Statistics of Resonances and of Delay Times in Quasiperiodic Schrödinger Equations

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We study the distributions of the resonance widths \( P(\Gamma) \) and of delay times \( P(\tau) \) in one-dimensional quasiperiodic tight-binding systems at critical conditions with one open channel. Both quantities are found to decay algebraically as \( \Gamma^{-\alpha} \) and \( \tau^{-\gamma} \) on small and large scales, respectively. The exponents \( \alpha \) and \( \gamma \) are related to the fractal dimension \( D_E^b \) of the spectrum of the closed system as \( \alpha = 1 + D_E^b \) and \( \gamma = 2 - D_E^b \). Our results are verified for the Harper model at the metal-insulator transition and for Fibonacci lattices.

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Quantum mechanical scattering has been a subject of a rather intensive research activity during the last years. This interest was motivated by various areas of physics, ranging from nuclear [1], atomic [2], and molecular [3] physics to mesoscopics [4] and classical wave scattering [5]. The most fundamental object characterizing the process of quantum scattering is the unitary scattering matrix, i.e., the matrix and of delay times \( \Phi(E) \) of the scattering matrix, i.e., \( \tau(E) = \frac{d\Phi(E)}{dE} \). The resonances represent long-lived intermediate states to which bound states are converted due to coupling to continua. On a formal level, resonances show up as poles of the scattering matrix \( S(\mathcal{E}) \) occurring at complex energies \( \mathcal{E}_n = E_n - \frac{i}{\hbar} \Gamma_n \), where \( E_n \) and \( \Gamma_n \) are called position and width of the resonances, respectively.

Recently, the interest in quantum scattering has extended to systems showing localization. For this case, there are analytical results about the distribution of phases of the S matrix and of delay times [9–13]. The former depends drastically on the disorder strength and energy [12], while for the latter a universal power law tail was found to hold [10–13]. Moreover, in [14] a first analytical result about the distribution of resonances appeared.

In the present paper we study delay time and resonance width statistics in a new setting, namely, a class of systems whose closed analogs have fractal spectra. The latter exhibit energy level statistics that are in strong contrast to the level repulsion predicted by random matrix theory [15]. Their level spacing distribution follows inverse power laws \( P(s) \sim s^{-\beta} \) which is a signature of level clustering. The power \( \beta \) was found to be related with the fractal dimension of the spectrum \( D_E^b \) (box-counting dimension) as \( \beta = 1 + D_E^b \) [16]. Realizations of this class are quasiperiodic systems with metal-insulator transition at some critical value of the on-site potential like the Harper model [16,17], Fibonacci chains [16,18] or quantum systems with chaotic classical limit as the kicked Harper model [19]. Here, for the first time we present consequences of the fractal nature of the spectrum in open systems. We consider open systems with one channel (the simplest possible scattering problem) and report the appearance of a new type of resonance width and delay time statistics. These distributions show inverse power law behavior dictated by the fractal dimension \( D_E^b \) of the spectrum. Specifically, we show that the probability distributions of resonance widths \( P(\Gamma) \) and of delay times \( P(\tau) \) when generated over different energies behave as

\[
P(\Gamma) = \Gamma^{-\alpha}, \quad \alpha = 1 + D_E^b, \\
P(\tau) = \tau^{-\gamma}, \quad \gamma = 2 - D_E^b.
\]

For the calculation of \( P(\Gamma) \) and \( P(\tau) \) we employed two independent approaches. Our results (1) are confirmed for two different types of quasiperiodic tight-binding models and are supported by analytical arguments.

We consider a one-dimensional (1D) quasiperiodic sample of length \( L \) with one semi-infinite perfect lead attached on the left side. The system is described by the tight-binding Hamiltonian

\[
H = \sum_n |n\rangle V_n \langle n | + \sum_n (|n\rangle \langle n + 1| + |n + 1\rangle \langle n |),
\]

where \( V_n \) is the potential at site \( n \). In the sequel we will consider examples where, for \( 0 \leq n \leq L \), \( V_n \) is given by a quasiperiodic sequence. For \( n < 0 \), \( V_n = 0 \) and we
impose Dirichlet boundary conditions at the edge $\psi_{L+1} = 0$. Therefore, for $n \leq 0$, scattering states of the form $\psi_n = e^{ikn} + Se^{-ikn}$ represent the superposition of an incoming and a reflected plane wave. Here, $k = \text{arccos}(E/2)$ is the wave vector supported at the leads. Since there is only backscattering, the scattering matrix $S(E) \equiv e^{i\Phi(E)}$ is of unit modulus and the total information about the scattering is contained in the phase $\Phi(E)$. One can write the scattering matrix in the form [7,14,20]

$$S(E) \equiv e^{i\Phi(E)} = 1 - 2iw^2\sin k\hat{e}^T \frac{1}{E - \mathcal{H}_{\text{eff}}} \hat{e}. \quad (3)$$

$\mathcal{H}_{\text{eff}}$ is an effective non-Hermitian Hamiltonian given by

$$\mathcal{H}_{\text{eff}} = H_L - w^2e^{ik}\hat{e} \otimes \hat{e}. \quad (4)$$

$H_L$ is the part of the tight-binding Hamiltonian (2) with $n = 0,\ldots,L$ corresponding to the quasiperiodic

$$\tau_{L+1} = G_L^{-1}\left(\tau_L + \frac{1}{\sin k}\right) + \frac{A_L \cot k}{1 + [\tan(\phi_L - k) + A_L]^2},$$

$$G_L = 1 + A_L\sin[2(\phi_L - k)] + A_L^2\cos^2(\phi_L - k), \quad (5)$$

where $A_L = V_L/\sin k$. Iteration relation (5) has proved to be very convenient for numerical calculations since it anticipates the numerical differentiation which is a rather unstable operation. Moreover, it allows us to go to large system sizes.

We motivate and numerically verify our results using first the well-known Harper model which is a paradigm of a quasiperiodic 1D system with metal-insulator transition [16,17]. It is described by the tight-binding Hamiltonian (2) with on-site potential given by

$$V_n = \lambda \cos(2\pi\sigma n). \quad (6)$$

This system effectively describes a particle in a two-dimensional periodic potential in a uniform magnetic field with $\sigma = a^2eB/\hbar c$ being the number of flux quanta in a unit cell of area $a^2$. When $\sigma$ is an irrational number the period of the effective potential $V_n$ is incommensurate with the lattice period. We consider generic irrationals which cannot be approximated "too well" by rationals. To this end we take $\sigma$ as the limit of successive rationals $p/q$, so that the potential becomes commensurate with the lattice with period $q$. Then we can define a scaling procedure where the incommensurate limit $q \rightarrow \infty$ becomes equivalent with the thermodynamic limit. The states of the corresponding closed tight-binding system are extended when $\lambda \leq 2$, and the spectrum consists of bands (ballistic regime). For $\lambda > 2$ the spectrum is pointlike and all states are exponentially localized (localized regime). The most interesting case is the critical point $\lambda = 2$ where we have a metal-insulator transition. At this point, the spectrum is a zero measure Cantor set with fractal dimension $D_0^E \leq 0.5$ [21] while the states are critical, sample and $\hat{e} = (1,0,0,\ldots,0)^T$ is an $L + 1$ dimensional vector that describes at which site we couple the lead with our quasiperiodic sample. The strength of the coupling is given by $w$. In the sequel we will always consider $w = 1$. Moreover, since $\text{arccos}(E/2)$ changes only slightly in the center of the band, we put $E = 0$ and neglect the energy dependence of $\mathcal{H}_{\text{eff}}$. The poles of the $S$ matrix are equal to the complex eigenvalues $\mathcal{E}$ of $\mathcal{H}_{\text{eff}}$. The latter are computed by direct diagonalization of $\mathcal{H}_{\text{eff}}$. We note here that numerical diagonalization of complex non-Hermitian matrices is a time consuming process and imposes limitations on the system size due to limited storage capacity. The size of the matrices that we used in our analysis below was up to rank 5000.

For the calculation of the Wigner delay time $\tau$ we have developed a simple iteration relation in [12]

$$\mathcal{P}_{\text{int}}(x) = \int_x^\infty \mathcal{P}(x') dx' \quad (7)$$

whose derivatives $\mathcal{P}(x) = -d\mathcal{P}_{\text{int}}/dx$ determine the probability density of resonance widths $\mathcal{P}(x = \Gamma)$ and delay times $\mathcal{P}(x = \tau)$. In all our calculations we will take approximants of the golden mean $\sigma_G = (\sqrt{5} + 1)/2$. For this case it is known that $D_0^E \approx 0.5$ [21].

Figure 1 shows $\mathcal{P}_{\text{int}}(\Gamma)$ for two different rational approximants $\sigma$ of the golden mean $\sigma_G$. It clearly displays an inverse power law

$$\mathcal{P}_{\text{int}}(\Gamma) \sim \Gamma^{1-\alpha} \quad (8)$$

and thus the resonance width distribution behaves as stated in (1) with $\alpha = 1.5 = 1 + D_0^E$. The integrated resonance width distribution cuts off at a small value of $\Gamma$’s (see Fig. 1), since for all rational approximants of $\sigma_G$ the total number of $\mathcal{E}_n$ is finite. This cutoff, however, can be shifted to arbitrarily small values for higher approximants.

Next we investigated the delay time statistics $\mathcal{P}(\tau)$. In Fig. 2 we report the integrated $\mathcal{P}_{\text{int}}(\tau)$ for three different rational approximants of the golden mean. Because of the efficiency of our iteration relation (5) we can approximate $\sigma_G$ by increasing the periodicity $q$ of the potential as much
proximants of $s$ with a value of $g$ squares DE fractal dimension $4428$

\[ P_{\text{int}}(\Gamma) \]

Fig. 1. $P_{\text{int}}(\Gamma)$ of the Harper model ($\lambda = 2$) for three approximants of $\sigma_i$: $\sigma_1 = \frac{907}{1597}$; $\sigma_2 = \frac{1597}{2584}$; $\sigma_3 = \frac{2584}{3181}$. An inverse power law $P_{\text{int}}(\Gamma) \sim \Gamma^{1-\alpha}$ is evident. A least squares fit yields $\alpha \approx 1.5$ in accordance with $D_0^E = 0.5$ and Eq. (1). As is seen the lower cutoff of the scaling region decreases for higher approximants.

as we like. Our numerical data are in agreement with an inverse power law, i.e.,

$$ P_{\text{int}}(\tau) \sim \tau^{1-\gamma} \quad (9) $$

with a value of $\gamma = 1.5 = 2 - D_0^E$ given by a best least squares fit, in perfect agreement with Eq. (1).

The connection between the exponents $\alpha$, $\gamma$ and the fractal dimension $D_0^E$ of the closed system calls for an argument for its explanation. The following heuristic argument, similar in spirit to [16,22], provides some understanding of the power laws (1). We consider successive rational approximants $\sigma_i = p_i/q_i$ of the continued fraction expansion of $\sigma$. On a length scale $q_i$, the periodicity of the potential is not manifest and we may assume that the variance of a wave packet spreads as $\text{var}(t) \sim t^{2D_0^E}$ [23].

We attach the lead at the end of the segment $q_i$ which results in broadening the energy levels by a width $\Gamma$. The maximum time needed for a particle to recognize the existence of the leads is $\tau_{q_i} \sim q_i^{1/D_0^E}$. The latter is related to the minimum level width $\Gamma_{q_i} \sim 1/\tau_{q_i}$. The number of states living in the interval is $\sim q_i$, and thus determines the number of states with resonance widths $\Gamma > 1/\tau_{q_i}$. Thus $P_{\text{int}}(\Gamma_{q_i}) \sim q_i^{-1} \sim \Gamma^{-D_0^E}$. By repeating the same argument for higher approximants $\sigma_{i+1} = p_{i+1}/q_{i+1}$ we conclude that $P(\Gamma) \sim \Gamma^{-(1+D_0^E)}$, in agreement with (1). Although the numerical results support the validity of the above argument, a rigorous mathematical proof is still lacking.

Next, we present another argument, which allows us to understand the relation between the power law decay exponent $\gamma$ and the fractal dimension $D_0^E$, i.e., $\gamma = 2 - D_0^E$. Our starting point is the well-known relation

$$ \tau(E) = \sum_{n=1}^L \frac{\Gamma_n}{(E - E_n)^2 + \Gamma_n^2/4} \quad (10) $$

which connects the Wigner delay times and the poles of the $S$ matrix. It is evident that anomalously large time delay $\tau(E) \sim \Gamma_n^{-1}$ corresponds to the cases when $E = E_n$ and $\Gamma_n \ll 1$. In the neighborhood of these points, $\tau(E)$ can be approximated by a single Lorentzian (10). Sampling the energies $E$ with step $\Delta E \ll \Gamma_{\text{min}}$ we calculate the number of points for which the time delay is larger than some fixed value $\tau$. Assuming that the contribution of each Lorentzian is proportional to its width one can estimate this number as $\sum_{\Gamma_n < 1/\tau} \Gamma_n / \Delta E$. For the integrated distribution of delay times we obtain $P_{\text{int}}(\tau) = \int^{1/\tau} d\Gamma P(\Gamma) \Gamma \sim \tau^{-(2-\alpha)}$ in the limit $\Delta E \rightarrow 0$ where we used the small resonance width asymptotics given by Eq. (1) (for similar argumentation see also [7,25]). Then for the asymptotic distribution

\[ P_{\text{int}}(\tau) \]

Fig. 2. $P_{\text{int}}(\tau)$ of the Harper model ($\lambda = 2$) for three approximants of the golden mean: $\sigma_1 = \frac{233}{1597}$; $\sigma_2 = \frac{1597}{233}$; $\sigma_3 = \frac{832040}{5342040}$. An inverse power law $P_{\text{int}}(\tau) \sim \tau^{1-\gamma}$ is evident. A least squares fit yields $\gamma \approx 1.5$ in accordance with $D_0^E = 0.5$ and Eq. (1). As is seen the upper cutoff of the scaling region increases for higher approximants.

\[ V \]

Fig. 3. Power law exponents $\alpha$, $\gamma$ (plotted as $\alpha - 1$ and $2 - \gamma$) of the resonance widths and of the delay time distributions, respectively, as a function of the potential strength $V$ for the Fibonacci model. We also plot the fractal dimension $D_0^E$ of the spectrum (the solid line is to guide the eye). Our numerical data show that $\alpha$ and $\gamma$ are related to the Hausdorff dimension $D_0^E$ according to Eq. (1).
of delay times we get \( P(\tau) \sim \tau^{-(2-D_F^0)} \) in agreement with (1) and our numerical findings.

The validity of the heuristic arguments [and thus of Eq. (1)] can be verified in more cases in the Fibonacci chain model of a one-dimensional quasicrystal where other scaling exponents can be obtained. Here the potential \( V_n \) only takes the two values \(+V \) and \(-V \) arranged in a Fibonacci sequence [18]. It was shown that the spectrum is a Cantor set with zero Lebesgue measure for all \( V > 0 \). We again find inverse power laws for the integrated distributions \( P(\Gamma) \) and \( P(\tau) \). Here the exponent depends on the potential strength \( V \), while Eq. (1) still relates the corresponding statistics to the fractal dimension \( D_F^0 \). Our results for various \( V \) values are summarized in Fig. 3 and show a nice agreement between the exponents \( \alpha, \gamma, \) and \( D_F^0 \) according to Eq. (1).

Because of a lack of space we defer the discussion of other results, such as the fractal nature of the resonance widths and the behavior of the delay time autocorrelation function to a later publication [26].

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[23] When averaged over different initial positions, the variance of a packet is believed to behave as \( \text{var}\{r(t)\} \sim t^{2D-1} \) [24] instead of \( \text{var}\{r(t)\} \sim t^{2D-2} \) as assumed here [16]. However, there is no clear conclusion yet and one may consider our assumption on the spread of the wave packet as a good approximation. Our numerical results were not conclusive at this point since \( D_0 \approx D_{-1} \).