TRANSFER MATRICES AND GREEN FUNCTIONS FOR THE STUDY OF ELEMENTARY EXCITATIONS IN MULTILAYERED HETEROSTRUCTURES

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ABSTRACT
This article is concerned with a mathematical tool, the Associated Transfer Matrix **T**, which proves useful in the study of a wide class of physical problems involving multilayer heterostructures. General properties of linear, second order differential matrix Sturm Liouville operators are discussed as a basis for establishing general properties of **T**, which is also generally related to the Green function **G**. Some identities satisfied by **T** are derived, which prove useful in practice to monitor the numerical quality of computational processes.

Key words: Transfer Matrix, Green function, heterostructure.

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RESUMEN
Este artículo trata de una herramienta matemática, la Matriz de Transferencia Asociada **T,** la cual resulta de utilidad en el estudio de una clase amplia de problemas físicos que involucran heteroestructuras multicapas. Se discuten propiedades generales de los operadores diferenciales lineales, de segundo orden matriciales de Sturm-Liouville como base para establecer las propiedades generales de **T**, que también se relaciona de manera genera con la Función de Green **G**. Se derivan ciertas identidades satisfechas por **T** que demuestran ser útiles en la práctica para supervisar la calidad numérica de procesos computacionales.

Palabras clave: Matriz de Transferencia, Función de Green, heteroestructura.

I. INTRODUCTION

Problems concerned with multilayer systems arise very often in different fields of physics. One has to integrate differential equations across some sequence of different domains, which raises the question of repeated matching at all interfaces involved. In particular, the development of efficient techniques of epitaxial crystal growth originated a great deal of work of this nature in solid state physics, notably -but not only- in the field of semiconductor quantum heterostructures[1,2].

A great deal of activity has also been concerned with *Quasiregular Heterostructures*[3] which follow some non periodic self-replicative sequence, of which the best known is the *Fibonacci sequence*[4]. In these cases the number of interfaces can be very large.

It is therefore of practical value to have mathematical tools available which can be useful in the study of such systems. Among these, the Surface Green Function Matching[1] has been extended to an arbitrarily large number of interfaces[5]. Green functions were generally related to a transfer matrix[6] which transfers amplitudes and normal derivatives -of which more will be said presently- but it was found later[7,8] that it is physically more appealing to introduce a different kind of transfer matrix, here denoted **T** and termed the *Associated Transfer Matrix* which is even simpler to operate with and is directly related to the physically interesting magnitudes of the problem under study.

The purpose of this article is to expound on the general relationship between **T** and the Green function **G**, to discuss some basic formal properties of **T** and to derive from this some general identities satisfied by **T** which can prove useful in practice. We shall deal explicitly with the case of planar geometry, although the analysis can also be adapted to other tractable geometries –e.g. spherical or cylindrical.

Irrespective of the specific physical nature of the states, modes, waves or quasiparticles we may be concerned with, the general setup is the following. We start from 3D linear, second order differential system and Fourier transform in the 2D (x,y) plane of the interfaces, thus introducing a 2D wavevector κ. We then have a system of N coupled, κ-dependent ordinary differential equations in the variable z, in the

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direction perpendicular to the interfaces. We stress that in practice N can be sufficiently large that an analytical study is impracticable. For instance, in electronic band structure calculations one can find multiband envelope function calculations of electronic band structure with N = 8[9] and N = 14[10] and pseudo-potential calculations with up to N = 65[11]. Thus, it is interesting to study in some detail the formal properties of an object, **T**[7], which is a useful tool for numerical computation.

The general formulation of the problem is setup in Section 2 and basic questions related to the hermiticity of linear, second order matrix differential Sturm-Liouville operators are discussed in Section 3. This provides a basis to study infinite domains and regularity at infinity –Section 4- after which the general relationship between **T** and the Green function **G** is established in Section 5. Finally, general properties and identities satisfied by **T** are derived in Section 6.

II. FORMULATION OF THE PROBLEM

The N coupled differential equations involve N coupled amplitudes corresponding to the physical model under study -e.g. the components of an electronic wavefunction in an N-band envelope function model or coupled elastic vibration amplitudes and electrostatic potential in piezoelectric waves. Loosely speaking, we shall refer to the 'primary field', for reasons presently explained.

The N amplitudes of the primary field will be condensed in an object, **F**(z), denoted for convenience as 'N-vector', which need not imply that it transforms literally as a vector.

We now consider the vast class of physical problems for which the differential system can be cast in a compact matrix form as

$$\mathbf{L}(z)\cdot\mathbf{F}(z) = \frac{d\mathbf{A}(z)}{dz} + \mathbf{Y}(z)\cdot\frac{d\mathbf{F}(z)}{dz} + \mathbf{W}(z)\cdot\mathbf{F}(z) = 0, \tag{1}$$

where we have defined another N-vector, namely

$$\mathbf{A}(z) = \mathbf{B}(z)\cdot\frac{d\mathbf{F}(z)}{dz} + \mathbf{P}(z)\cdot\mathbf{F}(z). \tag{2}$$

We denote this linear differential form, derived from **F**, as the *secondary field*. For instance, if **F** describes elastic strains, then **A** describes stresses. More precisely, normal stress components[1]. Furthermore, we are concerned with eigenvalue problems. The eigenvalue parameter, henceforth denoted Ω, is contained in **W**. The dependence on κ and Ω is understood throughout.

The z dependence of some, or all, of the (matrix) coefficients of (1) and (2) is an essential feature of heterostructures, even if piecewise homogeneous domains are involved.

Now, **F**(z) is obviously continuous everywhere and, furthermore, integration across any of the interfaces of the heterostructure proves that **A**(z) is also continuous, which bears out the convenience of this compact formulation. Since both, the primary field and the secondary field are continuous, this suggests the convenience of defining, instead of a transfer matrix **M**[1,6] which transfers **F**(z) and **F'**(z), a different one, here denoted as the Associated Transfer Matrix (ATM) **T**, which transfers the two fields that are continuous everywhere. Thus we define the 2N – vector

$$\Psi(z) = \begin{vmatrix}\mathbf{F}(z)\\ \mathbf{A}(z)\end{vmatrix} \tag{3}$$

and then, starting from any initial point z_0, we define **T**(z, z_0) which transfers Ψ from z_0 to any z by

$$\Psi(z) = \mathbf{T}(z, z_0)\cdot\Psi(z_0) \tag{4}$$

Unlike the *coefficient transfer matrix*, often used for systems with piecewise constant coefficients[12,13], **M**(z, z_0) and **T**(z, z_0) do not depend on knowing a basis of 2N linearly independent solutions. Both, **M**(z, z_0) and **T**(z, z_0), pertain to initial value problems, while the Green function **G**(z, z') depends on the choice of boundary conditions. Thus, for a given differential system **M** and **T** are unique, while **G** is not. The relationship between **G** and **M** was discussed in[1,6,15]. Here we discuss the relationship between **G** and **T**, for which we first study the general properties of the latter, for which first some observations concerning the differential system are in order.

III. THE HERMITICITY OF THE DIFFERENTIAL OPERATOR

The differential matrix **L**(z) of (1) is the representation of a linear differential operator which we now discuss. We recall[14] that the full definition of the operator requires the specification of the manifold **S** of functions –here termed 'vectors' **F**(z)- on which it acts.

Let $\hat{p}$ be an operator represented by the operating rule

$$p = -i\frac{d}{dz}. \tag{5}$$

So far, $\hat{p}$ is formally Hermitean[14], [Chapter 3]. Now let $\hat{\mathbf{L}}$, represented by the operating rule (1), be an operator defined to act on a given manifold **S** and let **F** denote the generic function of this particular manifold. We write the system (1) explicitly as

$$\mathbf{L}(z)\cdot\mathbf{F}(z) = \frac{d}{dz}\left[\mathbf{B}(z)\cdot\frac{d\mathbf{F}(z)}{dz}+\mathbf{P}(z)\cdot\mathbf{F}(z)\right] + \mathbf{Y}(z)\cdot\frac{d\mathbf{F}(z)}{dz}+\mathbf{W}(z)\cdot\mathbf{F}(z). \quad (6)$$

Thus, the operator $\hat{\mathbf{L}}$ represented by this equation is

$$\hat{\mathbf{L}} = -\hat{p}\,[\mathbf{B}\cdot\hat{p}+i\mathbf{P}\cdot] + i\mathbf{Y}\cdot\hat{p}+\mathbf{W}\cdot \quad (7)$$

where the dots indicate that, as a matrix, this is to act on vectors **F**. Furthermore, in most physical problems related to heterostructures the matrix coefficients satisfy the conditions

$$\mathbf{B}=\mathbf{B}^{\dagger},\qquad \mathbf{P}=-\mathbf{Y}^{\dagger}\qquad \mathbf{W}=\mathbf{W}^{\dagger}, \quad (8)$$

Thus, for the large class of problems we are concerned with we assume (8) to hold. Then it is easily seen that the *Hermitean* adjoint of $\hat{\mathbf{L}}$ is

$$\hat{\mathbf{L}}^{\dagger} = -\hat{p}^{\dagger}\mathbf{B}^{\dagger}\cdot\hat{p}^{\dagger}+i\hat{p}^{\dagger}\mathbf{Y}^{\dagger}\cdot+i\mathbf{P}^{\dagger}\cdot\hat{p}^{\dagger}+\mathbf{W}^{\dagger}\cdot, \quad (9)$$

which so far only ensures that $\hat{\mathbf{L}}$ is *formally Hermitean*.

We now, more specifically, define **S** as the manifold of functions defined in a given interval [a, b] -provisionally assumed to be finite- and satisfying given boundary conditions at its extremes. A physical example could be a quantum well with infinite barriers –vanishing amplitudes- in the external media. Let us then consider another operator $\hat{\mathbf{L}}_2$, acting on another manifold $\mathbf{S}_2$ of functions $\mathbf{F}_2$ defined in the same interval [a, b] but otherwise satisfying so far unspecified boundary conditions.

We define $\hat{\mathbf{L}}_2$ to be represented by

$$\mathbf{L}_2(z)\cdot\mathbf{F}_2(z) = \frac{d}{dz}\left[\mathbf{B}^{\dagger}(z)\cdot\frac{d\mathbf{F}_2(z)}{dz}-\mathbf{Y}^{\dagger}(z)\cdot\mathbf{F}_2(z)\right] - \mathbf{P}^{\dagger}(z)\cdot\frac{d\mathbf{F}_2(z)}{dz}+\mathbf{W}^{\dagger}(z)\cdot\mathbf{F}_2(z) \quad (10)$$

and then at every point z of the interval [a, b], by assumption common to **S** and $\mathbf{S}_2$, we define the residual **R**(z) by

$$\mathbf{R}(z)=\left[\frac{d\mathbf{F}^{\dagger}(z)}{dz}\cdot\mathbf{B}^{\dagger}(z)\cdot\mathbf{F}_2(z)-\mathbf{F}^{\dagger}(z)\cdot\mathbf{B}^{\dagger}(z)\cdot\frac{d\mathbf{F}_2(z)}{dz}+\mathbf{F}^{\dagger}(z)\cdot\mathbf{P}^{\dagger}(z)\cdot\mathbf{F}_2(z)+\mathbf{F}^{\dagger}(z)\cdot\mathbf{Y}^{\dagger}(z)\cdot\mathbf{F}_2(z)\right]^{\dagger}. \quad (11)$$

We then study the integral

$$\left\langle F_2\middle|\hat{\mathbf{L}}\mathbf{F}\right\rangle = \int_a^b dz\,\mathbf{F}_2^{\dagger}(z)\cdot\mathbf{L}(z)\cdot\mathbf{F}(z) \quad (12)$$

which, after partial integration, is

$$\left\langle F_2\middle|\hat{\mathbf{L}}\mathbf{F}\right\rangle = \left\langle F\middle|\hat{\mathbf{L}}_2\mathbf{F}_2\right\rangle^{\dagger}+\mathrm{R(b)}-\mathrm{R(a)}. \quad (13)$$

Now, since the matrix coefficients satisfy the conditions (8), the operating rule for $\hat{\mathbf{L}}_2$ is the same as for $\hat{\mathbf{L}}$, whence follows that the residual is

$$\mathbf{R}(z)=\mathbf{F}_2^{\dagger}(z)\cdot\mathbf{A}(z)-\mathbf{A}_2^{\dagger}(z)\cdot\mathbf{F}(z) \quad (14)$$

and thus the residual difference appearing in (13) is

$$\mathbf{R}(b)-\mathbf{R}(a)=\mathbf{F}_2^{\dagger}(b)\cdot\mathbf{A}(b)-\mathbf{A}_2^{\dagger}(b)\cdot\mathbf{F}(b) - \mathbf{F}_2^{\dagger}(a)\cdot\mathbf{A}(a)+\mathbf{A}_2^{\dagger}(a)\cdot\mathbf{F}(a). \quad (15)$$

The mathematical definition of **R** acquires a physical meaning in terms of the primary and secondary fields, the two objects transferred by **T**.

This is the central point of the analysis. The operators $\hat{\mathbf{L}}$ and $\hat{\mathbf{L}}_2$ are not yet fully defined, as the boundary conditions have not been specified. If we assume only that **S** and $\mathbf{S}_2$ are such that the combined effect of their boundary conditions is such that R(b) - R(a) vanishes, then

$$\left\langle F_2\middle|\hat{\mathbf{L}}\mathbf{F}\right\rangle = \left\langle F\middle|\hat{\mathbf{L}}_2\mathbf{F}_2\right\rangle^{\dagger} \quad (16)$$

and $\hat{\mathbf{L}}_2$ is the Hermitean adjoint of $\hat{\mathbf{L}}$.

If, furthermore, the boundary conditions are the same in **S** and $\mathbf{S}_2$, then $\hat{\mathbf{L}}_2$ -the Hermitean adjoint of $\hat{\mathbf{L}}$- is also equal to $\hat{\mathbf{L}}$ and it is then that $\hat{\mathbf{L}}$ is really Hermitean, that is to say, technically, it is *totally Hermitean*[14]. Such is the case, for instance, for electronic states with external infinite barriers, where all amplitudes vanish, or for elastic waves with external free surfaces, where all normal stresses vanish.

It seems reasonable to put forward this type of analysis to justify the basis of standard calculations for physical models with N > 1. Furthermore, this is the starting point to analyze a question directly relevant to the physical models employed in practice to study heterostructure.

IV. INFINITE DOMAINS: CAUSALITY AND REGULARITY AT INFINITY

This situation arises if the external media are semiinfinite or, simply, if one studies a bulk medium. So far it has been implicitly assumed that the eigenvalues are real, which is formally correct if the interval [a, b] is finite. We must now analyse the situation when this is infinite, for which a brief reminder of some basic facts is at this stage convenient. In order to fix ideas it suffices to consider a simple case with N = 1.

Firstly, we must define a sign convention for the description of stationary amplitudes F(z, t). We adopt the convention

$$F(z,t) = F_0\, e^{i(kz - wt)} \qquad (17)$$

for a wave travelling to the right. Then, when in the time dependent picture $t \to \infty$, in the stationary state time independent amplitude,

$$F(z) = F_0\, e^{ikz} \qquad (18)$$

the variable $z \to \infty$. In order for this to be a physically acceptable regular solution, it cannot blow up for $z \to \infty$, which requires formally (i) that the real wave-vector k, corresponding to the allowed eigenvalue of a stationary propagation eigenstate, be defined as

$$k = \lim_{\varepsilon \to 0}(k + i\varepsilon) \qquad (19)$$

and (ii) that we define the limit of F(z) for $z \to \infty$ as the *regular limit.*

$$\lim_{\varepsilon \to 0} \lim_{z \to \infty} F_0\, e^{i(k+i\varepsilon)z} = 0 \qquad (20)$$

The same analysis holds obviously for waves travelling to the left and $z \to -\infty$ and the same basic facts hold for less simple cases, e.g. for any N > 1.

Let us now return to the standard operator $\hat{\mathbf{L}}$ on which the analysis of the class of problems here considered is based. Since this is defined to act on the manifold **S** of functions which are regular at infinity, the second and fourth terms of the residual difference (15) vanish. However in order for (15) to vanish entirely, the condition on the adjoint of $\hat{\mathbf{L}}$ is that the boundary conditions of regularity at infinity must hold for the $\mathbf{F}_2^{\dagger}$, not the $\mathbf{F}_2$. In fact, in order for (15) to vanish the $\mathbf{F}_2$ must be precisely irregular at infinity, as only then the $\mathbf{F}_2^{\dagger}$, are regular. Therefore the manifold $\mathbf{S}_2$ is not the same as **S** and we reach the non trivial conclusion that $\hat{\mathbf{L}}$, the operator normally used in the description of infinite -or, in the event- semiinfinite regular media is *not totally Hermitean*.

Although a full analysis in general terms([16], §7.5) of the conditions at infinity is outside the scope of this article, it is in order to recall that while regularity at infinity is the physical requirement in the stationary state -time independent- picture, causality is the condition required in standard physical theory, and this in turn requires ω to be defined as the limit of $(\omega + i\eta)$ for $\eta \to 0$. Now, for the class of problems here considered ω bears a direct relation to the eigenvalue variable Ω. For instance, for electronic states Ω is the energy and ω is $\Omega/\hbar$;; for most wave problems ω is $\Omega^{1/2}$, etc. Then the causal formulation amounts to requiring that Ω is to be read everywhere as

$$\Omega = \lim_{\eta \to 0}(\Omega + i\eta). \qquad (21)$$

Even for bound states, for which the eigenvalue is real, a small imaginary part may have to be added in practice, for instance, when calculating spectral functions numerically with a computer code. The point to stress is that (21) must be kept as such everywhere and this has a direct bearing on the foregoing analysis.

It is correct to define $\hat{\mathbf{L}}^{\dagger}$, the *Hermitean conjugate* of an operator $\hat{\mathbf{L}}$ as has been done, but in the matrices resulting in the z-representation, where Ω appears explicitly, it must always be kept $\Omega + i\eta$, whether η stays small but finite or it tends to zero as in (21). In other words, while the standard *Hermitean conjugate* of a matrix of the general form

$$\mathbf{m}(\Omega) = \mathbf{m}_1(\Omega) + i\mathbf{m}_2(\Omega) \qquad (22)$$

is

$$\mathbf{m}^{\dagger}(\Omega) = \mathbf{m}^{\,t}_1(\Omega^*) - i\mathbf{m}^{\,t}_1(\Omega^*), \qquad (23)$$

this is not the concept required for an explicit matrix analysis of the problems here considered. The concept of *transconjugate* matrix

$$\mathbf{m}^{c}(\Omega) = \mathbf{m}^{\,t}_1(\Omega) - i\mathbf{m}^{\,t}_2(\Omega) \qquad (24)$$

was used in[6] where the relationship between the standard transfer matrix **M** and the Green function **G** was established. This was further developed in[1]. If

one used $\mathbf{m}^{\dagger}$ instead of $\mathbf{m}^{c}$, then one would obtain a negative density of states. We now relate **G** to **T**, defined in (4), while extending significantly the analysis.

V. THE RELATIONSHIP BETWEEN G AND T

We now start from

$$\mathbf{L}(z) \cdot \mathbf{G}(z, z') = \mathbf{I}_N \, \delta(z - z'), \tag{25}$$

where $\mathbf{I}_N$ is the N × N unit matrix and **L**(z) is the differential matrix of (1) but, instead of **A**(z) of (2), the differential form is now

$$\mathbf{A}(z , z') = \mathbf{B}(z) \cdot \frac{\partial \mathbf{G}(z,z')}{\partial z} + \mathbf{P}(z) \cdot \mathbf{G}(z, z'). \tag{26}$$

Defining

$$\mathbf{A}^{\pm}(z) = \lim_{z' \to z \pm 0} \mathbf{A}(z, z'), \tag{27}$$

a first integration of (25) yields the identity

$$\mathbf{A}^{+}(z) - \mathbf{A}^{-}(z) = -\mathbf{I}_N . \tag{28}$$

Furthermore, a detailed formal analysis of (25) shows[16] that if we define

$$\mathbf{Z}(z, z') = \frac{\partial \mathbf{G}(z,z')}{\partial z'} \cdot \mathbf{B}^{c}(z') + \mathbf{G}(z, z') \cdot \mathbf{P}^{c}(z'). \tag{29}$$

and hence

$$^{\pm}\mathbf{Z}(z) = \lim_{z' \to z \mp 0} \mathbf{Z}(z, z'), \tag{30}$$

then there is another identity, namely

$$^{+}\mathbf{Z}(z) - {}^{-}\mathbf{Z}(z) = -\mathbf{I}_N . \tag{31}$$

It is now convenient to display T in the form

$$\mathbf{T} = \begin{Vmatrix} \mathbf{T}_{AA} & \mathbf{T}_{AD} \\ \mathbf{T}_{DA} & \mathbf{T}_{DD} \end{Vmatrix}, \tag{32}$$

where the submatrices $\mathbf{T}_{\alpha,\beta}$ (α, β = A, D) are N × N. Then, similarly to (3), we define the rectangular 2N × N matrix

$$\Gamma(z, z') = \begin{vmatrix} \mathbf{G}(z, z') \\ \mathbf{A}(z, z') \end{vmatrix}, \tag{33}$$

and thus

$$\Gamma(z, z') = \mathbf{T}(z, z_0) \cdot \Gamma(z_0, z'), \tag{34}$$

that is to say, for fixed z' Γ(z, z ') is transferred like Ψ(z) and, in particular

$$\mathbf{G}(z, z') = \mathbf{T}_{AA}(z, z_0) \cdot \mathbf{G}(z_0, z') + \mathbf{T}_{AD}(z, z_0) \cdot \mathbf{A}(z_0, z'). \tag{35}$$

A similar analysis can be carried out with the Green function of the Hermitean conjugate differential system, which has the same ATM. This leads to a formula analogous to (35) in which $\mathbf{T}^{c}(z', z_0)$, acting from the right, transfers in z´ with z fixed.

Following this line of argument and recalling that the definition of **T** does not depend on the choice of z_0, we arrive -details in[16]- at a general expression for **G** in terms of **T** of the form

$$\mathbf{G}(z, z') = \begin{cases} \Sigma_{\alpha\beta} \mathbf{T}_{A\alpha}(z, z_0) \cdot \mathbf{C}^{<}_{\alpha\beta} \cdot \mathbf{T}^{c}_{A\beta}(z', z_0) & z \le z' \\ \Sigma_{\alpha\beta} \mathbf{T}_{A\alpha}(z, z_0) \cdot \mathbf{C}^{>}_{\alpha\beta} \cdot \mathbf{T}^{c}_{A\beta}(z', z_0) & z \ge z' \end{cases} \tag{36}$$

for any pair of values of (z, z´) irrespective of the position of z_0. Hence

$$\mathbf{A}(z, z') = \begin{cases} \Sigma_{\alpha\beta} \mathbf{T}_{D\alpha}(z, z_0) \cdot \mathbf{C}^{<}_{\alpha\beta} \cdot \mathbf{T}^{c}_{A\beta}(z', z_0) & z \le z' \\ \Sigma_{\alpha\beta} \mathbf{T}_{D\alpha}(z, z_0) \cdot \mathbf{C}^{>}_{\alpha\beta} \cdot \mathbf{T}^{c}_{A\beta}(z', z_0) & z \ge z' \end{cases} . \tag{37}$$

Not all the eight (matrix) coefficients $\mathbf{C}^{>}_{\alpha\beta}, \mathbf{C}^{<}_{\alpha\beta}$ are independent. Firstly, whether we proceed from the first or the second row of (36), we must obtain

$$G(z) \equiv \mathbf{G}(z, z') = \mathbf{C}^{<}_{AA} = \mathbf{C}^{>}_{AA} \equiv \mathbf{C}_{AA} \tag{38}$$

Then, from (28) and (37):

$$\mathbf{C}^{<}_{DA} - \mathbf{C}^{>}_{DA} = -\mathbf{I}_N . \tag{39}$$

Furthermore, an expression for **Z**(z, z') (29) can be obtained similar to (37) and then, from (31)

$$\mathbf{C}^{>}_{AD} - \mathbf{C}^{<}_{AD} = -\mathbf{I}_N . \tag{40}$$

Now, consider the configuration $z \le z_0 \le z'$, Then[1]

$$\mathbf{G}(z, z') = \mathbf{G}(z, z_0) \cdot [G(z_0)]^{-1} \cdot G(z_0, z') . \tag{41}$$

From this and the above equalities -together with the similar expressions for Z(z, z ')- we obtain

$$\mathbf{C}^{<}_{DD} = \mathbf{C}^{<}_{DA} \cdot \mathbf{C}^{-1}_{AA} \cdot \mathbf{C}^{<}_{AD};$$
$$\mathbf{C}^{>}_{DD} = \mathbf{C}^{>}_{DA} \cdot \mathbf{C}^{-1}_{AA} \cdot \mathbf{C}^{>}_{AD}. \quad (42)$$

These relationships hold quite generally and reduce the independent coefficients. The rest of the analysis depends on the domain under study.

For the finite internal domains of a heterostructure, it was shown in[15] that one can define any arbitrary extended pseudomedium with a Green function satisfying arbitrary boundary conditions -except for infinite barriers- at the extremes of the said domains. In practice a considerable simplification of the algebra can be achieved in this way. The external domains are different. Sometimes they are terminated by infinite barriers, which is part of the model. The algebra is then fairly simple. A different situation arises if the external domains are assumed to extend to infinity. We now consider an infinite regular medium, which is in any case always a valid description for any domain, even if it is finite or semiinfinite.

We take $z_0 = 0$ and abbreviate $\mathbf{T}_{\alpha\beta}(z, z_0)/\mathbf{T}_{\alpha\beta}(z', z_0)$ as $\mathbf{T}_{\alpha\beta}(z)/\mathbf{T}_{\alpha\beta}(z')$. Consider the first row of (36) and take $z' = 0$. Then

$$\mathbf{G}(z, 0) = \mathbf{T}_{AD}(z) \cdot \left\{ [\mathbf{T}_{AD}(z)]^{-1} \mathbf{T}_{AA}(z) \cdot \mathbf{C}_{AA} + \mathbf{C}^{<}_{DA} \right\} \quad (43)$$

Regularity at $-\infty$ requires the vanishing of the *regular limit* of (43). To this effect we note that even if the coefficients of the differential system are variable, for sufficient large |z| these can be asymptotically "flattened" -i.e. replaced by their average values- at sufficiently large distances without essential loss of accuracy. Then **T** can be written as $\mathbf{T}(\in, z)$ and regular limits taken in the manner of (19)-(20), so we define the regular limits

$$\mathbf{T}_{\pm} = \lim_{\in \to 0} \lim_{z \to \pm\infty} \left\{ [\mathbf{T}_{AD}(\in, z)]^{-1} \cdot \mathbf{T}_{AA}(\in, z) \right\}$$

$$\Theta_{\pm} = \lim_{\in \to 0} \lim_{z \to \pm\infty} \left\{ \mathbf{T}^{c}_{AA}(\in, z) \cdot [\mathbf{T}^{c}_{AD}(\in, z)]^{-1} \right\}. \quad (44)$$

Now, the first factor of (43) has asymptotic oscillatory behaviour. Thus the regular vanishing of $\mathbf{G}(-\infty, 0)$ requires the vanishing of the second factor in the regular limit. Following this line of argument and using the general identities just presented, we obtain the full set of parameters for the regular Green function

$$\mathbf{C}_{AA} = [\mathbf{T}_{-} - \mathbf{T}_{+}]^{-1},$$

$$\mathbf{C}^{<}_{DA} = -\mathbf{T}_{-} \cdot \mathbf{C}_{AA}, \; \mathbf{C}^{>}_{DA} = -\mathbf{T}_{+} \cdot \mathbf{C}_{AA},$$

$$\mathbf{C}^{<}_{AD} = -\mathbf{C}_{AA} \cdot \Theta_{+}, \; \mathbf{C}^{>}_{AD} = -\mathbf{C}_{AA} \cdot \Theta_{-},$$

$$\mathbf{C}^{<}_{DD} = -\mathbf{T}_{-} \cdot \mathbf{C}_{AA} \cdot \Theta_{+}, \; \mathbf{C}^{>}_{DD} = \mathbf{T}_{+} \cdot \mathbf{C}_{AA} \cdot \Theta_{-} \quad (45)$$

The regular Green function is thus fully determined from **T**. The latter is always an ultimate resort if the analytical solution is not viable, while **G** is a natural object to extract physical information directly from it. As indicated above, the set of parameters $\mathbf{C}^{<}_{\alpha\beta}, \mathbf{C}^{>}_{\alpha\beta}$ can be considerably simplified by the convenient choice of simpler boundary condition.

VI. THE SYMPLECTIC CHARACTER AND GENERAL PROPERTIES OF T

Firstly we note that, due to the fact that the two fields transferred by **T** are continuous everywhere, on crossing interfaces separating different media **T** is obtained by simple chain multiplication of the corresponding different matrices. This is a practical useful feature for the description of heterostructures, not shared by M[15]. Furthermore, let us define the 2N $\times$ 2N auxiliary matrix

$$\mathbf{J} = \begin{Vmatrix} \mathbf{O}_N & -\mathbf{I}_N \\ \mathbf{I}_N & \mathbf{O}_N \end{Vmatrix}. \quad (46)$$

Then

$$\Psi^{c} \cdot \mathbf{J} \cdot \Psi = -\mathbf{F}^{c} \cdot \mathbf{A} + \mathbf{A}^{c} \cdot \mathbf{F}. \quad (47)$$

Now, the general definition of the flux density is

$$j(z) = i[\mathbf{F}^{c}(z) \cdot \mathbf{A}(z) - \mathbf{A}^{c}(z) \cdot \mathbf{F}(z)] = -i\, \Psi^{c}(z) \cdot \mathbf{J} \cdot \Psi(z) \quad (48)$$

On the other hand, the second order differential system for **F** is transformed in the standard way into the first order differential system for Ψ,

$$\frac{d\Psi(z)}{dz} = \mathbf{D}(z) \cdot \Psi(z) \quad (49)$$

with

$$\mathbf{D}(z) = \begin{Vmatrix} -\mathbf{B}^{-1}(z) \cdot \mathbf{P}(z) & \mathbf{B}^{-1}(z) \\ \left[\mathbf{Y}(z) \cdot \mathbf{B}^{-1}(z) \cdot \mathbf{P}^{-1}(z) \cdot \mathbf{W}(z) \right] & -\mathbf{Y}(z) \cdot \mathbf{B}^{-1}(z) \end{Vmatrix}. \quad (50)$$

It is easily seen that

$$\frac{d}{dz}[\mathbf{F}^c \cdot \mathbf{A} - \mathbf{A}^c \cdot \mathbf{F}] = -\Psi^c \cdot [\mathbf{D}^c \cdot \mathbf{J} + \mathbf{J} \cdot \mathbf{D}] \cdot \Psi. \quad (51)$$

Then, since

$$\mathbf{D}^c \cdot \mathbf{J} + \mathbf{J} \cdot \mathbf{D} = \mathbf{O}_{2N} \quad (52)$$

it follows that j(z) is constant everywhere, which is a general expression of the continuity equation.

Now consider any arbitrary pair of points (z_0, z), transfer Ψ from z_0 to z, write $\mathbf{T}(z, z_o)$ for brevity as **T** and equate j(z) to j(z_0). This yields

$$\mathbf{J} = \mathbf{T}^c \cdot \mathbf{J} \cdot \mathbf{T} \quad (53)$$

Thus **T** is a symplectic matrix in a general sense[17]. Since **J** has unit determinant, it follows that

$$|\,\mathrm{Det}[\mathbf{T}]\,|^2 = 1 \quad (54)$$

This provides a concise practical rule which can be used to monitor the quality of the numerical computations as z grows away from z_0. Furthermore, by equating the submatrices of (53) we obtain the three independent identities

$$\mathbf{T}_{AA}^c \cdot \mathbf{T}_{DA} - \mathbf{T}_{DA}^c \cdot \mathbf{T}_{AA} = \mathbf{O}_N \quad (55)$$

$$\mathbf{T}_{DD}^c \cdot \mathbf{T}_{AD} - \mathbf{T}_{AD}^c \cdot \mathbf{T}_{DD} = \mathbf{O}_N \quad (56)$$

$$\mathbf{T}_{AA}^c \cdot \mathbf{T}_{DD} - \mathbf{T}_{DA}^c \cdot \mathbf{T}_{AD} = \mathbf{I}_N . \quad (57)$$

These can also prove useful in two ways, namely: (i) they can help simplify the algebra in the analytical formulation of a problem and (ii) other concise rules for numerical monitoring can also be extracted from them.

Further details and different ways to combine **T** and **G** for the study of multilayer heterostructures are given in[16].

VII. CONCLUSION

The Associated Transfer Matrix **T** appears to be both, formally appealing and practically useful. It suggests itself in a natural way from the physics of the problem. It is unique and does not depend on having an analytical basis, so it can always be an ultimate resort, obtainable by numerical integration. It satisfies some general identities, not satisfied by other transfer matrices, which provides useful rules to monitor the numerical quality of computational processes. Finally, it is directly related to the Green function, from which direct physical information follows in a natural way.

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