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A general theory of matching for layered systems

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Abstract. The problem of matching Green functions is studied for one or more coupled interfaces for those cases of physical interest, like quantum wells or superlattices, in which differential calculus is involved, e.g. Schrödinger equations. The Green functions are related to the transfer matrices of the constituent media and these can be evaluated by efficient numerical algorithms. One can then obtain the matched Green function of the composite system without having to directly evaluate any Green function or derivative thereof. The formulae for the matched wavefunction are also derived and practical aspects are discussed.

1. Introduction

This paper discusses the mathematical basis of a formalism which can be used to study matching problems when differential calculus is involved for configurations of physical interest, ranging from one interface—the free surface being a particular case—to the infinite periodic sequence of coupled interfaces constituting a superlattice. A significant intermediate case is that of two coupled interfaces, which may correspond to a thin film, a layer on a substrate, a sandwich configuration or a quantum well. All these systems are the subject of very active current research, on account of the considerable physical and practical interest they have.

Matching problems can be formulated in terms of Green functions. One of these techniques, the surface Green function matching (SGFM) method, has been reviewed recently [1]. Similar concepts can also be found in [2]. While this gives an appealing physical picture in terms of scattering theory, the method depends on the evaluation of Green functions and their normal derivatives. This can entail a formidable numerical task in cases of physical interest. Consider, for instance, electronic structure calculations based on some fairly realistic model. After effecting a two-dimensional Fourier transform we are left with a system of N coupled ordinary differential equations in z , the space coordinate normal to the surface. The corresponding Green function is an $N \times N$ matrix $\mathbf{G}(E, \boldsymbol{\kappa}; z, z')$, where $\boldsymbol{\kappa}$ is a two-dimensional wavevector and N may be a largish number. Even in cases where only one differential equation suffices, as in a one-band model, the evaluation of the \mathbf{G} matrices and their derivatives may become a forbidding practical difficulty. In a situation similar to that depicted in figure 1, for instance, even the question of what is \mathbf{G}_A or \mathbf{G}_B is none too clear.

Another possible approach to these problems is based on the concept of the transfer matrix, which can be defined in different ways, depending on whether it transfers

amplitudes [3] or amplitudes and derivatives [4, 5]. We shall follow the lead of the general analysis of [5], which has been used in several applications [6–8].

Now, these two approaches have complementary attractive features. The transfer matrix algorithms are very useful in practice for numerical calculations, while the SGFM method yields a more transparent physical picture and provides a good scheme for organising and obtaining physical information. The purpose of this paper is to blend the two methods and to establish the formal basis for a hybrid approach which provides an efficient scheme for the calculation of the Green functions needed for matching problems. A first step in this direction was taken in [9], which was limited to the secular equation for bound states in a parabolic quantum well. In this case $N = 1$. More recently the case $N = 1$ has been fully analysed and the complete matched Green function $G_s(z, z')$ has been obtained for the composite systems, with practical applications to the study of image potential states on metal surfaces and a simple self-consistent treatment of inversion layers in semiconductor interfaces [10]. The extension just from $N = 1$ to $N = 2$ poses new questions, as the objects involved become then non-commuting matrices. This extension has also been recently carried out, and has applications to the study of elementary excitations in superconductors and to electronic states in lead salt superlattices [11]. In all these cases the results have been satisfactory and it now seems interesting to study the problem with full generality. This is the purpose of this paper.

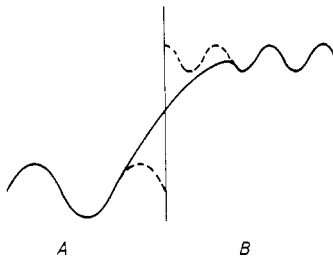


Figure 1. Matching of A and B . Broken curves represent ideal matching. Solid curves represent non-ideal matching, e.g. a self-consistent potential profile. The question is: what is G_A or G_B ?

The general relationship between Green function and transfer matrix is given in section 2. There and thenceforth the two-dimensional Fourier transform is implied, the dependence on E and κ is understood and only the dependence on z and/or z' is explicitly displayed. Section 3 gives the surface Green function matching analysis in terms of transfer matrices for one interface, while section 4 discusses the important cases of the quantum well and superlattice structures. The wavefunction is discussed in section 5 and then the practical aspects and the scope of applications are discussed in section 6.

2. The transfer matrix and the Green function

We start from the work of Mora *et al* [5], who discussed in detail the mathematical properties of the matrix $\mathbf{M}(z, z_0)$ to be presently discussed. They studied a system of N ordinary, linear, differential equations of arbitrary order. Here we shall consider, specifically, second-order differential systems. Let $\Psi(z)$, an N -component vector with components $\psi_1(z), \dots, \psi_N(z)$, be one solution of the system under study for a given value of the energy—or any other eigenvalue variable in general. The basis of this

system consists of $2N$ linearly independent solutions labelled $j = 1, 2, \dots, 2N$. From the j th solution we define the $2N$ -component vector

$$\Phi_j(z) = \begin{bmatrix} \phi_{1,j}(z) \\ \vdots \\ \phi_{N,j}(z) \\ \phi_{N+1,j}(z) \\ \vdots \\ \phi_{2N,j}(z) \end{bmatrix} = \begin{bmatrix} \psi_{1,j}(z) \\ \vdots \\ \psi_{N,j}(z) \\ \psi'_{1,j}(z) \\ \vdots \\ \psi'_{N,j}(z) \end{bmatrix}. \tag{2.1}$$

The $2N \times 2N$ transfer matrix $\mathbf{M}(z, z_0)$, which transfers amplitudes and derivatives from z_0 to z is then defined by

$$\Phi(z) = \mathbf{M}(z, z_0)\Phi(z_0). \tag{2.2}$$

Here we are interested in discussing the general relationship between $\mathbf{M}(z, z_0)$ and the associated Green functions $\mathbf{G}(z, z')$, in this case $N \times N$ matrices. The essential difference between these two objects is that \mathbf{M} is solely determined by the differential system, while \mathbf{G} requires also the specification of boundary conditions (BC). Thus we can anticipate that any relationship between \mathbf{M} and \mathbf{G} must involve parameters to be determined by the BC.

Now, consider the spectral representation of \mathbf{G} in the form

$$\mathbf{G}(E; z, z') = \sum_k \frac{\chi_k(E_k, z)\chi_k^\dagger(E_k, z')}{E - E_k}. \tag{2.3}$$

This may include discrete and continuous parts, for which the sum actually means an integral. The labels k , e.g. the quantum numbers in a physical application, could in general be vectors, or include discrete indices like a spin quantum number, but the concise form of (2.3) suffices to discuss the problem of interest here. Every χ_k has an expansion in terms of a basis:

$$\chi_k(E_k, z) = \sum_{i=1}^{2N} L_{ki}\Psi_i(E_k, z) \tag{2.4}$$

which can be used in (2.3). Note that (2.3) is only a formal expression which, for the physical theory, must be evaluated by prescribing some appropriate limit. We choose the standard causal prescription in which, with our sign convention, E is $\lim_{\epsilon \rightarrow 0}(E + i\epsilon)$. Evaluation of (2.3) according to this picks out the contributions from poles where $E_k = E \forall k$. In the final result this holds also for the basis functions of (2.4) and this finally leads to the general form

$$\mathbf{G}(z, z') = \sum_{i,j=1}^{2N} \Psi_i(z)C_{ij}\Psi_j^\dagger(z') \tag{2.5}$$

where \mathbf{G} and the Ψ vectors depend on the energy variable E . This dependence will be understood everywhere.

In general there is one set of parameters, $C_{ij}^<$, for $z \leq z'$ and another one, $C_{ij}^>$, for $z \geq z'$. This accounts for the change in functional form that $\mathbf{G}(z, z')$ must have depending on $\text{sgn}(z - z')$, subject to the continuity of \mathbf{G} and the discontinuity of its first derivative, which is uniquely determined by the differential system. The form of (2.5) is easily seen to remain invariant under a change of basis, so we choose a basis of vectors $\Phi_i^{\bar{z}_0}(z)$ defined to be canonical at some fixed point z_0 , i.e.

$$\phi_{ij}^{\bar{z}_0}(z_0) = \delta_{ij}. \tag{2.6}$$

It is convenient to define the N -component vectors $\Phi_{A_j}(z)$, which represent $\Psi_j(z)$, and $\Phi_{D_j}(z)$, which represent $\Psi'_j(z)$, so that

$$\Phi_j(z) = \begin{bmatrix} \Phi_{A_j}(z) \\ \Phi_{D_j}(z) \end{bmatrix} \tag{2.7}$$

where A and D denote amplitude and derivative respectively. The $2N \times 2N$ matrix \mathbf{M} is consequently partitioned into four $N \times N$ matrices \mathbf{M}_{AA} , \mathbf{M}_{AD} , \mathbf{M}_{DA} , \mathbf{M}_{DD} so (2.2) is cast as

$$\Phi_\alpha(z) = \sum_{\beta=A,D} \mathbf{M}_{\alpha\beta}(z, z_0) \Phi_\beta(z_0) \quad \alpha = A, D. \tag{2.8}$$

The amplitudes appearing in (2.5) are to be read as $\Phi_A(z)$ terms which, by (2.8) and (2.6), are combinations of $\mathbf{M}_{AA}(z, z_0)$ and $\mathbf{M}_{AD}(z, z_0)$. The postfactors $\Phi_A^\dagger(z)$ require careful treatment to account for the formal properties of adjoint operators. It is also convenient to group together the $2N \times 2N$ matrix of C_{ij} coefficients into four $N \times N$ blocks $\mathbf{C}_{\alpha\beta}$ ($\alpha, \beta = A, D$), consistently with (2.7) and (2.8). Everything is then compacted into terms involving only $N \times N$ matrices labelled by A and D. This leads to the final form

$$\mathbf{G}(z, z') = \begin{cases} \sum_{\alpha\beta} \mathbf{M}_{A\alpha}(z, z_0) \mathbf{C}_{\alpha\beta}^< \bar{\mathbf{M}}_{cA\beta}(z', z_0) & z \leq z' \\ \sum_{\alpha\beta} \mathbf{M}_{A\alpha}(z, z_0) \mathbf{C}_{\alpha\beta}^> \bar{\mathbf{M}}_{cA\beta}(z', z_0) & z \geq z'. \end{cases} \tag{2.9}$$

Here \mathbf{M}_c is defined in the following manner. Let \mathbf{M} be any matrix which in general can be a complex function of a complex variable ω (e.g. $E + i\epsilon$, or $E + i\Gamma$ for a resonance, with Γ finite). If

$$\mathbf{M}(\omega) = \mathbf{a}(\omega) + i\mathbf{b}(\omega) \tag{2.10}$$

then we define the transposed matrices $\bar{\mathbf{M}}$, $\bar{\mathbf{a}}$ and $\bar{\mathbf{b}}$. Then

$$\bar{\mathbf{M}}_c(\omega) = \bar{\mathbf{a}}(\omega) - i\bar{\mathbf{b}}(\omega) \tag{2.11}$$

Note that ω is not conjugated. The matrices $\bar{\mathbf{M}}_{cA\beta}$ of (2.9) are defined according to (2.11).

The form (2.9) can be proved independently and directly by studying in detail the formal properties of differential operators and their adjoints and the consequences for their respective matrix representations, while using only the general properties of the transfer matrix acting directly on \mathbf{G} with proper account of the ordering of z and z' to guarantee that the same functional form is preserved. The point is that (2.9) yields \mathbf{G} in terms of the submatrices of \mathbf{M} if the unknown matrices $\mathbf{C}_{\alpha\beta}$ can be obtained. These clearly depend on the specific choice of boundary conditions.

Some general relationship can be established right away. We define the surface objects

$$\begin{aligned} \mathcal{G} &= \mathbf{G}(z_0, z_0) \\ {}^{(\pm)}\mathcal{G}' &= \lim_{z' \rightarrow z_0 \pm 0} \left[\frac{\partial \mathbf{G}(z, z')}{\partial z} \right]_{z=z_0} \\ {}^{(=)}\mathcal{G}' &= \lim_{z \rightarrow z_0 = 0} \left[\frac{\partial \mathbf{G}(z, z')}{\partial z'} \right]_{z'=z_0}. \end{aligned} \tag{2.12}$$

Their inverses, when they exist, are defined in the subspace $z = z_0$. Moreover

$$\frac{d\mathbf{M}_{A\alpha}(\xi, z_0)}{d\xi} = \mathbf{M}_{D\alpha}(\xi, z_0). \tag{2.13}$$

Then, from (2.9), \mathcal{G} is given by

$$\mathcal{G} = \mathbf{C}_{AA}^> = \mathbf{C}_{AA}^< = \mathbf{C}_{AA} \tag{2.14}$$

and

$$\begin{aligned} {}' \mathcal{G}^{(+)} &= \mathbf{C}_{DA}^< & {}' \mathcal{G}^{(-)} &= \mathbf{C}_{DA}^> \\ {}^{(+)} \mathcal{G}' &= \mathbf{C}_{AD}^> & {}^{(-)} \mathcal{G}' &= \mathbf{C}_{AD}^<. \end{aligned} \tag{2.15}$$

By performing a first integration of the differential system one finds that, for systems with continuous coefficients,

$${}' \mathcal{G}^{(+)} - {}' \mathcal{G}^{(-)} = \mathbf{s} \qquad {}^{(+)} \mathcal{G}' - {}^{(-)} \mathcal{G}' = \mathbf{s}. \tag{2.16}$$

For instance, for a Schrödinger equation with a given pseudopotential, cast in the matrix differential form described in section 1, \mathbf{s} is $-(2m/\hbar^2)$ times the $N \times N$ unit matrix. However, \mathbf{s} need not be a multiple of the unit matrix. Quite generally we are interested in systems where the second derivative usually appears only in the main diagonal and is multiplied by a real coefficient. Then \mathbf{s} is a real, diagonal—and therefore symmetric—matrix. This fact will be used in the subsequent analysis.

Consider now the logarithmic derivatives

$$\begin{aligned} \mathcal{L}^{(+)} &= {}' \mathcal{G}^{(+)} \mathcal{G}^{-1} = \mathbf{C}_{DA}^< \mathbf{C}_{AA}^{-1} \\ \mathcal{L}^{(-)} &= {}' \mathcal{G}^{(-)} \mathcal{G}^{-1} = \mathbf{C}_{DA}^> \mathbf{C}_{AA}^{-1}. \end{aligned} \tag{2.17}$$

These are determined by the BC on the left and on the right of z_0 , respectively, as will be seen presently.

3. Surface Green function matching from the transfer matrices

Consider the one-interface matching problem in which medium 1 on the left is matched at z_0 to medium 2 on the right. We take $z_0 = 0$. The first question to decide is the matching rule. For a Schrödinger equation with a pseudopotential we must ensure the continuity of the logarithmic derivatives. More generally one must account for different effective masses or one must replace the derivative by some linear differential form appropriate for the different physical problems under study [1]. For the present purpose it suffices to consider matching of logarithmic derivatives. Then the composite Green function \mathbf{G}_s , resulting from the matching of \mathbf{G}_1 and \mathbf{G}_2 , has a surface projection \mathcal{G}_s given by

$$\mathcal{G}_s^{-1} = \mathbf{s}_1^{-1} \mathcal{L}_1^{(+)} - \mathbf{s}_2^{-1} \mathcal{L}_2^{(-)}. \tag{3.1}$$

The BC away from the matching plane must now be specified. Suppose 1 is a semi-infinite medium. For any $z < 0$, (2.9) yields

$$\mathbf{G}_1(z, 0) = [\mathbf{M}_{AA}(z, 0)\mathbf{C}_{AA} + \mathbf{M}_{AD}(z, 0)\mathbf{C}_{DA}^<]_1. \tag{3.2}$$

We then impose regularity at $-\infty$, i.e.

$$\lim_{\epsilon \rightarrow +0} \lim_{z \rightarrow -\infty} \mathbf{G}_1(E + i\epsilon; z, 0) = 0. \tag{3.3}$$

Put

$$\mathbf{M}_{\alpha\beta}(\pm) = \lim_{\epsilon \rightarrow +0} \lim_{z \rightarrow \pm\infty} \mathbf{M}_{\alpha\beta}(z, 0). \tag{3.4}$$

Then, from (3.2),

$$[\mathbf{M}_{AA}(-)\mathbf{C}_{AA} + \mathbf{M}_{AD}(-)\mathbf{C}_{DA}^<]_1 = 0 \tag{3.5}$$

whence, by (2.17),

$$\mathcal{L}_1^{(+)} = \mathbf{T}_1^{-1} = -[\mathbf{M}_{AD}(-)^{-1}\mathbf{M}_{AA}(-)]_1. \tag{3.6}$$

Likewise, by imposing regularity at ∞ if 2 is a semi-infinite medium, we find

$$\mathcal{L}_2^{(-)} = \mathbf{V}_2^{-1} = -[\mathbf{M}_{AD}(+)^{-1}\mathbf{M}_{AA}(+)]_2. \tag{3.7}$$

The causal limit $\epsilon \rightarrow +0$ is unnecessary (i) for bound states and (ii) when the condition of vanishing amplitude is imposed at some finite distance, in which case the variable z of (3.3) and (3.4) stops right there. Physically this would correspond to studying the interface problem by putting the system inside two infinite barriers away from the interface, which can be a good approximation if this distance is sufficiently large. Note that both $\mathbf{M}_{AA}(\pm)$ and $\mathbf{M}_{AD}(\pm)$ diverge separately, but (3.6) and (3.7) converge. In practice the numerical evaluation of these terms is carried out for growing z until the result shows stable convergence. The point is that \mathcal{G}_s^{-1} , (3.1), is explicitly evaluated in terms of the corresponding transfer matrices of each constituent medium.

Now for the complete $\mathbf{G}_s(z, z')$. Let $p = 1, 2$ denote one of the two parts and \bar{p} the other one. For z and z' on the same side, \mathbf{G}_s can be expressed as the sum of two terms:

$$\mathbf{G}_s(z, z') = \mathbf{G}_{p\infty}(z, z') + \mathbf{G}_{pm}(z, z') \quad z, z' \in p. \tag{3.8}$$

The first one is the *hard wall part*

$$\mathbf{G}_{p\infty}(z, z') = \mathbf{G}_p(z, z') - \mathbf{G}_p(z, 0)\mathcal{G}_p^{-1}\mathbf{G}_p(0, z') \tag{3.9}$$

and the second is the *matching part*

$$\mathbf{G}_{pm}(z, z') = \mathbf{G}_p(z, 0)\mathcal{G}_p^{-1}\mathcal{G}_s\mathcal{G}_p^{-1}\mathbf{G}_p(0, z'). \tag{3.10}$$

These are the analogues of the hard core and potential scattering terms in ordinary scattering theory.

The hard wall term describes medium p bounded in its own domain by an infinite barrier at $z = 0$. The BC on the left/right, as the case may be, is identically the same and so is the differential system—e.g. the potential—while the condition of vanishing amplitudes must be imposed at $z = 0$. Proceeding from (2.9) this yields, for side 1,

$$G_{1x}(z, z') = \begin{cases} -(\mathbf{M}_{AA}(z, 0) + \mathbf{M}_{AD}(z, 0)\mathbf{T}_1^{-1})\mathbf{s}_1\bar{\mathbf{M}}_{cAD}(z', 0) & z \leq z' \\ -\mathbf{M}_{AD}(z, 0)\mathbf{s}_1^{-1}(\bar{\mathbf{M}}_{cAA}(z', 0) + \mathbf{U}_1^{-1}\bar{\mathbf{M}}_{cAD}(z', 0)) & z \geq z' \end{cases} \tag{3.11}$$

where \mathbf{T}_1 is given by (3.6),

$$\mathbf{U}_1^{-1} = -[\bar{\mathbf{M}}_{cAA}(-)\bar{\mathbf{M}}_{cAD}(-)^{-1}]_1 \tag{3.12}$$

and the transfer matrices appearing in (3.11) are of course evaluated with the coefficients and potentials of the actual semi-infinite medium 1 of the real system.

Likewise, for side 2,

$$G_{2x}(z, z') = \begin{cases} \mathbf{M}_{AD}(z, 0)\mathbf{s}_2(\bar{\mathbf{M}}_{cAA}(z', 0) + \mathbf{Q}_2^{-1}\bar{\mathbf{M}}_{cAD}(z', 0)) & z \leq z' \\ (\mathbf{M}_{AA}(z, 0) + \mathbf{M}_{AD}(z, 0)\mathbf{V}_2^{-1})\mathbf{s}_2\bar{\mathbf{M}}_{cAD}(z', 0) & z \geq z' \end{cases} \quad (3.13)$$

where \mathbf{V}_2 is given by (3.7) and

$$\mathbf{Q}_2^{-1} = -[\bar{\mathbf{M}}_{cAA}(+) \bar{\mathbf{M}}_{cAD}(+)^{-1}]_2 \quad (3.14)$$

with the transfer matrices of (3.14) belonging to the real part 2 of the matched system.

If z and z' are on opposite sides, then

$$\mathbf{G}_s(z, z') = \mathbf{G}_p(z, 0)\mathcal{G}_p^{-1}\mathcal{G}_s\mathcal{G}_{\bar{p}}^{-1}\mathbf{G}_{\bar{p}}(0, z') \quad z \in p, z' \in \bar{p}. \quad (3.15)$$

Clearly \mathbf{G}_s in this case consists only of a matching term, of the same form as (3.8), except that both \mathbf{G}_1 and \mathbf{G}_2 are involved. Thus we must study terms of the form $\mathbf{G}_p\mathcal{G}_p^{-1}$ and $\mathcal{G}_p^{-1}\mathbf{G}_p$. We proceed again from (2.9) and find

$$\begin{aligned} \mathbf{G}_1(z, 0)\mathcal{G}_1^{-1} &= [\mathbf{M}_{AA}(z, 0) + \mathbf{M}_{AD}(z, 0)\mathbf{T}_1^{-1}] & z \leq 0 \\ \mathcal{G}_1^{-1}\mathbf{G}_1(0, z') &= [\bar{\mathbf{M}}_{cAA}(z', 0) + \mathbf{U}_1^{-1}\bar{\mathbf{M}}_{cAD}(z', 0)] & z' \leq 0 \\ \mathbf{G}_2(z, 0)\mathcal{G}_2^{-1} &= [\mathbf{M}_{AA}(z, 0) + \mathbf{M}_{AD}(z, 0)\mathbf{V}_2^{-1}] & z \geq 0 \\ \mathcal{G}_2^{-1}\mathbf{G}_2(0, z') &= [\bar{\mathbf{M}}_{cAA}(z', 0) + \mathbf{Q}_2^{-1}\bar{\mathbf{M}}_{cAD}(z', 0)] & z' \geq 0. \end{aligned} \quad (3.16)$$

The problem is thus fully solved: (3.1), (3.6) and (3.7) yield \mathcal{G}_s and (3.8)–(3.16) yield $\mathbf{G}_s(z, z')$ for all possible configurations of (z, z') . For each partial constituent the final result is obtained only and exclusively in terms of its own real transfer matrices and only the asymptotic bc away from the matching plane need be used. These determine the logarithmic derivatives $\mathcal{L}_1^{(+)}$ and $\mathcal{L}_2^{(-)}$, i.e. \mathbf{T}_1^{-1} and \mathbf{V}_2^{-1} . One can define the dual logarithmic derivatives

$${}^{(\pm)}\mathcal{L} = \mathcal{G}^{-1(\pm)}\mathcal{G}'. \quad (3.17)$$

It is easily seen that

$${}^{(+)}\mathcal{L}_1 = \mathbf{U}_1^{-1} \quad {}^{(-)}\mathcal{L}_2 = \mathbf{Q}_2^{-1}. \quad (3.18)$$

This provides an interpretation for the four parameters appearing in \mathbf{G}_s in terms of the four logarithmic derivatives.

The two points to stress are: (i) we need only to know the differential system on each side and the corresponding asymptotic bc (ii) any \mathbf{G}_p obeying the same conditions of (i) and otherwise satisfying any arbitrary bc at the matching plane yields identically the same solution of the matching problem. This was proved in [9] on general grounds. The question of knowing the real Green function of each constituent medium need not arise. Any arbitrary *extended pseudomedium* satisfying the conditions of (i) can equally be used instead. This will be used in the next section.

4. Quantum wells and superlattices

Consider a system with the structure 1-l-2-r-3, meaning that l is the interface where media 1 and 2 match, while 2 and 3 match at r. Such structures occur frequently in systems of physical interest. For electronic states this would correspond to a quantum well (qw), if medium 2 is a well, or to a tunnelling configuration if it is a barrier. Even

if they consist of the same material, media 1 and 3 need not be equal, as there may be inhomogeneities due either to self-consistency or to one-sided modulation doping, for instance. The theory developed here does not rest on the assumption that they are equal, or even that they are specular images of each other. Also important is the superlattice (SL) . . . 1-2-1-2 . . . Both QWs and SLs are the subject of intense current attention and one of the aims of the present work is to build up a formalism which can be applied to such systems with full generality, including possible complexities of the models employed and/or of inhomogeneities which may be present.

All these problems involve simultaneous matching at the different interfaces and can be treated by an extension of the SGFM analysis so that the Green function \mathbf{G}_s of the composite system is obtained in terms of the \mathbf{G}_p matrices involved [1, 9]. We first summarise the basic formulae for this case and then give the solution in terms of the corresponding transfer matrices.

We first consider the 1-2-3 system. The symbols l, r will be used indistinctly either as labels or to denote the unit of the corresponding interface, which is part of the matching domain with unit

$$\mathcal{I} = l + r. \tag{4.1}$$

We define the *external* medium (e), consisting of 1 on the left and 3 on the right, and the internal medium (i) consisting of 2 inbetween. We define the entire projection $\tilde{\mathbf{G}}_i$ as a 2×2 supermatrix

$$\tilde{\mathbf{G}}_i = \mathcal{I} \mathbf{G}_i \mathcal{I} = \begin{vmatrix} \mathcal{G}_{i1} & \mathbf{G}_i(l, r) \\ \mathbf{G}_i(r, l) & \mathcal{G}_{ir} \end{vmatrix}. \tag{4.2}$$

The diagonal terms are the corresponding projections at the l and r surfaces. Likewise we define

$$\tilde{\mathbf{S}}_i = \begin{vmatrix} \mathbf{s}_2 & \mathbf{0} \\ \mathbf{0} & \mathbf{s}_2 \end{vmatrix} \quad \tilde{\mathbf{G}}_i = \begin{vmatrix} \prime \mathcal{G}_2^{(-)} & \prime \mathbf{G}_2(l, r) \\ -\prime \mathbf{G}_2(r, l) & -\prime \mathcal{G}_2^{(+)} \end{vmatrix}. \tag{4.3}$$

The prime on the left denotes derivative with respect to z and $\prime \mathbf{G}(l, r)$ indicates that z is at l while z' is at r , and likewise for $\prime \mathbf{G}(r, l)$. For the external part we define

$$\tilde{\mathbf{G}}_e = \begin{vmatrix} \mathcal{G}_{11} & \mathbf{0} \\ \mathbf{0} & \mathcal{G}_{3r} \end{vmatrix} \quad \tilde{\mathbf{S}}_e = \begin{vmatrix} \mathbf{S}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{S}_3 \end{vmatrix} \quad \tilde{\mathbf{G}}_e = \begin{vmatrix} \prime \mathcal{G}_{11}^{(+)} & \mathbf{0} \\ \mathbf{0} & -\prime \mathcal{G}_{3r}^{(-)} \end{vmatrix}. \tag{4.4}$$

The entire projection of \mathbf{G}_s is defined as in (4.2) with \mathbf{G}_i replaced by \mathbf{G}_s . Then the matching formula is

$$\tilde{\mathbf{G}}_s^{-1} = \tilde{\mathbf{S}}_e^{-1} \tilde{\mathbf{G}}_e \tilde{\mathbf{G}}_e^{-1} - \tilde{\mathbf{S}}_i^{-1} \tilde{\mathbf{G}}_i \tilde{\mathbf{G}}_i^{-1}. \tag{4.5}$$

We now use the freedom to choose extended pseudomedia. For 1 we choose that \mathbf{G}_1 for which

$$\prime \mathcal{G}_1^{(+)} = \mathbf{s}_1 \quad \prime \mathcal{G}_1^{(-)} = 0 \tag{4.6}$$

while for 3 we choose that \mathbf{G}_3 for which

$$\prime \mathcal{G}_{3r}^{(+)} = 0 \quad \prime \mathcal{G}_{3r}^{(-)} = -\mathbf{s}_3. \tag{4.7}$$

Then $\tilde{\mathbf{S}}_e^{-1} \tilde{\mathbf{G}}_e$ is the $2N \times 2N$ unit matrix and

$$\tilde{\mathbf{G}}_e = \begin{vmatrix} \mathbf{T}_1 \mathbf{s}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{V}_3 \mathbf{s}_3 \end{vmatrix}. \tag{4.8}$$

\mathbf{T}_1 is given by (3.6) with $z = 0$ at 1 and \mathbf{V}_3 is \mathbf{V}_2 of (3.7) with 2 replaced by 3 and $z = 0$ at r .

For the internal part we can likewise choose a convenient pseudo \mathbf{G} , as was done in [9]. We choose that \mathbf{G}_2 for which

$$' \mathcal{G}_{2l}^{(+)} = 0 \quad ' \mathcal{G}_{2l}^{(-)} = -\mathbf{s}_2 \quad ' \mathcal{G}_{2r}^{(+)} = \mathbf{s}_2 \quad ' \mathcal{G}_{2r}^{(-)} = 0. \quad (4.9)$$

The merit of this choice lies in the fact that

$$\begin{aligned} ' \mathbf{G}(l, r) &= ' \mathcal{G}_l^{(+)} ' \mathcal{G}_l^{-1} \mathbf{G}(l, r) \\ ' \mathbf{G}(r, l) &= ' \mathcal{G}_r^{(-)} ' \mathcal{G}_r^{-1} \mathbf{G}(r, l). \end{aligned} \quad (4.10)$$

Then $-\tilde{\mathbf{S}}_i^{-1} \tilde{\mathbf{G}}_i$ is also the $2N \times 2N$ unit matrix and the matching formula becomes

$$\tilde{\mathbf{G}}_s^{-1} = \tilde{\mathbf{G}}_e^{-1} + \tilde{\mathbf{G}}_i^{-1} = \tilde{\mathbf{G}}_e^{-1} (\tilde{\mathbf{G}}_e + \tilde{\mathbf{G}}_i) \tilde{\mathbf{G}}_i^{-1}. \quad (4.11)$$

The secular equation yielding the eigenvalues of the matching states of the QW or sandwich structures can then be expressed as

$$\det[\tilde{\mathbf{G}}_e(E, \boldsymbol{\kappa}) + \tilde{\mathbf{G}}_i(E, \boldsymbol{\kappa})] = 0. \quad (4.12)$$

$\tilde{\mathbf{G}}_e$ has been given in (4.2). $\tilde{\mathbf{G}}_i$ is likewise obtained by working from (2.9) and imposing the BC (4.9), together with (2.14) and (2.16). The reference point, z_0 of (2.9), is now at l , so \mathcal{G} , (2.14) for instance, means \mathcal{G}_l and so on. Of course the continuity of \mathcal{G} and the discontinuity of $' \mathcal{G}^{(\pm)}$ or $'^{(\pm)} \mathcal{G}$ must also be obeyed at r .

We define

$$\mathbf{m}_{\alpha\beta} = \mathbf{M}_{\alpha\beta}(r, l) \quad \boldsymbol{\mu}_{\alpha\beta} = \bar{\mathbf{M}}_{\alpha\beta}(r, l). \quad (4.13)$$

Then evaluation of \mathcal{G}_r from (2.9) yields

$$\mathbf{m}_{AD} (\mathbf{C}_{DD}^< - \mathbf{C}_{DD}^>) \boldsymbol{\mu}_{AD} = \mathbf{m}_{AA} \mathbf{s} \boldsymbol{\mu}_{AD} - \mathbf{m}_{AD} \mathbf{s} \boldsymbol{\mu}_{AA} \quad (4.14)$$

while from the discontinuity of $' \mathcal{G}_r^{(\pm)}$:

$$\mathbf{m}_{DD} (\mathbf{C}_{DD}^< - \mathbf{C}_{DD}^>) \boldsymbol{\mu}_{AD} = \mathbf{m}_{DA} \mathbf{s} \boldsymbol{\mu}_{AD} - \mathbf{m}_{DD} \mathbf{s} \boldsymbol{\mu}_{AA} + \mathbf{s} \quad (4.15)$$

whence the identity

$$\mathbf{m}_{DA} - \mathbf{m}_{DD} \mathbf{m}_{AD}^{-1} \mathbf{m}_{AA} = -\mathbf{s} \boldsymbol{\mu}_{AD}^{-1} \mathbf{s}^{-1}. \quad (4.16)$$

By determining the $\mathbf{C}_{\alpha\beta}$ coefficients of (2.9) corresponding to the choice of BC (4.6), (4.7) and using (4.11), we obtain

$$\begin{aligned} \mathcal{G}_l &= \mathbf{m}_{DA}^{-1} \mathbf{m}_{DD} \mathbf{s} \quad \mathcal{G}_r = \mathbf{m}_{AA} \mathbf{m}_{DA}^{-1} \mathbf{s} \\ \mathbf{G}(l, r) &= \mathbf{m}_{DA}^{-1} \mathbf{s} \end{aligned} \quad (4.17)$$

and

$$\mathbf{G}(r, l) = (\mathbf{m}_{AA} \mathbf{m}_{DA}^{-1} \mathbf{m}_{DD} - \mathbf{m}_{AD}) \mathbf{s}. \quad (4.18)$$

The formula for $\mathbf{G}(r, l)$ can be cast in a simpler alternative form by defining each \mathbf{m}_r as a submatrix of the reverse transfer matrix $\mathbf{M}_r = \mathbf{M}(l, r)$, from r to l . Then

$$\mathbf{G}(r, l) = -\mathbf{m}_{rDA}^{-1} \mathbf{s}. \quad (4.19)$$

The above formulae are to be applied to \mathbf{G}_i , i.e. \mathbf{G}_2 . The four terms of $\tilde{\mathbf{G}}_i$ have been obtained in terms of transfer matrices across the finite domain inside the matching interfaces. It is easily seen that in the $N = 1$ case this reproduces the result first obtained in [9].

For the SL we use the labelling ... 2-*m*-1-1-2-*r*-1-*n*-2- ... meaning that *m* is the 2-1 interface on the left of the domain defined as internal and bounded by *l* and *r*, while *n* is the 1-2 interface on the right. The difference from the sandwich configuration is that the external domain now consists of two finite domains. The matching formula is similar to (4.5) with the difference [1] that the external terms $\hat{\mathbf{G}}_e$ and $\tilde{\mathbf{G}}_e$ are now replaced by

$$\begin{aligned} \hat{\mathbf{G}}_e &= \left\| \begin{array}{cc} \mathcal{G}'_{1l}^{(+)} & f^{-1} \mathbf{G}_1(l, m) \\ -f \mathbf{G}_1(m, l) & -\mathcal{G}'_{1m}^{(-)} \end{array} \right\| \\ \tilde{\mathbf{G}}_e &= \left\| \begin{array}{cc} \mathcal{G}_{1l} & f^{-1} \mathbf{G}_1(l, m) \\ f \mathbf{G}_1(m, l) & \mathcal{G}_{1m} \end{array} \right\| \end{aligned} \tag{4.20}$$

where

$$f = \exp(iqd) \tag{4.21}$$

is the phase factor associated with the superperiod $d = d_1 + d_2$ and 1D superwavevector *q*. We have used the fact that the (*m*, *l*) and (*r*, *n*) slabs are equivalent, so that, for instance, \mathcal{G}_{1m} is equal to \mathcal{G}_{1r} , and $\mathcal{G}_1(m, l)$ is equal to $\mathbf{G}_1(r, n)$. As before, the prime indicates differentiation with respect to the first argument. We now make for \mathbf{G}_1 the choice of BC analogous to that made in (4.4) for \mathbf{G}_2 , i.e.

$$\mathcal{G}'_{1m}^{(+)} = 0 \quad \mathcal{G}'_{1m}^{(-)} = -\mathbf{s}_1 \quad \mathcal{G}'_{1l}^{(+)} = \mathbf{s}_1 \quad \mathcal{G}'_{1l}^{(-)} = 0. \tag{4.22}$$

Then

$$\tilde{\mathbf{G}}_s^{-1} = \hat{\mathbf{G}}_e^{-1} + \tilde{\mathbf{G}}_i^{-1} = \hat{\mathbf{G}}_e^{-1} (\hat{\mathbf{G}}_e + \tilde{\mathbf{G}}_i) \tilde{\mathbf{G}}_i^{-1}. \tag{4.23}$$

All the formulae are as in the previous case, with the terms of the internal domain identical and those of the external domain now embodied in $\hat{\mathbf{G}}_e$. The four terms of this are of the same form as (4.17), (4.19) but the transfer matrices involved require new specification. Thus, defining now \mathbf{m} as the transfer matrix which transfers from *l* to *m*, i.e. across the potentials of medium 1, we have

$$\begin{aligned} \mathcal{G}_{1l} &= \mathbf{m}_{DA}^{-1} \mathbf{m}_{DD} \mathbf{s}_1 & \mathcal{G}_{1m} &= \mathbf{m}_{AA} \mathbf{m}_{DA}^{-1} \mathbf{s}_1 \\ \mathbf{G}(l, m) &= \mathbf{m}_{DA}^{-1} \mathbf{s}_2 \end{aligned} \tag{4.24}$$

while defining \mathbf{m}_r as that matrix which transfers from *m* to *l*, i.e. the reverse of the above

$$\mathbf{G}(m, l) = \mathbf{m}_{rDA}^{-1} \mathbf{s}_1. \tag{4.25}$$

With this the secular matrix $\tilde{\mathbf{G}}_s^{-1}$ of the SL is also evaluated only and exclusively in terms of transfer matrices which transfer across the potentials of the two constituent slabs.

The complete $\mathbf{G}_s(z, z')$ of the laminar system can now also be obtained in terms of transfer matrices. For the sandwich structure when *z* and *z'* are in the external domain, $\mathbf{G}_s(z, z')$ is given by the formulae of section 3 with the reference point at *l* when they are on the left and at *r* when they are on the right. When both arguments are inside

$$\mathbf{G}_s(z, z') = \mathbf{G}_2(z, z') + [\mathbf{G}_2(z, l), \mathbf{G}_2(z, r)] \tilde{\mathbf{G}}_2^{-1} (\tilde{\mathbf{G}}_s - \tilde{\mathbf{G}}_2) \tilde{\mathbf{G}}_2^{-1} \begin{bmatrix} \mathbf{G}_2(l, z') \\ \mathbf{G}_2(r, z') \end{bmatrix}. \tag{4.26}$$

The intervening Green function elements for the variables z and z' can be obtained from (2.9) once the chosen BC have been used to determine the parameters. With the choice (4.9) these are

$$\begin{aligned}
 \mathbf{C}_{DA}^{\leftarrow} &= \mathbf{C}_{DD}^{\leftarrow} = \mathbf{0} \\
 \mathbf{C}_{DA}^{\rightarrow} &= -\mathbf{s} \\
 \mathbf{C}_{AA}^{\rightarrow} &= \mathbf{m}_{DA}^{-1} \mathbf{m}_{DD} \mathbf{s} = \mathbf{C}_{AA}^{\leftarrow} \\
 \mathbf{C}_{AD}^{\rightarrow} &= -\mathbf{m}_{DA}^{-1} \mathbf{m}_{DD} (\mathbf{s} \boldsymbol{\mu}_{AA} \boldsymbol{\mu}_{AD}^{-1} - \mathbf{m}_{AD}^{-1} \mathbf{m}_{AA} \mathbf{s}) \\
 \mathbf{C}_{AD}^{\leftarrow} &= \mathbf{C}_{AD}^{\rightarrow} + \mathbf{s} \\
 \mathbf{C}_{DD}^{\rightarrow} &= \mathbf{s} \boldsymbol{\mu}_{AA} \boldsymbol{\mu}_{AD}^{-1} - \mathbf{m}_{AD}^{-1} \mathbf{m}_{AA} \mathbf{s}.
 \end{aligned}
 \tag{4.27}$$

Another case of physical interest is that in which z and z' are on opposite sides of the external domain. For instance, for z on the left and z' on the right

$$\mathbf{G}_s(z, z') = \mathbf{G}_1(z, 0) \mathcal{G}_{1l}^{-1} \tilde{\mathbf{G}}_s(l, r) \mathcal{G}_{3r}^{-1} \mathbf{G}_3(r, z')
 \tag{4.28}$$

which again can be obtained in terms of transfer matrices by using the results of this and the previous section.

Finally, the case of the SL is equally treated by means of the corresponding SGFM formulae [1] and the required Green function elements obtained in terms of transfer matrices by treating a slab of medium 1 in the same manner as one of medium 2.

5. The wavefunction of a matched system

Many properties of physical interest—notably dispersion relations and spectral functions—can be evaluated directly from the Green function. Others explicitly require the wavefunctions to calculate, say, some matrix elements. Having obtained the complete Green function of the matched system from the transfer matrices of the consistent media, one can also obtain the wavefunctions in the same way.

Consider first a one-interface problem. The formulae for the Green functions have their counterparts in formulae for the wavefunctions, just as in ordinary scattering theory the Lipmann–Schwinger and the Dyson equations are in correspondence. This can be formally proved in the SGFM analysis by using the reflection and transmission amplitudes, which can be written down in terms of \mathcal{G}_s . For instance, consider a scattering state ψ corresponding to an incident state ϕ_1 , an eigenstate of medium 1. Then

$$\psi(z) = \phi_1(z) + \mathbf{G}_1(z, 0) \mathcal{G}_1^{-1} (\mathcal{G}_s - \mathcal{G}_1) \mathcal{G}_1^{-1} \phi_1(0) \quad z \leq 0
 \tag{5.1}$$

whence

$$\psi(0) = \mathcal{G}_s \mathcal{G}_1^{-1} \phi_1(0)
 \tag{5.2}$$

and

$$\psi(z) = \mathbf{G}_2(z, 0) \mathcal{G}_2^{-1} \mathcal{G}_s \mathcal{G}_1^{-1} \phi_1(0) \quad z \geq 0
 \tag{5.3}$$

whence

$$\psi'(0+) = \mathcal{L}_2^{-1} \mathcal{G}_2^{-1} \psi(0).
 \tag{5.4}$$

Thus, for one given medium

$$\phi'(0) = \mathcal{L}_2^{-1} \phi(0).
 \tag{5.5}$$

If we define \mathcal{L} as the logarithmic derivative of the wavefunction, so that $\mathcal{L}\phi(0)$ is $\phi'(0)$ by definition, then this is related to the logarithmic derivative of the Green function by

$$\mathcal{L} = \mathcal{L}^{(\mp)} \tag{5.6}$$

depending on whether the wavefunction corresponds to a state propagating to the right (-) or to the left (+), as is easily seen by repeating the above analysis for the latter case.

We note that for one given medium, ϕ' is always continuous, but for a matched system it might or might not be. It is therefore in order to specify that the counterpart of (5.4) is

$$\psi'(-0) = \mathcal{L}_1^{(+)}\psi(0) \tag{5.7}$$

when ψ corresponds to incidence from the right, in which case

$$\psi(0) = \mathcal{G}_s \mathcal{G}_2^{-1} \phi_2(0). \tag{5.8}$$

The formulae always contain a reference to the incident amplitude.

Now consider a bound matching state, often called a surface state. For z and z' on side p , the formula for \mathbf{G}_s can be identically cast as

$$\mathbf{G}_s(z, z') = \mathbf{G}_p(z, z') + \mathbf{G}_p(z, 0) \mathcal{G}_p^{-1} (\mathcal{G}_s - \mathcal{G}_p) \mathcal{G}_s^{-1} \mathbf{G}(0, z'). \tag{5.9}$$

Take residues at the energy of a surface state. Then \mathbf{G}_p has no residue at this energy and we obtain

$$\psi_s(z) = \mathbf{G}_p(z, 0) \mathcal{G}_p^{-1} \psi_s(0) - \mathbf{G}_p(z, 0) \mathcal{G}_s^{-1} \psi_s(0). \tag{5.10}$$

But the matching equation is precisely

$$\mathcal{G}_s^{-1} \psi_s(0) = \mathbf{0}. \tag{5.11}$$

Thus

$$\psi_s(z) = \mathbf{G}_p(z, 0) \mathcal{G}_p^{-1} \psi_s(0) \quad z \in p. \tag{5.12}$$

with no reference, of course, to any incident amplitude.

It is easy to relate these results to the definition of the transfer matrix. For one given medium we find

$$\mathbf{K}(z, 0) = \mathbf{G}(z, 0) \mathcal{G}^{-1} = \mathbf{M}_{AA}(z, 0) + \mathbf{M}_{AD}(z, 0) \mathcal{L}^{(\mp)}. \tag{5.13}$$

This defines $\mathbf{K}(z, 0)$. For propagating states the (-/+ sign is associated with propagation to the right/left, while for bound states it is associated with evaluation of the wavefunction on the right/left of the reference point $z = 0$. This result relates the two concepts of transfer matrix used in the literature. \mathbf{M} is a full transfer matrix which transfers amplitudes and derivatives. \mathbf{K} is a matrix which transfers amplitudes only. In practice this is a useful object only for cases like homogeneous media with simple models, when it can be easily evaluated. But (5.13) gives a formula which can be used in all cases and only requires a suitable numerical algorithm for evaluating \mathbf{M} .

The qw or sandwich structure can be likewise studied by taking, say, l as the reference point $z = 0$. Bound states of the well are particularly important. These are matching solutions. Let ψ_l indicate the amplitude at l . Then for $z \in l$ (5.12) holds with $p = l$ for ψ_l and $\psi_s(0)$. It is convenient to define

$$\tilde{\psi}_s = \begin{bmatrix} \psi_l \\ \psi_r \end{bmatrix} \quad \tilde{\mathbf{D}}_s(r, l) = \begin{bmatrix} \mathcal{L}_l & \mathbf{0} \\ \mathbf{0} & \mathbf{K}_s(r, l) \end{bmatrix}. \tag{5.14}$$

Then, for $z \in 2$, i.e. inside the well or barrier,

$$\psi_s = [\mathbf{G}_2(z, l), \mathbf{G}_2(z, r)] \tilde{\mathbf{G}}_2^{-1} \tilde{\mathbf{D}}_s(r, l) \begin{bmatrix} \psi_1 \\ \psi_1 \end{bmatrix} \quad (5.15)$$

while for $z \in 3$:

$$\psi_s(z) = \mathbf{K}_3(z, r) \mathbf{K}_s(r, l) \psi_1. \quad (5.16)$$

Thus everything is expressed in terms of the reference amplitude ψ_1 only. The Green function elements entering these formulae can be evaluated from the corresponding transfer matrices by using the results of section 4.

The dependence on energy and 2D wavevector κ is understood everywhere, but the SL has additional distinct features. The wavefunctions now have a 1D wavevector q , corresponding to propagation in the z direction. However, all the SL states are matching states given by the matching equation

$$\tilde{\mathbf{G}}_s^{-1} \tilde{\psi}_s = 0. \quad (5.17)$$

This holds for both the SL and the QW cases, but in the latter $\tilde{\mathbf{G}}_s^{-1}$ depends on κ while in the former it depends on κ and q . The z dependence of $\psi_s(z)$ for all SL states can be written down in terms of formulae with the same form as for bound states of the QW. Thus

$$\psi_s(z) = \begin{cases} \mathbf{K}_1(z, l) \psi_1 & m \leq z \leq l \\ \mathbf{K}_1(z, r) \mathbf{D}_s(r, l) \psi_1 & r \leq z \leq n \end{cases} \quad (5.18)$$

while (5.15) yields $\psi_s(z)$ for $l \leq z \leq r$. In both cases

$$\mathbf{K}_s(r, l) = \tilde{\mathbf{G}}_s(r, l) \mathcal{G}_s^{-1}. \quad (5.19)$$

In the SL case the q dependence enters through (i) $\mathbf{K}_s(r, l)$ and (ii) ψ_p , as this is the l part of $\tilde{\psi}_s$ given by (5.17). The wavefunction for the SL can now be calculated again in terms of the constituent transfer matrices.

6. Practical aspects

For the sake of clarity and conciseness, we have often referred to electronic states and to the matching of logarithmic derivatives of the wavefunction, but the formal theory given here holds quite generally provided the derivative is replaced by the linear differential form appropriate to each different physical problem [1].

The case of a standard Schrödinger equation with given crystal potential, or pseudopotential, constitutes an important field of application. Another practical example is that of effective mass or envelope function models, which in spite of their limitations are frequently used because of their comparative flexibility. In this case the form of the differential matrix, which entails the form of the boundary conditions for matching problems, has been abundantly discussed. A recent study, with references to earlier work, can be found in [12]. Here we are only concerned with the question of how to handle a given starting differential matrix. In practice one is faced with a problem of the form

$$\mathbf{A}\Psi'' + \mathbf{B}\Psi' + \mathbf{C}\Psi = E\Psi \quad (6.1)$$

where Ψ is an N -component vector and \mathbf{A} , \mathbf{B} and \mathbf{C} are in general z -dependent $N \times N$ matrices. These may depend, for instance, on the procedure one chooses to ensure

the Hermitian character of the Hamiltonian, but this does not change the form of (6.1). It is trivial to see that this is equivalent to the first-order differential system

$$\left\| \begin{array}{cc} \mathbf{0} & \mathbf{1}_N \\ \mathbf{A}^{-1}(\mathbf{E}\mathbf{1}_N - \mathbf{C}) & -\mathbf{A}^{-1}\mathbf{B} \end{array} \right\| \Phi(z) = \frac{d}{dz} \Phi(z) \quad \Phi(z) = \begin{bmatrix} \Psi(z) \\ \Psi'(z) \end{bmatrix} \quad (6.2)$$

where $\mathbf{1}_N$ is the $N \times N$ unit matrix. This is the system for which one evaluates the transfer matrix. One could define the supervector Φ in a different way in which ψ' is replaced by the linear form $\mathbf{A}\psi' + \mathbf{B}$ [13], as (6.1) leads to the continuity of this form. When the matrices \mathbf{A} and \mathbf{B} are z dependent this becomes rather more complicated, while (6.2) holds whether they are constant or z dependent. Although some envelope function models may involve up to fourth-order derivatives [14]—a case which is also easily reduced to a first-order system—the second-order differential system is by far the most frequent and important case, not only for electronic states but also for other types of elementary excitations.

The formalism presented here shows how, once the model has been defined, both \mathbf{G}_s and ψ_s can be written down in terms of the transfer matrices of the constituent media so that all the effects of the matching are exactly included. Note that due to (2.13) the problem of evaluating normal derivatives is reduced to evaluating the submatrices of \mathbf{M} . Efficient numerical algorithms exist for this which are explained in [1]. Thus ultimately one has an expedient way of calculating the Green function of the wavefunction of layered systems, whence the desired physical information can be extracted in the standard way.

Especially interesting is the applicability to problems involving significant inhomogeneities. These may arise, for instance, in epitaxially grown structures like graded walls, QWs with parabolic or other z -dependent profiles, $n-i-p-i$ SLs or z -dependent image potential wells. All these problems can be studied with this method, and some have actually been studied in the preliminary applications quoted above. But the most interesting aspect is the new inroad this opens into performing self-consistent calculations at surfaces or interfaces by matching Green functions. Suppose one starts with the ideal interface (broken curves in figure 1) so \mathbf{G}_A^0 and \mathbf{G}_B^0 are the Green functions of the infinite perfect media A and B . Even if these can be easily obtained and used for the matching calculation, the problem is that the charge density profile one obtains from this is not consistent with the starting potential profile V (broken curves in figure 1). One then has a different potential profile V' (solid curves in figure 1) and the matching calculation must be repeated. The question is what are then \mathbf{G}_A and \mathbf{G}_B and how does one evaluate them? The method presented here, and used in [10] for $N = 1$, shows how this can be done. Once the numerical algorithm for the evaluation of the transfer matrix has been set up, it can be used for any potential profile as input. This opens a very attractive possibility of the self-consistent calculation of interface or layered structures.

The use of the transfer matrix \mathbf{M} , which transfers amplitudes and derivatives, to study matching problems appears to be very scarce altogether. We have already mentioned the work of Ram-Mohan *et al* [13], where \mathbf{M} is used to solve the eigenvalue problem for superlattices. The practical question of evaluating \mathbf{M} numerically is solved there by repeated multiplication of matrices of the form

$$\mathbf{M}(z_{n-1}, z_n) = \exp(\mathbf{P}_n \Delta_n). \quad (6.3)$$

The double-sized first-order differential system is defined as in (6.2) with the Ψ' part

of Φ replaced by $\mathbf{A}\Psi' + \mathbf{B}$, as mentioned above. \mathbf{P} is then the matrix multiplying Φ in the first-order differential system. The integration interval is divided into small increments $\Delta_n = z_{n+1} - z_n$ and \mathbf{P}_n is the value of \mathbf{P} in the n th interval. While the matrix \mathbf{P} can be diagonalised by means of standard subroutines, it is well known that the calculation of the exponential of an arbitrary matrix can be a tricky numerical problem [15]. The method is also inherently not very accurate, as it amounts to replacing the potential by discrete steps evaluated in the one-point approximation. Other numerical techniques are being implemented in the practical applications, currently in progress, of the formalism presented here.

The method of [13] has been used in [16] to study the quantum well problem as the limit of a superlattice when the thickness of one of the constituent slabs is very large. The approach developed here is different. Green functions and wavefunctions are obtained in complete form for either the superlattice or the quantum well. In the latter case this provides a natural way of giving proper distinct treatments to bound and scattering states from the beginning. This could be a suitable setting for studying problems of actual reflection or transmission across a barrier. The matching analysis presented here holds for wells or barriers equally.

The concept of the transfer matrix is a natural one for studying transmission across barriers and it has been abundantly used for these problems in the form defined in [3], i.e. the matrix which transfers amplitudes. Usually this is done in the context of one-band models. The most advanced analysis in this line is a recent study [17] of resonant tunnelling of holes in double-barrier heterostructures in a four-band envelope function model. With piecewise constant coefficients, and in the envelope function approximation, one can obtain analytically the eigenfunctions for the Hamiltonians of the constituent media. The wavefunctions of the matched system are then expressed as linear combinations of the said eigenfunctions. The form is the same in all domains but the coefficients change. The transfer matrix is defined to transfer the coefficients of these linear combinations. If one knows the analytical form of the amplitudes one can then also write down the form of the derivatives and thus complete matching can be effected. This method works well provided one knows the basis functions explicitly. The analysis presented here does not require this and can be used by proceeding directly from the z -dependent potential, or coefficients of the differential system, as numerical input. This can also have some practical advantages. Sometimes one may know the eigenfunctions of the constituent media, but these can be numerically rather intractable. A case in point is the image potential often used to study image states on metal surfaces [18–20]. The eigenfunctions of a potential going like $(z - z_0)^{-1}$ and converging at infinity are known. They are Whittaker functions, which are rather cumbersome for numerical work. Thus one often resorts to an approximation [21] in which these are approximated in terms of Bessel and Neumann functions, which are also non-trivial to handle numerically. One may gain in accuracy by proceeding directly from the potential [10] which, on the other hand, need not be known analytically.

Various applications of the formalism presented here are currently in progress.

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