# Effective resistance of systems with hopping conductivities in the case of many neighbors

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In a framework of self-consistency effective medium approximation, we derive an expression for the effective resistivity of the Miller-Abrahams resistor networks with hopping conductivities [$\sigma \propto \exp(-\kappa r)$, where $\kappa$ is a measure of disorder, and $r$ is a random number, $0 \leq r \leq 1$], and we compare it with the results of numerical simulations of such networks. When the number of neighbors is greater than four, the numerical results agree with the expression derived in this paper and not with the expression obtained in the percolative approach. In the case of four neighbors both results are in agreement.

Nanoscopic granular materials cannot be treated as classical composites,[1] since the typical size of their grains (of the order $\sim 15$–$20$ nm) demands the quantum-mechanical description. The most popular and convenient expression for the intergranular hopping conductivity $\sigma_{ij}$ (between the $i$th and $j$th grains) is the formula well-known for more than 40 years:[2,3] $\sigma_{ij} = \sigma_0 \exp(-r_{ij}/r_0 - \epsilon_{ij}/k_B T)$, where $r_{ij}$ is the distance between two grains, $r_0$ is the scale over which the wave function decays outside the grain, $\epsilon_{ij}$ is the activation energy, and $\sigma_0$ is the dimension coefficient. At sufficiently high temperatures $T$, the thermal hopping term $\epsilon_{ij}/k_B T$ is small compared to the spatial one $r_{ij}/r_0$. This is the situation of the so-called "$r$ percolation," when the conductivity $\sigma_{ij}$ is governed by the spatial term only.[4] For the sake of simplicity, we are interested only in this regime and will omit the activation energy $\epsilon_{ij}$.[5] In order to perform numerical simulations, we express the random distance between grains as $r_{ij} = 2\bar{l} \cdot rand_{ij}$, where $rand_{ij}$ is a random number taken from a uniform distribution in the range $(0,1)$, $\bar{l} \sim 1/\sqrt[D]{q}$ is the mean distance between metallic grains, $q$ is the density of the grains, and $D$ is the dimensionality.[6,7] Therefore, the expression for $\sigma_{ij}$ can now be rewritten as follows (Refs. 6 and 7):

$$\sigma_{ij} = \sigma_0 \exp(-\kappa \cdot rand_{ij}), \tag{1}$$

where $\kappa \equiv 2\bar{l}/r_0$ can be interpreted as the dimensionless mean hopping distance or as the degree of disorder (the smaller is density of the deposited grains $q$ the larger is $\kappa$).

The further treating of the system can be performed by the construction of a Miller-Abrahams resistor network,[2] where the resistances $R_{ij} \sim 1/\sigma_{ij}$ of the resistors are determined by the formula (1).

In Refs. 3, 8, and 9 an analytical expression (derived in the percolation approach[10]) is presented for the average effective conductivity $\sigma_e$ of such resistor networks. In the two-dimensional (2D) case, in terms of the effective resistivity $\rho_e = 1/\sigma_e$, it takes the form:

$$\rho_e \simeq \rho_0 e^{p_c \kappa}, \tag{2}$$

where $\rho_0 = 1/\sigma_0$ and $p_c$ is the percolation threshold.

In Ref. 11 it was shown that in 2D, in the limit $\kappa \to \infty$,

Eq. (2) is exact (see also Ref. 12). It is easy to show[7] that in the case of the 2D random resistor bond network (for which $z=4$ and $p_c=0.5$), Eq. (2) follows immediately from the Keller-Dykhne theorem[13] and is exact for an arbitrary $\kappa$.[7]
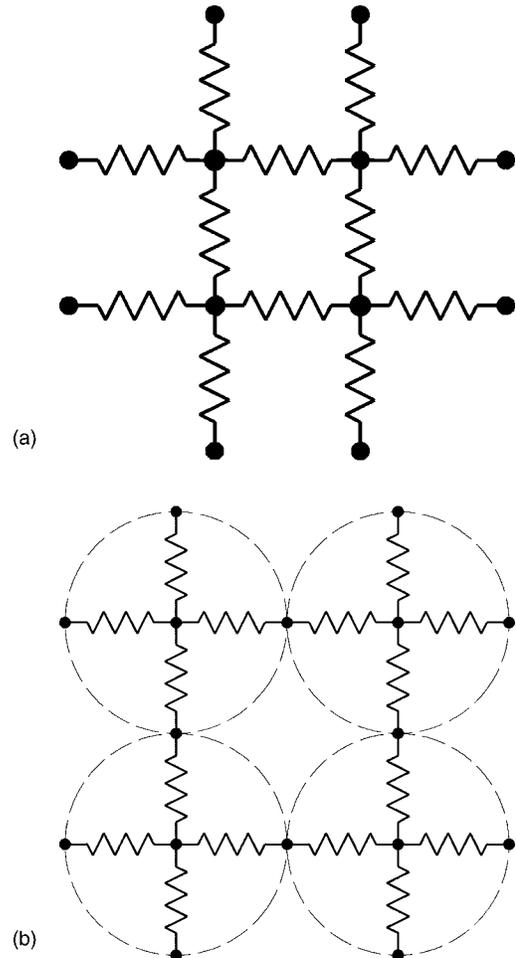


FIG. 1. (a) A square bond percolation network of resistors with a random resistivity given by Eq. (1), where ($ij$) denotes the bond between sites $i$ and $j$. (b) A site percolating network. The resistivity of all four resistors within a dashed circle is determined by a single random number $rand_{ij}$, where $ij$ denotes the labeling of the grid point $i, j$.
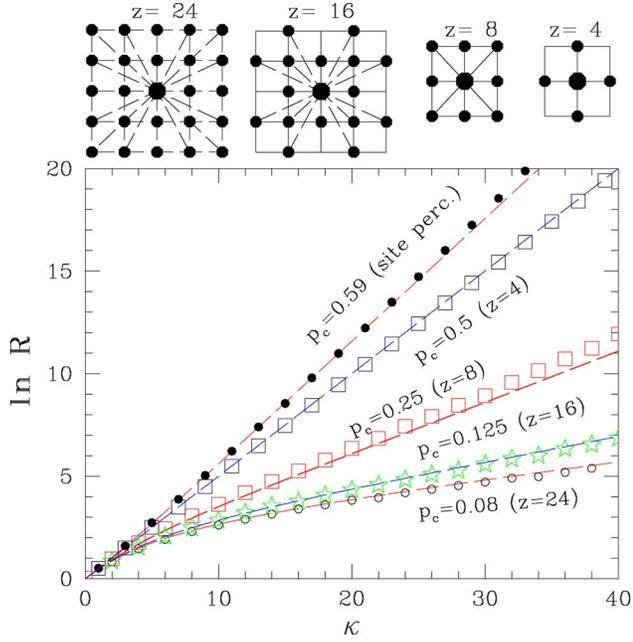
FIG. 2. (Color online) A semi-logarthmic plot of the effective resistance $\rho_e$ vs $\kappa$ for lattices with a different number of neighbors $z$. The results of numerical simulations (shown by empty and filled symbols) are in agreement with the analytical expression (4) obtained with EMA (shown by the lines). The case of the site percolation (with $p_c=0.59$) is calculated on the lattice shown in Fig. 1(b). The other cases are calculated on the lattices which unite cells [with $z=24$ ($p_c=0.08$), $z=16$ ($p_c=0.125$), $z=8$ ($p_c=0.25$), and $z=4$ ($p_c=0.5$), respectively] and are shown in the upper parts of this figure. The central grain in each unit cell (shown by larger filled circles) is connected with $z$ neighbors (shown by smaller circles) by solid and dashed lines denoting the trajectories of the hopping charged particles.

Effective resistivity $\rho_e$ can be found also in a framework of the symmetric self-consistency effective-medium approximation (EMA) rewritten for a many component composite.[14] If the local resistivities, $\rho$, are distributed continuously in a range $\rho_{min} \leq \rho \leq \rho_{max}$ according to some distribution function $f(\rho)$, then $\rho_e$ can be found by taking the integral

$$\int_{\rho_{min}}^{\rho_{max}} f(\rho)\left(\frac{\rho-\rho_e}{a\rho+\rho_e}\right)d\rho = 0, \qquad (3)$$

where $a=z/2-1$ and $z$ is the number of bonds (neighbors) at each node of the network. If $rand_{ij}$ in Eq. (1) is uniformly distributed between 0 and 1, then $f(\rho)=1/\kappa\rho$ (see e.g., Ref. 9). Taking the integral (3), we obtain $\ln\left[(a\rho+\rho_e)^{(1+a)/a}/\rho\right]\big|_{\rho_0}^{\rho_0 e^\kappa}=0$, and, therefore,

$$\rho_e = \rho_0 e^{\kappa p_c}\left(\frac{1-p_c}{p_c}\right)\left[\frac{1-e^{-\kappa p_c}}{1-e^{-\kappa(1-p_c)}}\right], \qquad (4)$$

where $p_c=1/(1+a)=2/z$. In the limit $p_c \rightarrow 1$, Eq. (4) reduces to $\rho_e=\rho_0(e^\kappa-1)/\kappa$, and the latter tends to $\rho_0$ when $\kappa \rightarrow 0$. For a square lattice $z=4$, and Eq. (4) coincides with Eq. (2).
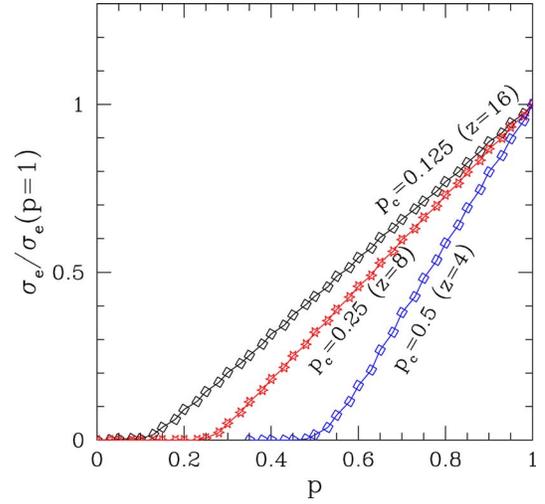


FIG. 3. (Color online) Normalized effective conductivity, $\sigma_e$, vs volume fraction $p$ (which conforms to the expression for the percolation threshold $p_c=2/z$). The lattices here are the same as in Fig. 2, but in calculations only two values of the local conductivities were used: $\sigma_{ij}=0$ and $\sigma_{ij}=1$.

However, for a granular hopping system the number of bonds can be much greater than four (see the sketches in the upper part of Fig. 2), due to the fact that hops can occur between nonneighbor grains. For these cases $z>4$, and Eq. (4) differs essentially from Eq. (2).

To determine whether Eq. (4) or Eq. (2) is correct, we performed large-scale Monte Carlo simulations. We built bond- and site-percolating Miller-Abrahams-like resistor networks (see Fig. 1 and Refs. 2 and 6), but assumed the conductivity of each resistor to have the form given in Eq. (1). Following Refs. 15 and 16, we wrote the Kirchhoff equations for each site, solved the system of coupled linear equations, using standard sparse solver subroutines accommodated for Cray supercomputers, and calculated the total effective resistance $\rho_e$ for two-dimensional (2D) networks.[6]

In Fig. 2, we show a semi-logarithmic plot of the dependences $\rho_e$ vs $\kappa$, obtained from both numerical simulations and analytical expressions (4). The results of the numerical simulations conform to Eq. (4) but not to Eq. (2). Only in the case when $z=4$ do the numerical results conform to Eq. (2).

In Fig. 3 we also examined the simple expression $p_c=2/z$ (see Ref. 15). The lattices are the same as in Fig. 2, but in the calculations only two values of the local conductivities, $\sigma_{ij}=0$ and $\sigma_{ij}=1$, were used. We plot $\sigma_e$ vs volume fraction $p$ of the resistors with conductivity $\sigma_{ij}=1$. The results of the numerical simulations conform to the expression for the percolation threshold $p_c=2/z$.

In summary, the numerical simulations show that the effective resistance of the systems with hopping conductivity obeys (in the case of the many neighbors, $z>4$) our Eq. (4) and does not obey Eq. (2). Only in the case of four neighbors both results are in agreement.

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