

Available online at www.sciencedirect.com



Annals of Physics 320 (2005) 1-20

ANNALS of PHYSICS

www.elsevier.com/locate/aop

# Eigenvalues, eigenfunctions, and surface states in finite periodic systems ☆

Pedro Pereyra \*

Física Teórica y Materia Condensada, UAM-Azcapotzalco, Av. S. Pablo 180, C.P. 02200, México D. F., Mexico

> Received 20 October 2004; accepted 26 May 2005 Available online 15 August 2005

### Abstract

Using a simple approach that requires neither the Bloch functions nor the reciprocal lattice, new, compact, and rigorous analytical formulas are derived for an accurate evaluation of resonant energies, resonant states, energy eigenvalues and eigenfunctions of open and bounded *n*-cell periodic systems with arbitrary 1D potential shapes, provided the single cell transfer matrix is given. These formulas are applied to obtain the energy spectra and wave functions of a number of simple but representative open and bounded superlattices. We solve the fine structure in bands and exhibit unambiguously that the true eigenfunctions do no not fulfill the periodicity property  $|\Psi_{\mu,\nu}(z+l_c)|^2 = |\Psi_{\mu,\nu}(z)|^2$ , with  $l_c$  the single cell length. We show that the well known surface states and surface energy levels come out naturally. We analyze the surface repulsion effect and calculate exactly the surface energy levels for different potential discontinuities an the ends. © 2005 Elsevier Inc. All rights reserved.

PACS: 03.65.Ge; 03.65.Nk; 71.15.-m; 72.20; 73.63; 78.67.Pt

Keywords: Eigenvalues; Eigenfunctions; Surface states; Intraband states in superlattices

0003-4916/\$ - see front matter © 2005 Elsevier Inc. All rights reserved. doi:10.1016/j.aop.2005.05.010

 $<sup>^{*}</sup>$  This work was partially supported by CONACyT, Mexico (Project 29026-E) and the Abdus Salam ICTP, Trieste, Italy.

Fax: +525553189540.

E-mail address: ppereyra@correo.azc.uam.mx.

# 1. Introduction

The calculation of eigenvalues and eigenfunctions is, undoubtedly, one of the most important and crucial objectives in physics, for they open up the possibility of evaluating other quantities and facilitate the understanding of the physical properties. Consequently, the advance of analytical methods for an accurate calculation of these quantities has been one of the most sustained aims of theoretical research in physics, specially in quantum and electromagnetic theories. Even though different techniques and approaches have been developed to derive compact formulas for an easy evaluation of these fundamental quantities, only in a small number of cases has it been possible to deduce analytical, closed expressions. In the present paper, we will show that this limited class of systems can in some sense be extended to include 1D *finite* periodic systems, *provided* that the single-cell transfer matrix is obtained [1]. We will report simple formulas for the evaluation of resonant energies, resonant wave functions, energy eigenvalues and eigenfunctions in open, bounded and quasi-bounded superlattices. These formulas are written in terms of the single-cell transfer matrix elements and are valid independently of the potential shape and the number of cells n. To illustrate the use of these formulas, we will discuss a number of specific and simple examples of open and bounded periodic systems.

In the current solid state theory the knowledge of the wave functions and the energy spectrum of *finite* periodic systems is still far from complete, though it has been regarded as completely understood [2], quite a while ago. The Bloch functions and the continuous energy bands obtained by applying standard methods (such as the tight-binding, pseudopotential, orthogonalized plane-wave, envelope function method, etc.) are congruent with the presumption of *infinite* periodic systems [3]. Eventhough it is known that the number of energy levels in bands and subbands of finite systems should be finite, the band energies and Bloch functions are often mistaken for the energy eigenvalues and eigenfunctions of *finite* periodic systems [4]. On the other hand, Ledermann [5] considered that a rigorous treatment of the frequency problem in the physical theory of crystals was *impracticable*. Therefore approximation methods, like the cyclic condition, were developed [6]. The Born's statement on the frequency distribution has been also deemed valid, when the number of boundary points is much less than the lattice points [5]. Lately, as the quantum structures size (experimentally achieved) moved toward the fundamental limits, the contention between discrete and continuous energy bands description becomes more evident. Nevertheless, most of the actual discussion of the transport and optical properties of semiconductor devices and superlattices rest on numerical calculations within the continuous energy band theory [7–13,4]. It is worth recognizing however that, in spite of the lack of intraband information, this theory (fully justified in the macroscopic domain) has been useful to build up the conceptual foundation of the present low dimensional physics.

In the last years, fairly accurate experiments [14–17] and fanciful applications using superlattices in the mesoscopic and nanoscopic domains stimulated the development of *ad rem* theoretical approaches to account for the fine structure inside

energy bands. The full quantization of electrons and photons in these systems becomes a focal characteristic, relevant in a number of attractive applications as the foreseen "zero-threshold lasers," where the electron-hole transitions couple with a single spontaneous emission mode [18,19]. The transfer matrix method that has been useful to study wave propagation and electronic structure in 1D alloys [20,21], and later to study resonant tunnelling and transmission coefficients in heterostructures and superlattices [14,15,22–29], has opened the possibility of determining *intraband* resonant energies in 1D finite periodic systems. Recently, Griffiths and Steinke [30] reviewed the theory of waves propagation in different kind of 1D locally periodic media using the transfer matrix approach. Sprung et al. [31] studied the relation between localized continuum bound states and surface states in finite periodic systems. Further developments of the transfer matrix approach were successfully applied to calculate optical transitions in the active region of (blue) laser devices [32]. To our knowledge, with the exception of a brief introduction to resonant energies and wave functions in [29] and the 'ictp' reprint [33], rigorous analytical expressions for the evaluation of eigenvalues and eigenfunctions in *bona fide* finite periodic systems, do not exist. This paper aspires to contribute to this purpose.

Early in the 1930s, Tamm [34] and Fowler [35] discussed for the first time the appearance of surface states when semi-infinite and finite systems are considered. Some years later Shockley [36] studied surface states associated with a finite periodic potential as functions of the lattice constants. The greatly increased experimental evidence for surface states in the late 1940s [37–39] spurred huge interest in the surface state theory [40–44] and specifically on various aspects of the Tamm and Shockley states. Even though the Schrödinger equation was solved only approximately, with the nearest-neighbor and tight-binding approximations, the one-electron resolvent method in the linear-combination-of-atomic-orbitals [43] and the pseudopotential method [45] were successful in treating various kinds of localized states on ideal crystal surfaces. Recently, Stęślicka et al. [46] studied quite extensively the localized states in binary and polytype *infinite* and *semi-infinite* semiconductor superlattices. As will be seen below (Eqs. (14) and (18)), surface energy levels emerge in a natural way within the theory of finite periodic systems further developed here.

The theory of finite periodic systems (TFPS) [23–29], originally proposed to calculate scattering amplitudes and related properties in open superlattices, is expanded here to deduce rigorous and compact analytical expressions for a precise calculation of the energy eigenvalues  $E_{\mu,\nu}$  and the corresponding eigenfunctions  $\Psi_{\mu,\nu}(z)$  (Sections 3 and 4) in bounded superlattices. For completeness, we enlarge in Section 2 the discussion on resonant energies  $E_{\mu,\nu}^*$  and resonant wave functions  $\Psi_{\mu,\nu}^*(z)$  presented in [29]. To encompass most of the various types of systems of current interest, classed by boundary conditions (see Fig. 1), we will refer separately to open and bounded (by finite and infinite height walls) periodic systems. The universal formulas reported here, written in terms of Chebyshev polynomials  $U_s$  (which order depends on the number of cells *n*) and the single-cell transfer matrix elements, allow to solve completely the fine structure in the bands, and can easily be applied to calculate intraband states, photo-transitions [32], and other transport and optical properties of



Fig. 1. Specific examples of (A) open, (B) bounded, and (C) quasi-bounded 1D *n*-cell periodic systems. Some parameters used in the text are also shown.

finite periodic systems described either by the electromagnetic or the quantum theories. All the expressions reported below, except for a few equations like (5) and (16), are valid for *any shape* of the single-cell potential and, are valid also for systems with an arbitrary number *n* of repetitions of the unit cell. In the limit of  $n \to \infty$ , these formulas reproduce the well known results of current theories. In order to illustrate the application of the principal results, we will consider representative examples of *n*-cell superlattices with sectionally constant potentials. It will be seen here that the assumption  $|\Psi(z + l_c)|^2 = |\Psi(z)|^2$ , is not correct for finite periodic systems, especially when the physical systems contain a small number of cells. New insights on the localization effect induced by phase coherence and level repulsion effects in bounded systems will also be presented.

Although we will be concerned in this paper with the simplest and widely used one channel (1D) approximation, our experience with transmission coefficients in multichannel systems, shows us that for open systems with uncoupled channels the transmission resonances for channel k > 1 occur at  $E_{\mu,\nu}^{(k)}$ , which coincides with the resonant energies in the one channel problem  $E_{\mu,\nu}^{(1)}$ , plus the corresponding energy threshold  $E_{\text{th}}^{(k)}$ , i.e.,  $E_{\mu,\nu}^{(k)} = E_{\mu,\nu}^{(1)} + E_{\text{th}}^{(k)}$ . For coupled-channels systems, however, the transmission coefficient  $T_{j,l}$  presents many more resonances (with amplitudes  $\leq 1$ ) [29], but they occur at  $E_{\mu,\nu}^{(l)}$  and  $E_{\mu,\nu}^{(l)}$ . This suggests that the multichannel spectrum consists of an appropriate combination of the independent-channels energy levels.

### 2. Resonant energies and resonant states in open systems

It is well established in scattering theory that a resonant transmission occurs precisely when the incident particle energy coincides with a bound-state energy in the scatterer system, which for our purpose is a locally periodic *n*-cell system. For this kind of systems, independent of the single-cell potential shape, the transmission amplitudes are obtained from [29]

$$t_{N,n}^{T} = \frac{1}{p_{N,n} - \beta^{-1} \alpha \beta p_{N,n-1}},$$
(1)

where N is the number of propagating modes (number of physical channels) and the functions  $p_{N,n}$  are  $N \times N$  matrix polynomials of order n, fully determined in terms of the single-cell transfer matrix M, which for time reversal invariant systems has the structure

$$M = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix}.$$
 (2)

In the one channel (one propagating mode) approximation  $\alpha$  and  $\beta$  are complex scalars and  $p_{1,n}$  is the Chebyshev polynomial of the second kind,  $U_n(\alpha_R)$ , evaluated at the real part of  $\alpha = \alpha_R + i\alpha_I$ . Note that it is precisely through this function that the specific single-cell potential shape parameters (or the single-cell refraction indices) enter into the universal formulas. The close relation between the resonant structure and the spectral properties, allows to determine simple expressions for the resonant energies. If we use the identity  $U_n U_{n-2} = U_{n-1}^2 - 1$ , we can rewrite the whole *n*-cell system transmission coefficient  $T_n = |t_n|^2 = |t_{1,n}|^2$  as

$$|t_n|^2 = \frac{|t|^2}{|t|^2 + U_{n-1}^2(1 - |t|^2)},$$
(3)

where  $|t|^2 = 1/|\alpha|^2$  is the single-cell transmission coefficient. It is clear from this expression that the transmission resonances occur precisely when the polynomial  $U_{n-1}(\alpha_R)$  becomes zero. Therefore, the vth resonant energy in the  $\mu$ th band [29] is the solution of

$$\left(\alpha_{\rm R}\right)_{\nu} = \cos\frac{\nu\pi}{n}.\tag{4}$$

Here  $(\alpha_R)_v$  represents the vth zero of the Chebyshev polynomial with v = 1, 2, ..., n - 1. The specific functional form of  $\alpha_R$  depends on the specific single-cell potential function. It is clear that the number of resonant states per subband equals the order of the Chebyshev polynomial in Eq. (3) and corresponds to the number of confining wells in the periodic system; in this case n - 1. It is important to notice that by solving the trascendental equation (4) all the subbands and the whole set of resonant energies  $E^*_{\mu,v}$ , in the selected energy interval, are straightforwardly obtained.

Let us now consider an example. In Fig. 2, we plot the energy spectra and level densities for the superlattice  $GaAs(Al_{0.3}Ga_{0.7}As/GaAs)^n$ , assuming sectionally



Fig. 2. The energy spectrum and the corresponding level densities  $\rho(E_{\mu,\nu})$  of the first three subbands of a GaAs(Al<sub>0.3</sub>Ga<sub>0.7</sub>As/GaAs)<sup>n</sup> superlattice, with a = 100 nm, b = 30 nm, and  $V_0 = 0.23$  eV. In the upper part, we show the resonant energies  $E_{\mu,\nu}^*$  for n = 14. In the lower part, the level density  $\rho(E_{\mu,\nu})$  for n = 7.70 is compared with the level density  $\rho(E)$  predicted by the Kronig–Penney model, which is reached only when the number of cells  $n \to \infty$ .

constant potential profile with GaAs layers of 10 nm, barrier height  $V_0 = 0.23$  eV and Al<sub>0.3</sub>Ga<sub>0.7</sub>As layers of 3 nm. In this case, the resonant energies are obtained from

$$\cos k_{\nu}a \cosh q_{\nu}b - \frac{k_{\nu}^2 - q_{\nu}^2}{2k_{\nu}q_{\nu}} \sin k_{\nu}a \sinh q_{\nu}b = \cos \frac{\nu\pi}{n}, \tag{5}$$

where  $k_{\nu}^2 = 2m_{\nu}^* E_{\mu,\nu}^* / \hbar^2$  and  $q_{\nu}^2 = 2m_b^* (V_0 - E_{\mu,\nu}^*) / \hbar^2$ . In the upper frame of Fig. 2 we show the resonant energies inside the first three conduction subbands for n = 14. In the lower frame we plot the subband level densities, for n = 7 and n = 70. As mentioned in Section 1, the continuous level density  $\rho(E)$  predicted by the familiar Kronig–Penney model [8] is reached only when the number of cells  $n \to \infty$  (see the lower part of Fig. 2).

For completeness, it is worth recalling that, in the transfer matrix approach, the allowed and forbidden continuous energy intervals are obtained from the well known Kramer's condition [29]

$$|\alpha_{\mathbf{R}}| \leqslant 1. \tag{6}$$

Let us now turn to the wave functions issue for open systems, in particular to deducing of exact formulas for the evaluation of resonant states. We shall start establishing the notation employed. As shown in Fig. 1, the coordinates  $z_j = jl_c$  (with j = 0, 1, 2, ..., n), define a lattice of points separated by multiples of  $l_c$ . If we are interested in evaluating functions at any point z in the (j + 1)th cell, it is useful to define the difference  $z_p = z - z_j = z'_o - z_o \leq l_c$ . Taking into account this

7

and the transfer matrix multiplicative property, it is easy to see that the transfer matrix  $M_z(z, z_o)$  relating the state vectors  $\Phi(z_o)$  and  $\Phi(z)$ , can be factorized either as

$$M_{z}(z, z_{o}) = M_{j}(z, z'_{o})M_{p}(z'_{o}, z_{o})$$
<sup>(7)</sup>

or, as

$$M_{z}(z, z_{o}) = M_{p}(z, z_{j})M_{j}(z_{j}, z_{o}).$$
(8)

Here  $M_j$  is the full *j*-cells transfer matrix

$$M_j = egin{pmatrix} lpha_j & eta_j \ eta_j^* & lpha_j^* \end{pmatrix} = M^j$$

with  $\alpha_j = U_j - \alpha^* U_{j-1}$ ,  $\beta_j = \beta U_{j-1}$ .  $M_p$  is a partial cell transfer matrix which, in general, we write as

$$M_p = egin{pmatrix} lpha_p & eta_p \ \gamma_p & \delta_p \end{pmatrix}.$$

Therefore, the state vector at any point z (inside the j + 1 cell) is obtained from

$$\Phi(z) = M_p M_j \begin{pmatrix} \vec{\varphi}(z_o) \\ \overleftarrow{\varphi}(z_o) \end{pmatrix} = M_j M_p \begin{pmatrix} \vec{\varphi}(z_o) \\ \overleftarrow{\varphi}(z_o) \end{pmatrix},\tag{9}$$

where  $\vec{\varphi}(z_o)$  and  $\overleftarrow{\varphi}(z_o)$  are the right and left propagating functions at  $z_o$ . Assuming incidence from only the left-hand side, we have

$$\stackrel{\leftarrow}{ \phi}(z_o) = -rac{eta_n^*}{lpha_n^*} \stackrel{
ightarrow}{ \phi}(z_o) = r_n \stackrel{
ightarrow}{ \phi}(z_o)$$

with  $\alpha_n$  and  $\beta_n$  being the whole *n*-cell system transfer matrix elements, and  $r_n$  the total reflection amplitude. Hence, the wave function is given by

$$\Psi(z,E) = \vec{\varphi}(z_o) \left[ \left( \alpha_j - \beta_j \frac{\beta_n^*}{\alpha_n^*} \right) (\alpha_p + \gamma_p) + \left( \beta_j^* - \alpha_j^* \frac{\beta_n^*}{\alpha_n^*} \right) (\beta_p + \delta_p) \right].$$
(10)

It is obvious that by evaluating this function at  $E^*_{\mu,\nu}$ , we get the desired vth resonant wave function in the  $\mu$ th subband, i.e.

$$\Psi_{\mu,\nu}^{*}(z) = \Psi(z, E_{\mu,\nu}^{*}).$$
(11)

In 1D periodic systems the resonant wave function  $\Psi_{\mu,\nu}^*(z)$  is a simple but not trivial combination of Chebyshev polynomials. It is easy to verify that Eq. (10) implies:

$$\begin{split} \Psi(z_n, E) &= \frac{1}{\alpha_n^*} \, \vec{\varphi}(z_o) = t_n \, \vec{\phi}(z_o) = \vec{\phi}(z_n), \\ \Psi(z_o, E) &= \left(1 - \frac{\beta_n^*}{\alpha_n^*}\right) \vec{\phi}(z_o) = (1 + r_n) \, \vec{\phi}(z_o) = \vec{\phi}(z_o) + \vec{\phi}(z_o) \end{split}$$



Fig. 3. Resonant wave functions at different points of the energy spectrum of the open superlattice GaAs(Al<sub>0.3</sub>Ga<sub>0.7</sub>As/GaAs)<sup>*n*</sup>. All squared wave-function amplitudes are plotted using arbitrary units. To get an idea of the relation between the eigenfunction amplitude and the energy, we plot in (A), using the same scale, the resonant functions  $|\Psi_{1,1}^*(z)|^2$  and  $|\Psi_{2,1}^*(z)|^2$  with different subband indices. (B and E) The resonant functions  $|\Psi_{2,2}^*(z)|^2$  and  $|\Psi_{3,4}^*(z)|^2$ , at  $E_{2,2}^* = 0.11761667862$  eV and  $E_{3,4}^* = 0.24557249944$  eV (first and last arrow), respectively. (C) The function evaluated at the arbitrary energy indicated by the second arrow. This function is partially transmitted and partially reflected. (D) We have a wave function *in* a gap, stationary in the left-hand side and exponentially decreasing inside the superlattice.

9

with  $t_n$  and  $r_n$  the *n*-cell transmission and reflection amplitudes, respectively. We plot in Fig. 3 several wave functions for the superlattice GaAs(Al<sub>0.3</sub>Ga<sub>0.7</sub>As/ GaAs)<sup>12</sup> mentioned before. In the upper part we have the spectrum of resonant energies and a sketch of the superlattice potential profile which, to visualize the regions where particles are piled up, is drawn in gray trace alongside the wave functions in the other frames. To get an insight of the relation between the eigenfunction amplitude and the energy, we plot in Fig. 3A (using the same vertical scale), the eigenfunctions  $|\Psi_{1,1}^*(z)|^2$  and  $|\Psi_{2,1}^*(z)|^2$  for different subband-index  $\mu$ . It is evident from this figure that as the energy (and the subband index  $\mu$ ) increases, the wave function amplitude gets smaller. To see the wave functions at qualitatively different energy values, we plot the wave functions shown in Figs. 3B-E for the energies indicated with arrows in the upper frame. The first and last arrow point to resonant energies, the second indicates an arbitrary point inside the second subband, and the third arrow any point in a gap. At these points the transmission coefficients take different values. While for the wave functions shown in Figs. 3B and E, the transmission coefficient is 1, in Figs. 3C and D it is 0.2419 and  $1.7284 \times 10^{-9}$ , respectively.

In Figs. 3A, B, and D, we have the resonant functions:  $|\Psi_{\mu,1}^*(z)|^2$ ;  $|\Psi_{2,2}^*(z)|^2$ and  $|\Psi_{3,4}^*(z)|^2$ . It is evident that these functions are remarkably modulated by an oscillating envelope function with v - 1 minima, in the inner part, plus two minima at the superlattice surface, i.e., at  $z_o = 0$  and  $z_n = nl_c$ . It is worth noticing their space and intraband symmetries. We will comment more on these symmetries below. Notice also that, as mentioned in Section 1, none of these functions fulfills the periodicity relation  $|\Psi_{\mu,v}(z + l_c)|^2 = |\Psi_{\mu,v}(z)|^2$ . Furthermore, the resonant states are extended wave functions with particle density different from zero throughout and at the ends of the system. This will not be the case, of course, for bounded systems.

The wave function  $|\Psi_2(z, E)|^2$ , at E = 0.125 eV, compared with the resonant functions in Figs. 3A, B, and E, looks rather irregular with a complicated behavior along the superlattice. As can be seen in Fig. 3C,  $\Psi_2(z, E)$  is a partially transmitted and partially reflected extended wave function.

In Fig. 3D we plot the gap function  $|\Psi_g(z, E)|^2$  for E = 0.16 eV, which lies in the gap between the second and the third subbands. The behavior of this wave function agrees with the vanishing of the transmission coefficient, and makes evident an interesting localization effect induced by phase coherence, as was in some sense insinuated by Kohn [7]. This is a very suggesting result that deserves further analysis.

# 3. Energy eigenvalues and eigenfunctions for bounded systems

An important extension of the scattering approach is accomplished when the transfer matrix method is applied to study stationary properties of bounded periodic systems. For this type of problems we will obtain general expressions for the evaluation of their eigenvalues and eigenfunctions, i.e., formulas that will be valid independent of the specific single-cell potential parameters. We shall also discuss some specific examples.

If we have a periodic system with exactly *n*-cells between  $z = z_o^+$  and  $z = z_n^-$ , the state vectors at these points are related by

$$\begin{pmatrix} \vec{\varphi}(z_n^-) \\ \overleftarrow{\varphi}(z_n^-) \end{pmatrix} = \begin{pmatrix} \alpha_n & \beta_n \\ \beta_n^* & \alpha_n^* \end{pmatrix} \begin{pmatrix} \vec{\varphi}(z_o^+) \\ \overleftarrow{\varphi}(z_o^+) \end{pmatrix},$$
(12)

where [28]:

 $\alpha_n=p_n-\alpha p_{n-1},$ 

 $\beta_n = \beta p_{n-1},$ 

are, in the general case of N propagating modes,  $N \times N$  matrices. The vanishing of the wave functions

$$\psi(z_o) = \sum_{i=1}^N ( ec{\phi_i}(z_o) + ec{\phi_i}(z_o))$$

and

$$\psi(z_n) = \sum_{i,j=1}^{N} [(\alpha_n + \beta_n^*)_{i,j} \vec{\varphi_j}(z_o) + (\beta_n + \alpha_n^*)_{i,j} \vec{\varphi_j}(z_o)],$$

required by the boundary conditions, leads straightforwardly to the implicit eigenvalues equation

$$\alpha_n - \alpha_n^* + \beta_n^* - \beta_n = 0. \tag{13}$$

In the 1D one-mode approximation (where  $\alpha_n = U_n - \alpha^* U_{n-1}$  and  $\beta_n = \beta U_{n-1}$ ), this matrix equation takes the simpler form

$$U_{n-1}(\alpha_{\rm I} - \beta_{\rm I}) = 0. \tag{14}$$

Here the subscript I refers to the imaginary part. This is another of our main results. A number n - 1 of the energy eigenvalues, in each subband of the bounded system [29], constitute the zeros of the Chebyshev polynomial  $U_{n-1}$ , the other two eigenvalues come from the factor ( $\alpha_I - \beta_I$ ). This is a non-trivial result; it leads to recognize the remarkable *surface level-repulsion effect* (SLRE), responsible of the well-known Tamm and Shockley states. The hard walls push upwards two of the n + 1 energy levels of each subband. As is also well-known and will be seen below, these are localized surface wave functions. To illustrate this effect with an specific example, we consider the superlattice ((GaAs)<sup>1/2</sup>Al<sub>0.3</sub>Ga<sub>0.7</sub>As(GaAs)<sup>1/2</sup>)<sup>12</sup> bounded by infinite hard walls. In the upper part of Fig. 4, we plot its electron energy spectrum in the effective mass approximation. The large arrows indicate the two (almost degenerate) energy levels pushed out from each energy subband. The fourth arrow, at 0.16815 eV, indicates the position of two levels driven out from the second subband. Focusing at this point, we find out that these levels are separated from each other by approximately 0.6  $\mu$ eV.

Before discussing the bounded system eigenfunctions, let us see what happens with the energy eigenvalues and the energy spectrum when the thickness of the



Fig. 4. Energy eigenvalues and eigenfunctions  $|\Psi_{\mu,\nu}^{b}(z)|^{2}$  for a system bounded by infinite hard walls as in Fig. 1B, but of length  $L = nl_{c}$ . The potential parameters are the same as in Fig. 2. The larger arrows, around 0.1681 and 0.364 eV, indicate the quasi-degenerated energy levels pushed up by the surface hard walls. The small arrows indicate the energy eigenvalues  $E_{2,2}$  and  $E_{2,3}$ , whose eigenfunctions are plotted in (A and B). It is interesting to compare these functions with the corresponding ones in Fig. 5, where the system length is  $L = nl_{c} + a$ .

quantum wells, at the ends of the superlattice, are slightly modified. Suppose that we have a system of length  $nl_c + a$  instead of  $nl_c$ , which we can obtain by adding, for example, two layers of thickness a/2 at the ends of the *n*-cell superlattice. The implicit equations is then slightly modified and, instead of equation (13), we now have

$$(\alpha_n \mathbf{e}^{\mathbf{i}ka} - \alpha_n^* \mathbf{e}^{-\mathbf{i}ka}) + \beta_n^* - \beta_n = 0 \tag{15}$$

and instead of (14), we have

$$U_n \sin ka + (\alpha_{\rm I} \cos ka - \alpha_{\rm R} \sin ka - \beta_{\rm I}) U_{n-1} = 0.$$
<sup>(16)</sup>

In the upper part of Fig. 5, we plot the energy spectrum for the superlattice  $GaAs(Al_{0.3}Ga_{0.7}As/GaAs)^{12}$ , whose length is  $L = nl_c + a$ . Whereas the energy spectra of this and the *n*-cell system are quite similar (see the upper parts of Figs. 4 and 5), their eigenfunctions present some differences, which we will discuss now.

Once the energy eigenvalues are known, it is easy to obtain the corresponding eigenfunctions. As for open systems, we start by finding the wave function at any point z in the (j + 1)th cell, with j = 0, 1, 2, ..., n - 1. Using the transfer matrix properties and the boundary conditions we easily obtain, for a system of length  $L = nl_c$ , the wave function

$$\Psi^{b}(z,E) = A \left[ (\alpha_{p} + \gamma_{p}) \left( \alpha_{j} - \beta_{j} \frac{\alpha_{n} + \beta_{n}^{*}}{\alpha_{n}^{*} + \beta_{n}} \right) + (\beta_{p} + \delta_{p}) \left( \beta_{j}^{*} - \alpha_{j} \frac{\alpha_{n} + \beta_{n}^{*}}{\alpha_{n}^{*} + \beta_{n}} \right) \right].$$
(17)



Fig. 5. Energy eigenvalues and eigenfunctions  $|\Psi_{\mu,\nu}^{b}(z)|^{2}$  for a system of length  $L = nl_{c} + a$  bounded by infinite hard walls like in Fig. 1B. The small arrows indicate the energy eigenvalues  $E_{2,2}$  and  $E_{2,3}$ , whose eigenfunctions are plotted in (A and B). The larger arrows indicate the energy levels pushed up by the *surface repulsion effect*. The corresponding eigenfunctions of these levels  $|\Psi_{2,12}^{b}(z)|^{2}$  and  $|\Psi_{2,13}^{b}(z)|^{2}$ , concentrate the particles near the surface and the high symmetry characteristic of the other eigenfunctions is broken. *None of these functions is periodic in the Bloch sense*  $|\Psi_{\mu,\nu}(z + l_{c})|^{2} = |\Psi_{\mu,\nu}(z)|^{2}$ .

Here A is a normalization constant. Evaluating this function at  $E = E_{\mu,\nu}$ , we obtain the corresponding eigenfunction

$$\Psi^b_{\mu,\nu}(z) = \Psi^b(z, E_{\mu,\nu}).$$

This is a rigorous solution of the Schrödinger equation for 1D finite periodic systems, bounded by infinite hard walls. In the particular case of a superlattice with length  $nl_c + a$ , the wave function gets an overall factor  $e^{ika/2}$ , and the phase  $(\alpha_n + \beta_n^*)/(\beta_n + \alpha_n^*)$  is replaced by  $(\alpha_n + \beta_n^* e^{-ika})/(\beta_n + \alpha_n^* e^{-ika})$ . This phase has the

P. Pereyra / Annals of Physics 320 (2005) 1-20



Fig. 6. Eigenfunctions  $|\Psi_{\mu,v}^{b}(z)|^{2}$  in the *first* subband of a GaAs(Al<sub>0.3</sub>Ga<sub>0.7</sub>As/GaAs)<sup>n</sup> superlattice, with n = 12 and the potential parameters as in Fig. 2. The eigenfunctions in this column, exhibit remarkable spatial and intraband symmetry. The spatial parity symmetry has the center of the periodic system as a symmetry point. Looking at the whole set of eigenfunctions in a band, the intra band symmetry is quite apparent. The first and the upmost eigenfunctions have similar envelope shapes, the same happens with the second and the last but one eigenfunctions, and so on. This symmetry has a symmetry point in the middle of the band.



Fig. 7. Eigenfunctions  $|\Psi_{\mu,\nu}^{b}(z)|^{2}$  in the *second* subband of a GaAs(Al<sub>0.3</sub>Ga<sub>0.7</sub>As/GaAs)<sup>n</sup> superlattice, with n = 12. Comparing with the eigenfunctions in Fig. 6, we notice that the oscillation frequency in the second subband is twice the frequency of the first subband. In general, the oscillations frequency in the  $\mu$ th subband is  $\mu$  times the frequency of the first subband. However, the envelope functions for the same excitation level  $\nu$  are equal and independent of  $\mu$ .

interesting effect of shifting the maxima of the envelope functions by  $\pi/2$ . In Fig. 5, we plot the same eigenfunctions  $|\Psi_{2,2}^b(z)|^2$ ,  $|\Psi_{2,3}^b(z)|^2$  as in Fig. 4, plus the wave functions  $|\Psi_{2,12}^b(z)|^2$ ,  $|\Psi_{2,13}^b(z)|^2$  corresponding to the energy levels pushed upwards because of the SLRE. While the envelope functions of the *n*-cell system of length  $L = nl_c + a$  have a *sine*-like shape (see Figs. 5A and B), the envelope functions of the system of length  $L = nl_c$  are *cosine*-like (see Figs. 4A and B). It is interesting to notice that the eigenfunctions  $\Psi_{2,12}^b(z)$ ,  $\Psi_{2,13}^b(z)$  describe particles localized at the ends of the superlattice. These are explicit realizations of Tamm and Shockley's surface wave functions, which up to now were calculated only in an approximate fashion.

In order to expose similarities and symmetries of the superlattice eigenfunctions, we plot in Figs. 6 and 7 two comparable sets of eigenfunctions for: the first and second subbands, respectively. In each band of a bounded periodic system we have finally n-1 energy levels, excluding the two levels displaced upwards by the surface repulsion. We show on each of these graphs the eigenfunctions for: the first two, three intermediate and the last two subband levels. We show also in these figures, in gray a sketch of the superlattice potential profile. The envelope of the wave functions with the same index v, in Figs. 6 and 7, is similar. Comparing both sets of eigenfunctions, we notice that each oscillation in the first subband gets splitted in the second and so on, as we go to higher energy subbands. Looking at the eigenfunctions of a given subband, a surprising intraband symmetry, with respect to the subband center, can be observed. Accordingly  $\Psi^b_{\mu,\nu}(z) \simeq \Psi^b_{\mu,(n-\nu)}(z)$ . As is well known, the most important difference between a periodic potential and a constant potential both flanked by infinite hard walls, is the presence (in the periodic potential case) or absence (in the infinite well case) of phase interference effect responsible for the energy levels splitting, that leads to the band structure.

It is important to remark again that none of the bounded eigenfunctions fulfill the periodicity relation  $|\Psi_{\mu,\nu}^{b}(z+l_{c})|^{2} = |\Psi_{\mu,\nu}^{b}(z)|^{2}$ . For Bloch functions confined within an infinite square well, Ren [47] reached recently a similar conclusion.

#### 4. Energy eigenvalues and eigenfunctions for quasi-bounded systems

Another and more realistic type of bounded periodic systems are the *n*-cell superlattices confined by cladding layers with finite potential walls. A potential profile of this type is shown in Fig. 1C) and in the upper part of Fig. 8. Assuming  $E < V_w$  and a superlattice of length  $nl_c$  (i.e., a finite periodic system with exactly *n* cells between the two walls of finite height at  $z_o$  and  $z_n$ ), and performing a simple calculation, we can deduce the following general implicit eigenvalues equation:

$$h_w U_n + f_w U_{n-1} = 0 (18)$$

with

$$h_w = 1 \tag{19}$$

and



Fig. 8. Quasi-bounded eigenfunctions  $|\Psi_{\mu\nu}^{ab}(z)|^2$  in the *second* subband of a GaAs(Al<sub>0.3</sub>Ga<sub>0.7</sub>As/GaAs)<sup>n</sup> superlattice, with AlAs cladding layers and n = 12. These functions are rather similar to the corresponding functions in Figs. 5 and 7. For the confining potential height  $V_w$  equal to 0.44 eV, indicated in the superlattice sketch, the repulsion effect is weak and the effect slightly visible.

$$f_{w} = \alpha_{\rm I} \frac{q_{w}^2 - k^2}{2q_{w}k} - \alpha_{\rm R} - \beta_{\rm I} \frac{q_{w}^2 + k^2}{2q_{w}k}.$$
 (20)

Here  $q_w^2 = 2m(V_w - E)/\hbar^2$  and k is the wave vector at  $z_o^+$ , and  $z_n^-$ ,  $\alpha_R$  and  $\alpha_I$  are the real and imaginary parts of the single-cell transfer matrix element  $\alpha$ .

For a system of length  $nl_c + a$ , like the superlattice in Fig. 8, the coefficients in Eq. (18) become

$$h_w = \frac{q_w^2 - k^2}{2q_w k} \sin ka + \cos ka$$
(21)

and

$$f_{w} = \frac{q_{w}^{2} - k^{2}}{2q_{w}k} (\alpha_{\rm I} \cos ka - \alpha_{\rm R} \sin ka) - \alpha_{\rm R} \cos ka - \alpha_{\rm I} \sin ka - \beta_{\rm I} \frac{q_{w}^{2} + k^{2}}{2q_{w}k}.$$
 (22)

To illustrate these formulas we consider again the AlAs/GaAs(Al<sub>0.3</sub>Ga<sub>0.7</sub>As/GaAs)<sup>12</sup>/AlAs heterostructure, and plot in Fig. 8 its energy spectra and several eigenfunctions in the lower bands. For this system the superlattice confining potential is  $V_w = 0.44$  eV. The surface repulsion effect is in this case negligible. Therefore, each subband contains n + 1 energy levels, which correspond to the same number of wells between the *AlAs* cladding layers. We shall see below that the uppermost two levels of each band become closer to each other and separate from the others as the confining potential  $V_w$  grows.

Quite similar structures are used in the active region of laser devices. Even though the real systems are not as precise and perfect as the theoretical model might be, the main qualitative and quantitative features of photoluminescence experiments are correctly accounted for when the energy spectra (for the valence and conduction subbands) is calculated by using the transcendental eigenvalue equation and the corresponding eigenfunctions (see [32]). Eigenfunctions of quasi-bounded 1D periodic systems can be obtained following the same procedure explained for open and bounded systems. Using the transfer matrices introduced in previous sections, it is easy to show that the wave function, at any point z in the j + 1 cell, is given by

$$\Psi^{qb}(z,E) = \frac{A}{g_n} \left\{ \left[ (\alpha_p + \gamma_p)\alpha_j + (\beta_p + \delta_p)\beta_j^* \right] \left( 1 - i\frac{q_w}{k} \right) + \left[ (\alpha_p + \gamma_p)\beta_j + (\beta_p + \delta_p)\alpha_j^* \right] \left( 1 + i\frac{q_w}{k} \right) \right\}.$$
(23)

Here A is a normalization constant and

$$g_{n} = \alpha_{nI} \frac{q_{w}^{2} + k^{2}}{2q_{w}k} - \beta_{nI} \frac{q_{w}^{2} - k^{2}}{2q_{w}k} - \beta_{nR}$$

with  $\alpha_{nI} = \alpha_n - \alpha_n^*$ ,  $\beta_{nr} = \beta_n + \beta_n^*$  and  $\beta_{nI} = \beta_n - \beta_n^*$ . Again, evaluating the wave function at  $E = E_{\mu,\nu}$ , we obtain the corresponding eigenfunction

$$\Psi^{qb}_{\mu,\nu}(z) = \Psi^{qb}(z, E_{\mu,\nu}).$$
(24)

With this formula we complete the set of rigorous solutions of the Schrödinger or Maxwell equations for 1D finite periodic systems with different boundary conditions. In Fig. 8, we plot the eigenfunctions  $\Psi_{2,5}^{qb}(z)$ ,  $\Psi_{2,12}^{qb}(z)$ , and  $\Psi_{2,13}^{qb}(z)$  that should be compared with those in Figs. 7 and 5. The eigenfunction  $\Psi_{2,5}^{qb}(z)$  looks rather similar to  $\Psi_{2,5}^{b}(z)$  in Fig. 7C). In Figs. 8B and C) the surface functions start to build on. Although imperceptibly, the wave functions decrease exponentially inside the potential walls. As in the previous figures, two main characteristics can be distinguished: (i) a remarkable symmetry with respect to the center of the superlattice and (ii) rapid

17

oscillations modulated by envelope functions, symmetric with respect to the middle of the subband. We have plotted here three egienfunctions for the indicated energy values in the second subband.

The eigenfunctions  $\Psi_{\mu,\nu}^{qb}(z)$  are useful and must be used for precise calculations of phototransition probabilities. Recently, we have successfully applied this formula to calculate photoluminiscence (PL) in the active region of blue emitting devices, and an extremely good agreement with the PL results obtained by Nakamura et al. is found [25]. We believe that most of the formulas reported here can be useful to describe and to design new optoelectronic devices.

To conclude this work, we shall refer to the interesting surface repulsion effect (the Tamm and Shockley states), manifest in the nicely factorized structure of the eigenvalue equation (14), and clearly observed in the energy spectra of Figs. 4 and 5. As mentioned before, the separation of the repelled energy levels, from the residual bands or subbands, increases as the potential height at the surface grows up. To visualize this property we plot in Fig. 9 the energy spectra of periodic systems which only differ on the confining potential height  $V_w$ . In the sequence energy-spectra shown there, we can clearly follow the displacement of the two uppermost levels of each subband, towards the gaps. Notice also that, while these levels move away from the band, they approach each other. A deficient eigenvalue equation cannot split



Fig. 9. The surface repulsion effect. Increasing the confining potential  $V_w$  two levels of each subband are pushed up. We show here the spectrum of the second and third subbands. The two repelled energy levels move inside the gaps and become closer as  $V_w$  increases.

these energy levels. They are present in the band structure of all bounded crystalline systems: metals, semi-metals and semiconductors. It is possible that they are hidden or mixed up with impurity levels. At any rate they deserve further attention.

## 5. Conclusions

In this paper several new, simple, and general formulas for the exact evaluation of fundamental quantities like the resonant energies, resonant states, energy eigenvalues and eigenfunctions of finite 1D periodic systems, with arbitrary single-cell potential shape, and distinct boundary conditions have been presented. With these formulas one can completely resolve the fine structure in bands and subbands and calculate numerous physical quantities. Plotting the wave functions for specific and illustrative examples, we exhibit conclusively that the widely accepted Bloch function property  $|\Psi(z + l_c)|^2 = |\Psi(z)|^2$ , correct for infinite periodic systems, is erroneous and inaccurate for finite size systems. All resonant states and eigenfunctions posses well defined parity symmetries and interesting intraband symmetry perceptible in the shape of envelope wave functions. Because of this symmetry the envelope of  $\Psi^b_{\mu,\nu}(z)$  resembles the envelope of  $\Psi^b_{\mu,\nu}(z)$ . The well known surface functions come across and manifest themselves in the nicely factorized structure of the eigenvalues equation (14), clearly observed in the energy spectra of Figs. 4, 5, and 9.

#### Acknowledgments

I acknowledge Project 29026-E from CONACyT, Mexico and the Abdus Salam ICTP, Trieste, Italy. I benefited from comments and discussions with H. Simanjuntak, A. Kunold, J. Grabinsky, and A. Robledo.

# References

- [1] In some cases, analytical methods are known to obtain exact single-cell transfer matrices. In general, there is a number of methods to obtain analytically (in a rather good approximation) or numerically single-cell transfer matrices.
- [2] H.M. James, Phys. Rev. 76 (1949) 1602.
- [3] F. Bloch, Z. Physik 52 (1928) 555.
- [4] E.L. Ivchenko, G.E. Pikus, in: Superlattices and other Heterostructures, Symmetry and Optical PhenomenaSpringer Ser. Solid-State Sci., vol. 110, Springer, Heidelberg, 1997.
- [5] W. Ledermann, Proc. Roy. Soc. Ser. A 182 (1944) 362.
- [6] M. Born, Atomtheorie des festen Zustandes Encykl. Math. Wiss. 25 (5) (1921) 532;
   M. Born, Proc. Roy. Soc. Ser. A 180 (1942) 397;
  - M. Born, W. Ledermann, Nat. Lond. 151 (1943) 197.
- [7] W. Kohn, Phys. Rev. 115 (1959) 809.
- [8] R.de.L. Kronig, W.G. Penney, Proc. Roy. Soc. (London) A 130 (1931) 499.
- [9] C. Kittel, Introduction to Solid State Physics, fifth ed., Wiley, New York, 1976.
- [10] O. Maddelung, in: Introduction to Solid State TheorySpringer Ser. Solid-State Sci., vol. 2, Springer, Heidelberg, 1981.

- [11] P.Y. Yu, M. Cardona, Fundamentals of Semiconductors, Springer, Heidelberg, 1996.
- [12] V. Mitin, V.A. Kochelap, M.A. Strocio, Quantum Heterostructures, Cambridge University Press, New York, 1999.
- [13] G. Bastard, Acta Electron. 25 (1993) 147.
- [14] L.L. Chang, L. Esaki, R. Tsu, Appl. Phys. Lett. 24 (1974) 593.
- [15] E.E. Mendez, W.I. Wang, B. Ricco, L. Esaki, App. Phys. Lett. 47 (1985) 415.
- [16] L.F. Luo, R. Beresford, W.I. Wang, Appl. Phys. Lett. 55 (1989) 2023;
   E.E. Mendez, H. Ohmo, L. Esaki, W.I. Wang, Phys. Rev. B. 43 (1991) 5196.
- [17] H. Kroemer, in: Proceedings of the Second International Conference on Modulated Semiconductor Structures, Kyoto, 1985, Surf. Sci 174 (1989) 299;
  B. Deveaud, J.Y. Emery, A. Chomette, B. Lambert, M. Baudet, Superlattices Microstruct. 1 (1985) 205.
- [18] Shuji Nakamura, Masayuki Senoh, Shin-ichi Nagahama, Naruhito Iwasa, Takao Yamada, Toshio Matsushita, Hiroyuki Kiyoku, Yasunobu Sugimoto, Jpn. J. Apl. Phys. 35 (1996) L217; Yukio Narukawa, Yoichi Kawakami, Shizuo Fujita, Shigeo Fujita, Shuji Nakamura, Phys. Rev. B 55 (1997) R1938.
- [19] F.A. Ponce, D.P. Bour, Nature 386 (1997) 351.
- [20] J.M. Luttinger, Philips Res. Rep. 6 (1951) 303.
- [21] R.L. Agacy, R.E. Borland, Proc. Phys. Soc. 84 (1964) 1017.
- [22] B. Ricco, M.Ya. Azbel, Phys. rev. B 29 (1984) 1970.
- [23] R. Pérez-Alvarez, H. Rodriguez-Coppola, Phy. Stat. Sol. (b) 145 (1988) 493.
- [24] T.H. Kolatas, A.R. Lee, Eur. J. Phys. 12 (1991) 275.
- [25] D.J. Griffiths, N.F. Taussing, Am. J. Phys. 60 (1992) 883.
- [26] D.W. Sprung, H. Wu, J. Martorell, Am. J. Phys. 61 (1993) 1118.
- [27] M.G. Rozman, P. Reineker, R. Tehver, Phys. Lett. A 187 (1994) 127.
- [28] P. Pereyra, Phys. Rev. Lett 80 (1998) 2677;
   P. Pereyra, J. Phys. A 31 (1998) 4521.
- [29] P. Pereyra, E. Castillo, Phys. Rev. B 65 (2002) 205120.
- [30] D.J. Griffiths, C.A. Steinke, Am. J. Phys. 69 (2001) 137.
- [31] D.W.L. Sprung, P. Jagiello, J.D. Sigetich, J. Martorel. Phys. Rev. B 67 (2003) 085318.
- [32] A. Kunold, P. Pereyra, J. Appl. Phys. 93 (2003) 5018.
- [33] P. Pereyra. Available from: <cond-mat/0009064>; IC/2000/124, ICTP, Trieste, Italy.
- [34] I. Tamm, Z. Physik 76 (1932) 849.
- [35] R.H. Fowler, Proc. Roy. Soc. A 141 (1933) 56.
- [36] W. Shockley, Phys. Rev. 56 (1939) 317.
- [37] J. Bardeen, Phys. Rev. 71 (1947) 717.
- [38] W.E. Meyerhof, Phys. Rev. 71 (1947) 727.
- [39] W. Shockley, G. Pearson, Phys. Rev. 74 (1948) 232.
- [40] K. Artmann, Z. Physik 131 (1952) 244.
- [41] T.A. Hoffmann, Acta Phys. Acad. Sci. Hung. 2 (1952) 195.
- [42] B.A. Lippmann, Ann. Phys. 2 (1957) 16.
- [43] J. Kouteck, Phys. Rev. 108 (1957) 13;
  - J. Kouteck, Tomsěk, Phys. Rev. 120 (1960) 1212.
- [44] S.G. Davison, J.D. Levine, Solid State Physics Suppl. 3, Academic Press, New York, 1971.
- [45] A.W. Maue, Z. Physik 94 (1935) 717.
- [46] M. Stęślicka et al., Surf. Sci. Rep. 47 (2002) 93.
- [47] Y. Ren, Phys. Rev. B 64 (2001) 035322.