Coupled spinors orthonormalization criterion in multiband systems

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Some fundamental physical quantities are determined by solving the eigenvalue problem that comes from a system of N coupled second order linear differential equations. An uncommon scenario evolves from the second order derivatives that appear in most multiband Hamiltonians, which leads to wave function spaces with non orthogonal axes. This notorious property has often been ignored by many authors. In this paper we discuss a possible criterion for the orthonormalization of eigenspinors (N×1) derived from the eigenvalue quadratic problem associated to the differential equation system. Such eigenspinors are taken as the basis on which the propagating wave modes system is built. When the norm of the new space is reformulated, the non-standard character of the weighted internal product comes to the forefront. This scheme has been successfully applied to the study of hole tunneling as it is described by the (4×4) Kohn Lüttinger model.

Keywords: Quadratic eigenvalue problem; normalization; polynomial matricial equation.

Varias magnitudes físicas fundamentales, son determinadas a través de la solución de problemas de autovalores, derivados de sistemas de N ecuaciones diferenciales lineales, acopladas y de segundo orden. Un escenario inusual, es el que evoluciona a partir de las derivadas de segundo orden, que aparecen, en la mayoría de los Hamilltonianos multibandas, lo cual conduce a espacios de Hilbert, de ejes no-ortogonales para la función de onda. Esta notoria propiedad, ha sido ignorada frecuentemente por muchos autores. En este artículo, discutimos un posible criterio de ortonormalización de los auto-espinores (N×1), derivados del problema cuadrático de valores propios, asociado a la ecuación dianámica del sistema. Tales autoespinores, son tomados como base para expandir los modos propagantes a través de una heteroestructura. Cuando se reformula la norma del nuevo espacio, el cáracter no estándar del producto interno pesado -sobre el que descansa la nueva norma-, pasa a un primer plano. El presente esquema, ha sido aplicado con éxito, en el estudio del tunelaje de huecos, cuyo marco teórico es el modelo de dos bandas de Kohn-Lüttinger (4×4).

Descriptores: Problema cuadrático de autovalores; normalización; ecuación polinomial matricial.

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1. Introduction

Several relevant physical quantities are convincingly determined through the solution to the eigenvalue problem that stems from a second order differential system of N coupled equations. In this paper, we will briefly go through the quadratic (QEP), generalized (GEP) and standard eigenvalue problems (SEP). Currently, the QEP is the one receiving more attention because of its applications to several fields such as dynamic structural mechanism analysis, acoustic systems, electric circuit simulation, fluid mechanics, linear algebra problems, signal processing and, lately, nano(micro) electrical system modeling [1], and the study of hole quantum transport [2,3]. These two last applications seem to be the most enticing, because of their contribution to the emerging fields of Optoelectronics and Nanotechnology.

The benefits of the QEP we have just mentioned do not include a comprehensive presentation of all the fields where this complicated problem could be applied. As a matter of fact, the number of practical applications persistently grows as the methods to solve the QEP [4,5] and the GEP [4,5] increase and become more diverse. This report is a contribution to that trend, since it presents a criterion for the orthonormalization of the eigenvectors (eigenspinors) of the SEP obtained from a $\boldsymbol{k}\cdot\boldsymbol{p}$ multiband Hamiltonian.

The most relevant algebraic distinction between the QEP and the GEP/SEP is that the quadratic problem has $2N$eigenvalues, with their respective $2N$ eigenvectors (left and right) which, strictly speaking, do not form an independent linear set. Within the wide range of problems whose systems are properly described by the envelope function approximation (EFA), the QEP has hardly been explored to our knowledge, and certainly it has not been dealt with as often as the GEP and the SEP. Certainly, the orthonormalization procedure in relation to the EFA for multiband Hamiltonians is not trivial, and its difference from routine procedures fundamentally comes from the presence of first derivative terms (linear elements of momentum) in the Hamiltonian. This difference is quite relevant when it comes to the electronic problem within the effective mass approximation (EMA) to a band.

Even if here we are addressing the general problem of Ncoupled components, our implicit goal is dealing with the QEP associated to the Kohn-Lüttinger model (KL) [6-9], where $N=$4.

2. QEP linearization

We understand linearization as the process whereby the QEP (which is non-linear by definition) is transformed into its corresponding GEP and SEP, that is, into equivalent linear problems with the same eigenvalues. The properties of second order differential equation systems have been thoroughly analyzed by Lancaster [10] and, later on, by Ghoberg, Lancaster and Rodman [11]. In their studies, the algebraic problem coming from the attempt to solve a system such as the ones we have mentioned is dealt with from a mathematical perspective. In a later date, F. Tisseur and K. Meerbergen [1] worked on a detailed study on this topic. They start by mentioning a wide range of technological and academic problems leading to systems for which an associated QEP can be defined, *i.e.* an eigenvalue problem where there is a square eigenvalue and terms in a first derivative.

The movement equation in multiband systems, which does not vary in relation to movements in the $[x, y]$ plane is [12,13]

$$\frac{d}{dz}\left[\mathrm{B}(z)\frac{d\mathbf{F}(z)}{dz} + \mathbf{P}(z)\mathbf{F}(z)\right] + \mathbf{Y}(z)\frac{d\mathbf{F}(z)}{dz} + \mathbf{W}(z)\mathbf{F}(z) = \mathbf{O}_{Nx1}, \qquad (1)$$

where $\mathrm{B}(z)$, $\mathbf{P}(z)$, $\mathbf{Y}(z)$, $\mathbf{W}(z)$ are (N × N) matrices mostly hermitian in the formal sense, and whose detailed form in specific cases might be found in references [12-14]. Here and in the rest of the paper $\mathbf{O}_N/\mathbf{I}_N$, will represent the N null/identity matrix. The N unknown functions are called *envelope* functions and may be collected in an N component vector which we will represent as $\mathbf{F}(z)$ being z the coordinate in the quantization direction.

Thus, by proposing a solution to the differential problem (1) of the form

$$\mathbf{F}(z) = \sum_{j=1}^{2N} \alpha_j e^{i\lambda_j z}\varphi_j = \sum_{j=1}^{2N} \alpha_j \mathbf{F}_j(z) \qquad (2)$$

where α_j contains the linear combination quotients and the corresponding normalization constants of the $\mathbf{F}_j(z)$ in the configuration space, λ_j is real or complex and φ_j is a (N×1) spinor, we get the following algebraic problem which determines the QEP associated to (1)

$$\mathbf{Q}(\lambda)\varphi = \{\lambda^2\mathbf{M} + \lambda\mathbf{C} + \mathrm{K}\}\varphi = \mathbf{O}_{Nx1} \qquad (3)$$

where λ is the eigenvalue, and the φ spinors are the eigenvectors (eigenspinors). Here $\mathbf{M}$, $\mathbf{C}$ and $\mathbf{K}$ are (N × N) matrixes which usually depend on z. The general properties of the Eq. (3) are displayed in Table I of Ref. 1. We will focus to the case where $\mathbf{M}$, $\mathbf{C}$ and $\mathbf{K}$ are hermitians and, therefore, λ are real or appear in coupled pairs (λ, λ^*), since it is the one that corresponds to the systems being studied by us; those described by Hamiltonians in the different methods for the widely-known $\mathbf{k}\cdot\mathbf{p}$ approximation [8,15-28].

If $\{\mathbf{A} - \lambda\mathbf{B}\}$ is a linear (2N×2N) matrix in λ and is taken as the *linearization* of $\mathbf{Q}(\lambda)$ [1,11]; a simple way to build the linear form found in (3) with identical eigenvalues is using the substitution $\mu = \lambda\varphi$ in (3) and reformulating the equation as [1]

$$\{\lambda\mathbf{M} + \mathbf{C}\}\,\mu + \mathbf{K}\phi = \mathbf{O}_{Nx1} \qquad (4)$$

which then leads to the associated GEP [1]

$$\begin{bmatrix} \mathbf{O}_N & \mathbf{N} \\ -\mathrm{K} & -\mathbf{C} \end{bmatrix}\begin{bmatrix} \phi \\ \mu \end{bmatrix} - \lambda\begin{bmatrix} \mathbf{N} & \mathbf{O}_N \\ \mathbf{O}_N & \mathbf{M} \end{bmatrix}\begin{bmatrix} \phi \\ \mu \end{bmatrix} = \{\mathbf{A} - \lambda\mathbf{B}\}\begin{bmatrix} \phi \\ \mu \end{bmatrix} = \mathbf{O}_{2Nx1} \qquad (5)$$

Usually $\mathbf{N} = \mathbf{I}_N$ or one of its multiples are to be chosen [1]. Other authors have used other ways to linearize the matricial polynomial $\mathbf{Q}(\lambda)$ [10].

In order to obtain physical observable data associated to (5) one must make the simultaneous diagonalization of matrices $\mathbf{A}$ and $\mathbf{B}$. There is a known solution for this problem in the case of vibrating mechanical systems, under a small oscillation regime. [29]. Nevertheless, the test of the GEP (5) for quantum systems described by $\mathbf{k}\cdot\mathbf{p}$ Hamiltonians may end up being a failed procedure, even when powerful symbolic calculation applications are used.

Therefore, the next step may be convenient. There, the GEP would be reduced to a solvable SEP. In order to do this $\mathbf{B}$ must be non-singular. Then, the following cases are possible:

$$(\mathbf{A}\mathbf{B}^{-1} - \lambda\mathbf{I}_{2N})\mathbf{B}\begin{bmatrix} \varphi \\ \mu \end{bmatrix} = \mathbf{O}_{2Nx1} \qquad (6)$$

$$(\mathbf{B}^{-1}\mathbf{A} - \lambda\mathbf{I}_{2N})\begin{bmatrix} \varphi \\ \mu \end{bmatrix} = \mathbf{O}_{2Nx1} \qquad (7)$$

The eigenvalues in (6) and (7) are the same as those in the QEP (3). But, on the other hand, the eigenvectors in both problems are different as it may be easily seen; nevertheless it is easy to obtain ϕ from (6) and (7), where ϕ is the eigenspinor of the original QEP.

It is worth noting that solutions to this problem have proved to be quite stable. These solutions have been studied for vibrating systems with different parameters [5]. In the case of quantum transport of carriers, which is one of the problems we have taken into consideration for this study, stability is strongly determined by the properties of the QEP's eigenspinors (we will address this issue in the following section) and by the features of the eigenvalues. The solutions obtained within a certain range of energies are complex or, being real, lack physical meaning for the given problem. Nevertheless, when studying tunneling phenomena both kinds of solutions are valid, and the evanescent ones represent a decisive contribution to channel interference mechanisms, both for electrons [30] and for holes [2,9,31].

3. QEP Eigenspinor orthonormalization

In order to get unitary flux solutions when a multichannel-multiband quantum transport problem is being solved [2,9] it is vital to build a space with orthogonal and normalized axes where independent linear solutions may be expanded. Some authors have invoked alternative procedures to face this question [32,33]. We will address that problem in this section.

Once we have obtained the GEP associated to the QEP it will be useful to define the right and left (2N×1) dimension vectors, which will be noted as ω_i and ψ_i respectively [1]

$$\omega_i = \left[\begin{array}{c} \varphi_i \\ \lambda_i \varphi_i \end{array} \right] \tag{8}$$

$$\psi_i = \left[\begin{array}{c} \vartheta_i \\ \lambda_i^* \vartheta_i \end{array} \right] \tag{9}$$

when substituting those in the QEP (3) and in the equations:

$$\mathbf{Q}(\lambda_i)\varphi_i = \mathbf{O}_{Nx1},$$

$$\vartheta_i^\dagger \mathbf{Q}(\lambda_i) = \mathbf{O}_{Nx1}$$

after a first linearization has been made, we get

$$\psi_i^\dagger(\mathbf{A} - \lambda_i \mathbf{B})\omega_i = 0. \tag{10}$$

This leads us to

$$\psi_i^\dagger \mathbf{A}\omega_i - \lambda_i \psi_i^\dagger \mathbf{B}\omega_i = 0, \tag{11}$$

whose simplest option

$$\left\{ \begin{array}{c} \psi_i^\dagger \mathbf{A}\omega_i = \lambda_i \\ \psi_i^\dagger \mathbf{B}\omega_i = 1 \end{array} \right\}, \tag{12}$$

can be generalized to the $2N$ eigenvalues λ_i. Let us introduce first

$$\begin{aligned} \mathbf{\Lambda} &= \text{diag}(\lambda_1, \lambda_2, ..., \lambda_{2N}) \\ &= \text{diag}\left(\psi_1^\dagger \mathbf{A}\omega_1, ..., \psi_{2N}^\dagger \mathbf{A}\omega_{2N}\right), \end{aligned} \tag{13a}$$

and the identity matrix

$$I_{2N} = \text{diag}\left(\psi_1^\dagger \mathbf{B}\,\omega_1, \psi_2^\dagger \mathbf{B}\,\omega_2, ..., \psi_{2N}^\dagger \mathbf{B}\,\omega_{2N}\right). \tag{13b}$$

Next we represent

$$\mathbf{\Psi} = \text{diag}(\psi_1, \psi_2, ..., \psi_{2N}), \tag{13c}$$

$$\mathbf{\Omega} = \text{diag}(\omega_1, \omega_2, ..., \omega_{2N}), \tag{13d}$$

and also include the ($4N^2 \times 4N^2$) diagonal matrices

$$\tilde{\mathbf{A}} = \text{diag}(\mathbf{A}, \mathbf{A}, ..., \mathbf{A}), \tag{13e}$$

$$\tilde{\mathbf{B}} = \text{diag}(\mathbf{B}, \mathbf{B}, ..., \mathbf{B}). \tag{13f}$$

Finally, we may re-write (12) and conclude that the normalization conditions imposed on $\mathbf{\Psi}$ and $\mathbf{\Omega}$ [1] can be quoted as

$$\mathbf{\Psi}^\dagger \tilde{\mathbf{A}} \mathbf{\Omega} = \mathbf{\Lambda}, \tag{14}$$

$$\mathbf{\Psi}^\dagger \tilde{\mathbf{B}} \mathbf{\Omega} = \mathbf{I}_{2N}. \tag{15}$$

Therefore it is straightforward for each eigenvector (left and right) that

$$\psi_i^\dagger \mathbf{A}\omega_j = \lambda_i \delta_{ij}, \tag{16a}$$

$$\psi_i^\dagger \mathbf{B}\omega_j = \delta_{ij}, \tag{16b}$$

and we remark how Eqs. (14) and (15) entail a change of base yielding simultaneously diagonalized matrices.

If we now substitute $\mathbf{A}$ and $\mathbf{B}$ in (16a) and (16b) by each of their own linearization forms (5), then we can easily obtain the conditions that should be satisfied by the eigenspinors in the original QEP (3)

$$\vartheta_i^\dagger \left(\lambda_i \mathbf{I}_N - \lambda_i \mathbf{K} + \lambda_i \lambda_j \mathbf{C}\right) \phi_j = \vartheta_i^\dagger \mathbf{L}^{\langle ij \rangle} \phi_j = \lambda_i \delta_{ij} \tag{17}$$

$$\vartheta_i^\dagger (\mathbf{I}_N + \lambda_i \lambda_j \mathbf{M})\varphi_j = \vartheta_i^\dagger \mathbf{D}^{\langle ij \rangle} \varphi_j = \delta_{ij}, \tag{18}$$

with the particular outcome

$$\mathbf{L}^{\langle ij \rangle} = \lambda_j \mathbf{I}_N - \lambda_i \mathbf{K} + \lambda_i \lambda_j \mathbf{C} \tag{18a}$$

$$\mathbf{D}^{\langle ij \rangle} = \mathbf{I}_N + \lambda_i \lambda_j \mathbf{M}. \tag{18b}$$

For the kind of systems we have defined in Section 1, the formal hermitian character of the matrices of the corresponding QEP establishes that $\vartheta_i^\dagger = \varphi_j^\dagger$ $(\forall \lambda_{i,j} \ \in \mathrm{R})$, therefore the matricial arrangements $\mathbf{L}^{\langle ij \rangle}$ and determine the internal product of the space we have generated departing from the original QEP.

We should note that, when solving a multichannel-multiband quantum transport problem, the matricial arrangements $\mathbf{L}^{\langle ij \rangle}$ and $\mathbf{D}^{\langle ij \rangle}$ determine the internal product of the space we have generated departing from the original QEP.

We should note that, when solving a multichannel-multiband quantum transport problem, the matricial arrangements $\mathbf{L}^{\langle ij \rangle}$ and $\mathbf{D}^{\langle ij \rangle}$ are not standard; since (18a) and (18b) are explicitly dependent upon the eigenvalues and therefore change along with them.

The expressions (17) and (18) have been deduced from the QEP [1]. For the sake of simplicity, from this point onwards we will use the expression (18b) to reformulate the norm of the new space, which will be justified further on.

In general, the norm for the new space will be established by the weighted internal product defined by:

$$\langle \varphi_j | \varphi_j \rangle = \sum_{kl} (\varphi_j^\dagger)_k (\mathbf{D}^{\langle \varphi_i | \varphi_j \rangle})_{kl} (\varphi_j)_l = \|\varphi_i\|^2 = 1 \tag{19}$$

Where the superindexes $\langle ij \rangle$ in the matricial arrangements determine the labels of what we shall call *spinorial weighted internal product of associated eigenvalues*. Notice that the eigenspinors satisfy

$$\langle \varphi_i | \varphi_j \rangle = \varphi_i^\dagger \mathbf{D}^{\langle ij \rangle} \varphi_j = \delta_{ij}; \quad \forall\, i, j;\ i < j \tag{20}$$

If we assume, for completeness, that the weighted internal product (19) is non commutative

$$\langle\varphi_j|\varphi_i\rangle - \langle\varphi_i|\varphi_j\rangle = \varphi_j^\dagger\left(\mathbf{D}^{\langle ji\rangle}\right)\varphi_i - \varphi_i^\dagger\left(\mathbf{D}^{\langle ij\rangle}\right)\varphi_j \neq 0,$$

given the character of the dynamic equation quotients and the form of the matricial arrangement $\left(\mathbf{D}^{\langle ij\rangle}\right)^\dagger = \left(\mathbf{D}^{\langle ji\rangle}\right)^\dagger$, the condition for the commutability of the weighted internal product should demand that

$$\left[\mathbf{D}^{\langle ji\rangle} - \left(\mathbf{D}^{\langle ji\rangle}\right)^\dagger\right] = 2iIm\left\|\lambda_j\lambda_i\right\|\mathbf{M} = \mathbf{O}_{Nx1}, \quad (21)$$

which is only fulfilled when $\lambda_i = \lambda_j^*$. Normalization (20) is not affected by this mimicked "leak" in the orthogonality of the φ_i –which we had assumed for completeness in our analysis-, because of the features of the space that has been built.

We should note that the $\mathbf{D}^{\langle ij\rangle}$ matricial arrangement (18b) is not only commutative as it has already been proved above, but it is also defined as positive if: $\mathbf{I}_{2N}+\lambda_i\lambda_j\mathbf{M}>\mathbf{0}$, for every vector $\mathbf{X} \neq \mathbf{0}$ with $\mathbf{X} \in \mathrm{R}^{2N}$, that yields $\mathbf{X}^\dagger\,\mathbf{D}^{\langle ji\rangle}\mathbf{X} > 0$. Since $\mathbf{D}^{\langle ij\rangle}$ is hermitian, its eigenvalues are real; and if we consider that $\mathbf{M}$ is diagonal by construction, then

$$1 + \lambda_i\lambda_j m_{ii} > 0 \;\rightarrow \lambda_i\lambda_j > -\left(\frac{1}{m_{ii}}\right).$$

Despite the non-standard weighting-function (18b), the commutability of $\mathbf{D}^{\langle ij\rangle}$, together with its positive-defined character, assure a well-defined and non-degenerate weighted internal product for the spinorial space.

If we are dealing with electric charge conservation processes for multiband-multicomponent quantum transport of charge carriers, it would be convenient not to depart from an orthonormal basis. We can orthonormalize the $\{\phi_1, \phi_2, \ldots \phi_{2N}\}$ set of eigenvectors from the SEP (6), by the Gram-Schmidt procedure; where the weighting-function role is played by the matricial arrangement (18b) and $\{\mathbf{\Phi}_1, \mathbf{\Phi}_2, \ldots \mathbf{\Phi}_{2N}\}$ is a set of orthogonal eigenvectors, *i.e.*

$$\begin{aligned}
\mathbf{\Phi}_1 &= \varphi_1\\
\mathbf{\Phi}_2 &= \varphi_2 - \frac{\langle\varphi_2|\mathbf{\Phi}_1\rangle}{||\mathbf{\Phi}_1||^2}\mathbf{\Phi}_1\\
\mathbf{\Phi}_3 &= \varphi_3 - \frac{\langle\varphi_3|\mathbf{\Phi}_1\rangle}{||\mathbf{\Phi}_1||^2}\mathbf{\Phi}_1 - \frac{\langle\varphi_3|\mathbf{\Phi}_2\rangle}{||\mathbf{\Phi}_2||^2}\mathbf{\Phi}_2\\
\mathbf{\Phi}_i &= \varphi_i - \frac{\langle\varphi_i|\mathbf{\Phi}_1\rangle}{\|\mathbf{\Phi}_1\|^2}\mathbf{\Phi}_1 - \frac{\langle\varphi_i|\mathbf{\Phi}_2\rangle}{\|\mathbf{\Phi}_2\|^2}\mathbf{\Phi}_2\\
&\quad - \frac{\langle\varphi_i|\mathbf{\Phi}_3\rangle}{\|\mathbf{\Phi}_3\|^2} - \ldots - \frac{\langle\varphi_i|\mathbf{\Phi}_{i-1}\rangle}{\|\mathbf{\Phi}_{i-1}\|}\mathbf{\Phi}_{i-1}. \quad (22)
\end{aligned}$$

Since the (N×1) ϕ_i eigenvalues are linearly independent, each orthonormalized (N × 1) eigenspinor has the following shape

$$\tilde{\mathbf{\Phi}}_i = \frac{\mathbf{\Phi}_i}{||\mathbf{\Phi}_i||^2}; \quad i = 1, 2, \ldots 2N. \quad (23)$$

The matricial arrangement (18b), we have chosen to discuss and reformulate the norm of the new spinorial space is trustworthy; since there are known numerical results for several physical phenomena which may be experimentally confronted, as well as widely acknowledged theoretical predictions which have been successfully obtained from (18b) in the study of hole tunneling. For the sake of consistency, we will briefly comment on this issue in short.

For instance, when Sánchez and Proetto [24] introduced the so-called pseudo-unitarity of the scattering matrix as

$$\mathbf{S}^\dagger\mathbf{J}\mathbf{S} = \mathbf{J},$$

they developed their problem departing from an orthonormalized base in the configuration space only. However, when a totally orthonormalized base is considered (configuration space and spinorial space), the

$$\mathbf{S}^\dagger\mathbf{S} = \mathbf{I}_N$$

standard unitarity is fully recovered [2]. Experimentally E. Méndez, Leo Esaki, *et al.* [34], had obtained the hole levels of a quantum well embedded in a semiconductor heterostructure from photoluminiscence data. On the other hand, Wessell and Altarelli [32] were able to appropriately determine most of these levels through their model. Sometime later, L. Diago-Cisneros *et al.* managed to reproduce those very levels with more accuracy (some of them with extremely good precision), through their multicomponent scattering approximation (MSA) [2]. With their model, P. Mello, P. Pereyra, and N. Kumar [35] obtained an expression for the probability flux density within the effective mass approximation (case N=1), in a model where the standard unitarity of the scattering matrix, was proved even for a stochastic metallic model. It is possible to prove that the results of P. Mello *et al*. are reproduced within the (N $\geq$2) MSA, when uncoupled modes are properly considered [36].

On the other hand D. Dragoman and M. Dragoman [37], proposed a single–chip device involving electrons and holes. In their experiment, they measured a 10^{-13} s order tunneling time for light and heavy holes. Within the MSA [2], it can be obtained the same order for the phase transmission time for light and heavy holes where no external magnetic fields were considered. A long time ago, T.E Hartman [38] had foreseen the autonomy of tunneling time, regarding the thickness of the potential scatterer for almost opaque barriers. Experimental evidences for Hartman's classical prediction for photons and electrons have been published elsewhere. Numerical simulations for Hartman's prediction have been obtained within the MSA, for coupled [2] as well as for uncoupled holes [6] by the phase time formalism. A. Kadigrobov *et al.* [39], N.K. Allsop *et al.* [40], and P. Pereyra [41] have also reported giant conductance conditions (maximum resonant transmittance) in different physical systems. Evidences

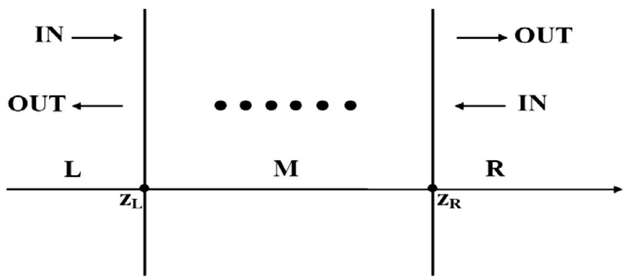

FIGURE 1. General scattering scheme of the system under study. Noteworthy implicit cases are: (i) simple interface between layers L and R; (ii) compound layers directly on top of each other or (iii) any intermediate embedded structure that might exist between them.

of giant conductance for uncoupled holes have been obtained in relation to the MSA [42] as well. Experimental measurements by A.P. Heberle *et al.* [43] for electron and hole tunneling time through semiconductor layered system, have been nicely reproduced for holes in the framework of the MSA [2]. Numerical evidences of superluminal events were obtained for the transmitted phase time [44], while appealing phase time dependencies for electrons traversing a simple cell, and a superlattice were also reported [44]. That phenomenology was found for the quantum transport of heavy and light holes, modeling in the framework of the MSA [42].

4. Real eigenvalues

In this subsection we will present a study where we will take the case of coupled incident/emerging states (see Fig. 1)^i as they are described in relation to the EFA as a point of departure. We will also explicitly demand the specific orthonormalization requirements adequate for the EFA case on the base of linearly independent functions (LI). Therefore, we will have to consider that the base has been fully orthonormalized. We will consider, *a priori*, that the LI solutions have been orthonormalized in the configuration space. We consider that the system is properly described at all times in relation to the EFA.

Let us start by determining certain orthonormality conditions in the function spinorial space which are far from being the only possible ones as already mentioned above. If we call $\mathbf{F}_j(z)$ the (N×1) LI vectors that form an orthonormal base to represent an envelope state (2) of the system (1), we can take, in particular

$$\mathbf{F}_j(z) = \mathbf{\Gamma}_j e^{iq_j z}, \tag{24}$$

for the L and R regions (see Fig. 1) of constant parameters, *i.e.* the matricial quotients $\mathrm{B}(z)$, $\mathbf{P}(z), \mathbf{Y}(z)$ and $\mathbf{W}(z)$ are no longer dependent on z and are constant in certain segments. Vectors $\mathbf{\Gamma}_j$ are (N×1) spinors and they do not depend on spatial coordinates, while q_j vectors are the corresponding $2N$ eigenvalues as a solution to the algebraic problem. If we substitute (24) in (1) we obtain

$$-q_j^2\mathbf{B}\cdot\mathbf{\Gamma}_j + iq_j\left(\mathbf{P}+\mathbf{Y}\right)\cdot\mathbf{\Gamma}_j + \mathbf{W}\cdot\mathbf{\Gamma}_j = \mathbf{O}_{Nx1} \tag{25}$$

This is a QEP [1] as the one we presented on (3), but has been formulated in the terms of the matricial quotients of the dynamic Eq. (1). Here we have introduced new symbols for several relevant quantities to highlight the fact that the reader should assume that these quantities coincide, in general, with the case discussed in Subsec. 3.1.

If $\mathbf{P}$ is hermitian, there is not a coupling term for the status in the first derivative in the field, and the analysis is rather simplified as we will see further on. Nevertheless that is not the case if that matrix is antihermitian $\left(\mathbf{P} = -\mathbf{P}^\dagger\right)$, and therefore $\mathbf{P} - \mathbf{P}^\dagger = 2\mathbf{P}$. That is the case which is interesting for us, because it keeps the coupling between propagating modes departing from the existence of a linear term in q_j. That situation happens in systems such as Kohn-Lüttinger, Kane and others where N $\geq$ 2 [6]. If we also use the property $\mathbf{Y} = -\mathbf{P}^\dagger$, then we can obtain from (25)

$$-q_j^2\mathbf{B}\cdot\mathbf{\Gamma}_j + 2iq_j\mathbf{P}\cdot\mathbf{\Gamma}_j + \mathbf{W}\cdot\mathbf{\Gamma}_j = O_{Nx1} \tag{26}$$

If we apply the complex transconjugate operation to (26) and using the properties of the matricial quotients of (1), we get

$$\mathbf{\Gamma}_j^\dagger\cdot\left[-(q_j^2)^*\mathbf{B} + 2i(q_j)^*\mathbf{P} + \mathbf{W}\right] = \mathbf{O}_{1xN}. \tag{27}$$

We multiply (26) by $\mathbf{\Gamma}_k^\dagger$ on the left. Then we re-write (27) for $\mathbf{\Gamma}_k^\dagger$ and multiply (28) by $\mathbf{\Gamma}_j$ on the right. Subtracting the new expressions, and doing a little algebra the result is

$$\mathbf{\Gamma}_k^\dagger\cdot\left[\left\{(q_k^2)^* - (q_j^2)\right\}\mathbf{B} - 2i(q_k^* - q_j)\mathbf{P}\right]\cdot\mathbf{\Gamma}_j = 0. \tag{28}$$

If now we consider $q_i$with $i = k, j$ as real and –in general-, that $(q_j \neq q_k)$, we may factorize this expression dividing it by $(q_k - q_j)$. We then get:

$$\mathbf{\Gamma}_k^\dagger\cdot\left[\left\{q_k + q_j\right\}\mathbf{B} - 2i\mathbf{P}\right]\cdot\mathbf{\Gamma}_j = 0. \tag{29}$$

Here, orthogonality conditions (29), suggest that the following orthonormalization conditions should be used:

$$\mathbf{\Gamma}_k^\dagger\cdot\left[\left\{q_k + q_j\right\}\mathbf{B} - 2i\mathbf{P}\right]\cdot\mathbf{\Gamma}_j = \delta_{jk}\beta, \tag{30}$$

for $q_i$with $i = k, j$ being real, and β an arbitrary constant.

It should be useful to note that the case in which $\mathrm{B} = \mathbf{I}_N$ and $\mathbf{P} = \mathbf{Y} = \mathbf{O}_N$ corresponds to the uncoupled electronic problem as it is described by one Schrödinger equation [32]. Under these particular conditions, Eq. (29) becomes

$$(q_k + q_j)\mathbf{\Gamma}_k^\dagger\cdot\mathbf{\Gamma}_j = 0, \tag{31}$$

where LI solutions are orthogonal in every case except when $q_i = -q_k$, where we know them to be equal [32] . This scheme has been successfully used in the study of hole tunneling described by the KL model [2,6] as we have already commented at the end of the previous section. In order to do this we obtained a base of eigenspinors (4×1) on which we built the envelope $\mathbf{F}(z)$, whose flow is unitary within an acceptable range of the physical parameters [2,32]. Unlike what is stated in previous reports [33,34], the introduction of arbitrary normalization constants in the transmission quotients has not been necessary.

5. Conclusions

Common QEP-GEP-SEP eigenvalues, along with the easy correspondence between derived eigenvectors, allows us to elaborate a useful way to associate these problems. The largest and upmost direct benefit of this way of doing is a less complicated SEP problem from the analytic and numerical perspectives to deal with.

The construction of an orthonormalized-metric solution space associated to a mixed-multicomponent QEP, demands a matrix weighting-function to be hermitian, and therefore leading to real eigenvalues. The non-standard character of the commutative weighted internal product, is highlighted as the new space norm is systematically reformulated, due to its explicit dependence on the QEP's eigenvalues. However this unusual scenario, weighted internal product is trustworthy, since there are strike numerical results related to several physical phenomena of hole tunneling described by the MSA model, that can be compared with experiments and with widely acknowledged theoretical predictions.

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