Symmetries and General Principles in the Multiband Effective Mass Theory: A Transfer Matrix Study.

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We study the time reversal and space inversion symmetry properties of those transfer matrices mostly used in the calculation of energy spectra and transport-process quantities. We determine the unitary transformation relating transfer matrices. We consider the Kohn-Luttinger model for a quasi-2D system and show that even though the system studied in the (4 × 4) scheme satisfies all the symmetry requirements, the (2 × 2) subspaces do not fulfill such constrains, except in the Γ point of the Brillouin Zone. We find new exchange properties between the (2 × 2) subspace quantities.

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I. INTRODUCTION

In the last years a large number of theoretical studies of multilayered semiconductor structures, using different schemes of \( k \cdot p \) multiband Hamiltonians, have been published\(^1\)–\(^17\). Besides the extensive application of these models, the symmetry problem in general, and the specific characteristics in particular, such as the time reversal invariance in the Kramer (2 × 2) subspaces of the Kohn-Luttinger (KL) model and the parity of heavy- \((hh)\) and light-hole \((lh)\) states, have been only partially considered in a small number of references\(^1\)–\(^12\),\(^12\)–\(^15\). The increasing interest in studying transport properties within the \( k \cdot p \) approximation puts forward the need of a simple procedure to obtain scattering amplitudes from Envelope Function Approximation (EFA) models, and to establish clear requirements to preserve the fundamental physical symmetries. Many physical properties, such as tunnelling and quantum coherence, depend strongly on the symmetries preserved by the system-particle interaction\(^18\). Recently, remarkable efforts have been done to study the breaking of discrete symmetries\(^12\),\(^13\),\(^19\)–\(^23\). However some issues remain to be studied. The lack of a theoretical analysis of whether the time reversal symmetry and the space inversion symmetry in the Kramer (2 × 2) subspaces are fulfilled or not, shows the need of a detailed and comprehensive analysis of symmetry problems in the KL and other EFA models. This is the aim of the present paper.

An important quantity, where the original Hamiltonian symmetries can be checked out in a simple way is the transfer matrix (TM). This object is being used with increasing frequency to study transport properties of different type of systems and within quite distinct approaches. Basically, two types of transfer matrices are being used in the literature. One of these transfer matrices, called here of the first kind, relates a field \( F(z) \) and its derivative \( F'(z) \) at any two points \( z_1 \) and \( z_2 \) of the scatterer system\(^26\)–\(^28\). Another transfer matrix, called here of the second kind, connects state vectors \( \Phi(z) \) that are expressed in the propagating modes representation\(^27\),\(^29\)–\(^34\). Because of its simple functional relation with the scattering amplitudes, the latter matrices were mainly used in the scattering approaches to deal with transport processes. The rigorous fulfillment of symmetry requirements, such as time reversal invariance (TRI), spin rotation (SR), space inversion invariance (SII) and flux conservation (FC) principle, were amply discussed in the literature in connection with these transfer matrices, both for 1-D one-channel and for 3-D multichannel systems\(^30\)–\(^33\). Transfer matrices of the first kind or their associated transfer matrices (which relate \( F(z) \) and a certain linear form \( G(z) = v(z)F'(z) + u(z)F(z) \), at any two points \( z_1 \) and \( z_2 \)), were mainly used in connection with the solution of EFA models\(^35\),\(^36\). The matrices \( u(z) \) and \( v(z) \) appear as coefficients in the matrix equation of motion\(^36\),\(^37\). To obtain the transfer matrix in the EFA one needs to build up the vector \( F(z) \), called the envelope (see Refs. 13,\(^27\),\(^35\),\(^38\)–\(^42\) and references therein). TM of the first kind have been widely used to study the hole spectrum in III-V, II-VI and IV semiconductors\(^24\),\(^25\),\(^43\)–\(^47\).

Since the multiband KL model in the \( k \cdot p \) approximation is amply used in the current solid state physics, and the understanding of the transport properties in heterostructure systems become of great interest, it is convenient to establish a clear bridge between the first and the second kind of transfer matrices. To this purpose the analysis of the

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symmetry requirements on the transfer matrices of the first kind and their relation with the scattering amplitudes and transfer matrices of the second kind, is very much called for. We apply our results to study with clear advantages and transparency the multichannel transport of heavy and light holes through III-V semiconductor heterostructures\textsuperscript{48,49}. However the results that we present here are to some extent also applicable to any EFA model.

Assuming the existence of $N$-coupled-differential-equations solutions, we define in Section II the transfer matrices of the first and second kind and determine the unitary transformation between them. In Section III, we derive the mathematical conditions that the transfer matrices of the first and second kind have to satisfy to fulfill the physical symmetries, and we also recall those for the TM of the second kind that are known. We focus our attention on the time reversal invariance, space inversion symmetry, and the flux conservation principle. In Section IV we consider the $(4 \times 4)$ KL Hamiltonian and derive an explicit representation of the unitary transformation determined in Section II. Next, we discuss the consequences of the various symmetry requirements obtained in Section II on the Hamiltonians and related quantities of the KL $(2 \times 2)$ subspaces. Finally we present some concluding remarks and comments.

II. TRANSFER MATRICES: AN OUTLINE OF BASIC DEFINITIONS

In this Section, we will outline the well known transfer matrix definitions. Based on these definitions, we will establish the relation between the transfer matrices of the first and second kind.

Solving the system of equations associated to an EFA Hamiltonian, one obtains a set of linearly independent eigenvectors. It is often convenient to consider, as will be the case here, an orthogonal set of eigenvectors. With these eigenvectors we can build the envelope function

$$F(z) = \sum_{j=1}^{2N} a_j f_j(z),$$

(1)

where $N$ is the dimension of the system of coupled differential equations, and the vector

$$\Psi(z) = \begin{bmatrix} F(z) \\ F'(z) \end{bmatrix}.$$  

(2)

Alternatively, we can write the eigenvectors in the propagating modes representation as

$$f_j(z) = \begin{pmatrix} g_{1j} \\ g_{2j} \\ \vdots \\ g_{Nj} \end{pmatrix} e^{iq_j z} = g_j e^{iq_j z}$$

(3)

and define, in the plane-wave basis, the state vectors

$$\Phi(z) = \begin{bmatrix} a \rightarrow \varphi (z) \\ b \leftarrow \varphi (z) \end{bmatrix}.$$  

(4)

where $\rightarrow \varphi (z)$ and $\leftarrow \varphi (z)$ represent the right and left moving modes (when $q_j$ is real). Both of them are $N$-dimensional vectors built in terms of the right- and left-travelling wave functions $\rightarrow \varphi_i (z)$ and $\leftarrow \varphi_i (z)$ in the $i$-th channel or propagating mode.

It is easy to see that, writing $\Phi(z)$ as

$$\Phi(z) = \begin{bmatrix} \rightarrow \varphi & 0 \\ 0 & \leftarrow \varphi \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix}$$

(5)

where $a$ and $b$ are $N$ dimensional vectors, and

$$\varphi (z) = \begin{pmatrix} \rightarrow \varphi_1 (z) & 0 & \ldots & 0 \\ 0 & \rightarrow \varphi_2 (z) & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \rightarrow \varphi_N (z) \end{pmatrix},$$

(6)

a simple and obvious unitary transformation can be established between $\Psi(z)$ and $\Phi(z)$. Since these vectors are used to define the transfer matrices of the first and second kind, one can determine such unitary transformation, i.e.

$$\Psi(z) = \mathcal{N} \Phi(z)$$

(7)

which is fundamental for the purpose of this paper. The specific structure of $\mathcal{N}$ depends on the particular Hamiltonian.
A. Transfer matrices of the first kind

Using the function $\Psi(z)$ it is common to define the transfer matrix of the first kind $M_{fd}$ such that

$$\Psi(z_2) = M_{fd}(z_2, z_1)\Psi(z_1).$$  \hspace{1cm} (8)

A slightly different definition for this type of transfer matrix is the associated transfer matrix $T_{36}$ defined by

$$\psi(z_2) = T(z_2, z_1)\psi(z_1)$$  \hspace{1cm} (9)

where

$$\psi(z) = \begin{bmatrix} F(z) \\ G(z) \end{bmatrix} \equiv \begin{bmatrix} F(z) \\ G(z) \end{bmatrix}.$$  \hspace{1cm} (10)

These two matrices are the first kind of matrices we use.

B. Transfer matrices of the second kind

Another TM that has been widely used in the literature that keeps a simple relation with the scattering amplitudes is the matrix defined by $31$

$$\Phi(z_2) = M_{sv}(z_2, z_1)\Phi(z_1).$$  \hspace{1cm} (11)

As for the first kind of transfer matrices, there is also a slightly different definition of the transfer matrix, usually called the coefficients transfer matrix defined by

$$\begin{pmatrix} c \\ d \end{pmatrix} = Q(z_2, z_1) \begin{pmatrix} a \\ b \end{pmatrix}.$$  \hspace{1cm} (12)

Based on the previous definitions and the transformation (7) it is clear that both types of transfer matrices are related by the system-dependent unitary transformation

$$M_{sv}(z_R, z_L) = N^{-1}M_{fd}(z_R, z_L)N.$$  \hspace{1cm} (13)

This is an important result. Based in the previous unitary transformation it is easy to obtain simple functional relations with the scattering amplitudes. The transformation matrix $N$, say

$$N = \begin{bmatrix} g_1 & g_2 & \ldots & g_{2N} \\ d_1g_1 & d_2g_2 & \ldots & d_{2N}g_{2N} \end{bmatrix},$$  \hspace{1cm} (14)

can be obtained when each linearly independent (LI) solution is written as a $(N \times 1)$ spinor, with no coordinate dependence (represented here by $g_j$), times a plane wave. By $d_j$ we denote the coefficient of $z$ in the exponent of the plane waves. In Section IV we will consider a particular KL Hamiltonian and we will obtain specific expressions for $M_{fd}$ and $M_{sv}$ and the unitary transformation in (13).

III. GENERAL FC, TRI AND SII REQUIREMENTS ON $M_{fd}$ AND $M_{sv}$

Let us now recall and deduce the constrains imposed on the transfer matrices by the fulfillment of flux conservation and the physical symmetries of time reversal and space inversion. For the sake of brevity, we report the most important relations and quote just some of the necessary and well known results.

A. Flux Conservation

To obtain the flux conservation requirements we need to write the current density

$$j(z) = -\frac{i\hbar}{2m^*} \left[ \Phi^\dagger \nabla \Phi - \Phi^T \nabla \Phi^* \right],$$  \hspace{1cm} (15)
in terms of any of the previously introduced $2N$-dimensional spinors. The method of derivation follows the usual calculation of the particle current in quantum mechanics. We thus have

$$j(z) = i \left[ F^\dagger G - G^\dagger F \right].$$  

(16)

It is found useful to emphasize that in the KL model this formula reduces to $j(z) = 2 \mathrm{Im} [F^\dagger v F] - 2 F^\dagger u^\dagger F$. In other interesting cases as the Schrödinger equation and the 1-D one-channel and for 3-D multichannel systems it reduces to the known expression $j(z) = F^\dagger F - F^\dagger F$.

When flux is conserved, which means $j(z_2) = j(z_1)$ at any two points, we immediately obtain the identity:

$$R^\dagger(z) \Sigma_y R(z) = M^\dagger_{fd}(z, z_0) R^\dagger(z_0) \Sigma_y R(z_0) M_{fd}(z, z_0),$$

(17)

where

$$R(z) = \begin{bmatrix} I_N & O_N \\ u(z) & v(z) \end{bmatrix},$$

and

$$\Sigma_y = \begin{bmatrix} O_N & -i I_N \\ i I_N & O_N \end{bmatrix}.$$  

Henceforth $O_N / I_N$ is the corresponding $(N \times N)$ null/identity matrix. In a completely similar way, one obtains the FC requirement for other transfer matrices. For the transfer matrices of the second kind the current conservation implies

$$dc^* - cd^* = ba^* - ab^*$$  

(18)

which, using the transfer matrix definition, leads to the well known relation

$$\Sigma_z = \sigma_z \otimes I_N,$$

(19)

where $\sigma_z = \otimes I_N$, is the enlarged $(2N \times 2N)$ Pauli $\sigma_z$ matrix (see Appendix B). This condition has been explicitly deduced in various references.

B. Time Reversal Invariance

TRI implies that the envelope function fulfills the relation

$$K \hat{C} F(z) = F(z),$$

(20)

where the usual notation for the complex-conjugation operator $\hat{C}$ is used, and $K$ is a model-dependent matrix. Using the definition (8) in equation (20) we obtain

$$M_{fd}(z, z_0) = \Sigma M^\dagger_{fd}(z, z_0) \Sigma^{-1}$$

(21)

with

$$\Sigma = \begin{bmatrix} K & O_4 \\ O_4 & K \end{bmatrix}.$$  

$T$, $M_{sv}$, and $Q$ fulfill similar identities. In the case of the matrix $T$, we obtain

$$T(z, z_0) = \Sigma T^*(z, z_0) \Sigma^{-1}.$$  

(22)

Concerning the transfer matrix of the second kind, it is well known that the TRI condition for systems with spin-independent interactions takes the form

$$M_{sv}(z, z_0) = \Sigma_z M^\dagger_{sv}(z, z_0) \Sigma_z^{-1},$$

(23)

while for systems with spin-dependent interactions, this relation changes slightly. The matrix $\Sigma_z$ is given in the Appendix B. In the particular case of systems of spin $1/2$ (see Ref.32), TRI implies the condition

$$M_{sv}(z, z_0) = KM^\dagger_{sv}(z, z_0) K^{-1}.$$  

(24)
C. Space Inversion

Let us now assume that the system possesses a space inversion symmetry with respect to the origin. It is convenient to emphasize that the space inversion we are interested here is the transformation that changes only the sign to the coordinate perpendicular to the interfaces of the Q2D system, leaving the signs of the in-plane wave vector components $k_x$ and $k_y$ unchanged. If $\hat{S}_i$ denotes such space inversion operator, the space inversion invariance implies

$$\hat{S}_i F(z) = ps F(-z)$$

(25)

where $p = \pm 1$ and $s$ is a model-dependent matrix.

As the derivatives change the parity of the functions, the action of the space inversion operator on the bi-field $\Psi(z)$ becomes

$$\hat{S}_i \psi(z) = S \psi(-z),$$

(26)

with

$$S = \begin{bmatrix} s & O_4 \\ O_4 & -s \end{bmatrix}.$$  

(27)

Therefore, the SII requirement on the transfer matrix $M_{fd}$ is

$$M_{fd}(z, z_0) = S^{-1} M_{fd}(-z, -z_0) S.$$  

(28)

Similar identities can be obtained for all the transfer matrices. In particular, for $M_{sv}$ we obtain:

$$M_{sv}(z, z_0) = S_{sv}^{-1} M_{sv}(-z, -z_0) S_{sv}.$$  

(29)

In the Appendix B, the explicit expression for $S_{sv}$ is given.

IV. TM PROPERTIES AND SYMMETRY REQUIREMENTS IN THE KOHN-LÜTTINGER HAMILTONIAN

The first part of this section is devoted to obtain an explicit form for $N$ in the case of the $(4 \times 4)$ KL model. In the second part we will focus our attention on the symmetries of the $(2 \times 2)$ subspaces of this model. For the sake of completeness we shall briefly recall some important and well-known results within the $(4 \times 4)$ KL model and we will describe explicitly the consequences of its TRI and SII symmetries on the $(2 \times 2)$ subspaces. These consequences have not received sufficient attention, however, because of their current interest concerning the elastic and assisted transmission studied within the $(2 \times 2)$ subspaces, deserve further clarification. We shall discuss these implications for the cases in which the wave vector $\kappa$ (defined in the interface planes) is either equal or different from 0.

A. Derivation of the transformation matrix $N$ in the $(4 \times 4)$ KL model

Dealing with the $(4 \times 4)$ KL model Hamiltonian it is usual to block-diagonalize it and to work then with $(2 \times 2)$ Hamiltonians. In this way, the mathematical difficulties are highly simplified. This method remains, nevertheless, a very useful tool to understand many of the intriguing physical properties of $hh$ and $lh$ valence bands near the band edge, and we use it for the derivation of the transformations (7) and (13) in the $(4 \times 4)$ space as our main objective.

In the block-diagonalizing procedure, a unitary transformation $U$ performs the splitting of the original $(4 \times 4)$ Hamiltonian $\hat{H}$ into two $(2 \times 2)$ blocks, which are labelled “up” (u) and “low” (l)

$$U \hat{H} U^\dagger F(z) = \begin{bmatrix} \hat{H}_u & O_2 \\ O_2 & \hat{H}_l \end{bmatrix} \begin{bmatrix} F_u(z) \\ F_l(z) \end{bmatrix} = E \begin{bmatrix} F_u(z) \\ F_l(z) \end{bmatrix},$$  

(30)

where the blocks are given by

$$\hat{H}_u = \begin{bmatrix} A_1\kappa^2 + B_2 \hat{k}_z^2 + V(z) & C_{xy} - iD_{xy}\hat{k}_z \\ C_{xy} + iD_{xy}\hat{k}_z & A_2\kappa^2 + B_1 \hat{k}_z^2 + V(z) \end{bmatrix}.$$  

(31)
\[ \hat{\mathcal{H}}_t = \begin{bmatrix} A_2 \kappa^2 + B_1 \hat{k}_z^2 + V(z) & C_{xy} - i D_{xy} \hat{k}_z \\ C_{xy} + i D_{xy} \hat{k}_z & A_1 \kappa^2 + B_2 \hat{k}_z^2 + V(z) \end{bmatrix}. \]  

(32)

For the definitions of \(A_1, A_2, B_1, B_2, C_{xy}, D_{xy}\) and \(\kappa^2\) see Appendix A. Thus, for each block and for each slab of material (with certain set of phenomenological parameters\(^5\)), we have an eigenvalue problem

\[
\begin{align*}
\{ \hat{\mathcal{H}}_{u,l} - E \mathbb{I}_2 \} F_{u,l}(z) &= O_2.
\end{align*}
\]

(33)

Solving this equation we have

\[
F(z) = U^\dagger \begin{bmatrix} F_u(z) \\ F_l(z) \end{bmatrix} = U^\dagger \begin{bmatrix} \alpha_j \begin{pmatrix} g_{1j} \\ g_{2j} \end{pmatrix} e^{iq_j \hat{z}} \\ \beta_j \begin{pmatrix} g_{3j} \\ g_{4j} \end{pmatrix} e^{iq_j \hat{z}} \end{bmatrix} = \begin{bmatrix} F_1(z) \\ F_2(z) \end{bmatrix}.
\]

(34)

The spinor components \(g_{ij}\) are given in the Appendix A. Here \(\alpha_j(\beta_j)\) stand for the linear combination coefficients of the LI solutions times the corresponding normalization constant in the “up” (“low”) subspaces, respectively. We remark that only two of the values of the momenta \(q_j\) are LI. They are obtained from the zeros of the secular fourth-order polynomial determinant of (33), which is the same for both \(u\) and \(l\) Hamiltonians and then, the energy eigenvalues of the subspace hole states are the same with different spatial trends. This is perhaps the most important consequence of the block-diagonalization (B-D) process from (30).

When considering the multichannel-multiband transport of $hh$ and $lh$ through, say, a III-V semiconductor heterostructures\(^{48,49}\), one should keep in mind the order of the basis components to assign correctly the transmission amplitudes. Assuming

\[
F(r) = F(z) \cdot u_0(r) \, e^{i \vec{q} \cdot (\vec{x} e_1 + \vec{y} e_0)},
\]

we shall choose for the periodic part of the Bloch function \(u_0(r) = (u_1, u_2, u_3, u_4) = (\{\frac{3}{2}, \frac{3}{2}\}, \{\frac{3}{2}, -\frac{1}{2}\}, \{\frac{3}{2}, \frac{1}{2}\}, \{\frac{3}{2}, -\frac{3}{2}\})\), in agreement with the order $hh_{3/2}, lh_{-1/2}, lh_{+1/2}, hh_{-3/2}$ given in Ref.5. Accordingly, the wave function \(\hat{\psi}(z)\) must be supplemented by identifying correctly each value of the momenta \(q_j\) to an $hh$ or $lh$ state. To perform this identification we refer to the levels of an infinite quantum well (iQW) at $\kappa = 0$ limit, given by previous calculations\(^6,11,13\). Considering a parabolic approximation to the dispersion law for the $hh$ and $lh$ bands in this limit, the energy can be cast as

\[
\begin{align*}
E_{hh} &= (\gamma_1 - 2 \gamma_2) q_z^2 \\
E_{lh} &= (\gamma_1 + 2 \gamma_2) q_z^2,
\end{align*}
\]

(35)

which unambiguously relates the uncoupled levels $hh(lh)$ to $q_3(q_1)$, respectively.

Before going forward, notice that both transfer matrices $M_{fd}$ and $T$ relate states in the quasi-particle representation characterized by a certain set of quantum numbers and describe the evolution along $z$ of these modes with no mention to their propagation direction. Nevertheless, as suggested above we can alternatively describe the system using the propagation modes representation\(^3\), \textit{i.e.} the representation where right and left moving states are resolved into separated components. This idea in combination with the mentioned adjustments lead us to express the wave function (34) and its derivative in terms of an eight-component state vector (5)

\[
\Psi(z) = W \begin{bmatrix} G \\ iG^*Q \\ (iG)^*Q \end{bmatrix} \begin{bmatrix} \varphi(z) \\ O_4 \varphi(z) \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix},
\]

(36)

where

\[
W = \begin{bmatrix} V & O_4 \\ O_4 & V \end{bmatrix}, \quad V = \begin{bmatrix} e^{i\phi} & 0 & 0 & 0 \\ 0 & e^{i\eta} & 0 & 0 \\ 0 & 0 & e^{-i\eta} & 0 \\ 0 & 0 & 0 & e^{-i\phi} \end{bmatrix},
\]

being

\[
\eta = \frac{1}{2} \left\{ \arctan \left( \frac{k_x}{k_y} \right) - \arctan \left( \frac{2 \gamma_3 k_y}{2 \gamma_2 k_x - k_y^2} \right) \right\} \quad \text{and} \quad \phi = \frac{1}{2} \left\{ \arctan \left( \frac{k_x}{k_y} \right) + \arctan \left( \frac{2 \gamma_3 k_y}{2 \gamma_2 k_x - k_y^2} \right) \right\}.
\]
The parameters $\eta$ and $\phi$ are taken in the form required by the unitary transformation $^5 U$ for block-diagonalization (30). Hereafter $\gamma_1$, $\gamma_2$ and $\gamma_3$ are the Luttinger parameters of the layer. We have defined

$$G = \begin{bmatrix} g_{13} & g_{11} & g_{41} & g_{43} \\ g_{23} & g_{21} & g_{31} & g_{33} \\ -g_{23} & -g_{21} & g_{31} & g_{33} \\ -g_{13} & -g_{11} & g_{41} & g_{43} \end{bmatrix}, \quad \text{and} \quad Q = \begin{bmatrix} q_3 & 0 & 0 & 0 \\ 0 & q_1 & 0 & 0 \\ 0 & 0 & q_1 & 0 \\ 0 & 0 & 0 & q_3 \end{bmatrix}.$$ 

In (36) the $(4 \times 1)$ vectors $a(b)$ contain the corresponding $a_j(b_j)$ linear combination coefficients of the LI solutions times the corresponding normalization constant of the configuration space in the “up” (“low”) subspaces, respectively. Defining

$$\mathcal{N} = W \begin{bmatrix} G & (G)^* \\ iGQ & (iG)^*Q \end{bmatrix},$$

we have

$$\Psi(z) = \left[ \begin{array}{c} \mathcal{N}_{11} \\ i\mathcal{N}_{11}Q \end{array} \right] \left[ \begin{array}{c} \mathcal{N}_{12} \\ (i)\mathcal{N}_{12}Q \end{array} \right] \left[ \begin{array}{c} \varphi(z) \\ \bar{\varphi}(z) \end{array} \right] \left[ \begin{array}{c} a \\ b \end{array} \right] = \mathcal{N} \Phi(z).$$

This relation is essential to achieve the purpose posted at the beginning of this section. Thus, from (38), the expression (8) that relates $\Psi(z)$ at any two points $z_1$ and $z_2$ of the scatterer system can be written as

$$\{\mathcal{N} \Phi(z_2)\}_2 = M_{fd}(z_2,z_2) \{\mathcal{N} \Phi(z_1)\}_1.$$ 

Hence the state vectors (5) in these regions are connected as

$$\Phi(z_2) = \mathcal{N}_{2}^{-1} M_{fd}(z_2,z_1) \mathcal{N}_{1} \Phi(z_1),$$

therefore

$$M_{sv}(z_2,z_1) = \mathcal{N}_{2}^{-1} M_{fd}(z_2,z_1) \mathcal{N}_{1}. \quad \text{(41)}$$

The convenience of this $(8 \times 8)$ matrix identity is likely found in the clear advantages of using both types of transfer matrices for the description of tunneling and related properties of particles moving through multilayered structures. This result becomes a profitable platform for block-diagonalization of quantum transport phenomena of heavy and light holes through heterostructures. For systems well-described within the EFA the orthonormalization procedure is not a trivial question and differs from routine process, basically, by the presence of linear $k_z$ terms in (31,32). A detailed study on that subject is published elsewhere.

### B. TRI and SII symmetries for the $\kappa \neq 0$ case in the $(2 \times 2)$ KL model

Let us analyze the implications of the TRI and SII symmetries (in the $(4 \times 4)$ KL model) on some physical quantities defined in the $(2 \times 2)$ subspaces. We shall start with the TRI symmetry. To exhibit this implications on the time reversal operator we will use its representation reported by Pasquarello et al. in Ref.1. Before block-diagonalizing the time reversal and space inversion operators, we need to transform them from the Pasquarello’s basis representation to the Broido and Sham basis representation. This transformation is done by means of

$$R = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & -i \end{bmatrix},$$

In the following, $\sigma_x, \sigma_y, \sigma_z$ are the three Pauli matrices and the coordinate origin will be placed in the inversion symmetry point ($z = 0$).
1. Time Reversal Invariance

The \((4 \times 4)\) time reversal operator in the Broido and Sham basis is given by

\[
\hat{T}_{BS} = K_{BS} \hat{C} = RK_{PB} \hat{C} R^{-1} = R \begin{bmatrix} O_2 & \sigma_y \\ \sigma_y & O_2 \end{bmatrix} R^T \hat{C} = \begin{bmatrix} O_2 & \sigma_z \\ -\sigma_z & O_2 \end{bmatrix} \hat{C}.
\] (43)

Hereafter subindexes BS and PB stand for Broido-Sham and Pasquarello-Bassani, respectively. After applying the transformation

\[
U = \frac{1}{\sqrt{2}} \begin{bmatrix} e^{-i\phi} & 0 & 0 & -e^{i\phi} \\ 0 & e^{-i\eta} & -e^{i\eta} & 0 \\ 0 & e^{-i\eta} & e^{i\eta} & 0 \\ e^{-i\phi} & 0 & 0 & e^{i\phi} \end{bmatrix},
\] (44)

the time reversal operator \(\hat{T}_{BS}\) becomes

\[
\hat{T}_{BS} = U R K_{PB} R^T U^T \hat{C} = \begin{bmatrix} O_2 & \sigma_x \\ -\sigma_x & O_2 \end{bmatrix} \hat{C}.
\] (45)

As a consequence the TRI requirement implies for the \((2 \times 2)\) subspace Hamiltonians the fulfillment of the following condition

\[
\sigma_x \hat{H}_u^*(z) \sigma_x = \hat{H}_l(z), \quad \sigma_x \hat{H}_l^*(z) \sigma_x = \hat{H}_u(z).
\] (46)

It is then clear that the TRI of the KL Hamiltonian in the \((4 \times 4)\) space does not imply the TRI of the Hamiltonians in the \((2 \times 2)\) subspaces. It is easy to show also that

\[
\sigma_x F^*_{u, l}(z) = F_{l, u}(z).
\] (47)

and hence

\[
\Gamma_x M^*_{u, l}(z) \Gamma_x = M_{l, u}(z),
\] (48)

here:

\[
\Gamma_x = \begin{bmatrix} \sigma_x & O_2 \\ O_2 & \sigma_x \end{bmatrix}.
\]

As can be seen from previous relations, the considered physical quantities of the subspaces \(u\) and \(l\) should be related to each other in order to satisfy the TRI requirement in the \((4 \times 4)\) space.

2. Space Inversion

It is convenient to emphasize that the space inversion symmetry we are dealing with is the one which changes only the sign to the coordinate perpendicular to the interfaces of the Q2D system. The usual space inversion\(^1\) makes \(\{x, y, z\} \rightarrow \{-x, -y, -z\}\) then, when taking 2D-Fourier transform in the \([x, y]\) plane, change the signs of \(k_x\) and \(k_y\) also.

As in the case of time reversal, we need to know first the space inversion operator (25) for the \((4 \times 4)\) KL space in the Broido and Sham basis\(^5\). This is obtained from

\[
\hat{S}_{BS} = R \hat{S}_{PB} R^{-1} = R \begin{bmatrix} -\sigma_z & O_2 \\ O_2 & -\sigma_z \end{bmatrix} R^{-1} = \begin{bmatrix} -I_2 & O_2 \\ O_2 & I_2 \end{bmatrix}.
\] (49)

It is easy to verify that the \((4 \times 1)\) wave function \(F(z)\) defined in (34), under this operator action, satisfies the symmetry condition (25). It can be seen also that the time reversal and space inversion operators satisfy \(\{\hat{T}_{BS}, \hat{S}_{BS}\} = 0\),
for the hole state. Taking advantage of (54) the following useful relation is obtained:

\[
\hat{S}_{\text{bs}} \begin{bmatrix} F_1(z) \\ F_2(z) \end{bmatrix} = p \begin{bmatrix} -F_1(-z) \\ F_2(-z) \end{bmatrix} = \begin{bmatrix} F_1(z) \\ F_2(z) \end{bmatrix}.
\]

Since

\[
U \hat{S}_{\text{bs}} U^\dagger = \begin{bmatrix} O_2 & \sigma_x \\ \sigma_x & O_2 \end{bmatrix},
\]

the space inversion invariance of the KL Hamiltonian leads us to

\[
\begin{bmatrix} O_2 & \sigma_x \\ \sigma_x & O_2 \end{bmatrix} \begin{bmatrix} \hat{H}_u(-z) & O_2 \\ O_2 & \hat{H}_l(-z) \end{bmatrix} = \begin{bmatrix} \hat{H}_u(z) & O_2 \\ O_2 & \hat{H}_l(z) \end{bmatrix}.
\]

Therefore

\[
\begin{align*}
\hat{H}_u(z) &= \sigma_z \hat{H}_l(-z) \sigma_x \\
\hat{H}_l(z) &= \sigma_z \hat{H}_u(-z) \sigma_x.
\end{align*}
\]

For the transfer matrices of the first kind and for the envelope wave functions we have

\[
M_{u, \ell}(z) = \Gamma_x M_{\ell, u}(-z) \Gamma_x,
\]

\[
\sigma_x F_{u, \ell}(-z) = p F_{\ell, u}(z).
\]

Here again the transfer matrices and wave functions, appearing in the first and second members of equations (53) and (54), belong to different subspaces. For \( \kappa \neq 0 \) the space inversion symmetry in the \((4 \times 4)\) space does not imply space inversion symmetry in the \((2 \times 2)\) spaces. Hence, the wave functions in both subspaces do not have a definite parity.

The mixing of \( hh \) with \( lh \) states increases as we go away from the center of the Brillouin Zone, i.e., as \( \kappa \) differs from \( 0 \). The square modulus of the wave function \((D_{u, \ell})\) was evaluated by using the representation for the TM of first kind for the hole state. Taking advantage of (54) the following useful relation is obtained:

\[
D_{\ell}(E, \kappa, z) = D_u(E, \kappa, -z).
\]

where \( D_{u, \ell} \) are defined as

\[
D_{u, \ell}(E, \kappa, z) = \left[ M_{12}^{u, \ell}(z, z_0) F_{u, \ell}(z_0) \right]^\dagger \left[ M_{12}^{u, \ell}(z, z_0) F_{u, \ell}^\prime(z_0) \right],
\]

where \( M_{12}^{u, \ell}(z, z_0) \) are blocks of the TM of first kind \( M_{u, \ell}^{u, \ell} \), respectively.

C. TRI and SII symmetries for the \( \kappa = 0 \) case in the \((2 \times 2)\) KL model

At \( \kappa = 0 \) the hole states decouple in the case of no external field or no strain, given independent series of levels (35) for the infinite quantum well boundary conditions. Both \( \hat{H}_u \) and \( \hat{H}_l \) are diagonal and thus invariant under time reversal and space inversion operations. The time reversal operator in this case is \( \sigma_z \hat{C} \), which commutes with the Hamiltonian, and the wave functions satisfy

\[
\sigma_z F_{u, \ell}(-z) = p F_{u, \ell}(z),
\]

then the \( hh \) and \( lh \) components of the vectors \( F_{u, \ell}(z) \) posses definite but opposite parities. At the \( \Gamma \) point the \( up \) and \( low \) subspaces satisfy FC, TRI and SII and belong to the \textit{symplectic universality class}\textsuperscript{32}, as the original \((4 \times 4)\) space of solutions.
V. CONCLUSIONS

We establish the relation between the TM of the first kind (frequently used to determine the energy spectra) and the TM of the second kind (widely used in the scattering approach) in general and for the specific case of KL Hamiltonian model. This relation allows us to take the advantage of using the appropriate transfer matrix according to the circumstances one is dealing with. It is possible to avoid the usual assumptions and restrictions that the current descriptions face in describing tunnelling of holes\textsuperscript{11,56–60}.

We deduce new symmetry requirements on the TM of the first kind $M_{fd}$ and SHI requirements on TM of the second kind $M_{sv}$ for $N > 1$ case of actual interest in quantum-transport problem. Any EFA model having a master equation like that of the References 36,37 are expected to have the same or similar properties. In fact, a great part of the analysis carried out in sections II and III can be extended to those problems with minor changes.

We made clear that the symmetry analysis in the reduced (2 × 2) subspaces of the KL model demand attention to prevent erroneous statements\textsuperscript{11}. We show that for $\kappa \neq 0$ the time reversal and space inversion invariance requirements of the (4 × 4) KL Hamiltonian does not imply the invariance of the “up” and “low” Hamiltonians and related objects, separately. However, to fulfill the whole Hamiltonian invariance they have to transform one to the other according to the corresponding expressions obtained here. It has been also deduced that for $\kappa = 0$, the “up” and “low” subspaces recover continuously the time reversal and space inversion symmetries, as expected.

Besides the basic interest of this topic, the relations obtained here are useful and convenient in controlling bothersome numerical calculations, as well as in studying the relevant quantities in the multichannel-multiband tunnelling of holes within a more realistic approach. Expressions of section III were verified numerically within computer uncertainty.

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APPENDIX A: PARAMETERS OF THE (2 × 2) $\hat{H}_u$ AND $\hat{H}_l$ KL HAMILTONIANS

\[
\begin{align*}
  k_\pm &= k_x \pm i k_y; \\
  A_1 &= \frac{\hbar^2}{2 m_0} (\gamma_1 + \gamma_2); \\
  B_1 &= \frac{\hbar^2}{2 m_0} (\gamma_1 + 2 \gamma_2); \\
  C_{xy} &= \sqrt{3} \frac{\gamma_2^2}{2 m_0} \sqrt{\gamma_2^2 + 4 \gamma_3^2 k_x^2 k_y^2}; \\
  D_{xy} &= \sqrt{3} \frac{\hbar^2}{2 m_0} \gamma_3 \kappa
\end{align*}
\]

(A1)

The non-ortonormalized spinor components $g_{ij}$

\[
\begin{align*}
  g_{11} &= A_2 \kappa^2 + B_1 q_1^2 + V(z) \\
  g_{13} &= A_2 \kappa^2 + B_1 q_3^2 + V(z) \\
  g_{22} &= -(C_{xy} + i D_{xy} q_2) \\
  g_{24} &= -(C_{xy} + i D_{xy} q_4) \\
  g_{31} &= A_1 \kappa^2 + B_2 q_1^2 + V(z) \\
  g_{33} &= A_1 \kappa^2 + B_2 q_3^2 + V(z) \\
  g_{42} &= -(C_{xy} + i D_{xy} q_2) \\
  g_{44} &= -(C_{xy} + i D_{xy} q_4)
\end{align*}
\]

(A2)
from $\hat{\mathcal{H}}_u$ and $\hat{\mathcal{H}}_l$ peculiarities follow

\[
\begin{align*}
q_2 &= -q_1 \\
q_4 &= -q_3 \\
g_{11} &= g_{12} \\
g_{13} &= g_{14} \\
g_{22} &= g_{21} \\
g_{24} &= g_{23} \\
g_{31} &= g_{32} \\
g_{33} &= g_{34} \\
g_{42} &= g_{41}^* \\
g_{44} &= g_{43}^* \\
\end{align*}
\]

(A3)

being

\[
\begin{align*}
\{g_{1j}, g_{3j} &\text{ real} \\
g_{2j}, g_{4j} &\text{ complex} \}
\end{align*}
\]

The Lüttinger parameters $\gamma_1, \gamma_2, \gamma_3$ typify each layer of the heterostructure.

**APPENDIX B: TRANSFORMATION SYMMETRY MATRICES**

Given the transformation between the matrices $M_{fd}(z, z_0)$ and $M_{sv}(z, z_0)$, it is easy to see that the FC constrain on $M_{sv}(z, z_0)$ (Sec.III) implies that

\[
\Sigma_z = (\mathcal{N}^{-1})^{-1} J_{fd} \mathcal{N}.
\]

(B1)

However, it is worth noticing that, whenever the basis of linearly independent KL Hamiltonian eigenvectors, is not an orthogonal basis, we will have

\[
J_{fd} = \begin{bmatrix}
    u^t(z) & -v(z) \\
    v(z) & O_4
\end{bmatrix}.
\]

For TRI and SII requirements on the TM $M_{sv}(z, z_0)$ (Sec.III) we used the matrices $\Sigma_x$ and $S_{sv}$, respectively, which read

\[
\Sigma_x = \mathcal{N}^{-1} \Sigma^{-1} \mathcal{N}^*, \quad S_{sv} = \mathcal{N} \Sigma \mathcal{N}^{-1}.
\]

(B2)

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