Why the effective-mass approximation works so well for nano-structures

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Abstract – The reason why the effective-mass approximation, derived using wave functions of infinite periodic systems, works so well with nanoscopic structures, has been an enigma and a challenge for theorists. To explain this issue, we first show that the essential “only-one-band” and “band-edge” assumptions that are behind the standard derivation of the effective mass approximation are better justified for nano-structures. We show then that the effective-mass approximation can also be derived using, instead of Bloch-type wave functions, the eigenfunctions and eigenvalues obtained in the theory of finite periodic systems, where the finiteness of the number of primitive cells in nanoscopic layers is a prerequisite and a crucial condition. We also show, with specific calculations of the optical response, that the rapidly varying eigenfunctions \( \Phi_{\epsilon_0,0}(z) \) of the one-band wave functions \( \Psi_{\epsilon_0,0}(z) = \Psi_{\mu,\nu}(z)\Phi_{\epsilon_0,0}(z) \), can be safely dropped out for the calculation of inter-band transition matrix elements.

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Introduction. – The effective-mass approximation (EMA) is, without a doubt, the most recurrent and widely used approximation in theoretical calculations involving semiconductor structures. The formal justification of why this approximation, derived using wave packets constructed in terms of wave functions of infinite periodic systems [1–7], works so well for finite micro- and nano-structures, has been an enigma and a challenge for theorists. Despite the various guises of the EMA, the correct explanation remained open. Along with the success of this approximation, the boundary condition problem, in heterostructures, and the breaking of validity conditions, such as the weak perturbation potential, the band parabolicity, the quantum confinement and mixing effects, among others, led to introduce multiband kp models [8,9], new formulations of the envelope-function equations [10,11], multiband effective-mass Hamiltonians and nonlinear response theories [12]. These and many other models, not mentioned here because of the lack of space, rely on the wave functions of infinite periodic systems.

The origin of the boundary condition problem has been the lack of explicit knowledge of the wave functions \( u_{l,k_0}(r) \) used to expand the heterostructure (HS) wave functions. Assuming identical or different unknown function \( u_{l,k_0}(r) \) in the HS layers, has, at the end, no meaning. The first contradiction emerges immediately because these functions are defined from \(-\infty\) to \(+\infty\). Now that the theory of finite periodic systems (TFPS) has evolved and shown its ability to obtain, bona fide, energy eigenvalues and eigenfunctions of finite periodic structures with a finite number of unit cells [13–21], we are in a better condition to justify or criticize the assumptions made in deriving the effective-mass approximation and to understand why it works so well. The wave functions \( \Psi(z,E) \) derived from the TFPS, depend strongly on the energy \( E \). As can be seen in refs. [21] they become eigenfunctions \( \Psi_{\mu,\nu}(z) \), when the energy is an eigenvalue \( E_{\mu,\nu} \), and localized (and exponentially decaying) functions when \( E \neq E_{\mu,\nu} \). We will show below that the boundary condition problem vanishes. It is then worth reviewing and re-deriving the EMA from an alternative point of view, using, instead of the practically unknown Bloch-type functions, the eigenfunctions and envelope functions obtained within the TFPS. Our purpose is to show that the main assumptions used in the standard derivation of the EMA are compatible and better justified when the layers widths become of the order of a few atomic layers and to re-derive the EMA taking into account the finiteness of the number of primitive cells.
account the finiteness of the HS layers as a fundamental requisite.

Superlattices (SLs) and layered structures are characterized by the simultaneous presence of two length scales: the primitive unit cells size of the semiconductor hosts, and the superlattice or heterostructure layers widths. This important difference between the primitive cells, which are of the order of 0.5 nm, and the layer widths, of the order of 5 nm, is behind the possibility to express the HS wave function as the product of rapid and slowly varying functions. The finiteness of the number of primitive cells \( n_X \) (in layer \( X \)) and the number of layers \( n_S \) (in the heterostructure) are important characteristics in the TFPS.

**Finiteness of periodic layers. An outline of the TFPS.** Soon after the semiconductor SLs were introduced [22,23], and the subband (or miniband) structures of direct and indirect band gap semiconductors were experimentally and theoretically confirmed [24–31], Leo Esaki noticed that whereas in reality SLs contain a finite number of layers, with a finite number of atomic cells each, the standard theoretical approaches tacitly assume that SLs are **infinite-periodic structures** with alternating layers containing also an infinite number of atomic cells [32]. In fact, the HS and SL wave functions are generally [2,3,33–38] written as \( \psi(r) = \sum u_n(r) f_I(r) \), with \( u_n(r) \) the periodic part of the host-semiconductor Bloch’s function at band \( n \), and \( f_I(r) \propto \exp[i\mathbf{k}_\perp \cdot \mathbf{r}_\perp] \chi_I(z) \) the envelope wave function, with \( \mathbf{k}_\perp = k_x + k_y \) the perpendicular wave number assumed, generally, a constant of motion [30]. At the end, it is common to assume that \( \psi(r) \) is set up only of one band, evaluated at the center of the Brillouin zone or at the subband edge \( k = 0 \). For SLs the envelope function is, again, written in terms of Bloch-type functions \( \chi_I(z) = \exp[iqz]u_I(z) \), characterized by a subband index \( \mu \) and a continuous wave number \( q \) that is then artificially discretized, via the cyclic boundary condition.

On the other side, the TFPS has grown, and has been generalized to include periodic structures with arbitrary potential profiles, arbitrary but finite number of unit cells \( n \) and arbitrary but finite number of propagating modes \( N \) for open, bounded and quasi-bounded periodic structures [19–21]. The TFPS is based on the transfer matrix properties and the rigorous fulfillment of continuity conditions, that make possible to express the \( n \)-cells transfer matrix \( M_n \) as \( M^n \), where \( M \) is the \( 2N \times 2N \) single-cell transfer matrix, which for time reversal invariant systems has the structure

\[
M(z_{i+1}, z_i) = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix},
\]

The accurate calculation of this matrix is crucial in this approach. In the single mode approximation, of interest here, it is easy to show that the \( n \)-cell transfer matrix elements, \( \alpha_n \) and \( \beta_n \), are given by

\[
\alpha_n = U_n - \alpha^* U_{n-1} \quad \text{and} \quad \beta_n = \beta U_{n-1},
\]

where \( U_n \) is the Chebyshev polynomial of the second kind of order \( n \), evaluated at the real part of \( \alpha = \alpha_R + i\alpha_I \). The eigenvalues of any quasi-bounded (qb) periodic system defined between \( z_L \) and \( z_R \), see fig. 1, with \( z_0 = z_L - z_n = d/2 \), are determined from

\[
\text{Re}(\alpha_n e^{i k d}) = -\frac{k^2 - q_n^2}{2q_n k} \text{Im}(\alpha_n e^{i k d}) = \frac{k^2 + q_n^2}{2q_n k} \beta_n = 0. \quad (3)
\]

\( q_n \) and \( k \) are the wave numbers at the left (right) and right (left) of the discontinuity point \( z_L \) (\( z_R \)) and \( \beta_n \) the imaginary part of \( \beta_n \). The eigenfunctions of the quasi-bounded superlattice are given by

\[
\Psi_{\mu,\nu} (z) = a_\mu e^{i k d/2} \left[ \left( (\alpha_p + \gamma_p) \alpha_j + (\beta_p + \delta_p) \beta_j^* \right) (k - i q_w) \right.
\]

\[
+ \left( (\alpha_p + \gamma_p) \beta_j + (\beta_p + \delta_p) \alpha_j^* \right) e^{-i k d(k + i q_w)} \left]_{E=E_{\nu,\nu}}, \quad (4)
\]

with \( a_\mu \) a normalization constant and \( z \) any point in the \( j + 1 \) cell. \( \alpha_j \), \( \beta_j \), ... are matrix elements of the transfer matrix \( M_j(z_j, z_0) \) that connects the state vectors at points separated by exactly \( j \) unit cells. \( \alpha_p \), \( \beta_p \), ... , where \( p \) stands for part of a unit cell, are the matrix elements of the transfer matrix \( M_p(z, z_j) \) that connects the state vectors at \( z_j \) and \( z \), for \( z_j \leq z \leq z_{j+1} \).

Our purpose here is to derive the effective mass approximation for the Schrödinger equation of a layered semiconductor heterostructure \( AB/C/\ldots \), using the eigenvalues and eigenfunctions obtained in the TFPS. We will assume, without loss of generality, that our system is a binary structure \( AB/A/\ldots B/A \), where the periodic semiconductor layers \( A = (a_A)^n \) and \( B = (b_B)^n \) contain \( n_A \) unit cells \( a_A \) and \( n_B \) unit cells \( b_B \) in the growing direction \( z \), respectively. We will show that the effective-mass approximation (EMA) can be derived when the heterostructure wave function \( \psi(z) \) is written as the product of the fast-varying function \( \Phi_{\alpha, \omega_0}(z) \), that could in principle be obtained from the TFPS, and the envelope function \( \Psi_{\mu, \nu}(z) \) evaluated, both, at the band-edges defined by the energy band index \( \omega_0 \) and the intra-band (or wave number) index \( \omega_0 \). In the particular case of periodic heterostructures, i.e., of SLs \((AB)^n = ((a_A)^n (b_B)^n)^n \), the envelope functions are straightforwardly obtained in

![Fig. 1: Parameters of a quasi-bounded superlattice whose unit cell has an arbitrary potential shape. The wave function in eq. (4) is defined at any point \( z \) of the \( j + 1 \) cell, with \( 0 \leq j \leq (n-1) \).](27003-p2)
the EMA and the TFPS. It is worth emphasizing that since the transfer matrices are the matrix representation of the continuity and boundary conditions and comprise the whole information on the phase evolution of the quantum states, the fast-varying and envelope wave functions, obtained in the TFPS, fulfill the continuity and boundary conditions. We will show also, for a specific example, that the optical response calculated with the matrix elements \((\Psi_{\mu'}^{0}|H_{\text{int}}|\Psi_{\mu}^{0})\) is practically the same as the optical response obtained with the matrix elements \((\Psi_{\mu',\nu'}^{0}|H_{\text{int}}|\Psi_{\mu,\nu}^{0})\), were the fast-varying wave functions \(\Phi_{c,k}(z)\) are ignored.

An alternative derivation of the effective-mass approximation. –

The one-dimensional approximation. Suppose now that for each layer \(X\) (with \(X\) standing for \(A\) or \(B\)) we can write the one-particle Schrödinger equation

\[
\left(\frac{p^2}{2m} + V_X^X(r)\right)\Phi_X^X(r) = E\Phi_X^X(r),
\]

where \(V_X^X(r) = V_p^X(x,y) + V_C^X(x,y)\) with periodic potential, which is zero for \(|x| < w_x/2\) and \(|y| < w_y/2\) and \(\infty\) elsewhere. \(V_C^X(x,y)\) is also the potential in the leads. To simplify this problem we can follow the confined geometry method in ref. [39] and the multichannel leads. To simplify this problem we can follow the confined geometry method in ref. [39] and the multichannel transfer matrix method in ref. [19]. In the leads, the set of orthonormal wave functions \(\chi_i(x, y)\), are solutions of

\[
\left(\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V_C^X(x,y)\right)\chi_j^X(x,y) = \varepsilon_j^X \chi_j^X(x,y).
\]

These functions can be used to express \(\Phi_X^X(r)\) as

\[
\Phi_X^X(r) = \sum_i \chi_i^X(x, y)\phi_i^X(z).
\]

If we replace this function in the Schrödinger equation (5), multiply the left by \(\chi_i^X(x, y)\) and integrate upon \(x\) and \(y\), we obtain the set of coupled equations

\[
-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} \phi_j^X(z) + \sum_{i=1}^{N_X} K_{ij}^X(z) \phi_i^X(z) = (E - \varepsilon_j^X) \phi_j^X(z),
\]

where \(N_X\) is the number of propagating modes or open channels in layer \(X\), defined by the condition \(E_F > \varepsilon_j^X\), where \(E_F\) is the Fermi energy, and

\[
K_{ij}^X(z) = \int_{-w_y}^{w_y} \int_{-w_x}^{w_x} \frac{dxdy}{2\pi^2} \chi_j^{X*}(x, y)V_P^X(x, y, z)\chi_i^X(x, y, z).
\]

the coupling-channels matrix elements. \(V_P^X(x, y, z)\) contains the interaction with external potentials, if any. The mixing of channels and the bands parabolicity depend, in general, on \(V_P^X(x, y, z)\). In actual semiconductor layers, the number of propagating modes depends on the Fermi energy and the cross section \(w_x, w_y\). When the multichannel problem for a specific semiconductor \(X\), with \(n_X\) unit cells is solved, one obtains, besides the corresponding eigenfuntions \(\phi_{c,\eta}^{A}(z)\), \(N_Xn_X\) energy eigenvalues \(E_{c,n_X}^{A}\) in each band, \(i.e.,\) in the valence, conduction and excited bands. For simplicity reasons we will restrict the discussion to the 1D one channel case, which natural extension is the 1D multichannel EMA, in the same way as the natural extension of the one-band EMA is the multiband EMA. This approximation has been particularly useful to describe valley-current values measured for resonant tunneling diodes [40–44], which are underestimated in the one-band EMA. In the multichannel EMA approach, the open channels contributions enhance the Landauer conductance and describes well the measured currents [45].

Assuming \(V_X^X(z) = K_{11}^X(z)\), \(E = E - \varepsilon_j^X\) and \(\phi_j^X(z) = \phi_j^X(z)\), eq. (8) becomes

\[
\left(\frac{p^2}{2m} + V_X^X\right)\phi_j^X(z) = E^X \phi_j^X(z).
\]

To solve this equation for the semiconductor layers \(A = (aA)^{n_A}\) and \(B = (bB)^{n_B}\), we need first to obtain the unit cell transfer matrices \(M_{A}A\) and \(M_{B}B\) and, applying the TFPS, determine the band structures \(E_{c,A}^X\) and \(E_{e,B}^X\) and the eigenfunctions \(\phi_{c,\eta}^{A}(z)\) and \(\phi_{e,\eta}^{B}(z)\). A very good approximation for the atomic potentials \(V_A(z)\) and \(V_B(z)\), are the effective potentials in the Hartree-Fock approximation. The quantum numbers \(\epsilon\) and \(\eta\), denote the bands and the intra-band energy levels, respectively. We will denote the valence and the conduction bands with \(\epsilon = v = 1\) and \(\epsilon = c = 2\), respectively. The intra-band energy levels correspond to \(\eta = 1, 2, \ldots, n_X + 1\). In terms of these energies the fundamental energy gap in layer \(X\) is given by

\[
E_g = E_{c,1}^X - E_{v,2n_AX+1}^X = E_{c,1}^X - E_{v,n_X+1}^X. \quad X = A, B
\]

with \(E_{c,1}^X\) the first energy eigenvalue of the conduction band, \(i.e.,\) the conduction band-edge denoted later as \(E_{c,1}^X\), and the upper-edge of the valence band is \(E_{c,1}^X\), the last energy eigenvalue of the valence band. As is well known, the band edges of layers \(A\) and \(B\) do not coincide, in general (see fig. 2), neither the energy spectra \(E_{c,1}^X\) and \(E_{c,1}^X\). Their difference gives rise to the conduction and valence band split offs, as well as, to piecewise constant superlattice or heterostructure potential in the EMA [36]. We will assume from here on that the semiconductor layers \(A\) and \(B\) are such that \(E_{c,1}^X < E_g^X\).

The boundary condition at layers’ interfaces. The boundary condition at the interface of two layers, particularly at the interface of atomic potentials with abrupt change, has been a difficult problem to materialize due to the lack of explicit knowledge of the layer wave functions. Below, the heterostructure wave function
ψ(z, E) will be written as in the standard derivation, as expansions in terms of rapidly varying functions, in our case the wave functions $\phi^A_{\epsilon, \eta_A}(z) = \phi^A(z, E)|_{E = E^A_{\epsilon, \eta_A}}$ and $\phi^B_{\eta_B, \eta_B}(z) = \phi^B(z, E)|_{E = E^B_{\eta_B}}$, with the envelope functions $\varphi^A(z, E) = \varphi^A_{\epsilon_A}(\eta_A, z)$ and $\varphi^B(z, E) = \varphi^B_{\epsilon_B}(\eta_B, z)$ as the expansion coefficients. The boundary conditions imply the fulfillment of energy-dependent relations like
\[
\varphi^A(z, E)\phi^A(z, E)|_{z = z_0} = \varphi^B(z, E)\phi^B(z, E)|_{z = z_0},
\]
\[
\frac{d\varphi^A(z, E)\phi^A(z, E)}{dz}|_{z = z_0} = \frac{d\varphi^B(z, E)\phi^B(z, E)}{dz}|_{z = z_0}
\]
at an interface $z = z_0$. When the energy coincides with the energy eigenvalues in layer $A$, i.e., when $E = E^A_{\epsilon, \eta_A}$ the eigenfunctions $\phi^A_{\epsilon, \eta_A}(z) = \phi^A(z, E)|_{E = E^A_{\epsilon, \eta_A}}$ are propagating functions while $\phi^B(z, E)|_{E = E^A_{\epsilon, \eta_A}}$ are evanescent.

For each value of the quantum number $\eta$ we have the wave number $k_\eta$. To keep some analogy with conventional notation, we can represent the energy eigenvalues $E_{c, \kappa}$, as $E_{c, \kappa}$ or just as $E_c$, that can be written also as $E_c(\kappa)$, keeping in mind that $\kappa$ is a discrete quantity.

It is worth stressing that the eigenfunctions $\phi^A_{\epsilon, \eta_A, \kappa}$, some of which are plotted in fig. 3(a), are continuous within the corresponding layers. These functions will be used to build the continuous heterostructure or SL wave functions.

Before focusing our attention on implications of the system size on the “only-one-band” and “band-edge” assumptions behind the derivation of the EMA, and its re-derivation in the TFPS, we need to build the continuous heterostructure or SL wave functions $\psi(z)$ along the whole structure based on the wave functions $\phi^A_{\epsilon, \eta_A}(z, E)$ and $\phi^B_{\epsilon, \eta_B}(z, E)$, defined inside the layers $A$ and $B$, respectively. To simplify the discussion let us assume that we have the SL $(AB)^nA$. If $\zeta = \text{mod}[l_c] - a$, with $a$ the layer $A$ width, $l_c = a + b$ the SL unit-cell length, we can write a rapidly varying wave function as (see fig. 3(b))
\[
\Phi_{\epsilon, \eta_A, \kappa}^A(z, E) = c_A H(-\zeta)\phi^A_{\epsilon, \eta_A, \kappa}(\text{mod}[l_c], E)
+ c_B H(\zeta)\phi^B_{\epsilon, \eta_B, \kappa}(\text{mod}[l_c], E),
\]
where $H(w)$ is the Heaviside function, $c_A$ and $c_B$ are coefficients fixed by the continuity conditions at the interfaces $A/B$ and $B/A$. These boundary conditions imply that for, say, $E = E^A_{\epsilon, \kappa}$ the function $\Phi_{\epsilon, \eta_A, \kappa}^A(z, E)|_{E = E^A_{\epsilon, \kappa}}$ reduces to $\phi^A_{\epsilon, \eta_A}(\text{mod}[l_c], E)|_{E = E^A_{\epsilon, \kappa}}$, within layers $A$, while, inside the layers $B$, they become the exponentially decaying functions $\phi^B_{\epsilon, \eta_B, \kappa}(\text{mod}[l_c], E)|_{E = E_B, \kappa}$, see fig. 3(b). A similar behavior occurs when $E = E^B_{\epsilon, \kappa}$.

As mentioned before, in the conventional derivations of the effective-mass approximation, the wave functions inside each layer are expanded in terms of the periodic parts of the band-edge Bloch functions, $u^A_{l, \kappa A}$ or $u^B_{l, \kappa B}$, which are generally assumed to be equal [46,47]. Setting up the SL wave function $\psi(z)$, the assumptions of only one-band and small $k$-vectors are also made [46]. In the theory of finite periodic systems, the bands and wave functions $\phi^A_{\epsilon, \eta_A}(z)$ and $\phi^B_{\epsilon, \eta_B}(z)$ are the energy eigenvalues and the eigenfunctions of the periodic systems $(a_A)^nA$ and $(b_B)^nA$.

In fig. 4 we show a simplified calculation in the TFPS of the energy spectrum\(^1\) and transmission coefficients for a specific (confined and open, respectively) semiconductor $A = (a_A)^nA$, with energy gap $E_{gA} \simeq 2.6$ eV and unit-cell length $l_A = 5.15$ nm. On the left-hand side of fig. 4, we show the valence and the conduction bands (VB and CB) of the periodic sequence $(a_A)^nA$ bounded by cladding layers, and, on the right-hand side, the transmission coefficients through the same semiconductor but open. At the top of the left-hand side column, we plot also the subbands (or minibands) in the conduction and valence bands of the SL $(AB)^n$ for $E_{gA} \simeq 2.6$ eV, $E_{gB} \simeq 2.9$ eV, $l_A \sim l_B = 5.15$ nm and $n = 10$. As the layers’ widths decrease, less and less host semiconductor states overlap with the superlattice subband states. For $n_A \simeq 5$, only the edge states overlap with the SL subbands. These graphs show also that as the layer width $n_A = l_A n_A$ gets thinner, the energy levels separation, $\Delta E_c$, increases. This behavior of the energy spectra, that leads to a weaker mixing of the spectrum and transmission coefficients in this figure were obtained for a simplified and approximate piecewise constant potential. The potential parameters were chosen to fit the accurate results published in refs. [48,49].

\(^1\)The spectrum and transmission coefficients in this figure were obtained for a simplified and approximate piecewise constant potential. The potential parameters were chosen to fit the accurate results published in refs. [48,49].
energy levels of envelope functions $\Psi$, eigenfunctions $\phi$, are larger separations increase and the level mixing decreases. It is also worth noticing that, in general, the edge levels mean-life times at the interfaces $A/B$ and the envelope wave function (black curve) is defined along the superlattice. In (b), after imposing the boundary conditions open SL (example of fig. 4, the level width $\Delta \Gamma_1$ the EMA works so well for nanostructures. In the specific relevance of the band-edge functions and reveals why energy levels, justifies the one-band "ansatz", strengthens the one-band $\langle \mu, \nu | \psi \rangle$. In terms of the envelope and the fast-varying functions, we shall also consider the expansion

$$\psi(z) = \sum_{\kappa_0, \kappa_B} \langle \epsilon_0, \kappa_0 | \psi \rangle \Phi_{\epsilon_0, \kappa_0}(z).$$  \hspace{1cm} (15)$$

Here and in the following, the quantum numbers $\epsilon_0$ and $\kappa_0$ represent the set $\epsilon_0^A, \epsilon_0^B$ and $\kappa_0^A, \kappa_0^B$, respectively. For a simple and compact notation, the expansion coefficient $\langle \epsilon_0, \kappa_0 | \psi \rangle$, known also as the envelope function, will be denoted as $\varphi^{\epsilon_0}(z)$ or $\varphi^{\epsilon_0}(\kappa_0, z)$. If we introduce the function

Fig. 3: Eigenfunctions $\phi^{A}_{\epsilon, \kappa, n_A}$, $\phi^{B}_{\epsilon, \kappa, n_B}$, a heterostructure wave function $\Phi^{n_A, n_B}_{A,B}(z, E)$ and an envelope function $\Psi^{\epsilon_0}_{\mu, \nu}(z)$. In (a) the eigenfunctions $\phi^{A}_{\epsilon, \kappa, n_A}(z; E)\big|_{z=E_{2n_A}}$ and $\phi^{B}_{\epsilon, \kappa, n_B}(z; E)\big|_{E=E_{B}}$ are defined within the corresponding layers $A$ and $B$ and the envelope wave function (black curve) is defined along the superlattice. In (b), after imposing the boundary conditions at the interfaces $A/B$ and $B/A$, the wave function $\Phi^{n_A, n_B}_{A,B}(z, E)$, evaluated here at $E = E_{2n_A}$, reduces to the eigenfunction $\phi^{A}_{\epsilon, \kappa, n_A}(z; E)\big|_{E=E_{2n_A}}$ inside layers $A$, and into an exponentially decaying functions inside the neighbor layers $B$. The envelope functions $\Psi^{\epsilon_0}_{\mu, \nu}(z)$ (see the black curves) are extended and continuous functions along the heterostructure.

Fig. 4: Layer widths and the band structure characteristics. In the left panel, the band structure of a bounded periodic semiconductor $C/(a_A)^n A/C$, with $E_{gA} = 2.6$ eV, $E_{gC} = 3.3$ eV, and, in the right panel, the transmission coefficient through the open SL $(a_A)^n A/C$, plotted for different layer widths $w_A = l_A n_A$. Here $l_A$ is the unit cell length and $n_A$ the number of unit cells in layer $A$ along the growing direction. In the upper graph of the left-hand side, we have also the subbands of the superlattice $C/(AB)^n C$ with $w_B \sim w_A$, $E_{gB} = 2.9$ eV and $n = 10$. It is clear that as the layer widths ($\propto n_A$) decrease, the energy levels separations increase and the level mixing decreases. It is also worth noticing that, in general, the edge levels mean-life times are larger

![Diagram showing band structure characteristics](image-url)
\[ \psi(z) \text{ of eq. (15) into the SL Schrödinger equation} \]
\[
\left( \frac{p^2}{2m} + V_{SL}(z) \right) \psi(z) = E \psi(z),
\]
where
\[ V_{SL}(z) = H(-\zeta)V_A(z \mod |l_0|) + H(\zeta)V_B(z \mod |l_0|), \]
(17)
multiply by \( \Phi_{\epsilon_0,\kappa_0}(z) \) and integrate, we have
\[
\sum_{\kappa_0, \kappa_0'} \left[ H(-\zeta)E_{\epsilon_0,\kappa_0}^A \delta_{\kappa_0,\kappa_0'} + H(\zeta)E_{\epsilon_0,\kappa_0}^B \delta_{\kappa_0,\kappa_0'} \right] \times (\epsilon_0, \kappa_0) = E (\epsilon_0, \kappa_0) \psi. \]
(18)

Since
\[ E_{\epsilon_0,\kappa_0}^A = E_{\epsilon_0,\kappa_0}^A + U_{\epsilon_0,\kappa_0}^A = E_{\epsilon_0,\kappa_0}^A + \langle \kappa_0^A | U_{\epsilon_0}(z) | \kappa_0^B \rangle, \]
(19)
the sectionally constant potential \( U_{\epsilon_0}(z) \), known as the split-off, appears here naturally as a consequence of the difference in the energy band structures of layers \( A \) and \( B \), both in the conduction \((\epsilon_0 = 2 = c)\) and valence \((\epsilon_0 = 1 = v)\) bands. Therefore, we are left with
\[
E_{\epsilon_0,\kappa_0}^A \psi_{\epsilon_0}^A(\kappa_0^A) + \sum_{\kappa_0^B} \langle \kappa_0^A | U_{\epsilon_0}(z) | \kappa_0^B \rangle \psi_{\epsilon_0}^B(\kappa_0^B) = E \psi_{\epsilon_0}^A(\kappa_0^A). \]
(20)

We can now, as usual, multiply by \((1/\Omega)e^{i\pi z}\) and sum the Fourier series to obtain
\[
E_{\epsilon_0}^A \left( -i \frac{\partial}{\partial \zeta} \right) \psi_{\epsilon_0}^A(z) + U_{\epsilon_0}(z) \psi_{\epsilon_0}^A(z) = E \psi_{\epsilon_0}^A(z). \]
(21)

If we further approximate \( E_{\epsilon_0}^A(-i\partial/\partial \zeta) \) by a quadratic function of \(-i\partial/\partial \zeta\), near the band-edge, assuming that the \( k \)-vector at the edge is small and an effective mass \( m_0^* \) defined as usual for each layer, we have
\[
\left[ \frac{p^2}{2m_{\epsilon_0}^*} + U_{\epsilon_0}(z) \right] \psi_{\epsilon_0}^A(z) = (E - E_{\epsilon_0,\eta_0}^A) \psi_{\epsilon_0}^A(z), \]
with \( \epsilon_0 = c \) and \( \eta_0 = 1 \) for the conduction band and \( \epsilon_0 = v \) and \( \eta_0 = n_A + 1 \) for the valence band. If we define the energy eigenvalues
\[ E_{\mu,\nu} = (E - E_{\epsilon_0,\eta_0}^A)_{\mu,\nu}, \]
(23)
measured from the band-edges, we can write the Schrödinger equation in the effective mass approximation
\[
\left[ \frac{p^2}{2m_{\epsilon_0}^*} + U_{\epsilon_0}(z) \right] \psi_{\epsilon_0}^{\mu,\nu}(z) = E_{\mu,\nu} \psi_{\epsilon_0}^{\mu,\nu}(z), \]
(24)
that we were looking for and was used for SLs and heterostructures, without a specific proof. For SLs, \( U_{\epsilon_0}(z) \) is periodic. In that case, we can use the TFPS to solve this equation and to determine the eigenvalues \( E_{\mu,\nu} \) and the eigenfunctions \( \psi_{\epsilon_0}^{\mu,\nu}(z) \), known as envelope functions. It is worth noting that this derivation of EMA does not require that the layered structure be periodic. Therefore, the EMA is valid for any layered heterostructure.

All the assumptions behind this derivation imply that the wave functions \( \psi(z) \) can be written as
\[ \psi(z) \rightarrow \psi_{\mu,\nu}^{\epsilon_0}(z) \Phi_{\epsilon_0,\eta_0}(z) \]
(25)
with \( \psi_{\mu,\nu}^{\epsilon_0}(z) \) the SL eigenfunction (envelope functions) and \( \Phi_{\epsilon_0,\eta_0}(z) \) the rapid oscillating wave functions. In fig. 5 we plot the functions \( \psi_{\mu,\nu}^{\epsilon_0}(z) \) and \( \Phi_{\epsilon_0,\eta_0}(z) \), in the conduction band, and the functions \( \psi_{\mu,\nu}^{\epsilon_0}(z) \) and \( \Phi_{\epsilon_0,\eta_0}(z) \) of the valence band. These functions can in principle be determined within the TFPS. Dealing with transport properties, one can neglect the function \( \Phi_{\epsilon_0,\eta_0}(z) \), however, for calculations involving two bands, the whole wave function \( \psi(z) \) should, in principle, be considered. According with the mean value theorem for definite integrals, the relation between the transition matrix elements \( H_{\Phi,\psi} = \langle \Phi_{0, n_A + 1}(z) \psi_{\mu,\nu}^{\epsilon_0}(z) | H_{\text{int}} | \Phi_{0, n_A + 1}(z) \psi_{\mu,\nu}^{\epsilon_0}(z) \rangle \) and \( H_{\psi,\Phi} = \langle \psi_{\mu,\nu}^{\epsilon_0}(z) | H_{\text{int}} | \Phi_{\mu,\nu}^{\epsilon_0}(z) \rangle \) evaluated with and without the fast-varying functions (FVFs), can be written as
\[ H_{\Phi,\psi} = \sum_{\nu,\nu'} \phi_{\nu,\nu'}^{\epsilon_0}(z_0) H_{\psi,\Phi} \]
(26)
Fig. 6: The fast-varying functions effect. (a) The mean value factor \( \phi_{\mu'\nu'}(z_0) \) of the FVFs for transitions from levels \((\mu, \nu) = (1, 1), (1, 2), \ldots, (1, 11)\), in the the CB, to \((\mu', \nu') = (2', 1'), (2', 2'), (2', 3')\) and \((2', 4')\), in the VB. (b) The optical reponse of a blue emitting superlattice with and without FVFs.

Conclusions. – We have shown that as the layers widths get thinner, the energy levels separation increases and the energy levels mixing gets weaker, the “ansatz” of only one-band approximation is better justified and reinforces the relevance of the band-edge functions. We have re-derived the effective mass approximation for the Schrödinger equation of layered heterostructures, based on the energy eigenvalues and rapidly oscillating eigenfunctions obtained in the theory of finite periodic systems. This derivation, based on better justified assumptions for nano-structures and true eigenfunctions and eigenvalues obtained from the theory of finite periodic systems, explains why the EMA works so well when applied to this kind of systems. We have shown also that, in order to evaluate matrix elements of interband transitions, the rapidly oscillating wave functions \( \Phi_{\alpha,\beta}(z) \) that should multiply the envelope functions, \( \psi_{\mu,\nu}(z) \), can safely be ignored.

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