Volume 7, Number 3
1004-423X/98/07030196-07

ACTA PHYSICA SINICA
(Overseas Edition)

March, 1998
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# QUANTUM DIFFUSION IN TWO-DIMENSIONAL OCTAGONAL QUASICRYSTALS*

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(Received 4 May 1997; revised manuscript received 22 October 1997)

We have studied the quantum diffusion in an octagonal quasiperiodic tiling. Paticular attention is paid to the analysis of long-time behavior of the autocorrelation function $C(t)$ and the relationship between diffusion and fractal dimensions of energy spectrum. For the pure hopping model, numerical calculations show that $C(t) \sim t^{-1}$, which corresponds to the case of periodic systems. For the combined model, in which the contribution of site potentials is considered, $C(t) \sim t^{-\delta}$ with $0 < \delta \leqslant 1$. The scaling factor $\delta$ is related to Hamiltonian parameters and the type of site where electron is initially located. Moreover, we find a crossover from $\delta = 1$ to $0 < \delta < 1$ with increasing site potentials.

PACC: 7125; 7290

## I. INTRODUCTION

Since the experimental discovery of quasicrystals(QC) by Shechtman *et al.*[1], a large amount of work has been done concerning the electronic nature of QC. Experiments show[2] that QC have special electronic transport properties, which mainly display the increase of conductivity with the increase of disorder and temperature. It is then of fundamental interest to understand such transport law theoretically.

Theoretical investigations on the electronic properties of QC in the earlier stage have been focused on their energy spectra and eigenstates.[3] Recently, more attention has been paid to the quantum diffusion[4-9], which aims at revealing the electronic dynamic feature and the relationship between diffusion and fractal dimensions of energy spectrum. Due to the particular structure of QC, their spectra are different from those of periodic and nonperiodic systems. For higher-dimensional QC, numerical calculations[3,10-12] suggest that the energy spectrum can be one band or band-like with a finite number of gaps, fractal-like with zero band width, or a mixture with some parts band-like and some parts fractal-like. Considering the peculiar spectrum, one thus expects that the electronic dynamics in QC lattices may exhibit new feature, which is related to the unusual transport properties of QC. In this paper, we study the electronic motion in two-dimensional(2D) Penrose tiling.

## II. QUANTUM DIFFUSION

In order to study the diffusion of an electron in a quasiperiodic system, one consid-

* Project supported by the National Natural Science Foundation of China and by the QC Science Foundation of Hunan Province.

ers the following time-dependent Schrödinger equation

$$i\frac{d}{dt}\Psi(t) = H\Psi(t), \tag{1}$$

where $\Psi(t) = (\cdots, \Psi_{n-1}, \Psi_n, \Psi_{n+1}, \cdots)^{\dagger}$ is the wave function at time $t$. $\Psi_n(t)$ is the coefficient of $\Psi(t)$at the $n$th site. The initial condition is as follows

$$\Psi_n(t=0)| = \delta_{n,0}. \tag{2}$$

Equation (1) with the initial condition (2) can be sloved by using the finite step Runge-Kutta method or by solving the static Schrödinger equation

$$H\Phi(E) = E\Phi(E), \tag{3}$$

where $E$ is the eigenenergy and $\Phi(E)$ is the eigenvector, $\Phi(E) = (\cdots, \phi_{n-1}, \phi_n, \phi_{n-1}, \cdots)^{\dagger}$. By solving Eq. (3), one can get all the eigenenergies $E_j (j = 1, 2, \cdots, N)$ and the corresponding eigenstates $\Phi(E_j)$. Since $\Phi(E_j)$ is an orthonormal complete set, the wave function $\Psi(t)$ can be given by

$$\Psi(t) = \sum_j C_j \Phi(E_j)\exp(-iE_j t). \tag{4}$$

From the initial condition (2), it follows that

$$C_j = \phi_0^*(E_j). \tag{5}$$

Then, the wave function $\Psi_n(t)$ is given as

$$\Psi_n(t) = \sum_j \phi_0^*(E_j)\phi_n(E_j)\exp(-iE_j t). \tag{6}$$

Two quantities have been used to describe the electronic diffusion. One is the mean square displacement $d(t)$ of the wave packet, defined as [4-7]

$$d(t) = <\Delta r|^2>^{1/2} = \left(\sum_n |r_n - r_0|^2 |\Psi_n(r_n, t)|^2\right)^{1/2}. \tag{7}$$

The other is the temporal autocorrelation function $C(t)$[8,9],

$$C(t) = \frac{1}{t}\int_0^t P(t')dt', \tag{8}$$

where $P(t) = |\Psi_0(t)|^2$. Evidently, $C(t)$ is the time-averaged version of the probability of the wave packet which is in the initial position at time $t$. One can only treat finite-size system numerically. In order to study the long-time evolution, one considers the behavior of $C(t)$ and $d(t)$ before the wave packet approaches the boundary.

The autocorrelation function $C(t)$ is directly related to the spectrum measure of the system.[8,9] The probability $P(t)$ can be written as

$$P(t) = \left|\int \exp(-iEt)d\mu(E)\right|^2, \tag{9}$$

which is the square of the modulus of the Fourier-Stieltjes transform of measure $\mu(E)$ at the site where the electron is initially placed. From the theory of fractal, the fractal dimension $D_2$ can be defined as[8,9]

$$R(l) = \int d\mu(E)\int_{E-l/2}^{E+l/2} d\mu(E') \sim l^{D_2} \qquad (l \to 0), \tag{10}$$

where $R(l)$ is the spectral probability and $D_2$ is the correlation dimension of the spectrum.

It can be proved[8,9] that

$$R(l) \sim l^{D_2} \quad (l \to 0) \quad \Leftrightarrow \quad C(t) \sim t^{-\delta} \quad (t \to \infty) \tag{11}$$

for $\delta = D_2$. Numerically, $D_2$ can be calculated by the box-counting technique.[8,9] Dividing the energy range into boxes $B_i$ of length $l$, $R(l)$ is then given by

$$R(l) = \sum_i \left[\int_{E \in B_i} \mathrm{d}\mu(E)\right]^2 \sim l^{D_2} \qquad (l \to 0). \tag{12}$$

The calculations of $d(t)$ for one-dimensional (1D) Fibonacci chain show that $d(t)$ obeys the asymptotic behavior as follows[4]

$$d(t) \sim t^{\beta}, \tag{13}$$

$0 < \beta < 1$. And $\beta = 1$ corresponds to the ballistic motion in periodic systems. Guarneri[5] has analytically proved that the power-law growth of $d(t)$ is a feature of 1D systems with singular continuous measures. Moreover, an inequality relation is found

$$\beta \geqslant D_1, \tag{14}$$

where $D_1$ is the information dimension of spectrum measure. Numerical results for the other 1D quasiperiodic systems[6] further confirm the above relation.

For 1D quasiperiodic systems, calculations show that $C(t)$ follows the inverse power-law[8,9]

$$C(t) \sim t^{-\delta}, \tag{15}$$

where $0 < \delta < 1$. In the periodic systems, $\delta = 1$.

For the higher-dimensional Fibonacci lattices, Ref.[9] found that $C(t) \sim t^{-\delta}$. Moreover, $C(t)$ exhibits a transition from a ballistic behavior to a non-ballistic behavior upon varying the modulation strength of the quasi-periodicity.

The electronic dynamics and the relationship between the dynamics and spectral measure in quasi-periodic lattices are far from being understood. To the best of our knowledge, there is not any report about the $C(t)$ in the complex higher-dimensional QC, such as the Penrose tiling. What law does the electronic dynamics follow in the higher-dimensional Penrose lattices? The calculations of $d(t)$ for 2D octagonal quasicrystals(OQC) performed by Passaro *et al*.[7] show $d(t) \sim t^{\beta}$. Moreover, it is found that $\beta = 0.78$ in the pure hopping case while the spectrum has a band-like structure.[10] The non-ballistic motion of an electron in a system with band-like spectrum was thought to be very surprising. In the following, we pay attention to the electronic diffusion in the 2D octagonal lattices. We calculate the $C(t)$ and analyze the relationship between $C(t)$ and energy spectral measure.

## III. ENERGY SPECTRUM AND QUANTUM DIFFUSION IN OCTAGONAL LATTICES

The Penrose lattices used here are generated by grid-dual method(see Fig.1), with atomic orbits located on the vertices. From Fig.1, we can see that the lattice is only composed of thin and fat rhombuses, and the local environments differ from the sites. In Fig.1, there exist seven types of vertices, respectively, with coordination number $Z_n = 2, 3, 4, 5, 6, 7, 8$, in which $Z_n = 2$ corresponds to the sites on the boundary. The frequency of each type of vertex in the infinite octagonal lattices occurs with: $v_1 = w$,

$v_4 = 2w^2$, $v_5 = 2w^3$, $v_6 = 2w^4$, $v_7 = w^5$, $v_8 = w^4$, where $w = \sqrt{2} - 1$.

Similar to Refs. [7, 10 - 12], we consider a system with the number of sites $N$. In the framework of single-particle tight-binding model, the Hamiltonian $H$ has the form

$$H\Phi_n = (1 - v)Z_n\Phi_n + v\sum_{m=1}^{Z_n}\Phi_m, \tag{16}$$

where the sum extends over the neighbors $m$ of the site $n$, and only the interactions along the edge of the rhombuses are cosidered in our work. To the above Hamiltonian, $v = 1$ corresponds to the pure hopping model, where the site potentials are equal to zero. However, when $v \neq 1$, both site potentials and hopping elements contribute simultaneously. This is named here as a combined model. For the latter, site potentials increase with the decrease of the parameter $v$, and the atoms become disconnected when $v \to 0$.

Numerically, we first use Household method to transform the original Hamiltonian to a tridiagonal matrix, then to compute the eigenvalues and eigenvectors. The energy spectra with various values of $v$ are shown in Fig.2($N = 1841$). One can see that the spectra are identical to those obtained by periodic approximants.[10] For the case of $v = 0$, the spectrum consists of discrete levels: $E_n = 2, 3, 4, 5, 6, 7, 8$, in which $E_n = 2$ corresponds to the level of sites on the boundary. Along with the increase of $v$, the energy levels begin to split successively and form a continuous spectrum. From Fig.2, we can also observe that the splitting and overlapping of levels are related to the coordination numbers. For $Z_n = 3, 4, 5$, their levels begin to overlap as $v \approx 0.3$; for $Z_n = 6$, the overlapping of levels occurs at $v$ near 0.4; while for $Z_n = 7$ and 8, we can find obvious intersection up to $v \approx 0.7$. For the pure hopping case ( $v = 1$ ), the spectrum becomes a continuous band-like structure.

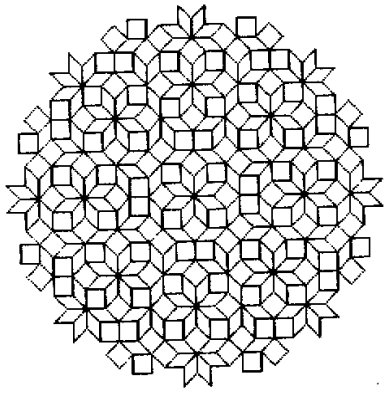

**Fig.1.** The Penrose lattice with an eightfold rotational symmetric axis.

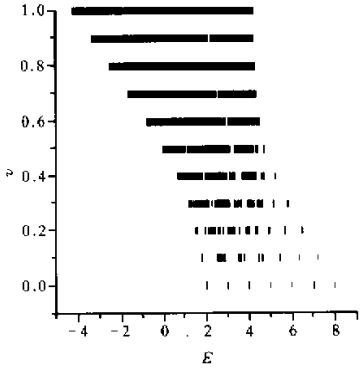


**Fig.2.** Energy spectra $E$ of the Penrose tiling ($N = 1841$), with $0 \leqslant v \leqslant 1$.

In Fig.3, we present $R(t)$ and $C(t)$ for the center site of the octagonal tiling de-

scribed in Fig.1 (pure hopping model ). In order to show whether $R(l)$ and $C(t)$ follow power-law (12) and (15) respectively, we plot them in double logarithm. Figue 3(a) indicates definitely that, for the case of long-time $t$ and small $l$, $R(l) \sim l^{D_2}$, $C(t) \sim t^{-\delta}$. Moreover, the curves of $R(l)$ and $C(t)$ are fairly parallel to each other, suggesting $\delta = D_2$. By translating the curve of $C(t)$ illustrated in Fig.3(a), we find that the curve of log $C(t)$ versus $\log t - 1.18$ coincides with the curve of log $R(l)$ versus-log$l$ (see Fig.3(b)), which clearly indicates $C(t) \sim R(1/t)$ and $\delta = D_2$. In addition, we have computed $C(t)$ and $R(l)$ for other types of sites. We find that the above conclusion is independent of the position where the electron is initially placed. As an example, $C(t)$ and $R(l)$ for the site around the center and with coordination number $Z_n = 3$ are given in Fig.4. One can see that $C(t)$ and $R(l)$ in Fig.4 exhibit the same behavior stated above.

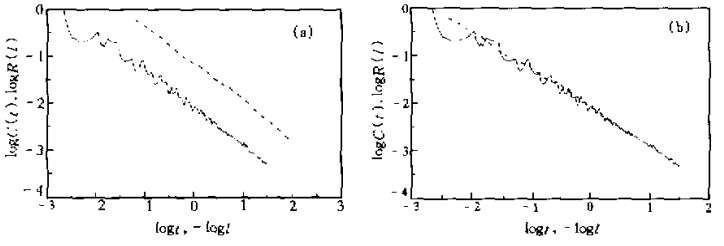


**Fig.3.** $C(t)$ and $R(l)$ for the center site of OQC (pure hopping model ). (a) The log-log plots of $C(t)$ and $R(l)$ are parallel to each other. (b) The plot of log $C(t)$ versus $\log t - 1.18$ coincides with the plot of log$R(l)$ versus-log$l$. Solid curve: log $R(l)$-(- log$l$); dashed curve: log $C(t)$-(log$t$ - 1.18)

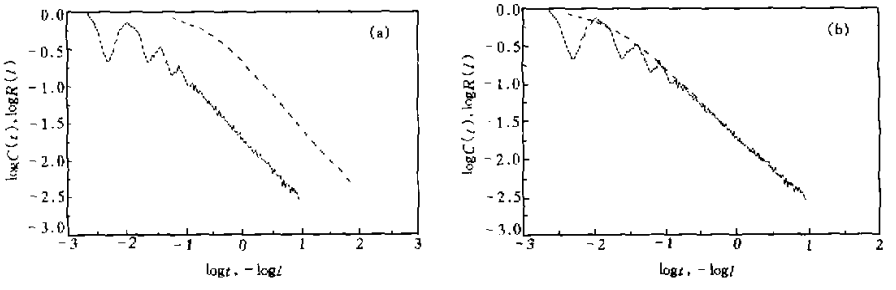


**Fig.4.** $C(t)$ and $R(l)$ for the site around the center and with coordination number $Z_n = 3$ (pure hopping model); (a) and (b) describe the same properties as shown in Fig.3. Solid curve: log$R(l)$-(- log$l$); dashed curve: log $C(t)$-(log$t$ - 1.16)

For periodic systems, one has found[9] $R(l) \sim l^{D_2} (l \to 0)$, $C(t) \sim t^{-\delta} (t \to \infty)$, and $\delta = D_2 = 1$. But it is rather difficult to extract $\delta = D_2 = 1$ directly from the log-log plot due to the limitation of finite-size effect. For instance, in the case of 1D periodic

chain, one usually measures $\delta = 0.84$ for $t < 1000$.[8,9] We also meet the same problem here. Measuring the slope in Figs.3 and 4 shows that $D_2$ and $\delta$ slightly depend on the region of the measurement. Considering $-\log l > -2$, we find $D_2 \approx 0.80$; for $-\log l > -1$, $D_2 \approx 0.81$; and in the case of $-\log l > 0$, we get $D_2 \approx 0.82$. In the following, we take the same way as it was done in the periodic system and Fibonacci chain[9] to deal with the scaling analyses of $R(l)$. For this, we replot $R(l)$ of Figs.3 and 4 in Fig.5. We found $R(l)$ can be fitted as $R(l) \sim l(1 - l^{\lambda})$, where $\lambda \approx 0.031$ for the center site ($Z_n = 8$) and $\lambda \approx 0.036$ for the site($Z_n = 3$) near the center. Because $\lambda > 0$, $R(l) \sim l$ when $l \to 0$. We have known from the above that $C(t) \sim R(1/t)$, hence $C(t) \sim t^{-1}$ when $t \to \infty$.

For the combined model, there is contribution of site potentials. How does $C(t)$ change as $v$ increases from 0 to 1? Figure 6 shows the decay of $C(t)$ for the center site with different values of $v$. Obviously, the results suggest that $C(t) \sim t^{-\delta}$. By a more detailed analysis, we find a crossover with increasing site potentials. Corresponding to $v > v_c \approx 0.7$, the curves of $C(t)$ are nearly parallel to each other with $\delta = 1$, which exhibit similar behavior to that of the periodic system. When $v < v_c$, $0 < \delta < 1$ and $\delta$ decreases with the decrease of $v$. Furthermore, $\delta$ decays more quickly especially when $v$ is relatively small. Apart from these, we have also calculated the correlation dimension $D_2$ for different $v$ and the results show that the relationship (11) still holds for the combined model. By analyzing the behavior of $D_2$, the same crossover stated above is found. For other types of sites, there exists the analogous crossover, but the critical value $v_c$ depends on the type of the site. Therefore, it is necessary to average $C(t)$ over all the sites in the system in order to eliminate the difference of $C(t)$ resulting from the different sites. But for high accuracy of calculation, this problem is left for further study.

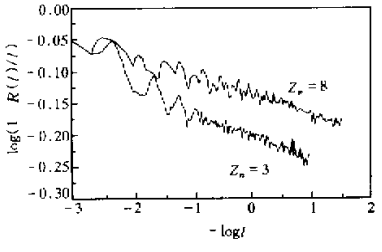


Fig.5. $\log(1 - R(l)/l)$ versus $-\log l$ for the center site ($Z_n = 8$) and the site ($Z_n = 3$) around the center respectively (pure hopping model).

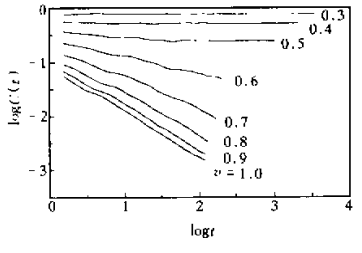


Fig.6. log-log plot of $C(t)$ versus $t$ for the center site($Z_n = 8$) corresponding to different values of $v$ (combined model).

Our numerical results indicate that the long-time behavior of $C(t)$ in the OQC is very similar to that in 2D Fibonacci lattices.[9] For the two models described above $C(t) \sim t^{-1}$, when they show band spectrum. We have known that $d(t) \sim t^{d}$ with

$\beta \geqslant D_1$ in the 1D QC. In the 2D octagonal tiling, Passaro[7] has found $d(t) \sim t^{0.78}$, but the spectrum is continuous. However, from the previous discussion of $C(t)$ and $R(l)$, we have obtained $D_2 = 1$. The value of $\beta$ must be 1 if $\beta \geqslant D_1$ in 2D QC since $D_1 \geqslant D_2$ generally. To be worthy pointing out, $\beta = 0.78$[7] only comes from the calculations of finite-size system, so it is fairly difficult to remove the possibility of $\beta \to 1$ as $t \to \infty$. Analyzing the long-time behavior of $d(t)$ appears particularly significant in order to make clear whether it is suitable or not to use Guarneri formula $\beta \geqslant D_1$ in 2D QC.

## IV. CONCLUSION

We have studied the autocorrelation function $C(t)$ and the spectral probability $R(l)$ for the Penrose lattices with eightfold rotational symmetry. It is found that $R(l) \sim l^{D_2}(l \to 0)$, $C(t) \sim t^{-\delta}(t \to \infty)$, and $\delta = D_2$. For the pure hopping model, the long-time behavior of $C(t)$ for different types of sites exhibits the same behavior as the periodic system, i.e. $\delta = 1$. For the combined model, numerical calculations for the center site show that $C(t) \sim t^{-\delta}$ with $0 < \delta \leqslant 1$. Moreover, there exists a critical value $v_c$. When the modulation parameter $v$ of the potential has $v > v_c$, we have $\delta = 1$. This corresponds to the case of periodic system. When $v < v_c$, we have $0 < \delta < 1$, and $\delta$ decays with decreasing $v$.

## ACKNOWLEGMENT

We are grateful to professors Liu You-yan, Dong Chang, Tian Dei-cheng for their helpful discussions. We also thank Dr. Liu Zheng-qiu for his procedure of generating Penrose lattices.

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