

Number of bound states of a Kronig-Penney finite-periodic superlattice

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Abstract. We calculate analytically the conditions that establish the number of bound states in finite superlattices as a function of the depth, width and separation of the wells. We consider a lattice of δ -wells and a set of rectangular wells. For this latter case, we show how for finite systems the energy levels already group together in bands separated by gaps.

PACS. 73.20.Dx Electron states in low-dimensional structures (superlattices, quantum well structures and multilayers)

1 Introduction

Since the appearing of the concept of heterostructure [1], a vast amount of scientific work in the field of condensed matter physics has been devoted to the theoretical and experimental study of such structures. The development and continuous improvement in growth techniques [2] allow to construct quasi-one dimensional systems in the direction of the growth of the heterostructure, forming structures such as single quantum wells, double barriers, coupled quantum wells and superlattices.

The envelope function method has become the most commonly employed theoretical tool for the study of electronic properties of heterostructures, such as transmission coefficients, bound state energies, or the behavior under the effect of electric and magnetic fields [3–11]. In this method, the effective mass approximation is usually considered, because the potential structures generated are near the bottom of the conduction band of the barrier and well material (typically, AsGa and AlAsGa). The standard model assumes that the potential wells and barriers are rectangular, due to the fast jump of the potential energy between successive materials.

An interesting problem that arises in the calculation of the bound states of a Kronig-Penney (KP) system formed by N identical rectangular wells (a finite periodic superlattice) is the number of bound states that this potential is able to hold. When a single well is considered, the result is well-known: the number of bound states depends on the

width and the depth of the well, and analytical conditions for the range of parameters corresponding to each number of bound states can be written down explicitly.

The aim of this paper is the calculation of the number of bound states for a finite periodic superlattice formed by N identical square wells. We will obtain analytical conditions for the appearance of each new bound states in the superlattice in terms of the width, depth and separation of the wells. These conditions can be considered as critical values of the interaction between the wells when they are coupled together to form a lattice.

The paper is organized as follows: in Section 2, we explain the method of calculation used to obtain the bound states of the systems considered. In Section 3, we solve the problem for a periodic system of δ -wells. For this system, the calculation is easier, because an isolated δ -well admits one and only one bound state, independently of its amplitude. Finally, in Section 4 we present the results for the more general case of a superlattice formed by square wells and barriers.

2 Method of calculation

We will calculate the number of bounds states sustained by a finite periodic lattice with the help of the characteristic determinant method. This is a very powerful technique that provides us with the relevant information contained in the Green function of the whole system [12,13]. The characteristic determinant method can be used in similar problems to the usually solved by the transfer matrix method, both providing the same results [14]. In this section we review the application of the method to the two

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models considered: δ -wells and rectangular potentials. The potential corresponding to a periodic finite chain of δ -wells is:

$$V(x) = - \sum_{n=1}^N V_0 \delta(x - na) \quad V_0, a > 0. \quad (1)$$

The second, more realistic, case that we will consider is a multilayered system, which we will restrict to only two types of layers forming identical square wells. Each layer is characterized by its width and its constant potential energy.

For both cases, the determinant, that in general is a complex function of the energy E , satisfies the following recurrence relationship

$$D_n = A_n D_{n-1} - B_n D_{n-2} \quad (2)$$

where the index n goes from 1 to N . This number N represents the total number of δ -wells for the first model, and the number of interfaces between different layers in the multilayered model. The initial conditions are:

$$\begin{aligned} D_{-1} &= 0 \\ D_0 &= 1. \end{aligned} \quad (3)$$

The magnitudes A_n and B_n depend on the model considered. For the δ -well case we have

$$A_1 = 1 + V_1 G_0(x, x)$$

$$A_n = 1 + V_n G_0(x, x)(1 - \lambda_{n-1}) + B_n \quad n > 1$$

$$B_n = V_n \lambda_{n-1} / V_{n-1} \quad n > 1 \quad (4)$$

where V_n is the amplitude of the n th well (in our case $V_n = -V_0$) and G_0 is just the GF for the free particle:

$$G_0(x, x') = \frac{1}{2\kappa} e^{-\kappa|x-x'|}. \quad (5)$$

In this equation $\kappa = \sqrt{-E}$, because we have to find the bound states in the region of negative energy. Note that, as in the rest of the paper, we use units derived from the convention $\hbar = 2m = 1$. The parameter λ_n is defined as:

$$\lambda_n = \exp\left(-\int_{x_n}^{x_{n+1}} \frac{1}{G_0(x, x)} dx\right). \quad (6)$$

For the multilayered case, the magnitudes A_n and B_n are defined as:

$$A_n = 1 + \lambda_{n-1,n} \frac{r_{n-1,n}}{r_{n-2,n-1}} (1 - r_{n-2,n-1} - r_{n-1,n-2}) \quad (7)$$

and

$$B_n = \lambda_{n-1,n} \frac{r_{n-1,n}}{r_{n-2,n-1}} (1 - r_{n-2,n-1}) (1 - r_{n-1,n-2}), \quad (8)$$

where $r_{n-1,n}$ is the reflection amplitude between layers $n-1$ and n , and in general is given by

$$r_{n-1,n} = \frac{G_{n-1} - G_n}{G_{n-1} + G_n} \quad (9)$$

where $G_n \equiv G_n(x, x)$ is the GF in layer n th at coinciding coordinates, which for a constant potential V_n is given by:

$$G_n = \frac{i}{2\sqrt{E - V_n}}. \quad (10)$$

Once D_N has been obtained the determination of the bound states is easy. It can be shown [13] that the poles of the GF of the whole system (which, as we know, correspond to the bound states) are just the zeroes of the characteristic determinant. Therefore, to find the bound states of the potential for both models we just will have to solve the equation:

$$D_N = 0. \quad (11)$$

3 δ -wells superlattices

In this section, we are going to obtain the number of bound states of a finite chain of N δ -wells. The reason for considering the δ -well case is that it can be solved analytically up to the end.

Let us remember first that for a single δ potential $V(x) = -V_0\delta(x)$, with $V_0 > 0$, we always have a single bound state, whose energy is given by:

$$E_1 = -\frac{V_0^2}{4}. \quad (12)$$

We can easily recast this result with the characteristic determinant method. As there is only one δ -function, we have a 1×1 determinant, $D_1 = 1 - V_0 G_0(x, x)$, where $G_0(x, x)$ is given by equation (5). The zero of the determinant corresponds to the solution of the equation:

$$1 - V_0 G_0 = 0 \quad (13)$$

which, of course, is the same given by equation (12).

Let us now consider two δ -wells, *i.e.*, a potential of the form $V(x) = -V_0(\delta(x) + \delta(x-a))$, where $V_0, a > 0$. We can obtain easily the bound spectrum of this potential either solving Schrödinger equation directly or with the help of the characteristic determinant solving the equation $D_2 = 0$, where D_2 is given by equation (2). The result for the bound spectrum of this potential is well-known (see, *e.g.* [15]): there exist at least one bound level, independent of the values of V_0 and a , and a second bound level appears when the condition

$$V_0 a > 2 \quad (14)$$

is satisfied. As we will see in the case of many δ -wells, and following the trend already established for two δ -wells, the number of bound states explicitly depends on the value of

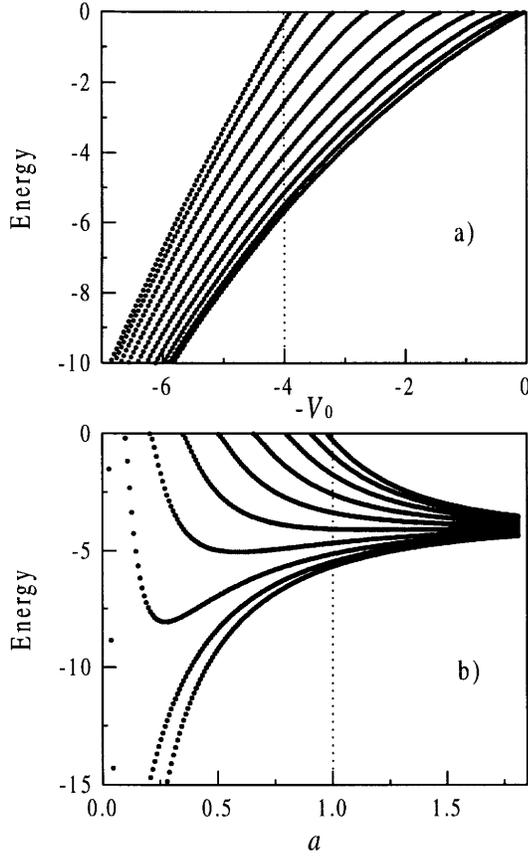


Fig. 1. Plot of the bound spectrum of a system formed by 10 δ -wells. In part (a) we show the behavior of the eigenenergies as a function of V_0 for $a = 1$. In part (b), we show the bound states as a function of the distance a between wells for $V_0 = 4$. The condition $V_0 a = 4$ is shown in both cases as a vertical dotted line.

the product $V_0 a$, which we will define as the interaction strength between the wells.

Our purpose now is to generalize the previous result to a periodic system consisting of an arbitrary number N of wells, whose potential is given by equation (1). The main aim is to obtain the number of bound states in terms of the interaction strength $V_0 a$.

Before entering into the details of the calculation, let us show, as an example, the numerical results for a system formed by $N = 10$ wells. In Figure 1a, we show the bound energies obtained for such a system as a function of the amplitude V_0 for a fix distance a (which we take $a = 1$). In Figure 1b, we represent the same bound energies as a function of the distance a between the wells for a fix amplitude V_0 (numerically $V_0 = 4$). In both cases, we show the condition $V_0 a = 4$ as a vertical dotted line. The number of bound states allowed in the band depends on the value of the product $V_0 a$.

For a system with N wells, there are $N - 1$ conditions of $V_0 a$ (excluding the trivial value $V_0 a = 0$ for the appearance of the first bound state) for the appearance of every new bound state in the band. It is important to point out that a new state always arises at an energy $E = 0$, which

facilitates our calculation. Let us denote by $(V_0 a)_i$, where $i = 1, 2, \dots, N - 1$, the value of the interaction strength for which the $(i + 1)$ th bound state appears at $E = 0$. When we finally reach the value $(V_0 a)_{N-1}$ no new bound state appears and the band is complete, *i.e.*, there are the same number of bound states as wells in the lattice.

For the δ -well periodic lattice, we can solve analytically the determination of the conditions $(V_0 a)_i$. The recurrence relation for our characteristic determinant, equation (2), can be summed for this system by making use of its periodicity, and the result can be written as [12]:

$$D_N = e^{-N\kappa a} \{T_N(\cos \beta a) - Z(\kappa a)U_{N-1}(\cos \beta a)\} \quad (15)$$

where N is the number of wells. The magnitude β plays the role of the quasimomentum, and its dispersion relationship is given by

$$\cos(\beta a) = \cosh(\kappa a) - \frac{V_0}{2\kappa} \sinh(\kappa a) \quad (16)$$

where $\kappa = \sqrt{-E}$ (we are in the range $E < 0$). The function $Z(\kappa a)$ is defined as:

$$Z(\kappa a) = \frac{V_0}{2\kappa} \cosh(\kappa a) - \sinh(\kappa a). \quad (17)$$

Finally, the functions $T_N(\cos \beta a)$ and $U_{N-1}(\cos \beta a)$ are the Chebyshev polynomials of the first kind of order N and of the second kind of order $N - 1$, respectively.

As we commented in the previous section, the bound energies of the system are obtained by solving the equation $D_N = 0$, and every new bound state appears at an energy infinitesimally small. Therefore, we have to look for the zeroes of D_N when the energy tends to 0, *i.e.*, when $\kappa \rightarrow 0$. In this limit, the function $Z(\kappa a)$ diverges and the sign of this divergence is determined by the sign of the function $U_{N-1}(\cos \beta a)$. Whenever $U_{N-1}(\cos \beta a)$ crosses zero, it changes its sign and so does the characteristic determinant D_N , indicating the appearance of a new bound state. Thus, the divergence of $Z(\kappa a)$ as κ goes to zero, ensures that the change in sign of D_N at very small energies and so the number of solutions of $D_N = 0$, *i.e.*, the number of bound states, is entirely dominated by the changes in sign of $U_{N-1}(\cos \beta a)$.

The polynomial $U_{N-1}(\cos \beta a)$ presents $N - 1$ zeroes given by [16]

$$\cos \beta a^{(m)} = \cos \frac{m\pi}{N}, \quad m = 1, 2, \dots, N - 1. \quad (18)$$

In the limit $\kappa \rightarrow 0$, the dispersion relationship given by equation (16) is reduced, in first order in κa , to:

$$\cos \beta a = 1 - \frac{V_0 a}{2}. \quad (19)$$

Substituting these values of $\cos \beta a$ in equation (18), we finally obtain the $N - 1$ critical values of the interaction strength $V_0 a$ for the appearance of a new bound state:

$$(V_0 a)_m = 2 \left(1 - \cos \frac{m\pi}{N} \right). \quad (20)$$

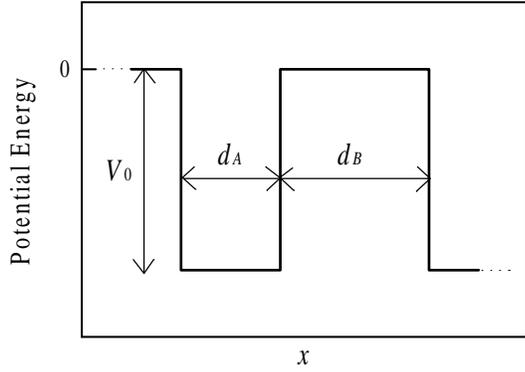


Fig. 2. Schematic plot of the potential energy profile of a piece of our system formed by square wells and barriers, where the parameters used (d_A , d_B and V_0) are indicated.

It is interesting to see what happens when N is large. In this case, the last state appears for $m = N - 1 \approx N$ and therefore the limiting condition for the completeness of the band is

$$(V_0 a)_{N-1} = 4. \quad (21)$$

This is the value shown as a vertical dotted line in Figures 1a and 1b. (The exact value for $N = 10$ is $(V_0 a)_9 = 3.902$.)

4 Square wells superlattice

We now want to solve the problem of the number of bound states of a finite Kronig-Penney model of square wells and barriers frequently used as a relatively realistic representation of superlattices. The effective mass approximation is often included in the model. We pass to generalize for this model the results previously obtained for the δ -wells lattice.

First of all let us summarize the well-known results for a single square well of width d_A and depth $-V_0$. For this potential there are n bound states when the value of the product $V_0 d_A^2$ is in the range:

$$\frac{(n-1)^2 \pi^2 \hbar^2}{2m} < V_0 d_A^2 < \frac{n^2 \pi^2 \hbar^2}{2m}. \quad (22)$$

Equivalently, the state number $n + 1$ appears at $E = 0$ when the condition

$$(V_0 d_A^2)_{n+1} = \frac{n^2 \pi^2 \hbar^2}{2m} \quad (23)$$

is satisfied. The previous equation can be written in our units as $(V_0 d_A^2)_{n+1} = n^2 \pi^2$.

Let us now consider a system formed by N identical square wells, of width d_A and depth $-V_0$, separated by identical flat barriers, of width d_B and $V = 0$, as it is shown in Figure 2. It corresponds to a periodic KP superlattice built with layers of two different materials, A and B , for which there is an energy shift in the bottom of their conduction bands. Let us call A the wells material,

and B the barriers material. The system is surrounded by two layers of material B of semi-infinite size. The problem is to know how many bound states exist in such a superlattice.

Again, the periodicity of the system allows us to solve the recurrence relation for the characteristic determinant, for which the following analytical expression can be deduced:

$$D_{2N} = e^{-N k_B d_B} \{T_N(\cos \beta a) - Z(E) U_{N-1}(\cos \beta a)\}. \quad (24)$$

The index of the determinant ($2N$) is the number of interfaces in the system, which is clearly equal to twice the number of wells, N . The magnitude β plays the role of the quasimomentum, and its dispersion relationship is given by:

$$\begin{aligned} \cos \beta a &= \cos k_A d_A \cosh k_B d_B \\ &\quad - \frac{k_A^2 - k_B^2}{2k_A k_B} \sin k_A d_A \sinh k_B d_B \end{aligned} \quad (25)$$

where

$$k_A = \sqrt{V_0 + E}, \quad k_B = \sqrt{-E} \quad (26)$$

since we are in the range $E < 0$. The function $Z(E)$ is now defined as:

$$\begin{aligned} Z(E) &= \cos k_A d_A \sinh k_B d_B \\ &\quad - \frac{k_A^2 - k_B^2}{2k_A k_B} \sin k_A d_A \cosh k_B d_B. \end{aligned} \quad (27)$$

We follow the same strategy as for the δ -lattice. Every new bound state appear in the limit $E \rightarrow 0$, where the dispersion relation given by equation (25) becomes:

$$\cos \beta a = \cos \sqrt{V_0} d_A - \frac{\sqrt{V_0} d_B}{2} \sin \sqrt{V_0} d_A. \quad (28)$$

As before, the function $Z(E)$ diverges as E goes to 0 and there is a new solution of the equation $D_{2N} = 0$ whenever U_{N-1} changes sign, *i.e.*, it becomes zero. Thus, a new bound state appears whenever the argument of the function U_{N-1} is equal to $\cos(m\pi/N)$, where $m = 1, 2, \dots, N - 1$. Using equation (28) the zeroes of U_{N-1} correspond to the condition:

$$\cos \frac{m\pi}{N} = \cos \sqrt{V_0} d_A - \frac{\sqrt{V_0} d_B}{2} \sin \sqrt{V_0} d_A \quad (29)$$

where $m = 1, 2, \dots, N - 1$. Let us define $F(V_0, d_A, d_B) \equiv \cos \sqrt{V_0} d_A - \frac{\sqrt{V_0} d_B}{2} \sin \sqrt{V_0} d_A$. From now on, we do not write the explicit dependence of F for brevity. In fact, this function depends on only two variables $\sqrt{V_0} d_A$ and $\sqrt{V_0} d_B$.

Equation (29) points out the physical difference between the parameters $\sqrt{V_0} d_A$ and $\sqrt{V_0} d_B$. For fixed values of $\sqrt{V_0} d_A$, the only $N - 1$ values of d_B for which a new bound state appears are:

$$(d_B)_m = 2 \frac{\cos \sqrt{V_0} d_A - \cos \frac{m\pi}{N}}{\sqrt{V_0} \sin \sqrt{V_0} d_A}. \quad (30)$$

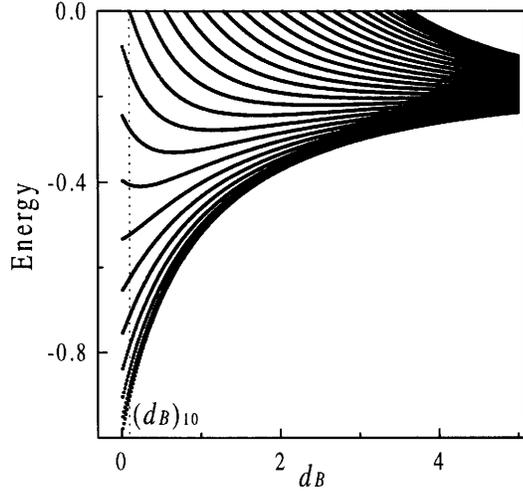


Fig. 3. The behavior of the bound states of a system formed by 30 identical square wells as a function of the distance between wells, d_B . We have taken $V_0 = d_A = 1$. The first physically acceptable value of d_B for the appearance of a new bound state $(d_B)_{10}$ is shown as a vertical dotted line.

We can note that for a range of values of $\sqrt{V_0}d_A$ it is possible to find negative values of $(d_B)_m$, which are not physically acceptable. Let us consider the limit $d_B \rightarrow 0$, in which the system is equivalent to a single well of width Nd_A and depth $-V_0$. Let us suppose that this well can maintain m_0 ($m_0 < N$) bound states. Then for positive values of d_B , only $N - m_0$ bound states can appear. There are only $N - m_0$ positive values of d_B that are solutions of equation (30). Note also that when $d_B = (d_B)_m$ the $(m + 1)$ th bound state appears at $E = 0$.

As an example of the previous result, we show in Figure 3 the energy spectrum of a system formed by 30 identical quantum wells as a function of d_B , for the case $V_0 = d_A = 1$. In the limit $d_B \rightarrow 0$ the equivalent “total” well has a depth of 1 and a width of 30, so it can maintain (see Eq. (22)) 10 bound states. Therefore, equation (30) only produces 20 physically acceptable (positive) values of $(d_B)_m$, corresponding to $m = 10, 11, \dots, 29$ for which a new state appears. The first positive solution $(d_B)_{10} = 9.58 \times 10^{-2}$ is represented in Figure 3 as a vertical dotted line, and gives the appearance of the bound state that firstly appears when we begin to separate the wells of the system.

The dependence of the number of bound states on the magnitude $\sqrt{V_0}d_A$ is very rich, since this magnitude enters as the argument of trigonometric functions. There are multiple sets of values of $\sqrt{V_0}d_A$ for which equation (29) is satisfied. This is natural, because when the depth or the width of a well is increased, the well admits more bound states, and the lattice must reflect the same behavior.

To illustrate the problem graphically, we represent in Figure 4 the energy bound spectrum as a function of $\sqrt{V_0}d_A$ for a system with 30 wells. Note that, as d_A is increased (we fix numerically $d_B = 1$ and $V_0 = 2$), new bound states appear (at $E = 0$), forming the well-known superlattice minibands separated by gaps. Our purpose

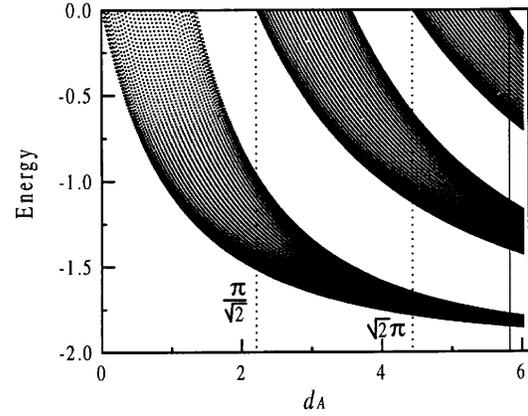


Fig. 4. The bound states of a system formed by 30 identical square wells as a function of d_A with $V_0 = 2$ and $d_B = 1$. The values $d_A = n\pi/\sqrt{V_0}$ for $n = 1, 2$ are shown as vertical dotted lines, and indicate the appearance of the first bound state of a new miniband. The solid line is used for reference in Figure 5.

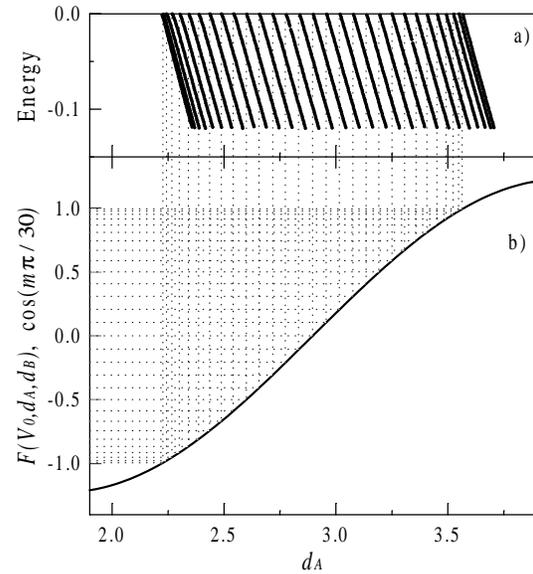


Fig. 5. In part (a), we show the spectrum of the same system as in Figure 4, but in the region of small energy (in absolute value) and the range of values of d_A corresponding to the appearance of the states of the second miniband. In part (b), we show the function $F(V_0, d_A, d_B)$ in a solid line, and in horizontal dotted lines we show the functions $\cos m\pi/30$ for $m = 1, 2, \dots, 29$. The crossings of these functions with F gives the appearance of new bound states, as we show with vertical dotted lines connecting (a) and (b).

here is the *exact* determination of the values of $\sqrt{V_0}d_A$ for which new bound states appear in the spectrum and, as a consequence, we will also explain the reason for the appearing of the gaps.

The general and exact solution of the problem of the appearing of new bound states is encountered by solving equation (29). We show a graphical solution of this equation in Figure 5. In part (a) we represent the bound

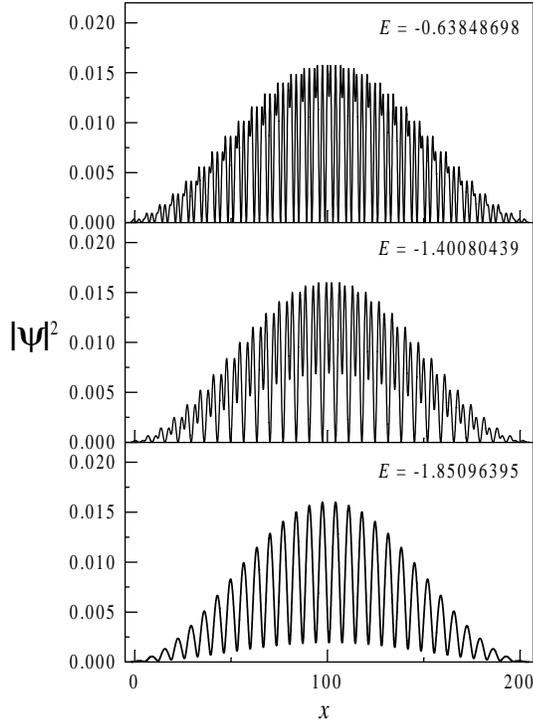


Fig. 6. The probability density of the three bound states corresponding to the ground states of the three minibands of the system, obtained for the parameters $V_0 = 2$, $d_B = 1$ and $d_A = 5.825$. These values correspond to the vertical solid line in Figure 4.

spectrum of the same system as in Figure 4, but only in the region of small energy (in absolute value) and for a range of values of d_A for which the 30 bound states of the second miniband appear. In Figure 5b, we show in a solid line the function $F(2, d_A, 1)$ for the same range of values of $\sqrt{V_0}d_A$ as in part (a). The horizontal dotted lines correspond to $\cos(m\pi/30)$ for $m = 1, 2, \dots, 29$. The crossings of these values with the function $F(2, d_A, 1)$ give the values of $\sqrt{V_0}d_A$ for which a new bound state appears. We represent these values with vertical dotted lines connecting parts (a) and (b) of Figure 5. Although we only show in Figure 5 the case of the second miniband, the crossings of $\cos m\pi/N$ and the oscillating function F will give the values of $\sqrt{V_0}d_A$ for which new bound states will appear in all the minibands.

The gaps between minibands (see Fig. 4) arise because there are intervals of $\sqrt{V_0}d_A$ for which F is bigger (in absolute value) than 1, and therefore the general equation (29) has no solution in these intervals. Note that, for $\sqrt{V_0}d_B$ constant, we can rewrite the function F as:

$$F = \sqrt{1 + \frac{V_0 d_B^2}{4}} \sin \left(\sqrt{V_0} d_A + \arctan \left(\frac{2}{\sqrt{V_0} d_B} \right) \right) \quad (31)$$

F is a sine function whose amplitude is always greater than 1. For certain intervals of $\sqrt{V_0}d_A$ we will have that $F > 1$, and no new bound states will appear at $E = 0$ in this region. Since the energy of the bound states are con-

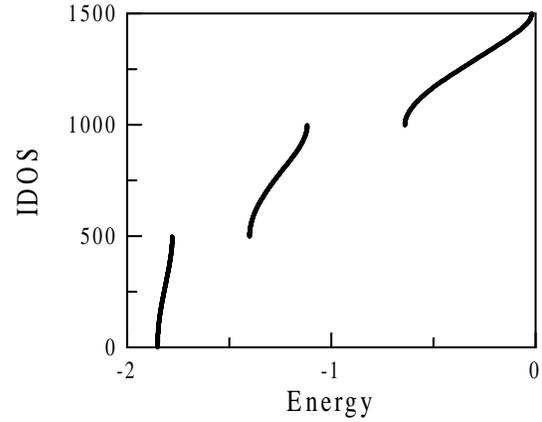


Fig. 7. Integrated density of states for a superlattice with 500 wells and for $V_0 = 2$, $d_B = 1$ and $d_A = 5.825$. Note that the three minibands are complete. The parameters correspond to the solid line at the right of Figure 4.

tinuous functions of $\sqrt{V_0}d_A$, the previous absence of states propagates to other energies, forming the well-known energy gaps for a fix value of $\sqrt{V_0}d_A$.

An additional remaining question is that we have determined only $N - 1$ conditions (per band) for the appearance of new states. But each band is formed by N bound states, and therefore there is still one undetermined condition. It corresponds to the existence of the first state of each band. A new band begins whenever all the wells of the system as a whole satisfy the well-known conditions for the appearance of a state in a single square well, equation (23). In particular, when $\sqrt{V_0}d_A = n\pi$, the first state of the $(n + 1)$ th band appears. As an example, the beginning of the second and third bands, at $\sqrt{V_0}d_A = \pi$ and $\sqrt{V_0}d_A = 2\pi$ (with $V_0 = 2$) respectively, are shown as vertical dotted lines in Figure 4.

The determinant method, which is based on a Green function formalism, can also provide the wave functions corresponding to the bound states. Note that the method yields the information of the total Green function in all the layers of the system, and also the transmission and reflection in each interface can be obtained (see Ref. [13] for more details). Therefore, the wave functions can be obtained directly. In Figure 6, we show the wave functions for three bound states corresponding to the ground states of the three bands obtained for the values $V_0 = 2$, $d_A = 5.825$ and $d_B = 1$. These values corresponds to the solid line at the right of Figure 4. Note how the envelope of the three states is the same, but they present a different oscillation pattern, as expected. In addition, the determinant method is very powerful when calculating the spectrum of bigger systems, because in general is a well-behaved function of energy whose zeroes (if the system is closed) are directly the bound states. These advantages, together with the numerical facilities derived from the recursion relationship (2) make this method very appropriated in the study of this kind of phenomena. As an example, and for the same parameters as in Figure 6, we show in Figure 7 the integrated density of states (IDOS) obtained for a superlattice

formed by 500 wells. Note that for the parameters that we are using, the three bands are complete, each one with 500 states.

Finally, we would like to comment that although, for the sake of simplicity, we have considered in all the calculations that $\hbar = 2m = 1$, our equations are also correct when the envelope function method is considered with the effective mass approximation included. Our results can be directly generalized to a binary superlattice with a well material A (like GaAs), with an effective mass m_A , and a barrier material B (like GaAlAs), with a different effective mass m_B . In this case, the corresponding wave vectors (26) in the effective mass formalism are just:

$$k_A = \sqrt{2m_A(V_0 + E)/\hbar^2}, \quad k_B = \sqrt{-2m_BE/\hbar^2}. \quad (32)$$

Therefore, from (29, 32), the general equation for the appearance of new bound states (at $E = 0$) in a superlattice formed by N wells becomes explicitly:

$$\cos \frac{m\pi}{N} = \cos \sqrt{\frac{2m_AV_0}{\hbar^2}} d_A - \sqrt{\frac{m_AV_0}{2\hbar^2}} d_B \sin \sqrt{\frac{2m_AV_0}{\hbar^2}} d_A, \quad (33)$$

where we have now abandoned our unit convention.

5 Conclusions and remarks

We have obtained conditions for the appearance of bound states in finite periodic Kronig-Penney structures. In particular we have considered the cases of δ -well potentials and rectangular wells and barriers. From these conditions one can easily deduce the number of states for any given range of the parameters of the problem. We solved the problem with the help of the characteristic determinant method, which is an exact and non-perturbative method that has established itself as a very powerful tool for the study of wave phenomena.

For the δ -well case, the relevant parameter is V_0a . The number of states increases with this parameter and ranges between 1, for very small values of V_0a , and the number of wells, for V_0a very large.

For rectangular wells and barriers, the relevant parameters are $\sqrt{V_0}d_A$ and $\sqrt{V_0}d_B$. The states are divided into bands. The number of states in each band ranges, depending on the parameters, between 1 and the number of wells, as it was the case for the δ -wells potential (which only has one band). The number of states bound by the single effective well obtained by considering $d_B = 0$ gives us the number of bands.

Finally, we would like to point out that the problem studied in this paper, apart from its evident academic interest, is important also from the experimental point of view in order to study or design real superlattices. Note that, although for mathematical convenience we have restricted ourselves to bound states, our results can be directly applied to transmission minibands in open systems, which will appear practically at the same energies as the

bands of bound states in a closed potential. If we are in a range of the parameters for which new states are able to appear (given in general by Eq. (33)), this means in the open case that there is a transmission miniband in the energy region around the top of the barriers (equivalent to $E = 0$ in the closed case). This region is in general more difficult to study, specially by using simple methods. The reason is that, in this case, the energy range is far away from the bottom of the conduction band of the well material, and non-parabolicity effects in the dispersion relation has to be taken into account. On the contrary, if we are in a range of the parameters for which no new states can appear, this means that the transmission minibands are well inside the well material of the superlattice. In this region, the envelope function method with the effective mass formalism gives reasonable good results in spite of its simplicity, even for parabolic dispersion relationship. In any case, our results can be helpful in order to select the wells width, the distance between wells or, if possible by changing the materials, V_0 , in the construction of a real superlattice.

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