Electronic spectra of quasi-regular Fibonacci systems: Analysis of simple 1D models

V.R. Velasco*

Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, 28049 Madrid, Spain

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Abstract

The electronic spectra of quasi-regular systems grown following the Fibonacci sequence are investigated via simple one-dimensional tight-binding, one-band models. Different models are considered and the influence of the model parameters and the number of atoms entering the different blocks on the electronic spectrum are discussed.

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1. Introduction

The quasi-regular systems have been intensively studied in the last years [1–36]. The interest was triggered from the theoretical side by the prediction that these systems should manifest non-conventional electron and phonon states [9,11,23,25], and exhibit energy spectra with a high fragmentation and fractal character [7,17,24]. The experimental growth of Fibonacci [2,3] and Thue–Morse [4] multilayer structures has provided the practical realization of these systems. The Fibonacci system, a linear lattice constructed recursively, is the one-dimensional (1D) version of the quasi-crystals [5,6,37,38], and has been the subject of many theoretical studies.

The electronic structure of the Fibonacci system has been investigated mainly in the single-band tight-binding limit. In these studies, it was found that the energy spectrum is self-similar, in the sense that the energy bands divide into three subbands, each of which further subdivides into three, and so on [13–16], thus producing a singular continuous spectrum [21], which in the infinite limit reduces to a Cantor-like spectrum with dense energy gaps everywhere [7–10]. More realistic studies, using an empirical tight-binding (ETB) $sp^3s^*$ Hamiltonian [39], were presented in [28–34]. In these works, the Fibonacci spectrum was only estimated for certain energy ranges and for wave vectors in the vicinity of the superlattice $\Gamma$ point.

We delve here into the properties arising from the simple models, by considering possible variations in the basic structure of these models, as a parallel to the more sophisticated and realistic $sp^3s^*$ Hamiltonians.

In Section 2, a brief description of the theoretical models is given and conclusions are provided in Section 3.

2. Theoretical 1D models

In theoretical and experimental studies of the real heterostructures grown following different quasi-regular sequences [2–4], obviously one does not study a full infinite quasi-regular sequence $S_\infty$, but attains only some high, but finite generation $S_N$, after repeated application of a generating rule. A reasonable assumption is then to expect that the systems for sufficiently high $N$ will display the essential features of the ideal infinite sequence. Thus, one takes $S_N$ as an acceptable numerical approximation.

We shall concentrate on the Fibonacci sequence, which is the most popular one, and embodies all the basic features of the quasi-regular structures. The Fibonacci heterostructures are grown by recursive stacking along one direction (e.g. the $x$ direction), with two generators, blocks $A$ and $B$, mapping...
the mathematical rule in the Fibonacci sequence

\[ S_1 = \{A\}, S_2 = \{AB\}, S_3 = \{ABA\}, S_4 = \{ABAAB\}, \ldots, \]
\[ S_n = S_{n-1} S_{n-2}. \tag{1} \]

The simple models usually considered are the 1D tight-binding ones defined by

\[ E \psi_n = \varepsilon_n \psi_n + t_{n,n+1} \psi_{n+1} + t_{n,n-1} \psi_{n-1}, n = 1, 2, \ldots, N, \tag{2} \]

where \( \varepsilon_n \) and \( \psi_n \) are, respectively, the on-site energy and amplitude probability of an electron being at the \( n \)th site, while \( t_{n,n+1} \) (\( t_{n,n-1} \)) is the hopping transition amplitude associated with the bond between site \( n \) and site \( n+1 \) (site \( n \) and site \( n-1 \)).

The most frequently studied cases, for this kind of model, are the following: (a) the on-site energies are constant, and then they can be absorbed into the eigenenergy \( E \), while the hoppings take two values \( t_S \) (strong) and \( t_W \) (weak), arranged in a Fibonacci sequence; (b) the same situation as in case (a), but interchanging \( t_S \) and \( t_W \); (c) the hoppings are constant, but the on-site energies take two values \( \varepsilon_A \) and \( \varepsilon_B \) arranged in a Fibonacci sequence.

We now discuss the results obtained with the simple 1D models frequently used in the study of the properties of quasi-regular systems.

As explained above, they are based on (2) and the varieties come from the on-site or hopping values being constant or following the Fibonacci sequence. It is clear that these are perfectly sound mathematical models, but they are not very good descriptions of the physical situation corresponding to the experimental samples [2-4].

We shall analyze in the first place the 15th Fibonacci generation, as a representative case, with periodic boundary conditions, that is, a superlattice having as period this Fibonacci generation. We consider, as in the usual studies, that we have only one atom of the different materials. These models satisfy the conditions of the theorems in [17,21]. Now, our system contains 987 atoms, 610 \( A \) atoms and 377 \( B \) atoms, respectively. The energy eigenvalues are obtained by direct diagonalization of the eigenvalue equation.

If the on-site values are constant, and the hopping values \( t_S \) and \( t_W \) follow the Fibonacci sequence, then we have

\[ t_S t_W t_S t_W t_S t_W \ldots \tag{3} \]

It is clear that this situation does not physically represent the two different materials \( A \) and \( B \) very well from the experimental point of view [2-4], even if we consider a simple model with a single orbital.

In Fig. 1, we present the eigenvalues versus their increasing ordering number \( k \), for the \( t_S = 0.5, t_W = 0.1 \) case. It is seen that there is an important fragmentation of the spectrum represented by the opening of primary and secondary gaps.
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