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The influence of phason disorder on the electronic spectrum and eigenstates of Fibonacci lattices

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Abstract

The electronic properties of a Fibonacci lattice with one mistake (phason flip) is studied. The phason is treated as a perturbation of the perfect chain, and we show that it is equivalent to the presence of two substitutional impurities. The effects of the phason on the electronic spectrum are that localized and resonant eigenstates are observed all over the whole spectrum and the distribution of energy level-spacing is modified by reducing the tendency of lever-clustering. On the contrary, it is also shown that phasons applied at certain sites of the chain left the spectrum unaffected. © 1998 Published by Elsevier Science B.V.

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With the advent of high-quality quasicrystalline samples, there has been clear evidence that quasicrystals have singular electronic properties. Some remarkable properties are that quasicrystals have abnormal high electrical resistivity [1] and that the conductivity is improved with impurities, structural defects and temperature [2]. It is obvious that many of these unusual properties of quasicrystals will be cleared up if we achieve a full understanding of the properties of quasiperiodic Hamiltonians. The study of one-dimensional quasiperiodic lattices for instance has provided important information on the nature of the spectrum and eigenstates. It is now clear that the spectrum is singular continuous [3,4] and the eigenstates are critical [5], with self-similar wave functions in real space. It seems, however, that the one-dimensional case is trivial but it is the only analytically tractable and it is justified to pursue work on this case since it may be an important guide to behavior in more dimensions, where critical states is an still unsettled question.

Of particular importance is the effect of phason disorder on the electronic properties of quasicrystals which has not been completely understood. In this letter we address this problem for a Fibonacci chain. As we shall see, despite of its simplicity, this model is capable of displaying the essential effects of phason disorder on the electronic spectrum of quasiperiodic structure.

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For that goal, using a tight-binding Hamiltonian, we shall consider that a single phason flip is considered a perturbation of the perfect chain. It should be remarked that we shall not consider phasons as long wavelength hydrodynamic modes [6]. Instead, what we mean by a phason (or a phason flip) is a single rearrangement of tiles at a certain site of the quasiperiodic structure which, in the hyper-space approach, corresponds to a localized fluctuation or tear along the perpendicular space.

The problem is first addressed analytically by noticing that one phason in the Fibonacci sequence is equivalent to the presence of two substitutional impurities on contiguous sites. As it will be seen, the two impurities create localized states in the whole spectrum of the unperturbed system due to the self-similar structure of gaps. This is a singular property of self-similar structures since in a diatomic periodic chain, with the same defect, only two localized states appear while the continuum of extended states remains unchanged. This change of localization properties of wave functions affects also the spectrum since they are closely related. For instance, extended wave functions correspond to continuous spectra while localized functions are characteristic of pure point spectra. In addition, critical states are associated with singular continuous spectra. Thus, when localized states appear all over the spectrum, the statistic of energy-levels in the spectrum must be modified. Here, using transfer matrices, numerical calculations are carried out to support these predictions and quantify the change on the level-spacing statistics. Contrary to these results, we will also show that there are special sites on the chain where phasons have no effect on the spectrum.

The Hamiltonian H_0 that we consider in this paper is defined, in the diagonal problem, by

$$H_0 = \sum_i \left(\epsilon_i |i\rangle \langle i| + t |i\rangle \langle i+1| + t |i\rangle \langle i-1|\right) , \tag{1}$$

where ϵ_i is the single site-energy and t is the nearest-neighbor hoping integral (set to one in this work). The site energies ϵ_A and ϵ_B are given by a Fibonacci sequence. We now introduce a phason flip in (1). Assume that we have an energy ϵ_A at site $|l\rangle$ and ϵ_B at $|l+1\rangle$, switching these values is equivalent to a phason flip at site $|l\rangle$. The perturbed Hamiltonian can be written as $H = H_0 - \left(\epsilon_A |l\rangle \langle l| + \epsilon_B |l+1\rangle \langle l+1|\right) + \left(\epsilon_B |l\rangle \langle l| + \epsilon_A |l+1\rangle \langle l+1|\right)$, or

$$H = H_0 + \Delta |l\rangle \langle l| - \Delta |l+1\rangle \langle l+1| , \tag{2}$$

where $\Delta = (\epsilon_B - \epsilon_A)$. This situation can be thought as a substitution of the host atoms at sites $|l\rangle$ and $|l+1\rangle$ by impurities with a level lying Δ times higher (or lower) than the original values. Eq. (2) can be written as $H = H_0 + H_l + H_m = H_{0l} + H_m$, where $m = l+1$ and H_{0l} is the Hamiltonian with a single impurity.

In order to study (2), we start considering the effect of a single impurity at site $|l\rangle$, that is, $H_{0l} = H_0 + H_l$. Following a perturbative approach, the task consist of expressing $G_{0l}(E)$ (the Green function of H_{0l}) in terms of G_0 (the Green function of H_0) and obtain information about eigenfunctions and eigenvalues of H_{0l} from $G_{0l}(E)$, defined as $G_{0l}(E) = (E - H_{0l})^{-1}$. Using a Dyson expansion, we have

$$G_{0l} = G_0 + G_0 S G_0 , \tag{3}$$

where

$$S = \frac{\Delta}{1 - \Delta \langle l| G_0 |l\rangle} |l\rangle \langle l| . \tag{4}$$

The discrete eigenvalues of H are obtained from $\langle l| G_0 |l\rangle = 1/\Delta$, that is, when the imaginary part of G_0 is zero. Since the imaginary part of G_0 is proportional to the local density of states, if new states appear due to the impurity at $|l\rangle$, they must lie inside a gap of the original spectrum. The presence of a single defect can therefore create impurity states all over the original spectrum since the spectrum of a Fibonacci lattice contains an infinite number of gaps [3] (actually, a similar effect is observed when the ends of a finite chain are taken into account [8,9]). Note that in a finite lattice the number of states is fixed and the apparition of

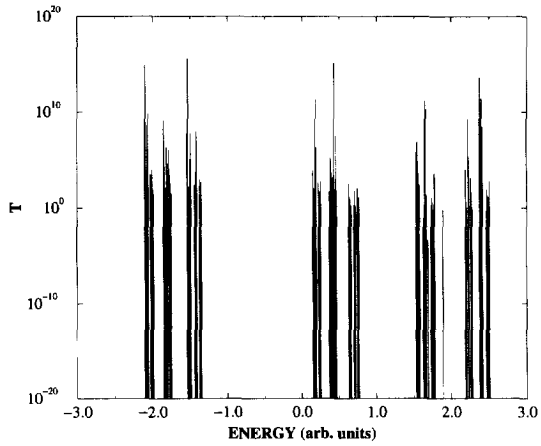

Fig. 1. T is plotted as function of the energy for the lattice with the phason flip. States fall in three categories: $T > 1$, localized at the phason site; $T \approx 1$, resonant (not scattered by the phason); $T \approx 0$, critical (scattered by the phason).

impurity states can be viewed as a shifting of the original states toward the spectral gaps, as it is expected from Rayleigh's theorem [10].

Now let us consider H_{0l} as the unperturbed part and H_m as the perturbation. From the previous equation, the Green function of the lattice with the phason flip is

$$G = G_{0l} - \frac{\Delta}{1 + \Delta \langle l+1 | G_{0l} | l+1 \rangle} G_{0l} | l+1 \rangle \langle l+1 | G_{0l} . \tag{5}$$

In this case impurity states are created when $1 + \Delta \langle l+1 | G_{0l} | l+1 \rangle = 0$. In order to find the new eigenvalues, let us consider the quantity

$$T = \frac{1}{| 1 + \Delta \langle l+1 | G_{0l}^{+}(E) | l+1 \rangle |^2} = \frac{1}{(1 + \Delta \mathrm{Re} \langle l+1 | G_{0l}^{+}(E) | l+1 \rangle)^2 + [\pi \rho(E, l+1)]^2} ,$$

which is directly related to the scattering of critical states since the eigenstates of H are given by $|\psi(E)\rangle = |\phi(E)\rangle + G_{0l}^{+}(E) S^{+}(E) |\phi(E)\rangle$, where $|\phi(E)\rangle$ are the eigenfunctions of H_{0l} and the plus exponents stand for the retarded Green function [11]. The amplitude at site $l+1$ is given by $\langle l+1 | \psi(E) \rangle^2 = T \langle l+1 | \phi(E) \rangle^2$.

T has its maximum value where $\rho(E, l)$ is small and $1 + \Delta \mathrm{Re} \langle l+1 | G_{0l}^{+}(E) | l+1 \rangle$ approaches zero, which is indicative of a resonant eigenstate. In these states T approaches one, and are the less scattered by the impurity. For impurity modes localized at the phason site T tends to infinity since $\rho(E, l+1)$ and $1 + \Delta \mathrm{Re} \langle l+1 | G_{0l}^{+}(E) | l+1 \rangle$ are both zero.

In Fig. 1, T is shown as a function of the energy for a Fibonacci chain of generation 19 with a phason flip. Observe that there are several states with $T \gg 1$; these are localized at the phason site. States with $T \approx 1$ are resonant and are not scattered by the phason, having nearly the same Landauer conductivity as in the perfect lattice (as a matter of fact, using the formalism of renormalized transfer matrices [12], it can be proved that these resonant states correspond to energies such that the commutator of the transfer matrices is nearly zero.) It should be pointed out that in the case where just one impurity is present, resonances are observed for a wide range of self-energies of the impurity [13]. Fig. 1 shows also states with $T \approx 0$ which correspond to critical states scattered by the phason.

The localization properties affects also the statistics of energy-levels. In the present case, the level statistics of the eigenvalue spectrum can be carried out by following the procedure described in Ref. [14]. Observe first that in a singular continuous spectrum all the states are bounded and the number of energy gaps larger than

some size s can be counted and an integrate level spacing distribution can be obtained by varying s. It is given, up to normalization, by

$$P_{\rm int}(s) = \int_s^\infty P(s')\,{\rm d}s',$$

with which the distribution function of level spacings s is given by $P(s) = -{\rm d}P_{\rm int}/{\rm d}s$.

The use of transfer matrices provide a efficient way of numerically obtaining the levels and their spacings. In this method, the wave equation is written in matrix form as

$$\begin{pmatrix} \psi_{i+1} \\ \psi_i \end{pmatrix} = M(i) \begin{pmatrix} \psi_i \\ \psi_{i-1} \end{pmatrix},$$

where

$$M(i) = \begin{pmatrix} E - \epsilon_i & -1 \\ 1 & 0 \end{pmatrix}.$$

Wave functions at any site are obtained, in terms of ψ_0 and ψ_1, by multiplying successively the transfer matrices in each site. The eigenenergies of the lattice are those which satisfy the condition

$$\mathrm{Tr}\left(\prod_{i=1}^{N-1} M(i) \right) \leqslant 2.$$

The site energy ϵ_i of the Fibonacci lattice take the two values ϵ_A and ϵ_B, and the sequence of $M(i)$'s is a Fibonacci sequence with two matrices. This allows the use of a renormalization procedure since the following relation holds [4],

$$M_n \equiv M(F_n) = M(F_{n-1})M(F_{n-2}), \tag{6}$$

where F_n is a Fibonacci number of generation n.

A Fibonacci chain with a phason flip near the center can be also generated using transfer matrices as follows. Eq. (6) is written as $M_n = M_{n-2}M_{n-3}M_{n-2}$, and in this expression M_{n-3} is replaced by M'_{n-3}, which contains a phason flip at the beginning of the sequence. Explicitly, we know that $M_3 = M_2M_1$, $M_4 = M_3M_2$, $M_5 = M_4M_3$, etc., defining $M'_3 = M_1M_2$, then we have $M'_4 = M'_3M_2$, $M'_5 = M'_4M_3 = M'_3M_2M_3$, etc. In this way, the n-step is given by $M^p_n = M_{n-2}M'_{n-3}M_{n-2}$ which yields a Fibonacci lattice with a single phason in the central section. Here, the superscript p indicates that the chain has a phason flip.

Fig. 2a shows a log–log plot of the integrated level spacing distribution of a Fibonacci chain of generation $n = 20$ (dashed line) and a chain with a phason flip (solid line) where all level spacings were normalized to mean spacing 1. In the former case, the curve displays an inverse power law $P_{\rm int}(s) \sim s^{1-\beta}$ (thus $P(s) \sim s^{\beta}$) and we found that, for $\epsilon_A = -1$ and $\epsilon_B = 1$, $1 - \beta = -0.6928 \pm 0.0011$. The fractal dimension (d_f) of the spectrum is related with β by [14] $d_f = \beta - 1$. The case of the lattice with the phason flip shows some differences; the curve follows nearly the same behavior as the perfect case but only for spacings greater than the average. For lower spacings, the curve deviates considerably showing a lower probability for these level-spacings. Albeit $P_{\rm int}(s)$ is not an exact power law in this region, we tried a power law fitting which gives $1 - \beta = -0.2056 \pm 0.0031$.

The power law observed in the Fibonacci lattice is associated with a level clustering regime [15,14], where the conditional probability of finding a level between x_0 and $x_0 + {\rm d}x$, provided that there is a level in x_0, is $\mu(x) \sim (\beta - 1)x^{-1}$. We can therefore conclude that according to our results, the levels tend to be less clustered when a phason flip is applied. This result turns out to be in agreement with the fact that the spectrum

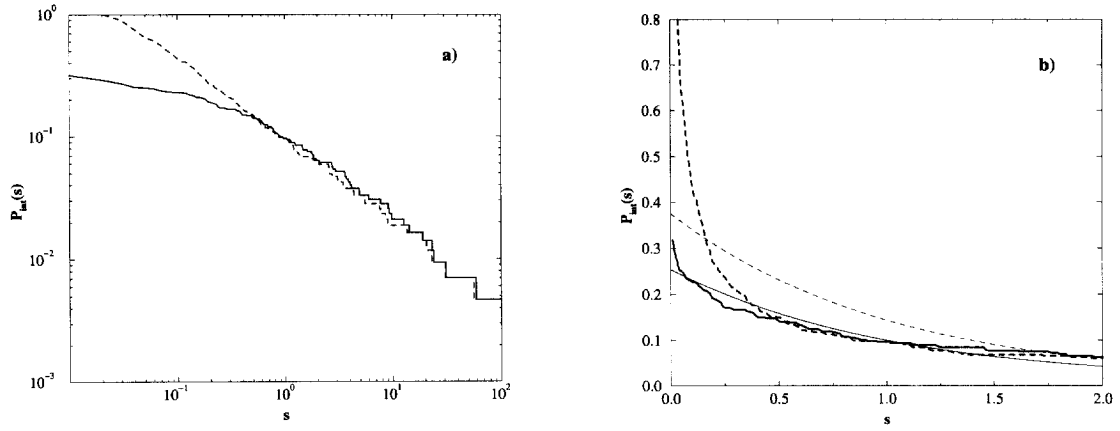

Fig. 2. Integrated level spacing distribution of chains of generation $n = 20$. (a) Logarithmic plot of a Fibonacci chain (dashed line) and a chain with a phason flip (solid line). (b) The same as in (a) but in linear scale. In order to compare with a Poisson distribution, each curve was fitted to a function of the form $A + B\,e^{-x}$, shown as thinner lines. All level spacings were normalized to mean spacing 1.

of disordered lattices is pure point; $P(s)$ follows a Poisson distribution [16] and $\mu(x) = \text{const}$. In order to illustrate this point, Fig. 2b shows the same graph as in 2a but in linear scale. Each curve was fitted to a Poisson-like equation shown as thinner lines. As it can be seen, the best fit is obtained for the curve that corresponds to the chain with the phason flip.

The above discussed effects depend, however, on the site where the phason flip is applied. For instance, the spectrum remains unchanged if a phason is applied in a site where two previous generations of the chain are joined or at the end of the chain. To support this affirmation, we observe that such a phason is generated by switching two previous generations of the chain, i.e., if $M_n = M_{n-1}M_{n-2}$, the chain with only one phason flip at the end is written as $M_n^p = M_{n-2}M_{n-1}$. Then, by using the cyclic properties of the trace, we have

$$\mathrm{Tr}(M_{n-2}M_{n-1}) = \mathrm{Tr}(M_{n-2}M_{n-2}M_{n-3}) = \mathrm{Tr}(M_{n-2}M_{n-3}M_{n-2}) = \mathrm{Tr}(M_{n-1}M_{n-2})\,. \tag{7}$$

Thus, $\mathrm{Tr}(M_n^p) = \mathrm{Tr}(M_n)$ and the spectrum is not affected. Also $T = 1$, since the original eigenstates are not scattered by the phason. Observe that the cyclic property of the trace provides a way for constructing chains containing more that one phason but with the same spectrum as the perfect Fibonacci chain.

Summarizing, considering a phason flip as a perturbation, and using transfer matrices, we have carried out a study of the effect of phason disorder on the electronic spectrum of a Fibonacci chain that can be applied to any singular continuous spectrum. From this analysis, we conclude that a singular continuous spectrum turns out to be quite unstable against phason disorder; the energy-level statistics changes due to the self-similarity of the spectrum. The new statistics shows less clustering than in the Fibonacci chain and many localized states appear inside the original spectrum. This can explain large changes in the spectrum observed when a small concentration of phasons is added to a Fibonacci lattice [17], although the introduction of phason disorder in some sites of the chain does not change the original spectrum. Also, it was found that resonant eigenstates are not scattered by phasons, having nearly the same Landauer conductivity as in the unperturbed lattice. We have to mention that all these effects are expected to be observed in the one impurity problem, where all the eigenvalues are shifted toward higher energies [10]. Nevertheless, in this work we centered our attention in phasons in quasiperiodic sequences, which are central to understanding the growth and electronic properties of quasicrystals.

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