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Quantum diffusion in semi-infinite periodic and quasiperiodic systems*

Zhang Kai-Wang(张凯旺)†

Department of Physics, Xiangtan University, Hunan 411105, *China*

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This paper studies quantum diffusion in semi-infinite one-dimensional periodic lattice and quasiperiodic Fibonacci lattice. It finds that the quantum diffusion in the semi-infinite periodic lattice shows the same properties as that for the infinite periodic lattice. Different behaviour is found for the semi-infinite Fibonacci lattice. In this case, there are still $C(t) \sim t^{-\delta}$ and $d(t) \sim t^{\beta}$. However, it finds that $0 < \delta < 1$ for smaller time, and $\delta = 0$ for larger time due to the influence of surface localized states. Moreover, β for the semi-infinite Fibonacci lattice is much smaller than that for the infinite Fibonacci lattice. Effects of disorder on the quantum diffusion are also discussed.

Keywords: quantum diffusion, semi-infinite, periodic lattice, quasiperiodic Fibonacci lattice
PACC: 7320D, 7125, 7215

1. Introduction

Stimulated by the discovery of quasicrystals[1] and the fabrication of Fibonacci superlattices,[2] we have paid much attentions to the study of electronic properties of quasicrystals and other related low-dimensional systems.[3−12] Experimental results show that quasicrystals have unusual electronic transport properties.[3] In order to understand these special properties, the study of quantum diffusion in quasiperiodic Hamiltonian systems has attracted considerable interests in recent years.[13−35]

To study the electronic properties of quasiperiodic systems, one always considers the following tight-binding Hamiltonian H:

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

where u_i is site potentials at the ith site, and v_{ij} are hopping matrix elements. In this work, only the nearest-neighbour interactions are considered.

Suppose the electron is initially localized at the site n_0 inside the system. The time evolution of wavefunction $\Psi_n(t)$ can be given by

$$\Psi_n(t) = \sum_j \phi^*_{n_0}(E_j)\phi_n(E_j)\exp(-\mathrm{i}E_j t), \qquad (2)$$

where E_j and $\phi(E_j)$ are the eigenenergies and eigenstates of the static Schrödinger equation respectively.

Two quantities have been introduced to describe the motion of an electron. One is the autocorrelation function $C(t)$,[13−29] the other is the mean square displacement $d(t)$,[21−35] which can be respectively defined as

$$C(t) = \frac{1}{t}\int_0^t P(t)\mathrm{d}t', \quad \text{where} \quad P(t) = \left|\Psi_{n0}(t)\right|^2, \qquad (3)$$

$$d(t) = \langle \Delta r^2 \rangle^{1/2} = \left[\sum_n (n-n_0)^2 \left|\Psi_n(t)\right|^2\right]^{1/2}. \qquad (4)$$

For convenience, we call the diffusion of electron initially located inside an infinite system as body diffusion. On the contrary, when the initial site n_0 is located on the surface of a semi-infinite system, we name it surface quantum diffusion.

In general, one has $C(t) \sim t^{-\delta}$ and $d(t) \sim t^{\beta}$ for body diffusion in periodic and aperiodic systems. In the case of periodic systems, the motion of an electron is ballistic with $\delta = 1$[14] and $\beta = 1$.[28] One-dimensional quasiperiodic systems commonly have singular continuous spectra, and it was shown that already in this case spectrum undergoes a transition from singular to absolute continuous spectrum.[14] For one-dimensional (1D) Fibonacci lattices, calculations show that $0 < \delta < 1$[14] and $0 < \beta < 1$.[25,26] However, it is found that, for higher-dimensional quasiperiodic systems, $C(t)$ exhibits a transition from $\delta = 1$ to $0 < \delta < 1$ upon increasing the modula-

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†E-mail: kwzhang@xtu.edu.cn

tion strength,[14,15,24] but $d(t)$ is still anomalous with $0 < \beta < 1$.[29]

We noticed that all existing studies for quantum diffusion are for the infinite systems, where electrons are initially located at a position inside the system. Thus, an interesting question is: what new feature will occur as to the quantum diffusion in semi-infinite systems? In this paper, we study the surface quantum diffusion in 1D semi-infinite periodic chain and Fibonacci lattices.

2. Surface quantum diffusion in 1D periodic systems

Surface quantum diffusion in a 1D systems is to study the time evolution of a wave packet initially located at the first site of a semi-infinite chain. Here, we investigate the surface quantum diffusion of 1D periodic chain with parameter $u_i = 0$ and $v_{ij} = 1$. From matrix theory, one can directly get the eigenenergies E_j and corresponding eigenstates $\phi(E_j)$ of the Hamiltonian matrix H.

$$E_j = 2\cos\left(\frac{j\pi}{N+1}\right), \quad (j = 1, 2, \cdots, N), \tag{5}$$

$$\phi_n(E_j) = \left(\frac{2}{N+1}\right)^{1/2} \sin\left(\frac{nj\pi}{N+1}\right), \tag{6}$$

where N is the size of systems. Actually, N should tend to ∞. From the initial condition, one can get

$$\begin{aligned}\Psi_n(t) &= \sum_j \phi_1^*(E_j)\phi_n(E_j)\mathrm{e}^{-\mathrm{i}E_j t} \\ &= \sum_j \left(\frac{2}{N+1}\right)\sin\left(\frac{nj\pi}{N+1}\right) \\ &\quad \times \sin\left(\frac{j\pi}{N+1}\right)\mathrm{e}^{(-\mathrm{i}2t\cos(\frac{j\pi}{N+1}))} \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} 2\sin(nx)\sin(x)\mathrm{e}^{-\mathrm{i}2t\cos(x)}\mathrm{d}x \\ &= \frac{(-\mathrm{i})^{n-1}nJ_n(2t)}{t}, \end{aligned} \tag{7}$$

where $J_n(t)$ is the nth-order Bessel function. For $N \to \infty$, one can change the sum into an integral in the above formula.

Then, the autocorrelation function $C(t)$ for surface quantum diffusion can be written as

$$\begin{aligned} C(t) &= \frac{1}{t}\int_0^t |\Psi_1(t')|^2 \mathrm{d}t' \\ &= \frac{1}{t}\int_0^t \left(\frac{J_1(2t')}{t'}\right)^2 \mathrm{d}t'. \end{aligned} \tag{8}$$

Since $|J_1|(t) \leq 1$, the integral in Eq.(8) is convergent for long-time t. Then, one has

$$C(t) \sim t^{-1}. \tag{9}$$

The mean square displacement $d(t)$ can be written as

$$\begin{aligned} d(t) &= \left(\sum_n (n-1)^2 |\Psi_n(t)|^2\right)^{1/2} \\ &= \frac{1}{t}\left[\sum_n (n-1)^2 n^2 J_n^2(2t)\right]^{1/2}. \end{aligned} \tag{10}$$

From the properties of Bessel function, we can get

$$d(t) \sim t. \tag{11}$$

Through the above analysis, one can find that the surface quantum diffusion for the semi-infinite periodic system shows the same behaviour as the body diffusion.[14] In Fig.1, we present the numerical results for the surface quantum diffusion of 1D periodic chain. One can find that the numerical results are in agreement with the analytical results.

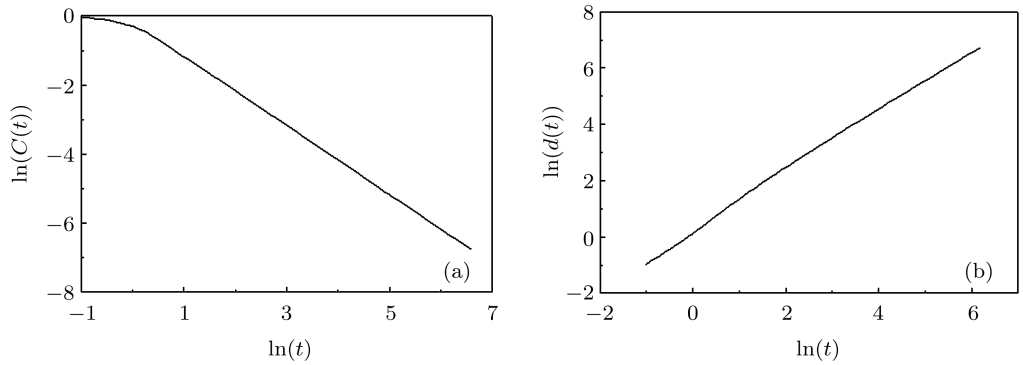


Fig.1. Surface quantum diffusion for 1D periodic chain. (a) Log–log plot of $C(t)$ vs t shows $C(t) \sim t^{-1}$. (b) Log–log plot of $d(t)$ vs t shows $d(t) \sim t$.

3. Surface quantum diffusion in 1D Fibonacci chain

In this section, we investigate the surface quantum diffusion for the semi-infinite 1D diagonal Fibonacci model. Without loss of generality, we assume that $v_{ij} = 1$ and u_i take u and $-u$ according to a Fibonacci sequence. In Fig.2, we show the log–log plots of surface quantum diffusion $C(t)$ versus t for 1D Fibonacci lattices. One can see that the behaviour of $C(t)$ in Fig.2 is different from the body diffusion. With the increase of time t, $C(t)$ firstly decays as $C(t) \sim t^{-\delta}$

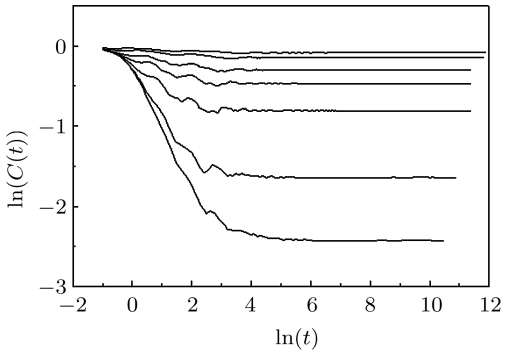


Fig.2. Surface quantum diffusion $C(t)$ for 1D Fibonacci lattices. $u = 0.3$, 0.5, 1.0, 2.0, 3.0, 4.0 from bottom to top, respectively.

with $0 < \delta < 1$, then $C(t)$ equals a constant for larger time, which shows some electrons diffuse toward the systems, but some electrons are always localized at the initial site. The probability staying at the initial site sharply increases with the modulation strength u, which can be found in Fig.3. Moreover, our numerical results show that the behaviour of $C(t)$ is independent on the size of 1D Fibonacci lattices, only related to the parameter u, which further proves the localization of surface electrons.

By more detailed analysis, we find that there exist surface localized states in 1D Fibonacci chain (in Fig.4). The behaviour of surface quantum diffusion $C(t)$ stated above is related to these surface localized states, which can be understood by the following analysis. Suppose that there exists a surface localized state at some eigenenergy E_k of a continuous spectrum, and the eigenstates for other eigenenergies are well-distributed.Let the square of modulus of surface localized states and other eigenstates equal A and B respectively, then the wavefunction $\Psi_1(t)$ at the surface site at time t can be given by:

$$\begin{aligned}\Psi_1(t) &= \sum_j |\phi_1(E_j)|^2 \exp(-\mathrm{i}E_j t) \\ &= |\phi_1(E_k)|^2 \exp(-\mathrm{i}E_k t) \\ &\quad + \sum_{j\neq k} |\phi_1(E_j)|^2 \exp(-\mathrm{i}E_j t) \\ &= A\exp(-\mathrm{i}E_k t) + \sum_{j\neq k} B\exp(-\mathrm{i}E_j t). \quad (12)\end{aligned}$$

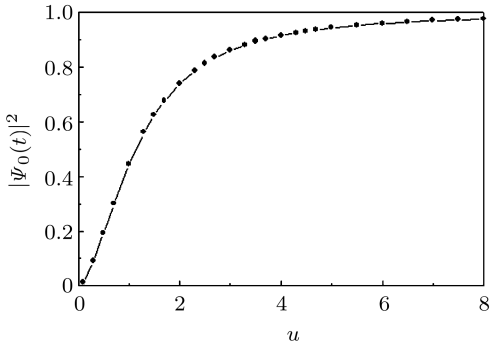


Fig.3. The probability of electron staying at the initial site at large time t for different parameter u.

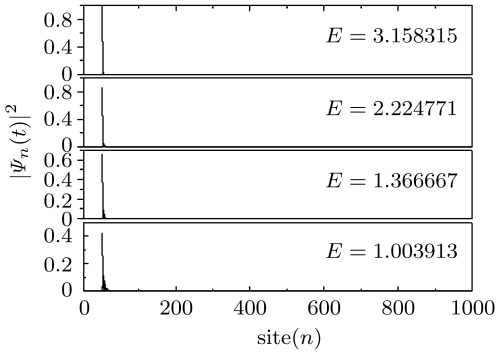


Fig.4. The surface localized states of 1D Fibonacci lattices. From bottom to top, $u = 0.5$, 1.0, 2.0, 3.0, respectively.

The probability $P(t)$ can be written as

$$\begin{aligned}P(t) &= |\Psi_1(t)|^2 \\ &= \left(A\cos(E_k t) + \sum_{j\neq k} B\cos(E_j t)\right)^2 + \left(A\sin(E_k t) + \sum_{j\neq k} B\sin(E_j t)\right)^2\end{aligned}$$

$$= \left(A\cos(E_k t) + \int_{E_0}^{E_k-\varepsilon} B\cos(Et)\mathrm{d}E + \int_{E_k+\varepsilon}^{E_1} B\cos(Et)\mathrm{d}E\right)^2$$
$$+\left(A\sin(E_k t) + \int_{E_0}^{E_k-\varepsilon} B\sin(Et)\mathrm{d}E + \int_{E_k+\varepsilon}^{E_1} B\sin(Et)\mathrm{d}E\right)^2$$
$$= A^2 + \frac{2AB}{t}[\sin((E_1-E_k)t) + \sin((E_k-E_0)t)] + \frac{4B^2}{t^2}\sin^2\left(\frac{(E_1-E_0)t}{2}\right), \quad (13)$$

where ε is an infinitesimal quantity, and we replace the sum by an integral.

Since the integral $\int_0^t \frac{\sin x}{x}\mathrm{d}x$ is convergent, then one can derive the following results from Eq.(13) for the surface quantum diffusion $C(t)$:

$$C(t) = A^2 + ct^{-1}, \quad (14)$$

where c is a constant related to A and B. Equation (14) shows that $C(t)$ decays as $C(t) \sim t^{-1}$ for smaller time t. When t is larger, $C(t)$ is close to A^2. To be worthy pointing out, for 1D Fibonacci lattices, the energy spectrum is a Cantor set and the eigenstates are critical,[4−7] so one get $C(t) \sim t^{-\delta}$ with $0 < \delta < 1$ and $C(t)$ shows weak oscillation for small time t as exhibited in Fig.2. From Fig.4, one can see that the square of modulus A for surface localized states increases with the increase of parameter u, which leads to the exponent-like increase of electronic probability staying at the initial site.

In Fig.5, we show the mean square displacement $d(t)$ for surface quantum diffusion and body diffusion of 1D Fibonacci lattices. One can see that $d(t) \sim t^{\beta}$ with $0 < \beta < 1$ for these two cases. However, the value of β for surface quantum diffusion is much less due to the influence of surface localized states. These suggest that the motion of surface electron is much slower than the one inside the systems, but there still exist partial surface electrons that diffuse toward the system infinitely. Furthermore, one can find obvious self-similar oscillations for the body diffusion, but not for the case of surface quantum diffusion.

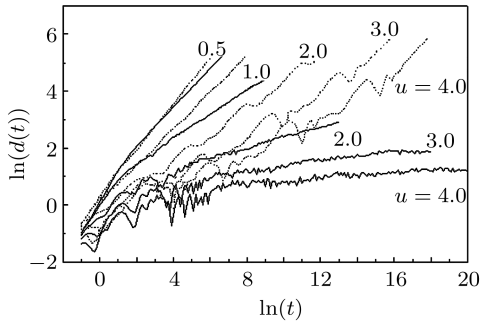


Fig.5. The mean square displacement $d(t)$ for surface quantum diffusion (solid line) and body diffusion (dotted line) of 1D Fibonacci lattices with u = 0.5, 1.0, 2.0, 3.0, 4.0, respectively.

From the above discussion, one can find that the surface quantum diffusion of 1D semi-infinite Fibonacci lattices is different from the body diffusion due to the influence of surface localized states, which is different from the cases of periodic systems.

4. The effect of disorder on surface quantum diffusion

It is well known that the electron is localized in 1D disordered systems. In recent years, large amount of results on the 1D Fibonacci quasilattice shows that its eigenstates are critical[4−7] and the disorder will dramatically change the property of the eigenstates.[5,6] How does disorder affect the motion of an electron in quasiperiodic systems? Here, we take account into the effect of site potential disorder on the surface quantum diffusion in 1D semi-infinite Fibonacci lattices.

Now, let us consider such site potentials $u_i + w_i$, where u_i take value u and –u according to a Fibonacci sequence, and w_i is a random variable homogeneously distributed in the interval $[-w/2, w/2]$. In this case, our numerical calculations show that the electron is localized around the initial site. Figure 6 describes the influence of disordered site potentials on the surface quantum diffusion $d(t)$ of 1D Fibonacci lattices. In Fig.6(a), we fix disorder parameter w and change u, from which one can find that the electron is localized and $d(t)$ tends to a localization length when adding disorder to the site potentials. The localization length decreases with the increase of parameter u. Figure 6(b) presents surface quantum diffusion $d(t)$ varied

with disorder parameter w. Analogously, the disorder results in localization of electron, and the strength of localization increases with the increase of disorder parameter w. Moreover, we also find that the electronic probability staying at the initial site increases with the increase of parameter u or w. All this shows that the surface electrons are completely localized around the initial site, and there is not any electron to diffuse infinitely towards the systems after introducing disorder of site potentials.

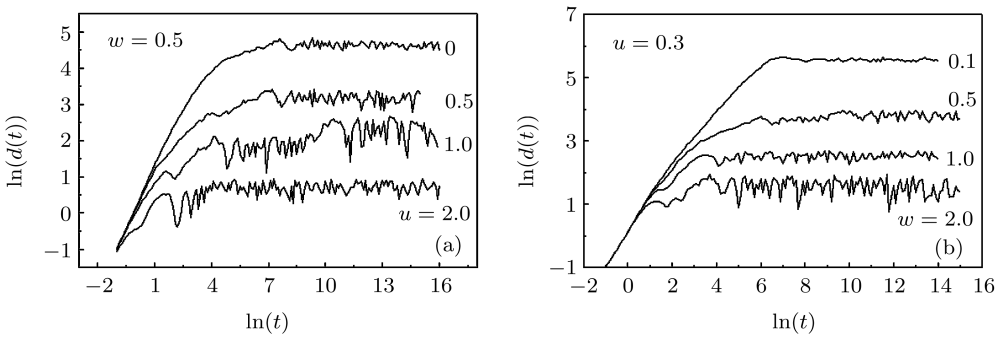


Fig.6. $d(t)$ for surface quantum diffusion when introducing disorder to the site potentials. (a) $w = 0.5$, and $u = 0.0$, 0.5, 1.0, 2.0, respectively (b) $u = 0.3$, and $w = 0.1$, 0.5, 1.0, 2.0, respectively.

5. Conclusions

We have studied the surface quantum diffusion in the semi-infinite periodic chain and the semi-infinite Fibonacci lattice. The surface quantum diffusion for the semi-infinite periodic chain shows $C(t) \sim t^{-1}$ and $d(t) \sim t$, which are the same as the body quantum diffusion. Different behaviour is found for the semi-infinite Fibonacci lattice. In this case, one still has $C(t) \sim t^{-\delta}$ and $d(t) \sim t^{\beta}$. However, one finds $0 < \delta < 1$ for smaller time t, and $\delta = 0$ for larger time due to the influence of surface localized states. β for surface diffusion is much smaller than that for body diffusion. Moreover, we find that surface electrons become localized when adding disorder to the site potentials.

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