Percolation Calculation of Hopping Conduction in Disordered Systems

Chien-Han Lin and G. Y. Wu

Abstract

We have developed a percolation calculation method for hopping conduction in disordered systems. The method incorporates the assumption that coherent hopping to non-nearest neighbor sites takes place via intermediate sites. To assess numerical accuracy of the method, the result is compared with that of a corresponding resistor circuit simulation, for the case of a bcc lattice with hopping up to next nearest neighbors, and good agreement is obtained between the two. The method is useful for the study of low-temperature hopping transport in disordered systems.

Key Word: disordered system, percolation, hopping transport, lattice

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I. Introduction

The electrical hopping conductivity of disordered system in low temperature has been observed widely to obey a "fractional temperature dependence", with $\sigma \propto \exp\left[-\left(T_0/T\right)^n\right]$, where the exponent $n=1\sim1/4$. The well-known granular metal have been many theoretical studies on the origin of the $n=1/2$ behavior in disordered systems[1-11]. In one of the frequently discussed models, a granular metal is regarded as a resistor network, with each resistor corresponding to a hopping between two sites. Within this model, the system resistance can be obtained by circuit simulations which solve Kirchoff equations.[8,11] However, in the simulation, the network size must be adjusted accordingly to ensure that the calculation is free of finite size effects. For example, if the linear size required for the nearest-neighbor (n.n.)-hopping-dominated transport equals N sites, then that for the next-nearest-neighbor (n.n.n.)-hopping-dominated transport must be at least 2N, since the relevant microscopic scale is doubled when going from n.n. hoppings to n.n.n. hopping. Therefore, for the low temperature range where long-range hopping are important, the size consideration imposes the requirement of large computer memory and CPU time.

Fortunately, in many cases, the networks of granular metal consist of distributions of widely varying resistances, and a good approximation, i.e. the critical percolation path method developed for variable-range-hopping problems,[12] offers a useful solution to the computational problem. This method has been applied to granular systems with only n.n. hopping included[3,11] and with non-nearest-neighbor hopping included as well. [5] While the latter study is able to cover a broad range of temperatures, it neglects possible intrusion of other sites into the path of tunneling between two sites.

In this paper, we shall remove the foregoing approximation and develop a percolation calculation suitable for disordered systems, in which case a tunneling

path between non-nearest neighbors often traverses through intermediate sites. In Sec. II, we shall present a percolation method, which incorporates the foregoing constraint. In Sec. III, the result of percolation calculation shall be compared to the corresponding circuit simulation for assessment of its accuracy. In Sec. IV, we conclude the study.

II. Percolation theory

We shall demonstrate our theoretical method with a calculation including hopping up to n.n.n. Firstly, we consider the charge transfer in a 3-site system with oxide barriers between the sites, as shown in Figure 1(a). There are two ways for an electron to transport from site 1 to site 3. One consists of two consecutive n.n. hopping during which the electron relaxes by inelastic scattering in site 2. This can be regarded as two resistors, R_{12} and R_{23}, in series, denoted as "$\sim+\sim$". The other is a coherent n.n.n. hopping, corresponding to a resistor R_{13}, denoted as "$\sim\sim$". For "$\sim+\sim$", we have[15]

$$
\begin{aligned}
R("\sim+\sim") &= R_{12} + R_{23} \\
&= R_0 \exp[2\alpha S_{12} + E_{12}/k_B T] + R_0 \exp[2\alpha S_{23} + E_{23}/k_B T],
\end{aligned}
\tag{1}
$$

where α is the wave function decay constant, and the activation energy[2], k_B is the Boltzmann's constant. E_1, E_2 and E_3 are charging energies, S_{12} and S_{23} are inter-site spacing, R_{12}, R_{23}, and R_{13} are hopping resistances, R_0 is a pre-factor of exponent resistance.

$$
E_{ij} = \frac{E_i + E_j + |E_i - E_j|}{2} = Max[E_i, E_j].
\tag{2}
$$

The resistance of "$\sim\sim$" is

$$
R("\sim\sim") = R_0 \exp[2\alpha(S_{12} + S_{23}) + E_{13}/k_B T],
\tag{3}
$$

Overall, we have "~+~" and "~~" in parallel, as shown in Figure 1(*b*), and the equivalent circuit resistance is taken to be the minimum of the two, that is,

$$(R_{12} + R_{23}) // R_{13} \sim Min[R("\sim + \sim"), R("\sim\sim")]. \tag{4}$$

The result of eq. (4) can be viewed as a competition between the two types of conduction paths, "~+~" and "~~". Because the variation in R_{12}, R_{23} and R_{13} is exponential, the equivalent resistance is dominated by either "~+~" or "~~", implying that the approximation in eq. (4) is sufficient for the purpose of calculating ln$R$ of a system. Assessment of the accuracy of eq. (4) shall be provided by the numerical result presented in Sec. III.
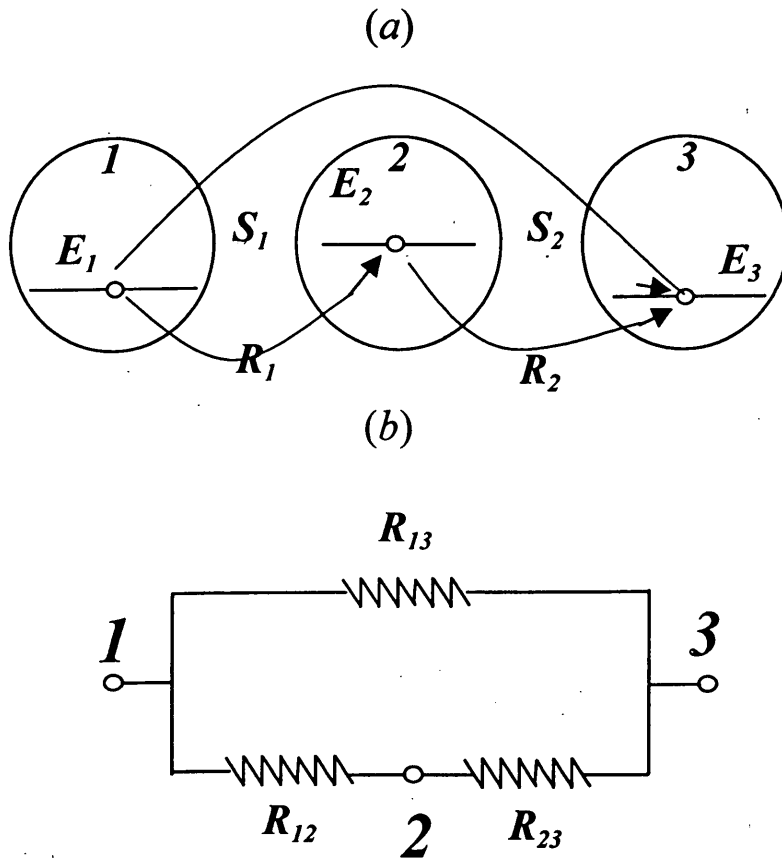

Figure 1. (a) A three-site system showing the initial, intermediate, and final states for both n.n. and n.n.n. hoppings. (b) The equivalent circuit – the serial resistance $R_{12}+R_{23}$ and the resistance R_{13} in parallel.

Next, we perform the critical path analysis. For illustration, here we use a 2-dimensional (2D) triangular lattice of sites to sketch the idea. We consider the lattice as consisting of the clusters shown in Figure 2. Each cluster contains a center site (site I), the shell of n.n. (site A), and the shell of n.n.n.(sites B and C). An n.n.n. here is defined as the site which can be reached from site I by two consecutive n.n. hopping. For each B, we have only one path connecting I to B which consists of two n.n. hopping, and its path number P_B is defined as 1. Correspondingly, there are one "~+~" and one "~~" between I and each B. Other paths to B involve more than 2 n.n. hopping, and are unaccounted for here, as they probably give much higher resistances. Inclusion of these paths, however, is straightforward within our framework.
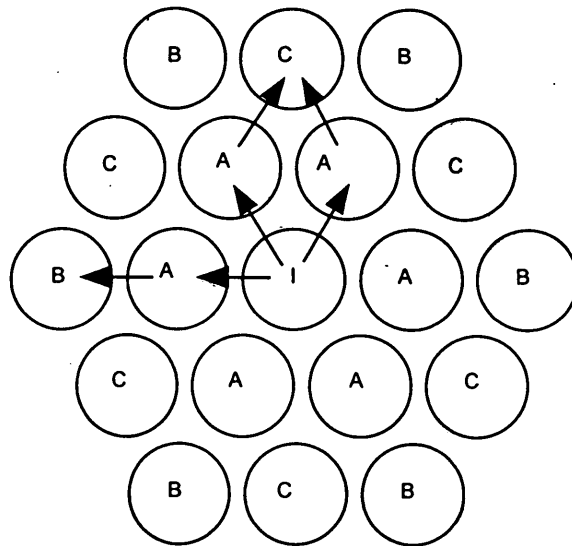

Figure 2. A cluster illustrating the percolation model. There are 6 n.n. sites ("A") and 12 n.n.n. sites ("B" and "C") surrounding the center site ("I"). For "B", there are $Z_B=6$ sites, and the path number $P_B=1$. For "C", there are $Z_C=6$ sites, and the path number $P_C=2$.

The minimum of the foregoing two resistances is taken to be the equivalent resistance between I and B, denoted as R^B and described in eq. (4). For each C, there are two paths connecting I to C as shown in the figure, and, correspondingly, two "$\sim + \sim$" and two "$\sim\sim$" between I and C. Therefore, we have 4 resistances in parallel, and the equivalent resistance, R^C , between I and C, is taken to be the minimum of the 4 resistances

$$R^c \sim Min\left[R^{Pc1}\left(" \sim + \sim "\right), R^{Pc1}\left(" \sim\sim "\right), R^{Pc2}\left(" \sim + \sim "\right), R^{Pc2}\left(" \sim\sim "\right)\right], \qquad (5)$$

where P^{c1} and P^{c2} denote the two paths connecting I to C, respectively. Again, as eq. (4), this equation is accurate enough for the calculation of $\ln R$. Now, consider the percolation problem for the 2D lattice with the clusters as building blocks. We suppress the internal structure of each cluster, and regard each one as nothing but a radial structure with resistors R^B and R^C. If we denote the critical resistance of the 2D system as $R_{critical}$, the percolation condition is that the fraction of resistances in a cluster that are less than $R_{critical}$ must, on the average, be equal to the critical threshold value b_c in the corresponding classical bond percolation problem. In short,

$$b_c \approx \frac{d}{d-1}$$

$$= Z_B \frac{\int dE_1 \rho(E_1) \int dE_2 \rho(E_2) \int dE_3 \rho(E_3) \int dS_{12} P(S_{12}) \int dS_{23} P(S_{23}) \Theta\left(R_c - R^B\right)}{\int_0^{E_m} dE_1 \rho(E_1)}$$

$$+ Z_C \frac{\int dE_1 \rho(E_1) \int dE_2 \rho(E_2) \int dE_3 \rho(E_3) \int dS_{12} P(S_{12}) \int dS_{23} P(S_{23}) \Theta\left(R_c - R^C\right)}{\int_0^{E_m} dE_1 \rho(E_1)}$$

$$(6)$$

where d is the dimensionality of the lattice, Z_B and Z_C are the total numbers of B and C sites, respectively, $E_m = k_B T \ln(R_{critical}/R_0)$, $\rho(E)$ is the energy distribution, and $P(S)$ is the inter-site spacing distribution. $\Theta\left(R_c - R^B\right)$ is a Heaviside step function. The last equation can be solved with numerical simulations to obtain $\ln R_{critical}$ in the following way. For example, in the case of the particular cluster structure shown in Figure 2, we firstly set up the charging energies of I, A, B, and C, and the spacings between I and A, A and B, and A and C, according to some prescribed distributions, and associate resistors according to eq. (1) and (3) with all the paths connecting I to B and I to C (both via A). We then calculate the effective resistances, R^B and R^C according to eq. (4) and (5), respectively. Finally, we require that the fraction of R^B and R^C, which are less than the critical resistance $R_{critical}$ is equal to b_c, as described in eq. (6). This allows us to find $R_{critical}$. We take $R_{critical}$ as the system resistance R.[13]

The above method can be extended to any random or regular lattice, e.g., sc, bcc, fcc, and so on, with corresponding coordination number Z and path number P. In addition, the method can include the next-next-nearest-neighbor (n.n.n.n.) hopping and etc. In the case of n.n.n.n. hopping, for example, three types of resistances appear in the cluster, the serial resistance, "~+~+~", consisting of three consecutive n.n. hoppings, the mixed resistances, "~+~~" and "~~+~", consisting of one n.n. hopping and one coherent n.n.n. hopping, and the coherent resistance "~~~" consisting of a coherent n.n.n.n. hopping.

III. Results and discussion

To assess whether the presented percolation theory is accurate, we have calculated the hopping resistance for a 3-dimensional bcc lattice, and compared it with the corresponding resistor circuit simulation. The calculation includes hoppings up to n.n.n. We take α =0.7A^{-1} from general case of granular metal system, and critical threshold value b_c=d/(d-1)=1.5 for a 3-dimensional bcc lattice. Both the charging energy and the intersite spacing are taken to obey log-normal distributions[2] with the means E_c=159 *meV* and S_{av}=12A, and the widths $\mu_E = 0.6$ and $\mu_S = 0.6$, respectively.

In the resistor circuit simulation, the lattice size is fixed at 15x15x15. We average over a total number of 10 configurations for each resistance calculation, and have checked that the lattice size and the number of configurations are sufficient to give a convergent result.

In the percolation simulation, there are three types of n.n.n. sites on the cluster, B sites in the direction of (1,0,0), S sites in the direction of (1,1,0), and C sites in the direction of (1,1,1). The calculation is done with 20,000 cluster configurations to ensure numerical convergence.

The results of ln(R/R_0) versus $1/\sqrt{T}$ are presented in Figure 3. The result with only n.n. hoppings is included for reference. As shown here, when the temperature lowers, the n.n. hopping-only results begin to bend upwards, showing deviation from the n=1/2 law towards a thermal activation behavior due to the pinning of hopping at n.n. The numerical difference between the n.n. hopping-only and the n.n.n. hopping-included results is substantial at low temperatures. With the n.n.n. hopping, we avoid the hopping-pinning problem. We also note that the percolation

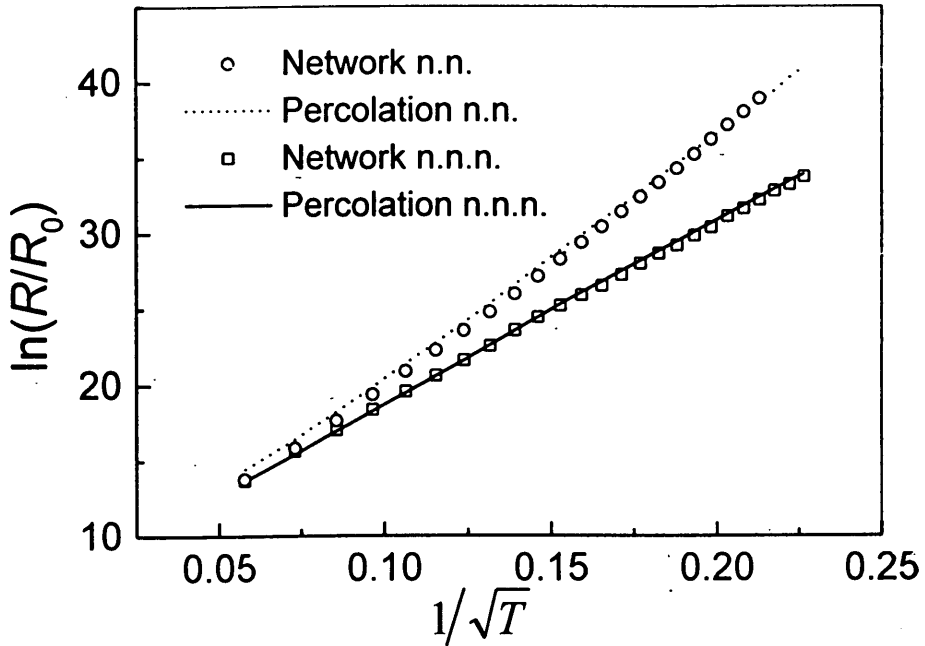result is in remarkable agreement with the corresponding network simulation.

Figure 3. $\ln(R/R_0)$ versus $1/\sqrt{T}$. "$\bigcirc$" - the result of resistor network simulation with only n.n. hoppings. "$\square$" - resistor network simulation with hoppings up to n.n.n. Dotted line - percolation calculation with only n.n. hoppings. Solid line - percolation calculation with hoppings up to n.n.n.

IV. Conclusion

We have demonstrated a percolation method, which includes a local constraint for the calculation of hopping resistance in disordered systems. This constraint is based on the assumption that the effective barrier width for a coherent hopping between non-nearest neighbor sites is the sum of barrier widths between n.n. sites. Good numerical agreement is obtained between the percolation calculation and the corresponding resistor circuit simulation. Because a percolation calculation takes only a small cluster of sites, it has the advantage of saving memory and computer CPU time, and is easily adapted to the problem of a random structure of sites, in contrast to the circuit simulation. It is our hope that this method will aid future theoretical studies of hopping transport in disordered systems.

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無序系統躍遷電導的滲流計算

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中文摘要

　　我們發展出一套應用在無序系統躍遷電導的滲流計算方法。這個方法包含有假設非最鄰近相參性躍遷。此一計算方法在 bcc 晶格上的次鄰近躍遷電導的計算結果，將與電阻網路模擬計算做比較，以評估其此方法計算結果的精確性,結果獲得即佳的一致性。　此一方法將可運用在低溫範圍下，無序系統躍遷電導傳輸的研究上。

關鍵字：：無序系統，滲流，躍遷傳輸，晶格

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