

# The electronic spectrum of a quasiperiodic potential: From the Hofstadter butterfly to the Fibonacci chain

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## Abstract

We show that an electronic tight-binding Hamiltonian, defined in a quasiperiodic chain with an on-site potential given by a Fibonacci sequence, can be obtained using a superposition of Harper potentials. Since the spectrum of the Harper equation as a function of the magnetic flux is a fractal set, known as the Hofstadter butterfly, we follow the transformation of the butterfly to a new one that contains the Fibonacci potential and related approximants. As a result, the equation in reciprocal space for the Fibonacci case has the form of a chain with long range interaction between Fourier components. Then, the structure of the resulting spectrum is analyzed by calculating the components in reciprocal space of the related potentials. As an application, the correlator of each potential and some localization properties are obtained.

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## 1. Introduction

Although the discovery of quasicrystals [1], which are alloys with a structure neither periodic, nor disordered, launched an extensive investigation on quasiperiodic Hamiltonians, in fact the study of such Hamiltonians goes back to the old Frenkel–Kontorova model [2] and to the pioneer research made in the 70s [3,4]. Here the word quasiperiodic means that in the system there are incommensurate periods; and as a result, the dimension of the Fourier space is always bigger than the dimensionality of the system. One of the most famous quasiperiodic Hamiltonians was obtained by Harper in connection with a problem proposed by Peierls [3]. The idea was to find the spectrum and the wave-functions of an electron in a square lattice with a perpendicular magnetic field. Two periods are involved in the problem, the electron motion in the lattice and the cyclotron frequency [3]. The spectrum as a function

of the ratio between these two periods turned out to be a complex set known as the Hofstadter butterfly [3]. Since then, the Harper model has been very useful to investigate the transition from localized to extended eigenstates, as the spectrum passes from pure point to continuous [3–5]. Between both limits, there is a new type of spectrum which is known as singular continuous [4]. The corresponding eigenstates are called critical and display self-similar properties. For certain parameters of the Harper equation, the distribution of level spacings follows an inverse power law [6], which is a new type of spectral statistics [6], explained as a level clustering tendency [7]. Also, it has been possible to find analytical expressions for the wave-functions using quantum groups [8]. More recently, the quantum phase diagrams [9] and the electronic correlation effects have been analyzed [10].

Another quasiperiodic system that has been extensively studied is the Fibonacci chain (FC). This chain is the simplest model of a quasicrystal [11]. The importance of the FC arises because the nature of the physical properties of quasicrystals is still not well understood [12–14]. Even in

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the theoretical side there is a lack of understanding in how electrons propagate in two and three dimensions [15], although the situation is more clear in one dimension. As is well known, a periodic potential satisfies the Bloch's theorem, which tells that the eigenstates of the Schrödinger equation are plane waves of delocalized nature, and the energy spectrum is continuous [16]. For disordered systems, like in the one dimensional (1D) Anderson model, all the states are localized corresponding to isolated eigenvalues [17], although long-range correlations can produce extended states due to resonance effects, as in the random dimer model [18]. In more dimensions, there is a mobility edge which separates extended from localized states [17]. For most of the quasiperiodic systems in 1D, the spectrum is neither continuous nor singular, instead a new type of spectrum, called singular continuous is obtained [19]. This spectral type is similar to a Cantor set, and presents a multifractal nature. The corresponding eigenfunctions are called critical, and also show self-similarity and multifractality. In two and three dimensions, the nature of the spectrum is not known, although there seems to be a kind of mobility edge [20,21]. However, even in 1D, where large amount of work has been done, there are many unsolved questions, like the nature of conductivity [22] or diffusivity [5], the spectral statistics and the shape of many of the eigenfunctions [23,24]. Even in the FC, there are no analytical expression for the wave-functions, except for few energies [11].

The Harper and Fibonacci potentials share many characteristics; for example, both can present a multifractal spectrum with self-similar wave-functions, although the Harper equation can also present pure point and continuous spectrum. An interesting question is why Fibonacci does not show pure point or continuous spectrum. An understanding of these questions will serve to give a better picture of the electronic properties of quasiperiodic systems. For example, it can suggest a way to construct analytical solutions for the FC in terms of those solutions from Harper.

In this article, we show that in fact, the Fibonacci potential can be approximated as a superposition of Harper potentials. Then, we can follow the evolution of the Hofstadter butterfly to the equivalent in the Fibonacci case. This allows to explore the equations in reciprocal space of the FC. The layout of this work is the following, in Section 2 we show how to obtain the Fibonacci potential in terms of Harper. Section 3 is devoted to a discussion of the corresponding spectra using the properties in reciprocal space, while Section 4 is devoted to study the localization in terms of the correlators of the potential. Finally, in Section 5 the conclusions are given.

## 2. The Fibonacci and Harper models

As a general model we will use a tight-binding Hamiltonian of the type,

$$(E - V(n))\psi_n = t_n\psi_{n+1} + t_{n-1}\psi_{n-1}, \quad (1)$$

where  $\psi_n$  is the wave-function at site  $n$ ,  $t_n$  is the resonance integral between sites  $n$  and  $n+1$ . For the present purposes,  $t_n$  is set to 1 for all sites.  $V(n)$  is the atomic on-site potential and  $E$  are the allowed energies. The generalized Harper equation is obtained when  $V(n) = V_H(n)$ , with  $V_H(n)$  defined as [3],

$$V_H(n) \equiv 2\lambda \cos(2\pi\phi'n + v), \quad (2)$$

where  $\lambda \geq 0$  is the strength of the potential,  $\phi'$  is a parameter that contains the ratio between the electron cyclotron frequency and the elementary quantum flux, and  $v$  is a phase shift. For a rational  $\phi'$ , Eq. (1) can be solved by Bloch's theorem, although its value is very limited since the coefficients in Fourier space of the solution form a dense set [3]. For  $\phi'$  irrational, the spectrum depends on the value of  $\lambda$ . For  $\lambda < 1$ , the spectrum is continuous with extended wave-functions, when  $\lambda > 1$  the spectrum is made from pure points and localized solutions. At  $\lambda = 1$  the spectrum is singular continuous with self-similar wave-functions.

The other potential that we will consider here, is the simplest model of a quasicrystal, called the diagonal model, obtained when  $V(n)$  has two possible values, that we denote by  $V_A$  and  $V_B$ , following the Fibonacci sequence (FS). The FS is build as follows: consider two letters,  $A$  and  $B$ , and the substitution rules,  $A \rightarrow B$ , and  $B \rightarrow AB$ . If one defines the first generation sequence as  $\mathcal{F}_1 = A$  and the second one as  $\mathcal{F}_2 = B$ , the subsequent chains are generated using the two previous rules, for instance,  $\mathcal{F}_3 = AB$ . Starting with an  $A$ , we construct the following sequences,  $A$ ,  $B$ ,  $AB$ ,  $BAB$ ,  $ABBAB$ ,  $BABABBAB$ , and so on. Each generation obtained by iteration of the rules is labeled with an index  $l$ . The number of letters in each generation  $l$  is given by the Fibonacci numbers  $F(l)$  of generation  $l$ , which satisfy:  $F(l) = F(l-1) + F(l-2)$  with the initial conditions:  $F(0) = 1, F(1) = 1$ . There are other choices for building a model quasicrystal, since for example, one can set  $V(n)$  as a constant and use the FS to define a sequence in the transfer integrals  $t_n$ . Such problem is known as the off-diagonal model. The mixed model is obtained when the FS is used both in  $V(n)$  and  $t_n$ . A vast literature is available for such potentials [15], but since the results are very similar for all of these models, in the present article we will only consider the diagonal one, although the techniques presented here are also useful tools for analyzing other cases.

Our first task in order to compare the FC and the Harper potential, is to find an analytical expression for the Fibonacci potential. This can be done in the following way. By using the cut and projection method, it is very easy to prove that the position  $y_n$  of the  $n$ -esim atom in a chain determined by a FS is given by [25],

$$y_n = [n\phi],$$

where the function  $[x]$  denotes the greatest integer lower than  $x$ ,  $\phi$  is a parameter which turns out to be the tangent of the angle between the real space subspace and a higher dimensional periodic lattice [25]. To obtain the Fibonacci

case,  $\phi$  must be equal to the inverse of the golden mean  $\tau^{-1} = (\sqrt{5} - 1)/2$ . For other values of  $\phi$ , one gets structures that have different kinds of quasiperiodicity, or rational approximants of quasiperiodic chains, since the main effect of  $\phi$  is to change the sequence of the binary potential, i.e., the sequence and statistics of letters  $A$  and  $B$ . For example, if  $\phi = 1$ , the resulting sequence is  $AAAAAA \dots$ , for  $\phi = \frac{1}{2}$ , we have  $ABABABAB \dots$  and for  $\phi = \frac{2}{5}$ ,  $ABAABAABA \dots$ . As a matter of fact, the parameter  $\phi$  is very important to understand crystal–quasicrystal transitions [26,27], since  $\phi$  is the inclination of the subspace in the cut and projection method. It provides a symmetry order parameter for the Landau free energy and thus contains information about the thermodynamics [26]. A relevant case is obtained when  $\phi = F(l)/F(l + 1)$ , which are the rational approximants of the golden mean.

The next step for building the potential consists in the observation that the separation between atoms in the chain is  $y_{n+1} - y_n$ . It is easy to show that the separation takes only two values,  $l_A$  and  $l_B$ . Thus, we can make a potential with the sequence of spacings to get,

$$V(n) = V_B + V_A(\lfloor(n + 1)\phi\rfloor - \lfloor n\phi\rfloor). \quad (3)$$

Using the identity  $x = \lfloor x \rfloor + \{x\}$ , where  $\{x\}$  is the decimal part of  $x$ , we obtain that  $V(n)$  can be written as,

$$V(n) = \langle V \rangle + \delta V(\{n\phi\} - \{(n + 1)\phi\}), \quad (4)$$

where  $\langle V \rangle = V_A\phi + V_B(1 - \phi)$  is an average potential that shifts the zero of the energies, and  $\delta V$  is the strength of the quasiperiodicity, measured by the difference between site-energies  $\delta V \equiv V_A - V_B$ . In what follows, without any loss of generality, we set  $V_A$  and  $V_B$  in such a way that  $\langle V \rangle = 0$ . A note of caution: is clear that our method gives the potential for all values of  $\phi$ , and not only for the FS. To avoid confusions, here we will call “square wave potential” to all of the potentials generated from Eq. (4), since if the integer variable  $n$  is replaced by a continuous one, say  $x$ , the resulting  $V(x)$  is just a square wave as shown in Fig. 1. The potential stays at  $-\delta V\phi$  for an interval of length  $1 - \phi$ , and then it jumps to  $\delta V(1 - \phi)$  for a length  $\phi$ . The Fibonacci potential is just a particular case for  $\phi = \tau^{-1}$ .

The decimal part function  $\{x\}$  has period 1, and can be developed as a Fourier series,

$$\{x\phi\} = \frac{1}{2} - \frac{1}{\pi} \sum_{s=1}^{\infty} \frac{1}{s} \sin(2\pi\phi sx).$$

It follows that,

$$V(n) = \bar{V} + 2\delta V \sum_{s=1}^{\infty} \tilde{V}(s) \cos(\pi s\phi(2n + 1)), \quad (5)$$

where  $\tilde{V}(s)$  is the  $s$  harmonic of the Fourier series,  $\tilde{V}(s) = \sin(\pi s\phi)/\pi s$ . The first terms of this series are shown in Fig. 1, and in fact, we are approximating a square wave by a sum of cosines. In Fig. 1 we can see the slow convergence of the series due to the  $1/s$  factor of each harmonic. This potential can be further reduced if a proper phase  $\chi$  is used

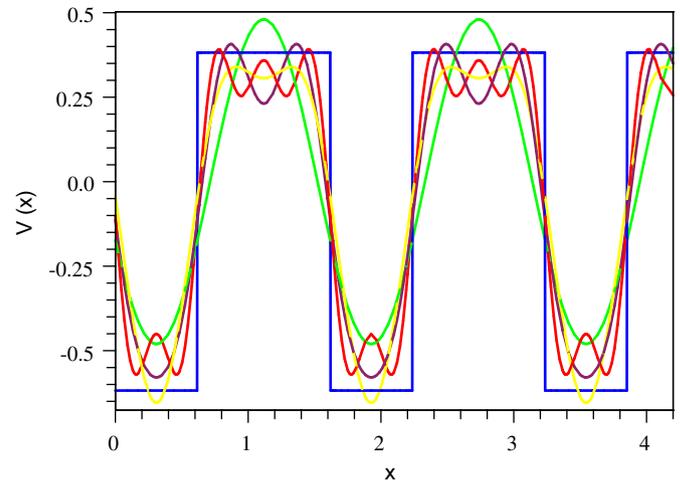


Fig. 1. The Fibonacci potential can be obtained by evaluating a square wave of period  $\tau$  at integers values. The approximations with one, two and three harmonics, obtained from Eq. (6), are shown in the figure. Notice the asymmetry in the steps.

in Eq. (4), in such a way that the terms  $\{x\phi\}$  are replaced by  $\{x\phi + \chi\}$ . The phase  $\chi$  is only an horizontal translation of the potential. For  $\chi = -\phi/2$ , the Fibonacci potential is simply written as,

$$V(n) = 2\delta V \sum_{s=1}^{\infty} \tilde{V}(s) \cos(2\pi s\phi n). \quad (6)$$

It is also worthwhile mentioning that for  $s = l\phi^{-1}$  (where  $l$  is an integer),  $\tilde{V}(s) = 0$ . This condition can only hold when  $\phi$  is a rational. When this is not the case,  $\tilde{V}(s) \approx 0$  for integers  $s$  and  $l$  such that  $\phi \approx l/s$ , and thus  $l/s$  is a rational approximant of  $\phi$ . Such rationals are obtained from the continuous fraction development of  $\phi$ . The corresponding potentials are just rational crystalline approximants. For the FS,  $s \approx l\tau$  from where it follows that  $l$  and  $s$  are successive Fibonacci numbers. The most important Fourier components in Eq. (6) are those where  $s \approx (r + \frac{1}{2})\phi^{-1}$  for an arbitrary integer  $r$ . Using the decomposition in integer and decimal parts, this happens whenever  $\{(r + \frac{1}{2})\phi^{-1}\}$  is nearly 0 or 1. Comparing Eq. (2) with Eqs. (5) and (6), we observe that in fact, the Fibonacci potential can be approximated as a superposition of Harper potentials if we set  $\phi' = \phi$ , so this situation can be thought as an applied effective modulated magnetic field [28]. This leads to many questions. The first is how the transition from Harper is done. To answer this, we will cut the sum in Eq. (6) at a finite number of harmonics, denoted by  $S$ , and the resultant potential will be called  $S$ -harmonic potential. In Fig. 2(a), we plot the energy spectrum of the Harper equation for the case  $\lambda = 1$ . This spectrum, as well as the others discussed in this article, were obtained by using the transfer matrix formalism [29]. Fig. 2(a) is the well known Hofstadter butterfly [3]. Notice that here  $v = \pi\phi$ , and thus our figure does not match exactly the original butterfly, since therein, a sweep for all values of  $v$  between 0 and  $2\pi$

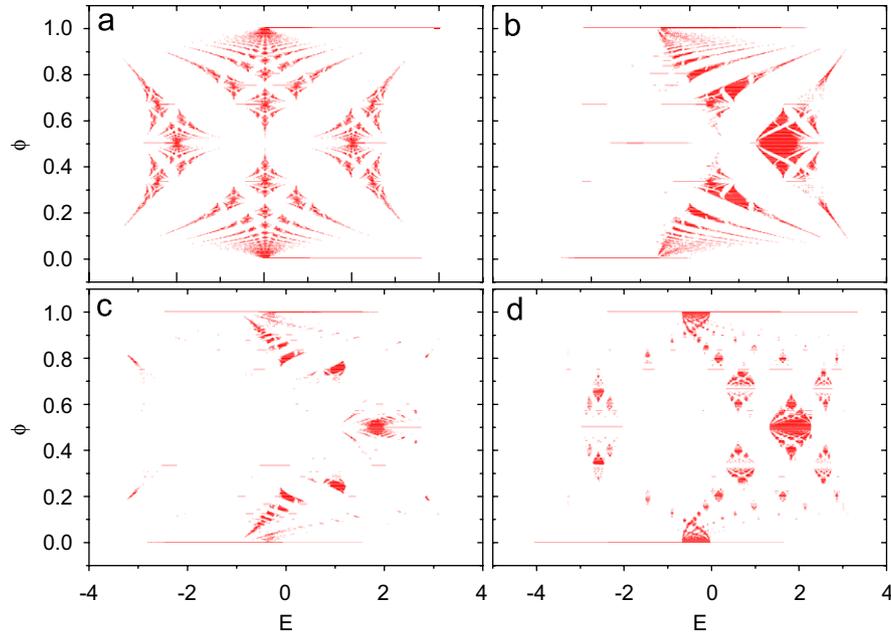


Fig. 2. The energy spectrum as a function of the parameter  $\phi$  for  $\delta V = \pi/\sin(\pi\tau^{-1})$ , corresponding to  $\lambda = 1$  in the pure Harper equation, using (a) one harmonic (similar to the Hofstadter butterfly), (b) two harmonics, (c) three harmonics, and (d) the square wave potential, that contains the Fibonacci potential for  $\phi = \tau^{-1}$ . Notice that in case (a), the Hofstadter butterfly is not exactly the usual one reported in the literature, since here we do not consider all the possible values of the phase  $v$ . As a result, the spectrum is not symmetric around  $E = 0$ , and some points are missing.

was made, and thus the spectrum has more points and is symmetric around  $E = 0$ . Our spectrum is not symmetric around  $E = 0$  since the phase  $v$  produce a shift of the spectrum. We have verified that in our computer program, we reproduce the original butterfly when such sweep is made, and also that the symmetry around  $E = 0$  is recovered when  $v = \pi/2$ . The reason of not considering all possible values of  $v$  is that we want to compare with the FC, which is defined only for a given phase. A sweep in  $v$ , is equivalent to make a sweep in  $\chi$  in the  $S$ -harmonic case, which produces new chains in the same isomorphism class. If  $\phi$  is taken as a parameter in Eq. (6), then the spectrum of Fig. 2(a) is also the  $S$ -harmonic potential for  $S = 1$ . The parameter used is  $\delta V = \pi/\sin(\pi\tau^{-1}) \approx 3.3706$ , chosen to correspond to  $\lambda = 1$  in the Harper equation. In Figs. 2(b) and (c) we show the effects of adding harmonics  $s = 2$  and 3 in the development of the potential, and Fig. 2(d) presents the result for the square wave potential. There is an important change between the pure Harper case and the second harmonic case. Mainly the left part of the Hofstadter butterfly is washed out. Also, is clear that with only three harmonics, the structure for  $\phi = \tau^{-1}$  is already very similar to the pure Fibonacci case. This wash out due to the second harmonic has its origins in the difference of lengths in the steps of the square wave potential. For the first harmonic, this change is not observed. By looking at Fig. 1, one can see that with two harmonics there is an asymmetry in the upper part of the series. This effect is more notorious when  $\delta V > 1$ , and can be translated in an almost split band limit when  $\delta V \rightarrow \infty$ , around self-energies  $V_A$  and  $V_B$ . In fact, this is one of the main differences between the Harper and Fibonacci potentials.

In Fig. 3, a similar set of figures presents what happens when  $\delta V = 1$ . This corresponds to  $\lambda = \sin(\pi\tau^{-1}) \approx 0.2967$  in the pure Harper case, and thus the spectrum is continuous. Figs. 3(b) and (c) are the cases with two and three harmonics. Finally Fig. 3(d) shows the case of Eq. (4), which is a beautiful fractal. Since it is known that the FC presents a singular continuous spectrum [19], it is open the question for which harmonic there is the transition from one type of spectrum to the other.

In all of the previous cases,  $\phi$  was studied between 0 and 1 since using the following identity,

$$\cos(2\pi x) = \cos(2\pi(\lfloor x \rfloor + \{x\})) = \cos(2\pi\{x\}),$$

we have that  $\cos(2\pi\phi sn + k) = \cos(2\pi\{\phi\}sn + k)$ . Thus, the problem has periodicity 1 in  $\phi$ . It only depends on  $\phi$  only through  $\{\phi\}$ . For rational  $\phi$  of the form  $P/Q$ , with  $P$  and  $Q$  integers, this means  $P < Q$ .

### 3. Structure of the spectrum

In this section we will discuss the main features that arises from the previous figures. The spectral properties of the pure Hofstadter butterfly has been discussed by many others using diverse techniques [3,4,30], but in order to understand the transformation between butterflies, here we will explain the main features using the structure in reciprocal space of the potential. Let us first study the tight-binding equation in the usual approach. We propose that the wave-function can be written as [4],

$$\psi_n = e^{ikn} \sum_{m=-\infty}^{\infty} d_m e^{im(2\pi\phi n + v)},$$

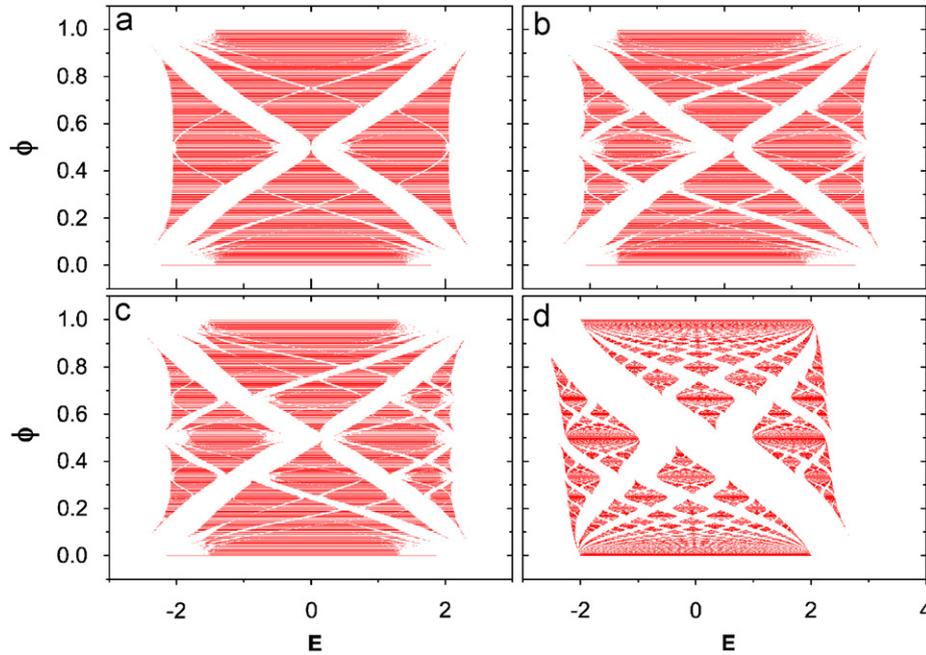


Fig. 3. The energy spectrum as a function of the parameter  $\phi$  for  $\delta V = 1$  using (a) one harmonic (corresponding to the Harper model at  $\lambda = 0.2967$ ), (b) two harmonics, (c) three harmonics, and (d) square wave potential using Eq. (4).

where  $d_m$  is the  $m$  Fourier component of the wave-function. If we introduce this solution into Eq. (1), when  $S$  harmonics are present in the potential, the following set of equations are obtained,

$$(E^* - 2\delta V^* \cos(2\pi\phi m + k))d_m = d_{m+1} + d_{m-1} + \sum_{s=2}^S \tilde{V}^*(s)(d_{m-s} + d_{m+s}), \quad (7)$$

where the parameters are defined as  $E^* = 2E/(V(1)\delta V)$ ,  $\delta V^* = 2/(V(1)\delta V)$ , and,

$$\tilde{V}^*(s) = \frac{\tilde{V}(s)}{\tilde{V}(1)} = \frac{1 \sin(\pi s \phi)}{s \sin(\pi \phi)}.$$

The other parameter is  $k = v$  for the pure Harper equation, and  $k = v = \pi\phi$  for the general case. If only the first harmonic  $s = 1$  is used, then Eq. (7) shows that a Harper equation in the reciprocal space is also a Harper equation with a renormalized set of parameters [30]. In the case of Fibonacci, Eq. (7) proves that the Schrödinger equation in reciprocal space has a different form, since each site interacts with infinite many others. The interaction between Fourier components decreases as  $1/s$ . It is a long range interaction that can be thought as a modulating field. Observe that in the transformation of the Hofstadter butterfly, the limitation to  $S$  harmonics in the potential is equivalent in Fourier space to a cut-off at range  $S$  of the interaction.

When  $\phi$  is a rational number, say  $P/Q$ , the potential with any number of harmonics has periodicity  $Q$ , as has been discussed in the previous section. The corresponding

wave-functions are given by,

$$\psi_n = e^{ikn} \sum_{m=0}^Q d_m e^{im(2\pi n(P/Q) + \pi(P/Q))}, \quad (8)$$

where  $-\pi/Q < k \leq \pi/Q$ . The only difference between the Harper and the Fibonacci case, is in the values of the  $Q$  coefficients  $d_m$ . Since the set  $d_m$  can be obtained in the Harper case using quantum groups [8], the present work suggests the possibility of finding an analytical solution for the Fibonacci potential.

Also, we can show that an effective potential can be written in the reciprocal space for periodic approximants of the  $S$ -harmonic potential. According to Eq. (8), the solution must have periodicity  $Q$ , with  $l$  an integer. Such result can also be obtained from  $V(n)$  when  $\phi$  is the rational  $P/Q$ . In this case, the factor  $\cos(2\pi s \phi n)$  in Eq. (6) is repeated for the harmonics  $s'$  that has the form  $s + lQ$  where  $l$  is a positive integer. By grouping all the harmonics module  $Q$ , the potential is written as,

$$V(n) = \bar{V} + 2\delta V \sum_{s=1}^Q \tilde{V}_{P/Q}(s) \cos\left(2\pi s \frac{P}{Q} n\right), \quad (9)$$

where  $\tilde{V}_{P/Q}(s)$  is an effective potential,

$$\tilde{V}_{P/Q}(s) = \frac{Q \sin(\pi s P/Q)}{P} \left( \sum_{l=0}^{\infty} \frac{(-1)^{lp}}{s + lQ} \right). \quad (10)$$

The equation in reciprocal space is then reduced as follows:

$$(E' - 2\delta V' \cos(2\pi\phi m + k))d_m = \sum_{s=1}^Q \tilde{V}_{P/Q}(s)(d_{m-s} + d_{m+s}), \quad (11)$$

which shows that for a periodic approximant, the range of the interaction in reciprocal space is  $Q$ .

Concerning the spectrum, the band edges are obtained from Eq. (7) when  $k = 0$  and  $\pi/Q$ . Instead of following this path, we will look at how the structure of the potential in the *lattice reciprocal space* determines the spectrum for  $\delta V \ll 1$ . A much more physical insight can be obtained in this way. This approach is different from the one realized in others works [4,30], since usually the potential is projected in the base  $e^{im(2\pi\phi n + v)}$ . Here we will project into the reciprocal “vectors” of the lattice ( $G$ ). The main idea is that for a 1D crystal, it is known that each reciprocal “vector”  $G$  with component of the potential ( $\tilde{V}(G)$ ), opens a gap of size,

$$\Delta_G \approx 2\|\tilde{V}(G)\|,$$

at reciprocal vectors  $q = G/2, G, 3G/2, \dots$ . It is possible to follow the opening of the gaps by the effect of  $\tilde{V}(G)$ . The reciprocal components are

$$\tilde{V}(G) = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} V(n)e^{-iGn},$$

where  $G$  can be chosen among the wave vectors  $q = 2\pi t/N$ , with  $t = 0, \dots, N-1$ , in a lattice with  $N$  sites, where periodic boundary conditions are used. The first Brillouin zone is the interval  $-\pi \leq q < \pi$ , although to simplify the algebra we take  $q$  between 0 and  $2\pi$ . Consider first the Fourier components of the Harper potential ( $\tilde{V}_H(G)$ ) for a given parameter  $\phi$ ,

$$\tilde{V}_H(G) \equiv \tilde{V}_H(t) = \frac{2\lambda}{\sqrt{N}} \sum_{n=0}^{N-1} \left( \frac{e^{i2\pi\phi n} + e^{-i2\pi\phi n}}{2} \right) e^{-i2\pi t n/N}. \quad (12)$$

If  $(\phi - t/N)$  is an integer, the problem is almost solved, because  $\tilde{V}(t) = \lambda\delta(\phi - t/N)$ . This happens whenever  $\phi = P/Q$  and

$$\frac{P}{Q} = \frac{m}{N},$$

so when  $N$  is chosen as a multiple of  $Q$ , as for example  $N = lQ$  with  $l = 0, 1, 2, \dots$ , then the harmonic  $m = P$  is the only one that has a contribution. This solution is very simple compared with other complex approaches, since what most of the people do is fix  $N$  and then a sweep of the  $\phi$  is made. In other words, the Hofstadter butterfly is built for a fixed  $N$ . However, the present approach shows that if we fix a rational  $\phi$  and move  $N$  for each  $\phi$  until  $N = lQ$ , the potential is much more tractable. In the limit of big  $l$ ,  $N \gg Q$  so there are many vectors  $k$  that fulfill the condition  $N = lQ$ ; in other words, there is a continuum of  $q$  such that  $e^{i2\pi\phi n}$  has a “possible periodicity” of the system.

The problems arise when  $\phi$  is an irrational or  $N$  is not a multiple  $Q$ , since the previous trick is not valid. Eventually, the sum in Eq. (12) can be made when  $\phi - t/N$  is not an

integer to give

$$\tilde{V}_H(G) \equiv \tilde{V}_H(t) = \frac{\lambda}{\sqrt{N}} \left( \frac{1 - e^{i2\pi\phi N}}{1 - e^{i2\pi(\phi - t/N)}} + \frac{1 - e^{-i2\pi\phi N}}{1 - e^{-i2\pi(\phi + t/N)}} \right).$$

The corresponding norm is

$$\|\tilde{V}_H(t)\|^2 = \frac{\lambda^2 A}{N B}, \quad (13)$$

where

$$A = (1 - \cos 2\pi\phi N)^2 + [\cos 2\pi\phi - \cos 2\pi\phi(N-1)]^2 - 2\cos(2\pi\phi t/N)[1 - \cos 2\pi\phi/N][\cos 2\pi\phi - \cos 2\pi\phi(N-1)],$$

and

$$B = [1 - \cos(2\pi(\phi - t/N))][1 - \cos 2\pi(\phi + t/N)].$$

Notice how  $\tilde{V}_H(t) \rightarrow \lambda\delta(\phi - t/N)$  as  $\phi \rightarrow t/N$ . The gaps width depend upon these components, and the maximum of  $\tilde{V}_H(G)$  occurs when  $G \approx \pm\phi$ . Now let us propose the solution,

$$\psi_n = \sum_{q=-\infty}^{\infty} c_q e^{iqn}$$

for Eq. (1). The resulting equation in reciprocal space is

$$(E - 2\cos q)c_q = \sum_G \tilde{V}_H(G)c_{q-G}.$$

Since the main contribution to  $\tilde{V}_H(G)$  comes from  $G \approx \pm\phi$ , a mixing of wave vectors  $G \approx \phi$  and  $G \approx -\phi$  occurs at  $q = \pm\phi/2$ . Using perturbation theory, this means that for  $\lambda \ll 1$ , the main gaps are open around,

$$E \approx \pm\lambda \cos(2\pi(\phi/2)) = \pm\lambda \cos(\pi\phi).$$

Fig. 4 compares this prediction with the Hofstadter butterfly, showing an excellent agreement. Other band gaps are obtained at  $q = \pm r\phi/2$  with  $r \in \mathbb{N}$ . The general  $p$ th-order perturbation term is of the form,

$$V_q = V(q_0 - q_1)V(q_1 - q_2)\cdots V(q_{N-1} - q_N),$$

where  $q_t$  labels the vector  $2\pi t/N$ . For small  $\lambda$ , gaps will be open at

$$E \approx \lambda^r \cos(\pi\phi r).$$

These cosine branches are also plotted in Fig. 4, compared with the Hofstadter butterfly, showing that the basic structure of the spectrum is determined by these branches. When  $\lambda$  is near 1, around each gap there are many wave vectors that mix together, so the present approximation breaks out. A detailed observation of the case of the potential with harmonics, given by Eq. (6), shows that the main effect is an asymmetry of the cosine branches. This is very clear in Figs. 3(b) and (c). The same analysis performed to the Harper equation is valid for these cases, specially for low  $S$ . The equivalent rough approximation

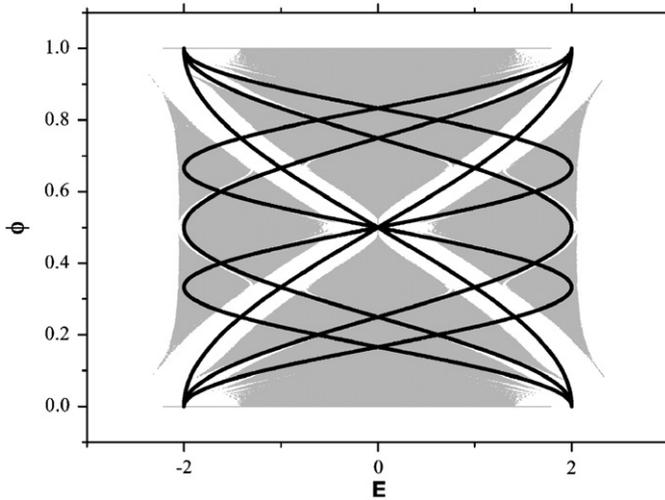


Fig. 4. General structure of all the obtained spectra. The Hofstadter butterfly is compared with the cosine branches given by  $E = \lambda \cos(\phi m)$  for  $m = 1, 2$  and  $3$  for  $\lambda = 0.2967$ .

for the position of the band gaps is,

$$E \approx \pm \left( \delta V \sum_{s=1}^{\infty} \frac{\sin(\pi s \phi)}{\pi s} \right) \cos(\pi \phi).$$

What is behind the process of gap opening, is a self-similar folding of the bands in the reciprocal space, as revealed by following the sequence of approximants for  $\phi$  in all the obtained spectra. For  $\phi = 0$ , the spectrum is continuous and goes from  $-2\delta V$  to  $2\delta V$ . The next most simple spectrum corresponds to  $\phi = \frac{1}{2}$ , which gives two bands. If the lattice has period 2, then the first Brillouin zone of the zero approximant ( $\phi = 0$ ) is folded around half the original Brillouin zone limit,  $k = \pi/2$ . As usual, an energy gap of size  $\Delta_G \approx 2|\tilde{V}(G)|$  is open in the zone boundary due to a mixing of waves with reciprocal vectors  $G/2$  and  $-G/2$ . In this case,  $G = \pi/2$  and  $\tilde{V}(G) = 2\lambda$ . For the Harper equation we get,

$$\Delta_G = 4\lambda.$$

In the Harper equation, there is a symmetry around  $E = 0$ , thus the bands limits are  $E = \pm 2\lambda$ . For the pure FC first approximant ( $\phi = \frac{1}{2}$ ),  $\tilde{V}(G)$  produces a different gap, and the central gap limits are

$$\Delta_G = \pm \delta V.$$

This gap is clearly in the horizontal lines at  $\phi = \frac{1}{2}$  in Fig. 3(d). The process of folding in reciprocal space can be repeated in a similar way for other rationals like  $\phi = \frac{2}{3}$  and  $\frac{1}{3}$ . In this case, the periodicity is 3, and the folding around the first Brillouin zone limit occurs at  $k = \pi/3$ . Three bands are produced in this case, and the gaps are centered at  $\pm \lambda \cos(\pi/3)$  and  $\pm \lambda \cos(2\pi/3)$ . The process is repeated for other approximants.

#### 4. Localization properties using correlators

As a simple example of the utility of having an expansion for the FC, we will obtain the potential correlator. This can serve to understand how the addition of harmonics leads to different localization properties. For  $\lambda = 1$  the eigenstates of the Harper equation are critical, i.e., the wave-functions decay as a power law, while they are localized for  $\lambda > 1$  and extended for  $\lambda < 1$ . This comes from Eq. (7). Therein, if the square of the components is finite,

$$\sum_{m=-\infty}^{\infty} |d_m|^2 < \infty,$$

the corresponding wave-function is non-localized. In the pure Harper equation, when  $\lambda \rightarrow \infty$ , the solutions in real space are localized wave-functions, since they correspond to the dual of solutions with  $\lambda \rightarrow 0$  in reciprocal space, which are known to be extended. In the FC, for all values of  $\delta V$  the eigenstates are critical [29]. An interesting question is how many harmonics are needed to produce the transition from the extended states in the Harper equation to the critical behavior observed in the FC. To measure localization in one dimension, the Lyapunov exponent (LE) is used ( $L^{-1}$ ). The LE is the inverse of the localization length ( $L$ ) for a localized state. Having the zero value of the LE, one can have a power law dependence of the wave-function. There are already many methods to treat the spectrum and the eigenfunctions, but the simplest one uses the pair correlation function of the potential [31]. This method requires that the potential must be bounded for any  $n$ , with  $V(n) \ll 1$ . Notice that the previous condition is the most interesting limit for quasiperiodic potentials, since for  $V(n) \gg 1$  one can use perturbation theory to obtain the spectrum and eigenfunctions [32]. Also, to get analytical expressions for the  $LE$ , the potential must be ergodic [31,33], a condition that is satisfied by the potential (5), since the obtained sequences of  $V_A$  and  $V_B$  are periodic or quasiperiodic. A second condition is that the correlation matrix of the potential ( $\xi_{kk'} \equiv \xi(k - k')$ ) must be semi-positive defined [31], where the correlator  $\xi(k)$  of any potential is defined as

$$\langle V(n)V(n+k) \rangle = \varepsilon_0^2 \xi(k), \quad \langle V(n)V(n) \rangle = \varepsilon_0^2.$$

For the Harper equation,  $\xi(k) = \cos(2\pi\phi k)$ , and for a Fibonacci-like potential, by using Eq. (6), the correlator can be written as,

$$\xi(k) = 4\delta V \sum_{s=1}^S \frac{\sin^2(\pi s \phi)}{(s\phi)^2} \cos(2\pi s \phi k), \quad (14)$$

which satisfies the conditions for a proper correlation in order to get the analytical LE. For a 1D Hamiltonian, the inverse localization length is given by [31],

$$L^{-1} = \frac{\varepsilon_0 \varphi(\mu)}{8 \sin^2(\mu)}; \quad \varphi(\mu) = 1 + 2 \sum_{k=1}^{\infty} \xi(k) \cos(2\mu k).$$

Here, the function  $\varphi(\mu)$  is given by the Fourier series with the coefficients  $\xi(k)$ . For the Harper equation,  $\xi(k) = \cos(2\pi\phi k)$ , which gives  $\varphi(\mu) = 0$  and thus all states are nonexponentially localized. For Fibonacci-like,  $\xi(k)$  is given by Eq. (14), which also gives  $\varphi(\mu) = 0$  for all  $S$ . Thus, since the  $LE$  are 0, all states are non-localized for any number of harmonics. As a result, the states can have a power law dependence of the wave-function or they can be extended as in the Harper case. The question that remains to be answered, is how the transition from extended to critical states is achieved as the number of harmonics is increased from Harper to Fibonacci. To solve this question, an expression for the scaling exponents in terms of the correlators is needed [34]. In a forthcoming article, we will pursue such investigation.

## 5. Conclusions

In the present article, we have shown that the Fibonacci potential can be approximated as a sum of Harper potentials. As a consequence, one can follow the evolution of the spectral types as a function of the number of harmonics. In particular, a butterfly similar to the Hofstadter case is found, which contains the Fibonacci potential. The corresponding spectrum is a fractal object, and the Fourier components of the potential provide a simple explanation for the main features of the spectra. However, since the spectrum of the Fibonacci chain is singular continuous with power law localized states for any strength of the potential ( $\delta V$ ), and that the Harper potential has a continuous ( $\lambda < 1$ ), singular continuous ( $\lambda = 1$ ), and pure point spectrum ( $\lambda > 1$ ), with non-localized, power law, and localized states, respectively, this leads to many interesting questions, as for example, at which harmonic the spectral type is changed when the potential goes from Harper to Fibonacci. This is equivalent to ask for which harmonic the eigenfunctions of the Fibonacci case become critical.

It is worthwhile mentioning that  $\phi$  controls the transition from periodic to quasiperiodic sequences, and thus, the present approach also leads to the possibility of studying the electronic properties as a function of such parameter. Furthermore, it can be proved that the parameter  $\phi$  can also be related with a magnetic field, as happens in the Harper potential. In that case, instead of having a constant magnetic field in space, one has a space modulated magnetic field [35]. In real systems, the changes in  $\phi$  are simple to study using many different devices, since its effect is only a change in the sequence of the binary potential. For example, one can use microwaves in a cavity, a dielectric superlattice or a space modulated magnetic field in a semiconductor.

Finally, the present approach also leads to the possibility of building analytical solutions for a FC. We hope that

other researchers will try to answer some of the intriguing questions posed by this paper.

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