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Quantum diffusion in the generalized Harper equation

Gun Sang Jeon, Beom Jun Kim, Sang Wook Yi†, and M Y Choi
Department of Physics and Center for Theoretical Physics, Seoul National University, Seoul 151-742, Korea

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Abstract. We study numerically the dynamic and spectral properties of a one-dimensional quasi-periodic system, where site energies are given by $\epsilon_k = V \cos 2\pi f x_k$ with x_k denoting the kth quasiperiodic lattice site. When $2\pi f$ is given by the reciprocal lattice vector $G(m, n)$ with n and m being successive Fibonacci numbers, the variance of the wavepacket is found to grow quadratically in time, regardless of the potential strength V. For other values of f, there exists a critical value of V beyond which the growth of the wavepacket variance is bounded. In particular an anomalous diffusion takes place for $2\pi f$ corresponding to $G(m, n)$ with generic integers m and n. The level-spacing distribution is also examined, and the corresponding exponent β is observed to decrease with V.

1. Introduction

Incommensurate [1] and quasiperiodic [2] systems, which can be considered to be intermediate between periodic and disordered systems, display interesting electronic properties, and have attracted much attention during the past decades. Among the typical incommensurate systems is the one-dimensional (1D) model described by the Harper equation

$$\Psi_{k+1} + \Psi_{k-1} + V \cos(2\pi f k + \theta)\Psi_k = E\Psi_k \tag{1}$$

with an irrational f, where Ψ_k represents the amplitude of the wavefunction at the kth site and θ is an arbitrary phase. This equation describes the system of a Bloch electron on a square lattice in a magnetic field [3], which can be mapped into the two-dimensional periodic superconducting networks and arrays under transverse magnetic fields [3, 4]. Unless f is a Liouville number, the system is known to have a critical potential strength $V_c = 2$: for the potential strength V below V_c all the eigenstates are extended, displaying an absolutely continuous energy spectrum, whereas for $V > V_c$ there exist only localized states with a pure-point spectrum. At the critical strength V_c all states are critical and the energy spectrum is singular continuous. One of the interesting features in the system is that for $V = V_c$ the level-spacing distribution (LSD), which has been studied mainly in connection with quantum chaos [5] and localization [6], follows an inverse-power law [7–9]

$$p(s) \sim s^{-\beta} \tag{2}$$

with $\beta = \frac{3}{2}$, indicating level clustering. On the other hand, the quasiperiodic system studied the most is the 1D Fibonacci chain, where the on-site potential takes the two values $+V$ and

† Present address: Department of Philosophy, Logic and Scientific Methods and Center for Philosophy of Natural and Social Sciences, London School of Economics and Political Science, London WC2A 2AE, UK.

$-V$ in a Fibonacci sequence. Regardless of V, the system has been shown to be always critical, which is manifested by the inverse-power-law behaviour of the integrated LSD [8, 9]. Further, the LSD exponent β has been found to vary from 2 to 1 as V is increased from zero to infinity.

It is generally believed that the dynamics of these systems is closely related to their spectral properties. The criticality of the 1D Fibonacci chain produces interesting dynamic properties such as the anomalous diffusion of the wavepacket [8]: the variance σ^2 of the wavepacket increases algebraically

$$\sigma^2(t) \sim t^{2\Delta} \tag{3}$$

where the dynamical exponent Δ is a decreasing function of V. In contrast, in the Harper system, the variance of the wavepacket grows linearly ($\Delta = \frac{1}{2}$) only at $V = V_c$, which separates the extended regime ($V < V_c$) with quadratic growth ($\Delta = 1$) from the localized regime ($V > V_c$) with bounded spread of the wavepacket [7, 8]. An early conjecture that the dynamical exponent Δ is equal to the Hausdorff dimension D_0 of the spectrum, which is given by $\beta - 1$ with the LSD exponent β, turned out to be incorrect [10]. Nevertheless the intimate relationship between dynamics and spectral properties is reflected by the fact that the information dimension D_1 of the spectrum provides a lower bound for Δ [11].

In this work we study another interesting quasiperiodic system described by the equation [3, 12]

$$\Psi_{k+1} + \Psi_{k-1} + V\cos(2\pi f x_k + \theta)\Psi_k = E\Psi_k \tag{4}$$

which we call the *generalized Harper equation* (GHE). Here the position of the kth site is given by $x_k \equiv k + [k\tau]\tau$, where $\tau \equiv (\sqrt{5} - 1)/2$ and $[k\tau]$ denotes the integer part of $k\tau$. Note that for irrational f this system is *both incommensurate and quasiperiodic*, since the incommensurate potential modulates the energies of the lattice sites which have Fibonacci quasiperiodicity. In the study of quasiperiodic superconducting networks [13] and arrays [14], which corresponds to equation (4) with $V = 2$, the transition temperature has been revealed to vary with the magnetic field in a complicated and non-monotonic manner. The perturbation theory for small V [12] predicts that essentially all states are critical when $2\pi f$ corresponds to a reciprocal lattice vector $G(m, n)$ of the quasiperiodic lattice. In this quasiperiodic system, the reciprocal lattice vector is given by $G(m, n) \equiv 2\pi(m + n\tau)/(1 + \tau^2)$ with m and n being integers. Particularly in case that n and m are two successive Fibonacci numbers, the system approaches a commensurate one, as the two numbers grow large, and exhibits only extended-like critical states. On the other hand, for other (generic) values of f it was found that there is a novel transition between critical and localized states: for $V < V_c$ critical and localized states coexist, while all states are localized for $V > V_c$, where the value of V_c in general depends on f. Such a peculiar transition associated with the eigenstate properties raises a question as to the nature of the transition in dynamics and diffusive properties, which are intimately connected to the characteristics of the level statistics. It is thus of interest to investigate the diffusion properties and the level statistics of the system, with emphasis on the connection between them.

2. Generalized Harper equation

2.1. Spread of the initially localized wavepacket

We first study numerically the time evolution of the wavepacket in the system described by the GHE (4). The initial wavepacket is chosen to be localized at the centre of the system and its time evolution is described by the time-dependent Schrödinger equation

$$\Psi_{k+1} + \Psi_{k-1} + V\cos(2\pi f x_k + \theta)\Psi_k = \mathrm{i}\frac{\partial \Psi_k}{\partial t}. \tag{5}$$

To calculate the variance of the wavepacket defined by

$$\sigma^2 \equiv \sum_k (x_k - \bar{x})^2 |\Psi_k|^2 \tag{6}$$

with the mean position $\bar{x} \equiv \sum_k x_k |\Psi_k|^2$, we integrate directly the Schrödinger equation (5) in the chain of length N with the free boundary conditions $\Psi_0 = \Psi_{N+1} = 0$. The fourth-order Runge–Kutta method is used in the numerical integration, with the time step $\Delta t = 0.05$. We have confirmed that the calculation with $\Delta t = 0.01$ yields the same results and, for simplicity, considered only the case $\theta = 0$. In most of the numerical results of this paper we employ a system of size $L = 10\,946$. However, a system of size $L = 28\,657$ has also been considered and found to display essentially the same results, so the main conclusions are believed to be correct at least qualitatively for larger systems.

Figure 1 displays the variance of the wavepacket as a function of time for several potential strengths V in the case of $2\pi f = 0.7$, which does not correspond to a reciprocal lattice vector of the system. At the beginning of the time evolution, the variances for all values of V follow a single curve and become separated from one another at time $t \approx 1$. In particular, for small V, the wavepacket shows almost-ballistic motion until the variance saturates due to the finiteness of the system. The spread of the wavepacket is suppressed as V is increased, and the variance is apparently bounded for V exceeding $V_c \approx 1.7$, at least up to time $t = 50\,000$.

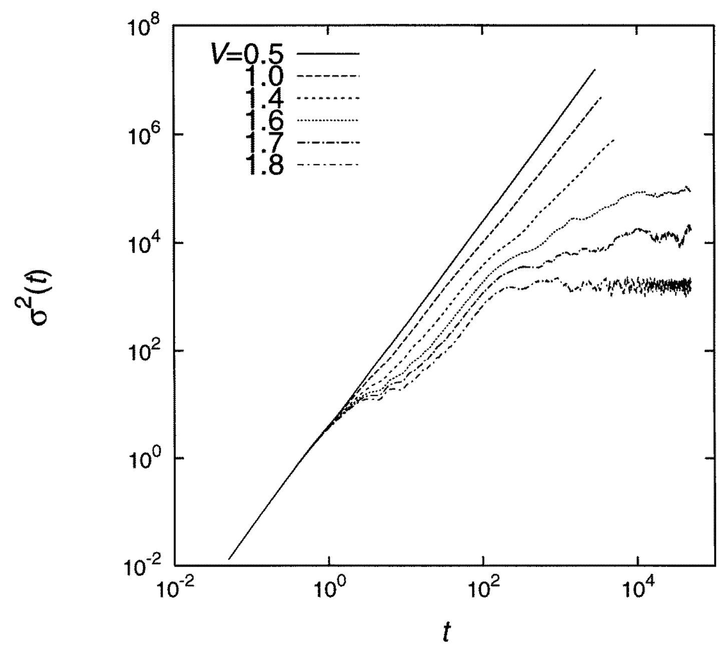

Figure 1. The log–log plot of the wavepacket variance σ^2 as a function of time t for several values of the potential strength V in the case $2\pi f = 0.7$. The initial wavepacket is chosen to be localized at the 5473rd site in the chain of length $N = 10\,946$.

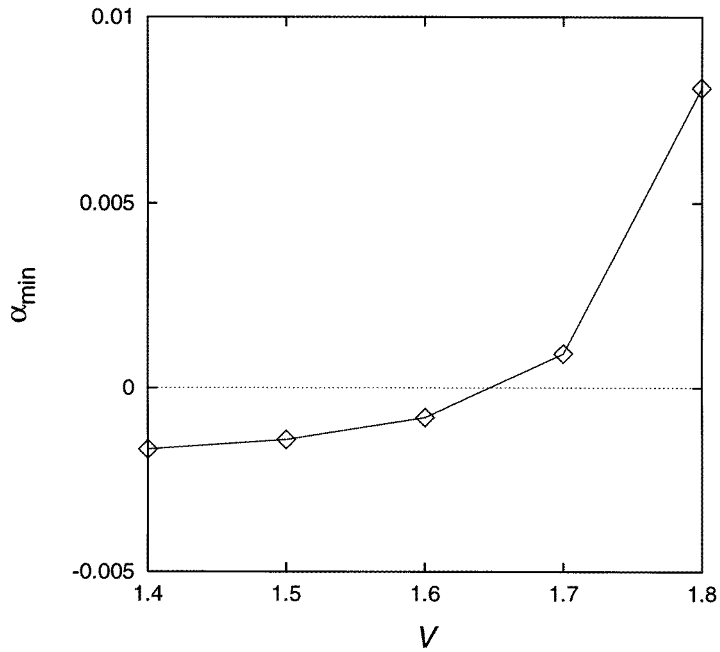

Figure 2. The minimum of the inverse localization length, $\alpha_{\min}$, for all eigenstates in the chain of length $N = 10\,946$ as a function of the potential strength V for $2\pi f = 0.7$. The full curve is a guide to the eye; the dotted line denotes $\alpha_{\min} = 0$.

The above dynamic behaviour can be easily understood in view of the eigenstate properties. In the GHE with $2\pi f \neq G(m, n)$, it is known that there exists the critical potential strength V_c, below which localized and critical states are coexistent [12]: it is this existence of critical states for $V < V_c$ which leads to the unbounded diffusion. As the potential strength V gets larger, the percentage of the critical states decreases relative to the localized states, resulting in the reduction of the diffusion rate. When V reaches V_c, no critical states exist in the system and the wavepacket can no longer diffuse unboundedly.

To confirm this, we also calculate the inverse localization length

$$\alpha \equiv \frac{1}{N} \sum_{k=1}^{N-1} \ln \left| \frac{\Psi_{k+1}}{\Psi_k} \right| \tag{7}$$

for each eigenstate, in the chain of length $N = 10\,946$. The minimum value $\alpha_{\min}$ of the inverse localization length over all eigenstates is plotted in figure 2 as a function of the potential strength V. This curve clearly shows that for the system size $N = 10\,946$ the critical potential strength V_c, above which critical states do not exist, is indeed consistent with the value at which the diffusion begins to be bounded.

Note here that the apparent value of V_c is significantly larger than that obtained in the equilibrium study [12], which is 1.361 ± 0.001 for $2\pi f = 0.7$. This discrepancy presumably does not reflect the difference between statics and dynamics of the system, but can be attributed to the finite-size effects: the previous reported value 1.361 in statics was obtained in the thermodynamic limit, whereas the larger value in dynamics has been obtained in the system of finite size $N = 10\,946$. We thus consider systems of various sizes, and the minimum values of the inverse localization length as functions of the potential strength. The

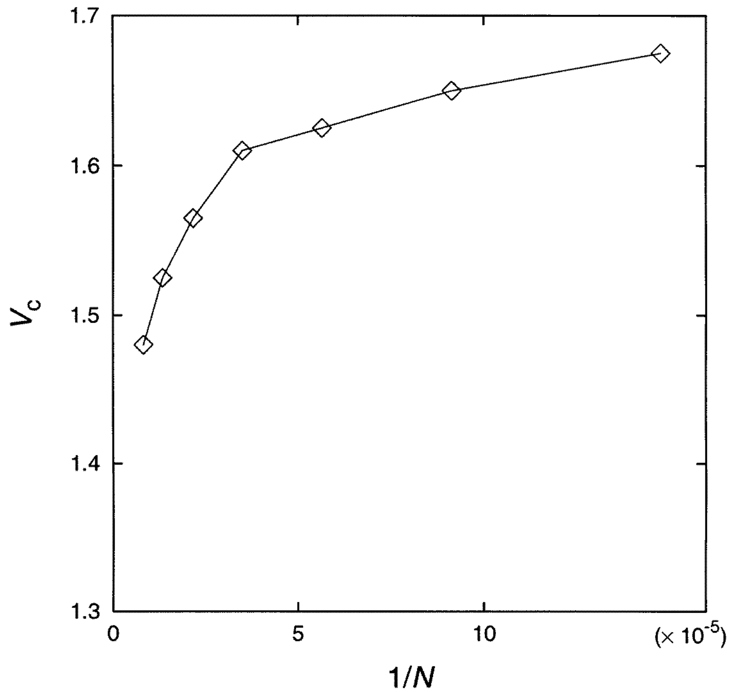

Figure 3. The critical potential strength, where all eigenstates become localized, as a function of the inverse system size $1/N$ ($N = 6765, 10\,946, 17\,711, 28\,657, 46\,368, 75\,025, 121\,393$). The full curve is a guide to the eye, and the typical error is less than the symbol size.

resulting values of the critical potential strength V_c, which can be identified with the zero of $\alpha_{\rm min}$, for various system sizes are displayed in figure 3, which demonstrates the reduction of the critical strength with the system size N. In particular, rather a sharp decrease of V_c can be observed for large N, manifesting the approach of V_c toward the equilibrium value (1.361) in the limit $N \to \infty$.

When $2\pi f$ corresponds to a reciprocal lattice vector $G(m, n)$, the system is more or less close to the commensurate system, resulting in the ubiquity of critical states. Such dependence of the eigenstate properties on the value of $2\pi f$ naturally leads us to expect rather different dynamic behaviour for $2\pi f$ given by a reciprocal lattice vector. In particular, when $2\pi f = G(m, n)$ with n and m being successive Fibonacci numbers, the potential becomes almost constant at (quasiperiodic) lattice sites and accordingly, extended-like states are expected. Indeed, figure 4 shows that the variance of the wavepacket for $(n, m) = (8, 13)$ grows quadratically in time, regardless of the potential strength. The quadratic growth of the variance signifies ballistic motion of the wavepacket, which is characteristic of the extended states. Of course, truly extended states are not allowed in the quasiperiodic system and it is concluded that there exist extended-like critical states in the case $2\pi f = G(m, n)$ with successive Fibonacci numbers n and m, which is in agreement with the previous equilibrium results [12].

In the case $2\pi f = G(m, n)$ with n and m not being successive Fibonacci numbers exhibits more interesting features. In figure 5, we plot the variance of the wavepacket as a function of time for several potential strengths in the system with $2\pi f = G(1, 3)$. As in other cases, the variance shows an unbounded quadratic growth for small V while it

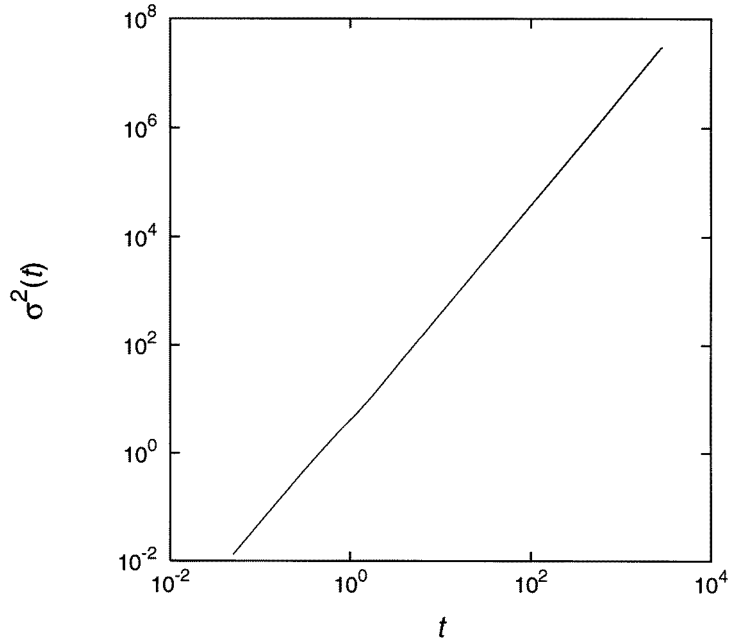

Figure 4. The log–log plot of the wavepacket variance σ^2 as a function of time t for several potential strengths $V = 0.5$, 1.0, 1.5, and 2.0 in the case $2\pi f = G(13, 8)$. For those values considered here, all data curves are shown to collapse into a single curve which is proportional to t^2; this corresponds to the ballistic motion. The initial wavepacket is chosen to be localized at the 5473rd site in the chain of length $N = 10\,946$.

is bounded for V larger than the critical strength V_c. It is of particular interest that the variance of the wavepacket displays the power-law increase, with the dynamical exponent Δ defined in equation (3) decreasing continuously from 1 to 0 as V is increased toward V_c. It is well known that such anomalous diffusion of the wavepacket also takes place in the 1D Fibonacci chain and persists for large V [8]. In the GHE, in contrast, it occurs only for V smaller than the critical strength V_c since critical states no longer exist above V_c. These phenomena reflect the quasiperiodicity and incommensurability of the potential: the quasiperiodicity results in anomalous diffusion whereas the existence of a critical potential strength has its origin in incommensurability.

2.2. Level statistics

We next examine the level statistics of the GHE to obtain its spectral properties. The allowed energy structure of the GHE is very complicated as shown in figure 6. The absolutely continuous energy band for $V = 0$ is subdivided into many subbands with increasing V. As in the Harper equation, energy levels in each subband arrange in clusters at a certain potential strength and a further increase of the potential strength yields the pure-point spectrum indicative of the localized regime. In the GHE, however, the clustering potential strength varies with each subband in contrast to the Harper equation, and tends to be larger in the inner subband. (The single isolated level, which appears at very low V, is presumably an artifact due to the free boundary conditions [9].) In order to investigate the spectral property in a quantitative manner, we consider the level statistics in this system. As

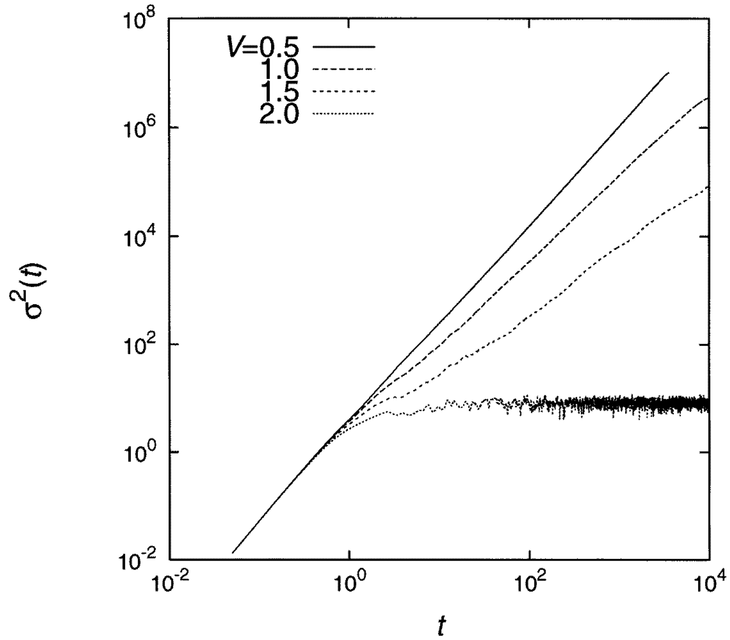

Figure 5. The log–log plot of the wavepacket variance σ^2 as a function of time t for several potential strengths V in the case $2\pi f = G(1, 3)$. The initial wavepacket is chosen to be localized at the 5473rd site in the chain of length $N = 10\,946$.

shown in figure 6, all energies are bounded, and we can count the number of energy-level spacings larger than a given value s. The integrated level-spacing distribution (ILSD) is then obtained

$$p_{\text{int}}(s) \equiv \int_s^\infty p(s')\,\mathrm{d}s' \tag{8}$$

where $p(s)$ is the probability density of level spacing s.

Figure 7 shows the ILSD for several potential strengths in the system with $2\pi f = G(1, 3)$. Each distribution consists of two parts: the exponentially decaying part for small s and the power-law decaying part for large s. It is known that localized states in general exhibit the LSD of Poisson type, which has been proved in the Anderson model [15] and also observed numerically in the Harper equation [9]. It is thus reasonable to attribute the exponentially decaying part to the contribution of the localized states. On the other hand, the power-law decaying part is associated with the critical states, as is known in the case of the Harper equation. This interpretation is strongly supported by the fact that the portion of the exponentially decaying part grows larger as V is increased.

Here it is of interest to note that the exponent β of the power-law decaying part is dependent on the potential strength V. We estimate the exponent β by fitting the power-law decaying part of the ILSD to the form $s^{1-\beta}$, and show in figure 8(a) that β decreases continuously from 2 with increasing V. Although we are unable to estimate β numerically for $V > 1.5$ where very few critical states exist, β is expected to approach unity as V is increased toward V_c. Similar dependence of β on V also appears in the 1D Fibonacci chain [9] except for the fact that a finite V_c does not exist.

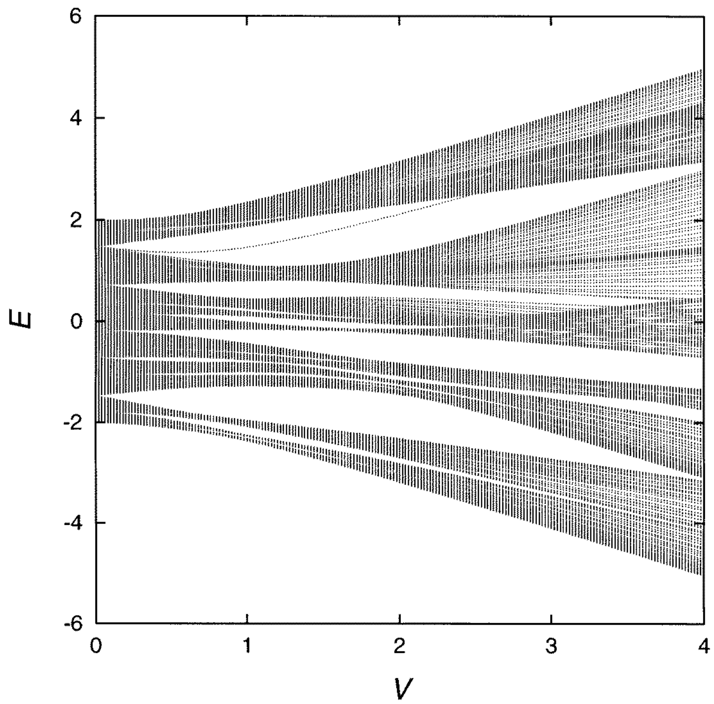

Figure 6. Allowed energies as a function of the potential strength V in the chain of length $N = 377$ for $2\pi f = G(1, 3)$.

It is known that between the LSD exponent β and the dynamical exponent Δ the simple relation

$$\Delta = \beta - 1 \tag{9}$$

holds approximately in the Harper equation with $f = \tau$ as well as in the 1D Fibonacci chain [7, 8]. We thus estimate the value of Δ from the time evolution of the wavepacket spread and plot the ratio of 2Δ to $\beta - 1$ in figure 8(b), which shows that equation (9) is satisfied only for small V. As V is increased, the relation between Δ and β begins to deviate from equation (9), presumably due to the coexistence of the localized states with the critical ones. For larger V there appear more localized states in the system, and the deviation grows larger. Consequently, it is concluded that the generalized Harper system is another example which suggests no simple relation between the spectral dimension and the dynamical exponent [10].

2.3. Autocorrelation function

Finally we consider the autocorrelation function, which is another useful quantity in the study of quantum chaos. In the Harper system the autocorrelation function $C(t)$ was shown to display a power-law decay with logarithmic correction [16]:

$$C(t) \sim f(\log t)t^{-\delta} \tag{10}$$

at the critical point, where $\delta \approx 0.13$ and $f(x)$ is a periodic function. In the extended regime the autocorrelation function $C(t)$ behaves as

$$C(t) \approx (c_0 + c_1 \log t)t^{-1} \tag{11}$$

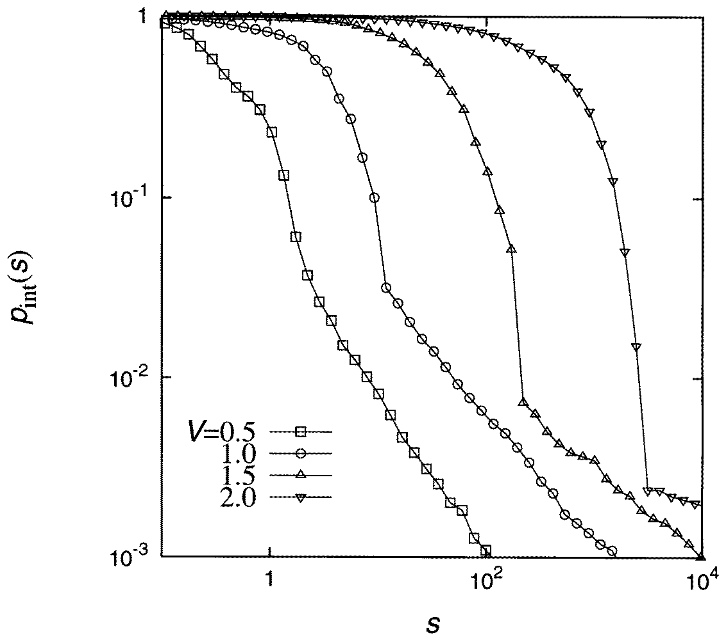

Figure 7. Integrated level-spacing distribution $p_{\rm int}(s)$ for several potential strengths in the chain of length $N = 10\,946$ with $2\pi f = G(1, 3)$. These distributions are normalized in such a way that the mean spacing is equal to unity. For a clear comparison, the curves for $V = 1.0$, 1.5, and 2.0 are shifted by 10, 10^2, and 10^3, respectively, along the horizontal axis.

with $c_0 \approx 0.30$ and $c_1 \approx 1.65$, which reflects the ballistic motion of the electron. In the localized regime the autocorrelation function $C(t)$ decays to a finite value, as expected. In the 1D Fibonacci chain, in contrast, the exponent δ of the autocorrelation function $C(t)$, which takes the extended-state value ($\delta = 1$) for $V = 0$, decreases continuously with V, approaching zero in the limit $V \to \infty$ [16].

In the GHE the autocorrelation function $C(t)$ of the diffusing wavepacket, shown in figure 9, manifests the interplay between the localized and the critical states. The time evolution of the autocorrelation can be explained in terms of the superposition of the two contributions: the power-law decaying term from the critical-state components and the non-decaying term from the localized-state components. Figure 9 shows that the saturation value grows with V, indicating the increase of the localized-state components. On the other hand, for $2\pi f = G(13, 8)$ the autocorrelation function exhibits almost the same behaviour as the extended case in the Harper equation, which is consistent with the behaviour in figure 4.

3. Summary

We have investigated numerically dynamic and spectral properties of the 1D quasiperiodic system described by the generalized Harper equation. For $2\pi f = G(m, n)$ with n and m being successive Fibonacci numbers, the wavepacket has been found to show ballistic motion regardless of the potential strength V. For other values of $2\pi f$, there exists a finite potential strength V_c above which the growth of the wavepacket variance is bounded. The critical strength appears naturally to be the same as the transition potential strength beyond which all states are localized, as found in the equilibrium study. Further, anomalous diffusion has

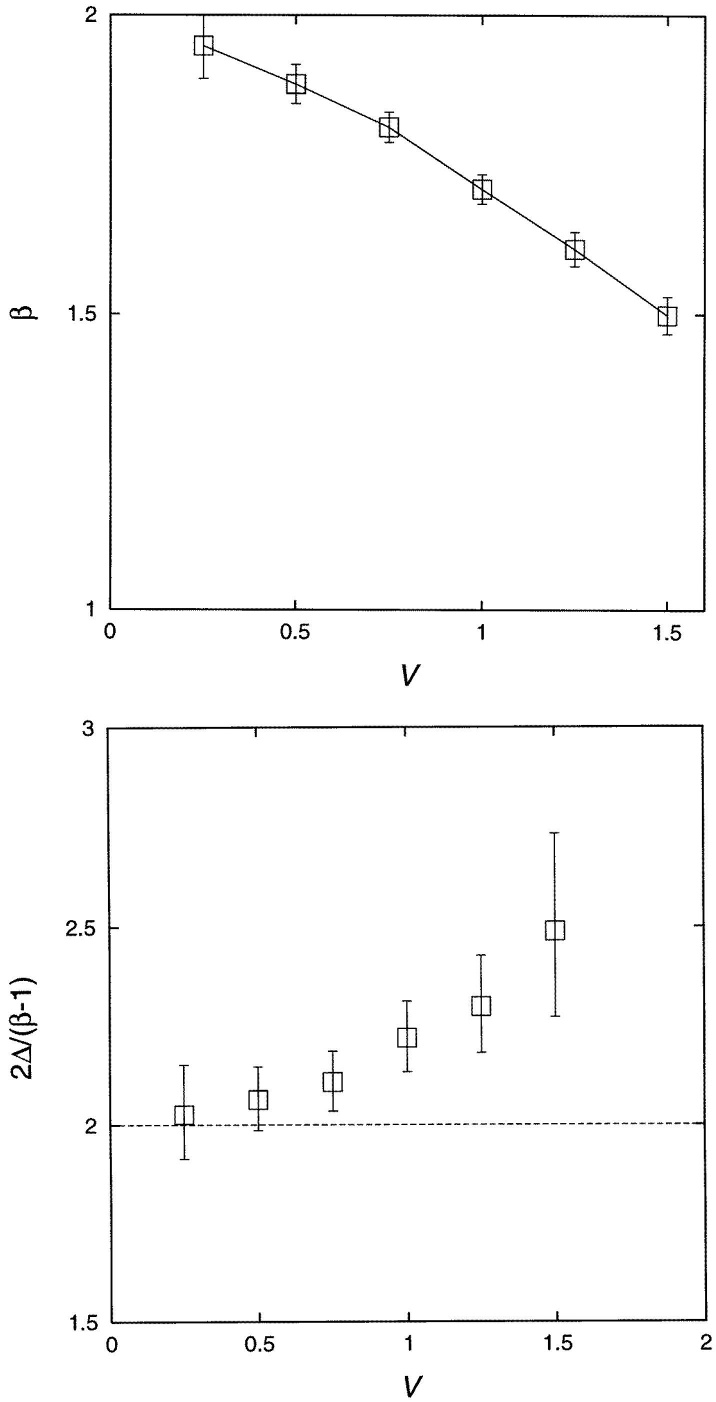

Figure 8. (*a*) The exponent β of the power-law decaying part of the ILSD, as a function of the potential strength. (*b*) The ratio of 2Δ to $\beta - 1$ as a function of the potential strength. The estimated error bars correspond to three standard deviations.

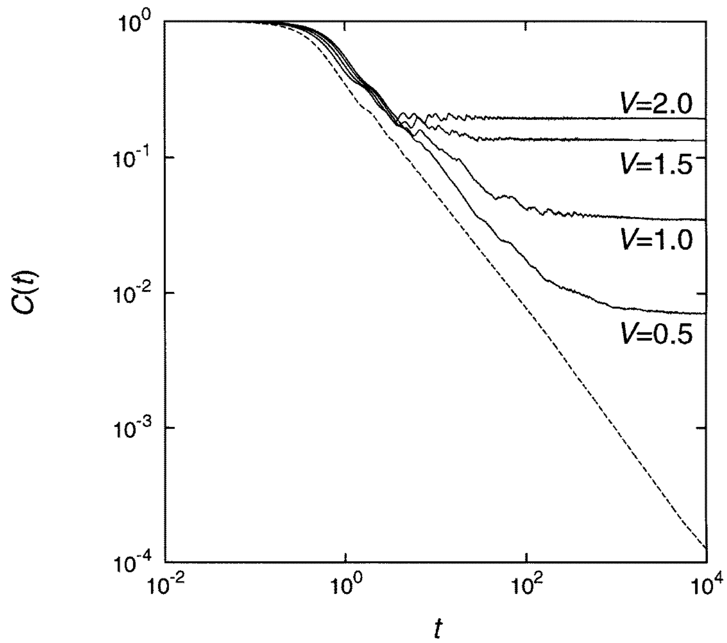

Figure 9. The autocorrelation function $C(t)$ as a function of time for several potential strengths in the chain of length $N = 10\,946$ with $2\pi f = G(1, 3)$. For comparison, $C(t)$ for $2\pi f = G(13, 8)$ is also plotted as a broken curve.

been observed below the finite critical potential strength for $2\pi f = G(m, n)$ where n and m are not successive Fibonacci numbers. In this case the ILSD has been shown to consist of two parts: the exponentially decaying part for small spacings arising from the contribution of localized states and the power-law decaying part for large spacings from the contribution of critical states. Here the exponent β of the level-spacing distribution has been found to decrease with V, similarly to the 1D Fibonacci chain model. We have also considered the autocorrelation function, which is again indicative of the interplay between the localized and the critical states. It may be possible to fabricate the superlattices of electronic systems with appropriate structures, which are described by the generalized Harper model for generic V; experiments performed on such systems are expected to display a variety of interesting phenomena.

Acknowledgments

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