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Simultaneous surface Green function matching for N interfaces

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Abstract. The method of surface Green function matching (SGFM) is extended to the case of an arbitrary number N of interfaces so that all the SGFM formulae are obtained in a compact $N \times N$ matrix (or supermatrix) form ready for practical calculations. As an example, shear (surface horizontal) waves in a Ni–W–Al–Ni structure are studied by a straightforward application of the general formulae. The range of applications of physical interest is stressed.

1. Introduction

In the most common types of heterostructures one has to solve a matching problem at one (single heterojunction) or two (quantum well or superlattice) physically distinct interfaces. However, there are more complicated heterostructures of physical interest for which one has to match at a larger number N of different interfaces. Some examples of heterostructures are a polytype superlattice, an arbitrary sequence of wells and barriers or a multilayer system of Fibonacci or Thue–Morse type.

In the surface Green function matching (SGFM) method the extension from one to two interfaces is made by defining the simultaneous bi-projection on the two-surface domain [1], which is the entire interface domain where matching is effected. For a given bulk medium the Green function is a matrix of order n, depending on the model or the physical problem under study. Then the bi-projection is of order $2n$, i.e. a 2×2 supermatrix in which each element is an $n \times n$ matrix. We shall refer to these as 'matrix elements', or simply as 'elements', on the understanding that they may be matrices (a point which is irrelevant for the analysis to follow).

The purpose of this paper is to present the extension of the SGFM method to the N-interface problem embodied in a compact algebra in terms of $N \times N$ supermatrices that result from the simultaneous N-projection at all interfaces involved. This allows for a concise formulation which yields a systematic algorithm that can be used for practical calculations.

The SGFM method can be equally developed for continuous systems, described in terms of differential equations, or for discrete systems, described in terms of matrices, such as discrete lattice dynamics or electronic structure calculations based on tight-binding models [1]. The case of continuous systems will be explicitly discussed here, although the way to do the same for discrete systems is obvious. Section 2 presents the formulation of the problem, giving the general form of the total Green function of the entire structure in terms of the Green functions of the constituent media. Section 3 describes how the simultaneous matching is done, leading to the matching formula. Section 4 demonstrates with some applications how the method works in practice and final comments are made in section 5.

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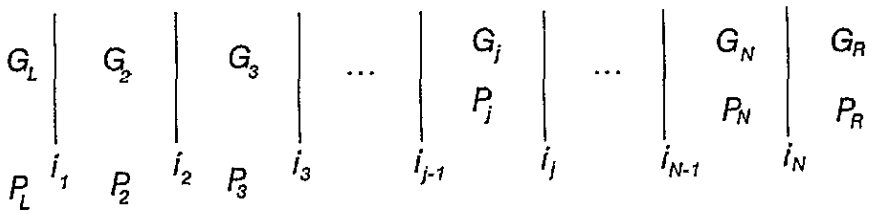

Figure 1. A general heterostructure with N interfaces and N domains. Note that domain 1 is disjoint and consists of L on the left and R on the right. The symbols i_j denote the projections on the different interfaces.

2. Formulation of the problem for continuous systems

Figure 1 displays the structure under study and part of the notation. The unit projectors on the different interfaces are denoted by i_j. Each constituent medium has an extended *bulk* Green function G_j. We stress that each G_j is the Green function of an *extended pseudomedium* [1, 2] which satisfies the same differential equations in domain j and arbitrary boundary conditions at its interfaces. In simple cases these can be just the G_j of the regular bulk media j, but sometimes it may be convenient in practice to use the flexibility provided by the arbitrary choice of boundary conditions in order to effect some practical simplifications [1, 2–4]; in any case we stress that all the G_j are *bulk* Green functions. The purpose of the analysis is to match all these Green functions at the N interfaces and thus obtain the Green function G_s of the full structure in terms of the given G_j. One technical point should be noted (figure 1). On the left we have a medium L with bulk Green function G_L and on the right a medium R with G_R, so we have N interfaces and $N+1$ physically different media. As in the case of the quantum well [1] it is convenient to define formally domain 1 to consist of L/R on the left/right. Then medium 1 is, by definition, medium L/R on the left/right and G_1 is G_L/G_R in L/R. We then have formally N interfaces and N media.

Consider now domain j, bounded by the interfaces i_{j-1} and i_j. We define the partial surface projector

$$\mathcal{I}_j = i_{j-1} + i_j \tag{1}$$

which spans the space of 2×2 supermatrices. Consequently we define, out of G_j, the projection

$$\tilde{G}_j = \mathcal{I}_j G_j \mathcal{I}_j. \tag{2}$$

The total surface projector is

$$\mathcal{I} = \sum_{j=1}^{N} i_j. \tag{3}$$

In the matrix representation $\mathcal{I}$ is the $N \times N$ unit supermatrix matrix, i.e. all diagonal elements are equal to 'unity', which simply means the number one if $n = 1$ (a scalar problem, like a one-band Schrödinger equation) or the $n \times n$ unit matrix if $n > 1$. We shall henceforth denote this as 'unity' without the need for further explanation. Thus, in the supermatrix format of $\mathcal{I}$, the partial projector i_j has 'unity' in the jth diagonal element

and zero elsewhere and $\mathcal{I}_j$ has 'unity' in the $(j-1)$th and jth diagonal elements and zero elsewhere. In the space of $\mathcal{I}_j$ the projection $\tilde{G}_j$ is the 2×2 supermatrix

$$\tilde{G}_j = \begin{Vmatrix} \langle i_{j-1}|G_j|i_{j-1}\rangle & \langle i_{j-1}|G_j|i_j\rangle \\ \langle i_j|G_j|i_{j-1}\rangle & \langle i_j|G_j|i_j\rangle \end{Vmatrix} \equiv \mathcal{I}_j\tilde{G}_j\mathcal{I}_j. \tag{4}$$

When this is represented in the $N \times N$ supermatrix format of I, the four non-vanishing elements of $\mathcal{I}\tilde{G}_j\mathcal{I}$ are those of (4) in the positions labelled $(j-1, j-1)$, $(j-1, j)$, $(j, j-1)$ and (j, j) as row and column indices of the $N \times N$ supermatrix. We note that with the present notation $\tilde{G}_1$ is a particular case. In the space of $\mathcal{I}_1$ (which, by definition, is $i_1 + i_N$) this is the 2×2 diagonal supermatrix

$$\tilde{G}_1 = \begin{Vmatrix} \langle i_1|G_L|i_1\rangle & 0 \\ 0 & \langle i_N|G_R|i_N\rangle \end{Vmatrix} \equiv \mathcal{I}_1\tilde{G}_1\mathcal{I}_1. \tag{5}$$

Any G_j for $j > 1$ is a propagator which can propagate from i_{j-1} to i_j, or *vice versa*, through a medium j. The topology of domain 1 is different, as it consists of two disconnected subdomains. The block diagonal form of (5) corresponds to the fact that there is no propagation from, say, i_1 to i_N with propagator G_L or *vice versa*. Thus when $\tilde{G}_1$ is represented in the $N \times N$ supermatrix format of $\mathcal{I}$, it has the non-vanishing elements (1, 1) and (N, N) and the rest are all zero.

Now in the final results all intervening elements are put together in the large $N \times N$ supermatrix format, but many algebraic steps, *including matrix inversions*, are carried out in the smaller space of 2×2 supermatrices. Obviously the large matrix $\mathcal{I}\tilde{G}_j\mathcal{I}$ cannot be inverted, but the small matrix $\mathcal{I}_j\tilde{G}_j\mathcal{I}_j$ can, in the space of $\mathcal{I}_j$, and after inversion the result can be put in its place in the large $N \times N$ supermatrix format. Symbols like $\tilde{G}_j^{-1}$ will be often used in this sense. Strictly speaking this is to be understood as $\mathcal{I}_j\tilde{G}_j^{-1}\mathcal{I}_j$ so that by definition

$$\mathcal{I}_j\tilde{G}_j^{-1}\mathcal{I}_j\mathcal{I}_j\tilde{G}_j\mathcal{I}_j = \mathcal{I}_j\tilde{G}_j^{-1}\tilde{G}_j\mathcal{I}_j = \mathcal{I}_j \tag{6}$$

which can be conveniently abbreviated as

$$\tilde{G}_j^{-1}\tilde{G}_j = \mathcal{I}_j. \tag{7}$$

It is understood that there is everywhere a dependence on the eigenvalue variable, say energy E or frequency ω, and on the 2D wavevector κ introduced by the 2D Fourier transform, so that only the dependence on the position variable z is explicitly displayed. A symbol like $\langle i_{j-1}|G_j|i_j\rangle$ denotes the value of $\langle z|G_j|z'\rangle$ when z is at the position corresponding to the $(j-1)$th interface and z' at that of the jth interface. We shall indicate by z_j that z is in the domain j, so that $\langle z_j|G|z_k\rangle$ when $j \neq k$ is zero if G is any of the G_m, but is just what we want to obtain if G is G_s. Again, $\langle z_1|G_1|z_1'\rangle$ requires special consideration, depending on whether 1 means L or R. Thus

$$\begin{aligned} &\langle z_L|G_1|z_L'\rangle = \langle z_L|G_L|z_L'\rangle \\ &\langle z_L|G_1|z_R'\rangle = 0 = \langle z_R|G_1|z_L'\rangle \\ &\langle z_R|G_1|z_R'\rangle = \langle z_R|G_R|z_R'\rangle. \end{aligned} \tag{8}$$

We then define N-supervectors as follows:

$$\langle z_j|G_j|\mathcal{I}_j\rangle = [0, 0, \ldots, 0, \langle z_j|G_j|i_{j-1}\rangle, \langle z_j|G_j|i_j\rangle, 0, \ldots, 0]. \tag{9}$$

We note the following. (i) This is , $\langle z_j|G_j|\mathcal{I}_j\rangle$ when put in the large format of N-supervectors. In the space of $\mathcal{I}_j$ it would be only a 2-supervector. (ii) Each component is an $n\times n$ matrix. This is a row supervector. Likewise, we define the column N-supervector , $\langle\mathcal{I}_j|G_j|z'_j\rangle$ with the two non-vanishing components , $\langle i_{j-1}|G_j|z'_j\rangle$ and , $\langle i_j|G_j|z'_j\rangle$. As particular cases we have again

$$\begin{aligned}\langle z_L|G_1|\mathcal{I}_1\rangle &= \langle z_L|G_L|\mathcal{I}_1\rangle = [\langle z_L|G_1|i_1\rangle, 0, \ldots, 0, 0]\\ \langle z_R|G_1|\mathcal{I}_1\rangle &= \langle z_R|G_R|\mathcal{I}_1\rangle = [0, 0, \ldots, 0, \langle z_R|G_R|i_N\rangle].\end{aligned} \tag{10}$$

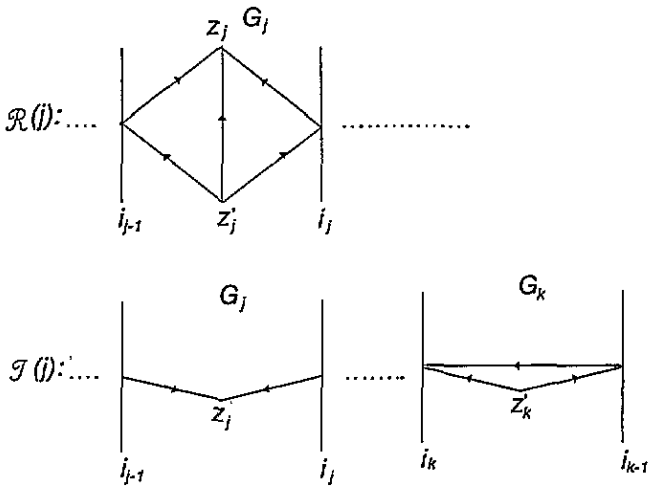

Figure 2. Illustrating the physical meaning of the reflection and transmission objects defined in the text.

Then the form of the generic elements of G_s is

$$\begin{aligned}\langle z_j|G_s|z'_j\rangle &= \langle z_j|G_j|z'_j\rangle + \langle z_j|G_j|\mathcal{I}_j\rangle\langle\mathcal{I}_j|\mathcal{R}(j)|\mathcal{I}_j\rangle\langle\mathcal{I}_j|G_j|z'_j\rangle\\ \langle z_j|G_s|z'_k\rangle &= \langle z_j|G_j|\mathcal{I}_j\rangle\langle\mathcal{I}_j|\mathcal{T}(j,k)|\mathcal{I}_k\rangle\langle\mathcal{I}_k|G_k|z'_k\rangle\end{aligned} \tag{11}$$

as in the usual SGFM analysis [1]. The meaning of the reflection, $\mathcal{R}(j)$, and transmission, $\mathcal{T}(j,k)$, objects is displayed in figure 2 and we recall that, by definition, these have the nature of T-matrices in the sense of scattering theory. This is why the propagators after interaction with the interfaces are the known 'unperturbed' bulk propagators, so the problem is reduced to finding the reflection and transmission objects. It is clear by inspection of (10) and of figure 2 that the four non-vanishing elements of $\mathcal{R}(j)$ in the large $N\times N$ supermatrix format are those labelled $(j-1,j-1)$, $(j-1,j)$, $(j,j-1)$ and (j,j), while those of $\mathcal{T}(j,k)$ are $(j-1,k-1)$, $(j-1,k)$, $(j,k-1)$ and (j,k). The case j or $k=1$ has again a special form. Firstly, $\langle\mathcal{I}_1|\mathcal{R}(1)|\mathcal{I}_1\rangle$ consists only of the two disjoint elements $(1,1)$ and (N,N), the rest being zero. Secondly, $\langle\mathcal{I}_1|\mathcal{T}(1,j)|\mathcal{I}_1\rangle$ consists of two disjoint pairs of elements, one formed by those with labels $(1,j-1)$, $(1,j)$ in row 1 and another one formed by those with labels $(N,j-1)$, (N,j) in row j, the rest being zero. Likewise $\mathcal{T}(j,1)$ consists of two disjoint pairs of elements, one constituted by elements $(j-1,1)$, $(j,1)$ in column 1 and the other one by elements $(j-1,N)$, (j,N) in column N, the rest being also zero.

From the first of equations (11) we obtain the projection

$$\langle \mathcal{I}_j|\tilde{G}_s|\mathcal{I}_j\rangle = \langle \mathcal{I}_j|\tilde{G}_j|\mathcal{I}_j\rangle + \langle \mathcal{I}_j|\tilde{G}_j|\mathcal{I}_j\rangle\langle \mathcal{I}_j|\mathcal{R}(j)|\mathcal{I}_j\rangle\langle \mathcal{I}_j|\tilde{G}_j|\mathcal{I}_j\rangle. \tag{12}$$

Note that this is part of the $N \times N$ supermatrix $\tilde{G}_s$ but, as it stands, (11) is strictly an equality between 2×2 supermatrices and in their own space we can carry out the desired matrix algebra, including matrix inversion as explained above.

In this space, this yields

$$\mathcal{R}(j) = \tilde{G}_j^{-1}(\tilde{G}_s - \tilde{G}_j)\tilde{G}_j^{-1}. \tag{13}$$

Although $\tilde{G}_s$ appears here, the fact of having $\tilde{G}_j^{-1}$ on the left and on the right automatically carries the corresponding projector $\mathcal{I}_j$ on both sides, so the $\tilde{G}_s$ appearing in a formula like (13) is, by definition, identically the LHS of (12). Therefore

$$\langle z_j|G_s|z_j'\rangle = \langle z_j|G_j|z_j'\rangle + \langle z_j|G_s|\mathcal{I}_j'\rangle\tilde{G}_j^{-1}(\tilde{G}_s - \tilde{G}_j)\tilde{G}_j^{-1}\langle \mathcal{I}_j|G_j|z_j'\rangle. \tag{14}$$

Likewise from the second of equations (11) we obtain the projection

$$\langle \mathcal{I}_j|\tilde{G}_s|\mathcal{I}_k\rangle = \langle \mathcal{I}_j|\tilde{G}_j|\mathcal{I}_j\rangle\langle \mathcal{I}_j|\mathcal{T}(j,k)|\mathcal{I}_k\rangle\langle \mathcal{I}_k|\tilde{G}_k|\mathcal{I}_k\rangle \tag{15}$$

which is again an equality between 2×2 supermatrices, from which we obtain

$$\mathcal{T}(j,k) = \langle \mathcal{I}_j|\tilde{G}_j^{-1}|\mathcal{I}_j\rangle\langle \mathcal{I}_j|\tilde{G}_s|\mathcal{I}_k\rangle\langle \mathcal{I}_k|\tilde{G}_k^{-1}|\mathcal{I}_k\rangle \tag{16}$$

whence

$$\langle z_j|\tilde{G}|z_k'\rangle = \langle z_j|G_j|\mathcal{I}_j\rangle\tilde{G}_j^{-1}\langle \mathcal{I}_j|\tilde{G}_s|\mathcal{I}_k\rangle\tilde{G}_k^{-1}\langle \mathcal{I}_k|\tilde{G}_k|z_k'\rangle. \tag{17}$$

The results (14) and (17) constitute the formal extension to the N-interface case of the standard SGFM results for $N = 2$, as do (13) and (16). If we can calculate $\tilde{G}_s$, then (14) and (17) yield all desired elements $\langle z|G_s|z'\rangle$ for z and z' anywhere. This can be obtained by imposing the matching conditions at the interfaces, whereby the scattering problem of calculating the reflection and transmission objects $\mathcal{R}$ and $\mathcal{T}$ is transformed into an exact matching analysis. This will be done in the next section.

3. The matching formula for continuous systems

The details of the matching formula for $\tilde{G}_s$ depend on the matching conditions to be imposed, which in turn depend on the physical problem under study. To fix ideas we shall first discuss one specific case and then give the general result. Consider, for instance, the one-band effective-mass model for a medium j with Green function G_j. The discontinuity of its derivative is

$$'\mathcal{G}_j^{(+)} - '\mathcal{G}_j^{(-)} \equiv s_j = -\frac{2m_j}{\hbar^2} \tag{18}$$

where

$$'\mathcal{G}_j^{(\pm)} = \lim_{z' \to \pm 0}\left(\frac{\partial\langle z|G|z'\rangle}{\partial z}\right)_{z=0}. \tag{19}$$

In this case in wavefunction terms one has to match the amplitude ψ and the derivative ψ' divided by m. This can be cast as the matching of $s^{-1}\psi'/\psi$, which is a weighted logarithmic derivative. In Green function terms the matching formula for $\mathcal{G}_s$ involves quantities of the form

$$\mathcal{L}_j^{(\pm)} \equiv s_j^{-1\prime}\mathcal{G}_j^{(\pm)}\mathcal{G}_j^{-1} \tag{20}$$

which are weighted logarithmic derivatives in Green function language [1]. Allowing for some more generality we shall formally consider the case in which the G_j and s_j are matrices but the matching rules call for continuity of amplitudes and derivatives weighted with the prefactor s_j^{-1}, which can also be a matrix. In this way the analysis takes a form that is more suitable for the immediate extension to the general case, while keeping the form of the familiar analysis involving the matching of weighted logarithmic derivatives.

The script symbols involved in (18)–(20) denote projections at one single surface. Our task is to extend this analysis to the simultaneous projections introduced in section 2, for which it is necessary to introduce some further elements of notation. Given s_j for a medium j we define the 2×2 diagonal supermatrix $\mathcal{I}_j\tilde{S}_j^{-1}\mathcal{I}_j$ or, in abbreviated form, simply $\tilde{S}_j^{-1}$, which has s_j^{-1} in its two diagonal elements and zero in the two off-diagonal ones. Put in the large format of the $N\times N$ supermatrix this becomes $\mathcal{I}\tilde{S}_j^{-1}\mathcal{I}$, which has only two non-vanishing diagonal elements, namely $(j-1, j-1)$ and (j, j), both equal to s_j^{-1}. Obviously $\mathcal{I}\tilde{S}_1^{-1}\mathcal{I}$ has again a special form: the (1,1) element is s_L^{-1}, the (N, N) element is s_R^{-1} and the rest are zero. It is also convenient to abbreviate the notation for the derivatives so that $\langle z|'G|z'\rangle$ denotes the derivative with respect to z. Suppose z and z' are in the domain j, so G is G_j, and z and z' tend to the interfaces. If they tend to different interfaces, then the symbols $\langle i_j|'G_j|i_{j-1}\rangle$ and $\langle i_{j-1}|'G_j|i_j\rangle$ are self-explanatory. If both tend to the same interface, then $\langle i_j|'\mathcal{G}_j^{(\pm)}|i_j\rangle$ is defined with the same criterion of (19), the point at which the projection is made being the location of i_j instead of $z=0$.

Formulae (14) and (17) can now be used to choose appropriate domains for z and z' tending to the desired interface and thus express the matching conditions at this interface. We start, for instance, from the configuration (z_L, z_L'). Then from (14)

$$\begin{aligned} s_1^{-1}\langle z_L|'G_s|z_L'\rangle = {} & s_1^{-1}\langle z_L|'G_L|z_L'\rangle - s_1^{-1}\langle z_L|'G_s|i_1\rangle\langle i_1|\mathcal{G}_1|i_1\rangle^{-1}\langle i_1|G_L|z_L'\rangle \\ & + s_1^{-1}\langle z_L|'G_L|i_1\rangle\langle i_1|\mathcal{G}_L|i_1\rangle^{-1}\langle i_1|\mathcal{G}_s|i_1\rangle\langle i_1|\mathcal{G}_L|i_1\rangle^{-1}\langle i_1|G_L|z_L'\rangle. \end{aligned} \tag{21}$$

We first let $z_L \to z(i_1) - 0$. Then

$$\begin{aligned} s_1^{-1}\langle i_1|'G_s|z_L'\rangle = {} & s_1^{-1}\langle i_1|'G_L|z_L'\rangle - s_1^{-1}\langle i_1|'\mathcal{G}_L^{(+)}|i_1\rangle\langle i_1|\mathcal{G}_L|i_1\rangle^{-1}\langle i_1|G_L|z_L'\rangle \\ & + s_1^{-1}\langle i_1|'\mathcal{G}_L^{(+)}|i_1\rangle\langle i_1|\mathcal{G}_L|i_1\rangle^{-1}\langle i_1|\mathcal{G}_s|i_1\rangle\langle i_1|\mathcal{G}_L|i_1\rangle^{-1}\langle i_1|G_L|z_L'\rangle \end{aligned} \tag{22}$$

after which we let $z_L' \to z(i_1) - 0$. Then, using the fact that

$$s_1^{-1}(\langle i_1|'\mathcal{G}_L^{(+)}|i_1\rangle - \langle i_1|'\mathcal{G}_L^{(-)}|i_1\rangle) = i_1 \tag{23}$$

we obtain

$$s_1^{-1}\langle i_1|'\mathcal{G}_s^{(-)}|i_1\rangle = s_1^{-1}\langle i_1|'\mathcal{G}_L^{(+)}|i_1\rangle\langle i_1|\mathcal{G}_L|i_1\rangle^{-1}\langle i_1|\mathcal{G}_s|i_1\rangle - i_1. \tag{24}$$

The idea is to obtain the same quantity starting from the configuration (z_2, z_1') and then to express the equality of the two results. Thus, from (17)

$$s_2^{-1}\langle z_2|'G_s|z_L'\rangle = s_2^{-1}\langle z_2|'G_2|\mathcal{I}_2\rangle\langle\mathcal{I}_2|\tilde{G}_2^{-1}|\mathcal{I}_2\rangle\langle\mathcal{I}_2|\tilde{G}_s^{-1}|i_1\rangle\langle i_1|\mathcal{G}_L|i_1\rangle^{-1}\langle i_1|G_L|z_L'\rangle. \tag{25}$$

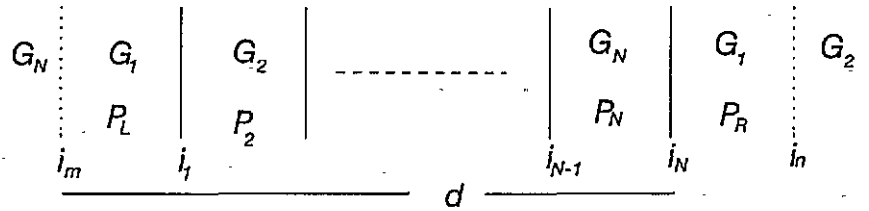

Figure 3. A polytype superlattice. The period consists of $G_1 - G_2 \ldots - G_N$. The interfaces i_m, i_n are physically identical to i_N, i_1, respectively. Note the difference with respect to figure 1: the domain P_1 consists of P_L and P_R in both cases, but now the L and R domains are physically identical and there is only one G_1 instead of having G_L in P_L and G_R in P_R, as in figure 1. The superlattice period is d.

Now consider explicitly the row N-supervector

$$\langle z_2|'G_2|\mathcal{I}_2\rangle = [\langle z_2|'G_2|i_1\rangle, \langle z_2|'G_2|i_2\rangle, 0, 0 \ldots]. \tag{26}$$

On letting $z_2 \to z(i_1) + 0$ we obtain

$$\langle i_1|'\tilde{G}_2|\mathcal{I}_2\rangle = [\langle i_1|'\mathcal{G}_2^{(-)}|i_1\rangle, \langle i_1|'G_2|i_2\rangle, 0, 0 \ldots]. \tag{27}$$

Carrying out this process in (25) and taking $z_L' \to z(i_1) - 0$, we have

$$s_2^{-1}\langle i_1|'\mathcal{G}_s^{(-)}|i_1\rangle = s_2^{-1}\langle i_1|'\tilde{G}_2\tilde{G}_2^{-1}|\mathcal{I}_2\rangle\langle\mathcal{I}_2|\tilde{G}_s|i_1\rangle. \tag{28}$$

Matching at i_1 is expressed by the equality of (28) and (24). Remembering the disjoint nature of domain 1 the result can be identically written as

$$\langle i_1|(\tilde{S}_1^{-1\,\prime}\tilde{G}_1\tilde{G}_1^{-1}|\mathcal{I}_1\rangle - \tilde{S}_2^{-1\,\prime}\tilde{G}_2\tilde{G}_2^{-1}|\mathcal{I}_2\rangle)\langle\mathcal{I}|\tilde{G}_s|i_1\rangle = i_1. \tag{29}$$

The same process can be repeated for all pairs of configurations of the type (z_j, z_k'), (z_{j+1}, z_k') or (z_j, z_j'), (z_j, z_k') with j fixed and $k = 1, \ldots, N$. After some algebra this yields the matching formula

$$\tilde{G}_s^{-1} = \mathcal{I}\left(\tilde{S}_1^{-1\,\prime}\tilde{G}_1\tilde{G}_1^{-1} - \sum_{j=2}^{N}\tilde{S}_j^{-1\,\prime}\tilde{G}_j\tilde{G}_j^{-1}\right)\mathcal{I} \tag{30}$$

which is the extension of the formula for $N = 2$ [1] to an arbitrary number N of interfaces.

More generally, the matching conditions require the continuity of a linear differential form [1]

$$\mathcal{A} = -\tilde{S}^{-1\,\prime}G + \tilde{P}\tilde{G}. \tag{31}$$

It is immediately obvious that the general matching formula is

$$\tilde{G}_s^{-1} = -\mathcal{I}\left(\mathcal{A}_1^{-1}\tilde{G}_1^{-1} - \sum_{j=2}^{N}\tilde{\mathcal{A}}_j^{-1}\tilde{G}_j^{-1}\right)\mathcal{I}. \tag{32}$$

The polytype superlattice (figure 3) can equally be studied by combining this analysis with the introduction of Bloch periodicity as in the binary superlattice [1]. When the extremes of the structure are open so L and R are semi-infinite, there are no cross terms between L and R. The off-diagonal elements, or blocks, of ${}'\tilde{G}_1$, or $\tilde{A}_1$, vanish and these supermatrices are block-diagonal. However, in the superperiodic structure of figure 3 the interfaces i_N and i_m are physically identical, as are i_n and i_1. Then the amplitudes at i_N/i_n are equal to those at i_m/i_1 except for the phase factor $f = \exp(iqd)$, where q is the superwavevector associated with the superperiod d. Then domains L and R appear as mathematically linked with the appropriate phase factor and the off-diagonal elements of the supermatrices ${}'\tilde{G}_1$ and $\tilde{A}_1$ no longer vanish.

In fact, they become [1]

$$
\begin{aligned}
{}'\tilde{G}_1 &= \begin{Vmatrix} \langle i_1|'\mathcal{G}_1^{(+)}|i_1\rangle & f^{-1}\langle i_1|'G_1|i_m\rangle \\ -f\langle i_N|'G_1|i_n\rangle & -\langle i_N|'\mathcal{G}_1^{(-)}|i_N\rangle \end{Vmatrix} \\
\tilde{A}_1 &= \begin{Vmatrix} \langle i_1|\mathcal{A}_1^{(+)}|i_1\rangle & f^{-1}\langle i_1|A_1|i_m\rangle \\ -f\langle i_N|A_1|i_n\rangle & -\langle i_N|\mathcal{A}_1^{(-)}|i_N\rangle \end{Vmatrix}.
\end{aligned}
\tag{33}
$$

The rest of the analysis proceeds exactly as above, and the matching formula is the same as that of (30) or (32) with the only difference that ${}'\tilde{G}_1$ or $\tilde{A}_1$ is now given by (33).

4. Examples

As an illustration of the practical use of the method here presented we shall study acoustic shear horizontal modes in a double sandwich. This is a simple but non-trivial case involving three interfaces, which provides a practical demonstration of the method in action.

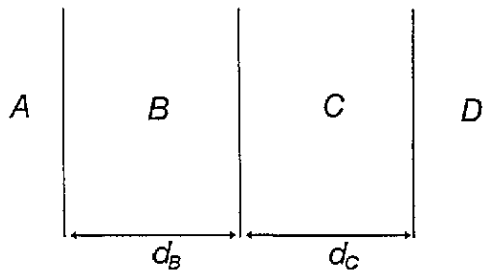

Figure 4. A double-sandwich structure A–B–C–D.

We shall consider the system sketched in figure 4. Each medium is characterized by its mass density ρ_ν and Lamé coefficient μ_ν ($\nu = A, B, C, D$).

In the case of shear horizontal modes the elements entering (32) are

$$
\begin{aligned}
\tilde{G}_1 &= \frac{1}{2}\begin{bmatrix} \mu_A\beta_A & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \mu_D\beta_D \end{bmatrix} \\
\tilde{G}_2 &= \frac{1}{2\mu_B\beta_B}\begin{bmatrix} 1 & e^{-\beta_B d_B} & 0 \\ e^{-\beta_B d_B} & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \\
\tilde{G}_3 &= \frac{1}{2\mu_C\beta_C}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & e^{-\beta_C d_C} \\ 0 & e^{-\beta_C d_C} & 1 \end{bmatrix}
\end{aligned}
\tag{34}
$$

Table 1. Mass densities and shear bulk velocities employed in the calculations.

	ρ (g cm^3)	v (10^5 cm s^{-1})
Ni	8.900	3.219
Al	2.703	3.110
W	19.300	2.860

and

$$\tilde{A}_1 = -\frac{1}{2}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\tilde{A}_2 = \frac{1}{2}\begin{bmatrix} 1 & -e^{-\beta_B d_B} & 0 \\ -e^{-\beta_B d_B} & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{35}$$

$$\tilde{A}_3 = \frac{1}{2}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & -e^{-\beta_C d_C} \\ 0 & -e^{-\beta_C d_C} & 1 \end{bmatrix}$$

where for each constituent medium

$$\beta = \sqrt{\kappa^2 - \frac{\omega^2 \rho}{\mu}} \tag{36}$$

and κ is the wavevector parallel to the surface.

Then (32) is

$$\tilde{G}_s^{-1} = \begin{bmatrix} \mu_A\beta_A + \frac{\mu_B\beta_B(1+e^{-2\beta_B d_B})}{1-e^{-2\beta_B d_B}} & \frac{-2\mu_B\beta_B e^{-\beta_B d_B}}{1-e^{-2\beta_B d_B}} & 0 \\ \frac{-2\mu_B\beta_B e^{-\beta_B d_B}}{1-e^{-2\beta_B d_B}} & \frac{\mu_B\beta_B(1+e^{-2\beta_B d_B})}{1-e^{-2\beta_B d_B}} + \frac{\mu_C\beta_C(1+e^{-2\beta_C d_C})}{1-e^{-2\beta_C d_C}} & \frac{-2\mu_C\beta_C e^{-\beta_C d_C}}{1-e^{-2\beta_C d_C}} \\ 0 & \frac{-2\mu_C\beta_C e^{-\beta_C d_C}}{1-e^{-2\beta_C d_C}} & \mu_D\beta_D + \frac{\mu_C\beta_C(1+e^{-2\beta_C d_C})}{1-e^{-2\beta_C d_C}} \end{bmatrix}. \tag{37}$$

After some algebra, this yields the dispersion relation in analytic form:

$$\begin{aligned} &\mu_A\beta_A\mu_D\beta_D[\mu_B\beta_B \tanh(\beta_C d_C) + \mu_C\beta_C \tanh(\beta_B d_B)] \\ &\quad + (\mu_A\beta_A + \mu_D\beta_D)\mu_B\beta_B\mu_C\beta_C + (\mu_A\beta_A\mu_C^2\beta_C^2 + \mu_D\beta_D\mu_B^2\beta_B^2) \\ &\quad \times \tanh(\beta_B d_B)\tanh(\beta_C d_C) + \mu_B\beta_B\mu_C\beta_C[\mu_B\beta_B \tanh(\beta_B d_B) \\ &\quad + \mu_C\beta_C \tanh(\beta_C d_C)] = 0. \end{aligned} \tag{38}$$

This can be further simplified in the particular case in which the medium D is the same as medium A. Then

$$\begin{aligned} &\mu_A^2\beta_A^2[\mu_B\beta_B \tanh(\beta_C d_C) + \mu_C\beta_C \tanh(\beta_B d_B)] \\ &\quad + 2\mu_A\beta_A\mu_B\beta_B\mu_C\beta_C + \mu_A\beta_A(\mu_B^2\beta_B^2 + \mu_C^2\beta_C^2)\tanh(\beta_B d_B)\tanh(\beta_C d_C) \\ &\quad + \mu_B\beta_B\mu_C\beta_C[\mu_B\beta_B \tanh(\beta_B d_B) + \mu_C\beta_C \tanh(\beta_C d_C)] = 0. \end{aligned} \tag{39}$$

It is easily verified that when B and C are equal this yields the dispersion relation for shear horizontal waves in the standard A–B–A sandwich [6].

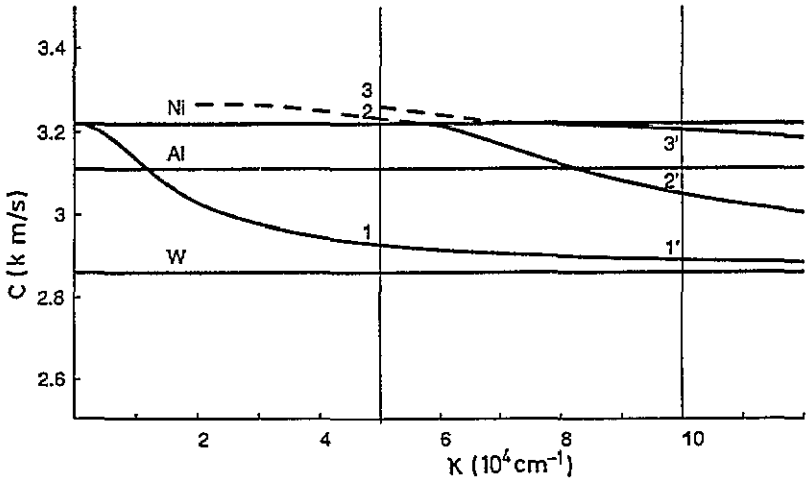

Figure 5. The horizontal lines give the bulk velocities of shear waves in Ni, Al and W employed in the calculation. The full curves give the real eigenvalues obtained from (39) for the Ni–Al–W–Ni structures. For the dotted lines see text. v is given in $\mathrm{km\,s^{-1}}$ and κ in $10^4\,\mathrm{cm^{-1}}$.

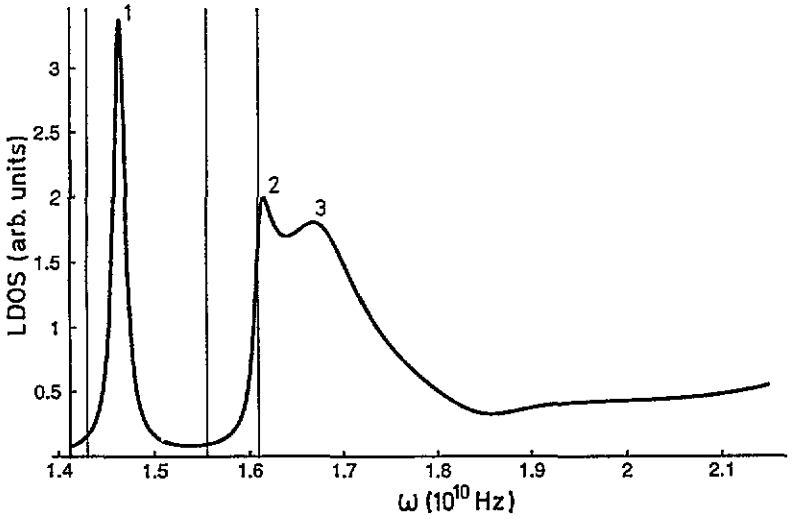

Figure 6. Local density of states projected at the interfaces of the Ni–W–Al–Ni structure as a function of ω in Hz, for $\kappa = 5 \times 10^4\,\mathrm{cm^{-1}}$.

Figure 5 shows the resulting phase velocities, ω/κ, obtained for the system Ni–Al–W–Ni with $d(\mathrm{Al}) = d(\mathrm{W}) = 100\,\mathrm{nm}$ and the input data given in table 1. The horizontal lines give the bulk values for Ni, Al and W. These lines separate allowed from forbidden frequencies ($\omega = v\kappa$), corresponding to oscillatory (propagating) or evanescent amplitudes, respectively, for each material. The curves give the velocities of the eigenvalues of (39) corresponding to matching solutions. The dotted lines above the Ni threshold will be commented upon presently. The thin vertical line at $\kappa = 5 \times 10^4\,\mathrm{cm^{-1}}$ crosses the eigenvalue curves at the frequencies indicated 1, 2 and 3. The first one corresponds to a mode localized in the W slab, where it has an oscillatory amplitude, while it is forbidden in Al and Ni, with an

evanescent amplitude in these materials. This is the only real eigenvalue of (39) for this value of κ. The nature of the solutions 2 and 3 is displayed in figure 6, which gives the local density of states, obtained from $\mathrm{Im}\,\mathrm{Tr}\,\tilde{G}_s$, projected at the interfaces as a function of frequency for $\kappa = 5 \times 10^4\,\mathrm{cm}^{-1}$. The thick vertical lines correspond to the horizontal thresholds of figure 5. The first peak, labelled 1, would be analytically a δ-function at the frequency of the confined mode labelled 1 in figure 5. The broadening is numerical, due to the addition of a small imaginary part to the real frequency, as one always does in practice for numerical convenience in order to obtain a smooth spectral function. The DOS rises again in the bulk continuum above the Ni threshold and shows the two humps corresponding to the modes labelled 2 and 3 in figure 5. As solutions of the secular equation (39) these would be complex eigenvalues. Physically they are resonances with the bulk continuum, as figure 6 displays. This is the meaning of the dotted lines of figure 5. The same type of resonances are found in the study of the electronic structure of quantum wells [7].

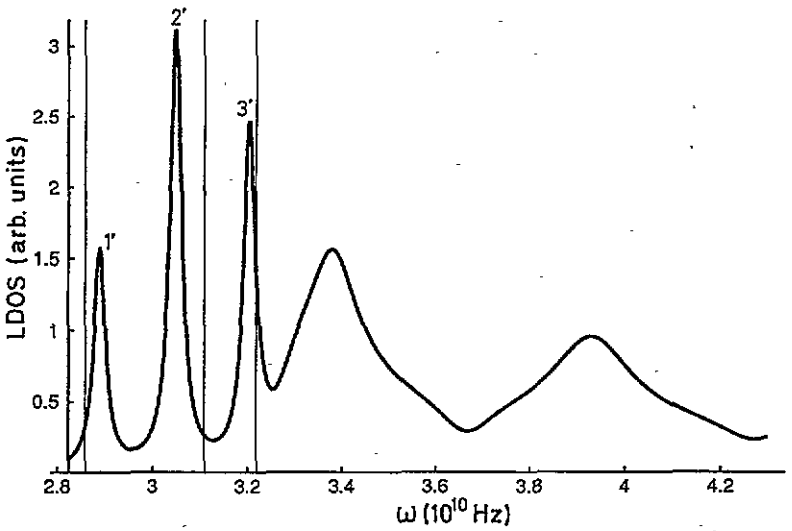

Figure 7. Same as figure 6, for $\kappa = 10^5\,\mathrm{cm}^{-1}$.

The picture changes as κ increases. More spectral strength tends to accumulate in the lower frequencies as the peaks and humps move down while new features appear in the Ni bulk continuum. This also entails changes in the physical nature of the solutions, as can be seen in figure 5 (the second vertical thin line) and figure 7, both for $\kappa = 10^5\,\mathrm{cm}^{-1}$. Peak 1 simply moves down to 1′ and retains its physical nature, but hump 2 becomes peak 2′ which is now a mode confined in the W slab. In figure 5 it is the real eigenvalue 2′. Likewise hump 3 becomes peak 3′ and this is confined in both the Al and W slabs. Furthermore, new humps appear above the Ni threshold, corresponding to two new resonances. This trend continues as κ increases. Thus the three-interface structure can be fully studied with great ease from (39), which is readily obtained by direct application of the simultaneous SGFM method.

5. Final comments

The mathematical form of the results presented here has some features worth noting. It provides a concise and compact algebra which affects the simultaneous matching at all

interfaces involved and allows for an algorithm with which practical calculations can be done in simple matrix form. The (super)matrix $\tilde{G}_s^{-1}$ has an appealing block-tridiagonal structure which reflects the physical fact that each slab is in contact with its immediate neighbours and is also advantageous when it comes to matrix algebra and, in particular, inversion.

The method can be readily used in practice to study rather complicated systems of real physical interest, such as those mentioned in the introduction, and others such as the modified multiple quantum well often used for laser action, in which a sizable number of interfaces can be involved. Another substantial problem arises in the double-barrier structures often used to study resonant tunneling, where the electron–polar-optical-phonon interaction is known to play a significant role [8]. Here one is interested in the long-wave modes of the double barrier, which involves four interfaces. Due to the coupling between the mechanical and electrical vibrations, the study of polar optical modes is already non-trivial even for a simple quantum well [9]. The study of a double-barrier structure of the type A–B–A–B–A, with five different media and four interfaces, is rather more involved due to the long-range nature of the Coulomb interactions. This is a problem which can be readily studied with the simultaneous coupling method presented here. Finally, this provides a basis for the solution of a practical problem of considerable importance. Suppose we want to do electronic structure calculations of layered structures like ordinary quantum wells or binary superlattices but using a fairly elaborate model, like an eight-band envelope function model. We have stressed above that the full transfer matrix [5] can be a useful device for calculating Green functions [1–3] or wavefunctions [10]. However, if the constituent slabs are sufficiently thick, then due to intrinsic mathematical reasons serious numerical problems soon appear in practice. The well known problem of the *stiffness* of differential systems [11] is an example of this type of problem.

The simultaneous matching method presented here provides a neat way to get round these practical difficulties. If a given slab is so thick that the integration of the differential system through it presents numerical problems, then it suffices to define arbitrary intermediate interfaces and effect the simultaneous matching as explained. The thicknesses of the partial slabs thus defined can be conveniently defined so that integration through them causes no problem. The practical difficulty of integrating through troublesome distances is thus totally avoided by throwing the weight of the calculation into a simple matrix algebra which presents no numerical difficulties. Work on this and on the polar optical modes of double-barrier structures is currently going on in our laboratories.

Acknowledgments

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