Energy minibands and analytical wave functions in semiconductor heterostructures

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We bring back the basic analytical results of our study of the electronic properties of semiconductor heterostructures. The one particle hamiltonian, the effective mass approximation, the Kroning-Penney potential and the method of the transfer matrix have been used to calculate the normalized analytical wave and functions and the minibands energy. The analytically current density calculated starting from the exact structure of minibands is the same as the one associated with the analytical wave functions. We also discuss the effect of the non-porabolicity of the superlattice conduction band on electronic properties and how to obtain the width of minibands in the tight binding approximation. Energy minibands and wave functions reproduce and consequently generalize those of the different limiting cases. The effective masses of the particle in the wells and barriers can be either different or equal. Our results can be directly used in the calculations of energies and functions specific to heterostructures where perpendicular and parallel movements are uncoupled and when there are no magnetic and an arbitrary magnetic fields in the direction of the deposit layers.

I. INTRODUCTION

Experimentally and especially due to modern techniques of growth MOCVD, and notably MBE, the composition, the thickness and the structure in the layers parallel to the surface of the crystal can be controlled [1] depending on the desired application[2]. Extensive studies of epitaxiated interfaces between different crystallin semiconductors and the realisation of new periodic structures like the superlattices allowed a better understanding of modern devices [2]. The discoveries of high mobilities [3], the quantum Hall effect [4] and the fractional quantum Hall effect [5] are among the principal motivations behind the study of the quasi-bidimensional systems. The electronic properties of these systems are summarized in Ref.[6].

In the calculations of electronic conductivity (optical phonon-assisted well to well hopping), the wave functions (GaAs-GaA1As superlattice) were taken to be linear combination of single well functions [7]. In other applications, energies and wave functions of the superlattices are approached through those corresponding to band borders [8], or those of infinite wells [9], or even calculated by variational method [10]. The study of the influence of functions on the conduction (hopping from one quantum well to another), in multiple quantum wells (A1As-InGaGs), has shown that the amplitude of the current depends strongly on the choice of wave functions (infinite wells, triangular wells, finite wells) [11].

In this article in addition to the structure of the energy minibands and the density of states, we are also interested in the analytical calculations of normalized wave functions and the reproduction of those given for the limiting cases with or without parobolicity of the conduction band [12, 13]. Using the standard techniques of transfer matrix, the Kroning-Penney potential and the effective mass approximation, we have calculated the energy minibands and analytical wave functions in semiconductor heterostructures. We have also evaluated the width of minibands in the tight binding approximation with or without effect of the non-parabolicity of the superlattice conduction band (effective masses in the wells and barriers can be different or equal). These envelope eigenfunctions and the eigenenergies can be used for obtaining those of the heterostructures and consequently in the calculations of the quantum transport coefficients [14]. The nature of the boundary conditions and the effective masse depend on the matching between the primitive Bloch functions of the two semiconductors (well and barrier) [15,16,17].

II. RECTANGULAR BARRIER SCATTERING

The investigated superlattice consists of one periodic repetition (along the axis z) of alternating layers of two semiconductors having different gaps, the same crystallin structure and parameters. In the different heterostructures the carrier movement in the perpendicular direction can be separated from that in the direction parallel to the layers.

In what follows, with the effective mass approximation and the Kroning-Penney potential type, we consider an electron in the conduction band of the superlattice. The potential in the direction of the latter is analyzed as a group of identical barriers ($Ga_{1-x}A1_xAs$, for example) of width 2a and height V_0 (depending on the atomic fraction x) measured from the bottom of identical quantum wells (GaAs, for example). The dependence of the effective mass on its position is justified from the fabrication method.

According to chosen Kroning-Penney potential type, we can write for the potential and effective mass:

$$\left[V(z), m^*(z)\right] = \begin{cases} \left[V_0, m_b^0\right]; \text{ in barriers} \\ \left[0, m_w^*\right]; \text{ in wells} \end{cases} \qquad (1)$$

The particle wave function $\psi(z)$ with an energy E, $0< E < V_0$ is the solution of the Schrödinger equation:

$$\frac{\hbar^2}{2m^*(z)}\frac{d^2}{dz^2}\psi(z)+[E-V(z)]\psi(z)=0 \qquad (2)$$

For each barrier of the superlattice (of period 1=2a+2b), there is a field of outgoing waves (amplitudes B and F) and a field of ingoing waves (amplitudes A and G). The wave functions in the wells and barriers are given by:

$$\begin{aligned}\psi_w(z) &= A_n e^{ikz_n} + B_n e^{-ikz_n};\ (a-1) < z_n < (-a)\\ \psi_b(z) &= C_n e^{-\rho z_n} + D_n e^{\rho z_n};\ (-a) < z_n < a\\ \psi_w(z) &= F_n e^{ikz_n} + G_n e^{-ikz_n};\ a < z_n < (1-a)\end{aligned} \qquad (3)$$

where $z_n=(z-nl)$

$$\hbar^2k^2 = 2m_w^*E;\ \hbar^2\rho^2 = 2m_b^*(V_0-E) \qquad (4)$$

k is the wave vector and A_n, B_n, C_n, D_n, F_n and G_n are amplitudes to be determined.

The continuity of $\psi(z)$ and $\frac{d\psi(z)}{m^*dz}$ which ensure the continuity of the current density at the interface (discontinuity of the potential (z-nl)=±a) leads to relationships between the amplitudes [15,16,17]. These conditions can be found directly by integrating the Schrödinger equation at the interface well-barrier. Expressions (1) and (2) can also be condensed into one in which the wave function is the solution of the Ben Daniel and Duke Hamiltonian [18]. The amplitude vectors are related by the following expressions:

$$\begin{pmatrix}A_n\\B_n\end{pmatrix}=\frac{1}{2}\begin{pmatrix}\Lambda^+e^{(\rho+ik)a} & \Lambda^-e^{-(\rho-ik)a}\\ \Lambda^-e^{(\rho-ik)a} & \Lambda^+e^{-(\rho+ik)a}\end{pmatrix}\begin{pmatrix}C_n\\D_n\end{pmatrix} \qquad (5\text{-a})$$

$$\begin{pmatrix}C_n\\D_n\end{pmatrix}=\frac{1}{2}\begin{pmatrix}M^-e^{(\rho+ik)a} & M^+e^{(\rho-ik)a}\\ M^+e^{-(\rho-ik)a} & M^-e^{-(\rho+ik)a}\end{pmatrix}\begin{pmatrix}F_n\\G_n\end{pmatrix} \qquad (5\text{-b})$$

$$\Lambda^{\pm}=1\pm i\lambda\frac{\rho}{k};\ M^{\pm}=1\pm i\frac{k}{\lambda\rho} \qquad (6\text{-a})$$

$$K^{\pm}=\frac{1}{2}\left(\frac{\lambda\rho}{k}\pm\frac{k}{\lambda\rho}\right);\ \lambda=\frac{m_w^*}{m_b^*} \qquad (6\text{-b})$$

The scattering matrix **M** of the barrier relates the amplitude vectors as follows:

$$\begin{pmatrix}A_n\\B_n\end{pmatrix}=M\begin{pmatrix}F_n\\G_n\end{pmatrix}=\begin{pmatrix}M_{11} & M_{12}\\ M_{21} & M_{22}\end{pmatrix}\begin{pmatrix}F_n\\G_n\end{pmatrix} \qquad (7)$$

$$M_{11}=M_{22}^*=\left[\cosh(2\rho a)+iK^-+\sinh(2\rho a)\right]=a_1+ib_1 \qquad (8\text{-a})$$

$$M_{12}=M_{21}^*=iK^+\sinh(2\rho a)=ib_2 \qquad (8\text{-b})$$

The quantities a_1, b_1 and b_2 are introduced here in order to simplify the notation. We note that $\mathrm{Det}(\mathbf{M}) = |M_{11}|^2-|M_{12}|^2 =1$ therefore $\mathbf{M}^{-1} = \mathbf{M}^+ \neq \mathbf{M}$. These properties of the matrix M characterize the case of symmetrical real potentials and invariance of Schrödinger equation with respect to time reversal and spacial reflection. The effect of the barrier on the particle is the same independently of its direction of incidence.

III. SCATTERING BY A FINITE NUMBER OF BARRIERS

In principle the number of layers which constitute the superlattice is finite, and thus the surfaces or interfaces effects are also of great importance and allow a sound comprehension of the surface states (localized states). In Ref.[19] where we derived analytical expressions for the envelope functions and the energy of electronic states, the effects of the dimensions of the supelattice (number of CdTe wells) and the conditions at the borders (heights of the barriers delimiting the CdMnTe-CdTe superlattice are different from those of CdMnTe on the surface states are studied in the superlattice with N periods. Wannier excitons binding energy in these finite superlattice is sensitive to the discontinuity in the potential barrier to the interface, the number of periods of the superlattice and the width of the wells CdTe [20]. The Green function methods (direct linking formalism and interface response theory) [21,22], have also been employed to calculate electronic structures of semi-finite $Ga_{1-x}Al_xAs$-GaAs superlattice in contact with $Ga_{1-y}Al_yAs$-GaAs substrat [23]. The localization and the position of the surface states (probability density calculations in the first and second minigaps) depend on the terminal potential (of the Kroning-Penney type) of the superlattice on the substrat [23].

A. Q transfert matrix

In the wells where the potential is taken as origin of energies, the amplitudes bellow the barrier (n): F_n and G_n are equal to those above barrier (n+1): A_{n+1} and B_{n+1} except for phase factors. The transfer matrix **Q** relates these amplitude vectors as follows:

$$\begin{pmatrix}A_n\\B_n\end{pmatrix}=\begin{pmatrix}M_{11} & M_{12}\\ M_{21}^* & M_{22}^*\end{pmatrix}\begin{pmatrix}e^{-ikl} & 0\\ 0 & e^{ikl}\end{pmatrix}\begin{pmatrix}A_{n+1}\\B_{n+1}\end{pmatrix}=Q\begin{pmatrix}A_{n+1}\\B_{n+1}\end{pmatrix} \qquad (9)$$

The elements of the scattering matrix **M** are defined through relations (7) and (8). We note that $\mathrm{Det}(\mathbf{Q}) = \mathrm{Det}(\mathbf{M}) = 1$ which means $\mathbf{Q}^{-1} = \mathbf{Q}^+ \neq \mathbf{Q}$. The non hermiticity of **Q** implies that its eigenvalues are complex (allowed energies). By iteration, Eq. (9) gives:

$$\begin{pmatrix}A_n\\B_n\end{pmatrix}=P^n\begin{pmatrix}A_0\\B_0\end{pmatrix} \qquad ;P=Q^+ \qquad (10)$$

It should be noted as we shall see in parts IV and V, that eigenvalues and eigenvectors of the transfer matrix **P**

determine the minibands energy and the wave functions of the superlattice respectively.

B. Transmission and reflection coefficients

The amplitude vector to the right of the last barrier will be $\begin{pmatrix} A \\ 0 \end{pmatrix}$. The null component of $\begin{pmatrix} A \\ 0 \end{pmatrix}$ translates of an absence of obstacle (barrier). Relations (5)-(7) and (10) lead to:

$$\begin{pmatrix} A \\ 0 \end{pmatrix} = \begin{pmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{pmatrix} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} ; \mathbf{X} = (\mathbf{Q}^n\mathbf{M})^{-1} \qquad (11)$$

The transmission (T) and reflection (R) coefficients defined in terms of the matrix elements are:

$$T = \left|\frac{A}{A_0}\right|^2 = \left|X_{11} - \frac{X_{12}X_{21}}{X_{22}}\right|^2 = \frac{1}{|X_{22}|^2} \qquad (12\text{-a})$$

$$R = \left|\frac{B_0}{A_0}\right|^2 = \left|\frac{X_{21}}{X_{22}}\right|^2 = 1 - T \qquad (12\text{-b})$$

In the case of a single barrier ($\mathbf{X}=\mathbf{M}^+$, see Eq.(7) and (8)),

$$T = \frac{1}{a_1^2 + b_1^2} = \frac{1}{1+b_2^2}; R = \frac{b_2^2}{1+b_2^2} \qquad (13)$$

The same holds for the case of two barriers $\mathbf{X} = (\mathbf{Q}\,\mathbf{M})^{-1}$:

$$T = \left\{2b_2^4 + 2b_2^2[1 + 2a_1b_1\sin(2kl)] + 1\right\}^{-1} \qquad (14)$$

For n wide identical barriers ($2\rho a \gg 1$), we have $T \approx \left|\frac{2\lambda\rho}{k^2+\lambda^2\rho^2}\right|^{2n} e^{-4n\rho a}$ therefore the attenuation of the wave function amplitude is translated by the exponential decrease of transmission T which generalizes the case where masses are equal [24].

IV. STRUCTURE OF ENERGY MINIBANDS AND DENSITY OF STATES

The eigenvalues of **P**, obtained from $\mathrm{Det}(\mathbf{P} - p\mathbf{1}) = 0$, are the solution to the equation: $p^2 - p\,\mathrm{trace}(\mathbf{P}) + 1 = 0$ and as the wave function must remain finite for $n \to \pm\infty$, the acceptable solutions [25] are such that $|\mathrm{trace}P| \le 2$. The two solutions are $p = e^{\pm ik_z l}$ with $\cos(k_z l) = \mathrm{trace}(\mathbf{P}/2)$.

With the Eq. (7)-(10), the eigenenergies are given by [12,13]:

$$\cos(k_z l) = \mathrm{Re}(M_{11}e^{-ikl}) = \cosh(2\rho a)\cos(2bk) + K^- \sin(2\rho a)\sin(2bk) \qquad (15)$$

where K^- is given by Eq.(6-b)

The Eq.(15) demonstrates that allowed energies correspond to solutions of $|(\mathrm{Re}\left(M_{11}e^{-ik_z l}\right) = \cos(k_z l))| \le 1$.

In particular for $2bk = m\pi$, $\cos(k_z l) = (-1)^m \cosh(2\rho a)$, the forbidden energies are such that $\cosh(2\rho a) > 1$ and in this case the transfer matrix becomes hermitian: $\mathbf{Q}^+ = \mathbf{Q}$ (its eigenvalues are real). Eq. (15) generalizes equation (6.72) of ref.25 valid for the usual electron mass. It is identical to equation (3) of ref.8, obtained differently, and similar to equation (12) of Ref.[15.]. If we employ the continuity of the wave function derivative instead of that of $\frac{1}{m^*}\frac{d\psi}{dz}$, we thus obtain Eq. (15) where λ will be replaced by λ^{-1} in K^{-1}, in agreement with Ref.[26].

For high and/or wide barriers, $y = 2\rho a \gg 1$, Eq.(15) reduce to $\mathrm{cotan}(2kb) \approx -K^-$ wich defined the eigenenergies of an isolated quantum well[27]. In particular when $V_0 \to \infty$, we find the case of the infinite well. For thin barriers, $2a \to 0$ and $V_0 \to \infty$ so that $2aV_0 = \frac{\hbar^2}{m^*}\frac{\alpha}{2b}$ is finite ($\rho \gg k$ and $2pa \ll 1$), Eq.(15) gives that of Kroning-Penney [28]:

$$\cos(k_z l) = \cos(2bk) + \alpha\frac{\sin(2bk)}{2kb} \qquad (16)$$

Let us note that this equation can be found also through resolution of the Schrödinger equation in the reciprocal space [29] or directly through the scattering matrix **T** related to the Green operators [30]. Another interesting limiting case of Eq. (15) is that of the tight binding approximation ($2pa \gg 1$). Using a perturbatif treatment, we have calculated energy bands corresponding to Eq. (15) starting from discrete levels of an isolated well [12]:

$$\varepsilon = E - E_0 = (-1)^{j+1}\frac{4\mu_0 E_0}{K_0^+}\left\{2b\rho_0 + 2\frac{1+\lambda\mu_0^2}{1+\lambda^2\mu_0^2}\right\}^{-1} \times \exp(-2\rho_0 a)\cos(k_z l); \mu_0 = \frac{\rho_0}{k_0} \qquad (17\text{-a})$$

Writing the factor of $\cos(k_z l)$ as $(\Delta_j / 2)$, $E_0 \to E_j^0$ and $E \to E_j(k_z)$ we obtain the dispersion in the tight binding approximation (E_j^0 is the j^{th} level energy and Δ_j is the j^{th} miniband width):

$$E_j(k_z) \approx E_j^0 + (-1)^{j+1}\left(\frac{\Delta_j}{2}\right)\cos(k_z l) \qquad (17\text{-b})$$

Expression (17) can be generalized when the non-parabolicity is taken in to account (for equal or different masses in the wells and barriers (see VI)) and generalize the Eq.(21-43) of Ref.[27] where the masses are taken to be equal.

From Eq.(15) , the one dimensional density of states is given by:

$$n(E)=\frac{2}{\pi}\left|\frac{dk_z}{dE}\right|=\frac{2m_w^*}{\pi l\hbar^2}\left|\left\{\frac{F_1}{\lambda\rho}+\frac{F_2}{k}\right\}\left[1-\cos^2(k_z l)\right]^{-\frac{1}{2}}\right|$$

$$F_1=2a\left\{\sinh(2\rho a)\cos(2bk)+\left[K^-\cosh(2\rho a)+\frac{K^+}{(2\rho a)}\sinh(2\rho a)\right]\sin(2bk)\right\} \qquad (18)$$

$$F_2=2b\left\{\cosh(2\rho a)\sin(2bk)+\left[-K^-\cos(2bk)+\frac{K^+}{(2ba)}\sin(2bk)\right]\sinh(2\rho a)\right\}$$

The Van Hove sigularities of D.O.S correspond to bands extrema where $\cos(k_z l) = \pm 1$. In the Kroning-Penney , Eq.(18) gives that of Ref.[28]:

$$n(E)=\frac{1}{\pi\hbar}\sqrt{\frac{2m^*}{E}}\left\{\sin(2bk)+\alpha\left[\frac{\sin(2bk)}{(2bk)^2}-\frac{\cos(2bk)}{(2bk)}\right]\right\}$$

$$\times\left\{1-\left[\cos(2bk)+\alpha\frac{\sin(2bk)}{2bk}\right]^2\right\}^{-\frac{1}{2}} \qquad (19)$$

Eq.(19) leads to the free electron one dimensional D.O.S. and the case of the tight binding approximation(see Eq.17)

V. NORMALIZED WAVES FUNCTIONS AND CURRENT DENSITY.

In the same wells and barriers, the wave functions are precedently given by relations (3)-(5). The coefficients C_n and D_n are related to coefficients A_n, B_n, A_0 and B_0 via relations (5) and (10). The two eigenvectors $\begin{pmatrix}A_0^{\pm}\\B_0^{\pm}\end{pmatrix}$ representing reference vector $\begin{pmatrix}A_0\\B_0\end{pmatrix}$ correspond to the eigenvalues $e^{\pm ik_z l}$ of the martix **P** [12,13] :

$$\frac{A_0^{\pm}}{B_0^{\pm}}=ib_2e^{ikl}\left\{(a_1-ib_1)e^{ikl}-e^{\pm ik_z l}\right\}^{-1}$$

$$=i\left[(a_1+ib_1)e^{-ikl}-e^{\pm ik_z l}\right]\frac{e^{ikl}}{b_2}=\begin{pmatrix}B_0^{\mp}\\A_0^{\mp}\end{pmatrix}^* \qquad (20)$$

As $e^{\pm 2ik_z l}-2e^{\pm ik_z l}\mathrm{Re}\left(M_{11}e^{-ikl}\right)+1=0$, Eq.(20) takes the following form:

$$\frac{A_0^{\pm}}{B_0^{\pm}}=\frac{b_2e^{ikl}}{\beta^{\mp}}=\beta^{\pm}\frac{e^{ikl}}{b_2};$$

$$\beta^{\mp}=\beta_0^{\mp}\sin(k_z l)$$

$$=\left[\sin(x)\cosh(y)-K^-\cos(x)\sinh(y)\right]\mp\sin(k_z l) \qquad (21)$$

These relations demonstrate that the coefficients(wave amplitudes) depend on the minibands energy.

Replacing $\begin{pmatrix}A_n\\B_n\end{pmatrix}$ by $\begin{pmatrix}A_n^{\pm}\\B_n^{\pm}\end{pmatrix}=e^{\pm inkzl}\begin{pmatrix}A_0^{\pm}\\B_0^{\pm}\end{pmatrix}$ in Eq.(3) and using Eq.(20)-(21), we obtain the normalized wave functions (in one period) [12,13] :

$$\psi_w^{\pm}(z)=\frac{e^{-\frac{ikl}{2}}e^{\pm ink_z l}}{\sqrt{N^{\pm}}}\left\{b_2e^{ik\left[z-\left(n-\frac{1}{2}\right)\right]}+\beta^{\mp}e^{-ik\left[z-\left(n-\frac{1}{2}\right)\right]}\right\} \qquad (22\text{-a})$$

$$(-l+a)\langle(z-nl)\langle(-a)$$

$$\psi_b^{\pm}(z)=\frac{e^{-\frac{ikl}{2}}e^{\pm ink_z l}}{\sqrt{N^{\pm}}}\left\{p^{\pm}\cosh\left[\rho(z-nl+a)\right]+\right. \qquad (22\text{-b})$$

$$\left.q^{\pm}\sinh\left[\rho(z-nl+a)\right]\right\}\quad,(-a)\langle(z-nl)\langle a$$

where

$$N^{\pm}=A'\left(b_2^2+(\beta\mp)^2\right)+B'\beta^{\mp}$$

$$=\left(2A'\beta_0+B'\beta^{\mp}\right) \qquad (23\text{-a})$$

$$=A'\sin^2(k_z l)\mp\left(2A'\beta_0+B'\right)\sin(k_z l)+C'$$

$$A'=1+a\Pi^+\left(\frac{\mathrm{sh}2y-2y}{2y}\right)=2b+a\left[\Pi^-+\Pi^+\frac{\mathrm{sh}2y}{2y}\right]; \qquad (23\text{-b})$$

$$\Pi^{\pm}=\frac{2k}{\lambda\rho}K^{\pm}$$

$$B'=2b_2\left\{2a\left[\frac{\Pi^+}{2}+\Pi^-\frac{\mathrm{sh}2y}{4y}\right]\cos(x)+\right. \qquad (23\text{-c})$$

$$\left.\left[\frac{1}{k}-\frac{k}{\lambda\rho}\frac{\mathrm{ch}(2y)-1}{2\rho}\right]\sin x\right\};C'=A'\left(b_2^2+\beta_0^2\right)+\beta_0B'$$

and

$$p^{\pm}=b_2e^{ikb}+\beta^{\mp}e^{-ikb};$$

$$q^{\pm}=(ik/\lambda\rho)\left\{b_2e^{ikb}-\beta^{\mp}e^{-ikb}\right\} \qquad (24)$$

In these expressions x=2kb , y=2ρa and β_O was given by Eq. (21). Defining $\beta^{\mp}$ as

$\beta^{\mp}\beta^{\pm}=b_2^2\Rightarrow\beta^+N^+=\beta^-N^-$,

$\left(p^{\pm^*},q^{\pm^*}\right)=\left(\beta^{\mp}/b_2\right)\left(p^{\mp},q^{\mp}\right)$ and $\left(N^+k_z\right)=N^-(-k_z)$

they satisfy:

$$\left(\psi^{\pm}{}_{k_z}(z)\right)^{*} = \psi^{\mp}{}_{k_z}(z); \psi^{+}{}_{-k_z}(z) = \psi^{-}{}_{k_z}(z) \qquad (25)$$

Similarly these analytical waves are Bloch functions: $\psi^{\pm}(z) = e^{\pm ik_z z} U^{\pm}(z)$. Indeed, from Eq.(22):

$$\psi^{\pm}_{w}(z) = \frac{e^{\pm ik_z z}}{\sqrt{N^{\pm}}} \left\{ e^{\frac{-ikl}{2}} e^{\mp ik_z (z-nl)} \left(b_2 e^{ik\left[z-\left(n-\frac{1}{2}\right)l\right]} \right) + \beta^{\mp} e^{-ik\left[z-\left(n-\frac{1}{2}\right)l\right]} \right\}$$
$$= e^{\pm ik_z z} U^{\pm}_{w}(z) \qquad (26)$$

As $U^{\pm}{}_{n+1}(z+l) = U^{\pm}{}_{n}(z) = U^{\pm}{}_{n-1}(z-l)$

the eigenfunctions are Bloch functions, product of plane waves with wave vectors $\pm k_z$ and periodic functions $U^{\pm}(z)$ having the periodicity of the superlattice potential. The same holds for $\psi^{\pm}{}_{b}(z) = e^{\pm ik_z z} U^{\pm}{}_{b}(z)$. We can also write (omitting the n index): $\psi^{\pm}(z+l) = e^{\pm ik_z l} \psi^{\pm}(z)$, a relations which reminds us of the matrix property $\mathbf{P} = \mathbf{Q}^{+}$.

In what follows, we study the behaviour of these wave functions at the bands border zone and in the barriers.

For $k_z l \to m\pi$, $\cos(k_z l) \to (-1)^m$, $\beta_0^2 = b_2^2$. Consequently

$$N^{\pm} \to N = 4b_2^2 \left\{ 1 + \frac{\sin(2bk)}{2bk} \right\} = 4b_2^2 \left\{ b + \frac{\lambda\rho}{k^2 + \lambda\rho^2} \right\}$$

$$\psi_w \approx \frac{2b_2}{\sqrt{N}} \begin{cases} \cos k\left[z - \left(n - \frac{1}{2} \right) l \right]; \beta_0 = b_2 \\ \sin k\left[z - \left(n - \frac{1}{2} \right) l \right]; \beta_0 = -b_2 \end{cases} \qquad (27\text{-a})$$

This expression is in agreement with Ref.[8] where the wave functions are not normalized. This behaviour of ψ_w remains valid also for $2\rho a \gg 1$ (as in this case $b_2/\beta^{\mp} \approx (-1)^{j+1}$, and for $\rho \gg k$). In these two cases, $N^{\pm}$ is reduced to $N \approx 4b_2^2 \left\{ b + \frac{1}{\lambda\rho} \right\} \approx 4b_2^2 b$. Qualitatively for $2\rho a \gg 1$ and with the function $\psi_b(z)$ null in the middle of the barrier, we deduce the relation providing energy levels for an isolated well ($\cot an(2kb) \approx -K^{-}$). Quantitatively for $2pa$ 1 so that $\cot an(2kb) \approx -K^{-}$, we can conclude that $(b_2/\beta^{\mp}) \approx (b_2/\beta_0) \approx (-1)^{(j+1)}$. The solution $b_2 = \beta_0$ corresponds to odd levels (j =1,3,...), while $b_2 = -\beta_0$ correspond to the even levels (j=2,4...). The wave functions of different parity are orthogonal. Relation (22) also provides the behaviour of the wave function in the barrier, (-a<z-nl), for uncoupled wells,

$$\psi_b \approx \frac{2b_2}{\sqrt{N}} e^{-\rho[z-nl+a]} \begin{cases} \cos(kb); & \beta_0 = b_2 \ (j\,odd) \\ \sin(kb); & \beta_0 = -b_2 \ (j\,even) \end{cases} \qquad (27\text{-b})$$

which becomes null for infinite wells ($2kb = j\pi$).

Now, we provide the current density and the links with the energy minibands, and the direct connection between parts IV and V. The proceeding wave functions $\psi^{\pm}(z)$ give for the current density:

$$J^{\pm}(k_z) = \frac{i\hbar e}{2} \int \left\{ \left[\psi^{\pm}(z)\right]^{*} \frac{\partial \psi^{\pm}(z)}{\partial z} - \psi^{\pm}(z) \frac{\partial \left[\psi^{\pm}(z)\right]^{*}}{\partial z} \right\} \frac{dz}{m^{*}(z)} =$$
$$\frac{el}{m^{*}_{w}} \hbar k \left[b_2^2 - (\beta^{\pm})^2 \right] / N^{\pm} = 2\frac{el}{m^{*}_{w}} \hbar k \beta^{\pm} \sin(k_z l) / N^{\pm} = \qquad (28)$$
$$2\frac{el}{m^{*}_{w}} \hbar k \frac{\sin(k_z l)}{(2A'\beta_0 + B')}$$

This expression can be deduced directly from the standard definition of the velocity ($J(k_z) \alpha V_{kz}$): $|V_k| = \frac{1}{\hbar} \left| \frac{\partial E}{\partial k_z} \right| = \frac{2}{\pi \hbar n(E)}$ with the D.O.S n(E) given by Eq.18 and $2\left\{ F_2 + \frac{k}{\lambda\rho} F_1 \right\} \equiv 2A'\beta_0 + B'$

Eq.28 demonstrates directly the dependence of the current density on the band structure of the superlattice. When there is no external electric field , we have : $J^{\pm}(k_z) + J^{\pm}(-k_z) = 0$. For the bands borders, there is no propagation ($k_z l = m\pi$, $J^{\pm} = 0$). The same holds for $2\rho a \gg 1$ (non-coupled wells: $\cot an(2k_0 b) = -K_0^{-}$). for a weak coupling of wells ($2\rho \bullet a \gg 1$), (18) results in:

$$J(k_z) \approx (-1)^{j+1} 4 \frac{elE}{\hbar K^{+}} \frac{\rho}{k} e^{-2\rho a} \sin(k_z l) \left\{ 2b\rho + 2\frac{k^2 + \lambda\rho^2}{k^2 + \lambda^2\rho^2} \right\}^{-1} \qquad (29\text{-a})$$

In particular, Eq.29 gives the miniband with Δ_j

$$E_j(k_z) = E_j^0 + \frac{\tilde{\Delta}_j}{2} \cos(k_z l);$$
$$J_j(k_z) \equiv \frac{-e}{\hbar} \left[\frac{\partial}{\partial k_z} E_j(k_z) \right] = \frac{el}{2\hbar} \tilde{\Delta}_j \sin(k_z l) \qquad (29\text{-b})$$

In comparison with the Eq.(29-a) , we find Eq.17 giving Δ_j obtained by perturbatif calculation(see Eq.(15). Eq.(29-a) also provides D.O.S. in the tight binding approximation ($2\rho a \gg 1$) where J and Δ present analitycally the same exponential decrease. In the Kroning-Penney limit and from equations (18) and (29-a), we obtain for $y = 2\rho a \ll 1$ ($x=2kb$):

$$J(k_z) \equiv -e \frac{\hbar k}{m^{*}_{w}} \sin(k_z l) \left\{ \sin(x) + \alpha \left[\frac{\sin(x)}{x^2} - \frac{\cos(x)}{x} \right] \right\}^{-1} \qquad (30)$$

VI. THE NON-PARABOLICITY EFFECT

A. Boundary conditions

According to the Kane two-band model [31,32,33], the eigenunctions of the Hamiltonian in the direction of the superlattice (with $k_x=k_y=0$) associated to a conduction band electron [35,36] with an energy $0 < E < V_0$, are solutions of the Schrödinger equation[13]:

$$\left[\hbar^2 a_2 \frac{\partial^2}{\partial z^2} + \hbar^4 a_4 \frac{\partial^4}{\partial z^4}\right]\psi(z) + [E - V(z)]\psi(z) = 0 \quad (31\text{-a})$$

$$a_2 = \frac{1}{2m^*(z)} \quad (31\text{-b})$$

$$a_4 = \frac{1}{E_g}\left(\frac{1}{2m^*(z)} - \frac{1}{2m_0}\right) \quad (31\text{-c})$$

The corrective term reflects the non-parabolicity effect (via a_4). When $a_4 = 0$, we find Eq.(3) where the non parabolicity is ignored. The integration of Eq.31 through an interface of small arbitrary thickness provides the new boundary conditions:

$$a_{2,w}\psi'_w + a_{4,w}\hbar^2\psi'''_w = a_{2,b}\psi'_b + a_{4,b}\hbar^2\psi'''_b \quad (32)$$

This expression which ensures the continuity of the local current density generalises that of Ref. [15,16,12] where $a_4 = 0$. In the case of non-parabolicity, the wave functions corresponding to the new condition (32), generalise those where the continuity of $\frac{1}{m^*}\frac{d\psi(z)}{dz}$ is used. As the first derivative of the wave function is discontinuous at the interface (which also holds for $\frac{1}{m^*}\frac{d\psi(z)}{dz}$), the derivative of order three of the wave function presents a singularity at the interface.

In the following we give the wave functions and the bands structure corresponding to the Schrôdinger equation (31) .

B. Effects on the electronic properties

As the last Hamiltonian term of (31) commutes with the Hamiltonian without parabolicity, the wave functions are given in the n^{th} well and barrier by expression (3) .

Due to the new conditions (32) on the derivative of the wave function , the analysis of the preceding sections can be used with λ replaced by μ which we define as follows.

From equations (31) and (3), expressions of k, ρ and μ are given by [13]:

$$\hbar^2 k^2 = 4m^*_w E^w_{max}\left\{1 - \sqrt{1 - \frac{E}{E^w_{max}}}\right\} \quad (33\text{-a})$$

$$E^w_{max} = \left(\frac{a_2^2}{4a_4}\right)_w \quad (33\text{-b})$$

$$E^b_{max} = \left(\frac{a_2^2}{4a_4}\right)_b \quad (33\text{-c})$$

$$\hbar^2\rho^2 = 4m^*_b\left(E^w_{max} - V_0\right)\left\{-1 + \sqrt{1 + \frac{V_0 - E}{E^b_{max} - V_0}}\right\} \quad (34\text{-a})$$

$$\mu = \frac{(a_{2,b} + \hbar^2\rho^2 a_{4,b})}{(a_{2,w} - \hbar^2 k^2 a_{4,w})} \quad (34\text{-b})$$

When the effect of the non-parabolicity becomes negligible ($a_4 \to 0$), $\mu \to \lambda = \frac{m^*_w}{m^*_b}$, defined in the parabolic case . Expressions (33) and (34) allow an explicit relationship of ρ in relation with k. For $E^b_{max} - V_0 = E^w_{max}$ (i.e. $k_0^2 = \lambda\rho_0^2$) insignificant values of ρ and k, we find the parabolic case given by relation (4).

VII. CONCLUSION

We have presented the analytical results of electronic properties of semiconductors heterostructures (superlattice,quantic wells) in the direction of the superlattice. This latter is described in its direction by a one-dimensional Kroning-Penney potential (wells separated by barriers) constituted by the extrema of the conduction band (which are not necessarily found in the same material as those of the valency band). The analytical wave functions which we have calculated are normalized in one period.

The general behaviour of the analytical wave functions is directly justified by that of the components of the current density. These results are directly predictable on the basis of the minibands structure. When there is no electric field, the total current density is null . These wave functions satisfy Bloch theorem and generalize those given in Ref.[25] where the masses are equal to that of the free electron. They reproduce the stationary states corresponding to boundaries of the Brillouin zone in agreement with Ref.8 and the case of an infinite well. They out in the middle of barriers in agreement with the case of an isolated well [7,25]. The current density calculated on the basis of the exact bands structure and the density of states, is the same as that associated to wave functions. We have also given these expressions in the two extreme cases of tight and weak binding (the effective masses in the wells and in the barriers can be equal or different).

When the effect of the non-parabolicity for the conduction band is included, all the preceding results are easily generalized. The corrections introduced to the miniband structure for a superlattice GaAs-GaAlAs are negligible [13,14].But this is not the case for materials with a weak energy gap or those whose growth direction is other than [100] (see Ref.[32]. The energy gap can be controlled, for example by introducing positive barriers in the wells of the superlattice or potential wells in the barriers of the superlattice[34]. The periodic one-dimensional potential model (Kroning-Penney) can be corrected by taking into account the non-homogeneity effects of the charge

distribution (self consistent calculation in the approximation of Hartree) along the superlattice[35,36].

The analytical envelope functions which we have calculated for the one-dimensional superlattice are Bloch functions. This is a consequence of the one-dimensional periodic potential considered. The electronic properties of the one-dimensional superlattice can be used directly to calculate those of a tri-dimensional superlattice whenever the parallel and perpendicular movements are uncoupled, and in the presence as well as in the absence of an arbitrary magnetic field [14].

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