Fibonacci superlattices of narrow-gap III-V semiconductors

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Abstract

We report theoretical electronic structure of Fibonacci superlattices of narrow-gap III-V semiconductors. Electron dynamics is accurately described within the envelope-function approximation in a two-band model. Quasiperiodicity is introduced by considering two different III-V semiconductor layers and arranging them according to the Fibonacci series along the growth direction. The resulting energy spectrum is then found by solving exactly the corresponding effective-mass (Dirac-like) wave equation using tranfer-matrix techniques. We find that a self-similar electronic spectrum can be seen in the band structure. Electronic transport properties of samples are also studied and related to the degree of spatial localization of electronic envelope-functions via Landauer resistance and Lyapunov coefficient. As a working example, we consider type II InAs/GaSb superlattices and discuss in detail

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our results in this system.

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I. INTRODUCTION

Heterostructures and superlattices (SL) consisting of semiconductors have been investigated as a source of novel physical properties as well as for their applications in devices. From the very beginning, most researchers have considered the Fibonacci sequence as a typical example of a quasiperiodic system [1,2] and, some years ago, due to the advances achieved in nanotechnology, mainly those techniques based on molecular beam epitaxy, it was possible to fabricate quasiperiodic semiconductor SL [3,4]. Since these progresses were made, there has been an increasing interest in the study of (quasiperiodic) Fibonacci systems, their electronic structure and transport properties. These studies have provided much information and several physical properties are now well established. One of the most conspicuous features is the occurrence of highly fragmented electronic spectra with a hierarchy of splitting subbands displaying self-similar patterns [5,6]. This exotic electronic spectrum strongly influences electron propagation [7,8] and dc conductance through the system, even at finite temperature [9]. In addition, electronic wave functions are neither extended in the Bloch sense, nor exponentially localised, but critical in Fibonacci lattices [10]. All these striking features make Fibonacci lattices good candidates in regard to investigation of their novel properties from a theoretical point of view as well as their potential technological applications in new devices.

Electronic properties of quasiperiodic SL have been studied by various methods, most of them being based on the envelope-function approximation [5], which is known to be quite successful for periodic structures [11]. Neglecting the nonparabolicity of the bands, the electron dynamics is described by a scalar Hamiltonian corresponding to decoupled bands in the host semiconductors. The wave equation is a Schrödinger-like equation for a particle of effective mass m^* in a one-dimensional potential, so that electron dynamics is studied only with a single envelope-function. Since the potential through which the electron moves is usually regarded as piecewise constant (Kroning-Penney potential), the solution of the wave equation is a superposition of plane waves in each layer with real or imaginary momentum,

corresponding to travelling or evanescent solutions respectively. Matching the solutions at the interfaces, one can obtain the envelope-function in the SL using, for instance, the transfer-matrix formalism. Isotropic and parabolic bands usually work well in some III-V semiconductors, like GaAs and AlAs. However, scalar Hamiltonians cannot adequately describe narrow-gap semiconductors [11] or those SL whose band modulation is comparable to the magnitude of the gap, as is the case in sawtooth-doped GaAs [12], since coupling of bands and non-parabolicity effects for such a situation are usually rather strong. Hence a more realistic band structure is indeed required to properly analyse electron states in superlattices of narrow-gap semiconductors. It is known that two-band models as we report here based on a Dirac-like equation represent narrow-gap III-V semiconductors quite well [13]. In this case, two envelope-functions are needed, one corresponding to the conduction-band (s like) and the other corresponding to the valence-band (p like).

The need for a general model like the two-band model poses the question as to whether the peculiar electronic properties obtained so far within the one-band model (highly fragmented and self-similar spectra and the allied transport properties) still remain in narrow-gap SL. As far as we know, this question has not been answered yet. The main aim of this work is to show that those *distinctive* characteristics also appear in more complex and realistic models, suggesting strongly that those features can be regarded as *universal* fingerprints of one-dimensional Fibonacci systems. As we have already mentioned, the equation governing the conduction- and valence-band envelope functions is a Dirac-like equation. We can find exact solutions via the transfer-matrix technique in view of the analogy existing between the two-band models and the relativistic Dirac theory of electrons. Transport properties of relativistic electrons in (quasiperiodic) Fibonacci as well as in (aperiodic) Thue-Morse one-dimensional lattice have been previously considered by the authors [8,14], and the transfer-matrix formalism for relativistic electrons is well established (see Refs. [15–19] to cite a few). The main difference between the two treatments is that, in the case of two-band models, the gap is also position-dependent and it enters in the equation of motion as a scalar-like potential, whereas our previous relativistic treatments only considered electrostatic-like

potentials (the time component of a Lorentz vector). Keeping this difference in mind, one can proceed in analogy with the relativistic treatment. Transport properties of the SL at zero temperature are discussed in the context of transmission coefficient and the Landauer resistance [20,21] and related to the possible critical nature of the electronic states. Spatial extension of the envelope-functions is determined by means of the Lyapunov coefficient, which is nothing but the inverse of the localization length. The nature of the electronic spectrum of our system is analysed by means of bandwidth-scaling techniques which suggest a underlying singular continuous character.

II. THE MODEL

The system we study in this work is a Fibonacci superlattice (FSL) made of two kind of layers of narrow-gap III-V semiconductors, hereafter denoted by A- and B-layers. Due to the offset between conduction- and valence-band at the interfaces, carriers move under the action of barriers and wells within the effective-mass approximation. For simplicity, we neglect band bending in the rest of the paper, so that the build-in potential is constant in each layer. This approximation simplifies our treatment while keeping the qualitative aspects of the physics involved. Without loss of generality, we consider that B-layers act as barriers for electrons and that their width b is the same for all layers. To generate our FSL we arrange two tiles a and a' (a and a' larger than b), which represent the distance between two consecutive points characterizing the centres of two consecutive barriers, according to the Fibonacci sequence (see Ref. [19] for further details on how to construct the FSL). A-layers are of thickness $a-b$ or $a'-b$ according to this arrangement. The number of barriers in the FSL is a Fibonacci number F_l, obtained from the recurrent law $F_l = F_{l-1} + F_{l-2}$ with $F_0 = F_1 = 1$.

After describing the way we construct the FSL, we turn to the dynamics of electrons in this system. We treat the resulting electronic structure by means of the effective-mass $\mathbf{k}\cdot\mathbf{p}$ approximation. The electronic wave function is written as a sum of products of band-edge

orbitals with slowly varying envelope-functions, assuming that the SL potential is also slowly varying. To proceed, let E_{gA} and E_{gB} be the gaps of semiconductors A and B respectively, and let us denote the relative offset between gap centres by V (in what follows we take the centre of the gap in A-layers as the origin of energies; V is then the energy of the gap centre in B-layers which could be positive or negative, depending of the kind of interfaces). As pointed out earlier, we will restrict ourselves to the case of two nearby bands. Thus, there are two coupled envelope-functions describing the conduction-band and valence-band states of the semiconductor, subject to an effective 2×2 Dirac-like equation. Assuming that both the gap and the gap centre depend only on x (the growth direction), the resulting equation for the envelope-functions in the conduction- and valence-band can be written as

$$\begin{bmatrix} \frac{1}{2}E_g(x) - E + V(x) & -i\hbar v\partial \\ -i\hbar v\partial & -\frac{1}{2}E_g(x) - E + V(x) \end{bmatrix} \begin{pmatrix} f_c(x) \\ f_v(x) \end{pmatrix} = 0, \tag{1}$$

where $\partial = d/dx$. Here, $E_g(x)$ is the position-dependent gap and $V(x)$ gives the energy of the gap centre. The velocity v is related to the Kane's momentum matrix elements and is given by $v^2 = E_g/2m^*$. In spite of the fact that both E_g and the effective mass m^* are in general position dependent, the value of v is almost constant in direct gap III-V semiconductors [22]. Hereafter, we assume this constancy in the SL. It should be mentioned that the non-zero in-plane momentum can be easily absorbed in the definition of parameters and we will henceforth ignore it.

Considering only electronic states below the barrier, which are of most interest to study quantum confinement effects, the solution of the Eq. (1) yields the following expression with reference to the nth barrier centered at x_n

$$\begin{pmatrix} f^A_{cn}(x) \\ f^A_{vn}(x) \end{pmatrix} = p_n \begin{pmatrix} 1 \\ \gamma \end{pmatrix} \exp[i\kappa(x - x_n - b/2)] + q_n \begin{pmatrix} 1 \\ -\gamma \end{pmatrix} \exp[-i\kappa(x - x_n - b/2)]$$
$$x_n + b/2 < x < x_{n+1} - b/2, \tag{2a}$$
$$\begin{pmatrix} f^B_{cn}(x) \\ f^B_{vn}(x) \end{pmatrix} = s_n \begin{pmatrix} 1 \\ i\lambda \end{pmatrix} \exp(-\eta x) + u_n \begin{pmatrix} 1 \\ -i\lambda \end{pmatrix} \exp(\eta x)$$
$$x_n - b/2 \leq x \leq x_n + b/2, \tag{2b}$$

where, for brevity, we have defined the following real parameters

$$\kappa = \left(\frac{1}{\hbar v}\right)\sqrt{E^2 - E_{gA}^2/4}, \tag{3a}$$

$$\gamma = \frac{E - E_{gA}/2}{\hbar v \kappa}, \tag{3b}$$

$$\eta = \left(\frac{1}{\hbar v}\right)\sqrt{E_{gB}^2/4 - (E-V)^2}, \tag{3c}$$

$$\lambda = \frac{E_{gB}/2 - E + V}{\hbar v \eta}. \tag{3d}$$

Assuming the continuity of the envelope-functions at the interfaces, we can eliminate (s_n, u_n), thus relating (p_n, q_n) with (p_{n-1}, q_{n-1}) via the 2×2 transfer-matrix $M(n)$ through the relationship

$$\begin{pmatrix} p_n \\ q_n \end{pmatrix} = M(n) \begin{pmatrix} p_{n-1} \\ q_{n-1} \end{pmatrix} \equiv \begin{pmatrix} \alpha_n & \beta_n \\ \beta_n^* & \alpha_n^* \end{pmatrix} \begin{pmatrix} p_{n-1} \\ q_{n-1} \end{pmatrix}, \tag{4}$$

where

$$\alpha_n = \left[\cosh(\eta b) + i\left(\frac{\gamma^2 - \lambda^2}{2\gamma\lambda}\right)\sinh(\eta b)\right]\exp[i\kappa(\Delta x_n - b)] \tag{5a}$$

$$\beta_n = -i\left(\frac{\gamma^2 + \lambda^2}{2\gamma\lambda}\right)\sinh(\eta b)\,\exp[-i\kappa(\Delta x_n - b)], \tag{5b}$$

with $\Delta x_n \equiv x_n - x_{n-1}$ and the convention $x_0 = 0$. Note that $\det[M(n)] = 1$. Letting N be the total number of barriers (B-layers), the transfer matrix $T(N)$ of the whole FSL is obtained as follows

$$T(N) = \prod_{n=N}^{1} M(n) \equiv \begin{pmatrix} A_N & B_N \\ B_N^* & A_N^* \end{pmatrix}. \tag{6}$$

The elements of the transfer matrix $T(N)$ can be easily calculated recursively taking into account the fact that $T(N) = M(N)\,T(N-1)$. In particular we find the expression [8,23]

$$A_N = \left(\alpha_N + \alpha_{N-1}^* \frac{\beta_N}{\beta_{N-1}}\right) A_{N-1} - \left(\frac{\beta_N}{\beta_{N-1}}\right) A_{N-2}, \tag{7}$$

supplemented by the initial conditions $A_0 = 1$, $A_1 = \alpha_1$.

Once we have calculated the matrix element A_N, some physically relevant entities can be readily obtained from it. Thus, the transmission coefficient τ at a given energy E is written as

$$\tau = \frac{1}{|A_N|^2}. \tag{8}$$

Also the single-channel, dimensionless Landauer resistance is given as [20]

$$\rho = \frac{1-\tau}{\tau} = |A_N|^2 - 1. \tag{9}$$

The dependence of the resistance with the system size is useful to study the spatial extension of the electronic states: Localized states lead to a nonhomic behaviour of the resistance which increases exponentially with the system size, whereas extended states show a bounded resistance. Apart from these two entities, there are other which can also be obtained from A_N. Indeed, the Lyapunov coefficient Γ is a nonnegative parameter given by [24]

$$\Gamma = -\frac{1}{2N}\ln\tau. \tag{10}$$

The Lyapunov coefficient represents the growth rate of the envelope-function and it is nothing but the inverse of the localization length in units of the SL period: The more localized the electronic state, the larger the value of Γ.

Finally, considering periodic boundary conditions at both edges of the FSL, one can obtain the following condition for an energy to lie in an allowed miniband

$$\left(\frac{1}{2}\right)|\mathrm{Tr}\,[T(N)]| \leq 1. \tag{11}$$

In particular, in the case of periodic SL ($a = a'$) with period L the Bloch theorem holds good and one then gets $\cos KL = \mathrm{Re}\,(\alpha_1)$; for this situation the dispersion relation $E(K)$, K being the crystal momentum, is found from

$$\cos KL = \cosh(\eta b)\cos[\kappa(L-b)] - \left(\frac{\gamma^2-\lambda^2}{2\gamma\lambda}\right)\sinh(\eta b)\sin[\kappa(L-b)]. \tag{12}$$

This expression will be used later to determine the miniband structure in periodic SL, in order to compare it with results obtained in FSL.

III. InAs/GaSb FSL

As an application of our results we consider nearly lattice-matched InAs/GaSb SL. Recently, much interest was centered on the use of these materials in resonant tunnelling devices which produce differential negative resistance with high peak-to-valley current ratio even at room temperature [25]. The band alignment is type II-staggered [26] in the InAs/GaSb interface, as shown in Fig. 1. Perhaps this is the most interesting feature because the conduction-band edge of the InAs is 0.15 eV lower in energy than the valence-bad edge of the GaSb [27], so that electrons can flow from the conduction-band of the InAs to the valence-band in GaSb. Moreover, these two semiconductors present a nearly equal Kane's matrix element leading to $\hbar v \sim 0.77\,\mathrm{eV\,nm}$, thus supporting our previous assumption that this parameter is constant through the whole SL. From Fig. 1 we conclude that $E_{gA} = 0.36\,\mathrm{eV}$, $E_{gB} = 0.67\,\mathrm{eV}$, and $V = 0.665\,\mathrm{eV}$. We set layer thickness leading to $a = 6.0\,\mathrm{nm}$, $a' = 6.2\,\mathrm{nm}$, and $b = 4.0\,\mathrm{nm}$ in our numerical computations.

Using the above set of parameters, we first studied the miniband structure using (12) in periodic SL with periods $L = a$ and $L = a'$. The corresponding dispersion relations are shown in Fig. 2. The most relevant feature is that, in both cases, there exists only one miniband between the conduction-band edges of InAs (0.18 eV) and GaSb (1.0 eV). As expected, the larger the SL period L, the deeper the miniband. Nevertheless, this is the only noticeable effect since the miniband-width is almost unchanged

Now we consider the most prominent features of the resulting electronic structure when quasiperiodicity is introduced ($a \neq a'$). Figure 3 presents a schematic diagram of the band-edge profile in the FSL. As we have already explained in the Introduction, one of the most characteristic properties of electronic spectra in (one-band) FSL is its highly fragmented, Cantor-like nature. We have confirmed this fragmentation in our (two-band) FSL, even when deviation from perfect periodicity is actually small. This deviation can be quantitatively measured from the ratio a'/a which, with our choice of parameters, is very close to unity. In fact, using the condition (11), we have found that the miniband of the periodic SL splits

into several sub-minibands, that is, small gaps appear. The origin of these small inner gaps are directly related to the loss of long-range quantum coherence of the electrons. Results corresponding to the fragmentation of the miniband are shown in Fig. 4 as a function of the Fibonacci order l, i. e., the number of GaSb layers in the FSL is F_l. Only short approximants of the FSL are displayed since on increasing l the spectrum becomes so fragmented that it is difficult to observe minor features in the plot. However, we have carefully analysed FSL spectra up to order $l = 15$ ($N = F_{15} = 987$ GaSb layers) and we have confirmed that the number of sub-minibands composing the whole spectrum is exactly F_l. The two outermost main sub-mibands present F_{l-2} subsub-minibands whereas the innermost sub-miniband presents F_{l-3} subsub-minibands so the total number of subsub-miniband is $F_{l-2} + F_{l-3} + F_{l-2} = F_{l-1} + F_{l-2} = F_l$. The number of subsub-minibands in each main cluster is a consequence of how the energy spectrum is fragmented, as we shall further discuss later. Since, strictly speaking, quasiperiodicity is only observable in the limit $N \to \infty$, our results provide information on the prefractal signature of the FSL energy spectrum. We have observed that both the position and widths of the main sub-minibands converge very rapidly to stable values with increasing the number or GaSb barriers. We shall refer to this behaviour as *asymptotic stability* of the spectrum; it implies that its global structure can be obtained in practice by considering very short approximants, as short as $F_9 = 55$ barriers, to very large FSL.

Another characteristic feature of Fibonacci systems is the self-similar pattern exhibited by their corresponding spectra. This self-similarity has been widely investigated within the tight-binding approximation and, to lesser extend, in wide-gap semiconductor FSL. Our results point out that self-similar spectra are also obtained in narrow-gap semiconductor FSL as shown in Fig. 5. It is clear that the whole electronic spectrum for a short approximant ($F_3 = 3$ in this case) is mapped onto a small portion of the spectrum of a higher approximants ($F_6 = 13$ and $F_9 = 55$ in Fig. 5). This is a consequence of how the FSL is constructed, based on a deterministic substitution sequence [28]. Our previous experience [9] has led us to the conclusion that the fragmentation scheme of a particular kind of Fibonacci lattice is very well

characterized by means of the Lyapunov coefficient. Hence, we undertook the study of this parameter in InAs /GaSb FSL. Results are displayed in Fig. 6 for a FSL with $N = F_{11} = 144$ barriers, although results are independent of the Fibonacci order. To be specific, in all cases we have considered we have observed a well-defined trifurcation pattern of the energy spectrum, characterized by the presence of three main sub-minibands separated by large minigaps. Inside each main sub-miniband, the fragmentation scheme follows a trifurcation pattern in which each sub-miniband further trifurcates obeying a hierarchy of splitting from one to three subsub-minibands. This fragmentation scheme is clearly observed in Fig. 6(a), in which the three main sub-minibands are detected as an overall decrease of the Lyapunov coefficient, whereas minigaps appear as local maxima. In Fig. 6(b), an enlarged view of the lower main sub-miniband shows the self-similar nature of the spectrum structure.

In the thermodynamical limit Fibonacci systems present singular continuous electronic spectrum [29]. In order to estimate the spectral type associated with our FSL, we have computed the so-called equivalent bandwidth S, defined as the sum of all allowed sub-minibands. As can be expected from the Cantor-like nature of Fibonaccian spectra, S vanishes as the number of barriers increases according to a power law of the form $S = F_N^{-\beta}$ with $\beta \sim 0.3$ (see Fig. 7). Earlier works [28] reported that such power-law scaling is characteristic of a singular continuous spectrum for which all the wave functions are critical, i.e., regarding localization properties, the functions are neither exponentially localized nor extended in the Bloch sense. Therefore, it should be expected that FSL present higher values of the Landauer resistance at zero temperature than periodic SL with the same number of barriers since, in the former case, electronic states are critical whereas in the later case electronic states are truly extended (Bloch states). To confirm this situation we have evaluated the Landauer resistance ρ by means of its definition (9) for the two kinds of SL with $N = F_8 = 34$ GaSb barriers, as shown in Fig. 8. Notice that, in addition to the occurrence of well-define inner gaps leading to a strong enhancement of ρ, the overall resistance is larger in the case of FSL. These results suggest that the overall resistance of the SL is directly connected with the decay rate of the electronic envelope-function along

the sample, as can be deduced from the comparison between Fig. 6 showing the inverse of the localization length, and Fig. 8(b). Hence, the spatial extension of envelope-functions controls the electrical transport of the sample, as is the case for wide-gap semiconductor FSL.

IV. SUMMARY

We have studied theoretically a new type of quasiperiodic SL made of narrow-gap III-V compounds, whose electron dynamics is described by means of an effective Dirac equation in the framework of an effective-mass $\mathbf{k}\cdot\mathbf{p}$ approach. The quasiperiodic SL is constructed arranging two kind of narrow-gap semiconductor layers following the Fibonacci sequence, assuming that barrier thickness is always the same while well thickness takes on two values according to the inflation rule of the Fibonacci series. By means of the transfer-matrix formalism, we obtain closed expressions to study electron transport through the Landauer resistance, localization length of electrons through the Lyapunov coefficient, and the spectral nature of the FSL. Those expressions are suitable for an efficient numerical treatment. Although the method is completely general even in the presence of band-inverted semiconductors as it is the case of some IV-VI heterostructures (e. g., $Pb_{1-x}Sn_xTe$), we have focused our attention on InAs/GaSb FSL. The corresponding electronic spectrum shows a highly fragmented, self-similar nature resembling that found for simpler tight-binding models. The spectral nature of our model Hamiltonian, obtained from bandwidth-scaling considerations, indicates that it is singular continuous in the thermodynamical limit, in agreement with the conjecture that the spectral type for almost all substitution sequences should be singular continuous [29]. Using the Lyapunov coefficient we have been able to demonstrate that the electronic spectrum follows a trifurcation scheme of fragmentation with increase of the Fibonacci order. In addition, investigations on the Landauer resistance indicate an overall increase of its value as compared to periodic SL. The relationship obtained in this regard suggests that the resistance of the FSL is directly connected with the decay rate of the

electron envelope-function along the sample.

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FIGURES

FIG. 1. Schematic band-edge diagram of InAs/GaSb type II interface, neglecting band bending at the heterojunction.

FIG. 2. Miniband structures for periodic InAs/GaSb superlattices with periods $L = 6.0\,\text{nm}$ (solid line) and $L = 6.2\,\text{nm}$ (dashed line) and barrier thickness $b = 4.0\,\text{nm}$. Energies are measured from the gap centre of InAs.

FIG. 3. Schematic band-edge diagram of a InAs/GaSb FSL. GaSb layers are of the same thickness b and they are centered at x_n. $x_n - x_{n-1}$ takes on two values a or a' according to the Fibonacci sequence.

FIG. 4. Allowed sub-minibands as a function of the Fibonacci order l, for a InAs/GaSb FSL. The number of sub-minibands is F_l for each order l. Thickness of GaSb layers is $b = 4.0\,\text{nm}$ and the distance between their centres is $a = 6.0\,\text{nm}$ or $a' = 6.2\,\text{nm}$, arranged according to the Fibonacci sequence.

FIG. 5. Self-similar spectrum of the InAs/GaSb FSLs with the same layer thickness as in Fig. 3. Left plot shows the whole spectrum of a FSL of order $l = 3$ whereas central and right plots show a detail of the spectrum of the FSL of order $l = 6$ and $l = 9$, respectively.

FIG. 6. (a) Lyapunov coefficient as a function of energy for InAs/GaSb FSL with the same layer thickness as in Fig. 3. The number of GaSb layers is $F_{11} = 144$. (b) An enlarged view of one of the main sub-mibands in which the self-similar character is more clearly observed.

FIG. 7. Equivalent bandwidth S as a function of the number of GaSb layers $N = F_l$ for a InAS/GaSb FSL with the same layer thickness as in Fig. 3.

FIG. 8. Landauer resistance as a function of energy for InAs/GaSb SLs for (a) periodic with $L = 6.0\,\text{nm}$ and $b = 4.0\,\text{nm}$ (b) Fibonacci with the same parameters as in Fig. 2. In both cases the number of GaSb layers is $F_8 = 34$.