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Effects of an impurity in the Harper model

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Abstract

The effects of one impurity in the spectrum of the Harper equation is studied. The results indicate that the spectral statistics changes by reducing the clustering tendency of the energy levels, and a reduction of the fractal dimension of the spectrum is observed. This can be explained as an induced transition in the localization, since many localized states appear all over the original spectrum, as a consequence of the self-similar structure of the spectrum.

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1. Introduction

After the discovery of quasicrystals [1], the spectrum of quasiperiodic Hamiltonians has been the focus of a very active research in order to understand the electronic properties of quasiperiodic potentials [2–8]. In particular, the Harper model has been a very useful tool to investigate the transition from localized to extended eigenstates, as the spectrum pass from pure point to continuous [2,9,10]. Between both limits, there is a new type of spectrum which is known as singular continuous and is a fractal like set [9]. The corresponding eigenstates are called critical and show self-similar properties. Other systems, like the Fibonacci chain, share many of these characteristics [3]. However, until now, many of the properties predicted for these kind of models are not observed in most of the real systems like quasicrystals [11]. Here we investigate the effect of disorder in a fractal spectrum as a possible explanation for this fact, since we observe that the effect of disorder is much bigger than in a random or periodic system. To do this, we first calculate the statistical distribution of energy levels. This field has been very active in the last years [12–14]. Now is well established that in disordered insulators, the eigenstates of the Schrödinger equation are localized, and the distribution of energy-levels spacing follows a Poisson statistics [12], due to the space localization of the eigenfunctions. Disordered metals present extended states with a correlation between levels, since there is a repulsion between them. These systems are characterized by the Wigner distribution, which also is observed in quantum systems that show chaotic classical dynamics [12]. In systems with a singular continuous spectrum, a new type of spectral statistics has been found [15], since Machida et al. observed that for certain parameters of the Harper equation, the distribution of level spacings follows an inverse power law [15]. This tendency was explained as a level clus-

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tering [16]. More recently, it has been argued that the clustering regimen of the distribution of level spacings was an artifice of an inappropriate way of making the unfolding [17].

Another parameter which serves to characterize the spectrum, specially for the case of fractal or Cantor like spectrums, is the fractal dimension of the set, and the corresponding distribution of scaling exponents. A system with extended states and a continuous spectrum has fractal dimension one, while a random system in one dimension has a pure point spectrum with fractal dimension zero [11]. A singular continuous spectrum has a fractal dimension between zero and one. Our numerical results show that the local disorder reduces the fractal dimension, and the tendency for clustering is reduced. This effect can be understood as a consequence of the fractal structure of the unperturbed spectrum, that produces localized states in a self-similar way. The layout of this Letter is as follows, in Section 2 we define the problem and the various statistical measures that we consider. In Section 3 we give a possible explanation for the observed results, and in Section 4 the conclusions are given.

2. Spectral properties of the Harper model with an impurity

In this Letter, we will consider the problem of a substitutional impurity inside a Harper chain,

$$E\psi_n = 2\lambda\cos(2\pi\sigma n + \nu)\psi_n + \psi_{n+1} + \psi_{n-1} + \epsilon\delta_{n,l}\psi_n, \tag{1}$$

where ψ_n is the wave-function of energy E at site n, and $\nu = 0$. The impurity is on site l of the chain, with self-energy ϵ. We can treat the impurity as a perturbation of the original chain, in the sense that the Hamiltonian can be subdivided as,

$$H = H_0 + \epsilon H_{l,l}, \tag{2}$$

where H_0 is the Hamiltonian of the Harper model, while $H_{l,l}$ is the local perturbation at site l, given by $H_{i,j} = \delta_{il}\delta_{jl}$. If $\epsilon = 0$, we recover the Harper equation. In this unperturbed equation, when σ is irrational, the spectrum is continuous for $\lambda < 1$, pure points for $\lambda > 1$ and singular continuous when $\lambda = 1$ [2,9].

To do the gap statistics, we define an integrated level-spacing distribution as follows [16],

$$p_{\text{int}}(G) = \int_G^\infty p(G')\,dG' \tag{3}$$

whose derivative, $p(G) = -dp_{\text{int}}(G)/dG$ determines the probability density of gaps G. The gaps are obtained numerically using the transfer matrix $\mathbf{M}(E,n)$ that we define below. We write Eq. (1) as,

$$\begin{pmatrix}\psi_{n+1}\\ \psi_n\end{pmatrix} = \mathbf{M}(E,n)\begin{pmatrix}\psi_n\\ \psi_{n-1}\end{pmatrix},$$

where

$$\mathbf{M}(E,n) = \begin{pmatrix}E - 2\lambda\cos(2\pi n\sigma + \upsilon) & -1\\ 1 & 0\end{pmatrix}.$$

The irrational number σ is approximated by successive rational convergent to the continued fraction expansion of σ. For $\sigma = P/Q$, the Harper potential has period Q. In such a case, we analyze the matrix product of only one period,

$$M_Q(E,n) = \prod_{n=0}^{Q-1}\mathbf{M}_n(E,n)$$

that corresponds to the unit cell of the supercrystal. Due to the periodicity of this supercrystal, the Bloch theorem shows that the allowed values of the energies are those which satisfy $|\text{tr}\,M_Q(E,n)| \leqslant 2$, from which one obtains the spectrum of the system. In this Letter, we consider that σ is the golden mean $(\sqrt{5}-1)/2$, and thus the rational approximants are given by the ratio of successive Fibonacci numbers. Fig. 1 shows the statistics of a chain with the approximant $\sigma = 375/610$, which corresponds to 610 sites in the unit cell of the supercrystal, with $\lambda = 1$. In the same figure, we illustrate the effect of one impurity at the middle of the chain, with different values of ϵ. As ϵ raises, the curve starts to change its behavior, since the inverse power law is not longer valid at all parts of the spectrum. For the chain without impurities, $P_{\text{int}} \approx G^{-1/2}$ and $p(G) \approx G^{-1.5}$, and thus the statistical distribution of gaps follows an inverse power law of the type $P(s) \approx s^{-\beta}$ when $\lambda = 1$. As impurities are added, the probability of small gaps decreases. Locally, this effect can be thought as a reduction in the exponent β. The decreasing probability of small

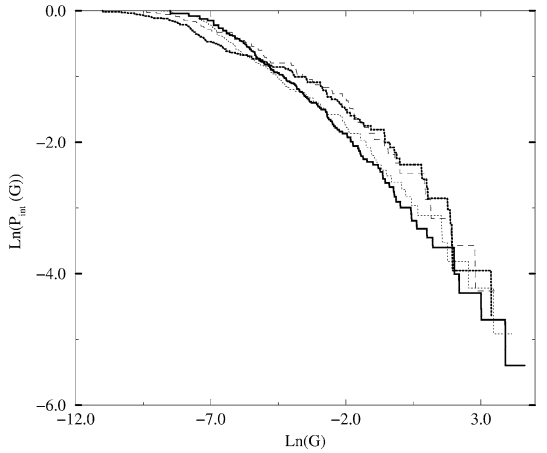

Fig. 1. Integrated distribution of gaps as a function of the gap sizes. The solid line corresponds to the Harper equation without an impurity. With thin dots, dashed lines and dots the respective statistics of chains with $\epsilon = 1.5, 5$ and 10 are shown.

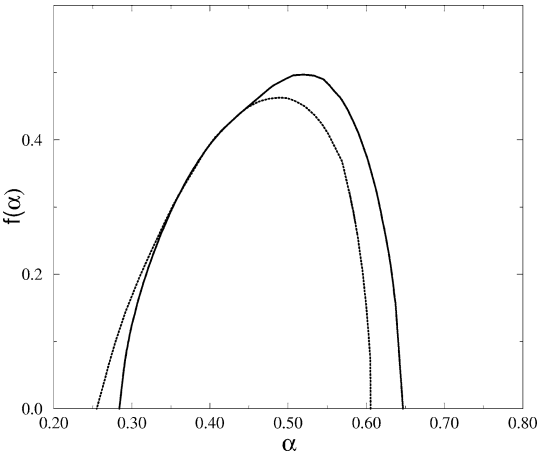

Fig. 2. Distribution of scaling exponents $f(\alpha)$ for the pure Harper model (solid line) and the same model with an impurity with $\epsilon = 2$.

spacings with respect to the original chain, indicates a reduction in the clustering of levels, since the conditional probability ($\mu(x)$) of finding a level in $[x, x + dx]$, if there is a level at x, goes as [16] $\mu(x) = (\beta - 1)x^{-1}$. If β is reduced from 1.5, this conditional probability is diminished. This means that the spectrum tends to recover the Poisson case, which corresponds to independent level positions since μ tends to be constant.

Another tool for studying the spectrum, is the multifractal analysis, which allows to determine the scaling properties of a set. In a pure fractal, as, for example, in the two-thirds Cantor set, there is only one scaling exponent. A multifractal has more than one scaling exponent (that we denote by α), and the distribution of these exponents is a very useful tool to determine the fractal dimension, the maximum and minimum exponents and the information dimension [18] of the set. To obtain this distribution, we use the tools of multifractal analysis. First we denote the bandwidth of the ith band of the spectrum by ΔE_i. Each band contains the same measure or density of states $1/N(Q)$, where $N(Q)$ is the number of bands for a given length Q of the chain. A partition function $\tau(q)$ is defined by [19],

$$\Gamma_Q(q,\tau) = \sum_{i=1}^{N(Q)} \left(\frac{1}{N(Q)}\right)^q \left(\frac{1}{\Delta E_i}\right)^\tau.$$

This function has a limit when l goes to infinity, which is either zero or infinity, unless τ and q are chosen in an appropriate way [19] such that $\Gamma_l(q,\tau) = 1$. This condition determines a function $\tau(q)$. The fractal dimension for a set of points with the scaling α, is obtained by a Legendre transformation of the partition function,

$$f(\alpha) = -\tau(q) + \alpha q,$$

where $\alpha = d\tau(q)/dq$. The maximum value of this curve is the Hausdorff dimension (d_f) and gives the fractal dimension d_f of the spectrum [18]. In Fig. 2 we plot $f(\alpha)$ for the Harper model with and without an impurity for $\epsilon = 2$ and $\lambda = 1$. For the unperturbed case, the curve is similar to the one obtained by Tang et al. [20], and d_f is equal to 0.5 as observed previously [20]. When the impurity is added, d_f is 0.46 for $\epsilon = 2$. This means that the spectrum is more point-like than in the Harper case. For a periodic chain, this effect is not observed (since the bandwidth of the unique band remains nearly equal when the impurity is added), and the same can be said in the case of a pure point spectrum (d_f is non-negative). Observe that the maximum exponent present in the perturbed system is lower than in the pure Harper system. The opposite is true for the minimum exponent: disorder shifts the exponent to lower values. As a result, one can conclude that the bands reduce their bandwidths at all the scales.

3. Apparition of localized states inside the spectral gaps

Since the spectral statistics and the distribution of scaling exponents are related to the localization of the wave-functions, the changes observed are related with the localization of states. This is illustrated in Fig. 3, where the inverse participation ratio (IPR), defined as,

$$\mathrm{IPR} = \sum_{n=1}^{q-1} |\psi_n|^4$$

is shown for a chain of 1597 sites with $\lambda = 1.0$. Observe that we choose the IPR for determining localization in favor of the Lyapunov coefficients, due to the inherent problems in detecting localization with such method, as showed by the author in a previous work [21]. A bigger IPR means more localization, and in the figure it can be seen that in the chain with an impurity there are many states that are much more localized than in the unperturbed chain.

We can understand this effect as follows: in a chain where all the self-energies are equal, an impurity produces a localized state outside the band. This fact is a consequence of the Rayleigh condition that satisfies an impurity mode for any system [22],

$$G_0(E,l,l) = \frac{1}{\epsilon}, \tag{4}$$

where $G_0(E,l,l)$ is the Green function of the unperturbed chain at the perturbed site l, defined as,

$$G_0(E,l,l) = \sum_n \frac{\psi_l(E_n)\psi_l^*(E_n)}{E + i\eta - E_n} \tag{5}$$

and E_n is an eigenvalue of the non-perturbed Hamiltonian H_0, and η is a small imaginary number.

The Rayleigh equation can only be satisfied when $G_0(E,l,l)$ has no imaginary part, which corresponds to energies that are spectral gaps [22]. In the present case, $G_0(E,l,l)$ is the Green function of the Harper model evaluated in the impurity site. However, for the singular continuous spectrum, the distribution of gaps is self-similar [23], thus, if we produce a localized state inside a gap at a certain scale, we will produce other localized states at different scales. This effect is illustrated in Fig. 7 where the real part of the Green function of the unperturbed chain is shown. The horizontal line corresponds to the line

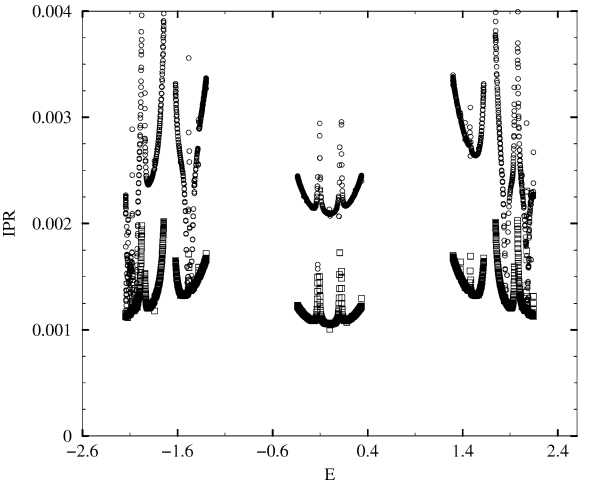

Fig. 3. Enlarged view of the lowest part of the IPR for a Harper chain of 1597 sites, $\lambda = 1.0$ and $\epsilon = 15$. In squares (circles), the IPR of the Harper equation without (with) an impurity. Eigenstates with a bigger IPR are more localized.

$1/\epsilon$. An impurity mode appears at the intersection of both functions. Notice that the Green function is self-similar as a consequence of the self-similar structure of the spectrum and the corresponding wave-functions [24]. The scaling of the Rayleigh condition, is more clearly seen if we assume that $G_0(E,l,l)$ has a certain scaling in the sense that after a change of scale δ in the energy, the Green function is scaled as,

$$G_0(\delta E,l,l) = \delta^{\gamma(E)} G_0(E,l,l),$$

where $\gamma(E)$ is an scaling exponent. Observe that $\gamma(E)$ depends on E, since the spectrum is a multi-fractal, with a certain distribution of scaling exponents. Thus, if in a certain scale the Rayleigh condition is valid for an energy E_c, for an energy given by $E_{c1} = \delta^{-\gamma(E_c)} E_c$ the condition is also satisfied since,

$$G_0\left(\delta^{-\gamma(E_c)} E_c, l, l\right) = \left(\delta^{-\gamma(E_c)}\right)^{\gamma(E_c)} G_0(E_c,l,l) = \frac{1}{\epsilon}.$$

The same argument can be applied again at different scales, and many impurity modes would appear at the energies $E_{c,m} = \delta^{-m\gamma(E_c)} E_c$, where m is an integer.

As usual, impurity modes are formed at the expense of the original spectrum, since the local density of states at site n of the perturbed system ($\rho_n(E)$) is related with the unperturbed density ($\rho_n^0(E)$) by [22],

$$\rho_n(E) = \rho_n^0(E) - \epsilon \frac{\mathrm{Im}}{\pi} \frac{G_0(E,n,l)G_0(E,l,n)}{1 - \epsilon G_0(E,l,l)}.$$

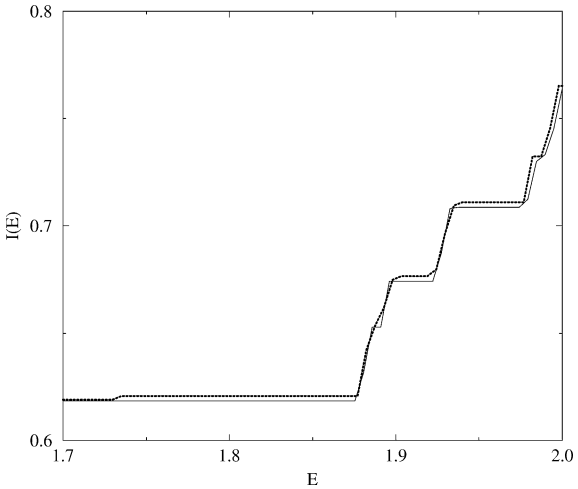

Fig. 4. Enlarged section of the integrated density of states of the Harper equation (solid line) and the same with an impurity $\epsilon = 15$ (dots) for a chain with 1597 sites.

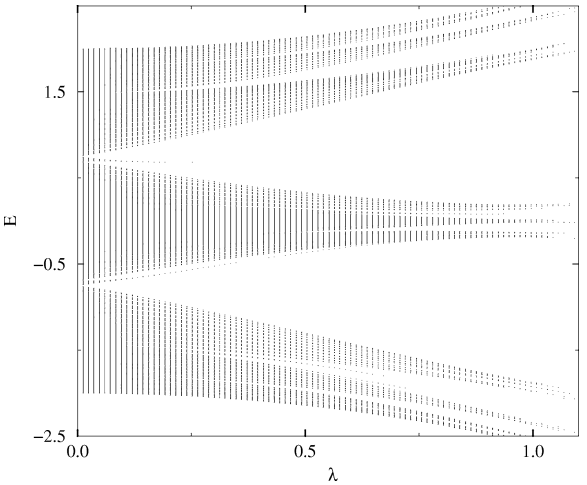

Fig. 5. Allowed bands as a function of λ of the Harper chain for an approximant of 310 sites.

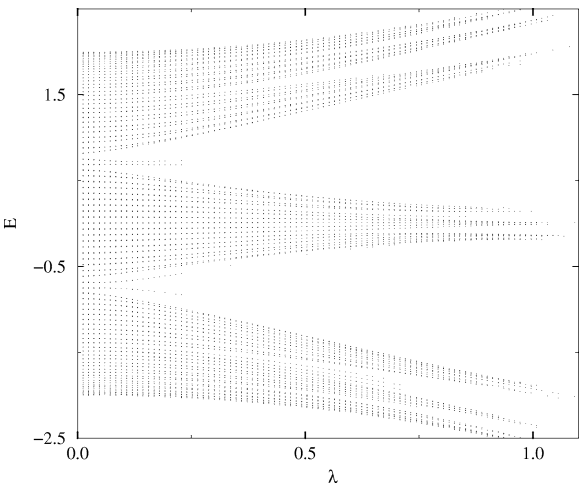

Fig. 6. Allowed bands as a function of λ of the Harper chain with an impurity $\epsilon = 10$ at the middle of the chain.

Using this fact, and by observing that the total number of states remains constant, one can conclude that the width of each band is reduced, as observed in the previous section from the distribution of scaling exponents. In general, the reduction of the bandwidth is related with the fact that the states are more localized, since the bandwidth depends on the overlap of the wave-function at the end of the unit cell considered [21].

In a finite lattice, with a fixed boundary condition, the effect consists in a displacement of the eigenvalues toward the gaps. As an example, in Fig. 4 a small portion of the integrated density of states of a Harper chain (obtained from diagonalization) is compared with a perturbed chain with an impurity $\epsilon = 15$. As it can be seen, there is a displacement of the eigenvalues at all the scales.

The same result can be observed using the transfer matrix formalism. In Figs. 5 and 6, we show the allowed bands as a function of the parameter λ. As it can be seen, there is a reduction in the bandwidth, which is achieved by a fragmentation of the bands.

Notice that the arguments given in this Letter for the self-similar generation of impurity states depend only in the self-similar nature of the Green function. Thus, one can expect this conclusion to be general for other quasiperiodic potentials. For example, similar observations of a localization transition due to an impurity were made in a previous work for a different quasiperiodic system: the Fibonacci chain [25]. Furthermore, in that paper it was discussed how the fixed boundary conditions produce effects at all scales, since each fixed end of a chain can be seen as an impurity, and also some resonant eigenstates were found [25]. Similar effects have been also observed in the study of the statistical properties of resonances in open quasiperiodic systems [26,27], where there is a strong analogy to the present work. In Refs. [26, 27], the quasiperiodic systems were opened by intro-

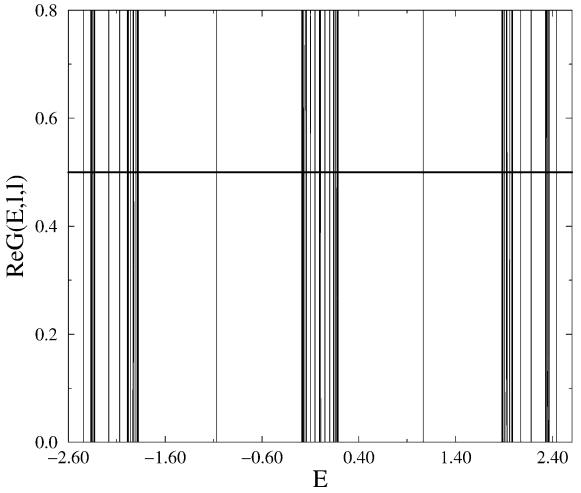

Fig. 7. Amplification of the real part of the Green function at the impurity site for a chain with $Q = 144$ sites, and the function $1/\epsilon$ for $\epsilon = 2$.

ducing an impurity (by adding an imaginary part to the on-site potential) at the leads of a finite Harper and Fibonacci chains. As a result, the Hamiltonian becomes non-Hermitian and the eigenvalues move to the complex part gaining an imaginary part (the resonance width Γ). The resulting probability distribution of resonance widths ($P(\Gamma)$) follows a power law as a function of the width $P(\Gamma) \approx \Gamma^{-\alpha}$, i.e., small resonances widths are more frequent. Since the resonance width is inverse proportional to the mean life-time (τ) of a state due to the Heisenberg principle, one expects more states with high τ. States of this type are local excitations that do not decay very fast, and thus the excitations remain inside the chain for a certain period of time, so they tend to be more localized than non-perturbed states. As can be seen, the observed abundance of these states is in agreement with the results found in this Letter.

4. Conclusion

We have studied the Harper chain with a local perturbation, and it was found that the spectral statistics changes by reducing the tendency for clustering observed in the case of a singular continuous spectrum. Also, the fractal dimension of the spectrum and the bandwidths are reduced, as is deduced from the distribution of scaling exponents. These changes are due to the apparition of localized impurity modes all over the gaps, which are distributed in a self-similar way. Other quasiperiodic systems follow this behavior, and thus it seems plausible to be a general feature of self-similar spectrums.

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