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Microelectronics Journal 36 (2005) 882–885

Microelectronics Journal

www.elsevier.com/locate/mejo

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

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Available online 11 July 2005

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.

Keywords: Quasi-regular heterostructures; Electron states

PACS: 73.21.-b

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 Γ 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_∞, 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_3 direction), with two generators, blocks A and B, mapping

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doi:10.1016/j.mejo.2005.05.021

the mathematical rule in the Fibonacci sequence

$$S_1 = \{A\}, S_2 = \{AB\}, S_3 = \{ABA\}, S_4 = \{ABAAB\}, \ldots,$$
$$S_n = S_{n-1}S_{n-2}. \quad (1)$$

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

$$E\psi_n = \varepsilon_n\psi_n + t_{n,n+1}\psi_{n+1} + t_{n,n-1}\psi_{n-1}, n = 1,2,\ldots,N, \quad (2)$$

where ε_n and ψ_n are, respectively, the on-site energy and amplitude probability of an electron being at the nth 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 ε_A and ε_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

$$t_S t_W t_S t_S t_W t_S t_W t_S \ldots \quad (3)$$

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.

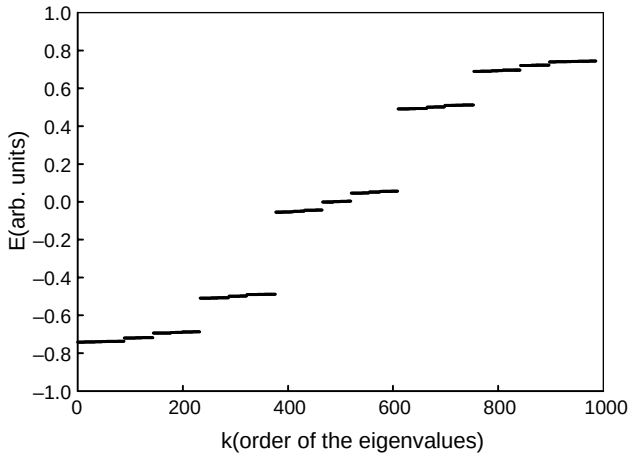

Fig. 1. Energy eigenvalues E (arbitrary units), ordered by increasing value, versus ordering number k for a 15th Fibonacci generation linear chain with $\varepsilon_A = \varepsilon_B = 0$, $t_S = 0.5$ and $t_W = 0.1$.

If we exchange the strong and weak bonds, then we have the following situation

$$t_W t_S t_W t_W t_S t_W t_S t_W \ldots \quad (4)$$

The results are analogous to those of the former case.

Another possibility is that in which the hopping parameters are constant and the on-site energies take the two values ε_A and ε_B, arranged in a Fibonacci sequence, which leads to the following situation

$$\varepsilon_A\varepsilon_B\varepsilon_A\varepsilon_A\varepsilon_B\varepsilon_A\varepsilon_B\varepsilon_A \ldots \quad (5)$$

From the standpoint of representing two different materials, this approach has no more physical meaning than the cases previously studied.

The eigenvalues versus their increasing ordering number are shown in Fig. 2, for the $t_S = t_W = 0.1$, $\varepsilon_A = -0.5$, $\varepsilon_B = 0.5$ case. The picture is similar to that in Fig. 1, but the details are clearly different, since the eigenvalues in the neighborhood of the energy origin, have disappeared.

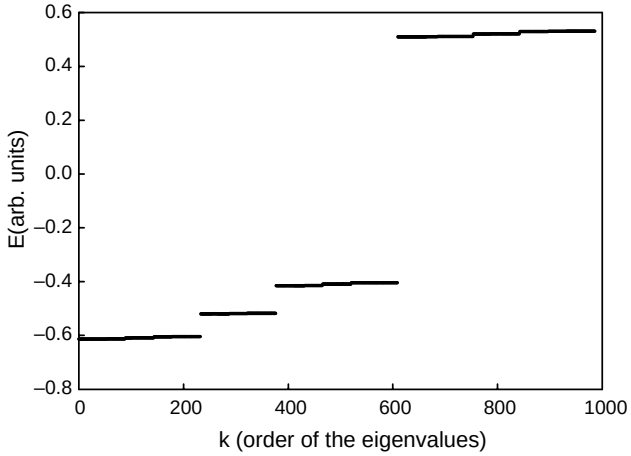

Fig. 2. As in Fig. 1 with $\varepsilon_A = -0.5$, $\varepsilon_B = 0.5$ and $t_S = t_W = 0.1$.