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August 2005

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Abstract

Based on the standard multiband Hamiltonians, the quadratic eigenvalue problem method and the multichannel transfer matrix technique, we develop a general approach to study multichannel-multiband transport properties through multilayered systems. In this approach we deal simultaneously with all the accessible physical channels. We are then able to distinguish and to calculate transmission amplitudes, $t_{ij}$, for each pair $j,i$ of incoming and outgoing propagating modes. We apply this approach to study hole tunnelling through a single-barrier and multiple-barrier semiconductor heterostructures, modelled by a zero-biased $(4 \times 4)$ Kohn-Luttinger Hamiltonian. We calculate transmission coefficients and the Landauer conductance for systems with coupled and uncoupled channels. Extremely good agreement with experimental results is found when applied to Double Barrier Resonant Tunnelling systems. We find interesting under-barrier interference and resonance effects.
I. INTRODUCTION

The transport and tunnelling processes of electrons and holes through semiconductor heterostructures are important topics in Solid State and Condensed Matter Physics. Compared with electrons, holes and the physical structures where these particles are the charge carriers have been much less studied because of the mathematical complexity characterizing the theoretical approaches to these systems. The importance of a complete characterization of holes passing through semiconductor systems is, very likely, based on the assumption that the characteristic times of optoelectronic devices, in which electrons and holes are involved, is limited by the last ones because of their larger effective mass. Nevertheless, transmission time experiments with GaAs – AlAs superlattices\textsuperscript{1} have shown that when the valence band is in resonance, the tunnelling of holes occurs more rapidly than that of electrons, in spite of the mass.

While the electron tunnelling can properly be described within the 1-D (single-mode) approximation (implicit in the WKB, transference Hamiltonian\textsuperscript{2}, Wannier\textsuperscript{5} and Wigner\textsuperscript{6} functions, and the 1-D transfer matrix\textsuperscript{3,4} approaches), the strongly coupled multi-mode (multichannel) systems, in general, and the strongly mixed non-parabolic band-states, in particular, cannot. Multimode problems have been considered with relative success in the framework of tight-binding approximations\textsuperscript{7} (for valence bands), and the $k \cdot p$ approach\textsuperscript{13,14}, for valence and conduction band mixing\textsuperscript{8}. In the tight binding and $k \cdot p$ approaches, some effective $N \times N$ Hamiltonians\textsuperscript{7,8,13,14} are built on and, eventually, the solutions described within the Envelope Function Approximation (EFA). Even though these solutions are multicomponent wave functions, it is usual to cancel arbitrarily all components, except one of them\textsuperscript{15–19}, to determine transmission coefficients. Besides this, it is also usual, after block diagonalizing, to work in reduced Hilbert spaces\textsuperscript{19,20}, which, taken separately, do not fulfill all the physical symmetries of the whole Hilbert space\textsuperscript{21}. It is clear then, that following the actual one-component flux approaches, important physical information is lost. Hence, the one-component flux description for a transport process characterized by mixed-multi-component flux is unreliable. We propose here an alternative approach where all the propagating modes are taken into account jointly and simultaneously, and a multi-component description of transmission amplitudes is carried out in a natural way. In this paper we combine the effective $N \times N$ Hamiltonians of the $k \cdot p$ approach with the multichannel (multimode) transfer matrix approach\textsuperscript{10–12}. To solve the second order differential equation associated to $N \times N$ Kohn-Luttinger-like Hamiltonians and to obtain the momentum eigenvalues, we follow the quadratic eigenvalue problem (QEP) method studied by Tisseur et al in Ref. \textsuperscript{9}. We show that using an orthonormal basis derived from QEP, the important flux conservation requirement is rigorously satisfied. Therefore, it is not necessary to introduce arbitrary factors to normalize transmission coefficients\textsuperscript{16,20,22}. For the calculation of transport properties of multichannel-multilayer systems, we follow the finite periodic systems theory\textsuperscript{23}.
On the experimental side, some interesting transport properties and features, such as the strong $\kappa_t$ dependence of the resonant hole transmission coefficients, have recently been reported\textsuperscript{15-19}. We are mainly interested here on the transmission amplitudes matrix, which like the scattering matrix $S$ contains full information on the scattering process described by the model Hamiltonian. Once the transmission amplitudes are obtained, one can readily determine transmission coefficients $T_{i,j}$, and specific transport properties, such as the channel interference characteristics, and global quantities like the Landauer conductance, as functions of the incoming Fermi energy, and the heterostructure’s parameters.

In Section II, assuming an arbitrary $N \times N$ Hamiltonian, we outline the principal theoretical methods incorporated in the present approach, basically the so-called quadratic eigenvalue problem (QEP)\textsuperscript{9} method (adjusted to obtain the momentum eigenvalues and an orthonormal basis), and the transfer matrix method brought in to establish an easy relation with the scattering amplitudes matrices. This approach will be applied, in Section III, to study hole’s transport properties through III-V semiconductor heterostructures described by the (4 $\times$ 4) Kohn-Luttinger (KL) model\textsuperscript{27}. It is worth noticing here that the hole tunnelling through III-V semiconductor heterostructures is beset also by the fact that most, though not all, of the descriptions of hole states have been obtained within the (2 $\times$ 2) Kohn-Luttinger (KL) model, which limits the possibility of observing transition probabilities between different angular momentum projection states and transmission between hole states with different Kramer’s sign (under time reversal symmetry operation). In Section IV, we will present several transmission coefficient results exhibiting, within other features, the mixing of light ($lh$) and heavy holes ($hh$)\textsuperscript{14,19,20,27}. We choose these quasi-particles not only because they were much less studied than the electrons, but also because they constitute intrinsically a multichannel physical system, whose relevance has been suggested in the performance of optoelectronic semiconductor devices\textsuperscript{1,29}. Finally, in Section V we present some conclusions.

II. THE MULTICOMPONENT SCATTERING APPROACH

The bare bones of our approach, which details will be given in the next subsections, are the following: We assume a system described by

$$\hat{H}(z)F(z) = \varepsilon F(z), \quad (1)$$

where the spin-dependent $N \times N$ Hamiltonian $\hat{H}(z)$, invariant to time reversal and space inversion\textsuperscript{28}, complies with physical systems of sectionally constant potentials. To obtain the solutions

$$F(z) = \sum_{j=1}^{2N} c_j \psi_j e^{i q_j z} = \sum_{j=1}^{2N} c_j F_j(z), \quad (2)$$

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FIG. 1: Schematic representation of multichannel \( hh \) and \( lh \) transport processes through a \((GaAs\text{-cladding layer (L)})/(AlAs/GaAs)^n/(GaAs\text{-cladding layer (R)})\) superlattice in the absence of external fields or strains. In the cladding layers, \( hh \) and \( lh \) modes mix due to the \( k \cdot p \) interaction. By complex-momentum valued states, holes propagate through classically forbidden Layer A, via the threshold effect, activating a closed path. In Layer B, holes are allowed to perform a resonant transport at energies of the quasi-bound states in the well. As we increase the energy and surmount the channel threshold, we increase the number of allowed propagating modes.

and particularly the ‘eigenvalues’ \( q_j \) and the ‘eigenvectors’ \( \psi_j \), we use the linearized QEP that will be explained below. Once these quantities are known and an orthonormal basis is obtained, we determine the transfer matrices \( M_{fd}(z_R, z_L) \) (relating functions and their derivatives at \( z_R \) and \( z_L \)) and \( M_{sv}(z_R, z_L) \) (relating state vectors in the propagating mode representation at the same points). We then use the well known relations between \( M_{sv} \) and the scattering amplitudes \( r \) and \( t \), to calculate the relevant transport theory quantities.

A. The Quadratic Eigenvalue Problem (QEP) and orthonormalization criterion

In the actual theoretical calculations dealing with multiband \( \kappa \cdot \mathbf{p} \) Hamiltonians for sectionally constant potentials, it is not usual to consider a complete set of orthonormal basis functions, instead the basis set of functions is normalized to Dirac’s delta function in the configuration space\(^7,8,13,14\) and arbitrary unitary conditions to the incident flux are enforced,\(^15-19\) with complementary normalization constants for the transmission coefficients.\(^16,22\)

The eigenvalue equation (1) for a multi-component system with translation symmetry in the transverse \([x, y]\) plane, can be written in the form

\[
\frac{d}{dz} \left[ B(z) \frac{dF(z)}{dz} + P(z)F(z) \right] + Y(z) \frac{dF(z)}{dz} + W(z)F(z) = O_N
\]

where \( B(z) \) and \( W(z) \) are, in general, \((N \times N)\) Hermitian matrices and \( Y(z) = -P^\dagger(z) \).
Assuming a solution like

\[ \psi e^{i q z} , \]

where \( q \) is a real or complex scalar and \( \psi \) is a \((N \times 1)\) spinor, we obtain the following \textit{quadratic eigenvalue problem}

\[ Q(q) = \{ q^2 M + q C + K \} \psi = O_N. \tag{4} \]

which solutions result in the eigenvalues \( q_j \) and the eigenvectors \( \psi_j \). The matrix coefficients in this equation bear a simple relation with those in (3). In the case discussed in Section IV, \( M = -B \), \( C = 2iP \) and \( K = W \). The specific symmetries of these coefficients determine the method to follow in each case. A summary of the possible QEP’s problems can be found in Table 1 of Ref. [9]. We will focus our attention in a case where matrices \( M, C \) and \( K \) are \((N \times N)\) Hermitian matrices and the \( q_j \) are all different real or complex numbers. Complex eigenvalues \( q_j \) occur together with their complex conjugated \( q^*_j \), while the real eigenvalues \( q_j \) occur together with their symmetric \(-q_j\). In the problem that will be discussed below, an equation like (4) is obtained for each layer of the heterostructure.

Following Ref. [9], we linearize the QEP to get finally the associated standard eigenvalue problem (SEP), with the same eigenvalues as the QEP. In this linearization process, we derive the orthonormality conditions for the eigenvectors of the QEP, namely:

\[ \psi_k \begin{bmatrix} q_j I_N - q^*_j K + q^*_j q_j C \end{bmatrix} \psi_j = \psi_k L^{kj} \psi_j = q_k \delta_{kj} . \tag{5a} \]

\[ \psi_k \begin{bmatrix} I_N + q^*_j q_j M \end{bmatrix} \psi_j = \psi_k D^{kj} \psi_j = \delta_{kj} . \tag{5b} \]

For real eigenvalues, the orthonormality condition can be written as

\[ \psi_k \begin{bmatrix} (q_k + q_j) B + 2iP \end{bmatrix} \psi_j = \psi_k R^{kj} \psi_j = \delta_{kj} . \tag{5c} \]

In the numerical calculations of Section IV, we follow the Gram-Schmidt procedure to orthonormalize the basis functions, using the weight function \( D^{kj} \) in (5b).

Finally it is important to emphasize that using this orthonormalized basis, the scattering matrix satisfies the usual unitarity condition:

\[ S^\dagger S = I_N . \tag{6} \]

We will refer again to this fundamental property at the end of subsection (IIC).

B. The \( N \)-component Hamiltonian and the Transfer Matrix formalism

To introduce the transfer matrices, let us now define the vector

\[ \Psi(z) = \begin{pmatrix} F(z) \\ F'(z) \end{pmatrix} , \tag{7} \]
which includes the wave vectors and their derivatives, and the \((2N \times 1)\) state vector

\[
\Phi(z) = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \begin{pmatrix} \vec{\varphi} \\ \vec{\varphi}' \end{pmatrix}
\]  

(8)

where \(a\) and \(b\) are \(N \times N\) diagonal coefficient matrices, and

\[
\vec{\varphi}(z) = \begin{pmatrix} \vec{\varphi}_1(z) \\ \vec{\varphi}_2(z) \\ \vdots \\ \vec{\varphi}_N(z) \end{pmatrix}.
\]  

(9)

Each component of \(\Phi\), depending on the energy, represents a propagating or evanescent mode.

Based on these definitions, it is possible to establish between \(\Psi\) and \(\Phi\) the important relation

\[
\Psi(z) = \mathcal{N}\Phi(z).
\]  

(10)

The matrix \(\mathcal{N}\) depends upon the specific \(N\)-component Hamiltonian. The vectors \(\Psi(z_L)\) and \(\Psi(z_R)\), at any two points \(z_L\) and \(z_R\) of the heterostructure, are related by

\[
\Psi(z_R) = M_{fd}(z_R, z_L)\Psi(z_L).
\]  

(11)

Similarly

\[
\Phi(z_R) = M_{sv}(z_R, z_L)\Phi(z_L).
\]  

(12)

\(M_{fd}\) and \(M_{sv}\), are the first and second kind transfer matrices respectively. The subscripts \(fd\) and \(sv\) stand because these matrices connect wave functions and their derivatives, in one case, and state vectors in the other. These matrices satisfy the relevant physical properties and symmetries of the Hamiltonian, such as flux conservation \(j(z_L) = j(z_R)\); time reversal, spin rotation and space inversion invariance. \(^{21,24}\) In principle all transfer matrices can be obtained using the transfer-matrix multiplicative property, however, it is frequent to find, evaluating transfer matrices \(M_{fd}\), numerical instabilities which lead to introduce particular calculation algorithms.

Using equations (10)-(12), we obtain the crucial transformation

\[
M_{sv}(z_R, z_L) = \mathcal{N}^{-1}M_{fd}(z_R, z_L)\mathcal{N}.
\]  

(13)

which relates the two types of transfer matrices, and opens the possibility of evaluating the scattering amplitudes. It is well-known from the scattering approach the relation between the transfer matrix \(M_{sv}\) and the scattering matrix \(S\). In the next subsection we summarize some of these relations and the relevant physical quantities defined in terms of the scattering amplitudes.
C. The $M_{sv}$ transfer matrix and the scattering amplitudes

Given the transfer matrix $M_{sv}$, in the propagating mode representation, it is easy to establish the relation with the scattering matrix $S$. For this purpose it is sufficient to use their definitions:

$$
\left( \begin{array}{c}
\varphi (z_L) \\
\varphi (z_R)
\end{array} \right) = M_{sv} \left( \begin{array}{c}
\varphi (z_L) \\
\varphi (z_R)
\end{array} \right) = \left( \begin{array}{cc}
\alpha & \beta \\
\gamma & \delta
\end{array} \right) \left( \begin{array}{c}
\varphi (z_L) \\
\varphi (z_R)
\end{array} \right),
$$

and

$$
\left( \begin{array}{c}
\varphi (z_L) \\
\varphi (z_R)
\end{array} \right)_{\text{out}} = S \left( \begin{array}{c}
\varphi (z_L) \\
\varphi (z_R)
\end{array} \right)_{\text{in}} = \left( \begin{array}{cc}
r & t' \\
t & r'
\end{array} \right) \left( \begin{array}{c}
\varphi (z_L) \\
\varphi (z_R)
\end{array} \right),
$$

where the $(N \times N)$ blocks $t$ and $r$ ($t'$ and $r'$) are the transmission and reflection amplitudes for left (right) incident particles. Assuming that both fluxes are fixed arbitrarily, the following relations are obtained:

$$
r = -\delta^{-1} \gamma, \\
t = \alpha - \beta \delta^{-1} \gamma, \\
t' = \delta^{-1}, \\
r' = \beta \delta^{-1}.
$$

These expressions together with (13) relate the physical properties with the scattering amplitudes.

Considering incidence of particles from the left only, the transmission coefficient from channel $j$ to channel $i$ will be given by

$$
T_{ij} = |t_{ij}|^2,
$$

and the total transmission probability to channel $i$ (channel conductance in units of $e^2/\pi h$) will be obtained from

$$
G_i = \sum_j |t_{ij}|^2.
$$

Here the sum runs over all the incident channels $j$. Another quantity that can be calculated from the transmission amplitudes is the well known two-probe Landauer conductance defined, in units of $e^2/\pi h$, as

$$
G = \text{Tr} \left( tt^\dagger \right),
$$

Once the transmission amplitudes $t_{ij} = t_{ijR} + i t_{ijI}$, and their phases

$$
\theta_{ij} = \arctan \left( t_{ijI}/t_{ijR} \right),
$$
are known, it is possible also to evaluate the transmission phase times:

\[
\tau_{ij} = \frac{\partial \theta_{ij}}{\partial \omega} = \frac{\hbar t_{ijR}^2}{t_{ijR}^2 + t_{ijI}^2} \frac{\partial}{\partial E} \left( \frac{t_{ijI}}{t_{ijR}} \right),
\]  

(20)

which we shall assume provides the traverse (or tunnelling) time, for a particle coming in channel \( j \) and leaving in channel \( i \).

Finally, a few comments on the orthonormal basis and its consequence on the flux conservation requirements and the scattering matrix unitarity. To show the fulfillment of this property we start from the current density in the EFA models,

\[
j(z) = -i \left[ A(z)^\dagger F(z) - F(z)^\dagger A(z) \right],
\]  

(21)

where \( A(z) = B(z)F'(z) + P(z)F(z) \), is a linear form from (3). Using some identities of the QEP, such as (5c), it is easy to show that the current in (21) can be expressed also in the form

\[
j(z) = -\sum_{j=1}^{2N} c_j^c c_j = -c^c c = -(a^b a - b^b b).
\]  

(22)

The coefficients \( a, b, \) and \( c \) were introduced in equations (2) and (8). This result and the flux conservation requirement leads, straightforwardly, to obtain the well-known flux conservation condition

\[
M_{sv} \Sigma_z M_{sv}^\dagger = \Sigma_z.
\]  

(23)

Here \( \Sigma_z = I_2 \otimes \sigma_z \), is the generalized Pauli matrix \( \sigma_z \). From (23) it is easy to obtain the cardinal unitarity property (6) of the scattering matrix \( S \). The pseudo-unitarity condition suggested by A. D. Sánchez and C. R. Proetto\cite{20} for “scattering matrices”, is just a particular way of amending the lack of an orthonormal basis (in the sense of (5)), which, otherwise, leads to a violation of flux conservation. Hereafter \( O_N/I_N \) stands for the corresponding \((N \times N)\) null/identity matrix.

### III. AN EXAMPLE. THE \((4 \times 4)\) KOHN-LUTTINGER MODEL

This model, widely used to study the electronic properties in III-V and II-VI semiconductor valence bands, considers in the \( \kappa \cdot p \) approximation the highest two valence bands degenerated in the \( \Gamma \)-point of the Brillouin zone. The usual \((4 \times 4)\) Kohn-Luttinger Hamiltonian is of the form:

\[
\hat{H}_{KL} = \begin{pmatrix}
H_{11} & H_{12} & H_{13} & 0 \\
H_{12}^* & H_{22} & 0 & -H_{13}^* \\
H_{13} & 0 & H_{22} & H_{12} \\
0 & -H_{13}^* & H_{12}^* & H_{11}
\end{pmatrix},
\]  

(24)
where

\[
\begin{align*}
H_{11} &= A_1 \kappa_1^2 + V(z) - B_2 \frac{\partial^2}{\partial z^2} \\
H_{12} &= \frac{\hbar^2 \sqrt{3}}{2 m_0} \left( \gamma_2 (k_y^2 - k_z^2) + 2i \gamma_3 k_x k_y \right) \\
H_{13} &= \frac{i \hbar^2 \sqrt{3}}{2 m_0} \gamma_3 (k_z - i k_y) \frac{\partial}{\partial z} \\
H_{22} &= A_2 \kappa_1^2 + V(z) - B_1 \frac{\partial^2}{\partial z^2}
\end{align*}
\]

with

\[
\begin{align*}
A_1 &= \frac{\hbar^2}{2 m_0} (\gamma_1 + \gamma_2) ; & A_2 &= \frac{\hbar^2}{2 m_0} (\gamma_1 - \gamma_2) \\
B_1 &= \frac{\hbar^2}{2 m_0} (\gamma_1 + 2 \gamma_2) ; & B_2 &= \frac{\hbar^2}{2 m_0} (\gamma_1 - 2 \gamma_2)
\end{align*}
\] (25)

In (24), the atomic-like states, which correspond to the valence band states of interest, are taken as \(hh_{+3/2}, lh_{-1/2}, lh_{+1/2}, \) and \(hh_{-3/2}\), after Ref [27]. Though in general the precise definition of physical channels depend on the physical problem envisioned, in this model each of the 4 components of \(F_{kl}(z)\), corresponding to one of the angular momentum components \(m_j = \pm 3/2\) and \(m_j = \pm 1/2\), are the physical channels to deal with. It is worth noticing that each \(F_{kl}(z)\) component is a linear superposition of right and left moving quasi-particle states.

It is easy to see that, independently of the specific parameters, the matrices \(M, C\) and \(K\) associated to the QEP of \(\hat{H}_{kl}\) are:

\[
M_{kl} = \begin{pmatrix}
B_2 & 0 & 0 & 0 \\
0 & B_1 & 0 & 0 \\
0 & 0 & B_1 & 0 \\
0 & 0 & 0 & B_2
\end{pmatrix},
\] (26)

\[
C_{kl} = \begin{pmatrix}
0 & 0 & \mathcal{H}_{13} & 0 \\
0 & 0 & 0 & -\mathcal{H}_{13} \\
\mathcal{H}_{13}^* & 0 & 0 & 0 \\
0 & -\mathcal{H}_{13}^* & 0 & 0
\end{pmatrix},
\] (27)

with \(\mathcal{H}_{13} = -\frac{\hbar^2 \sqrt{3}}{2 m_0} \gamma_3 (k_z - i k_y)\), and

\[
K_{kl} = \begin{pmatrix}
A_1 \kappa_1^2 + V(z) - E & H_{12} & 0 & 0 \\
H_{12}^* & A_2 \kappa_1^2 + V(z) - E & 0 & 0 \\
0 & 0 & A_2 \kappa_1^2 + V(z) - E & H_{12} \\
0 & 0 & H_{12}^* & A_1 \kappa_1^2 + V(z) - E
\end{pmatrix}.
\] (28)
An important role in our approach is played by the crucial relation (10), which is easily obtained when the envelope function (in the propagating modes representation)

\[
F_{kl}(z) = \sum_j^N \left( a_j \psi_j \bar{\varphi}_j(z) + b_j \psi_{N+j} \bar{\varphi}_j(z) \right)
\]  

is written as

\[
F_{kl}(z) = \mathcal{N}_{11} a \bar{\varphi}(z) + \mathcal{N}_{12} b \bar{\varphi}(z).
\]  

with

\[
\mathcal{N}_{11} = (\psi_1 \psi_2 \cdots \psi_4)
\]

\[
\mathcal{N}_{12} = (\psi_5 \psi_6 \cdots \psi_8).
\]

Therefore, we obtain the relation

\[
\Psi_{kl}(z) = \begin{pmatrix} \mathcal{N}_{11} & \mathcal{N}_{12} \\ i\mathcal{N}_{11}Q & -i\mathcal{N}_{12}Q \end{pmatrix} \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \begin{pmatrix} \bar{\varphi} \\ \bar{\varphi} \end{pmatrix}
\]

\[
= \mathcal{N} \Phi_{kl}(z).
\]  

for the 4 × 4 KL model. Here we have defined the matrix

\[
Q = \begin{pmatrix}
q_{hh} & 0 & 0 & 0 \\
0 & q_{lh} & 0 & 0 \\
0 & 0 & q_{lh} & 0 \\
0 & 0 & 0 & q_{hh}
\end{pmatrix}.
\]

containing the QEP eigenvalues. The spinors in (31) and (32) are the orthonormalized eigenvectors of the corresponding QEP. The order in which spinors are labelled should be consistent with the labelling of the scattering matrix elements. We are now able to distinguish incoming and outgoing channels, as well as all the possible transitions among them.

Given the transformation (33), relating the bulk-like plane wave states with well-defined right and left propagating modes, we have the similarity transformation (Eq. (13))

\section*{IV. NUMERICAL RESULTS}

To make clear the notation and terms used here, let us consider again the figure 1. We sketch there a multichannel hole transport process through a GaAs-cladding layer (L)/(AlAs/GaAs)^n/ GaAs-cladding layer (R) heterostructure. As is well-known, the alternation of AlAs and GaAs layers lead to a sequence of valleys and barriers in the conduction and valence bands. For systems...
with small number of layers like in the double barrier systems (DBS), or systems with a larger number of layers but locally periodic, the transmission process is resonant and occurs through a number of levels or subbands (where the transmission coefficient is close to one). Within the heterostructure, heavy and light holes ($hh$ and $lh$) can scatter to any of the energetically possible states. In this Section we will refer to crossed and direct transitions process (dashed and straight arrows, respectively in figure 1). For locally periodic (bi-component) systems $BABAB...$, with alternating wells $B$ of length $L_w$ and barriers $A$ of length $L_b$, we consider single cells of the form $B^{1/2}AB^{1/2}$ (with $B^{1/2}$ half layer $B$), of length $l_c = L_w + L_b$. In all examples considered here, we will have $L_w = 50 \text{ Å}$ and $L_b$ (ranging between 10 and 40 Å). The Luttinger parameters are taken after Ref. [39]. The incident and transmitted channels are labelled according to Ref.[27]. All numerical results presented in this Section were obtained for transmission processes along the growing direction.

A. Transmission probabilities in the limit of uncoupled modes ($\kappa_T = 0$)

In figure 2 we show the transmission probabilities for “direct path” processes, i.e. for $hh_{+3/2} \rightarrow hh_{+3/2}$ and $hh_{-3/2} \rightarrow hh_{-3/2}$ (solid lines) and $lh_{+1/2} \rightarrow lh_{+1/2}$ and $lh_{-1/2} \rightarrow lh_{-1/2}$ (dashed lines), when $\kappa_T = 0$. An interesting but not unexpected result is that, uncoupled holes with equal effective mass and opposite angular momentum components $m_j$, have exactly the same tunnelling probability, which means that reversing the total angular momentum orientation, the transmission rate remains invariant. Nevertheless, our model is able to solve between the four $in-out$ channels, which, in turn, allows to state that, in the uncoupled limit, the crossed paths $hh_{+3/2} \rightarrow hh_{-3/2}$ and $lh_{+1/2} \rightarrow lh_{-1/2}$, drawn in full horizontal line in figure 2, are closed in both directions. In this independent-modes limit, the 4 direct paths are the allowed transmission processes, while the crossed paths are forbidden. It can also be noticed that at low energies, the transition probabilities for light holes is larger than for heavy holes, in agreement to single-band model predictions. This characteristic changes in the presence of band mixing.

B. Transmission probabilities for coupled modes $\kappa_T \neq 0$. Strong dependence on $\kappa_T$

The coupling effects manifest themselves through an important number of different transmission probability features. We shall refer here only to the most relevant and apparent ones. In figures 3(a)–(b) we plot the direct process transmission coefficient $T_{ii}$ with $i = hh_{+3/2}$ for several transverse wave numbers. $\kappa_T = 0$ and $\kappa_T \neq 0$. The most visible characteristics in these figures are the gradual transfer of flux from direct to crossed paths at higher energies and the strong resonant interference phenomena at low energies. The remarkable reduction in the direct process transmission coefficient, contrasts with the increase of crossed processes probability (shown partially in figure 3(d)). For energies below the barrier height ($V_b = 0.48 eV$) the evanescent
FIG. 2: Transmission Probabilities $T_{ij}$ as functions of the incident-particles energy for the heterostructure GaAs-cladding layer ($L$)/(AlAs/GaAs)$^n$/GaAs-cladding layer ($R$) when $\kappa_T = 0$, $V_b = 0.498$ eV and $n = 1$. The solid-thick line curve describes the direct paths $hh_{\pm3/2} \rightarrow hh_{\pm3/2}$, and the solid-thin line $lh_{\pm1/2} \rightarrow lh_{\pm1/2}$. The solid-horizontal line represents the 12 crossed paths, which as expected are forbidden.

modes couple resonantly with negligible effects on the transport properties. From figure 3(d) we notice also that for larger Fermi energies, the crossed-paths transmission coefficients $T_{ij}$ drop to zero and the direct processes become, again, the dominant ones. The constructive interference between channels, in the finite $\kappa_T$ regime described by the KL model considered here, occurs with different characteristics for energies below and above the potential barrier.

In subsection IVB2, we will analyze the meaning of $E_{lh}^+$ and $E_{hh}^-$, as well as the relation between the resonant peaks in figures (a) and (c) and the threshold effects.

The similarities observed in the direct transitions from $hh$ and $lh$ at normal incidence, gradually fade as $\kappa_T$ grows even at low energies. This is a consequence of the anisotropy and
FIG. 3: Transmission coefficients as functions of the incoming energy. Panels (a) and (c) for energies below the barrier and panels (b) and (d) for energies above the barrier. In (a) $T_{ii}$ (with $i = hh_{3/2}$) for $V_b = 0.498$ eV, $n = 1$, several values of $\kappa_r$ and energies below 0.6 eV. Two vertical dashed lines indicate the reference energy window $(E_{lh})^+$ and $(E_{hh})^-$ at $\kappa_r = 0.01 \text{Å}^{-1}$. (b) $T_{ii}$ (with $i = hh_{3/2}$) for several values of $\kappa_r$ and energies above 0.6 eV. It is clear from this panel and (a) that, for energies above the barrier, increasing $\kappa_r$ the direct-processes transmission coefficient decreases. In (c) we have $T_{ij}$ for the crossed paths $hh_{3/2} \rightarrow hh_{-3/2}$ and $lh_{-1/2} \rightarrow hh_{-3/2}$ when $\kappa_r = 0.01 \text{Å}^{-1}$. We show also $T_{ii}$ for $i = hh_{3/2}$ and two values of $\kappa_r$: $\kappa_r = 0$ (solid thick) and $\kappa_r = 0.01 \text{Å}^{-1}$ (solid thin). (d) The crossed paths transmission coefficient $T_{ij}$ for $lh_{-1/2} \rightarrow hh_{1/2}$, $lh_{-1/2} \rightarrow lh_{+1/2}$ and $lh_{+1/2} \rightarrow hh_{3/2}$. All for the same value of $\kappa_r$. At larger energies the crossed paths transmission coefficients drop again to zero.
non-parabolicity, which lead on to an interfering process among channels.

It is important to notice that the potential “observed” by holes during their movement, changes as \( \kappa T \) changes too. To evaluate this effect qualitatively, the following calculation was performed: The matrix \( W \), in equation (3), includes the potential \( V(z) \), the energy eigenvalue and some terms of the KL Hamiltonian depending on \( \kappa T \). Diagonalizing this matrix, one can roughly assert that the “interaction eigenvalues” correspond, in some sense, to an effective potential seen by the heavy and light holes. After performing this type of exercise, we obtain the following results: the barrier height reduces and the band edge moves upward as \( \kappa T \) increases (see figure 4). This figure shows also, that for larger values of \( \kappa T \) the low energy particles might be below the band edge, leading (within other evanescent modes interference effects) to a reduction in the transmission probabilities of direct processes. As the model we are using is elastic, that reduction at low energies leads to the opening of crossed-paths in the same energy range as a balance mechanism. For the same reason the opposite occurs at the high energy range in which no strong dependence on \( \kappa T \) is observed (see panels (b) and (d)). On the other hand, the potential obtained for heavy and light holes are quite similar even though the dependence on \( \kappa T \), for each type of holes, is different. In these calculations we used the Luttinger parameters of Ref. [40]

1. Transitions between modes with Kramer-up (+) and Kramer-low (−) sign to time reversal operation

In Ref. [19], sensitive differences in the transmission quantities when comparing the \( (2 \times 2) \) \( u \) and \( l \) sub-spaces were reported. These differences, justify the existence of transitions between them. Figure 3(d) shows the transmission probabilities of the crossed-paths \( lh_{-1/2} \rightarrow lh_{+1/2} \) (dashed line) and the \( lh_{+1/2} \rightarrow hh_{+3/2} \) (dotted line) whose initial and final states belong to different sub-spaces, in the sense of the sign of Kramer degeneracy under the time reversal symmetry (a well defined symmetry within the \( (4 \times 4) \) KL model Hamiltonian). Crossed-path transmissions of this kind, cannot obviously be observed working separately in the usual \( (2 \times 2) \) \( u \) and \( l \) KL sub-spaces, since the Kramer (+) and Kramer (-) propagating modes are not related in the framework of such scheme. Even though we are not asserting that the early studies of these phenomena are wrong when using the \( (2 \times 2) \) KL subspaces, we consider that these transitions, are naturally absent from their analysis. We guess that the crossed-path resonances will be observed experimentally for high values of \( \kappa T \)

2. Threshold effect: Evanescent modes contribution to transmission

In the AlAs barrier (Layer A, figure 1) the longitudinal \( k_z \) eigenvalues (denoted as \( q_{lh} \) and \( q_{la} \)) can take imaginary, complex or real values, as reported before\(^1\). In the first two cases, we are in the presence of evanescent modes, which occur basically at low energies. To gain
FIG. 4: Qualitative approximation to the potential energy observed by holes for two different values of $\kappa_T$. The same potential $V(z)$ is used and the difference appears for the $\kappa_T$ terms. The calculation was performed for a symmetrical barrier and only one half is plotted.

some insight on the rather complicated resonant interference phenomena, let us consider the dispersion relation of the bulk\(^{20}\) (here $k_z = 0$)

\[
\begin{align*}
(E_{hh})^- &= R_y a_o^2 (\gamma_1 - 2\gamma_2)\kappa_T^2 + V_b \\
(E_{lh})^+ &= R_y a_o^2 (\gamma_1 + 2\gamma_2)\kappa_T^2 + V_b
\end{align*}
\]

which determine a reference energy window $[(E_{lh})^- \lesssim E \lesssim (E_{hh})^+]$, broader as $\kappa_T$ increases (see figure 5) and closes precisely at $E = V_b = 0.5eV$, when $\kappa_T = 0$. Here $R_y$ and $a_o$ stand for the Rydberg constant and the Bohr's radius, respectively. For a fixed transverse momentum $\kappa_T$, the resonances of direct and crossed transmission coefficients are correlated, as can be seen in figures 3(a) and 3(c) (for $\kappa_T = 0.01\text{Å}^{-1}$). As $\kappa_T$ departs from zero and the energy window opening broadens, the resonant peaks move away from $E = V_b$. In fact the spikes labelled 1, 2 and 3 above the window in figure 3(a), are the same resonance for three different values of $\kappa_T$ (for $3 \times 10^{-4}$, $4 \times 10^{-4}$ and $1 \times 10^{-2}$ Å$^{-1}$, respectively). The same is true for the resonances 1, 2 and 3 below the window.

Spikes like those shown in figure 3(c) were reported in multichannel electron tunnelling\(^{22,23}\) and in hole tunnelling.\(^{17,18,42}\). In this Figure, it is important to notice that there is no threshold
FIG. 5: Broadening of the reference window. The zero-contour curves of the eigenvalues $q_{lh}$ (full circles) and $q_{hh}$ (full rectangles) as a functions of $\kappa_T$. Here $V_b = 0.500$ eV for AlAs barriers. Below these curves the eigenvalues are purely imaginary (evanescent modes), and above are real (oscillatory modes).

response effect at $\kappa_T = 0$ and no spikes are expected inside the window since in the region between the boundaries $(q_{lh})^2$ and $(q_{mh})^2$, evanescent $q_{lh}$ and oscillatory $q_{mh}$ QEP components are simultaneously available to assemble envelope modes (2) for finite values of $\kappa_T$. These two facts are an alternative way of keeping the result in (34). An evidence of this sort is familiar as an interference phenomenon, when a closed path opens for non-zero coupling, with opened paths. This features emphasize the leading contribution of the evanescent modes -via the appearance of spikes during threshold response- to the holes transmission processes.

C. Partial conductance and the Landauer conductance at $\kappa_T = 0$

In this subsection we shall present and discuss results related to the total transmission probability to channel $i$, $G_i$, defined in equation (18), and the conductance $G$ defined in equation (19). We will analyze basically the barrier width and the coherence effects in the uncoupled channels limit $\kappa_T = 0$, for locally periodic structures. Some calculations have been carried out also for local periodic structures in the interacting modes regime, but for the sake of space and clarity we will present only a brief discussion of this case.
FIG. 6: Transmission Probabilities for the direct paths $hh_{+3/2} \rightarrow hh_{+3/2}$ (a) and $lh_{-1/2} \rightarrow lh_{-1/2}$ (b) as functions of the incident particle energy for several values of the barrier thickness. Here $\kappa_r = 0$, $V_b = 0.498$ eV and $n = 1$. The resonances move to lower energies and become thinner as $L_b$ increases.

1. The barrier width and the low energy conductance behavior

In Figures (6a) and (6b) we present the direct process transmission coefficients $T_{ii}$ (for $i = hh_{+3/2}$ and $i = lh_{-1/2}$, respectively) in the uncoupled regime, as functions of the incoming energy and for different values of the barrier width $L_b$. It can be seen that when the energy is less than $V_b$ the transmission coefficients $T_{ii}$ decreases as $L_b$ increases. We observe several local resonances in the crossed paths $T_{ij}$, which start to opening while raising $L_b$ in the range of $[479 - 491]$ meV, whose intensities, however, are too small and very little sensitive to variations of $L_b$ for values up to 40 Å. Conductance variations are reflected in the curves displayed in the
FIG. 7: Partial hole conductances as functions of the incident energy. Here $\kappa_t = 0$, $V_b = 0.498$ eV, $L_b = 20\,\AA$ and $n = 1$. Solid thick lines show the partial conductance $G_1$ ($G_4$) to channel $hh_{+3/2}$ ($hh_{-3/2}$) and the solid thin lines the partial conductance $G_2$ ($G_3$) to channel $lh_{-1/2}$($lh_{+1/2}$). The two-probe Landauer conductance $G$ is also shown as function of the barrier width.

upper part of the figure 7 for $\kappa_t = 0$ and $L_b = (10 - 40)\,\AA$. For $E < V_b$ we observe the same behavior for $G$ as for $T_{ii}$. However, for $E > V_b$ the resonances of $G$ shift to lower energies, but the peaks decrease their intensities at variance with what was found for $T_{ii}$. We guess that for $E > V_b$ in the uncoupled-modes regime, the barrier width is a parameter for the activation of the interference between channels. This strong dependence of the transmission on the barrier width can be used to set the threshold energy in the response of optoelectronics devices in a similar way to what is pursued with the hole absorption increment in semiconductor optical amplifiers for the reduction of the current threshold.\textsuperscript{8}

2. Homogeneity in the partial conductance of holes

In figure 7 we plotted also the total transmission probabilities $G_i$ (referred to also as partial conductance to channel $i$), as functions of the energy for several values of $L_b$ and for $\kappa_t = 0$. It can be noticed, that the partial conductances for holes with the same effective mass are equal. The $lh_{\pm 1/2}$ modes open first and provide the main contribution to $G_i$ (and $G$) at low energies. Comparing the four $G_i$ curves, it is easy to see that the transmitted wave is more or less homogeneously distributed between different outgoing channels. The physical interpretation is the following: The hole tunnelling through a single barrier in a multiband-multichannel problem
of 4-mixed components, described with the (4 × 4) KL model for a flat-band case, is a balanced phenomenon. The system does not grant any advantage either of the Kramer-up or the Kramer-low sub-spaces while it scatters the incoming hole stream. This homogeneous process, in a sense, is a consequence of the time reversal symmetry that the (4 × 4) KL model fulfills.\textsuperscript{21,41} This calculation was done in the framework of an elastic model, then the variations of $G$ for each energy value, must be appropriately included in the reflection wave and must be reflected in the charge conservation law. We have evaluated the flux conservation symmetry requirement (23) numerically to confirm its fulfillment -within the machine uncertainty- in a wide range of energies and values of $\kappa_T$ in the neighborhood of the $\Gamma$ point and good results were found.

3. Transmission isotropy

We have not observed remarkable differences in the $T_{ij}$ as well as in other transmission quantities while changing the in-plane direction along $\langle 10 \rangle$ to $\langle 11 \rangle$, for different values of the transversal quasi-momentum. This isotropy of hole quantum transport described by the KL model used here, contrasts with the well-known strong anisotropy of the valence band of layered heterostructures of III-V materials.\textsuperscript{20,27,41}

D. Spectral quantities in multilayer systems

At this point we shall introduce an outline apostrophe to mention one of the most significant concepts for the purpose of studying solid state systems: the energy spectrum. We will consider here heavy- and light-holes bandstructures from the point of view of the multicomponent scattering approach. The results obtained here agree with the well-known transmission-coefficients bandstructure of finite periodic systems (characterized by a finite number of intra-band energy levels\textsuperscript{23}), at variance with the continuous band structures predicted for infinite periodic systems.

1. Discrete quasi-stationary levels in a DBRT

In figures 8(a)-8(c) we plot several transmission coefficients $T_{ij}$ for a double barrier resonant tunnelling (DBRT) system, with $i$ and $j$ as indicated in each panel. Specifically we consider the heterostructure GaAs-cladding layer ($L$)/AlAs/GaAs)/GaAs-cladding layer ($R$) with $n = 2$. At low energies, $E < V_b$, discrete quasi-stationary hole levels in the quantum well of the DBRT heterostructure\textsuperscript{7,14,16,19,20,30} are correctly resolved into sharp individual resonances. The quasi-stationary levels are the same for all panels in figure 8 and, as shown in Table I, the agreement with those reported in Ref. [16] is rather good. Zero transmission in multiband systems\textsuperscript{45} occurs in between isolated Fano resonances\textsuperscript{46} when a bound state in the well is coupled to states in the continuum. Previous works report Fano resonances for $lh$ in tight-binding sp3s* calculations, in
FIG. 8: Discrete quasi-stationary bound levels in a 50Å GaAs quantum well within the DBRT GaAs-cladding layer \((L)/(AlAs/GaAs)^2/GaAs\)-cladding layer \((R)\). For \(E < V_b\), Fano-type transmission resonances of \(hh\) and \(lh\) through the double barrier resonant tunnelling system with AlAs barriers. In panel \((a)\) \(\kappa_t = 0\) and \(L_b = 10\ Å\). In \((b)\) The same as in panel \((a)\) but \(L_b = 20\ Å\). In \((c)\) and \(d\) \(\kappa_t = 0.01\ Å^{-1}\) for \(L_b = 10\ Å\) and \(L_b = 20\ Å\), respectively. In all cases, unbound hole levels are evident for \(E > V_b\) and they displace to lower energies with barriers broadening, as expected.

which, even at \(\kappa_t = 0\), the bands \(lh\), \(hh\) and spin split are coupled by symmetry breaking and spin-orbit interaction\(^{43}\). In figure 8, panels \((a)\) and \((b)\), we show isolated Fano resonances for \(hh\) and \(lh\) bands. In the uncoupled channels limit\(^{44}\) only the quasi-stationary states \(hh_j\) with \(j = 1, 2, 3, 4\) contribute to \(T_{ii}\) with \(i = hh_{+3/2}\) (solid line), while the main contributions to \(T_{ii}\) for \(i = lh_{1/2}\) (dashed line) come from the quasi-stationary light hole states \(lh_1\) and \(lh_2\).

In the uncoupled regime, the Hamiltonian \(\hat{H}_{kl}\) in (24) is diagonal, hence an independent band approximation is possible. The \(hh\) states must be closer to one another due to their greater effective mass. This is reflected in thinner resonance picks of heavy hole states in panels \((a)\) and \((b)\) of Figure 8. In \((a)\) the barriers for \(hh\) are more opaque than for \(lh\), therefore, the \(hh\) are strongly confined with larger lifetimes. The widths of \(hh_j\) peaks with \(j = 1, 2, 3, 4\) are 1.8 meV, 2 meV, 5 meV and 15 meV, respectively, while for the \(lh_j\) peaks with \(j = 1, 2\) are 34 meV and 67 meV.

For \(\kappa_t \neq 0\) we find strong band coupling with interfering effects absent in the actual one component approaches. In panel \((c)\) of Figure 8 we have the transmission coefficients for the same direct paths as in panel \((a)\). One of the most interesting results is the probability that a charge carrier incident as a \(hh\) or \(lh\) state, emerges on the other side as a different quasi-
FIG. 9: (a) The metamorphosis of the band spectrum profile for the $hh$ bands at $\kappa_x = 0$ as a function of the incoming particle’s energy and the number of cells. (b) The same as in figure (a) for the $lh$ bands. The single cell dimension was taken as 60 Å, for a fixed well thickness of $L_w = 50$ Å.
TABLE I: Comparison of resonant energies for a DBRT with \( V_b = 0.550 \text{ eV}, L_b = 10 \text{ Å} \) and \( L_w = 50 \text{ Å} \). Typical discrete-level structure of holes is indicated in the second column. The results in the last two-column were obtained in the framework of our approach using the same parameters as in Ref. [16] for two values of \( \kappa_T \).

<table>
<thead>
<tr>
<th>Levels</th>
<th>Resonances(eV) ( \kappa_T \approx 0.001 \text{ Å}^{-1} )</th>
<th>Resonances(eV) ( \kappa_T = 0 )</th>
<th>Resonances(eV) ( \kappa_T = 0.001 \text{ Å}^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( hh_1 )</td>
<td>0.028</td>
<td>0.028</td>
<td>0.020</td>
</tr>
<tr>
<td>( lh_1 )</td>
<td>0.073</td>
<td>0.071</td>
<td>0.081</td>
</tr>
<tr>
<td>( hh_2 )</td>
<td>0.111</td>
<td>0.110</td>
<td>0.109</td>
</tr>
<tr>
<td>( hh_3 )</td>
<td>0.245</td>
<td>0.247</td>
<td>0.245</td>
</tr>
<tr>
<td>( lh_2 )</td>
<td>0.299</td>
<td>0.309</td>
<td>0.318</td>
</tr>
<tr>
<td>( hh_4 )</td>
<td>0.432</td>
<td>0.434</td>
<td>0.431</td>
</tr>
<tr>
<td>( lh_3 )</td>
<td>-</td>
<td>-</td>
<td>0.481</td>
</tr>
<tr>
<td>( hh_5 )</td>
<td>-</td>
<td>-</td>
<td>0.542</td>
</tr>
</tbody>
</table>

*Labelling follows Ref. [43].

Ref. [16]

See Figure 8(a).

particle\(^{23,30}\). In panel (d) of Figure 8, we see that for such crossed-transition paths the charge carrier resonates with energy levels of the inner well having the same or different effective mass. For example, the crossed path \( lh_{-1/2} \rightarrow hh_{-3/2} \) (dashed-double dotted line) which involves a change in effective mass and in Kramer sign, is resonant at \( E = 0.0204 \text{ eV} \) corresponding to a \( hh_1 \) state, and at \( E = 0.5009 \text{ eV} \) through the \( lh_3 \) state. For the crossed-path \( lh_{+1/2} \rightarrow hh_{-3/2} \) (short dashed-dotted line), where only the effective mass changes while the Kramer sign is kept constant, the incident light hole resonates at \( E = 0.5009 \text{ eV} \), with a light hole state \( lh_3 \) to come out as a heavy hole state. It is important to highlight that the state \( lh_3 \) is seen only through crossed-paths and does not appear at \( \kappa_T = 0 \) (in panels (a) and (b) of figure 8). The constraints imposed to the incident flux could be the reason why this state does not appear in previous reports\(^{16,44}\) using similar parameters.

2. Bandstructure and superlattices

The purpose of the sequence of plots in Figure 9 is to illustrate the formation of the heavy-hole and light-hole band structures as the number of cells \( n \) grows\(^{23,30}\). In Figure 9(a) the heavy hole resonance splits and a band structure emerges. In the case of heavy holes the band spectrum reveals itself reasonably well defined, already for \( n \) of the order of 5. It is worth noticing that, even though the band structure is a consequence of and will emerge once the phase coherence
and the periodicity have been combined, the single-cell multichannel-multiband transfer matrix $M_{sv}$ already contains information of this fundamental property $^{23,47}$ (see Figure 2). Additional calculation are in progress for locally periodic systems and related physical quantities, such as the phase time.

V. CONCLUSIONS

A new approach that is able to resolve the multimode transport processes was developed. This approach is based on the standard multiband Hamiltonians, the quadratic eigenvalue problem method and the multichannel transfer matrix techniques. We applied this approach to study transmission of holes described by a multiband-multichannel model. In this approach we do not need to impose any restriction on the incident flux of holes, i.e., we study, at the same time, all amplitudes of heavy and light holes. Without disproving the input assumptions used in Refs.[15–19,44], in accordance with the general remarks of quantum mechanics, we can stress, that our approach has the benefit of identifying clearly, inter- and intra-band hole transitions, and even transitions between states with different Kramer sign to time reversal, which is not the usual case. Moreover, it allows the precise determination of the contribution from each input channel to the scattering process, boosted by the simultaneous presence of the rest of the channels, which are, in principle, equally accessible to the incident hole stream. We believe that this approach provides more realistic predictions and will be useful in describing forthcoming experiments.

The analysis presented here shows that the transmission probabilities are sensible to the transverse wave number $\kappa_T$, and geometrical parameters, like the barrier width.

Our approach puts forward the outstanding effect of the evanescent modes to the transmission mechanism and reveals explicitly the band spectrum profile metamorphosis. Appealing channel interference and threshold effects, interposed by bond and evanescent states, are clearly foreseen. The location of the quasi-stationary states of the well in the DBRT case are in good agreement with typical hole tunnelling experiments.

Acknowledgments

This work was developed under grant No. E120.1717 of CONACyT of Mexico and partially supported by the Departamento de Ciencias Básicas, UAM-A, Mexico, by the Catedra de Ciencia Contemporánea, Universitat “Jaume I”, Spain and also by the CYTED network IX.E of the CYTED Program of Microelectronics. The authors gratefully acknowledge V. Velasco, J. Gravinsky, A. Robledo and A. Anzaldo-Meneses for useful and clarifying comments. This work was done within the framework of the Associateship Scheme of the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy.
APPENDIX A: TRANSFER MATRIX PROPERTIES

To circumvent numerical instabilities of the TM formalism, found in structures longer than few tens of Å, several algorithms have been suggested. In our procedure one slab of the n-cell heterostructure is divided into adjustable-sized partitions over which the TM fulfills its general properties and can be successfully computed. For example, let us suppose Layer A to have a width \( z_2 - z_1 \) (see Figure 1). One can divide this length into \( m \) pieces of width \( \Delta z \) in which the matrix fulfills:

\[
M_{fd}(z_2, z_1) = M_{fd}(z_2, z_m - 1) \cdots M_{fd}(z_1, z_1) = [M_{fd}(z_1 + \Delta z, z_1)]^m,
\]

where \( m = (z_2 - z_1)/\Delta z \). Next, we match the corresponding transfer matrices, and then for a single cell we obtain

\[
M_{fd}(z_3, z_l) = M_3(z_3, z_2)C_2M_2(z_2, z_1)C_1M_1(z_1, z_l),
\]

hence for an \( n \)-cell heterostructure

\[
M_{fd}(z_n, z_l) = \{M_{fd}(z_3, z_l)\}^n.
\]

The matrices \( M_{1,2,3} \) correspond to the Layer L/Layer A/Layer R, respectively (from Figure 1 notice that for \( n = 1 \), layers R and B coincide). The matrices \( C_{1,2} \) are the matching matrices at points \( z_{1,2} \) respectively, where potentials and band parameters jump from one set of values in one layer to the other of the next layer.

\[
C(z) = \left( \begin{array}{cc}
-I_4 & O_4 \\
\frac{i}{2}(C_{KL})_+ & (M_{KL})_+
\end{array} \right)^{-1} \left( \begin{array}{cc}
I_4 & O_4 \\
\frac{i}{2}(C_{KL})_- & (M_{KL})_-
\end{array} \right).
\]

where matrices \( C \) and \( M \) are the \( 4 \times 4 \) matrices given in (27) and (26) respectively for the matrix equation of motion\(^{37}\) of the form (3), corresponding to the \( (4 \times 4) \) KL space considered in an homogeneous layer. The band parameters are evaluated at the right(+)/left(-) of the matching point.

We have verified for a \((GaAs/AlAs)^n\) superlattice\(^{21}\) with \( n = 11 \) (\( z_R - z_L = 660 \) Å) that the following general constrains fulfill for a wide range of the incident hole energy and in the neighborhood of \( \kappa_T = 0 \)

\[
\text{Re}\{\det\{M_{fd}(z_3, z_l)\}^n\} = 1, \quad \text{and} \quad \text{Im}\{\det\{M_{fd}(z_3, z_l)\}^n\} = 0.
\]

\[
\text{Re}\{M_{sv}(z_R, z_L)^\dagger \Sigma_z M_{sv}(z_R, z_L) - \Sigma_z\} = O_N, \quad \text{and} \quad \text{Im}\{M_{sv}(z_R, z_L)^\dagger \Sigma_z M_{sv}(z_R, z_L) - \Sigma_z\} = O_N.
\]
For an orthogonal basis of linearly independent propagating solutions, \( \Sigma_z = \sigma_z \otimes I_N \) is the enlarged Pauli matrix \( \sigma_z \). The identity (A5) is the well known flux conservation requirement on the TM \( M_{sv} \).\(^{24}\)

It may be convenient, to avoid the truncation error spreading in the numerical simulation and to diminish the computational effort for the calculation, to perform the diagonalization

\[
M_{fd}(z_R, z_L) [M_{fd}(z_3, z_L)]^T = T^{-1} J^n T.
\]

The diagonal matrix \( J \) is the Jordan matrix of \( M_{fd}(z_R, z_L) \).

To achieve consistency we have obtained the \((8 \times 8)\) TM to be used in this problem directly by its definition\(^{21,49}\) \( M_{fd}(z, z_0) = N(z) N(z_0)^{-1} \), being \( N(z) \) the matrix of the linearly independent solutions \((4 \times 1)\) \( F(z) \) and their derivatives. The continuity matrix at points where the potential and the Luttinger parameters jump, was obtained straightforwardly from the \((4 \times 4)\) KL Hamiltonian.
References

28. Systems of the so-called *symplectic universality class*.
36 The evaluation of transmission phase and tunnelling phase time is underway and will be published elsewhere.