Statistics of resonances and of delay times in quasiperiodic Schrödinger equations

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We study the statistical distributions of the resonance widths $P(\Gamma)$, and of delay times $P(\tau)$ in
one dimensional quasi-periodic tight-binding systems 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 $D_0^F$ of the spectrum of the closed system as $\alpha = 1 + D_0^F$, and $\gamma = 2 - D_0^F$. 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 characterising the process of quantum scattering is the unitary $S$-matrix relating the amplitudes of incoming waves to the amplitudes of outgoing waves. At present, there are two complementary theoretical tools employed to calculate statistical properties of the $S$-matrix, namely the semiclassical and the stochastic approach. The starting point of the first is a representation of the $S$-matrix elements in terms of a sum over classical orbits \[6\] while the later exploits the similarity with ensembles of Random Matrices (see \[7\] and references therein). Thus, for chaotic/ballistic systems, many results are known. Among the most interesting is the knowledge of the Wigner delay time statistics and of the resonance width statistics \[8\]. The former quantity captures the time-dependent aspects of quantum scattering. It can be interpreted as the typical time interval a scattering particle remains in the intermediate states to which bound states of a closed system 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 $\mathcal{E}_n = E_n - \frac{i}{2} \Gamma_n$, 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 \[9\]. The former depends drastically on the disorder strength and energy \[10\]. For the latter a universal power law tail was found to hold \[10\]. Moreover, in \[10\] 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 system analogues have fractal spectra. The latter exhibit energy level statistics that are in strong contrast to the level repulsion predicted by Random Matrix Theory (RMT) \[11\]. 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 $D_0^F$ as $\beta = 1 + D_0^F$ \[11\]. Realizations of this class are, quasi-periodic systems with metal-insulator transition at some critical value of the on-site potential like the Harper model \[12\]. Fibonacci chains \[12\], or quantum systems with chaotic classical limit as the Kicked Harper Model \[13\]. 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 resonances width and delay time statistics. These distributions show inverse power law behaviour dictated by the fractal dimension $D_0^F$ 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

$$
P(\Gamma) = \Gamma^{-\alpha} ; \quad \alpha = 1 + D_0^F$$

$$
P(\tau) = \tau^{-\gamma} ; \quad \gamma = 2 - D_0^F$$

For the calculation of $P(\Gamma)$ and $P(\tau)$ we employed two independent approaches. Our results \[14\] are confirmed for two different types of quasi-periodic tight-binding models and are supported by analytical arguments.

We consider a 1D quasi-periodic 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 quasi-periodic 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, \( k = \arccos(E/2) \) 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 \[ S(E) = 1 - 2iw^2 \sin k e^{iT} \frac{1}{E - H_{\text{eff}}} \varepsilon. \] (3)

\( H_{\text{eff}} \) is an effective non-hermitian Hamiltonian given by

\[ H_{\text{eff}} = H_L - w^2 e^{ik} \varepsilon \otimes \varepsilon. \] (4)

\( H_L \) is the part of the tight-binding Hamiltonian \( \{ \} \) with \( n = 0, \ldots, L \) corresponding to the quasi-periodic sample and \( \varepsilon = (1, 0, 0, \ldots, 0)^T \) is an \( L \)-dimensional vector that describes at which site we couple the lead with our quasi-periodic sample. The strength of the coupling is given by \( w \). In the sequel we will always consider \( w = 1 \). Moreover, since \( \arccos(E/2) \) changes only slightly in the center of the band, we put \( E = 0 \) and neglect the energy dependence of \( H_{\text{eff}} \). The poles of the \( S \)-matrix are equal to the complex eigenvalues \( E \) of \( H_{\text{eff}} \). The latter are computed by direct diagonalization of \( H_{\text{eff}} \). 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 [2]

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

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

\[ \tan(\phi_{L+1}) = \tan(\phi_L - k) + A_L \] (5)

where \( A_L = V_L / \sin k \). Iteration relation [2] 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 quasi-periodic 1D system with metal-insulator transition [14,17]. It is described by the tight-binding Hamiltonian with on-site potential given by

\[ V_n = \lambda \cos(2\pi \sigma n). \] (6)

This system effectively describes a particle in a two-dimensional periodic potential in a uniform magnetic field with \( \sigma = a^2 eB / hc \) 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 irrational 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 \( q \to \infty \) becomes equivalent with the thermodynamic limit. The states of the corresponding closed tight-binding system are extended when \( \lambda < 2 \), and the spectrum consists of bands (ballistic regime). For \( \lambda > 2 \) the spectrum is point-like 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.

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Next we investigated the delay time statistics \( \mathcal{P}(\tau) \). In Fig. 2 we report the integrated \( \mathcal{P}(\tau) \) for three different rational approximants of the golden mean \( \sigma_G \) 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 \( q \to \infty \) becomes equivalent with the thermodynamic limit. The states of the corresponding closed tight-binding system are extended when \( \lambda < 2 \), and the spectrum consists of bands (ballistic regime). For \( \lambda > 2 \) the spectrum is point-like 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.

First, we will investigate the statistical distribution of the resonance widths \( \Gamma \), and delay times for the Harper model at the critical point \( \lambda = 2 \). For this case it is known that \( D \approx 0.5 \) [24].

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

\[ \mathcal{P}(\Gamma) \sim \Gamma^{-\alpha} \] (8)

and thus the resonance width distribution behaves as stated in [1] with \( \alpha \simeq 1.5 = 1 + D \). 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 bands 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 \( \mathcal{P}(\tau) \) for three different rational approximants of the golden mean. Due to the efficiency of our iteration relation [2] we can approximate \( \sigma_G \) by increasing the periodicity \( q \) of the potential as much as we like. Our numerical data are in agreement with an inverse power law i.e.

\[ \mathcal{P}(\tau) \sim \tau^{-1-\gamma} \] (9)

with a value of \( \gamma \approx 1.5 = 2 - D \) given by a best least square fit, in perfect agreement with Eqn. [1].
The connection between the exponents $\alpha, \gamma$ and the fractal dimension $D^F_0$ of the close system calls for an argument for its explanation. The following heuristic argument, similar in spirit to [4,22] provides some understanding of the power laws [4]. We consider successive rational approximants $\sigma_i = q_i/p_i$ 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 a wave packet moves as $\text{var}(t) \sim t^{2D^F_0}$ [3]. 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 $\tau_{q_i} \sim q_i^{-1/D^F_0}$. 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 $\mathcal{P}_{\text{int}}(\Gamma_{q_i}) \sim q_i \sim \Gamma^{-D^F_0}$. By repeating the same argument for higher approximants $\sigma_{i+1} = q_{i+1}/p_{i+1}$ we conclude that $\mathcal{P}(\Gamma) \sim \Gamma^{-1+D^F_0}$, in agreement with [4]. 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 $D^F_0$, i.e. $\gamma = 2 - D^F_0$. Our starting point is the well known relation

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

(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 $E \approx E_n$ and $\Gamma_n \ll 1$. In the neighbourhood of these points, $\tau(E)$ can be approximated by a single Lorentzian [4]. 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 $\mathcal{P}_{\text{int}}(\tau) \sim \int \tau^{1/\tau} d\Gamma \mathcal{P}(\Gamma) \Gamma \sim \tau^{-(2-\alpha)}$ in the limit $\Delta E \to 0$ where we used the small resonance width asymptotics given by Eqn. (1) (for similar argumentation see also [23]). Then for the asymptotic distribution of delay times we get $\mathcal{P}(\tau) \sim \tau^{-(2-D^F_0)}$ in agreement with [4] and our numerical findings.

The validity of the heuristic arguments (and thus of Eqs. (4)) can be verified in more cases in the Fibonacci chain model of a one dimensional quasi-crystal 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 [43]. 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 $\mathcal{P}(\Gamma)$ and $\mathcal{P}(\tau)$. Here the exponent depends on the potential strength $V$, while Eqs. (4) still relate 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. (4).

Because of lack of space we defer the discussion of other results, like the fractal nature of the resonance widths, and the behaviour of the delay time autocorrelation function to a later publication [44].

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\[ P_{\text{int}}(\tau) \sim \tau^{1-\gamma} \]

\[ P_{\text{int}}(\Gamma) \sim \Gamma^{-0.5} \]

\[ P_{\text{int}}(\tau) \sim \Gamma^{1-\alpha} \]

\[ V \sim (\sigma_1, \sigma_2, \sigma_3) \]

\[ D_{E}^{(0)} \sim 2-\gamma \]

**FIG. 1.** \( P_{\text{int}}(\Gamma) \) of the Harper model (\( \lambda = 2 \)) for three approximants of the golden mean \( \sigma_1 = \frac{13977}{2584}, \sigma_2 = \frac{2584}{4181}, \) and \( \sigma_3 = \frac{4181}{6944}. \) 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 \( D_{E}^{(0)} \approx 0.5 \) and Eqn. (1). As is seen the lower cutoff of the scaling region decreases for higher approximants.

**FIG. 2.** \( P_{\text{int}}(\tau) \) of the Harper model (\( \lambda = 2 \)) for three approximants of the golden mean \( \sigma_1 = \frac{13977}{2584}, \sigma_2 = \frac{2584}{4181}, \) and \( \sigma_3 = \frac{4181}{6944}. \) 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 \( D_{E}^{(0)} \approx 0.5 \) and Eqn. (1). As is seen the upper cutoff of the scaling region increases for higher approximants.

**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 \( D_{E}^{(0)} \) 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 \( D_{E}^{(0)} \) according to Eqns. (1).