Eigenvectors of composite systems. I. General theory



1989 J. Phys.: Condens. Matter 1 1239

(http://iopscience.iop.org/0953-8984/1/7/007)

J. Phys.: Condens. Matter **1** (1989) 1239–1245. Printed in the UK

# Eigenvectors of composite systems: I. General theory

L Dobrzynski and H Puszkarski†

Equipe Internationale de Dynamique des Interfaces, Laboratoire de Dynamique des Cristaux Moléculaires (Unité associée au CNRS 801), Unité de Formation et de Recherche de Physique, Bâtiment P5, Université des Sciences et Techniques de Lille Flandres-Artois 59655 Villeneuve D'Ascq Cédex, France

Received 8 June 1988

**Abstract.** A composite system is a system formed out of different subsystems connected by interfaces. Any physical property of such a system can be described by an operator which can have a discrete matrix form or a continuous (e.g. differential) form. Some composite systems can even be formed of partly discrete and partly continuous subsystems. We present here a general unified theory enabling us to calculate the deformations of any composite system submitted to some action. It is then shown how this theory can be used for the calculation of eigenvectors related to the eigenvalues of a given operator.

## 1. Introduction

Let us define in a given $d$-dimensional space $D$ a composite system as a system formed out of $N$ subsystems defined in subspaces $D_i\,(1 \leqslant i \leqslant N)$ and bounded together by interface subspaces $M_i \in D_i$. The ensemble of all $M_i$ will be called the interface space $M$ of the composite under consideration. Under such a general and abstract definition can enter any system and in particular any physical system such as composite materials or multimaterials.

A general and unified interface response theory of discrete [1], continuous [2] and mixed [3] (partly continuous and partly discrete) composite systems was recently formulated. This theory gives general relations between the response function (also called the Green function) associated with a given operator and with a given composite system and the response function of a reference system out of which the composite can be built. We show here that similar general relations also exist between the deformations due to an applied action and the eigenvectors of the composite system and the corresponding entities of the reference system. In what follows, we shall consider respectively discrete, continuous and mixed composite systems. The corresponding general results will be illustrated by specific examples in the subsequent paper [4].

† Permanent address: Surface Physics Division, Physics Institute, A Mickiewicz University, Matejki 48/49, 60–769 Poznan, Poland.

## 2. Discrete composite systems

Consider a matrix operator

$$\mathbf{h} = E\mathbf{I} - \hat{\mathbf{h}} \tag{1}$$

defined for a composite system within a $d$-dimensional discrete space $D$. In equation (1), $\mathbf{I}$ is the unity matrix. Let us call $|u\rangle$ the vector of the deformations of this system when it is submitted to an action $|F\rangle$, such that

$$\mathbf{h}|u\rangle = |F\rangle \qquad \text{in } D \tag{2a}$$

or, equivalently,

$$\langle u|\,\mathbf{h} = \langle F| \qquad \text{in } D \tag{2b}$$

where we use in equation (2$b$) row vectors rather than column vectors as in equation (2$a$). When the action on the system is zero, then the diagonalisation of equations (2) provides the eigenvalues $E$ and the corresponding eigenvectors $|u\rangle$. However, the direct calculation from equation (2) of the deformation $|u\rangle$ due to $|F\rangle$ and that of the eigenvalues and eigenvectors can become a large numerical problem as $\mathbf{h}$ is in general a huge matrix for a composite system.

We propose in what follows an alternative, and in general simpler, solution of this problem, using the response function $\mathbf{g}$ defined by

$$\mathbf{gh} = \mathbf{hg} = \mathbf{I} \qquad \text{in } D. \tag{3}$$

It was shown [1] that this response function can be calculated from knowledge of the response function $\mathbf{G}$ of a reference system corresponding to this composite system. This reference response function $\mathbf{G}$ is a block diagonal matrix, each independent block $\mathbf{G}_i$ of which is formed out of either the elements $\mathbf{G}_{si}$ in $D_i$ of the response function $\mathbf{G}_{0i}$ of the corresponding infinite subsystem ($\mathbf{G}_{si}$ is a truncated part of the infinite matrix $\mathbf{G}_{0i}$) or the elements $\mathbf{g}_{si}$ in $D_i$ of the response function of the corresponding subsystem with ideally cleaved free surfaces.

These response functions $\mathbf{g}_{si}$ and $\mathbf{G}_{si}$ are related by the following relations:

$$\mathbf{g}_{si}(\mathbf{I} + \mathbf{A}_{si}) = \mathbf{G}_{si} \qquad \text{in } D_i \tag{4a}$$

or

$$(\mathbf{I} + \mathbf{A}'_{si})\mathbf{g}_{si} = \mathbf{G}_{si} \qquad \text{in } D_i. \tag{4b}$$

In these equations, $\mathbf{A}_{si}$ and $\mathbf{A}'_{si}$ are the truncated parts within $D_i$ of, respectively,

$$\mathbf{A}_{0i} = \mathbf{V}_{0i}\mathbf{G}_{0i} \tag{5a}$$

and

$$\mathbf{A}_{0i} = \mathbf{G}_{0i}\mathbf{V}_{0i} \tag{5b}$$

where $\mathbf{V}_{0i}$ is the cleavage operator which creates, within the infinite subsystem $i$, two independent parts, one of which is in $D_i$ the elementary brick that we need to build the composite system, such that

$$\mathbf{h}_{0i} = \mathbf{H}_{0i} + \mathbf{V}_{0i} \qquad \text{in } D_\infty. \tag{6}$$

$\mathbf{H}_{0i}$ is the corresponding operator of the infinite system.

Couple now all $N$ such ideally cleaved subsystems by a coupling operator $\mathbf{V}_\mathrm{I}$ and perturb the composite system by a perturbation $\mathbf{V}_p$ such that

$$\mathbf{h} = \mathbf{h}_s + \mathbf{V}_I + \mathbf{V}_p \qquad \text{in } D \tag{7}$$

where $\mathbf{h}_s$ is a block diagonal matrix formed out of the relevant parts of the $\mathbf{h}_{0i}$.

The response function $\mathbf{g}$ of the composite perturbed system and the reference response function $\mathbf{G}$ are related [1] by the universal equations

$$\mathbf{g}(\mathbf{I} + \mathbf{A}) = \mathbf{G} \qquad \text{in } D \tag{8a}$$

and

$$(\mathbf{I} + \mathbf{A}')\mathbf{g} = \mathbf{G} \qquad \text{in } D \tag{8b}$$

where the interface response operators $\mathbf{A}$ and $\mathbf{A}'$ are

$$\mathbf{A} = \mathbf{A}_s + (\mathbf{V}_I + \mathbf{V}_p)\mathbf{G} \qquad \text{in } D \tag{9a}$$

and

$$\mathbf{A}' = \mathbf{A}'_s + \mathbf{G}(\mathbf{V}_I + \mathbf{V}_p) \qquad \text{in } D. \tag{9b}$$

$\mathbf{A}_s$ and $\mathbf{A}'_s$ are block diagonal matrices formed out of the $\mathbf{A}_{si}$ and $\mathbf{A}'_{si}$ defined above. It is possible to use in $\mathbf{G}$ for some blocks the surface response function $\mathbf{g}_{si}$ of the bulk response function $\mathbf{G}_{0i}$; then the corresponding blocks $\mathbf{A}_{si}$ and $\mathbf{A}'_{si}$ are zero in $\mathbf{A}_s$ and $\mathbf{A}'_s$ respectively.

Note that the space $M$ of all interfaces includes also the space in which the perturbation $\mathbf{V}_p$ is defined.

The interface response operator $\mathbf{A}$ has non-zero elements only between a point of the interface space $M$ and any other point of $D$. It is useful then to define a rectangular matrix $\mathbf{A}(MD)$ and in the same manner $\mathbf{A}'(DM)$ and similar notation for all the other operators. Defining then within the interface space $M$, the square matrices

$$\boldsymbol{\Delta}(MM) = \mathbf{I}(MM) + \mathbf{A}(MM) \tag{10a}$$

and

$$\boldsymbol{\Delta}'(MM) = \mathbf{I}(MM) + \mathbf{A}'(MM) \tag{10b}$$

enables us to obtain from equations (8) the following matrix equations:

$$\mathbf{g}(DD) = \mathbf{G}(DD) - \mathbf{G}(DM)\boldsymbol{\Delta}^{-1}(MM)\mathbf{A}(MD) \tag{11a}$$

and

$$\mathbf{g}(DD) = \mathbf{G}(DD) - \mathbf{A}'(DM)\boldsymbol{\Delta}^{-1}(MM)\mathbf{G}(MD). \tag{11b}$$

When the response function $\mathbf{g}$ of the composite is known, its deformations can be obtained, using equation (2), from

$$|u(D)\rangle = \mathbf{g}(DD)|F(D)\rangle \tag{12a}$$

and

$$\langle u(D)| = \langle F(D)|\mathbf{g}(DD). \tag{12b}$$

Applying the same action on both sides of equations (11) then provides

$$\langle u(D)| = \langle U(D)| - \langle U(M)|\boldsymbol{\Delta}^{-1}(MM)\mathbf{A}(MD) \tag{13a}$$

or

$$|u(D)\rangle = |U(D)\rangle - \mathbf{A}'(DM)\boldsymbol{\Delta}'^{-1}(MM)|U(M)\rangle \tag{13b}$$

where

$$\langle U(D) = \langle F(D)|\mathbf{G}(DD) \tag{14a}$$

and

$$|U(D)\rangle = \mathbf{G}(DD)|F(D)\rangle \tag{14b}$$

are the deformations of the reference system. Note that the action can be localised, in particular in one subsystem and even at one single point.

So knowledge of the deformation $|U(D)\rangle$ of the reference system (formed for example from the bulk subsystems) and that of the scattering matrices $\boldsymbol{\Delta}^{-1}(MM)\mathbf{A}(MD)$ or $\mathbf{A}'^{-1}(DM)\boldsymbol{\Delta}'^{-1}(MM)$ enables us to obtain the deformation of the composite system.

Equation (13*b*) has already been given previously [1] but used only for a discussion of interface reflection and transmission.

Let us stress here the usefulness of equations (13) not only for the calculation of deformations of a composite system but also for the determination of the eigenvectors corresponding to the eigenvalues $E$ of the operator $\mathbf{h}$. In this case, $|U(D)\rangle$ is the corresponding eigenvector of the reference system. As the reference system consists of independent subsystems and as in equations (14) the action generating the eigenvectors can be localised in one single subsystem, it is very convenient to take for $|U(D)\rangle$ only a non-zero component for the eigenvector of one single subsystem. Equations (13) will nevertheless provide, because of the scattering matrices, the eigenvector $|u(D)\rangle$ corresponding to the chosen eigenvalue $E$ in the whole composite system.

When using equations (13) to calculate the eigenvectors, one has also to bear in mind that for a *finite* composite system all the eigenvalues $E$ are given by

$$\det[\boldsymbol{\Delta}(MM)] = \det[\boldsymbol{\Delta}'(MM)] = 0. \tag{15}$$

So, in order to avoid a divergence in the normalisation factor of the eigenvector, one *first* has to multiply equations (13) by this determinant. Then, *for a finite composite system*, the right space dependence in $D$ of the eigenvectors can be obtained just from

$$\langle u(D)| \propto \langle U(M)| \det[\boldsymbol{\Delta}(MM)]\,\boldsymbol{\Delta}^{-1}(MM)\mathbf{A}(MD) \tag{16a}$$

or

$$|u(D)\rangle \propto -\mathbf{A}'(DM)\det[\boldsymbol{\Delta}'(MM)]\,\boldsymbol{\Delta}'^{-1}(MM)|U(M)\rangle. \tag{16b}$$

For a composite system having semi-infinite subsystems, equations (16) can be used for the eigenvalues given by equation (15), e.g. for those corresponding to interface localised states. However, equations (13) have to be used for the eigenvalues of the semi-infinite subsystems which are not given by equation (15).

Rather than expanding here on these general and abstract results, the reader should consult the following paper [4] where the above expressions are used to calculate the eigenvectors of several composite systems in a simple analytical model, as it is often much easier to understand the general theory after having seen a few explicit applications.

Let us just stress here that the above expressions are exact and that no expansion is needed to calculate the deformations and the eigenvectors, as is often done for perturbed infinite systems. In that case, $\mathbf{A}_s = \mathbf{V}_I = 0$ and from equation (8*b*) one obtains the well known relation

$$|u\rangle = |U\rangle - \mathbf{GV}_p|u\rangle. \tag{17}$$

Successive iterations of the second term of this equation are then often used to calculate $|u\rangle$, starting from the $|U\rangle$ of the unperturbed system.

## 3. Continuous composite systems

The space variables of continuous composite systems are continuous and $\mathbf{h}(X)$ is in general a differential operator rather than a matrix as in § 2. The corresponding response function is defined by

$$\mathbf{h}(X)\mathbf{g}(X, X') = \mathbf{I}\delta(X - X'). \tag{18}$$

It has been shown [2] that this response function can be calculated for any continuous composite system from the following expression:

$$\begin{aligned}\mathbf{g}(DD) = \mathbf{G}(DD) - \mathbf{G}(DM)\mathbf{G}^{-1}(MM)\mathbf{G}(MD)\\ + \mathbf{G}(DM)\mathbf{G}^{-1}(MM)\mathbf{g}(MM)\mathbf{G}^{-1}(MM)\mathbf{G}(MD)\end{aligned} \tag{19}$$

with the same notation as above, bearing in mind that $D$ is now a continuous space. The reference response function $\mathbf{G}(DD)$ is formed here out of disconnected parts of bulk response functions for each subsystem. $\mathbf{G}(MM)$ is its value in the interface space and $\mathbf{G}^{-1}(MM)$ is defined as the inverse matrix of $\mathbf{G}(MM)$; this can always be achieved by taking a finite number of discrete points in the continuous $M$ space.

$\mathbf{g}(MM)$ is in the same manner the inverse matrix of $\mathbf{g}^{-1}(MM)$, which can be obtained from knowledge of the corresponding entities $\mathbf{g}_s^{-1}(M_iM_i)$ calculated for the independent subsystems with perfectly reflecting surfaces. These entities are also defined as the inverse matrices of the $\mathbf{g}_s(M_iM_i)$. Their calculation is easily achieved once the following are known: the bulk response function $\mathbf{G}_0(D_iD_i)$ and the cleavage operator $\mathbf{V}_{0i}(X)$ creating the independent subsystem $i$ with perfectly reflecting surfaces. Let us recall [2] it briefly here. First one has to calculate the operators

$$\mathbf{A}_{si}(X, X') = \mathbf{V}_{0i}(X'')\mathbf{G}_{0i}(X'', X')|_{X''=X} \qquad X', X'' \in D_i \qquad X \in M_i \tag{20}$$

and

$$\boldsymbol{\Delta}_s(M_iM_i) = \mathbf{I} + \mathbf{A}_{si}(\mathrm{M}_i\mathrm{M}_i). \tag{21}$$

Then

$$\mathbf{g}_s^{-1}(M_iM_i) = \boldsymbol{\Delta}_s(M_iM_i)\mathbf{G}_0^{-1}(M_iM_i). \tag{22}$$

Finally $\mathbf{g}_s^{-1}(MM)$ is obtained by superposition of the elements of the $\mathbf{g}_s^{-1}(M_iM_i)$. In what follows, $M_{ij}$ defines the subinterface space $j$ in the total interface space $M_i$ of subsystem $i$. With this notation,

$$\mathbf{g}^{-1}(M_{ij}M_{i'j'}) = \mathbf{0} \qquad M_{i'j'} \notin M_i \tag{23a}$$

$$\mathbf{g}^{-1}(M_{ij}M_{i'j'}) = \mathbf{g}_{si}^{-1}(M_{ij}M_{ij'}) \qquad j \neq j' \tag{23b}$$

$$\mathbf{g}^{-1}(M_{ij}M_{ij}) = \sum_{i'} \mathbf{g}_{si'}^{-1}(M_{i'j'}M_{i'j'}) \qquad M_{ij} \equiv M_{i'j'}. \tag{23c}$$

Considering equation (19) again, one sees easily in the same manner as for the discrete systems that the deformations $|u(D)\rangle$ of a continuous system are obtained from the deformations $|U(D)\rangle$ of the reference system from

$$|u(D)\rangle = |U(D)\rangle - \mathbf{G}(DM)\mathbf{G}^{-1}(MM)|U(M)\rangle + \mathbf{G}(DM)\mathbf{G}^{-1}(MM)\mathbf{g}(MM)\mathbf{G}^{-1}(MM)|U(M)\rangle. \tag{24}$$

Here also this expression can be used to calculate eigenvectors corresponding to given eigenvalues. In fact just the third term of this expression is necessary to obtain the unnormalised eigenvectors corresponding to the eigenvalues given by

$$\det[\mathbf{g}(MM)] = 0 \tag{25}$$

namely

$$|u(D)\rangle \propto \mathbf{G}(DM)|\mathbf{G}^{-1}(MM) \det[\mathbf{g}(MM)]\, \mathbf{g}(MM)\mathbf{G}^{-1}(MM)|U(M)\rangle. \tag{26}$$

Let us recall [2] that all the eigenvalues of finite systems are given by equation (25) and also the eigenvalues of modes localised at interfaces of semi-infinite parts of composite systems.

## 4. Mixed (discrete–continuous) composite systems

Calculation of the deformations and of the eigenvectors of mixed (partly discrete and partly continuous) composite systems can be done from the same equations (24) and (26) as for continuous composite systems. The only differences [3] are first that the reference response function $\mathbf{G}$ is now built out of respectively discrete and continuous blocks. The $\mathbf{g}(MM)$ will be still calculated as the inverse of the matrix $\mathbf{g}^{-1}(MM)$. The elements of this last matrix are obtained with the help of equations (23) for the interfaces between continuous subsystems and for the interfaces between continuous and discrete subsystems. For the interfaces between discrete subsystems, one has to use the following equation [1, 2]:

$$\mathbf{g}^{-1}(MM) = \mathbf{g}_s^{-1}(MM) + \mathbf{V}_I(MM) \tag{27}$$

where $\mathbf{V}_I$ is the corresponding interface coupling as defined by equation (7).

## 5. Discussion

This paper gives a general theory for the calculation of the deformations and the eigenvectors of any composite system. This general presentation will be followed by two papers [4, 5] showing simple specific examples of how to apply the general results given here. The first [4] of these papers deals with phonon eigenvectors in a few layered and discrete composite materials [6] (semi-infinite crystal, one slab, a double-layer slab and one adsorbed slab). It uses as reference the bulk subsystems. The second [5] of these papers uses as reference the response function and the eigenvectors of a single discrete slab and calculates the eigenvectors of double- and triple-layer discrete slabs, with specific applications for tight-binding electrons and magnons. This paper [5] also contains a comparison with an alternative method recently proposed [7] for solving the eigenvalue problem of layered composite systems (the so-called recurrent interface rescaling method). This approach [7] does not use the response function but performs a direct diagonalisation procedure, because the interface rescaling approach permits us to replace the eigenvalue problem of a whole layered composite system by an individual constituent subsystem. It is shown [5] that the three approaches outlined in [4, 5, 7] are equivalent for finite layered composite systems.

Finally an application of the theory developed in this paper to continuous and mixed (partly continuous and discrete) composite systems will be published for a tunnel junction made out of two discrete transition metals separated by a vacuum slab.

## Acknowledgments

One of the authors (HP) is indebted to the Centre National de la Recherche Scientifique for providing the necessary support for his sabbatical leave in Lille. Thanks are also due to the Members of Université des Sciences et Techniques de Lille Flandres-Artois for their hospitality and to the Institute of Low Temperatures and Structural Studies of the Polish Academy of Sciences for their support under Grant CPBP-01.12/2.8.

## References

[1] Dobrzynski L 1986 *Surf. Sci. Rep.* **6** 119; 1986 *Surf. Sci.* **175** 1
[2] Dobrzynski L 1987 *Surf. Sci.* **180** 489
[3] Akjouj A, Oleksy C and Dobrzynski L 1988 *Proc. 12th Int. Semin. Surface Physics (Piechowice) 9–14 May 1988; Surf. Sci.* at press
[4] Sylla B, Dobrzynski L and Puszkarski H 1989 *J. Phys. C: Condens. Matter* **1** 1247
[5] Puszkarski H and Dobrzynski L 1989 *Phys. Rev.* B at press
[6] Akjouj A, Sylla B, Zielinski P and Dobrzynski L 1987 *J. Phys. C: Solid State Phys.* **20** 6137
[7] Puszkarski H 1988 *Acta Phys. Pol.* at press