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Finite periodic and quasiperiodic systems in an electric field

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Abstract. We study several properties of Fibonacci and Thue-Morse sequences of square well potentials in the presence of an applied electric field and compare them with the results for periodic systems. We obtain integrated densities of states and show that Wannier-Stark ladders appear in all cases. We analyze the fractal properties and the energy level spacing distributions and show that the effect of the electric field is to make more regular the quasiperiodic systems. Finally, we obtain the wavefunctions of these systems.

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I. Introduction

The properties of independent electrons in a periodic lattice potential and with a uniform electric field applied have produced a great interest during many years. Frequently, to illustrate the features of these systems, one-dimensional periodic potentials are used. In this case, the electron Hamiltonian can be written as

$$H = T + V(x) + eFx, \tag{1}$$

where T is the kinetic energy operator, $V(x)$ is a one-dimensional periodic potential, e is the electron charge and F is the modulus of the electric field applied. When interband transitions are ignored, Zener [1] suggested a class of electron wave functions that exhibit time-periodic oscillations, now called Bloch oscillations. The period of these oscillations is given by $\tau_B = h/eFa$, where h is Planck's constant, and a is the lattice spacing.

Wannier [2] proposed that the eigenvalue spectra of periodic systems in an electric field are ladders of discrete and equally spaced levels, which are now called Wannier-Stark ladders (WSL). WSL and Bloch oscillations are not unrelated, because the equally spacing of the energy levels are prerequisite for the periodic oscillations. The energy levels in a ladder are given by $E_n = E_0 + neFa$, E_0 being the lower energy level of the band and n a positive integer. WSL have been also extensively studied from the experimental point of view [3, 4]. Often, semiconductor superlattices have been used to study WSL, the associated Bloch oscillations, and related phenomena, since the electric field needed to observe these phenomena are easily accessible due to the large effective lattice spacing [5, 6].

We study the electronic spectra and the existence of Wannier-Stark ladders in quasiperiodic systems with external electric fields applied over the length of the system (not between $-\infty$ and $+\infty$). Our systems consist in Fibonacci and Thue-Morse sequences of square potentials.

The Fibonacci lattice has become a standard model for the study of quasiperiodic systems. This structure is made by juxtaposing two different building blocks α and β arranged in a Fibonacci sequence. The Fibonacci sequence S_∞ is obtained by the recursion relation

$$S_{l+1} = \{S_l S_{l-1}\}, \quad l \geq 1 \tag{2}$$

with $S_0 = \{\beta\}$ and $S_1 = \{\alpha\}$. The Fibonacci number F_l is the total number of building blocks α and β in S_l, and obeys the recursion relation $F_{l+1} = F_{l-1} + F_l$ for $l \geq 1$ with $F_0 = F_1 = 1$. It is easy to obtain that in the limit $l \to \infty$, the ratio F_l/F_{l-1} tends to the golden mean $\tau = (1 + \sqrt{5})/2$.

A Thue-Morse sequence is a different type of aperiodic system, with a very different kind of aperiodicity from that of Fibonacci sequences. The Thue-Morse sequence is obtained by the recursion relation

$$M_{l+1} = \{M_l M_l^*\}, \quad l \geq 0 \tag{3}$$

with $M_0 = \{\alpha\beta\}$ and where M_l^* is the complement of M_l, obtained by interchanging α and β.

In Sect. 2, we describe the model used in the calculations and the numerical procedure employed to obtain the energy spectrum. The numerical procedure is based on the characteristic determinant method, whose main results are also described.

In Sect. 3, we study the properties of the energy spectra as a function of the electric field 1 applied via the integrated density of states. We show that Wannier-Stark ladders appear not only in the case of periodic potentials, but also in the case of quasiperiodic sequences. We study the effect of the electric field on the fractal properties of the energy spectra. We show that the electric field changes the fractal behavior of the spectra, making it more regular.

In Sect. 4, we study the energy level spacing distribution and show that the electric field behaves as a parameter that introduces 'order' in quasiperiodic systems. In Sect. 5, we obtain the wavefunctions for quasiperiodic systems, and we check that they are also localized by the electric field.

II. Construction of the chain and method of calculation

We want to study numerically how the presence of an electric field affects the properties of the electronic spectra of the two types of system considered, periodic and quasiperiodic. In the presence of the field, there are still well defined energies whose corresponding wavefunctions are localized. Our systems consist in sets of potential wells arranged following periodic or quasiperiodic sequences, surrounded by two semi-infinite media of constant potential energy. We choose our origin of energies as the energy of the lower semi-infinite medium. In the periodic case, all the wells have the same depth d_α, and the widths of each well and barrier have been set to unity. In Fibonacci and Thue-Morse cases, we use two different types of sequences. In sequences of type 1, the Fibonacci and Thue-Morse systems are obtained by using two different well depths, d_α and d_β, while the widths of the wells and barriers are equal, and have been set to unity in the numerical calculations. In sequences of type 2, the two quasiperiodic sequences are obtained by using two different well widths, w_α and w_β, while the depths of the wells are equal, and has been set to 5 in the numerical calculations. In our numerical study, the choice of the parameters d_α, d_β, w_α and w_β is made in such a way that there is only a bound state per well. The units of all the magnitudes correspond to consider that $\hbar = 2m = 1$. This convention is assumed in the rest of the paper.

To build the systems when we apply a uniform electric field along the longitudinal axis, instead of considering a linear increasing of the potential energy at the bottom of each well and top of each barrier, we have discretized this linear increasing into 10 small steps of constant potential energy. As an example of the systems under study, we plot in Fig. 1 two Fibonacci chains consisting in eight wells with the same electric field applied, $F = 0.06$. The upper plot corresponds to a type 1 sequence, meanwhile the lower one corresponds to a type 2 sequence. The Fibonacci sequence plotted is then $\alpha\beta\alpha\alpha\beta\alpha\beta\alpha$, corresponding to S_5, as defined in (2), where α and β represent either d_α and d_β for type 1, or w_α and w_β for type 2. The value of F, the electric field, is given by:

$$F = \frac{\Delta E}{L} \tag{4}$$

For energies smaller than 0, the system is closed, and has a discrete electronic spectrum forming a single band of

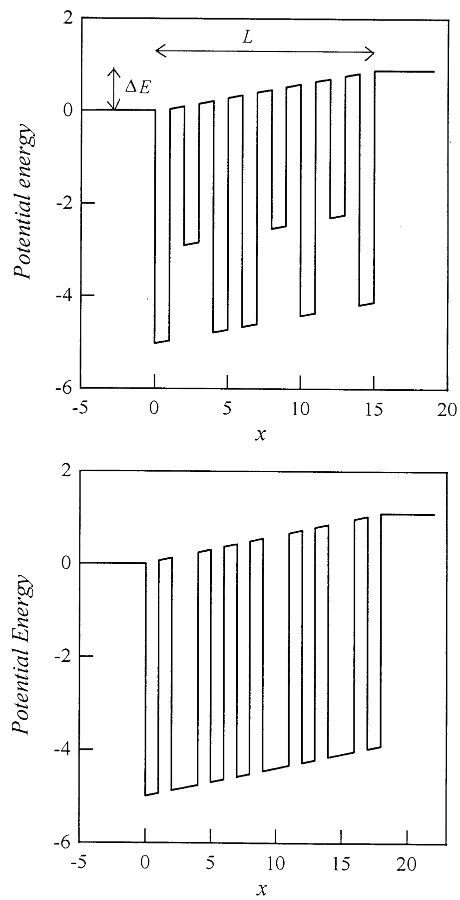

Fig. 1. A type 1 Fibonacci sequence (upper), and a type 2 Fibonacci sequence (lower), both consisting in eight wells and with the same electric field applied, $F = 0.06$. The systems are surrounded by two semi-infinite media of constant potential energy. In the type 1 system, the depths are $d_\alpha = 5$ and $d_\beta = 3$, and all the widths are set to unity. In the type 2 system, the widths are $w_\alpha = 1$ and $w_\beta = 2$, and all the depths are set to five. The electric field, which is given by $\Delta E/L$, does not affect to the media placed at the two sides of the systems

bound states. We will study how the electric field changes this spectrum for both periodic and quasiperiodic chains.

To calculate the electronic spectrum of our systems, we use the characteristic determinant method, firstly introduced by Aronov et al. [7]. The characteristic determinant is an exact and non perturbative method that provides the information contained in the Green function of the whole system. The determinant is calculated by using only the unperturbed Green function of each layer that forms the system. The information of each layer is incorporated into the determinant by integrating successively Dyson's equation (see [7] for more details). At the end of the calculation, a function written as a determinant is obtained, and that function is what we call the characteristic determinant, D. The determinant provides the transmission coefficient and the density of states when opened systems are considered, and gives the bound spectrum if the system is closed. For some cases of particular interest, like piecewise constant potentials, the characteristic determinant D satisfies the following recurrence relationship:

$$D_n = A_n D_{n-1} - B_n D_{n-2} \tag{5}$$

where the index n goes from 1 to the number of steps of potential energy. This recurrence relationship facilitates the numerical computation of the determinant. The initial conditions are:

$$A_1 = 1; \quad D_0 = 1; \quad D_{-1} = 0 \tag{6}$$

and we have for $n > 1$:

$$A_n = 1 + \lambda_{n-1,n} \frac{r_{n-1,n}}{r_{n-2,n-1}} (1 - r_{n-2,n-1} - r_{n-1,n-2}) \tag{7}$$

and

$$B_n = \lambda_{n-1,n} \frac{r_{n-1,n}}{r_{n-2,n-1}} (1 - r_{n-2,n-1})(1 - r_{n-1,n-2}) \tag{8}$$

The parameters $r_{n-1,n}$, which are the reflection coefficients between media $n-1$ and n, are given by:

$$r_{n-1,n} = \frac{G_{n-1}^{(0)} - G_n^{(0)}}{G_{n-1}^{(0)} + G_n^{(0)}} \tag{9}$$

and $r_{n-1,n} = -r_{n,n-1} \cdot G_j^{(0)}(x,x)$ is the unperturbed GF in layer j and is equal to

$$G_j^{(0)}(x,x) = \frac{i}{2\pi\sqrt{E - E_j}} \tag{10}$$

where E_j is the constant potential energy of layer j. The value of $\lambda_{n-1,n}$ is given by:

$$\lambda_{n-1,n} = \exp\left(- \int_{x_{n-1}}^{x_n} \mathrm{d}x \frac{1}{2G_n^{(0)}(x,x)} \right) \tag{11}$$

where x_{n-1} and x_n are the boundaries of layer $n-1$.

The determinant D above defined is in general a complex function of the energy E. The bound states of the system correspond to the poles of the GF for the whole system, which coincide with the zeroes of $D(E)$. Therefore, the numerical procedure used to obtain the energy bound spectrum is to calculate numerically $D(E)$ and to find simultaneous zeroes in its real and imaginary parts.

III. Densities of states and fractal properties

In order to study the properties of the energy spectra for both periodic and quasiperiodic systems, we use the integrated density of states as a function of energy. In Fig. 2, we represent the integrated density of states, $g(E)$, for periodic (a), Fibonacci (b), and Thue-Morse (c) systems without electric field. The periodic system is formed by 500 wells of depth 5. The quasiperiodic systems are of type 1 and are formed by 610 wells in the case of Fibonacci, and 512 wells in the case of Thue-Morse, and we use two depths $d_\alpha = 5$ and $d_\beta = 4.5$ in both cases. The width of each well and barrier is set to unity in all cases. The periodic $g(E)$ (curve (a)) has been shifted vertically 100 units to avoid overlapping.

It is well known that the energy spectrum of a Fibonacci sequence is a Cantor set [9]. It has been studied using renormalization group techniques [10] and with the characteristic determinant for δ-function potential [8]. The self-similarity and the fractal characteristics

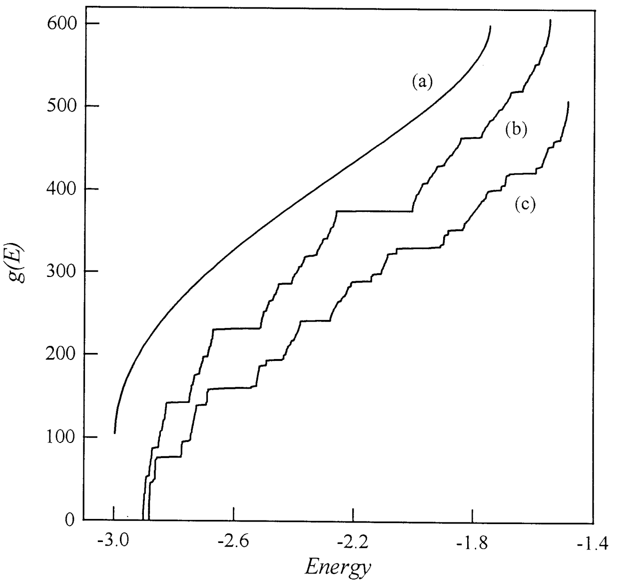

Fig. 2. Integrated densities of states for a periodic system consisting in 500 wells (*a*), a type 1 Fibonacci sequence formed by 610 wells (*b*), and type 1 Thue-Morse system with 512 wells. The value of the depth of the wells is 5 in the periodic case, and we use $d_\alpha = 5$ and $d_\beta = 4.5$ in Fibonacci and Thue-Morse cases. In all cases, the width of wells and barriers is 1. The integrated density of states of the periodic sequence has been shifted vertically to avoid overlapping

of the spectra can be clearly seen in Fig. 2b. The flat regions are the energy gaps, and the number of states between any two gaps in a Fibonacci number. For example, the number of states up to the bigger gap is 377, which is the previous Fibonacci number to the total number of states (610). Changing the values of the depth or the width of the wells, but keeping constant the total number of states, we vary the width of the gaps, but not the number of states between them. This integrated density of states as a function of energy resemble the devil's staircase found by Bak and Bruinsma [11] for the chemical potential as a function of the relative occupancy of a periodic interacting one-dimensional system. In a recent experiment in photonic Fibonacci superlattices, Hattori et al. [12] have found a magnitude closely related to the integrated density of states which behaves very similar to Fig. 2b.

The integrated densities of states as a function of energy for Thue-Morse chains, as in Fig. 2c, are similar to those of Fibonacci chains, showing a whole sequence of gaps. The only major difference between these densities of states is the position of the gaps, which reflects the structure of the corresponding lattice.

The structure of the integrated density of states, and therefore the properties of the corresponding electronic spectrum, changes when the electric field is applied. In this paper, we restrict ourselves to a range of electric field applied for which the eigenenergies are below the zero reference energy level (the energy of the left-side semi-infinite media). For this energies, the system is always closed, and the bound states does not not turn into resonances. In Fig. 3, we plot three densities of states for periodic (a), Fibonacci (b) and Thue-Morse (c), with

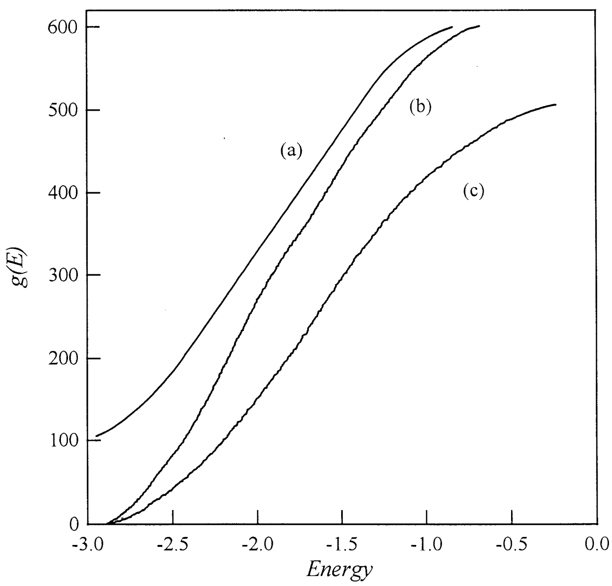

Fig. 3. Integrated densities of states for the same systems of Fig. 2, but with an electric field applied, $F = 0.005$. Again, the integrated density of states for the periodic sequence has been shifted vertically to avoid overlapping

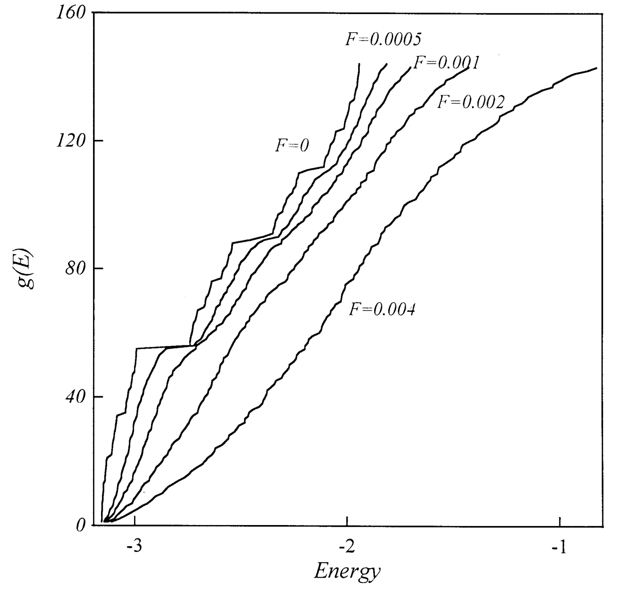

Fig. 4. Integrated densities of states for a type 2 Fibonacci sequence consisting in 144 wells, and for different values of F. The depth of all the wells is 5, and the widths are $w_\alpha = 1$ and $w_\beta = 1.5$. Note how the electric field smooths $g(E)$

a uniform electric field applied of value $F = 0.005$. The quasiperiodic systems are of type 1, and all the parameters have the same values that the ones used in Fig. 2. In the case of periodic sequences, for which $g(E)$ has been shifted vertically 100 units, the field produces a migration of levels from the edges of the band to its centre. The slope of the integrated density of states is almost constant, indicating a constant spacing between levels, reflecting the presence of the Wannier-Stark ladder. The electric field washes out the square root singularity in the integrated density of states.

For the quasiperiodic systems, the electric field smooths the integrated density of states. The small gaps disappear even with weak electric fields, and the large gaps require strong electric fields for them to disappear. The slope of the integrated density of states is again almost constant, indicating the presence of the Wannier-Stark ladder in quasiperiodic systems also.

The behavior of quasiperiodic systems of type 2 are qualitatively identical to the type 1 sequences. As an example, we plot in Fig. 4 the evolution of the integrated density of states of a type 2 Fibonacci sequence consisting in 144 wells to two different widths, $w_\alpha = 1$, and $w_\beta = 1.5$. The different electric fields applied can be seen in the plot. The depth of all the wells is set to 5. In this case, it can be seen again how the electric field smooths $g(E)$. Even the big gaps disappear when big enough electric fields are applied. The slope of $g(E)$ also tends to a constant, reflecting again the presence of the Wannier-Stark ladder. The behavior of type 2 Thue-Morse sequences is qualitatively the same, and we do not plot the corresponding figure to avoid redundance.

To carry out a quantitative study of how the structure of the electronic spectrum, reflected in the whole sequence of gaps, changes as a function of the electric field applied,

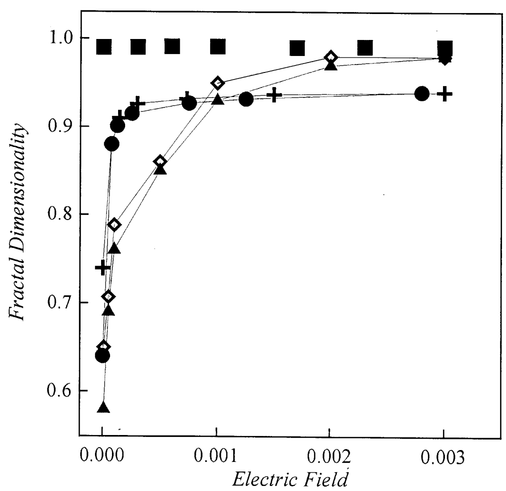

Fig. 5. Plot of the fractal dimensionality as a function of the electric field applied for periodic (solid squares), Fibonacci type 1 (crosses), Fibonacci type 2 (diamonds), Thue-Morse type 1 (solid circles), and Thue-Morse type 2 (triangles) systems

we use the fractal dimensionality. We perform a direct computation of the definition of fractal dimensionality [13], applied to the energy spectra. We consider line segments of different sizes and calculate how many of them are needed to cover the whole corresponding spectrum. The number of segments n is of the form:

$$n \propto \varepsilon^{-d} \tag{12}$$

where ε is the size of the line segment considered and d is the fractal dimensionality. The results are shown in Fig. 5, in which we plot the fractal dimensionality versus the electric field applied for periodic (squares), Fibonacci type 1 (crosses), Fibonacci type 2 (diamonds), Thue-Morse type 1 (circles), and Thue-Morse type 2 (tirangles) sequences. The results show that the structure of gaps, which is the fact that produces a low fractal dimensionality for zero electric field, decreases when the electric field increases. Therefore, we can conclude that the electric field makes the quasiperiodic spectra more uniform. The only difference between type 1 and type 2 sequences is that the former increase very fast their fractal dimensionality for small electric fields up to reach approximately 0.9, but then the electric field becomes inefficient as far as the dimensionality is concerned, meanwhile the latter increase more slowly the dimensionality, but a higher value is reached, which is very close to unity.

IV. Level statistics

The results for the integrated density of states indicates that we cannot properly normalize the nearest neighbor level spacings of quasiperiodic systems, since their infinite structure of gaps does not allow us to define an average separation that varies smoothly with energy. This is strictly true for zero electric field. The presence of the electric field smooths the density of states and removes this problem. This fact is reflected in Fig. 6, in which we plot four integrated densities of states, each one corresponding to a different value of the electric field applied, versus energy for type 1 Fibonacci sequences consisting in 610 wells. The parameters are $d_\alpha = 5$ and $d_\beta = 4.5$. All the widths are set to unity. The figure shows a region (around 377 on the vertical axis) where we know that there is a big gap when no electric field is applied (see Fig. 2b). The energy on the horizontal axis corresponds to the zero electric field case. The different lines correspond to $F = 0$ (thick line), $F = 0.0005$ (thin line), $F = 0.002$ (dotted line) and $F = 0.02$ (dashed line) electric field applied. We can observe how the big gap present in the zero electric field case is disappearing when the electric field increases.

We have obtained the distribution of energy spacings of periodic and quasiperiodic sequences of different values of the electric field applied. The results are shown in Fig. 7 for periodic (a), type 1 Fibonacci (b) and type 1 Thue-Morse (c) sequences, for two different values of the electric field applied in each case. In all cases, the solid line corresponds to zero electric field, and the dashed one corresponds to $F = 0.005$. In the periodic case it can be seen how the electric field produces a very sharp distribution, reflecting a constant level spacing which indicates the presence of WSL. In the cases of Fibonacci and Thue-Morse sequences, it can be seen that the spectrum changes from a Poisson-type distribution (decaying exponential), corresponding to a very disordered system, to a distribution in which there is level repulsion (see how $P(s) \to 0$

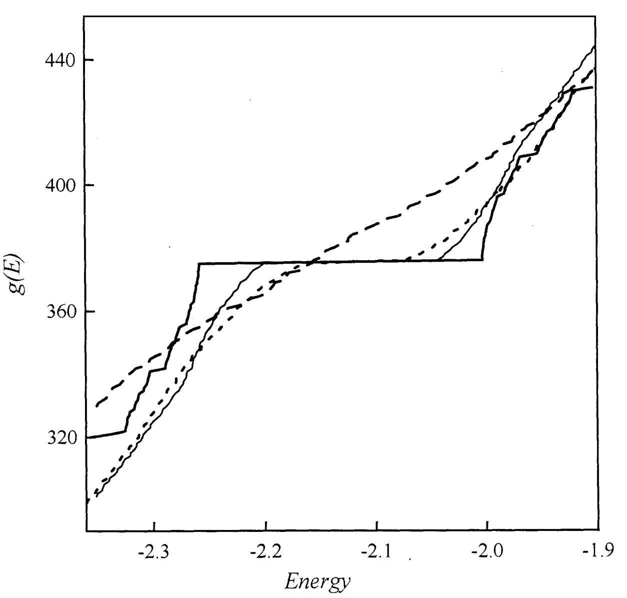

Fig. 6. Plot of the evolution of a gap in the integrated density of states for a type 1 Fibonacci sequence with 610 wells, when we apply different electric fields. The parameters are $d_\alpha = 5$, $d_\beta = 4.5$ and all the widths are set to 1. For zero electric field (thick line), we see a big gap. For low electric field, $F = 0.0005$, (thin line), we still see the gap, but it is smaller. For medium electric field, $F = 0.002$, (dotted line), the gap is even smaller, and for high electric field, $F = 0.02$, (dashed line), the gap has disappeared

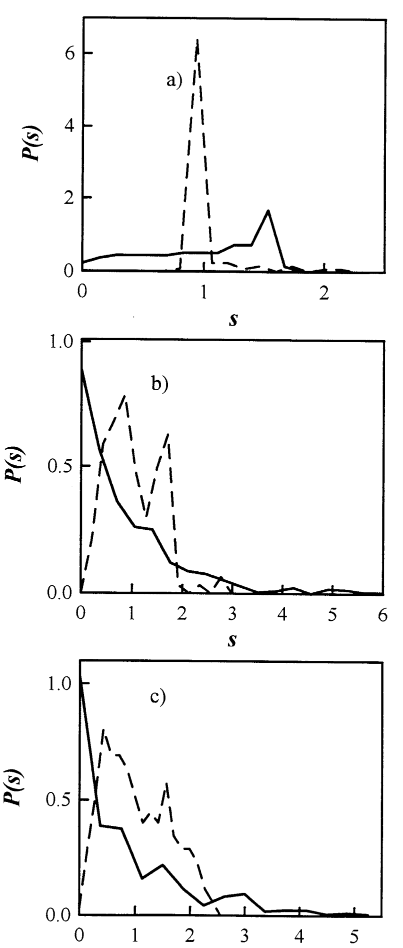

Fig. 7a–c. Plot of the energy level spacing distribution obtained from the integrated densities of states plotted in Figures 2 and 3, where **a** corresponds to the periodic, **b** to Fibonacci type 1, and **c** to Thue-Morse type 1 sequences. In all cases, the solid line corresponds to zero electric field, and the dashed line to $F = 0.005$

when $s \to 0$), which is a characteristic of low disordered systems [14]. The level statistics of type 2 sequences presents the same features as the ones just described for type 1 systems. Therefore, from this point of view, we can conclude that the electric field introduces 'order' in these systems.

V. Wavefunctions

The knowledge of the zeroes of the characteristic determinant allows us to calculate easily the corresponding eigenfunctions of the system. In the barrier region (right extreme in Fig. 1), where the potential energy is much bigger than the total energy, the only solution of Schrödinger equation physically acceptable is the decaying exponential. We start from this solution and construct the wave functions in successive regions away from the barrier by imposing the corresponding boundary conditions. For the correct energies (for which $D(E) = 0$) the wavefunction constructed in this way tends to zero also in the extreme opposite to the barrier (left, in Fig. 1).

In Fig. 8, we show the wavefunctions obtained for the ground state of a periodic sequence with 50 wells (a), a type 1 Fibonacci sequence with 55 wells (b), and a type 1 Thue-Morse sequence with 64 wells (c), for zero electric field in all cases. The parameters are $d_\alpha = 5$, $d_\beta = 4.5$ and all the widths are set of 1. For comparison, in Fig. 9 we plot the wavefunctions for the ground state of the same systems, but with an electric field applied of value $F = 0.001$, which is the same in all cases. We can appreciate how the wavefunctions become more localized when the electric field increases. The effect of localization is stronger in the case of quasiperiodic sequences, *i.e.*, when the electric field applied is the same, quasiperiodic wavefunctions are more localized than periodic ones, as can be seen in Fig. 9. This result, which is also obtained in type 2 sequences, agrees with the one reported recently by de Brito et al. [15] where they concluded that even weak fields destroy the superdiffusive motion encountered in quasiperiodic chains for zero electric field. This fact indicates a very fast localisation of the states even for small fields, or equivalently, that quasiperiodic states localize faster than periodic ones, which is the result we have obtained. For higher electric fields, the wavefunction corresponding to each eigenvalue tends to be completely localized in an individual well. The faster localization of

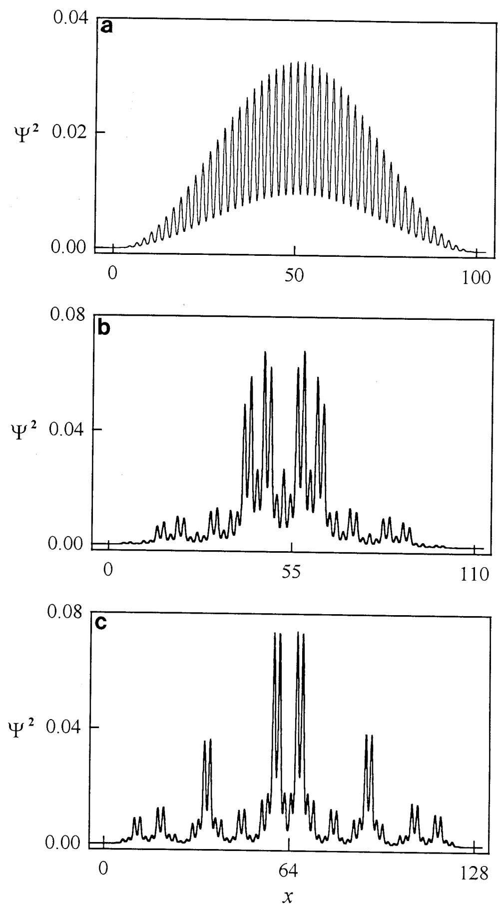

Fig. 8. Plot of the eigenfunctions corresponding to the ground states for a periodic system with 50 wells **a**, a type 1 Fibonacci sequence with 55 wells **b**, and a type 1 Thue-Morse sequence with 64 wells **c**. The parameters are $d_\alpha = 5$, $d_\beta = 4.5$, and all the widths are 1. There is no electric field applied

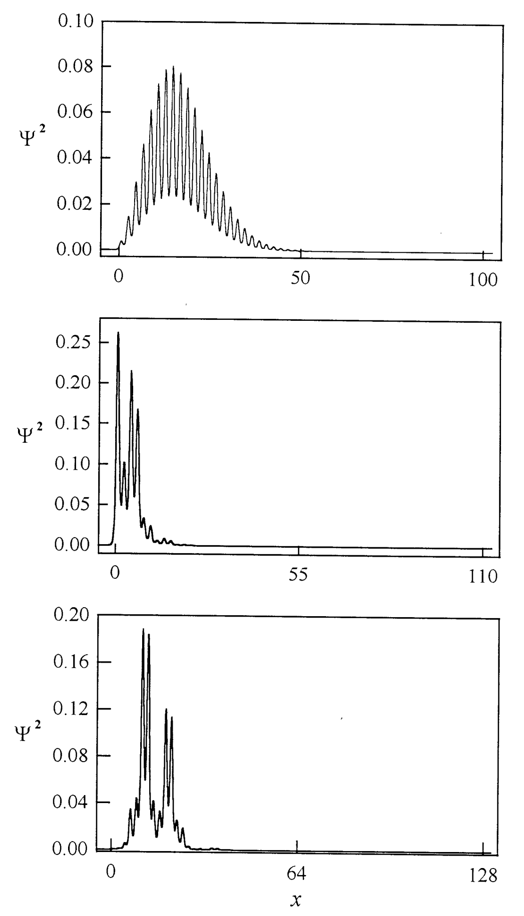

Fig. 9. The eigenfunctions corresponding to the ground state of the same systems of Fig. 7, but with an electric field applied, which is the same in all cases, $F = 0.001$. Note how the electric field localizes the electron, and how this localization is stronger in the quasiperiodic systems

quasiperiodic sequences could be observed experimentally by means of an experiment similar to the well-known carried out by Méndez et al. [3] with periodic superlattices. Although the behavior for quasiperiodic superlattices must reflect qualitatively the same properties that periodic ones, because the localization is present in both cases, smaller electric fields would be needed to reach the Stark-localization regime due to the faster localization of quasiperiodic lattices.

VI. Discussion

The characteristic determinant is an adequate tool to study the effects of electric fields. It allows us to obtain easily the energies and eigenfunctions of one-dimensional and layer systems in the presence of an electric field. We found that Wannier-Stark ladders also appear in quasiperiodic systems. We show that the effect of the electric field is to make more regular the quasiperiodic systems as long as their fractal properties and energy level spacing distributions are concerned.

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