Interface response and rescaling approach to the eigenvectors of layered composite systems. I. Double-layer slab

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We consider the eigenproblem of a composite system of two different layer subsystems, assumed to be coupled at their interface. General formulas for the eigenvectors and eigenvalues of the total system, as well as its response function, are derived and expressed in terms of matrix elements of the individual subsystem response functions and the interface coupling parameter. Explicit expressions for the case most frequently considered in the literature—that of homogeneous subsystems (with arbitrary asymmetrical boundary conditions)—are also given, illustrating the applicability of our general formulas to arbitrary double-layer systems.

I. INTRODUCTION

Recently, layered composite materials (multilayers, superlattices, etc.) have become of great interest. Such systems are produced by various technique, e.g., molecular-beam epitaxy, among others. The theoretical studies of such systems began only a few years ago. In such studies, when the physical properties are analyzed within a matrix representation, one is faced with the analysis of composite matrices formed out of homogeneous parts corresponding to individual subsystems related together through the interface interactions. For superlattices which are formed out of a periodic repetition of two or more slabs, such an analysis is simplified due to this periodicity. In this paper, we address mainly finite-layered composite materials (multilayers) which do not show a periodicity. For such materials, when studying their physical properties within a matrix representation approach, one is in general faced with the necessity to deal with *large* composite matrices. A direct numerical analysis of such a matrix would, in general, lead to huge numerical computations.[1] Alternative analytical approaches were recently proposed.

The first approach to the analysis of a composite matrix consists in the calculation of its inverse, called also a response function or Green's function. This can be achieved from the knowledge of the inverse bulk or slab matrices of individual constituent subsystems. The surface Green's-function matching method was used to obtain the eigenvalues for quantum wells and superlattices.[2] The interface response theory was formulated for performing eigenvalues[3] and eigenvectors[4] calculations for any composite system. These calculations can be done within the last theory from the knowledge of the bulk response function of each subsystem.[5] They can be done also from the knowledge of the *surface* response functions of each subsystem, as explicitly done in the present paper for a double-layer film.

The second approach calculates the eigenvalues and eigenvectors of the finite composite *system* by performing the reduction of its eigenproblem to that of *one* of its individual constituent subsystems. This approach was recently presented as a recurrential interface rescaling method of solving the eigenproblem of secular equation contraction[7] or composite systems.[6] Another method for searching eigenvalues of composite structures appeared also and was called matrix reduction formalism.[8]

Finally let us stress that the knowledge of the eigenvectors is essential in many physical investigations as, for example, in recently observed spin-wave resonances of magnetic multilayer films.

In the present paper, for the case of a double-layer slab, we use the interface response theory starting from the inverse matrices (or surface response functions) for each single slab. The results obtained for the eigenvectors of the double-layer slab enable us to express the *rescaling interface parameters* defined before[6] in function of a single interface element of the single-slab response functions. What emerges, then, is a clear physical picture of this interface rescaling as well as new explicit results for the eigenvectors of a double-layer slab.

The outline of this paper is as follows. In Sec. II we chose a simple model of layered composite system, namely the one composed of two subsystems separated by an interface; then the response function (or an inverse matrix) of the system is calculated in terms of the inverse matrices of individual subsystems (Sec. III). Finally, the formulas for the eigenfunctions and eigenvalues (i.e., characteristic equation) are presented in Secs. IV and V in general form, and in their explicit form (for some special cases) in Sec. VI. The paper concludes with some general remarks.

II. THE MODEL

We consider the following eigenvalue problem:

$$\vec{\vec{h}}\,\vec{\vec{u}} \equiv \begin{bmatrix} \vec{\vec{H}}_1 & \vec{\vec{V}}_{12} \\ \vec{\vec{V}}_{21} & \vec{\vec{H}}_2 \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ u_N \\ \\ u_{N+1} \\ \vdots \\ u_L \end{bmatrix} = \vec{\vec{0}}_{L\times 1} , \tag{2.1}$$

where

$$\overleftrightarrow{V}_{12}=\begin{bmatrix}\overleftrightarrow{0}_{(N-1)\times(L-N-1)} & \overleftrightarrow{0}_{(N-1)\times 1}\\ -\varepsilon & 0\end{bmatrix} \tag{2.1a}$$

and

$$\overleftrightarrow{V}_{21}=\begin{bmatrix}0 & -\varepsilon\\ \overleftrightarrow{0}_{(L-N-1)\times(N-1)} & \overleftrightarrow{0}_{(L-N-1)\times 1}\end{bmatrix}=(\overleftrightarrow{V}_{12})^{T} . \tag{2.1b}$$

The indices labeling the matrix elements take the following values [$\vec{u}$ is a $L\times 1$ (column) matrix; $\overleftrightarrow{h}$, $\overleftrightarrow{H}_1$, and $\overleftrightarrow{H}_2$ are square matrices]:

$H_1(n,n')$ for $n,n'=1,2,\ldots,N$;

$H_2(m,m')$ for $m,m'=N+1,N+2,\ldots,L$;

$h(l,l')$ for $l,l'=1,2,\ldots,L$;

$u(l)\equiv u_l$ for $l=1,2,\ldots,L$.

In the notation of (2.1) the eigenvalue E corresponding to eigenvector $\vec{u}$ is implicit in the diagonal elements of $\overleftrightarrow{H}_1$ and $\overleftrightarrow{H}_2$. We moreover define two matrices $\overleftrightarrow{H}_0$ and $\overleftrightarrow{V}_I$ fulfilling the following relation:

$$\overleftrightarrow{h}=\overleftrightarrow{H}_0+\overleftrightarrow{V}_I ; \tag{2.2}$$

$$\overleftrightarrow{H}_0=\begin{bmatrix}\overleftrightarrow{H}_1 & 0_{N\times(L-N)}\\ \overleftrightarrow{0}_{(L-N)\times N} & \overleftrightarrow{H}_2\end{bmatrix} , \tag{2.2a}$$

$$\overleftrightarrow{V}_I=\begin{bmatrix}\overleftrightarrow{0}_{N\times N} & \overleftrightarrow{V}_{12}\\ \overleftrightarrow{V}_{21} & \overleftrightarrow{0}_{(L-N)\times(L-N)}\end{bmatrix} . \tag{2.2b}$$

$\overleftrightarrow{V}_1$ has only two nonzero matrix elements: $V_I(N;N+1)=V_I(N+1;N)=-\varepsilon$. We also write the inverse matrices as

$$\overleftrightarrow{G}_1=(\overleftrightarrow{H}_1)^{-1},\quad \overleftrightarrow{G}_2=(\overleftrightarrow{H}_2)^{-1} ,$$

$$\overleftrightarrow{G}_0=(\overleftrightarrow{H}_0)^{-1},\quad \overleftrightarrow{g}=\overleftrightarrow{h}^{-1} .$$

The notation (2.2) enables us to reinterpret our problem as that of two *finite* subsystems (characterized by the matrices $\overleftrightarrow{H}_1$ and $\overleftrightarrow{H}_2$) entering into interaction described by the matrix $\overleftrightarrow{V}_I$ and forming a new system, the properties of which are described by the matrix $\overleftrightarrow{h}$. For convenience, we introduce the following indices for the spatial variables of the respective subspaces: in the subspace D_1, let $l\equiv n=1,2,\ldots,N$; in the subspace D_2, let $l\equiv m=N+1,N+2,\ldots,L$; in the whole space D, let $l=1,2,\ldots,L$; in the "interface" subspace M, let $l=N$ and $N+1$. Obviously, the subspace referred to as the interface is determined by those elements of the "interaction" matrix $\overleftrightarrow{V}_I$ that are nonzero.

With regard to the properties of the inverse matrix, we have

$$\overleftrightarrow{G}_0(DD)=\begin{bmatrix}\overleftrightarrow{G}_1(D_1D_1) & \overleftrightarrow{0}_{N\times(L-N)}\\ \overleftrightarrow{0}_{(L-N)\times N} & \overleftrightarrow{G}_2(D_2D_2)\end{bmatrix} . \tag{2.3}$$

We moreover define the following $L\times 2$ ("two-column") matrix, which is the "innermost" two columns extracted out of the full matrix $\overleftrightarrow{G}_0(DD)$:

$$\overleftrightarrow{G}_0(DM)=\begin{bmatrix}G_1(1,N) & 0\\ G_1(2,N) & 0\\ \vdots & \vdots\\ G_1(N,N) & 0\\ 0 & G_2(N+1,N+1)\\ 0 & G_2(N+2,N+1)\\ \vdots & \vdots\\ 0 & G_2(L,N+1)\end{bmatrix} . \tag{2.3a}$$

We shall show that if the inverse matrices $\overleftrightarrow{G}_1,\overleftrightarrow{G}_2$ of the *subsystems* and the matrix $\overleftrightarrow{V}_I$ coupling them to each other are available, we are fully able to determine the eigenvalues E and the eigenvectors $\mathbf{u}$ of the system as a whole. To this aim, we introduce a new matrix $\overleftrightarrow{A}(DD)$; the latter will be essential in proving our theorem. We define it as follows:

$$\overleftrightarrow{A}(DD)=\overleftrightarrow{V}_I(DD)\overleftrightarrow{G}_0(DD) . \tag{2.4}$$

By (2.2b), (2.1a), (2.1b), and (2.3), the matrix $\overleftrightarrow{A}(DD)$ possesses nonzero elements only in the two rows belonging to the interface subspace; these are $A(N;D_2)$ and $A(N+1;D_1)$. We denote by $\overleftrightarrow{A}(MD)$ the $2\times L$ ("two-row") matrix, projected out of the "innermost" two rows of the full matrix $\overleftrightarrow{A}(DD)$ so as to contain nonzero elements only,

$$\overleftrightarrow{A}(MD)=\begin{bmatrix}\overleftrightarrow{0}_{1\times N} & \overleftrightarrow{A}_{12}^{(MD)}\\ \overleftrightarrow{A}_{21}^{(MD)} & \overleftrightarrow{0}_{1\times(L-N)}\end{bmatrix} , \tag{2.5}$$

where

$$\overleftrightarrow{A}_{12}^{(MD)}=(-\varepsilon G_2(N+1,N+1)\quad -\varepsilon G_2(N+1,N+2)\quad \cdots\quad -\varepsilon G_2(N+1,L)) , \tag{2.5a}$$

$$\overleftrightarrow{A}_{21}^{(MD)}=(-\varepsilon G_1(N,1)\quad -\varepsilon G_1(N,2)\quad \cdots\quad -\varepsilon G_1(N,N)) . \tag{2.5b}$$

It will prove useful to further project the matrix $\overleftrightarrow{A}(MD)$ in a manner to retain only those of its elements that are strictly related with the interface subspace. In this way, we arrive at the following 2×2 matrix:

$$\overleftrightarrow{A}(MM)=\begin{bmatrix}0 & -\varepsilon G_2(N+1,N+1)\\ -\varepsilon G_1(N,N) & 0\end{bmatrix} . \tag{2.6}$$

III. THE INVERSE OF A MATRIX (RESPONSE FUNCTION)

We now proceed to calculate the inverse matrix $\overleftrightarrow{g}$ of the system as a whole. This can be done using Dyson's equation if $\overleftrightarrow{V}_I$ in Eq. (2.2) is dealt with as a perturbation in the system $\overleftrightarrow{H}_0$. Dobrzynski[3] has shown that Dyson's

equation, for composite systems, can be written in a form in which the only essential operations to be carried out shall take place within the interface subspace M. This leads to the relation

$$\vec{\vec{g}}(DD)=\vec{\vec{G}}_0(DD)-\vec{\vec{G}}_0(DM)\vec{\vec{\Delta}}^{-1}(MM)\vec{\vec{A}}(MD)\ , \tag{3.1}$$

where the essential role belongs to the following 2×2 matrix, defined in the interface space:

$$\vec{\vec{\Delta}}(MM)\equiv\vec{\vec{I}}_2+\vec{\vec{A}}(MM)=\begin{bmatrix}1 & -\varepsilon G_2(N+1,N+1)\\ -\varepsilon G_1(N,N) & 1\end{bmatrix}\ , \tag{3.2a}$$

$$\vec{\vec{\Delta}}^{-1}(MM)=\|\vec{\vec{\Delta}}(MM)\|^{-1}\begin{bmatrix}1 & \varepsilon G_2(N+1,N+1)\\ \varepsilon G_1(N,N) & 1\end{bmatrix}\ , \tag{3.2b}$$

$$\|\vec{\vec{\Delta}}(MM)\|\equiv\det\vec{\vec{\Delta}}(MM)=1-\varepsilon^2 G_1(N,N)G_2(N+1,N+1)\ , \tag{3.3}$$

where $\vec{\vec{I}}_2$ is the 2×2 unit matrix. With regard to (3.1), on performing the necessary operations and having recourse to (3.2b), (2.5), and (2.3a), we obtain $\vec{\vec{g}}$ in the form

$$\vec{\vec{g}}(DD)=\begin{bmatrix}\vec{\vec{g}}(D_1D_1) & \vec{\vec{g}}(D_1D_2)\\ \vec{\vec{g}}(D_2D_1) & \vec{\vec{g}}(D_2D_2)\end{bmatrix}\ , \tag{3.4}$$

where the elements of the respective submatrices are for $\vec{\vec{g}}(D_1D_1)$,

$$g(n,n')=G_1(n,n')+\|\vec{\vec{\Delta}}(MM)\|^{-1}[\varepsilon^2 G_2(N+1,N+1)G_1(n,N)G_1(N,n')]\ ; \tag{3.5a}$$

for $\vec{\vec{g}}(D_2D_2)$,

$$g(m,m')=G_2(m,m')+\|\vec{\vec{\Delta}}(MM)\|^{-1}[\varepsilon^2 G_1(N,N)G_2(m,N+1)G_2(N+1,m')]\ ; \tag{3.5b}$$

for $\vec{\vec{g}}(D_1D_2)$,

$$g(n,m)=\varepsilon\|\vec{\vec{\Delta}}(MM)\|^{-1}G_1(n,N)G_2(N+1,m)\ ; \tag{3.5c}$$

for $\vec{\vec{g}}(D_2D_1)$,

$$g(m,n)=\varepsilon\|\vec{\vec{\Delta}}(MM)\|^{-1}G_2(m,N+1)G_1(N,n)\ . \tag{3.5d}$$

IV. GENERAL FORMULA FOR THE EIGENVECTORS

Let us denote the eigenvectors of the unperturbed system $\vec{\vec{H}}_0$ by the $L\times 1$ (column) matrix $\vec{\vec{U}}_0(D)$. On the basis of (3.1) we can derive[4] a similar relation between the eigenvectors of the perturbed system $\vec{\vec{u}}(D)$ and the column vectors $\vec{\vec{U}}_0(D)$:

$$[\vec{\vec{u}}(D)]^T=[\vec{\vec{U}}_0(D)]^T-[\vec{\vec{U}}_0(M)]^T\vec{\vec{\Delta}}^{-1}(MM)\vec{\vec{A}}(MD)\ , \tag{4.1}$$

where $[\ ]^T$ symbolizes the transposed matrix, whereas $\vec{\vec{U}}_0(M)$ is the 2×1 (column) matrix containing only those two elements of the $L\times 1$ column vector $\vec{\vec{U}}_0(D)$ which belong to the interface subspace. For finite systems (such as our system $\vec{\vec{h}}$) Eq. (4.1) reduces to[4]

$$[\vec{\vec{u}}(D)]^T=-\|\vec{\vec{\Delta}}(MM)\|\,[\vec{\vec{U}}_0(M)]^T\vec{\vec{\Delta}}^{-1}(MM)\vec{\vec{A}}(MD)\ . \tag{4.2}$$

We immediately note that the presence of $\det\vec{\vec{\Delta}}(MM)$ in (4.2) is only apparent since it cancels out with the denominator of the inverse matrix $\vec{\vec{\Delta}}^{-1}(MM)$ [see Eq. (3.2b)]. The formula (4.2) presents the advantages of (i) permitting the calculation of the eigenvectors of the perturbed system from those of the unperturbed system, and (ii) involving operations bearing on the interface subspace only. However, it should be kept in mind that the vectors (4.2) are not normalized and still have to be multiplied by an appropriate constant; in practice, when it comes to using formula (4.2), this poses but a simple numerical problem.

Since the unperturbed system $\vec{\vec{H}}_0$ consists of two *noninteracting* subsystems $\vec{\vec{H}}_1$ and $\vec{\vec{H}}_2$, the eigenvectors $\vec{\vec{U}}_0(D)$ fall into two classes: the one belonging to the basis of eigenvectors of $\vec{\vec{H}}_1$ and the other to that of $\vec{\vec{H}}_2$. On representing $\vec{\vec{U}}_0(D)$ in the general form

$$\vec{\vec{U}}_0(D)=\begin{bmatrix}\vec{\vec{U}}_0(D_1)\\ \vec{\vec{U}}_0(D_2)\end{bmatrix} \tag{4.3}$$

we find that the eigenvectors of either class can be expressed as vectors possessing nonzero elements in only one of the subspaces D_1 or D_2:

$$\begin{bmatrix}\vec{\vec{U}}_0(D_1)\\ \vec{\vec{0}}_{(L-N)\times 1}\end{bmatrix}\quad(\text{basis }\vec{\vec{H}}_1)$$

or (4.4)

$$\begin{bmatrix}\vec{\vec{0}}_{N\times 1}\\ \vec{\vec{U}}_0(D_2)\end{bmatrix}\quad(\text{basis }\vec{\vec{H}}_2)\ .$$

Obviously, we are justified in writing quite generally

$$[\vec{\vec{U}}_0(M)]^T=[U_0(N),U_0(N+1)]\ . \tag{4.5}$$

On insertion of (4.5), (3.2b), and (2.5) into (4.2) we arrive at the following formulas for the eigenfunctions:

$$u_l=\begin{cases}\varepsilon G_1(N,n)[\varepsilon U_0(N)G_2(N+1,N+1)+U_0(N+1)] & \text{for } l=n\in D_1 \quad (4.6a)\\ \varepsilon G_2(N+1,m)[U_0(N)+\varepsilon U_0(N+1)G_1(N,N)] & \text{for } l=m\in D_2\ . \quad (4.6b)\end{cases}$$

Next, inserting—in conformity with formulas (4.4)—$U_0(N)\equiv 0$ or $U_0(N+1)\equiv 0$ into (4.6) (and omitting unessential constant factors shared by the subspaces D_1 and D_2) we obtain, respectively, for the eigenvector derived from the $\overleftrightarrow{H}_2$ basis,

$$u_l=\begin{cases}\varepsilon G_1(N,n) & \text{for } l=n\in D_1\ , \quad (4.7a)\\ \varepsilon^2 G_1(N,N)G_2(N+1,m) & \text{for } l=m\in D_2 \quad (4.7b)\end{cases}$$

and for the eigenvector derived from the $\overleftrightarrow{H}_1$ basis,

$$u_l=\begin{cases}\varepsilon^2 G_2(N+1,N+1)G_1(N,n) & \text{for } l=n\in D_1\ , \quad (4.8a)\\ \varepsilon G_2(N+1,m) & \text{for } l=m\in D_2\ . \quad (4.8b)\end{cases}$$

The next section will be devoted to the interpretation of our results.

V. INTERFACE RESCALING

Our initial set of equation (2.1) can be rewritten in the form of two mutually coupled subsets:

$$\overleftrightarrow{H}_1\begin{pmatrix}u_1\\u_2\\\vdots\\u_N\end{pmatrix}=\begin{pmatrix}0\\\vdots\\0\\\varepsilon u_{N+1}\end{pmatrix}, \quad (5.1a)$$

$$\overleftrightarrow{H}_2\begin{pmatrix}u_{N+1}\\u_{N+2}\\\vdots\\u_{N+M}\end{pmatrix}=\begin{pmatrix}\varepsilon u_N\\0\\\vdots\\0\end{pmatrix}. \quad (5.1b)$$

Elsewhere,[6] one of us has shown that applying a procedure referred to as "interface rescaling," the two subsets can be "split apart" and then solved independently. The procedure resides essentially in the introduction of interface rescaling parameters, defined as follows: $R(H_1\overleftarrow{|}H_2)$—the parameter rescaling the subset H_1 with respect to the subset H_2—fulfills the following equation:

$$\varepsilon u_{N+1}=R(H_1\overleftarrow{|}H_2)u_N\ , \quad (5.2a)$$

whereas $R(H_1\overrightarrow{|}H_2)$—that rescaling the subset H_2 with respect to H_1—fulfills the equation

$$\varepsilon u_N=R(H_1\overrightarrow{|}H_2)u_{N+1}\ . \quad (5.2b)$$

Quite obviously, once use is made of (5.2a) and (5.2b), the subsets (5.1a) and (5.1b) become accessible to solution independently of each other. Thus, the problem reduces to that of determining the *rescaling parameters* explicitly. We shall now show that the latter are determined completely by those elements of the inverse matrix $\overleftrightarrow{G}_0$ which belong to the interface subspace M. By (4.7) and with regard to the relation (5.2a) we obtain directly

$$R(H_1\overleftarrow{|}H_2)=\varepsilon^2 G_2(N+1,N+1) \quad (5.3a)$$

and similarly from (4.8) and (5.2b)

$$R(H_1\overrightarrow{|}H_2)=\varepsilon^2 G_1(N,N)\ . \quad (5.3b)$$

Very significantly, the formulas (5.3) state that in order to "carry over" *complete* information concerning one of the two subsystems into the other subsystem, it suffices to make use of *only one* inverse matrix element of the "information-giving" subsystem, namely, the element belonging to the interface subspace. The formulas (5.3) are equivalent to those derived by us earlier[6] using a recurrential procedure. In Ref. 6 we moreover show how to derive relations equivalent to (4.7) and (4.8) of the present paper by applying the *recurrential* procedure of interface rescaling.

We shall now apply the concept of interface rescaling parameters to interpret the formulas (4.7) and (4.8) derived by us in Sec. IV. We rewrite them as follows:

$$u_l=\begin{cases}\varepsilon G_1(N,n) & \text{for } l=n\in D_1 \quad (\text{basis } \overleftrightarrow{H}_2) \quad (5.4a)\\ R(H_1\overrightarrow{|}H_2)G_2(N+1,m) & \text{for } l=m\in D_2 \quad (\text{basis } \overleftrightarrow{H}_2)\ , \quad (5.4b)\end{cases}$$

$$u_l=\begin{cases}R(H_1\overleftarrow{|}H_2)G_1(N,n) & \text{for } l=n\in D_1 \quad (\text{basis } \overleftrightarrow{H}_1)\ , \quad (5.5a)\\ \varepsilon G_2(N+1,m) & \text{for } l=m\in D_2 \quad (\text{basis } \overleftrightarrow{H}_1)\ . \quad (5.5b)\end{cases}$$

We note that the eigenvectors of matrix $\overleftrightarrow{h}$ are "constructed" on elements of the inverse matrix $\overleftrightarrow{G}_0$ only which belong to the interface subspace; the elements in question can be symbolized as follows:

$$\overleftrightarrow{G}_0=\begin{pmatrix}\overleftrightarrow{G}_1 & \overleftrightarrow{0}_{N\times(L-N)}\\ \overleftrightarrow{0}_{(L-N)\times N} & \overleftrightarrow{G}_2\end{pmatrix}. \quad (5.6)$$

In Eqs. (5.4) and (5.5) these elements occur multiplied by the parameter ε of coupling between the subsystems and the respective interface rescaling parameter $R(H_1|H_2)$.

The eigenvalues of our problem are determined by the poles of the matrix $\overleftrightarrow{g}(DD)$. By (3.5), we find them to be determined by the equality $\|\overleftrightarrow{\Delta}(MM)\|=0$. In explicit form, this gives the following characteristic equation [we make use of Eq. (3.3)]:

$$1-\varepsilon^2 G_1(N,N)G_2(N+1,N+1)=0 \quad (5.7)$$

or, with regard to Eqs. (5.3),

$$R(H_1 \uparrow H_2)R(H_1 \downarrow H_2)=\varepsilon^2 \ . \tag{5.8}$$

Since the characteristic equation (5.8) makes the relations (5.4) and (5.5) go over into each other, each of the equations (5.4) and (5.5) obviously contains the *complete* set of eigenvectors. Thus, in one situation or another, we are free to choose among the formulas derived from the *nonperturbed* eigenvectors of one of the subsystems, i.e., formulas (5.4) *or* (5.5). In the next section we shall give a simple illustration of the use of the above derived rules for the case when the subsystems are bulk homogeneous and their sole inhomogeneity exists on their surfaces.

VI. AN EXAMPLE: APPLICATION TO HOMOGENEOUS SUBSYSTEMS

We assume the homogeneous system with asymmetric boundary conditions as described by the tridiagonal matrix:

$$\overleftrightarrow{H}_i=\begin{vmatrix} x_i-E-a_i & -\beta_i & & & & & \\ -\beta_i & x_i-E & -\beta_i & & & & \\ & -\beta_i & x_i-E & -\beta_i & & & \\ & & & \vdots & & & \\ & & & -\beta_i & x_i-E & -\beta_i & \\ & & & & -\beta_i & x_i-E-b_i & \end{vmatrix}_{L_i\times L_i} , \tag{6.1}$$

where the index $i=1,2$ labels the subsystems. The quantities a_i, b_i are the *surface* parameters, whereas x_i and β_i characterize the homogeneous bulk. E is an eigenvalue. On introducing the variable k_i (the wave number) defined as

$$x_i-E=2\beta_i\cos k_i \tag{6.2}$$

one readily finds that $\overleftrightarrow{G}_i\equiv\overleftrightarrow{H}_i^{-1}$, the inverse of $\overleftrightarrow{H}_i$, possesses the following matrix elements,

$$G_i(l,l')=\frac{1}{W(a_i,b_i)}\times\begin{cases} A_l(a_i)B_{l'}(b_i) & \text{for } l'\geq l \quad (6.3a)\\ B_l(b_i)A_{l'}(a_i) & \text{for } l'\leq l \ , \quad (6.3b)\end{cases}$$

where we have introduced the following notations:

$$A_l(a_i)\equiv\sin(lk_i)-\frac{a_i}{\beta_i}\sin[(l-1)k_i] \ , \tag{6.4a}$$

$$B_l(b_i)\equiv \sin[(L_i-l+1)k_i] -\frac{b_i}{\beta_i}\sin[(L_i-l)k_i] \ , \tag{6.4b}$$

$$W(a_i;b_i)\equiv(\sin k_i)\{\beta_i\sin[(L_i+1)k_i] -(a_i+b_i)\sin(L_ik_i) +\beta_i^{-1}a_ib_i\sin[(L_i-1)k_i]\} \ . \tag{6.4c}$$

Above, the indices l,l' take the values $1,2,\ldots,L_i$.

We can regard the system as a whole as constructed from the subsystems $i=1$ and 2. This is equivalent to construction of a "new" space D (see Sec. II) composed of the two subspaces D_1 and D_2. Accordingly, when applying Eq. (6.3) to the subsystem $i=2$, one should keep in mind that the indices l,l' of Eq. (6.3) have to be shifted by N, i.e., with respect to the subsystem $i=2$ the $G_2(l,l')$ become effective matrix elements $G_2(N+l,N+l')$. We shall now consider a simple example of the use of Eq. (6.3), assuming for the surface parameters such values as occur most commonly in the theory of electron states[9] and magnons, respectively;[10] for simplicity, we shall assume symmetric boundary conditions for the subsystems.

A. "Electron" case ($a_i=b_i=0$)

The interface response-rescaling parameters are, respectively [by Eqs. (5.3) and (6.3)],

$$R(H_1 \uparrow H_2)=\varepsilon^2\frac{\sin[(L-N)k_2]}{\beta_2\sin[(L-N+1)k_2]} \ , \tag{6.5a}$$

$$R(H_1 \downarrow H_2)=\varepsilon^2\frac{\sin(Nk_1)}{\beta_1\sin[(N+1)k_1]} \ . \tag{6.5b}$$

Thus, by (5.8), the characteristic equation takes the form

$$\varepsilon^2\frac{\sin(Nk_1)\sin[(L-N)k_2]}{\beta_1\beta_2\sin[(N+1)k_1]\sin[(L-N+1)k_2]}=1 \ , \tag{6.6}$$

and, with regard to Eqs. (5.4), the eigenfunctions in $\overleftrightarrow{H}_2$ basis become, respectively,

$$u_l=\begin{cases}\dfrac{\sin(lk_1)}{\sin(Nk_1)} & \text{for } l\in D_1 \quad (6.7a)\\ \dfrac{\varepsilon}{\beta_2}\dfrac{\sin[(L-l+1)k_2]}{\sin[(L-N+1)k_2]} & \text{for } l\in D_2 \ , \quad (6.7b)\end{cases}$$

with all common factors omitted.

B. "Magnon" case ($a_i=b_i=\beta_i$)

The interface response-rescaling parameters, respectively, equal, with regard to Eqs. (5.3) and (6.3)

$$R(H_1 \uparrow H_2)=\varepsilon^2\frac{\cos(\frac{1}{2}k_2)\cos[(L-N-\frac{1}{2})k_2]}{-\beta_2\sin(k_2)\sin[(L-N)k_2]} \ , \tag{6.8a}$$

$$R(H_1 \downarrow H_2)=\varepsilon^2\frac{\cos[(N-\frac{1}{2})k_1]\cos(\frac{1}{2}k_1)}{-\beta_1\sin(k_1)\sin(Nk_1)} \ . \tag{6.8b}$$

The characteristic equation (5.8) now takes the following form:

$$\varepsilon^2 \frac{\cos(\frac{1}{2}k_1)\cos(\frac{1}{2}k_2)\cos[(N-\frac{1}{2})k_1]\cos[(L-N-\frac{1}{2})k_2]}{\beta_1\beta_2\sin(k_1)\sin(k_2)\sin(Nk_1)\sin[(L-N)k_2]}=1 , \tag{6.9}$$

whereas the eigenfunctions in $\overleftrightarrow{H}_2$ basis take the form [by (5.4) and with constant factors omitted]

$$u_l=\begin{cases} \dfrac{\cos[(l-\frac{1}{2})k_1]}{\cos[(N-\frac{1}{2})k_1]} & \text{for } l\in D_1 \qquad (6.10a) \\ -\dfrac{\varepsilon}{\beta_2}\dfrac{\cos[(L-l+\frac{1}{2})k_2]}{2\sin(\frac{1}{2}k_2)\sin[(L-N)k_2]} & \text{for } l\in D_2 \ . \end{cases}$$

(6.10b)

The above formulas are equivalent to those derived by one of us in a separate paper[6] applying recurrential interface rescaling procedure. The corresponding case for "phonon" will be presented in a separate paper.[5]

The preceding expressions (6.5)–(6.10) involve two wave numbers k_1 and k_2. The two, however, are mutually dependent since they have to correspond to the same eigenvalue E for the system *as a whole*. The relation between k_1 and k_2 is obtained determining E from Eq. (6.2) for $i=1$ and 2 separately, and then equating the two expressions:

$$\tfrac{1}{2}(x_1-x_2)=\beta_1\cos k_1-\beta_2\cos k_2 \ . \tag{6.11}$$

The above relation permits the elimination of one of the wave numbers, if necessary.

VII. CONCLUDING REMARKS

Above, we have derived formulas for the following characteristics of a double-layer system: its interface response-rescaling parameters, eigenfunctions, and characteristic equation. The basis for their calculations resides in the knowledge of the *individual* response functions for the constituent subsystems. Equations (6.3) and (6.4) permit the expression of the above characteristics in explicit form for homogeneous subsystems with *arbitrary* asymmetric boundary conditions. The case of nonhomogeneous subsystems would first involve the calculation (for each concrete case separately) of the respective subsystem response functions.

Our next paper (paper II) will deal with triple-layer structures. There, we shall derive similar formulas, expressing the fundamental characteristics of the composite system by way of the response functions of the *subsystems*.

Finally, let us note that the preceding interface response-rescaling theory can be formulated even more generally on admitting the interactions between the subsystems as given by a *matrix* $\overleftrightarrow{\varepsilon}$ rather than by a scalar ε. This extension of the theory will be the subject of a separate paper. We also note that, in fact, from the mathematical point of view, our procedure can serve, in general, as a method for the calculation of the inverse of a *block* matrix.

In this presentation we have restricted ourselves to the case of finite one-dimensional systems only. However, the application of our method to realistic finite three-dimensional systems (layered structures) is straightforward. Due to translational invariance parallel to surfaces of the system, one can perform the usual Fourier transformation in the two in-plane directions, and all the quantities involved become functions of the in-plane wave vector $\mathbf{k}_\parallel$. Since this is the only difference which shows up, the dependence of $\mathbf{k}_\parallel$, for simplicity, has not been explicitly written down in our presentation.

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