Electronic spectra of GaAs/Ga$_x$Al$_{1-x}$As superlattice with impurities arranged according to a Fibonacci sequence

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Abstract

We study the electronic density of states (DOS) of a GaAs/Ga$_x$Al$_{1-x}$As superlattice with impurities arranged according to the Fibonacci sequence. Our theory uses a Green function method based on Dyson’s equation within the real-space renormalization-group approach in the framework of the tight-binding Hamiltonian for the Fibonacci quasiperiodic lattice. An exact decimation transformation has been done for the physical parameters characterizing the Fibonacci chain considering the scaling factor, under which the system is self-similar, equal to the golden mean $\tau = (1 + \sqrt{5})/2$. The electronic energy spectrum are then used to determine the electronic specific heat which, due to the localization of the electronic states, exhibits strong Schottky anomalies when the temperature goes to zero together with a log-periodic oscillation.

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In recent years, there has been considerable interest in understanding the physical properties of substitutional quasiperiodic structures. Quasiperiodic structures are composed of the superposition of two (or more) building blocks that are arranged in a desired manner. For example, the Fibonacci quasiperiodic superlattice (FSL), which is made by juxtaposing two different building blocks A and B arranged in a Fibonacci sequence, has become a standard model for the study of these systems since Merlin et al. [1,2] reported its realization and characterization considering layers of GaAs/Ga$_x$Al$_{1-x}$As grown by molecular-beam epitaxy.

The Fibonacci system is the archetypal one-dimensional version of the quasi-crystals, where the site and/or bond variables (site energies and hopping matrix elements), arranged in a Fibonacci sequence, can be generated by the rule $S_N = S_{N-1} S_{N-2}$, $N > 2$, where $S_1 = A$, $S_2 = AB$, and $N$ is the Fibonacci generation number. It is invariant under the transformation $A \rightarrow AB$ and $B \rightarrow A$. Its electronic structure has been the subject of intense theoretical investigation, mainly in
the single-band tight-binding limit (for a review see [3]).

In a recent work [4], we have calculated the density of states of a GaAs/Ga_xAl_{1-x}As superlattice whose ratio between the potential energy of the impurities and the potential energy of the atoms at the lattice is a \( n \)-th power of the golden mean \( \tau = (1 + \sqrt{5})/2, \ (n = 1, 2, 3, \ldots) \). Our theory used Dyson’s equation together with a transfer-matrix treatment, within the tight-binding Hamiltonian model. The electronic density of states was calculated stressing the regions of frequency where the transfer function is complex, which correspond to localized states.

On the other hand, the analysis of the FSL’s specific heat spectrum was recently done by a model based on the real electron’s multifractal energy spectra [5]. However, in these calculations an approximation was made, namely the consideration of a constant potential energy of the atoms at the lattice, within a tight-binding model, in which the transfer function is complex, which correspond to localized states.

We intend in this work to extend our previous results considering a Fibonacci quasiperiodic superlattice, within a tight-binding model, in which its nearest-neighbor-hopping matrix elements are distributed according to the Fibonacci sequence. The electronic DOS is then determined by using a Green function method based on Dyson’s equation within the real-space renormalization-group approach [6–9].

Let us consider a one-dimensional electronic chain described in terms of a localized basis by the tight-binding Hamiltonian

\[
H = \sum_n |n\rangle \varepsilon_n \langle n| + \sum_n \sum_{n'} |n\rangle V_{nn'} \langle n'|
\]  

(1)

where \( |n\rangle \) is the atomic-like orbital centered at site \( n \), and \( \varepsilon_n (V_{nn'}) \) denotes the site energies (nearest-neighbor-hopping matrix elements). In a Fibonacci chain \( V_{nn'} \) can assume only one of two values, \( V_A \) and \( V_B \), and they are distributed according to the Fibonacci sequence. Also, \( \varepsilon_n \) can have one of three values depending on the local environment of site \( n \), i.e.,

\[
\begin{align*}
\varepsilon_n & = \varepsilon_A \quad \text{if} \quad V_{n-1,n} = V_{n,n+1} + V_A \\
\varepsilon_n & = \varepsilon_B \quad \text{if} \quad V_{n-1,n} = V_A \quad \text{and} \quad V_{n,n+1} = V_B \\
\varepsilon_n & = \varepsilon_F \quad \text{if} \quad V_{n-1,n} = V_B \quad \text{and} \quad V_{n,n+1} = V_A
\end{align*}
\]  

(2)

Eq. (1) can be conveniently written within a Green function (Dyson) formalism as:

\[
\sum_{nn'} G_{nn'}^{-1} |n\rangle \langle n'| = 0
\]  

(3)

where

\[
G_{nn'}^{-1} = (\varepsilon_n - V_{nn'}) \delta_{nn'} - V_{n,n+1} \delta_{n+1,n'} - V_{n,n-1} \delta_{n-1,n'}
\]  

(4)

The Green function \( G_{nn'} \) can be found through the completeness relation:

\[
\sum_{nn'} G_{nn'}^{-1} G_{nn'} = \delta_{nn'}
\]  

(5)

yielding:

\[
G_{nn'} = G_{nn}^0 + \sum_{n''} G_{nn}^0 T_{nn''} G_{n''n'}
\]  

(6)

with

\[
G_{nn}^0 = (\varepsilon_n - V_{nn})^{-1}
\]  

(7)

and

\[
T_{nn'} = V_{n,n+1} \delta_{n+1,n'} + V_{n,n-1} \delta_{n-1,n'}
\]  

(8)

By iteration, Eq. (6) can be written as

\[
G_{nn'} = G_{nn}^0 + G_{nn}^0 T_{nn'} G_{n'n'}^0 + G_{nn}^0 \sum_{n''} T_{nn''} G_{n''n'}^0 T_{n''n'} G_{n'n'}^0 + \cdots
\]  

(9)

whose diagonal element is:

\[
G_{nn} = G_{nn}^0 + G_{nn}^0 \sum_n T_{nn'} G_{n'n'}^0 T_{n'n} G_{nn}^0 + \cdots
\]  

(10)

The electronic density of states can now be calculated in terms of the trace of the Green function, i.e.:

\[
\rho(\varepsilon) = \left(\frac{1}{2\pi}\right) \lim_{N \to \infty} \text{Im} G_{nn}(\varepsilon + iN)
\]  

(11)

Although straightforward, the numerical determination of the density of states defined above is a very complicated task, which can consume a large amount of computer time. Instead, we used an extremely efficient decimation method for numerical calculation of the density of states, based on the renormalization-group approach. The formalism is based on the successive elimination of the degrees of freedom of the system, through decimations of alternate sites on a chain. At each step (see Fig. 1) the degrees of freedom are eliminated by an appropriate projection technique of the Fibonacci linear chain, where the original
system can be related to a reduced version of itself in such a way that it must be recovered after each renormalization step. This process defines recursion relations connecting the site energies and the nearest-neighbor-hopping matrix elements, \( e_n, V_n, e_{n+1}, V_{n+1} \), under a length scaling factor. When iterated, such a transformation yields a system with a fraction of the original number of degrees of freedom and with renormalized parameters \( e_0, V_0, e_{n+1}, V_{n+1} \). In our case the scaling factor under which the system is self-similar is equal to the golden mean, \( \tau \), and the decimal transformation associated with this length rescaling factor, for the Fibonacci chain, is given by:

\[
\begin{align*}
  e' &= e + \frac{V_A^2 + V_B^2}{E - e}; \\
  e' &= e + \frac{V_A^2}{E - e}; \\
  V' &= \frac{V_AV_B}{E - e}; \\
  V' &= V_A
\end{align*}
\] (12)

Therefore, for a fixed set of system parameters \( \{V_A, V_B, e_x, e_y, e_z\} \) one has that \( n \) interactions of (12) take \( \{V_A, V_B, e_x, e_y, e_z\} \) to \( \{V'_A, V'_B, e'_x, e'_y, e'_z\} \), where, for example, \( V'_A \) denotes the renormalization interaction between two sites which are a distance \( \tau^n \) apart, measured in units of the original lattice spacing. In Fig. 1 we show schematically the renormalization-group approach procedure used here for a simple case of the Fibonacci chain with nine sites. Typically, only a few number of interactions (less than 20) of (12) are required to achieve a good precision for \( G_{nn} \), and therefore such a procedure is computationally very efficient.

Fig. 2 shows the density of states, as given by Eq. (11) as a function of the energy, considering initial physical parameters according to the scheme used in the experimental realization of a FSL [1,2]. In this way, the A block has 20 GaAs layers and 8 GaAl\(_{1-x}\)/As layers, while block B has 10 GaAs layers and 8 GaAl\(_{1-x}\)/As layers. The tight-binding parameters were chosen to give a band offset of 0.5 eV and the GaAs \( \Gamma \)-point conduction-band mass, i.e.: \( e_x = e_y = e_z = 14.45 \text{ eV} \), \( V_A = 7.225 \text{ eV} \) and \( V_B = 6.975 \text{ eV} \) [10]. The zero of the energy is taken to be the bottom of the conduction band of GaAs. This band offset is within experimentally accepted values for (0 0 1) interfaces [11], and correspond to a 66/34 band-offset rule [12]. We went up to the 15th generation number of the Fibonacci sequence, meaning a precision of one part in \( 10^8 \) for the diagonal element of the Green function.

We now use the electronic density of states shown in Fig. 2 to analyze the behavior of the specific heat in the small temperature regime. The partition function \( Z \) of this system is given by:

\[
Z = \int \rho(e) \exp \left( \frac{-e}{k_B T} \right) de
\] (13)

For simplicity we will consider the Boltzmann constant \( k_B \) equal to unity, and normalize the energy interval to \([0, 1]\), without loss of generality.

The specific heat, as a function of the temperature, for the \( N \)th generation of the Fibonacci sequence is given by:

\[
C_N = \beta^2 \frac{\partial^2 \ln Z_N}{\partial \beta^2}
\] (14)

Here \( \beta = 1/T \).
Fig. 2. Normalized integrated density of state $\rho(\varepsilon)$, vs. $\varepsilon/V_A$ for Fibonacci superlattice.

Fig. 3. Specific heat spectrum vs. temperature for the Fibonacci quasiperiodic sequence considered up to its 16th generation. The inset depicts the plot $C(T)$ vs. $\log(T)$ at low temperatures to show the log-periodicity effects in the Fibonacci structure.
In Fig. 3 we have plotted the specific heat as a function of the temperature. Overall speaking, the spectrum shows the superposition of $N$ Schottky anomalies corresponding to the scales of the electronic density of energy (DOS) spectra, $N$ being the Fibonacci generation number. At high temperatures ($T \to \infty$), the specific heat for all Fibonacci generation numbers converges and decays as $T^{-2}$, mainly due to the fact that we have considered our system bounded. More important however, is the oscillatory behavior of the specific heat for low temperatures. For the constant electronic DOS considered in [5] (see its Fig. 2) the oscillations are harmonic. Besides, they have two well-defined different profiles, one for the even and the other for the odd generation numbers of the sequence, the amplitudes of the latter being bigger than the amplitudes of the former, with the number of oscillations proportional to the Fibonacci generation number $N$. Now, due to the real electronic density of states, the specific heat spectrum displays quasi-uniform oscillations neither around the fractal dimensionality of the spectrum nor as an approximation of the constant DOS oscillations found in the previous work [5]. In the inset of Fig. 3 we have shown the log-periodic behavior of the specific heat at low temperatures, where we have plotted $C(T)$ versus $\log(T)$ for the Fibonacci sequence. The curves resemble the previous case, with a mean value $d$, around it $C(T)$ oscillates log-periodically, although this value is not related with the fractal dimension of the Fibonacci quasiperiodic structure. The reason for that is because our electronic DOS spectrum is not strictly invariant under changes of scales (as in the constant DOS case).

To summarize, we have proposed in this paper a more realistic and computational simple model to study the electronic density of states and the corresponding specific heat profiles from electrons in one-dimensional Fibonacci lattice. We are aware that our results, appropriated to one-dimensional structure, can be quite different from that obtained in real three-dimensional ones. However, one-dimensional system are widely investigated nowadays because of the growing importance of quasi-1D ordered and disordered materials in physics and biology. For instance, the effect of disorder on the properties of 1D system is qualitatively different from its two and three dimensions counterpart. Certainly the theoretical predictions shown here can be tested experimentally, and we expect that experimentalists get encouraged to face them.

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References