Quantum diffusion in bilateral doped chains*

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In this paper, we quantitatively study the quantum diffusion in a bilateral doped chain, which is randomly doped on both sides. A tight binding approximation and quantum dynamics are used to calculate the three electronic characteristics: autocorrelation function $C(t)$, the mean square displacement $d(t)$ and the participation number $P(E)$ in different doping situations. The results show that the quantum diffusion is more sensitive to the small ratio of doping than to the big one, there exists a critical doping ratio q_0, and $C(t)$, $d(t)$ and $P(E)$ have different variation trends on different sides of q_0. For the self-doped chain, the doped atoms have tremendous influence on the central states of $P(E)$, which causes the electronic states distributed in other energy bands to aggregate to the central band ($E = 0$) and form quasi-mobility edges there. All of the doped systems experience an incomplete transition of metal-semiconductor-metal.

Keywords: quantum diffusion, doped chain, metal semiconductor transition

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1. Introduction

With the increasing integration of the microelectronic circuit, the requirement for components that possess smaller volumes and better properties has become the main trend in technology development. Of all the materials, nanodevices, such as graphene,[3−5] nanotuber,[6−8] nanowires[9,10] and even one-dimensional chains[11,12], are found to be the most promising candidates and have attracted much attention[1,2] because they are small and have peculiar transport properties. In addition, the appearance of the scanning tuneling microscope (STM) makes it possible to dope and improve materials of this kind.[13]

Naturally, one-dimensional and quasi-one-dimensional chains have the simplest structures and also reflect the most essential things. Though it is still difficult to make an atomic chain that is both perfect and long, however research in this respect has never stopped. Paul Erdös and Herndon[11] discussed this problem in detail and several methods have been developed for this system, such as scattering matrix theory,[14,15] Green's function theory[16−18] and the elastic scattering quantum chemistry (ESQC) technique.[19,20] Dag *et al.*[21] used the density functional theory (DFT) based on the first-principles pseudopotential plane-wave and the generalized gradient approximation (GGA) to analyse the stability of linear chain structures and their magnetic and electronic properties. Time-resolved high resolution transmission electron microscopy (HRTEM) and molecular dynamics (MD) simulations are also used to analyse the atomistic aspects of the mechanical stretching of metallic nanowires of different compositions.[22−25] Zhong and Stocks[26,27] have found some significant results in quantum doping, e.g., in a shell-doped nanowire there are localization/quasi-delocalization transitions and quasi-mobility edges in the energy spectrum, which can be exploited experimentally through the control of electron concentration, carrier density and degree of disorder.[27]

It is well known that a one-dimensional chain will not have good conductance if there is a small disorder in it, which also limits its application. Research of many one-dimensional aperiodic or nonlinear systems have also confirmed this conclusion. For example, in the one-dimensional Anderson model, any diagonal disorder will lead to the localization of all the electronic states;[28] in Fibonacci and generalized Fibonacci chains, the electronic states are either localized or critical,[29,30] both of their transport properties are not good. Then, if there is a pure chain, in which electrons transport well, instead of displacing the atoms in the chain, we put foreign atoms on both

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sides randomly in the same plane, how then will its transport properties change? Hu *et al.*[31] have investigated the transport properties of a random binary side-coupled chain using the transfer-matrix technique and found resonant states in the systems. Until now, the transport properties of the bilateral doped chain under different doping ratios and potential energy modulations have not been discussed. This issue is worth studying.

In this paper we mainly use the tight binding (TB) approximation and quantum dynamics to calculate the transport properties of a single electronic wave packet in the above system. Emphasis is put on the autocorrelation function, mean square displacement and the participation number. To our surprise, a transition of electronic transport is found in all of our doped systems.

2. Model and methodology

There are 1000 atoms in our chain, and the total number of atoms will become even bigger when doping randomly beside the chain. The model is shown in Fig. 1.

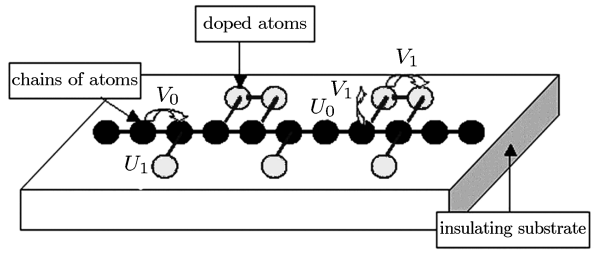


Fig. 1. Model of the bilateral doped chain, the black balls denote the original atoms in the chain, the white balls are the doped foreign atoms.

For this model, the tight-binding Hamiltonian can be expressed as

$$H = \sum_i u_i \left|i\right\rangle\left\langle i\right| + \sum_{i,j} v(i,j) \left|i\right\rangle\left\langle j\right|, \tag{1}$$

where u_i is the site energy for the i-th atom as shown in Fig. 1, with the values of u_i for the original atoms (OA) set to be U_0 and the foreign atoms (FA) assumed to be U_1; $v(i,j)$ is the hopping integral for the nearest neighbours, V_0 is the value for OA–OA bond, V_1 is the value for OA–FA bond and it is also assumed to be the value for FA-FA bond for convenience.

Because of the random doping, we can obtain different chain structures at different doping times. Figure 2 shows a part of the chain with parameter $U_0 = 0.0$, $U_1 = 0.0$, $V_0 = 1.0$, $V_1 = 1.0$ and with different doping atom numbers. Here we define the doping ratio $q = n/m$, n is the number of doped atoms and m is the length of the chain, which is 1000 in our system.

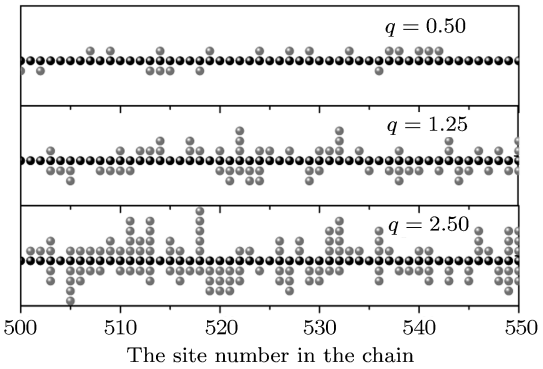


Fig. 2. A part of the chain with parameters $U_0 = 0.0$, $U_1 = 0.0$, $V_0 = 1.0$, $V_1 = 1.0$ under different values of doping ratio q.

When studying the diffusion of the electron wave packet with time, we need to consider the time-contained Schrödinger equation

$$\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\psi}(t) = H\boldsymbol{\psi}(t), \tag{2}$$

where $\boldsymbol{\psi}(t) = (\ldots, \psi_{n-1}(t),\ \psi_n(t),\ \psi_{n+1}(t), \ldots)^{\mathrm{T}}$, with $\psi_n(t)$ being the wave function of the site n at time t. Also, we suppose the initial condition[32] is

$$\left|\psi_n\left(t=0\right)\right| = \delta_{n,n_0}. \tag{3}$$

In other words, the electron is set at the site n_0 at the initial time ($t = 0$). By solving the static Schrödinger equation, one can easily obtain the eigenenergy E_j and the corresponding eigenvector $\boldsymbol{\psi}(E_j)$, $j = 1, \ldots, N$. Because $\boldsymbol{\psi}(E)$ has formed an orthogonal and complete set, the wave function can be expressed as

$$\psi_n(t) = \sum_j C_j \phi_n(E_j) \exp(-\mathrm{i}\,E_j t). \tag{4}$$

From initial condition (3), one can obtain

$$C_j = \varphi^*_{n_0}(E_j). \tag{5}$$

So at time t, the wave function $\psi_n(t)$ is given by

$$\psi_n(t) = \sum_j \varphi^*_{n_0}(E_j)\varphi_n(E_j) \exp(-\mathrm{i}\,E_j t). \tag{6}$$

In order to describe the diffusive motion, one usually introduces two functions: the autocorrelation function $C(t)$ and mean square displacement $d(t)$, which are defined as

$$C(t) = \frac{1}{t}\int_0^t P(t')\,\mathrm{d}t',$$

where

$$P(t) = |\psi_0(t)|^2, \tag{7}$$

and

$$d(t) = \sqrt{\sum_n |\boldsymbol{r}_n - \boldsymbol{r}_{n_0}|^2 |\psi_n(t)|^2}. \tag{8}$$

In addition, we also calculate the participation number $P(E)$, which measures the localization length of a certain state.[28] It is given by

$$P(E)^{-1} = \sum_n \varphi(E, \boldsymbol{r}_n)^4. \tag{9}$$

3. Results and discussion

In the following, the calculated results and the quantitative measurements of the electronic transport will be presented.

3.1. Auto-correlation function $C(t)$

The $C(t)$ is defined as the time-averaged value of the probability that the electron can be found at time t and initial site n_0. For a finite system, because of the boundary effect, we consider only the behaviours of the wave packet before it arrives at the edges.

In many cases, autocorrelation function $C(t)$ has a behaviour that power-law decays with time, which can be described as $C(t) \sim t^{-\delta}$, and the decay index δ is directly related to the transport properties of the system:[33] for ballistic motion, $\delta = 1$, the system is metalic; and for non-ballistic motion, $0 < \delta < 1$, because of ineluctable scattering, the system will be semiconducting. So the stronger the scattering in a system is, the smaller the index δ will be. Fitting the curves with the doping ratios $q = 0$, 0.02, 0.04, 0.10 in Fig. 3, we obtain $\delta_0 > \delta_{0.02} > \delta_{0.04} > \delta_{0.10}$. As expected, the decay index δ decreases with the increase of the doping ratio q, and this change trend continues until the doping ratio reaches 1.25. However, when there is a little more doping ($q > 1.25$), the value of $\ln C(t)$ suddenly increases, which is much different from our traditional views. In this doping period, the conductance of the system becomes better. The transition happens at the doping $q = 1.25$, which is called the critical doping. We calculate the chains with different site energies and hopping integers, and find the same critical doping ratio 1.25.

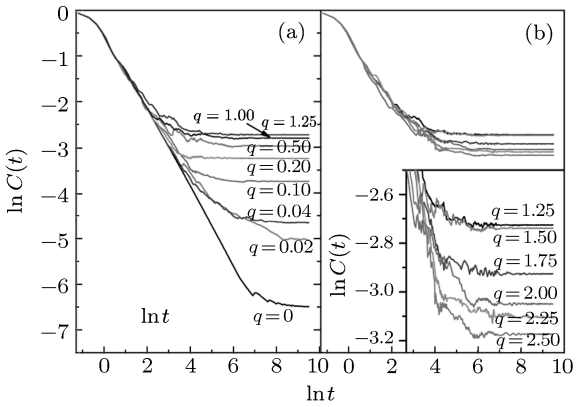


Fig. 3. Autocorrelation function $C(t)$ with initial site $n_0 = 500$ (in the centre of the chain), site energy $U_0 = 0$, $U_1 = 0.5$, hopping integer $V_0 = 1.0$, and $V_1 = 1.0$. (a) The time evolution of $\ln C(t)$ for the doping ratio $q \leq 1.25$. (b) The time evolution of $\ln C(t)$ for the doping ratio $q \geq 1.25$. Insert shows the enlarged plot of $\ln C(t)$ for $q \geq 1.25$.

To understand more about this conduction transition, the mean square displacement $d(t)$ and the participation number $P(E)$ are also discussed in the following.

3.2. Mean square displacement $d(t)$

The mean square displacement $d(t)$ is used to identify different electron dynamic properties, with ballistic motion $d(t) \approx t$, diffusion $d(t) \approx \sqrt{t}$ and localization $d(t \to \infty) = d_0$.[27] The d_0 is the dynamical localization length, which can be understood as the distance the electron moves away from its initial site n_0. Figure 4 exhibits the time evolution of $d(t)$ as a function of the doping ratio. The electron initially locates at the central site of the chain. To avoid a large fluctuation, we calculate the average value of 100 different configurations.

Based on the theory of electron localization in a one-dimensional system,[28] we expect that $d(t)$ is time-independent behaviour over a long time, namely, $d(t \to \infty) = d_0(n)$, where d_0 decreases as q increases. From Fig. 4, it is easily found that for the pure chain, $d(t)$ is linear with respect to t in the first period of time and the motion is ballistic; for the doping situation, $d(t)$ raises crookedly in the first period of time because the electron has been scattered. Then $d(t)$ indeed evolves to d_0 for both situations at a long time, and the electron is localized. At a certain degree of doping ($q = 0$–1.25), d_0 decreases with the increase of q, which is consistent with the traditional view. When the doping has reached a certain degree ($q > 1.25$), d_0 increases slowly with the increase of the doping ratio, which is beyond our expectation , the conductance becomes strong again. This result is consistent with the conclusion given by Zhong and Stocks in Ref. [27].

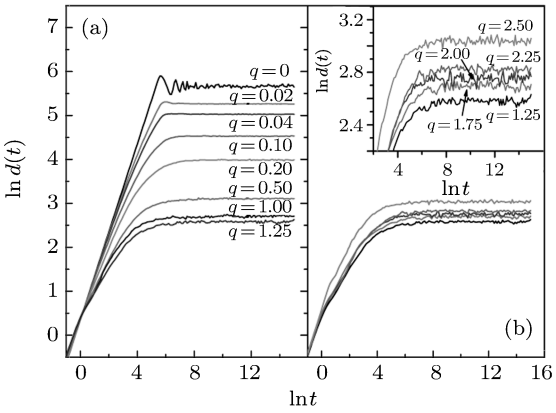


Fig. 4. Mean square displacement $d(t)$, for the chain with different degrees of doping at $U_0 = 0$, $U_1 = 0.5, V_0 = 1.0$, and $V_1 = 1.0$. (a) The time evolution of $\ln d(t)$ for the doping ratio $q \leq 1.25$. (b) The time evolution of $\ln d(t)$ for the doping ratio $q \geq 1.25$. Insert shows the enlarged plot of $\ln d(t)$ for $q \geq 1.25$.

3.3. Max mean square displacement d_0

Considering that d_0 is related to different kinds of dopant atoms, hence, we employ different values of site energy U and hopping integer V here and make a comparison between the results. Figure 5 shows the maxima of $d(t)$ ($d_{\rm m}(t)$) of six chains with different site energies and different hopping integers. The most obvious feature in Fig. 5 is that all the curves of $d_{\rm m}(t)$ we calculated fall by a big margin in the first period of doping, but when they arrive at a critical value, they begin to gradually rise again. This transition is found to take place at the doping ratio $q = 1.25$. It is also surprising that the transport for all of the chains changes at about the same value of q. At the same time, different site energies and hopping integers have different effects on the strength of the scattering, manifesting in different heights of the curves in Fig. 5. To be exact, when comparing the square, circle and inverted triangle curves, we can see that the bigger site energies of the doped atoms (U_1) lead to the larger values of $d_{\rm m}(t)$ in the system. So big values of U_1 are conducive to the electronic transport in the main chain. Comparing the triangle, inverted triangle, rhombus and star curves, again we know that the smaller the value of the hopping integer V_1 is, the stronger the electronic transport in the system is. Large values of V_1 just block the electronic transport here.

It is obvious that all of the above systems have experienced an incompatible transition of metal-semiconductor-metal. However, unlike the Anderson transition,[34,35] this transition is incomplete and occurs at the constant doping ratio $q = 1.25$. It exists in all of our doped chains with this special doped structure, and is modulated by the site energy and the hopping integer of the doped atoms. Then, if we choose the proper kind of atom, we may have a good control of this transition.

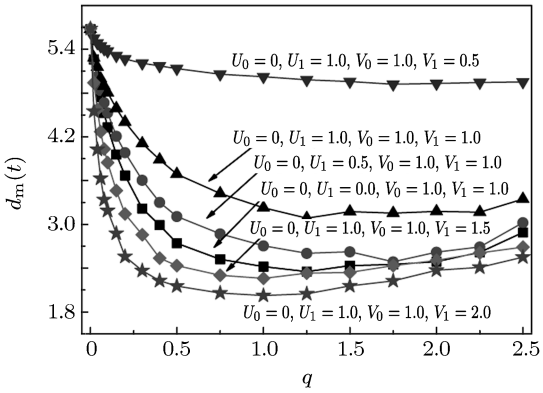


Fig. 5. Maxima of $d(t)$ in different chains, each as a function of the doping ration q.

3.4. Participation number $P(E)$

Similarly, $P(E)$ is also an index of the electronic transport. It reflects the localization length of an electronic eigenstate. Usually $P(E)$ is independent of the size of a system, but here we suppose $P(E) \propto N^D$, where D is the correlation dimension of the wave function and the largest $P(E)$ corresponds to the most extended states in the system.[36] For a localized state $D = 0$, $P(E)$ is small; and for a delocalized wave function that completely extends over the system, $D = 1$ and $P(E)$ is very large. In practice, because of the quantum fluctuation, we make a statistic of 100 models in each doping situation.

Figure 6 shows the participation number of the chain with parameters $U_0 = 0.0$, $U_1 = 0.0$, $V_0 = 1.0$, and $V_1 = 1.0$ (the doped atoms are the same kind atom in the host chain and this behaviour is named self-doping). An obvious fact in Fig. 6 is that $P(E)$ is symmetrical and more sensitive to a small quantity of doping. The $P(E)$ is a constant for a pure chain. For the case of little doping, $P(E)$ becomes fiercely fluctuated and forms a beautiful butterfly-like pattern. When the doping increases, the peaks on both sides come down quickly, while the peak in the centre, which is usually very small, grows higher and higher. At the highest doping, the central peak becomes even more narrow and its height reaches 300, which is the limit of our system. So the eigenstate at E=0 should be the most extended state in the system. The ratio of $P(E)$ between the central states and the bilateral states can be as high as 260 for the last model we doped. If the

width of the peak is $2E_c$, then all the states in the spectrum range $|E| < E_c$ can be considered to be extended and the states in the other ranges ($|E| > E_c$) to be localized. As a result, $P(E)$ undergoes a sharp transition around the energy E_c. So E_c can be considered as the quasi-mobility edge in this system.

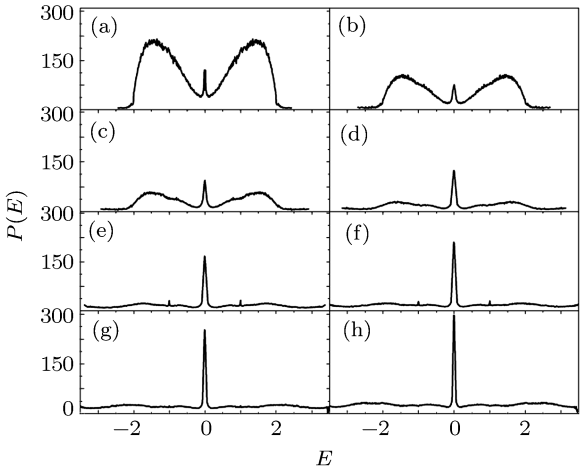


Fig. 6. Participation number of the chain with parameters $U_0 = 0.0$, $U_1 = 0.0$, $V_0 = 1.0$, and $V_1 = 1.0$ for different doping ratio q. (a) $q = 0.04$, (b) $q = 0.10$, (c) $q = 0.20$, (d) $q = 0.50$, (e) $q = 1.00$, (f) $q = 1.50$, (g) $q = 2.00$, and (h) $q = 2.50$.

It seems that $P(E)$ is smooth on both sides beyond the critical doping, but in fact it is not so. Figure 7 shows the enlarged $P(E)$ with doping ratio $q = 1.25$, 1.50, 2.00, and 2.50. The values of $P(E)$ oscillates fiercely between 10 and 33 besides the central states. We can find that the peaks of $P(E)$ on both sides rise up again with the augmentation of the doping ratio. The increasing of $P(E)$ indicates that the conductance is improving. This result confirms the above conclusion. At the same time, we also calculate the participation numbers of other chains and find the same

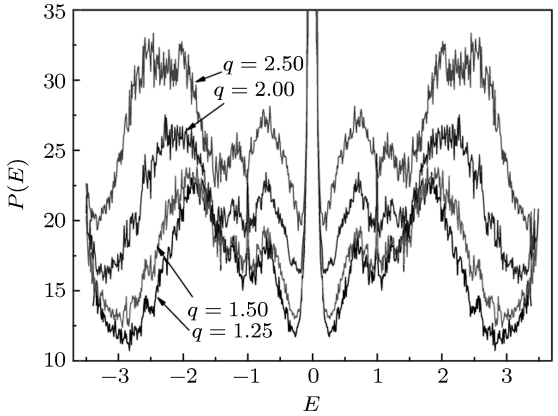


Fig. 7. Enlarged plot of $P(E)$ with doping ratios $q = 1.25$, 1.50, 2.00, and 2.50.

transition. Figure 8 shows the enlarged plot of $P(E)$ for a chain with the parameters $U_0 = 0.0$, $U_1 = 0.5$, $V_0 = 1.0$, and $V_1 = 1.0$. In this case, because of the asymmetrical values of the parameters, $P(E)$ is no longer symmetrical and is fiercely crooked instead.

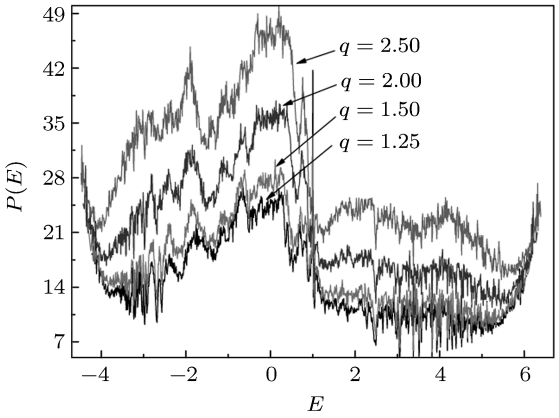


Fig. 8. Participation numbers of the chain with parameters $U_0 = 0.0$, $U_1 = 1.0$, $V_0 = 1.0$, $V_1 = 1.5$.

4. Summary and conclusion

In brief, we numerically investigate the quantum diffusion in a bilateral doped chain. We use the well-known tight binding approximation and quantum dynamics to calculate different chains with different dopings. Three characteristics of electronic transport are taken into account: the autocorrelation function $C(t)$, the mean square displacement $d(t)$ and the participation number $P(E)$. Our results show that the electronic transport becomes weaker and weaker in the first period of doping, but becomes stronger when the doping has reached a certain degree. However, unlike the Anderson transition, this transition is incompletable and happens at the constant doping ratio q=1.25. It exists in all of our doped chains with this special doped structure and is modulated by the site energy and the hopping integer of the dopant atoms. Also, for the symmetry doping, there is a quasi-mobility edge near the central energy spectrum, which separates the extended states from the localized states. The new peculiar properties in this kind of chain, together with the fast development of experimental fabrication,[21−25] could be conducive to the design of nanoscale electronic devices.

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