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Direct current hopping conductance in one-dimensional diagonal disordered systems*

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Based on a tight-binding disordered model describing a single electron band, we establish a direct current (dc) electronic hopping transport conductance model of one-dimensional diagonal disordered systems, and also derive a dc conductance formula. By calculating the dc conductivity, the relationships between electric field and conductivity and between temperature and conductivity are analysed, and the role played by the degree of disorder in electronic transport is studied. The results indicate the conductivity of systems decreasing with the increase of the degree of disorder, characteristics of negative differential dependence of resistance on temperature at low temperatures in diagonal disordered systems, and the conductivity of systems decreasing with the increase of electric field, featuring the non-Ohm's law conductivity.

Keywords: direct current hopping conductivity, diagonal disordered systems, the degree of disorder
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1. Introduction

Recently, electronic transport in low dimensional disordered systems has been a subject of intensive experimental and theoretical studies.[1−6] Mott and Davis[7] first figured out the electronic hopping transport mechanism in disordered systems, and then Miller and Abrahams[8] calculated the electronic mobility using a so-called resistor network model. Hunt[9] studied the hopping conductivity of spatially random systems using the theory of percolative transport. Liu *et al*[10] investigated the localized property of Bloch electrons with Coulomb interaction. At present more and more physicists are paying much attention to the effect of the long-range correlations on the physical properties of electron wavefunctions and electronic transport.[11,12] But a complete theory about the electronic transport of disordered systems has not been formed yet; especially, the role played by the degree of disorder in electronic transport of disordered systems has very seldom been studied.

In order to simplify the problem, we neglect the Coulomb interaction of electrons and the effect of correlations in this paper. And we establish a dc electronic hopping transport conductance model of one-dimensional diagonal disordered systems, and derive a dc conductance formulation. By calculating the dc conductivity of disordered systems with 10000 lattice sites, we probe the effects of temperature and electric field on the conductivity of disordered systems. Meanwhile, the role played by the degree of disorder in electronic transport is also analysed.

2. Model

In order to study the electronic properties of one-dimensional disordered systems, we use the simplest form of the tight-binding disordered model describing a single electron band. The Hamiltonian is

$$H = \sum_{i=1}^{N} \varepsilon_i |i\rangle \langle i| + \sum_{i=1}^{N} \sum_{j \neq i}^{N} t_{ij} |i\rangle \langle j| , \qquad (1)$$

where ε_i is the energy assigned to each lattice site i, and t_{ij} is the electronic overlap (hopping term) between the wavefunctions of electrons centred at two neighbouring sites i and j. For a perfectly ordered crystal, all site energies ε_i have the same value or fol-

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low a periodic pattern. For a disordered system, ε_i can be arbitrarily chosen to have a certain probability distribution, for example, a uniform or a Gaussian distribution. The probability distribution generating ε_i is characterized by a parameter W which quantifies the spread of the distribution, and thus the degree of disorder. Then, in the model of one-dimensional disordered systems, we need to consider only two parameters: the degree of disorder, W, and the interaction term between the nearest neighbours, t_{ij}. Thus the controlling parameter is the ratio W/t_{ij}. Typically, t_{ij} is fixed, thus the energy scale in the system is fixed, while W is changed in order to study the effects produced by different levels of disorder.

In the model, we assume the energy ε_i to be uncorrelated and random, the distribution is[13]

$$P(\varepsilon_i) = \begin{cases} 1/W, & |\varepsilon_i| < W/2, \\ 0, & |\varepsilon_i| > W/2. \end{cases} \tag{2}$$

Namely, ε_i is chosen to have a uniform distribution, and W is the distribution width. As for t_{ij}, we assume

$$t_{ij} = -2/\left(|i-j|+1\right), \quad |i-j| \leq 2. \tag{3}$$

If λ is the eigenvalue of the Hamiltonian, and φ is its relevant eigenvector, then

$$H\varphi = \lambda\varphi. \tag{4}$$

So the eigenvalue and eigenvector can be gained by solving the following equation:

$$\begin{bmatrix} \varepsilon_1-\lambda & -1 & -2/3 & & & 0 & \\ -1 & \varepsilon_2-\lambda & -1 & . & & & \\ -2/3 & -1 & \varepsilon_3-\lambda & . & . & & \\ & . & . & . & . & . & \\ & & . & . & \varepsilon_{N-2}-\lambda & -1 & -2/3 \\ & 0 & & . & -1 & \varepsilon_{N-1}-\lambda & -1 \\ & & & & -2/3 & -1 & \varepsilon_N-\lambda \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ . \\ . \\ . \\ b_N \end{bmatrix} = 0. \tag{5}$$

Based on Dean and Martin's negative eigenvalue theory[14] and Wu and Zheng's infinite order perturbation theory,[15] the eigenvectors of disordered systems can be obtained.[16] The method is not only accurate but also efficient. It can compute the matrix with about 10^5 orders, and the computing error is below 10^{-12}. As expected, the electron wavefunctions of the disordered systems present the property of localization. With the increase of degree of disorder, the electron wavefunctions change their characteristics from extended states to localized states. Meanwhile, the stronger the degree to which electrons localize, the shorter the extended length of the wavefunctions. After the electronic localized states are formed, each eigenvector has its own central localized position.[17]

3. Hopping conductivity formulation

In the following, we describe the electronic transport mechanism in one-dimensional diagonal disordered systems using the simplest approach. There are only three necessary conditions for characterizing the hopping process. Under these conditions the dc conductance can be derived, so it is referred to as electronic hopping transport conductance model of one-dimensional disordered systems. The three conditions are given as follows:

1) The electrons are transported through an incoherent hopping process between two localized states with the energy interval being equal to the energy provided by the phonon and the electric field.

2) The probability of the central position R_i of a certain localized state whose eigenvalue is E_i occupied by an electron is characterized by a Fermi distribution

$$f(E_i) = \frac{1}{\exp[(E_i - E_{\mathrm{F}})/k_{\mathrm{B}}T] + 1}. \tag{6}$$

3) The jump rate for an electron to hop from one localized state to another is assumed to be[8,18]

$$\begin{aligned} P =& \nu_{\mathrm{ph}} \exp(-2\gamma R_{ij}) \exp\left(-\frac{E_j - E_i}{k_{\mathrm{B}}T}\right) \\ =& \nu_{\mathrm{ph}} \exp(-2\gamma R_{ij}) \exp\left(-\frac{E_{\mathrm{ph}} + eE'R_{ij}}{k_{\mathrm{B}}T}\right), \end{aligned} \tag{7}$$

where ν_{ph} is the attempt-to-jump frequency which should be a typical phonon frequency, γ is the spatial

decay constant of the wavefunction, R_{ij} is the electron hopping distance, namely $R_{ij} = R_j - R_i$, $E_{\rm ph}$ is the energy of the phonon, and E' is the electric field strength.

Considering the interactions of electron–phonon and electron-electric field, we can obtain the positive current density in the process of the electron hopping from the state $|E_i\rangle$ to the state $|E_j\rangle$, namely,

$$\begin{aligned} j_{ij} =& eP f(E_i)[1 - f(E_j)] \\ =& e\nu_{\rm ph}\exp(-2\gamma R_{ij}) \\ & \times \exp\left(- \frac{E_{\rm ph} + eE'R_{ij}}{k_{\rm B}T}\right) f(E_i)[1 - f(E_j)]. \end{aligned} \tag{8}$$

On the other hand, the electron hops from the state $|E_j\rangle$ to the state $|E_i\rangle$, and the negative current density induced in this process is

$$\begin{aligned} j_{ji} =& eP f(E_j)[1 - f(E_i)] \\ =& e\nu_{\rm ph}\exp(-2\gamma R_{ij}) \\ & \times \exp\left(- \frac{E_{\rm ph} + eE'R_{ij}}{k_{\rm B}T}\right) f(E_j)[1 - f(E_i)]. \end{aligned} \tag{9}$$

So the net current density can be given by

$$\begin{aligned} j =& j_{ij} - j_{ji} \\ =& e\nu_{\rm ph}(E_{\rm ph} + eE'R_{ij}) \\ & \times \exp\left(- 2\gamma R_{ij} - \frac{E_{\rm ph} + eE'R_{ij}}{k_{\rm B}T}\right) \\ & \times \left(- \frac{\partial f(E)}{\partial E}\right). \end{aligned} \tag{10}$$

Then the total current density induced by the electronic transport is

$$\begin{aligned} j_{\rm total} =& \int e\nu_{\rm ph}(E_{\rm ph} + eE'R_{ij}) \\ & \times \exp\left(- 2\gamma R_{ij} - \frac{E_{\rm ph} + eE'R_{ij}}{k_{\rm B}T}\right) \\ & \times \left(- \frac{\partial f(E)}{\partial E}\right) {\rm d}E. \end{aligned} \tag{11}$$

Finally, in terms of the relationship between the current density and electric field strength, we can obtain the dc conductivity of the one-dimensional diagonal disordered systems induced by the electron hopping transport as follows:

$$\begin{aligned} \sigma_{\rm dc} =& \frac{j_{\rm total}}{E'} \\ =& \int \nu_{\rm ph}\left(\frac{eE_{\rm ph}}{E'} + e^2 R_{ij}\right) \\ & \times \exp\left(- 2\gamma R_{ij} - \frac{E_{\rm ph} + eE'R_{ij}}{k_{\rm B}T}\right) \\ & \times \left(- \frac{\partial f(E)}{\partial E}\right) {\rm d}E. \end{aligned} \tag{12}$$

As is well known, it is the electrons with an energy near to the Fermi energy that contribute mainly to the hopping transport conductance. Therefore, the difference in energy between the two localized states in which electrons hop is little, but the localized positions of the electrons can be different significantly. When the temperature is low, the hopping of electrons between the states mainly takes place near Fermi energy. Assuming the electron hopping energies to be equal to each other approximately, the dc conductive formula can be simplified as

$$\begin{aligned} \sigma_{\rm dc} =& \nu_{\rm ph}\left(\frac{eE_{\rm ph}}{E'} + e^2 R_{ij}\right) \\ & \times \exp\left(- 2\gamma R_{ij} - \frac{E_{\rm ph} + eE'R_{ij}}{k_{\rm B}T}\right) \\ & \times \left(- \frac{\partial f(E)}{\partial E}\right) N(E_{\rm F})k_{\rm B}T, \end{aligned} \tag{13}$$

where $N(E_{\rm F})$ is the electron states density near the Fermi energy.

4. Results and discussion

Based on the dc conductance formula, we calculate the conductivity of a one-dimensional diagonal disordered system with 10000 sites.

Figure 1 shows the relationship between the dc conductivity and the degree of disorder, in which the electric field strength is fixed in Fig1(a), while in Fig1(b), the temperature is fixed. It can be seen that the conductivity of the system decreases with the increase of the degree of disorder. It is known that with the increase of degree of disorder, an electron wavefunction changes from an extended state to a localized state, thus the electronic mean free path decreases. And the stronger the degree to which electrons localize, the shorter the extended length of the wavefunctions, then the hopping of electrons from one localized state to another becomes difficult and thus the jump rate decreases, which is the reason why the conductivity of systems decreases with the increase of the degree of disorder.

At the same time, when the degree of disorder is weak, the conductivity oscillates with the change in the degree of disorder in some range. For this phenomenon, we can assume that to a certain degree of disorder, the localized state's distribution is favourable for the hopping of electrons. We know

that the electronic hopping process is an electron–phonon interaction process, namely, a phonon-assisted hopping process. When the energy interval between the two localized states between which the hopping of electrons can take place is equal or near to the energy of phonon, the phonon's energy can be absorbed easily by the electron, then the hopping of electron becomes easy and the hopping probability increases, so we believe that the resonant hopping transport of electron–phonon takes place at this point. When the degree of disorder is strong, the oscillation characteristics of conductivity vanish, and the conductivity is rather low, which is due to the localization becoming dominant seriously, and the hopping probability between different localized states is rather low.

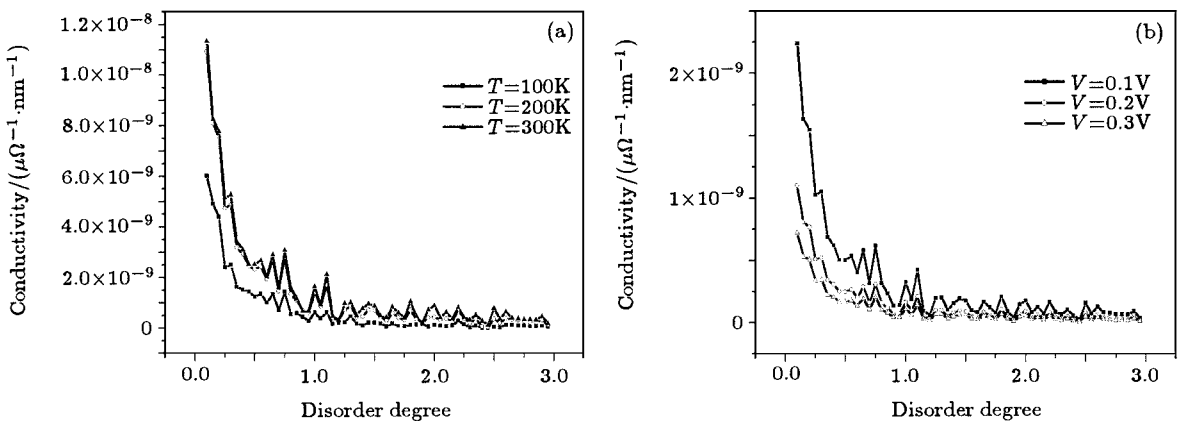


Fig.1. Relationship between dc conductivity and the degree of disorder.

Figure 2 shows the relationship between dc conductivity of a one-dimensional diagonal disordered system and the temperature, in which three curves are drawn at the same electric field strength but different levels of disorder. As can be seen from the curves, at low-temperatures, the disordered system exhibits the characteristics of negative differential dependence of resistance on temperature, namely, the conductivity first increases and then decreases with temperature rising. This fits well with the experimental results of Palasyuk *et al*[19] about the relationship between resistance and temperature of $Y_xMn_yAl_z$. This phenomenon is connected with the hopping of electrons between localized states and can be explained as follows. At low-temperatures, the thermal movement of atoms is not violent, and the electron–phonon scattering is rather weak. With the increase of the temperature, which corresponds to an increase in delocalization, the thermal movement of atoms will be stimulated gradually, which will be beneficial to the hopping of electrons, as a result, the conductivity of systems increases with the increase of temperature. But at high temperatures, the thermal movement of atoms is rather violent, and the inelastic electron–phonon scatterings are predominate, so full delocalization takes place, and the conductivity decreases with the increase of temperature.

Meanwhile, the temperature corresponding to the maximum of conductivity changes with the degree of disorder. We can see from the curves that the larger the degree of disorder in systems, the higher the temperature corresponding to the maximum of conductivity, namely, the conductivity in weakly disordered systems changes with the degree of disorder much more sharply. This phenomenon shows that at low temperatures, the scattering effect in weakly disordered systems increases with the increase of temperature more slowly than in strongly disordered systems, so the conductivity of the system can reach the maximum more quickly.

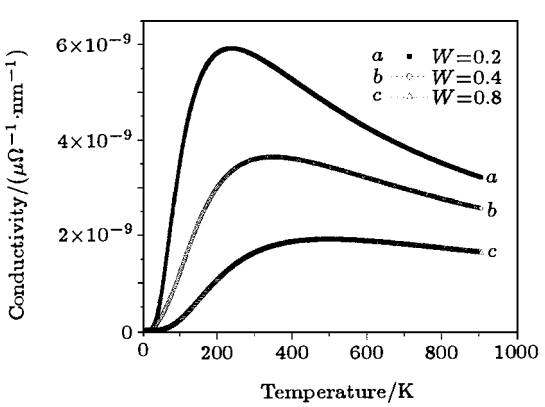


Fig.2. Relationship between dc conductivity and temperature.

Figure 3 shows the relationship between dc conductivity of a one-dimensional diagonal disordered system and the electric field strength, in which three curves are drawn at the same temperature but different levels of disorder. It can be seen that the conductivity of the system decreases with the increase of electric field strength. This characteristic does not coincide with the normal pattern of Ohm's law. We know that in a disordered system, the electron hopping probability varies with the applied electric field strength. And because the electron hopping energy is provided by phonons and the electric field, the dc conductivity in a disordered system varies with the electric field, featuring the non-Ohm law conductivity.

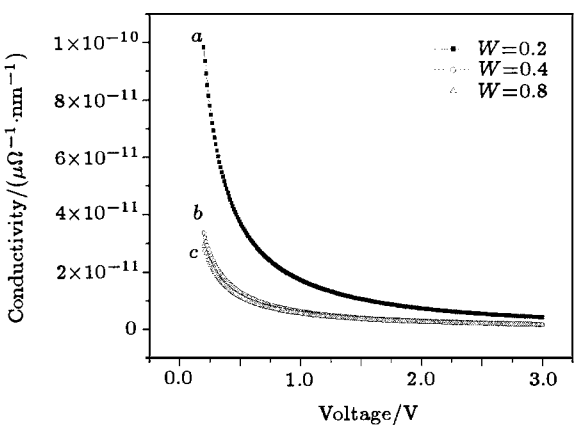


Fig.3. Relationship between dc conductivity and electric field.

5. Conclusions

From the above discussion, we can draw conclusions as follows:

1) The degree of disorder has a great effect on dc conductance of the system, and the conductivity of the system decreases with the increase of the degree of disorder.

2) The dc conductivity of a diagonal disordered system exhibits the characteristics of negative differential dependence of resistance on temperature. At low-temperatures, the dc conductivity of the system increases with the increase of temperature, but the dc conductivity of the system decreases with the increase of temperature at high-temperatures.

3) The temperature corresponding to the maximum value of conductivity varies with the degree of disorder, and the larger the disorder degree of the system, the higher the temperature corresponding to the maximum value of conductivity.

4) The conductivity of the system decreases with the increase of the applied electric field featuring the non-Ohm law conductivity.

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