 1) $\varepsilon_0/k_B T_{ES} = (T/T_{ES})[(1+T_{ES}/T)^{1/2}-1]$, one obtains that the appropriate inequality above is satisfied for $T_{ES}/T > 3.3$, using the choices $(C_M/C_E^3)^{1/2} \sim 1$, $T_{ES}=11.2$ K, and $T_M = 420$ K.[24] The latter parameter selection is conservative, since one expects a broader range of validity for our approach when C_E takes smaller values than predicted by percolation. The latter has been argued in Ref. 14 due to the effects of electron-electron interactions. On the other hand, the range of validity could also be reduced for samples where T_{ES}/T_M is very small. Using the same set of parameters

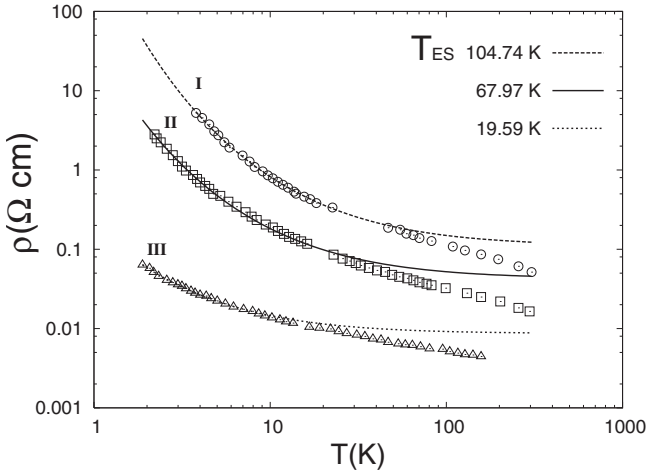

FIG. 5. Resistivity versus temperature derived from Ref. 13. Each data set shows the labeling indicated in Table I and differs from one another in the concentration of carriers, with III having the largest concentration and I the smallest. The original data set III was multiplied by 0.1 to avoid overlap of the data. The legend shows the values of the characteristic temperature T_{ES} for each curve. All the fits to the theory are consistent with the hopping criterion.

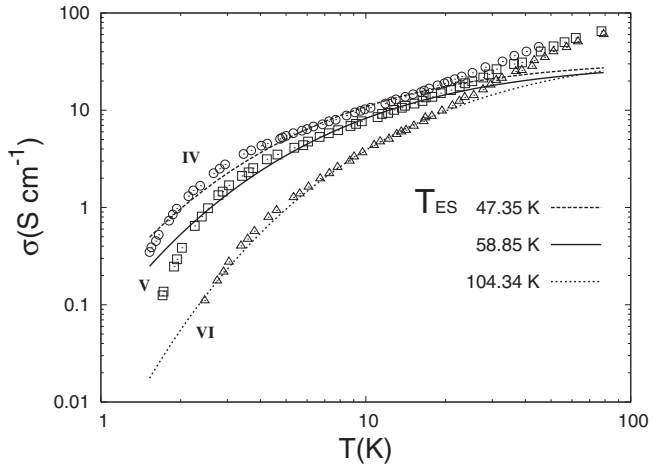

FIG. 6. Conductivity as a function of temperature from Shafarman *et al.* (Ref. 15). Each set of data is labeled as indicated in Table I. The data are only fitted to our theory in the range claimed to be ES by the authors. The legend shows the values of the characteristic temperature T_{ES} for each curve. All fits are consistent with the hopping criterion as indicated in Table I.

above to judge whether the energy scale for the Coulomb gap has not been exceeded (implying a crossover to the Mott regime), one finds $T_{ES}/T>3$; again an appreciable range of consistency for our approach.

B. Experimental support

To give some experimental support to this theory, we analyze data from various emblematic references that report anomalous VRH behavior in the sense that $R_{hop}/\xi<1$, in contradiction with basic assumptions of the theory. It is our intention to show that the formulation developed in this paper can be used to fit data previously interpreted as following standard ES law but leading to nonsensical values for the physical parameters. For simplicity, and in the absence of further information in the literature, we will assume impurity wave functions that decay with a hydrogenic, *s*-wave character.

In Fig. 5, we depict reference data of Rosenbaum,[13] and in Fig. 6, the most insulating samples from the work of Shafarman *et al.*[15] Table I displays the values of T_{ES} and R_{hop}/ξ that result from the fitting to the typical ES law (second and third columns) to samples I, II, and III of Ref. 13 and samples IV, V, and VI taken from Ref. 15. For the fitting to the regular ES law, the hopping condition is always violated ($R_{hop}/\xi<1$). The fourth and fifth columns of the table show the best values of the parameters obtained from a fit using our extended theory assuming only a hydrogenic decay ($n=0$) for the impurity wave function. The corresponding value for a_n in the theory is $a_0=1.84$ from the semianalytical approach explained in Sec. II. This latter value is applied to both sets of data chosen, so this is not a free parameter; it is dictated by the wave-function decay. Note the quality of the fit in Figs. 5 and 6, which is at least as good as that of the original papers. The only regions fitted are those where the original authors claim ES behavior. The parameters derived, according to Table I, are consistent with the hopping criterion. The temperature dependence of the prefactor is weak enough so that the fit is dominated only by the exponential of our semianalytical approximation. The resistivity prefactor is then the only parameter fitted to set the correct scale of the resistance. As a final example showing the broad applicability of our generalization, we show data derived from Ref. 25 for the crossover between Mott and ES. The original fit to the ES region with the standard theory has a consistent hopping cri-

TABLE I. Parameters derived from fitting data with source labels d, e, and f in Ref. 13 (our labels I, II, and III, respectively) and data with source labels 7.39, 7.3, and 6.98×10^{18} cm^{-3} (donor concentration) in Ref. 15 (our labels IV, V, and VI). The second and third columns show the values of T_{ES} and R_{hop}/ξ, respectively, when the exponential ES law is used, while the fourth and fifth columns display the corresponding values using the theory derived here, assuming hydrogenic wave functions. Note that the theory predicts a consistent value for R_{hop}/ξ with values of T_{ES} shifted to slightly higher values. The reported ratios R_{hop}/ξ in the table correspond to the temperatures: d→26.5 K, f→17.5 K, g→9.5 K, and, for Ref. 15, $T=10$ K. Such temperatures correspond to the lowest values possible for R_{hop}/ξ in the fitted ES range.

	ES law fit		Present theory	
Samples	T_{ES}	R_{hop}/ξ	T_{ES}	R_{hop}/ξ
I→d	49.9	0.35	104.74	1.14
II→f	40.9	0.38	67.97	1.13
III→g	8.9	0.24	19.59	1.04
IV→7.39	31.34	0.44	47.35	1.17
V→7.3	41.26	0.51	58.85	1.22
VI→6.98	104.34	0.81	104.34	1.38

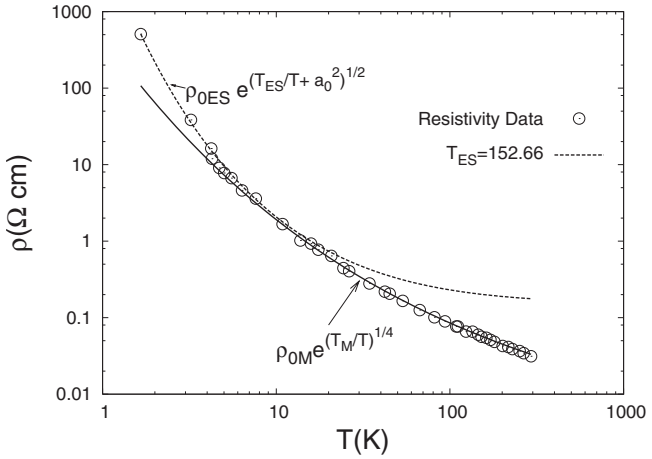

FIG. 7. Resistivity versus temperature from Ref. 25, where a transition between ES law and Mott is observed. The dotted line fits only the ES region according to the theory proposed using a hydrogenic decay and bears the T_{ES} indicated. The solid line is a fit according to the indicated Mott behavior.

terion. The fit of our theory is also excellent and also consistent with the hopping criterion as shown in the Fig. 7.

V. SUMMARY

In summary, we presented a theoretical model that incorporates the preexponential factor of the system's wave function into Mott's optimization procedure, generating corrections to the well-known percolation results. This procedure suggests that the hopping criterion $r_{hop}/\xi > 1$ is consistently valid in a broader range of temperatures even when $T_{ES} \sim T$. The derived relations for the crudest analytical model recover the conventional Efros-Shklovskii formulation in the limit $T \ll T_{ES}$. In this sense, the latter formulation is a particular case of our first approximation. Nevertheless, two refined models suggest prefactor corrections to the Efros-Shklovskii theory even when $T_{ES} \gg T$. The latter modifications, notwithstanding, will be difficult to assess in an exponentially dominated regime but should be very clear for $T_{ES} \sim T$. Our analysis suggests that violation of the hopping condition could be the signature of the nature of the decay of localized states in the material and/or the result of the relative importance of prefactor effects when *s*-wave-type wave functions are the case. Finally, the scenario suggested here brings about the possibility of nonmonotonic behavior of the resistance with temperature as seen in recent experimental systems.

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