Determination of the Structure of a 1-D Nano-Particle by Means of an Electric Field

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***Abstract*— In this paper, a method to determine the configurational structure of a chain of atoms, based in the application of an electric field is proposed. This method gives the possibility to detect the existence and localization of dislocations and the presence of impurities inside the particle. This is a simple example of the so-called inverse problems, which consist in specifying the configuration of a system from the knowledge of the spectrum. On the other hand, in the so-called direct problems, which are studied much more frequently in the literature, one must obtain the spectrum from the knowledge of the characteristics of the system.**

Keywords-quasiperiodic systems; electron states; Stark ladders.

I. INTRODUCTION

The study of the electronic properties of materials that do not have translational symmetry has been a very active field in the last years. Among the important properties of these structures are: the Anderson localization, the fractal properties of the spectrum of the quasi crystals, etc. In particular, the discovery of the Anderson localization phenomenon of quantum mechanics [1] gave origin to one of the most important subjects in condensed matter physics. On the other hand, the systems whose structural order is described by means of deterministic sequences like those of Fibonacci [2], Thue-Morse [3], Godreche-Luck [4], etc. can be seen as an intermediate case between periodic and disordered 1-D systems. It has been observed that the electronic spectra of some of these systems are self-similar, and the energy bands divide into several sub-bands, each of which further subdivides into more sub-bands and so on [5-7].

Most of these studies have been direct problems in the sense that they begin with a given system, and then the eigenvalues and eigenfunctions are obtained. Here, we consider a particular case of an inverse problem [8]. We follow here the same path at the beginning, but then, we return to the characteristics of the systems and we establish a correlation between the configuration of the system and the characteristics of the spectrum. We show that the configuration of the systems considered here can be deduced from the knowledge of the spectra. The main idea is to employ the capability of the electric field to produce well-separated eigenvalues. In particular, if the systems are periodic, the electric field produces the well-known Wannier-Stark Ladders (WSL), which consists of a series of equally spaced energy levels appearing in the spectrum [9]. The distance between the neighboring energies is proportional to the field intensity. This property of the electric field allows the prediction of the approximate configuration of the imperfect crystal, in spite of the chaotic appearance of the spectrum at first view.

The article is organized as follows: In Section II the model for a deformed crystal is described. The properties of the calculated spectra are discussed in Section III. Section IV is devoted to explain the main conclusions derived from this work.

II. MODEL FOR THE DEFORMED CRYSTAL

In order to show how an electric field can be used for the aforementioned objectives, we consider a one-dimensional crystal that has suffered a deformation under control. Then, the structure of the spectrum is analyzed and a correlation between the structure of the particle and the spectrum is established. The electrified imperfect crystal is modeled as follows. Let us suppose that the potential for one electron in a 1-D system can be described by means of the following expression (see Fig. 1).

$$V(x) = \sum_{i=1}^{N-1} \beta_i \delta(x - x_i) + \sum_{i=1}^{N-1} h_i \theta(x - x_i) \quad 0 < x < x_N \tag{1}$$

 ISBN: 978-1-61208-303-2

with $x_i \in [0, x_N]$, $i = 0,...,N$. The values of the potential at the ends of the interval $(0, x_N)$ are equal to infinite, in order to confine the movement of the electron inside this interval. Here, $\delta(x - x_i)$ and $\theta(x - x_i)$ are the Dirac delta function and the Heaviside step function, respectively [10]. The length of the interval (x_1, x_{i+1}) will be denoted as l_i. We note that when the lengths l_i and the intensities β_i of the delta potentials are set equal to constants l_0 and $\beta_1 \ \forall i$, respectively, the potential (1) can be seen as the superposition of a periodic potential, plus a linear term $f x$ due to a uniform applied electric field of intensity f. The relation between the parameters h_i and the intensity of the electric field is $h_i = l_i f = (x_{i+1} - x_i) f$.

The specific form of the potential $V(x)$ will be a superposition of blocks of type A_i and blocks of type B_i. The block A_i is a flat interval of height $V_i \equiv \sum_{m=1}^{i} h_m$ and length l_A independent of i. The block B_i is a delta potential of intensity β_i. When $f = 0$, we have $V_i = 0 \ \forall i$, and all the blocks A_i are equal to a given block A. In this case, we can obtain periodic structures, if we take, for example, all the blocks B_i equal to a given block B and we take the configuration $AB\,AB\,AB\,AB\,AB\ldots$.

We will study the evolution of the electronic spectrum when the potential (1) becomes disordered by changing the distribution of the blocks. We will start from perfect periodic structures and then we will gradually perturb them to obtain a quasi-periodic structure. Here, we will only consider the Fibonacci sequences [2] S_8. However, the use of this sequence is not restrictive and one can use the electric field to analyze any other type of imperfect crystals. For the case $f = 0$, we built these sequences using the blocks A and B defined above and using the Fibonacci rule $S_{j+1} = \{S_j, S_{j-1}\}$ [2], with the initial conditions $S_1 = A$ and $S_2 = AB$, being j the generation number. The eighth generation is

S_8=ABAABABAABAABABAABABAABAABABAABAAB. (2)

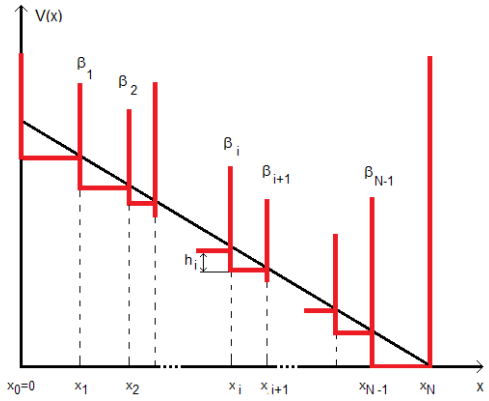

Figure 1. Potential $V(x)$ given by (1).

III. PROPERTIES OF THE SPECTRUM

Briefly, in the following, we use the phrase "periodic system" or "locally periodic system" to denote a section of a periodic system inside the potential well of Fig. 1. For future reference, we start by discussing the well-known effect of an electric field on the spectrum of a periodic system. By means of the transfer matrix method, we have calculated the energies and the results which are shown in Fig. 2. The figure shows the evolution of the energy levels as a function of the electric field intensity f. Each line corresponds with an energy level. The characteristics of a similar spectrum were discussed many years ago in [11]. On the left of these figures, we see that all the levels are grouped in bands, as must be for $f = 0$, since in this case, the system is periodic. Each band in Fig. 2 has 8 levels, because the potential considered in the figure has exactly 8 cells.

It is easy to prove that the upper limit of the $n-$th band of a finite periodic sequence is equal to the upper limit E_n of the $n-$th band of the infinite Kronig-Penney model [12]. Furthermore, it is also equal to the $n-$th level of an infinite well of length p, which is given by $E_n = n^2\pi^2/2p^2$.

 ISBN: 978-1-61208-303-2

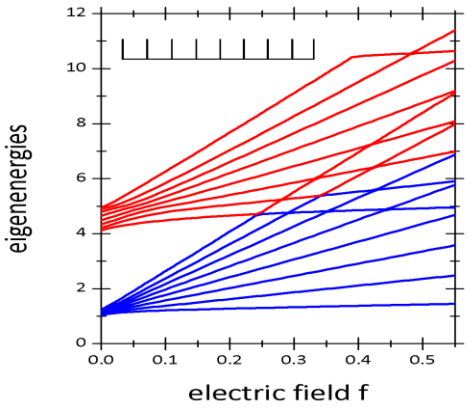

Figure 2. First and second bands of the electronic spectrum of a finite periodic structure with 8 cells (see inset) as functions of the electric field intensity.

For the lower level of the $n-$th band, there is not a closed expression, but it can be proved [13] that it is very close to the lower limit e_n of the $n-$th band of the infinite Kronig-Penney model, which satisfies the following expression [12]

$$\cos\left(\sqrt{2e_n}\,p\right)+\beta\frac{\sin\left(\sqrt{2e_n}\,p\right)}{\sqrt{2e_n}}=\pm 1. \qquad (3)$$

We have verified that E_1, E_2, e_1 and e_2 obtained from these formulas are in agreement with the plotted values on the left sides of Fig. 2, where we have used $p=2.$ On the right of this figure (corresponding with the value $f=0.55$), the levels appear separated due to the presence of the electric field. We clearly see that all the levels coming from the first band appear equally spaced (except the two levels of the extremes that are a little more separated). This structure is precisely the WSL predicted by Wannier [6]. According to Wannier, the nearest-neighbor energy level spacing ΔE is equal to pf. However, due to our systems being finite, the WSL are not perfect. So, the levels of the ladders are not exactly equally spaced. This is frequently more evident with the extreme levels of the ladders, as occurs with the first ladder of Fig. 2 at $f=0.55.$ If one neglects these two levels, the rest of the levels have a quite reasonable behavior.

A superficial analysis of Fig. 2 could yield to the conclusion that the second WSL comes from the second band. However, this is not true. Indeed, a detailed analysis of the lines shows that the fifth level of the first band is bending at $f=0.44,$ giving rise to the first level of the second ladder, etc. However, because a fast view of the lines induce to consider that the $n-$th ladder is generated by the $n-$th band, and in order to make the discussion of figures easier, we are taking this consideration valid.

On the other hand, it is well known [12] that, for the case $f=0,$ the level density in each band is not uniform. In contrast, when f is large enough and the WSL are well established, the level density is uniform for all values of f greater than a certain minimum value. As a consequence, the trajectories that the eigenvalues follow, as f increases, are slightly curved lines in the region of small values of f, as can be verified with a detailed analysis of each trajectory.

In the following, we analyze the effects of disorder. We show in the insets of Fig. 3 six configurations of potentials for the case $f=0.$ The inset of Fig. 3a shows a finite periodic potential with 8 wide cells and 8 thin cells distributed as

$$C_wC_t\,C_wC_t\,C_wC_t\,C_wC_t\,C_wC_t\,C_wC_t\,C_wC_t\,C_wC_t \qquad (4)$$

where C_w represents a wide cell of length l_w and C_t, a thin cell of length l_t. We are taking $l_w=2,\ \ l_t=1.$ Therefore, the period p is equal to 3 and the number of periods is equal to 8. The above sequence of cells can be constructed by assigning the sequence of blocks AAB with the cells C_w and the sequence AB with the cells C_t. So, the block sequence

$$AABAB\,AABAB\,AABAB\,AABAB\,AABAB\,AABAB\,AABAB\,AABAB \qquad (5)$$

is equivalent to the sequence of cells (4).

We now transform step by step the above periodic system into the system S_8, given by expression (2). In the inset of Fig. 3b, we have moved the eight thin cells to the right. For brevity, the corresponding configurations of cells and blocks are not written here.

In the inset of Fig. 3c, we have dropped three thin cells and in the inset (d), we have moved one of the thin cells to the place that it must have in a Fibonacci sequence of blocks. In the inset (e), we have moved a second thin cell to the place that it had in a Fibonacci sequence. At the end of this process, we obtain the inset of Fig. 3f, which corresponds with the configuration of blocks given by the sequence S_8 of expression (2).

The spectra associated with the insets of Fig. 3 are shown in the whole figures, respectively. The set of points at the left ends of the lines (at $f=0$) form the electronic

 ISBN: 978-1-61208-303-2

spectra associated with the potentials of the insets. The other points of the lines show, as before, the evolution of the energy levels as a function of f.

On the left of Fig. 3a, we see at least two groups of levels which evolve into a complex structure when the intensity f, is increased. Since the system has a total amount of 16 cells, each band must have 16 levels. However, because each period has an internal structure consisting of the two cells C_w and C_t, each band must have an internal structure consisting of two sub-bands, each of them having 8 levels. The 8 levels of lower energy shown in Fig. 3a are just the levels of the first sub-band of the first band $\mathbf{B_1}$. The other 8 levels forming the second sub-band of $\mathbf{B_1}$ are in the same zone as the first sub-band of the second band. The second sub-band of $\mathbf{B_2}$ is not shown in the figure. The first sub-band must be associated with the wide cells, and the second sub-band with the thin cells. The first sub-band of $\mathbf{B_1}$ generates the WSL shown by means of gross points on the right of the figure.

As mentioned, at $f = 0$, the second sub-band of $\mathbf{B_1}$ overlaps with the first sub-band of $\mathbf{B_2}$. In particular, one obtains that the upper level E_2^w of the second band of a periodic system formed uniquely of wide cells is equal to the upper level E_1^t of the first band of a periodic system formed uniquely of thin cells. Their value is $E_1^t = E_2^w = 4.934$, as can be seen on the left of Fig. 3a. However, the 16 levels of this group evolve to form two different Stark ladders. One of them is due to the thin cells and the other to the wide cells. We have attached crosses at the right ends of the levels forming one of these Stark ladders, and arrows to the levels forming the other WSL. We observe that each level associated with a cross is always beside a level associated with an arrow. So, we have a composed ladder in which each of its rungs are indeed coupled closely together. The most important point here, according with the objectives of this work, is to observe that this distribution of levels is similar to the distribution of the cells, that is, a wide cell is always beside a thin cell.

This last effect is shown more clearly in Fig. 3b, where we have put the 8 wide cells together and the 8 thin cells together, as depicted in the inset. On the right of this figure, we see a first WSL generated by the first band of the wide cells, with a nearest-neighbour level spacing of the order of 1.1 at $f = 0.55$. However, for higher energies, we observe a more complicated structure. It consists in two WSL separated at distance ΔS and each of them having 8 levels and 7 spaces. One can understand this characteristic if one observes that now the local period associated with the wide cells is equal to 2, and therefore, the levels associated with these cells must be separated a distance of the order of 1.1 at $f = 0.55$. Similarly, the local period associated with the thin cells is equal to 1, and therefore, their levels must be separated a distance of the order of .55 at $f = 0.55$. These two WSL ladders are separated one from each other because the cells are also distributed in that way.

When one continues moving the other thin cells to the place that they have in the final sequence S_8, one gets the corresponding spectrum shown in Fig. 3f. This figure shows a rather complex structure, which appears as chaotic. However, by using the reasoning above discussed, it is easy to deduce the configuration of the cells produced by these spectra.

IV. CONCLUSION

We have shown that an external electric field can be used as a tool to establish a close correlation between the spectrum of a small one-dimensional disordered quantum system and its geometric configuration. We have taken advantage of the capability of the electric field to produce sets of equally spaced levels in the spectrum of a periodic system, that is, the WSL. This property allows us to analyze the evolution of the energy levels as the system becomes gradually disordered. In this way, we were able to explain why the levels acquire the observed arrangement in the disordered systems. The use of Fibonacci sequences, as a particular case of non-periodic structure, was not crucial and one can analyze any other type of disordered sequences, provided the amount of disorder is large enough. Since the WSL have been observed in three dimensional systems [14], the use of an electric field to analyze the effect of disorder in real three dimensional systems could be a real possibility.

 ISBN: 978-1-61208-303-2

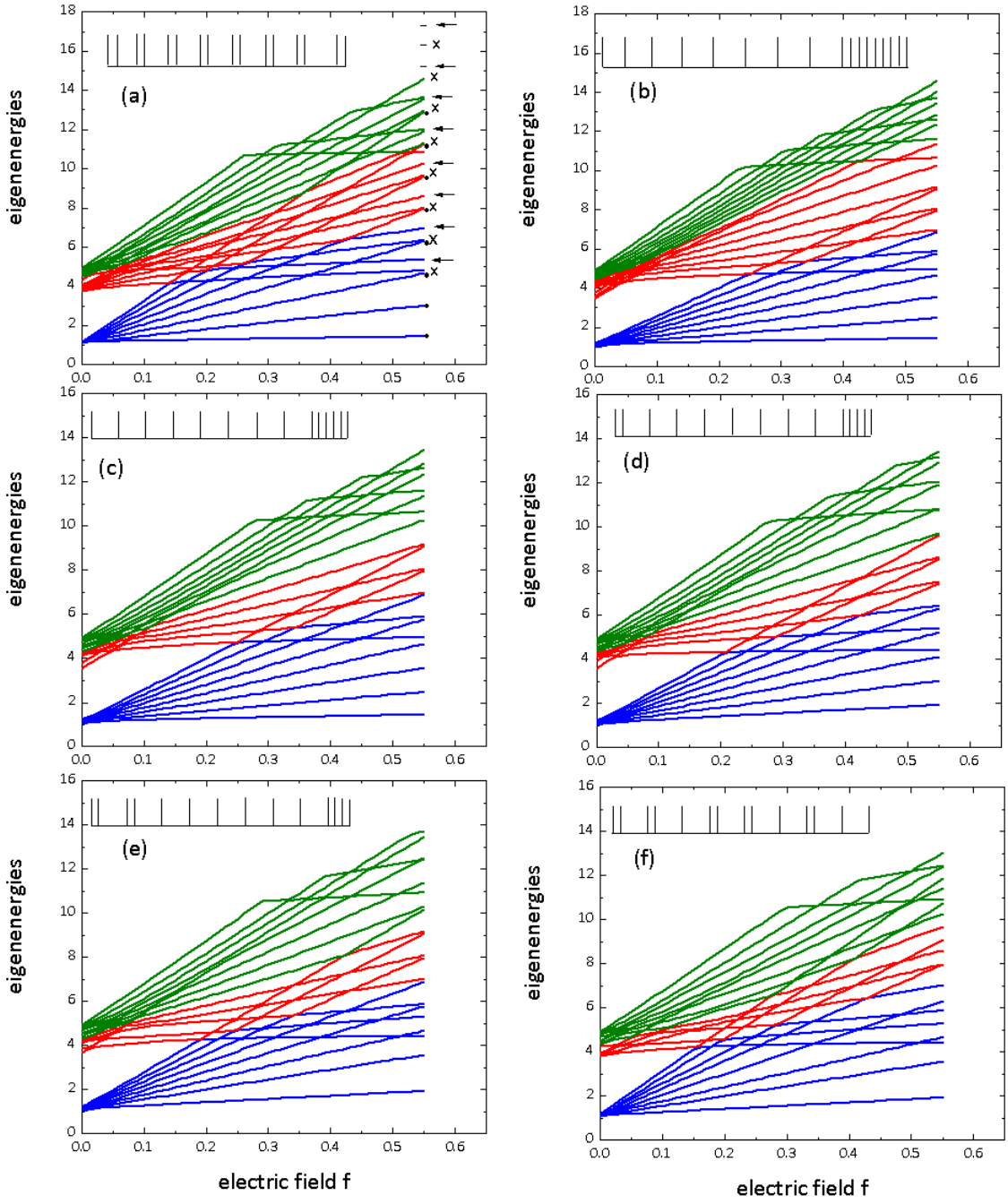

Figure 3. Effect of disorder on the electronic spectra of finite structures as functions of the electric field intensity. The structures are schematically shown in the insets.

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