

Quantum electron dynamics in periodic and aperiodic sequences

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(Received 24 June 1994)

We study the electron dynamics in one-dimensional periodic and aperiodic (Thue-Morse) crystals. For the periodic chain the mean-square displacement $\sigma^2(t)$ and the integrated autocorrelation function $C(t)$ of a quantum wave packet put on an initial site display unlimited ballistic motion defined by the asymptotic $\sigma^2(t) \sim t^2$ and the nonexponential $C(t) \sim t^{-1}$ laws. In the spatial distribution of the wave packet we find unexpected “phase chaos” features. For the aperiodic Thue-Morse sequence our numerical results show super-diffusion [$\sigma^2(t) \sim t^{3/2}$] and interesting self-similar oscillations for the “return to the origin” probability. The transmission coefficient of plane waves scattered from the aperiodic Thue-Morse sequence is shown to display self-similar band structure with completely transmissive modes which are related to the corresponding dynamics.

I. INTRODUCTION

The essential difference of periodic and nonperiodic quantum lattice structures mostly lies in the localization properties of their electronic states. In the periodic case all the states are perfectly extended Bloch waves, while in a strongly disordered sequence the states localize because of quantum interference effects.¹ In this respect the absence of quantum diffusion in one-dimensional disordered systems has been rigorously established.^{2,3} The corresponding spectral measure is absolutely continuous and purely pointlike for extended and localized states, respectively. After the experimental discovery of quasicrystals, attention has also been focused in quasiperiodic systems, such as the binary Fibonacci sequence, which lie between the periodic and the random. In this case the band structure becomes singular continuous Cantor-set-like, and the corresponding eigenstates are “critical.” The elucidation of these fractal measures has been the subject of a large number of studies.^{4–10} More recent works have been devoted to the aperiodic deterministic structures, beyond quasiperiodicity, such as the Thue-Morse sequence.^{11–15} The aperiodic sequences display sufficient homogeneity properties and are also believed to be relevant for the physics of quasicrystals. Apart from the purely theoretical interest in the aperiodic and quasiperiodic systems there is now available a large variety of experimental data concerning epitaxially grown superlattice structures by x-ray and neutron diffraction, Raman scattering, etc.^{16,17}

In parallel to the usual approach, which concerns the properties of the time-independent states in the last few years much interest has been focused on the corresponding electron dynamics.^{18–26} The essence of the localization phenomenon is that, if the electron is initially localized in one of the sites it can be found again on the same site after a long time has been elapsed. On the other hand, if the electronic states are extended, the probability of finding the electron again on the initial site decays with time. Recent advances in laser technology have made it possible to study atomic and molecular processes with a time resolution comparable to the quantum-mechanical

time scale.²⁷ From the theoretical viewpoint one can construct simplified models and study the dynamical processes using modern efficient computational techniques.

The problem of dynamics is best exemplified by considering the time-evolution properties of a quantum wave packet left to evolve in the lattice. The propagation is naturally characterized by the so-called mean-square displacement, which is defined as

$$\sigma^2(t) = \sum_n (n - n_0)^2 |\psi_n(t)|^2, \quad (1)$$

where n_0 is the initial site and $\psi_n(t)$ is the wave-packet amplitude on the n th site at time t . The values of $\sigma^2(t)$ give an estimate of the wave-packet spread in space, and, if we focus on the asymptotic long- t behavior, we expect the power-law form

$$\sigma^2(t) \sim t^\mu, \quad (2)$$

where $\mu < 1$ for localization, $\mu = 1$ for ordinary diffusion, $\mu > 1$ for super-diffusion and $\mu = 2$ for ballistic motion. Therefore, the global information about the dynamics of a system can be obtained by calculating $\sigma^2(t)$, either analytically or numerically.

In this paper we systematically investigate the dynamical properties of both periodic and aperiodic sequences. For a periodic sequence the mean-square displacement can be analytically obtained. The corresponding asymptotic behavior shows exact ballistic motion. We also show that the spatial distribution of the wave packet at a given time instant exhibits interesting “phase-chaos” features, despite the simplicity of the model. For the aperiodic Thue-Morse model, instead, via a numerical calculation of the mean-square displacement, for almost all the range of parameters we find super-diffusion. In order to further probe the properties of the aperiodic Thue-Morse sequence we also calculate the transmission coefficient of plane waves through the chain. Our results demonstrate the unambiguous presence of completely reflectionless modes, whose existence is discussed in connection to the dynamical behavior.

The paper is organized as follows: In Sec. II we present the analytical results for the mean-square displacement in the periodic chain and find several interesting figures for the corresponding dynamical process. In Sec. III we numerically calculate the dynamical properties of the Thue-Morse sequence. In Sec. IV the transmission coefficient for plane waves is calculated, and the main results are compared with the conclusions from the preceding sections. A brief summary and a discussion of our results are given in Sec. V.

II. DYNAMICS OF THE PERIODIC SEQUENCE

We start from the one-dimensional (1D) tight-binding Hamiltonian:

$$H = \sum_n \epsilon_n |n\rangle \langle n| + \sum_{\langle NN \rangle} V_{nm} |n\rangle \langle m|, \quad (3)$$

where $|n\rangle$ is the Wannier state of electron on the n th site, ϵ_n is the corresponding energy level, V_{nm} is the hopping matrix element between states $|n\rangle$ and $|m\rangle$ and only the nearest neighbor (NN) hoppings are taken into account. If we express the wave function of an electron in terms of linear combination of states $|n\rangle$

$$\psi = \sum_n \psi_n |n\rangle, \quad (4)$$

from the Hamiltonian of Eq. (3) we have the following set of difference equations for the coefficients ψ_n :

$$V_{n-1,n} \psi_{n-1} + (\epsilon_n - E) \psi_n + V_{n,n+1} \psi_{n+1} = 0, \quad (5)$$

for all n , where the lattice spacing is unity, and E is the corresponding eigenvalue.

For a periodic chain, we choose all site levels to be of zero energy and all the hopping matrix elements to be unity. The corresponding time-dependent wave functions have the Bloch form

$$\psi_k(t) = \frac{1}{\sqrt{N}} \exp(-iE_k t) \sum_n \exp(ikn) |n\rangle, \quad (6)$$

with energy

$$E_k = 2 \cos k, \quad (7)$$

where N denotes the total number of sites. If we put a wave packet on site $n=0$ at $t=0$, its wave function can be expressed as

$$\psi(t) = \frac{1}{\sqrt{N}} \sum_k \psi_k(t). \quad (8)$$

This is just $|0\rangle$ at $t=0$, and the corresponding coefficients are

$$\psi_n(t) = \sum_k \exp(-iE_k t) \exp(ikn). \quad (9)$$

By replacing the sum for k in Eq. (9) by an integral one has

$$\psi_n(t) = \exp\left[-\frac{in\pi}{2}\right] J_n(2t), \quad (10)$$

where $J_n(t)$ is the n th order Bessel function. From this simple calculation the mean-square displacement can be expressed as

$$\begin{aligned} \sigma^2(t) &= \sum_{n=-N/2}^{N/2} n^2 |\psi_n(t)|^2 \\ &= \sum_{n=0}^{N/2} n^2 J_n^2(2t), \end{aligned} \quad (11)$$

and using the properties of the Bessel functions it is easy to obtain the result

$$\sigma^2(t) = 2t^2. \quad (12)$$

Therefore, for an infinite periodic sequence the dynamical behavior is exactly ballistic. At the same time, the probability density $P_0(t)$ to find the particle at site 0 at time t is given by

$$P_0(t) = |\psi_0(t)|^2 = |J_0(2t)|^2, \quad (13)$$

whose asymptotic behavior for large t is⁶

$$P_0(t) \sim 0.39894 t^{-1} \cos^2(2t). \quad (14)$$

A temporal autocorrelation function $C(t)$ can be defined by smoothing $P_0(t)$:⁷

$$C(t) = \frac{1}{t} \int_0^t dt' P_0(t'), \quad (15)$$

and for the periodic chain we obtain the following power law:

$$C(t) \sim t^{-1}, \quad (16)$$

for large t .

In Fig. 1, we demonstrate the spatial variation of $|\psi_n(t)|^2$ for different time instants t . The value of the amplitude on a given site, at a given time, is represented by a dot. It is interesting that the dots seem to be randomly distributed under an envelope curve, and the peaks of the wave packet are at the two ends. In fact, the initial wave packet is a composition of all the plane waves within a continuous band. At time t , only the modes with group velocity s/t can reach the site having distance s away from the site 0. Thus, the envelope curve represents the density of states per group velocity as a function of s . For a plane wave, the group velocity is $2 \sin k$ and the envelope function is proportional to $1/\sqrt{1-(s/t)^2}$, which can be seen in the figures. Because for each group velocity, $2 \sin k$, two values of k correspond in the Brillouin zone, whose difference is $\delta k = \pi - 2|\arcsin(s/2t)|$, the probability amplitude at a given site is the result of the interference between the two modes depending on their phase difference. If $\delta k/\pi$ is an irrational number at a site, the dots on the nearby sites may take almost any value under the envelope and exhibit phase-chaos behavior. On the contrary, if $\delta k/\pi$ is rational at a site the dots on the nearby sites can only reach several isolated values, which opens windows in the chaotic structure, as it can be seen from the corresponding figures. Thus, if the initial wave packet consists of a continuous spectrum of modes, the dynamical process may display chaotic

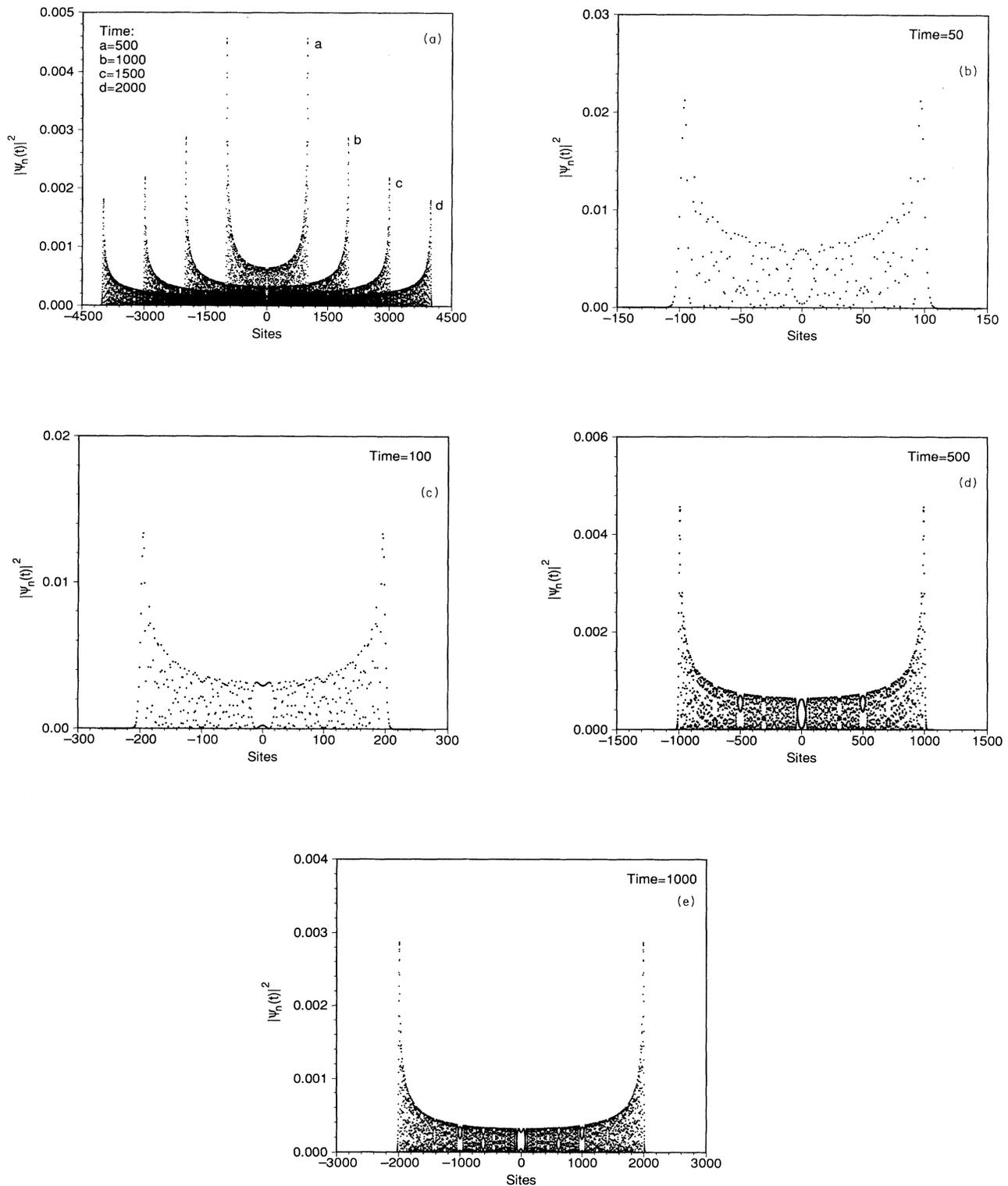


FIG. 1. (a) The variation of the spatial distribution of the wave packet in a periodic sequence for different times t . The probability amplitudes are indicated by the dots and set a is taken for $t = 500$, set b for $t = 1000$, set c for $t = 1500$, and set d for $t = 2000$. The units of time are \hbar/E_0 , where E_0 is the unit of energy taken to be the NN hopping. (b) The details of distribution at time $t = 50$. (c) The details of distribution at $t = 100$. (d) The details of distribution at $t = 500$. (e) The details of distribution at $t = 1000$.

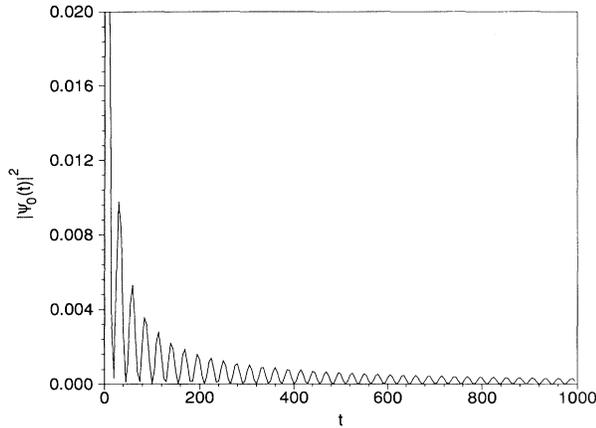


FIG. 2. The probability of finding at the initial site 0, as a function of time t , in the periodic sequence.

features, despite the linearity of the model.

In Fig. 2 we illustrate the variation of the amplitude $P_0(t) = |\psi_0(t)|^2$ on the initial site 0 versus time t . The oscillatory behavior reflects the quantum characteristics of the diffusion. In Fig. 3 we plot the integrated autocorrelation function $C(t)$. It is interesting to notice that the decay of $C(t)$ for long times is power-law-like. The slope of the log-log curve gives the corresponding exponent, which is seen to vary with time starting from 0.84 for short times and eventually approaching 1.0 for larger times.

III. DYNAMICS IN THE THUE-MORSE SEQUENCE

As an example of an aperiodic system we choose the Thue-Morse sequence. The corresponding eigenstates have a Bloch-like character and are clearly different from those of the quasiperiodic (e.g., Fibonacci) and the disor-

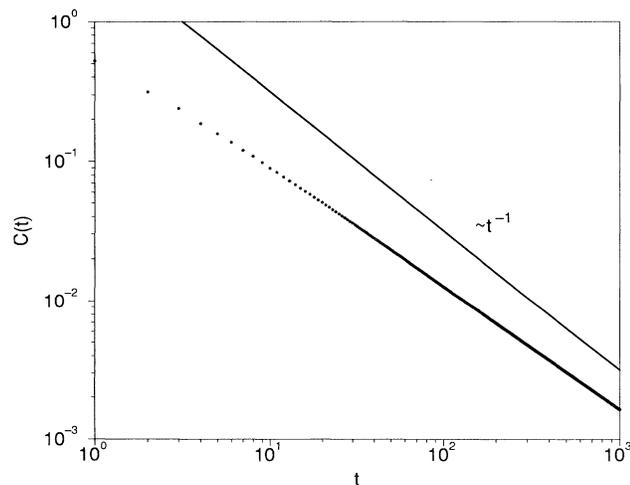


FIG. 3. The integrated autocorrelation function, as a function of time t , is plotted in a log-log scale. The ballistic limit $C(t) \sim t^{-1}$ is also shown by the continuous line, which is approached for long times.

dered chains. The 1D lattice consists of two species of the atoms, one denoted by A and the other denoted by B , arranged in aperiodic fashion according to the Thue-Morse sequence.¹¹ This construction can be achieved by appending to each sequence the complemented subsequence, as follows:

$$\begin{aligned} &A, \\ &AB, \\ &ABBA, \\ &ABBABAAB, \\ &ABBABAABBAABBA, \end{aligned}$$

which is equivalent to making the substitutions $A \rightarrow AB$ and $B \rightarrow BA$. If we use l to label the generations of this construction, the total number of sites N is 2^{l-1} for the l th generation. In the limit $l \rightarrow \infty$, the sequence is aperiodic and has the property that every second term in the sequence reproduces the sequence in a self-similar form. The Thue-Morse sequence has a singular continuous Fourier transform different from the quasiperiodic Fibonacci chain, whose Fourier transform is discrete and exhibits Bragg peaks.¹¹

We have used the tight-binding Hamiltonian of Eq. (3) to describe the electronic Thue-Morse sequence by taking the NN hopping to be 1 and the energy levels for the atoms A and B to be V and $-V$, respectively. Initially we put the wave packet at a central 0 site and investigate the dynamic behavior by numerical integration of the corresponding time-dependent Schrödinger equation

$$i \frac{\partial \psi(t)}{\partial t} = H \psi(t). \quad (17)$$

The fourth-order Runge-Kutta method is employed. Our results have also been checked via a direct numerical diagonalization of the Hamiltonian H .

In Fig. 4 we show our results for the mean-square dis-

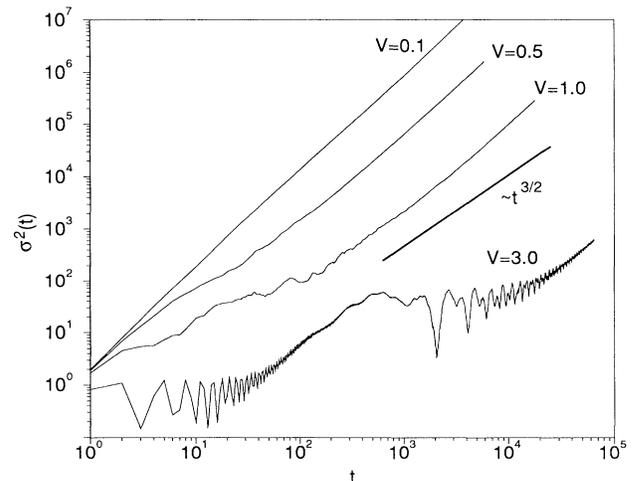


FIG. 4. The mean-square displacement of a wave packet in the Thue-Morse sequence, as a function of time and for different V values, plotted in log-log coordinates.

placement $\sigma^2(t)$ for various values of V . The asymptotic behavior for large t is of a power-law form, but the corresponding exponent μ is strongly dependent on the value of V . For small V , the difference in energy level between atoms A and B is small, and the behavior of the system is close to that of the periodic sequence. The value of μ is smaller than, but close to the ballistic limit of 2. If V is increased, the difference between Thue-Morse and the periodic chain sequence increases, while the corresponding exponent is decreased, being close to 3/2 for large V . Therefore, the wave-packet motion is of super-diffusive nature clearly different from the laws obtained for the periodic or the disordered chains. Moreover, it reflects the Bloch-like behavior of the corresponding eigenstates.

In order to further probe the dynamics we introduce the information entropy

$$S(t) = - \sum_n |\psi_n(t)|^2 \log_{10} |\psi_n(t)|^2, \quad (18)$$

which is an alternative measure to describe the character of the wave packet in the diffusion processes.²⁶ In Fig. 5 we plot $S(t)$ versus $\log_{10} t$ for the Thue-Morse sequences and various values of V . For small V , it increases almost monotonically with t , which means that the wave packet spreads out continuously, similarly to the situation in the periodic case. On the other hand, if V is large enough the information entropy exhibits heavy oscillatory features in time. This is due to the complicated transmissive and reflective behavior of the subsequences for different modes, which are included in the wave packet.

In Fig. 6 we plot the probability density for finding the particle at site 0, or the "return-to-the-origin" probability, at time t . It is shown to oscillate for all values of V decaying much more slowly than for the corresponding wave packet in the periodic sequence. Moreover, the oscillations exhibit some kind of self-similar structure, which becomes more evident for high values of V . The origin of this self-similar behavior in time arises from the

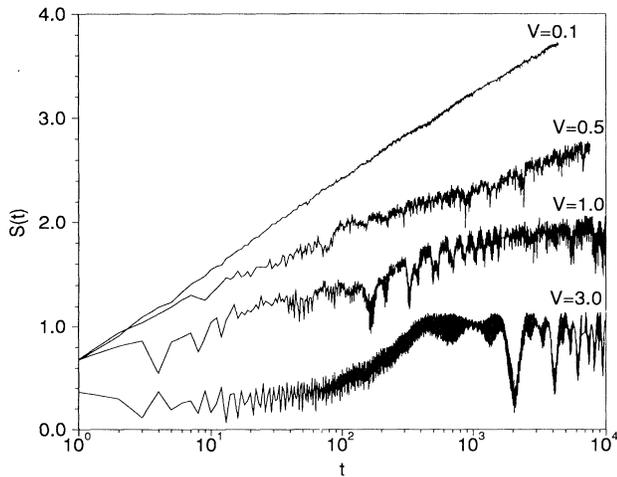


FIG. 5. The information entropy as a function of time for the diffusion of a wave packet in the Thue-Morse sequence.

self-similar structure of the sequence in space. This, in turn, produces self-similar structures of the transmission and the reflection coefficients versus the energy (or the frequency) of the corresponding modes.

In Fig. 7 we show the shape of the wave packet at different instants of time. By comparison with the corresponding periodic case (Fig. 1) it is interesting to notice that the chaotic features now disappear, while the two peaks at the edges are replaced by complicated peaks near the central site. This is due to the filtering effect of the subsequences for the plane-wave modes included in the wave packet. As will be seen in the next section, only the modes in several narrow bands or subbands are transmissive through the subsequences. Moreover, for a comparatively large distance only a few selected modes exist and the diffusion process does not exhibit the phase-chaos properties present in the purely periodic structure.

IV. TRANSMISSION COEFFICIENT OF PLANE WAVES THROUGH THE THUE-MORSE SEQUENCE

In the preceding sections we investigated the diffusion motion of a wave packet in periodic and aperiodic sequences. Since a wave packet can be decomposed into an infinite number of plane-wave modes of a continuous spectrum, the behavior of this diffusive motion is closely related to the transmission coefficient from the sequence for different modes. As the transmission coefficient in a periodic sequence is quite trivial (it is unity within the band and zero outside the band), we focus only on the transmission coefficient in the aperiodic case.

From the Hamiltonian of Eq. (3), the coefficients of a plane wave in adjacent sites are related by a transfer matrix via

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = \hat{T}_n \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}, \quad (19)$$

where \hat{T}_n is the 2×2 matrix

$$\hat{T}_n = \begin{pmatrix} E - \epsilon_n & -1 \\ 1 & 0 \end{pmatrix}.$$

If we insert a Thue-Morse sequence with N sites of species A and B into a periodic chain made of species A , and let a plane wave propagate towards the sequence from the left then the transmission coefficient, which measures the intensity of transmitted wave, is

$$|t|^2 = \frac{4 \sin^2 k}{[T_{21} - T_{12} + (T_{22} - T_{11}) \cos k]^2 + (T_{11} + T_{22})^2 \sin^2 k}, \quad (20)$$

where $T_{11}, T_{12}, T_{21}, T_{22}$ are the elements of matrix \hat{T} , defined by

$$\hat{T} = \begin{pmatrix} E - V & -1 \\ 1 & 0 \end{pmatrix} \prod_{i=1}^N \hat{T}_{N-i+1}.$$

The wave vector of the incident plane wave is k and for

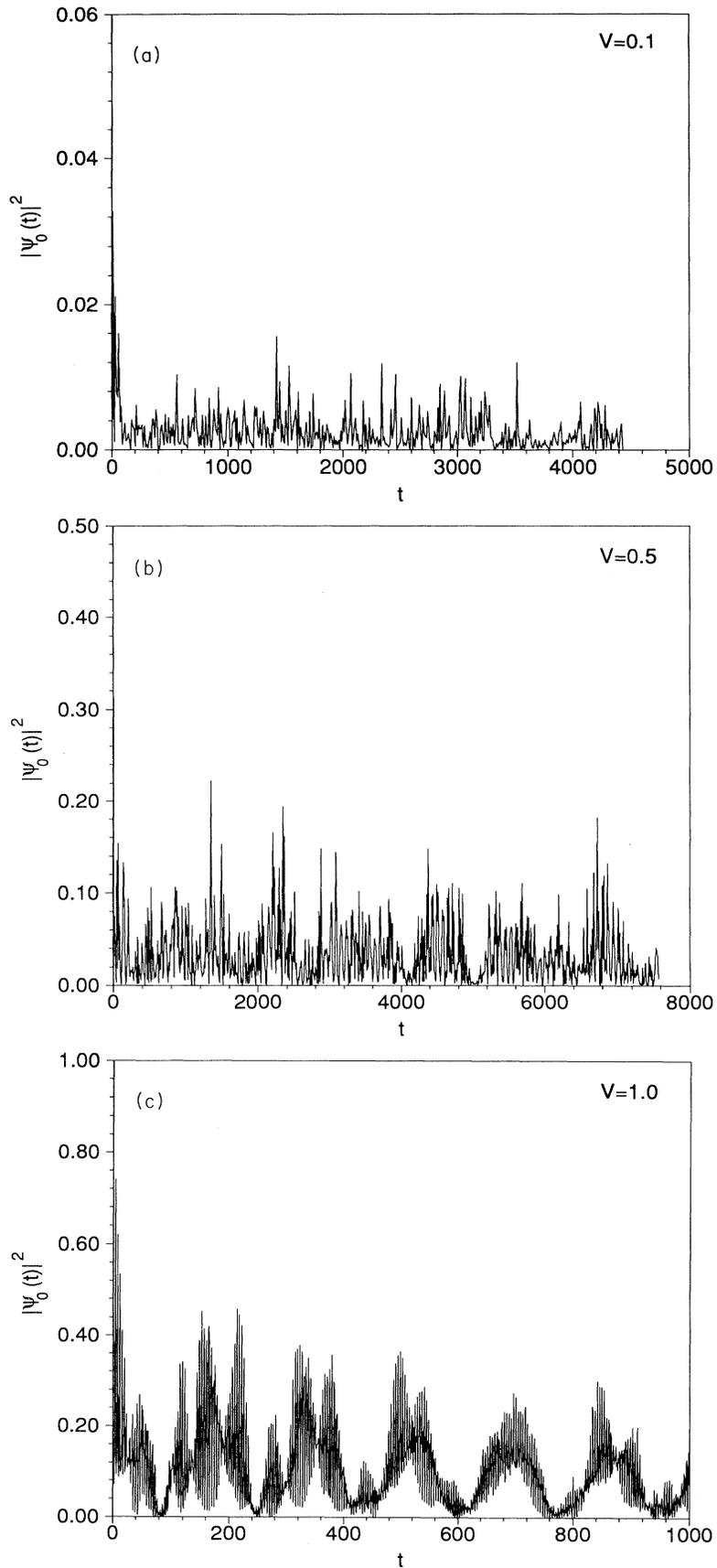


FIG. 6. The return-to-the-origin probability density $P_0(t)$, of finding the particle at site 0 as a function of time t , for the wave packet diffusion in the Thue-Morse sequence: (a) $V=0.1$, (b) $V=0.5$, (c) $V=1.0$, (d) $V=3.0$, and (e) $V=5.0$. For the cases (d) and (e) certain enlarged parts are shown in the inserted figures.

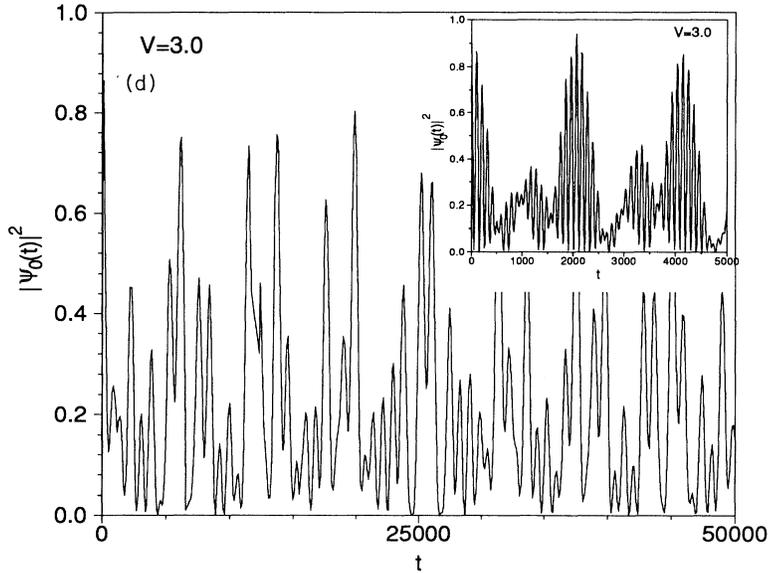
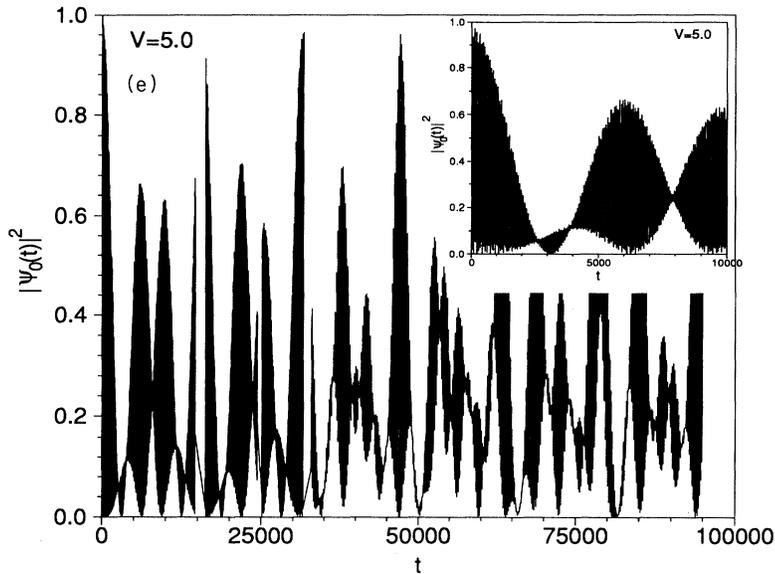


FIG. 6. (Continued).



the periodic chain is related to E by

$$E = 2 \cos k + V.$$

In Fig. 8 we plot the transmission coefficient as a function of energy for $V=0.5$ and 1.0 . Although most of the plane-wave modes are completely reflected by the sequence, we notice that there also exist several groups of modes, which remain completely unscattered ($|t|^2=1$). Unlike the isolated transmissive modes in Fibonacci sequence and in chains with correlated disorder^{8,25} in the Thue-Morse sequence these modes form a kind of band, which is fragmented into smaller subbands. In the self-similar band structure the main bands decompose into subbands whose width reduces when V increases. Such a transmissive band structure reflects the Bloch-like feature of the Thue-Morse sequence. For a further demonstra-

tion of this behavior, we have calculated the total bandwidth as a function of the number of sites imposing a periodic boundary condition to the two ends of the chain. The results are shown in Fig. 9, where it is seen that the band width is reduced and eventually reaches a finite limit when $N \rightarrow \infty$. This is consistent with the presence of absolutely continuous parts in the spectrum and also displays the Bloch-like character of the eigenstates. In quasiperiodic systems the total bandwidth vanishes as a power-law (singular continuous spectrum) and exponentially for localized states (pure point spectrum). For a given finite N the bandwidth becomes narrower when V is increased, which is also compatible with the results obtained from the transmission coefficient.

In the diffusion process the modes with zero transmission coefficient are resident within some subsequences and only the transmissive modes can return to the origin.

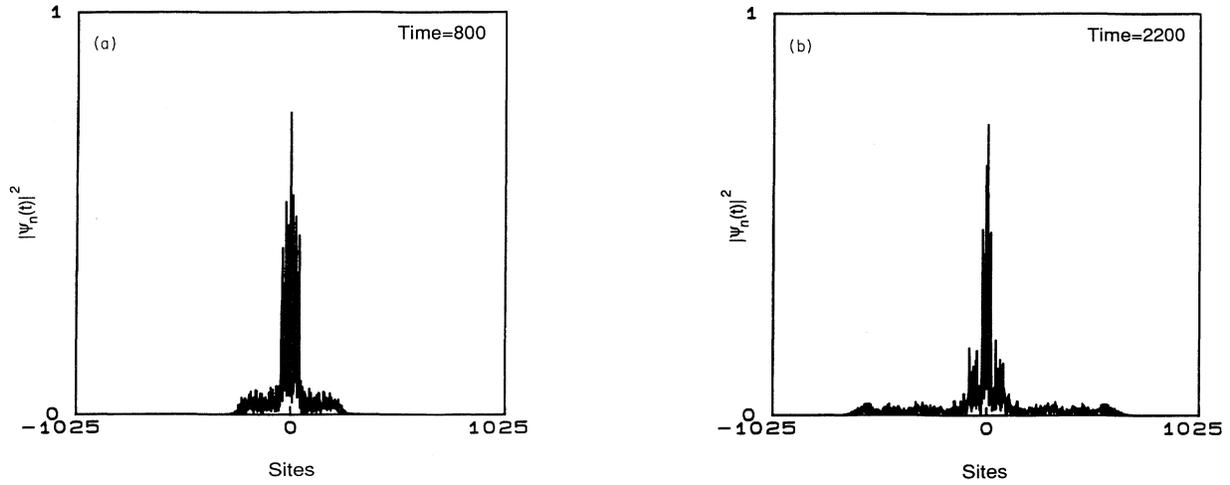


FIG. 7. The spatial distribution of a wavepacket in the Thue-Morse sequence for two different times: (a) $t = 800$ and (b) $t = 2200$.

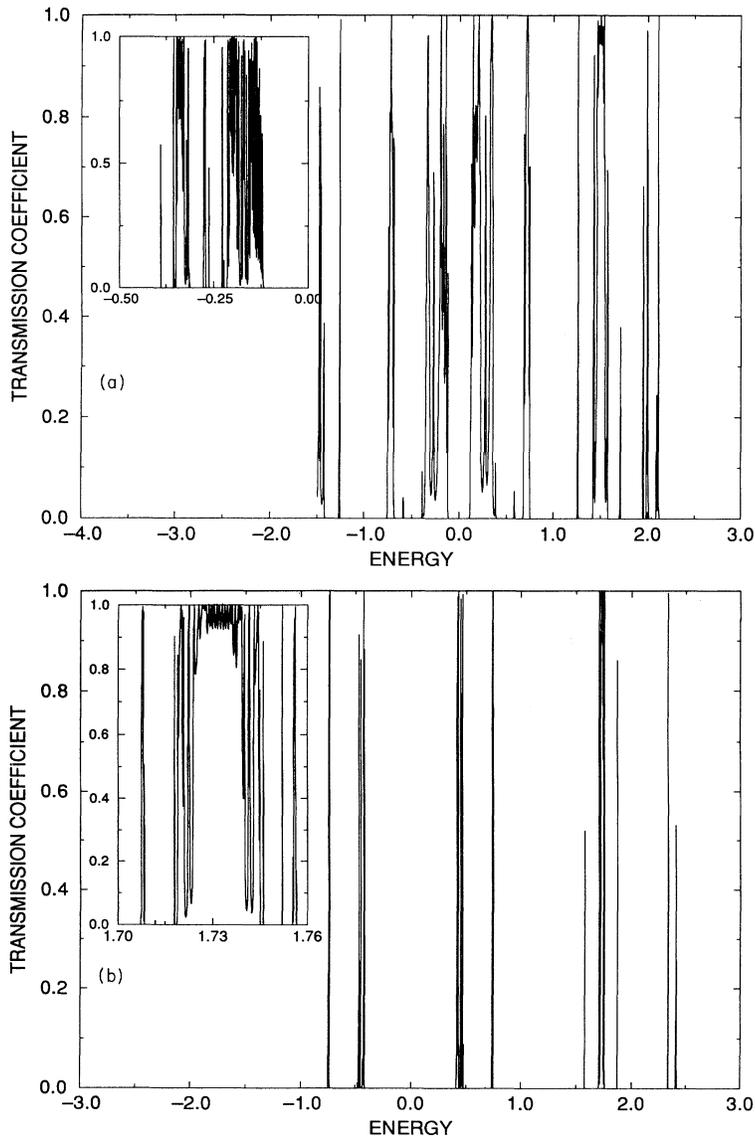


FIG. 8. The transmission coefficient $|t|^2$ as a function of energy E for the Thue-Morse sequence. Enlarged parts are shown in the inserted figures. The values of V are (a) $V = 0.5$ and (b) $V = 1.0$.

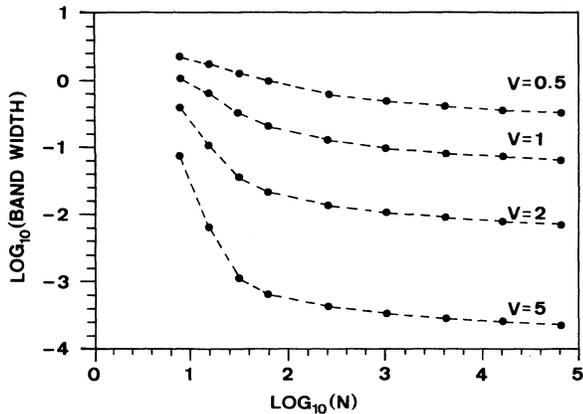


FIG. 9. The log-log plot of the total band width as a function of the number of sites of a Thue-Morse sequence for which periodic boundary conditions are imposed in the two ends. The value of V is indicated besides the curves. The absolutely continuous component of the spectrum can be concluded from the finite limit as $N \rightarrow \infty$.

As a result, the return probability density $P_0(t)$, defined in the last section, reflects the spectral character of the transmission coefficient. For $V=0$ and small V , the transmissive bands are wide, so that $P_0(t)$ behaves like a "white noise," as can be seen from Figs. 6(a) and 6(b). For larger V , the transmissive bands are very narrow, and $P_0(t)$ oscillates only with several selected frequencies, as can be seen from Figs. 6(c), 6(d), and 6(e). Thus, the self-similarity in the dynamical behavior of $P_0(t)$ can be traced back to the self-similar structure of the $|t|^2$ versus E curves.

V. DISCUSSION

We considered the dynamical properties of electrons in periodic and aperiodic lattice sequences. In the periodic case the time evolution of a wave packet performs an unlimited ballistic motion with constant velocity. The corresponding mean-square displacement behaves as

$\sigma^2(t) = 2t^2$ and the integrated autocorrelation function asymptotically decays as t^{-1} . Moreover, the spatial distribution of the wave packet at a given time exhibits interesting phase-chaotic properties, under a well-defined envelope curve. The origin of such a complicated dynamic behavior, in this simple model, is due to the continuous band of modes which are included in the initial wave packet and can be transmitted through the sequence. On the other hand, in the aperiodic Thue-Morse sequence only the modes within the very narrow bands or subbands can be transmitted so that in the corresponding diffusion process the phase-chaotic behavior disappears. However, the probability of finding a particle at the initial site $P_0(t)$ exhibits self-similarity in time, which reflect the spatial self-similarity of the model. The dynamic behavior in the Thue-Morse sequence is clearly shown to be consistent with the absence of localization, despite the slow spread of the wave packet in space.

The present dynamical study, which concerns the local spectral properties, in connection with our global spectral study allows the understanding of the dominant physically interesting questions concerning the aperiodic Thue-Morse system. The results can be easily extended to other kinds, such as the period doubling, or circle sequences, which are generated by different substitutions.¹¹ Moreover, a study of the higher moments of the wave packet is also possible, in order to specify the details of the evolution.²⁶ From the experimental side the importance of deterministic nonquasiperiodic structures has been increasingly recognized. Thue-Morse superlattice heterostructures have been grown on by molecular-beam-epitaxy techniques, and the singular continuous Fourier transform has been observed. Our results may contribute towards understanding the electronic structure properties of these materials.

ACKNOWLEDGMENTS

This work was supported in part from a HCM network and by a IIENEA research grant of the Greek Secretariat of Science and Technology.

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