Green's function formalism for phononic crystals

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We develop a Green's function multiple-scattering formalism for the calculation of the density of states and the local density of states of the elastic field in periodic and nonperiodic structures consisting of nonoverlapping scatterers in a homogeneous host medium. The formalism is based on concepts and techniques developed in relation to the similar problem of electrons in solids. We apply the method to a specific example which demonstrates the existence of virtual bound states of the elastic field localized about a plane of nonoverlapping steel spheres in polyester. These states are manifested as dips in the transmission spectrum of the monolayer. They develop into narrow frequency bands in a phononic crystal built by a succession of such planes.

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I. INTRODUCTION

The multiple-scattering Green's function method has been used extensively in the study of the electronic structure and related properties of materials (see, e.g., Ref. 1 and references therein). It has been very successful in calculations of the electronic structure of periodic solids, impurities, disordered alloys, surfaces, layered structures, low-dimensional systems, etc. In recent years, the propagation of electromagnetic or elastic waves in composite materials with dielectric or, respectively, elastic properties which are periodic functions of the position, with a period comparable to the wavelength of the corresponding field, has been the object of considerable attention (see, e.g., Ref. 2 and references therein). These materials, photonic and phononic crystals, respectively, whether they exist naturally or are artificially fabricated, exhibit a variety of physical properties of interest to fundamental and applied research. There are striking analogies between the propagation of electrons in ordinary crystals and electromagnetic or elastic waves in photonic or phononic crystals, so that a variety of multiple-scattering methods originally developed for electronic-structure calculations have been transferred to the field of photonic crystals[3–8] and some of them also to phononic crystals.[9–11]

The aim of the present paper is to develop a multiple-scattering Green's function formalism for phononic crystals and related structures. A knowledge of the Green's function is particularly useful in those situations where a knowledge of the density of states, or of the local density of states of the elastic field, is required rather than the wave functions of individual modes. Moreover, using the Lippmann-Schwinger equation and the Green's function of the periodic crystal to begin with, one can obtain in systematic manner the Green's function, and therefore the density of states of the displacement field, associated with defects of the crystal. A Green's function approach may also be very useful in the study of disorder in phononic structures, by using procedures analogous to those developed for the examination of disorder in relation to the electronic and vibrational structures of solids.[1]

As is usual in any multiple-scattering formalism, one combines the properties of the single scatterer with the geometrical properties of the structure to obtain the required Green's function for the system as a whole. In doing so the scattering transition matrices describing the individual scatterers and the propagator functions involving the geometry are expressed in the appropriate-in-each-case representation, involving plane-wave or spherical-wave expansions as required. In Sec. II we present some general formulas relating to the scattering of elastic waves. In Sec. III we derive explicit expressions for the Green's function of a homogeneous medium in the plane-wave and the angular-momentum representation. The scattering of elastic waves by a single sphere is explicitly treated in Sec. IV, while multiple scattering by (periodic or not) arrays of spheres is treated in Sec. V. In Sec. VI we consider the case of slabs consisting of a number of parallel planes of spheres with the same two-dimensional (2D) periodicity. Although we present the case of nonoverlapping homogeneous spherical scatterers in a homogeneous host medium, the formalism applies to the general case of arbitrary nonoverlapping scatterers as well, provided the quantities which describe the properties of the single scatterer are properly modified. Finally, in Sec. VII we demonstrate the applicability of the formalism by applying it to a specific example: a square array of steel spheres in polyester.

II. BASIC FORMULAS

The displacement vector $\mathbf{U}(\mathbf{r};t)$ associated with an elastic wave propagating in an inhomogeneous medium characterized by a mass density ρ and Lamé coefficients λ, μ, which depend on the position $\mathbf{r}$, satisfies the differential equation[12]

$$\rho\partial_t^2 U_i = \sum_{i''} \partial_{i''}\left[\lambda\,\delta_{ii''}\sum_{i'} \partial_{i'} U_{i'} + \mu(\partial_{i''}U_i + \partial_i U_{i''})\right], \tag{1}$$

where ∂_i denotes the partial derivative with respect to the ith component of $\mathbf{r}$ (throughout the paper the subscript i means Cartesian components x,y,z); ∂_t denotes the partial derivative with respect to time. We assume, to begin with, that the Lamé coefficients are real and positive quantities and that they do not depend on the frequency. In the case of a harmonic elastic wave of angular frequency ω, we have

$$\mathbf{U}(\mathbf{r};t)=\mathrm{Re}\{\mathbf{u}(\mathbf{r})\exp[-i\omega t]\} \tag{2}$$

and Eq. (1) reduces to the time-independent form

$$-\sum_{i'}\left\{\rho^{-1/2}\left[\partial_i(\lambda\partial_{i'})+\delta_{ii'}\sum_{i''}\partial_{i''}(\mu\partial_{i''})+\partial_{i'}(\mu\partial_i)\right]\rho^{-1/2}\right\}\rho^{1/2}u_{i'}=\omega^2\rho^{1/2}u_i, \tag{3}$$

which is an eigenvalue equation: $\sqrt{\rho(\mathbf{r})}\mathbf{u}(\mathbf{r})$ is an eigenvector, corresponding to the eigenvalue ω^2, of the linear (second rank) tensor differential operator $\mathbf{\Lambda}(\mathbf{r})$, defined by

$$\Lambda_{ii'}(\mathbf{r})=-\rho^{-1/2}\left[\partial_i(\lambda\partial_{i'})+\delta_{ii'}\sum_{i''}\partial_{i''}(\mu\partial_{i''})+\partial_{i'}(\mu\partial_i)\right]\rho^{-1/2}, \tag{4}$$

which operates on the Hilbert space of square integrable vector functions. The inner product of any two such functions, $\mathbf{v}$ and $\mathbf{w}$, is defined by

$$(\mathbf{v},\mathbf{w})=\int_V d^3r\,\mathbf{v}^*(\mathbf{r})\cdot\mathbf{w}(\mathbf{r}), \tag{5}$$

where V is the volume of the system and * denotes, as usual, complex conjugation. $\mathbf{\Lambda}(\mathbf{r})$ is Hermitian, i.e.,

$$(\mathbf{v},\mathbf{\Lambda}\mathbf{w})=(\mathbf{\Lambda}\mathbf{v},\mathbf{w}). \tag{6}$$

One can easily prove Eq. (6) using the definition of the inner product, Eq. (5), integrating by parts, and neglecting the surface terms (one assumes that the displacement field either vanishes at the boundaries of the system or satisfies appropriate boundary conditions).

The Hermiticity of $\mathbf{\Lambda}(\mathbf{r})$ means that its eigenvalues are real (and positive in the present case[13]) and that the corresponding eigenfunctions form a complete set, i.e.,

$$\sum_\alpha \sqrt{\rho(\mathbf{r})}u^*_{\alpha;i}(\mathbf{r})\sqrt{\rho(\mathbf{r}')}u_{\alpha;i'}(\mathbf{r}')=\delta_{ii'}\delta(\mathbf{r}-\mathbf{r}') \tag{7}$$

and an orthonormal set, i.e.,

$$\sum_i \int_V d^3r\,\rho(\mathbf{r})u^*_{\alpha;i}(\mathbf{r})u_{\alpha';i}(\mathbf{r})=\delta_{\alpha\alpha'}, \tag{8}$$

where the index α characterizes the eigenvalues and eigenfunctions of $\mathbf{\Lambda}(\mathbf{r})$.

Sometimes it is more convenient to express the above properties in the Dirac bra-ket notation.[14] In this notation, for example, the eigenvalue equation (3) is written as

$$\hat{\Lambda}|\alpha\rangle=\omega_\alpha^2|\alpha\rangle, \tag{9}$$

and the completeness and orthonormality properties take the form

$$\sum_\alpha |\alpha\rangle\langle\alpha|=\hat{I} \tag{10}$$

and

$$\langle\alpha|\alpha'\rangle=\delta_{\alpha\alpha'}, \tag{11}$$

where $\hat{I}$ is the identity operator. We use throughout the coordinate $(i\mathbf{r})$ representation in which $|\alpha\rangle$ becomes $\sqrt{\rho(\mathbf{r})}u_{\alpha;i}(\mathbf{r})$.

The Green's function associated with $\hat{\Lambda}$, as a function of a complex variable z, is defined by[1]

$$(z-\hat{\Lambda})\hat{G}(z)=\hat{I}, \tag{12}$$

which, in explicit form becomes

$$\sum_i [z\delta_{i''i}-\Lambda_{i''i}(\mathbf{r})]G_{ii'}(\mathbf{r},\mathbf{r}';z)=\delta_{i''i'}\delta(\mathbf{r}-\mathbf{r}'). \tag{13}$$

One can easily show that

$$G_{ii'}(\mathbf{r},\mathbf{r}';z)=\sum_\alpha \frac{\sqrt{\rho(\mathbf{r})}u_{\alpha;i}(\mathbf{r})\sqrt{\rho(\mathbf{r}')}u^*_{\alpha;i'}(\mathbf{r}')}{z-\omega_\alpha^2}. \tag{14}$$

It is clear, from Eq. (14) that the Green's function is analytic in the complex z plane, except at those points of the real positive axis which are eigenvalues of $\hat{\Lambda}$. There, following a standard procedure, we put $z=\lim_{\epsilon\to 0^+}(\omega+i\epsilon)^2$, which corresponds to the retarded Green's function.

We define the local density of states of the elastic field by

$$n(\mathbf{r};\omega)=\sum_\alpha |\mathbf{u}_\alpha(\mathbf{r})|^2\delta(\omega-\omega_\alpha)=-\frac{2\omega}{\pi\rho(\mathbf{r})}\mathrm{Im}\sum_i G_{ii}(\mathbf{r},\mathbf{r};\omega^2). \tag{15}$$

The density of states (number of states of the elastic field per unit frequency) for the system under consideration is obtained, accordingly, from

$$n(\omega)=\int_V d^3r\,\rho(\mathbf{r})n(\mathbf{r};\omega)=\sum_\alpha \delta(\omega-\omega_\alpha)=-\frac{2\omega}{\pi}\mathrm{Im\,Tr}\,\hat{G}(\omega^2)=\frac{2\omega}{\pi}\mathrm{Im\,Tr}\,\hat{G}^\dagger(\omega^2), \tag{16}$$

where † denotes, as usual, the adjoint operator.

In a number of applications one needs to obtain the eigenfunctions of a given system (described by $\hat{\Lambda}$), by reference to another system (described by $\hat{\Lambda}_0$) for which the Green's function $\hat{G}_0$ is easily determined. We put

$$\hat{\Gamma}=\hat{\Lambda}-\hat{\Lambda}_0. \tag{17}$$

One can show that, at a frequency ω which belongs to the eigenvalue spectra of both systems, the eigenfunction of the system under consideration is related to the corresponding eigenfunction of the reference system by the Lippmann-Schwinger integral equation[1]

$$|\alpha\rangle=|\alpha\rangle_0+\hat{G}_0\hat{\Gamma}|\alpha\rangle. \tag{18}$$

The so-called on-shell scattering transition operator $\hat{\mathcal{T}}(\omega)$ connects the eigenfunctions $|\alpha\rangle$ of the perturbed to those of the reference system, $|\alpha\rangle_0$, at a given common eigenfrequency ω, as follows:

$$\hat{\Gamma}|\alpha\rangle=\hat{\mathcal{T}}|\alpha\rangle_0, \tag{19}$$

in which case the Lippmann-Schwinger equation takes the form

$$|\alpha\rangle=|\alpha\rangle_0+\hat{G}_0\hat{\mathcal{T}}|\alpha\rangle_0. \tag{20}$$

We should further clarify the notation by writing Eq. (20) explicitly as follows:

$$\begin{aligned}\sqrt{\rho(\mathbf{r})}u_{\alpha;i}(\mathbf{r})=&\sqrt{\rho_0(\mathbf{r})}u_{0\alpha;i}(\mathbf{r})+\sum_{i',i''}\int_V\int_V d^3r'\,d^3r''\\&\times G_{0ii'}(\mathbf{r},\mathbf{r}')\mathcal{T}_{i'i''}(\mathbf{r}',\mathbf{r}'')\sqrt{\rho_0(\mathbf{r}'')}u_{0\alpha;i''}(\mathbf{r}'').\end{aligned} \tag{21}$$

It is easy to show that

$$\hat{\mathcal{T}}=\hat{\Gamma}+\hat{\Gamma}\hat{G}_0\hat{\mathcal{T}} \tag{22}$$

and

$$\hat{G}=\hat{G}_0+\hat{G}_0\hat{\Gamma}\hat{G}=\hat{G}_0+\hat{G}_0\hat{\mathcal{T}}\hat{G}_0. \tag{23}$$

From Eq. (22) and the Hermiticity of $\hat{\Gamma}$ we obtain

$$\hat{\mathcal{T}}-\hat{\mathcal{T}}^{\dagger}=\hat{\mathcal{T}}^{\dagger}(\hat{G}_0-\hat{G}_0^{\dagger})\hat{\mathcal{T}}, \tag{24}$$

which is the formal statement of the so-called generalized optical theorem.[1] Sometimes it is more convenient to work, instead of $\hat{\mathcal{T}}$, with the reaction operator $\hat{\mathcal{K}}$, defined by

$$\hat{\mathcal{T}}=\hat{\mathcal{K}}+\tfrac{1}{2}\hat{\mathcal{K}}(\hat{G}_0-\hat{G}_0^{\dagger})\hat{\mathcal{T}}. \tag{25}$$

Using Eq. (24) one can show that $\hat{\mathcal{K}}$ is a Hermitian operator, $\hat{\mathcal{K}}=\hat{\mathcal{K}}^{\dagger}$.

We can now introduce the $\hat{S}$ operator by

$$\hat{S}=\hat{I}+(\hat{G}_0-\hat{G}_0^{\dagger})\hat{\mathcal{T}}, \tag{26}$$

which, using Eq. (24), becomes

$$\hat{S}=[\hat{\mathcal{T}}^{\dagger}]^{-1}\hat{\mathcal{T}}. \tag{27}$$

$\hat{S}$ can be also expressed in terms of the reaction operator, using Eq. (25), as follows:

$$\hat{S}=[\hat{I}+\tfrac{1}{2}(\hat{G}_0-\hat{G}_0^{\dagger})\hat{\mathcal{K}}][\hat{I}-\tfrac{1}{2}(\hat{G}_0-\hat{G}_0^{\dagger})\hat{\mathcal{K}}]^{-1}. \tag{28}$$

Using $\hat{\mathcal{T}}$ we can obtain a useful formula for the difference $\Delta N(\omega)$ in the number of states up to a given frequency ω between the considered system and the reference one. According to Eq. (16), the difference between the densities of states of the two systems is

$$\begin{aligned}\Delta n(\omega)&=-\frac{2\omega}{\pi}\mathrm{Im\,Tr}[\hat{G}(\omega^2)-\hat{G}_0(\omega^2)]\\&=-\frac{\omega}{\pi}\mathrm{Im\,Tr}[\hat{G}(\omega^2)-\hat{G}^{\dagger}(\omega^2)-\hat{G}_0(\omega^2)+\hat{G}_0^{\dagger}(\omega^2)].\end{aligned} \tag{29}$$

Using the identity $2\omega\hat{G}(\omega^2)=-\partial\ln\hat{G}(\omega^2)/\partial\omega$, which follows directly from the definition of the Green's function [Eq. (12)], and Eqs. (23) and (27) we obtain

$$\begin{aligned}\Delta n(\omega)&=\frac{1}{2\pi}\mathrm{Im\,Tr}\frac{\partial}{\partial\omega}\ln\{\hat{G}(\omega^2)\\&\quad\times[\hat{G}^{\dagger}(\omega^2)]^{-1}\hat{G}_0^{-1}(\omega^2)\hat{G}_0^{\dagger}(\omega^2)\}\\&=\frac{1}{2\pi}\mathrm{Im\,Tr}\frac{\partial}{\partial\omega}\ln\{[\hat{\mathcal{T}}^{\dagger}(\omega)]^{-1}\hat{\mathcal{T}}(\omega)\}\\&=\frac{1}{2\pi}\mathrm{Im\,Tr}\frac{\partial}{\partial\omega}\ln\hat{S}(\omega),\end{aligned} \tag{30}$$

and therefore

$$\Delta N(\omega)=\int_0^{\omega}d\omega'\,\Delta n(\omega')=\frac{1}{2\pi}\mathrm{Im\,Tr}\ln\hat{S}(\omega). \tag{31}$$

Substituting in Eq. (31) the expression of $\hat{S}$ given by Eq. (28), using the equation $\mathrm{Im\,Tr}\ln[\hat{I}+\tfrac{1}{2}(\hat{G}_0-\hat{G}_0^{\dagger})\hat{\mathcal{K}}]=-\mathrm{Im\,Tr}\ln[\hat{I}-\tfrac{1}{2}(\hat{G}_0-\hat{G}_0^{\dagger})\hat{\mathcal{K}}]$ and Eq. (25) we finally obtain

$$\Delta N(\omega)=\frac{1}{\pi}\mathrm{Im\,Tr}\ln\left[\hat{I}+\frac{1}{2}(\hat{G}_0-\hat{G}_0^{\dagger})\hat{\mathcal{T}}\right]. \tag{32}$$

We should note that though $\Delta N(\omega)$ by itself may not be an important quantity in the case of the elastic field, its derivative is. Numerical differentiation of $\Delta N(\omega)$ obtained on the basis of Eq. (31) provides an effective means for the calculation of $\Delta n(\omega)$.

We should also note that, although the formulas of this section have been derived assuming λ and μ to be (real) constants independent of frequency, one can easily see that, for the purpose of calculating $\Delta n(\omega)$ at a given ω, we can use the same formulas even when λ and μ are functions of ω, because usually they can be replaced by constants over a small frequency region about ω.

III. THE HOMOGENEOUS MEDIUM

In the case of a homogeneous medium, characterized by ρ, λ, μ that do not depend on $\mathbf{r}$, Eq. (3) takes the form

$$-c_l^2\nabla(\nabla\cdot\mathbf{u})+c_t^2\nabla\times(\nabla\times\mathbf{u})=\omega^2\mathbf{u}, \tag{33}$$

where $c_l=\sqrt{(\lambda+2\mu)/\rho}$ and $c_t=\sqrt{\mu/\rho}$. The most general solution of Eq. (33) consists of longitudinal (irrotational) and transverse (divergenceless) waves, which propagate independently with velocities c_l and c_t, respectively. The eigenfunctions of the elastic field are longitudinal and transverse plane waves, which we shall often write in dimensionless form as follows

$$\sqrt{\rho V}\mathbf{u}_{\mathrm{p}\mathbf{q}}(\mathbf{r})=\exp[i\mathbf{q}\cdot\mathbf{r}]\hat{\boldsymbol{e}}_{\mathrm{p}}(\mathbf{q}), \tag{34}$$

in which case we shall refer to them as dimensionless eigenfunctions. The wave vector $\mathbf{q}$ can take any value. The subscript p takes the values $\mathrm{p}=1,2,3$. $\mathrm{p}=1$ defines a longitudinal wave: $\hat{\boldsymbol{e}}_1$ is the radial unit vector along $\mathbf{q}$ and the corresponding eigenfrequency equals c_lq. Correspondingly $\mathrm{p}=2,3$ define transverse waves (p and s polarized): $\hat{\boldsymbol{e}}_2$ and $\hat{\boldsymbol{e}}_3$ are the polar and azimuthal unit vectors, respectively, which are perpendicular to $\mathbf{q}$, and the corresponding eigenfrequency equals c_tq. Because the eigenfunctions $\sqrt{\rho}\mathbf{u}_{\mathrm{p}\mathbf{q}}(\mathbf{r})$ defined by Eq. (34) constitute a complete and orthonormal set, the Green's function for a homogeneous medium can be written as follows:

$$g_{ii'}(\mathbf{r},\mathbf{r}';\omega^2)=\frac{\rho V}{(2\pi)^3}\int d^3q\sum_{\mathrm{p}}\frac{u_{\mathrm{p}\mathbf{q};i}(\mathbf{r})u^*_{\mathrm{p}\mathbf{q};i'}(\mathbf{r}')}{\omega^2-\omega^2_{\mathrm{p}\mathbf{q}}}, \tag{35}$$

according to Eq. (14), where we put $z=\omega^2$, and we have substituted $\Sigma_{\mathbf{q}}$ by $V/(2\pi)^3\int d^3q$, which is valid in the limit $V\to\infty$. Obviously, in a homogeneous medium $g_{ii'}(\mathbf{r},\mathbf{r}';z)$ depends on $\mathbf{r}$ and $\mathbf{r}'$ only through their difference $\mathbf{r}-\mathbf{r}'$.

In the present paper we are concerned with phononic crystals consisting of nonoverlapping spheres, and with the multiple scattering of elastic waves between them. Accordingly, we employ the so-called spherical-wave solutions of Eq. (33). A set of longitudinal spherical-wave eigenfunctions corresponding to an eigenfrequency c_lq is given by

$$\sqrt{\rho V}\mathbf{u}_{Llmq}(\mathbf{r})=\frac{1}{q}\nabla[f_l(qr)Y_l^m(\hat{\boldsymbol{r}})], \tag{36}$$

where $Y_l^m(\hat{\boldsymbol{r}})$ are the usual spherical harmonics, and f_l may be any linear combination of the spherical Bessel function j_l and the spherical Hankel function h_l^+. A set of transverse spherical-wave eigenfunctions corresponding to an eigenfrequency c_tq is given by

$$\sqrt{\rho V}\mathbf{u}_{Mlmq}(\mathbf{r})=f_l(qr)\mathbf{X}_{lm}(\hat{\boldsymbol{r}}), \tag{37}$$

and

$$\sqrt{\rho V}\mathbf{u}_{Nlmq}(\mathbf{r})=\frac{i}{q}\nabla\times[f_l(qr)\mathbf{X}_{lm}(\hat{\boldsymbol{r}})]. \tag{38}$$

Again when the spherical-wave eigenfunctions are written in the above form we shall refer to them as dimensionless eigenfunctions, by analogy to Eq. (34). The vector spherical harmonics, denoted by $\mathbf{X}_{lm}(\hat{\boldsymbol{r}})$, are defined by $\sqrt{l(l+1)}\mathbf{X}_{lm}(\hat{\boldsymbol{r}})=\mathbf{L}(\mathbf{r})Y_l^m(\hat{\boldsymbol{r}})=-i\mathbf{r}\times\nabla Y_l^m(\hat{\boldsymbol{r}})$. By definition, $\mathbf{X}_{00}(\hat{\boldsymbol{r}})=0$; for $l\geqslant 1$ we have

$$\begin{aligned}\sqrt{l(l+1)}\mathbf{X}_{lm}(\hat{\boldsymbol{r}})=&[\alpha_l^{-m}\cos\theta e^{i\phi}Y_l^{m-1}(\hat{\boldsymbol{r}})-m\sin\theta Y_l^m(\hat{\boldsymbol{r}})\\&+\alpha_l^m\cos\theta e^{-i\phi}Y_l^{m+1}(\hat{\boldsymbol{r}})]\hat{\boldsymbol{e}}_2(\mathbf{r})\\&+i[\alpha_l^{-m}e^{i\phi}Y_l^{m-1}(\hat{\boldsymbol{r}})\\&-\alpha_l^m e^{-i\phi}Y_l^{m+1}(\hat{\boldsymbol{r}})]\hat{\boldsymbol{e}}_3(\mathbf{r}),\end{aligned} \tag{39}$$

where

$$\alpha_l^m=\tfrac{1}{2}[(l-m)(l+m+1)]^{1/2}, \tag{40}$$

and $\hat{\boldsymbol{e}}_2$, $\hat{\boldsymbol{e}}_3$ are the polar and azimuthal unit vectors, respectively, which are perpendicular to $\mathbf{r}$ in the chosen system of spherical coordinates.

Vector plane waves are expanded into vector spherical waves as follows:

$$\mathbf{u}_{\mathrm{p}\mathbf{q}}(\mathbf{r})=\sum_{Plm}a_{Plm}^{\mathrm{p}\hat{\mathbf{q}}}\mathbf{u}^0_{Plmq}(\mathbf{r}), \tag{41}$$

where $P=L,M,N$. A vector plane wave is finite everywhere, therefore $\mathbf{u}^0_{Plmq}(\mathbf{r})$ in Eq. (41) are given by Eqs. (36), (37), and (38) with $f_l=j_l$ (regular vector spherical waves); one can easily show that the nonzero coefficients in Eq. (41) are

$$a_{Llm}^{1\hat{\mathbf{q}}}=4\pi i^{l-1}Y_l^m{}^*(\hat{\mathbf{q}}),$$

$$a_{Mlm}^{2\hat{\mathbf{q}}}=-a_{Nlm}^{3\hat{\mathbf{q}}}=4\pi i^lX^*_{lm;2}(\hat{\mathbf{q}}),$$

$$a_{Mlm}^{3\hat{\mathbf{q}}}=a_{Nlm}^{2\hat{\mathbf{q}}}=4\pi i^lX^*_{lm;3}(\hat{\mathbf{q}}), \tag{42}$$

where the polar and azimuthal components of the vector spherical harmonics are given by Eq. (39). In the following, we use an index L (this should not be confused with the index L that characterizes longitudinal spherical waves) to denote collectively the indices Plm.

An expression of the Green's function in terms of spherical waves can be obtained from Eq. (35) as follows. We expand the plane waves into spherical waves using Eqs. (41) and (42); we integrate over all solid angles $\Omega_{\hat{q}}$: using the explicit expressions of the regular vector spherical waves [Eqs. (36), (37), and (38)] and the orthonormality properties $\int d\Omega_{\hat{q}}Y_l^m(\hat{\mathbf{q}})Y_{l'}^{m'}{}^*(\hat{\mathbf{q}})=\delta_{ll'}\delta_{mm'}$, $\int d\Omega_{\hat{q}}\mathbf{X}_{lm}(\hat{\mathbf{q}})\cdot\mathbf{X}^*_{l'm'}(\hat{\mathbf{q}})=\delta_{ll'}\delta_{mm'}$, $\int d\Omega_{\hat{q}}\mathbf{X}_{lm}(\hat{\mathbf{q}})\cdot[\hat{\mathbf{q}}\times\mathbf{X}^*_{l'm'}(\hat{\mathbf{q}})]=0$, we obtain

$$g_{ii'}(\mathbf{r},\mathbf{r}';\omega^2)=\frac{2}{\pi c_l^2}\sum_{lm}\boldsymbol{\nabla}_i\boldsymbol{\nabla}'_{i'}\times\left[Y_l^m(\hat{\boldsymbol{r}})Y_l^{m}{}^*(\hat{\boldsymbol{r}}')\int_0^\infty dq\frac{j_l(qr)j_l(qr')}{(\omega/c_l)^2-q^2}\right]+\frac{2}{\pi c_t^2}\sum_{lm}\frac{[\mathbf{r}\times\boldsymbol{\nabla}]_i[\mathbf{r}'\times\boldsymbol{\nabla}']_{i'}}{l(l+1)}\times\left[Y_l^m(\hat{\boldsymbol{r}})Y_l^{m}{}^*(\hat{\boldsymbol{r}}')\int_0^\infty dq\,q^2\frac{j_l(qr)j_l(qr')}{(\omega/c_t)^2-q^2}\right]+\frac{2}{\pi c_t^2}\sum_{lm}\frac{[\boldsymbol{\nabla}\times\mathbf{r}\times\boldsymbol{\nabla}]_i[\boldsymbol{\nabla}'\times\mathbf{r}'\times\boldsymbol{\nabla}']_{i'}}{l(l+1)}\times\left[Y_l^m(\hat{\boldsymbol{r}})Y_l^{m}{}^*(\hat{\boldsymbol{r}}')\int_0^\infty dq\frac{j_l(qr)j_l(qr')}{(\omega/c_t)^2-q^2}\right], \tag{43}$$

where we have also used the identity $i\boldsymbol{\nabla}\times[j_l(qr)\mathbf{X}_{lm}(\hat{\boldsymbol{r}})]=[l(l+1)]^{-1/2}\boldsymbol{\nabla}\times\mathbf{r}\times\boldsymbol{\nabla}[j_l(qr)Y_l^m(\hat{\boldsymbol{r}})]$.

It can be shown by contour integration that

$$\int_0^\infty dq\frac{j_l(qr)j_l(qr')}{\kappa^2-q^2}=-i\frac{\pi}{2\kappa}j_l(\kappa r_<)h_l^+(\kappa r_>)+\frac{\pi}{2(2l+1)\kappa^2}\frac{r_<^l}{r_>^{l+1}} \tag{44}$$

and

$$\int_0^\infty dq\,q^2\frac{j_l(qr)j_l(qr')}{\kappa^2-q^2}=-i\frac{\pi\kappa}{2}j_l(\kappa r_<)h_l^+(\kappa r_>), \tag{45}$$

where $r_<=\min(r,r')$, $r_>=\max(r,r')$. It is clear from Eqs. (43), (44), and (45) that, at *a given frequency* ω, the angular-momentum expansion of the Green's function involves both regular (incoming) and irregular (outgoing) vector spherical waves at this frequency. We denote them by $\mathbf{J}_{\mathrm{L}}(\mathbf{r})$ and $\mathbf{H}_{\mathrm{L}}(\mathbf{r})$, respectively; they are dimensionless spherical wave functions given by Eqs. (36), (37), and (38) with $q=\omega/c_l$ if $P=L$ and $q=\omega/c_t$ if $P=M,N$, and $f_l=j_l$ for $\mathbf{J}_{\mathrm{L}}$ and $f_l=h_l^+$ for $\mathbf{H}_{\mathrm{L}}$. For simplicity, in what follows we do not denote explicitly the dependence on the frequency of the various quantities. Using Eqs. (44) and (45) and the identity

$$\left[\boldsymbol{\nabla}_i\boldsymbol{\nabla}'_{i'}+\frac{[\boldsymbol{\nabla}\times\mathbf{r}\times\boldsymbol{\nabla}]_i[\boldsymbol{\nabla}'\times\mathbf{r}'\times\boldsymbol{\nabla}']_{i'}}{l(l+1)}\right]\times\left[\frac{r_<^l}{r_>^{l+1}}Y_l^m(\hat{\boldsymbol{r}})Y_l^{m}{}^*(\hat{\boldsymbol{r}}')\right]=0, \tag{46}$$

in Eq. (43), we obtain

$$g_{ii'}(\mathbf{r},\mathbf{r}')=-i\sum_{\mathrm{L}}\frac{\omega}{c_\nu^3}[J_{\mathrm{L};i}(\mathbf{r})\overline{H}_{\mathrm{L};i'}(\mathbf{r}')\Theta(r'-r)+H_{\mathrm{L};i}(\mathbf{r})\overline{J}_{\mathrm{L};i'}(\mathbf{r}')\Theta(r-r')], \tag{47}$$

where $\nu=l$ if $P=L$ and $\nu=t$ if $P=M,N$. $\Theta(x)$ is the Heaviside step function. The bar symbol over a vector spherical wave, $\overline{\mathbf{u}}_{Plm}(\mathbf{r})$, stands for $(-1)^f\mathbf{u}_{Pl-m}(\mathbf{r})$, where $f=m$ if $P=L,N$ and $f=m+1$ if $P=M$. Obviously, $\overline{\mathbf{J}}_{\mathrm{L}}(\mathbf{r})=\mathbf{J}_{\mathrm{L}}^*(\mathbf{r})$ but $\overline{\mathbf{H}}_{\mathrm{L}}(\mathbf{r})\neq\mathbf{H}_{\mathrm{L}}^*(\mathbf{r})$. Since $\Sigma_mY_l^m(\hat{\boldsymbol{r}})Y_l^{m}{}^*(\hat{\boldsymbol{r}}')=\Sigma_mY_l^{m}{}^*(\hat{\boldsymbol{r}})Y_l^m(\hat{\boldsymbol{r}}')$, in Eq. (43) complex conjugation can be applied to the spherical harmonics of either $\mathbf{r}$ or $\mathbf{r}'$. Consequently, in Eq. (47) the bar can be put over the vector spherical functions of $\mathbf{r}$ or over those of $\mathbf{r}'$. Having this in mind, we can see that $g_{ii'}(\mathbf{r},\mathbf{r}')=g_{i'i}(\mathbf{r}',\mathbf{r})$.

IV. A SPHERE IN A HOST MEDIUM

Let us consider a single homogeneous sphere of radius S centered at the origin of coordinates. The sphere, which is characterized by elastic constants ρ_s, λ_s, μ_s, is embedded in a homogeneous host medium characterized by elastic constants ρ, λ, μ, which are different from those of the sphere. A plane wave (longitudinal or transverse) of a given frequency ω incident on the sphere can be expanded into spherical waves: $\Sigma_{\mathrm{L}}a_{\mathrm{L}}^0\mathbf{J}_{\mathrm{L}}(\mathbf{r})$, where the expansion coefficients a_{L}^0 depend on the amplitude, polarization, and direction of propagation of the incident plane wave. Similarly, the wave scattered by the sphere is described by outgoing spherical waves, $\Sigma_{\mathrm{L}}a_{\mathrm{L}}^+\mathbf{H}_{\mathrm{L}}(\mathbf{r})$. The displacement field inside the sphere has the form $\Sigma_{\mathrm{L}}a_{\mathrm{L}}^I\mathbf{J}_{\mathrm{L}}^s(\mathbf{r})$, where $\mathbf{J}_{\mathrm{L}}^s(\mathbf{r})$ is given by Eqs. (36), (37), and (38) with $q=\omega/c_{sl}$ if $P=L$, and $q=\omega/c_{st}$ if $P=M,N$, and $f_l=j_l$. Imposing the appropriate boundary conditions, we obtain a system of linear equations, the solution of which gives us a_{L}^+, a_{L}^I in terms of a_{L}^0, as follows (see Appendix A):

$$a_{\mathrm{L}}^+=\sum_{\mathrm{L}'}T_{\mathrm{LL}'}a_{\mathrm{L}'}^0,\quad a_{\mathrm{L}}^I=\sum_{\mathrm{L}'}C_{\mathrm{LL}'}a_{\mathrm{L}'}^0, \tag{48}$$

where the matrices $\mathbf{T}$, $\mathbf{C}$ are diagonal in angular momentum (lm) and have nonzero elements for $PP'=MM,NN,NL,LN$ and $l\geqslant1$, and for $PP'=LL$ and $l\geqslant0$, as can be seen from Eqs. (A1) and (A2). Therefore, we define the regular at the origin dimensionless eigenfunction of $\boldsymbol{\Lambda}(\mathbf{r})$ for the system under consideration, which corresponds to an incident spherical wave of given L, as follows:

$$\mathbf{R}_{\mathrm{L}}(\mathbf{r})=\left[\mathbf{J}_{\mathrm{L}}(\mathbf{r})+\sum_{\mathrm{L}'}T_{\mathrm{L}'\mathrm{L}}\mathbf{H}_{\mathrm{L}'}(\mathbf{r})\right]\Theta(r-S)+\sqrt{\rho_s/\rho}\sum_{\mathrm{L}'}C_{\mathrm{L}'\mathrm{L}}\mathbf{J}_{\mathrm{L}'}^s(\mathbf{r})\Theta(S-r). \tag{49}$$

A property of $T_{\mathrm{LL}'}$ is worth noting. Using the Lippmann-Schwinger equations [Eqs. (18) and (20)] and the Green's function [Eqs. (47)] for the homogeneous host medium (taken as the reference system), we obtain for $\mathbf{R}_{\mathrm{L}}(\mathbf{r})$ the following expression:

$$\begin{aligned}\mathbf{R}_{\mathrm{L}}(\mathbf{r}) &= \mathbf{J}_{\mathrm{L}}(\mathbf{r}) - i\sum_{\mathrm{L}'} \frac{\omega}{c_{\nu'}^3}\mathbf{H}_{\mathrm{L}'}(\mathbf{r}) \\ &\quad \times \int_{r'\leqslant S} d^3r' \sum_{i'i''} \overline{J_{\mathrm{L}';i'}}(\mathbf{r}')\Gamma_{i'i''}(\mathbf{r}')R_{\mathrm{L};i''}(\mathbf{r}') \\ &= \mathbf{J}_{\mathrm{L}}(\mathbf{r}) - i\sum_{\mathrm{L}'} \frac{\omega}{c_{\nu'}^3}\mathbf{H}_{\mathrm{L}'}(\mathbf{r}) \\ &\quad \times \int\int_{r',r''\leqslant S} d^3r'\,d^3r'' \sum_{i'i''} \overline{J_{\mathrm{L}';i'}}(\mathbf{r}') \\ &\quad \times \mathcal{T}_{i'i''}(\mathbf{r}',\mathbf{r}'')J_{\mathrm{L};i''}(\mathbf{r}''),\end{aligned} \tag{50}$$

for $r \geqslant S$. Comparing Eq. (50) with Eq. (49), we obtain the following integral expressions for $T_{\mathrm{LL}'}$:

$$\begin{aligned}T_{\mathrm{LL}'} &= \frac{-i\omega}{c_\nu^3}\int_{r'\leqslant S} d^3r' \sum_{ii'} \overline{J_{\mathrm{L};i}}(\mathbf{r}')\Gamma_{ii'}(\mathbf{r}')R_{\mathrm{L}';i'}(\mathbf{r}') \\ &= \frac{-i\omega}{c_\nu^3}\int\int_{r',r''\leqslant S} d^3r'\,d^3r'' \\ &\quad \times \sum_{ii'} \overline{J_{\mathrm{L};i}}(\mathbf{r}')\mathcal{T}_{ii'}(\mathbf{r}',\mathbf{r}'')J_{\mathrm{L}';i'}(\mathbf{r}''),\end{aligned} \tag{51}$$

where the integral in Eq. (51) is the matrix element of the on-shell scattering transition operator in the L representation

$$\mathcal{T}_{\mathrm{LL}'} = \langle \mathrm{L}\omega|\hat{\mathcal{T}}|\mathrm{L}'\omega\rangle = \frac{ic_\nu^3}{\omega}T_{\mathrm{LL}'}. \tag{52}$$

We remember that

$$\langle \mathrm{L}\omega|\mathrm{L}'\omega'\rangle = \frac{\pi c_\nu^3}{2\omega^2}\delta(\omega-\omega')\delta_{\mathrm{LL}'}, \tag{53}$$

which one can prove using the explicit expressions for $|\mathrm{L}\omega\rangle$ in the coordinate representation, $\mathbf{J}_{\mathrm{L}}(\mathbf{r})$, obtained from Eqs. (36), (37), and (38).

We can obtain the matrix elements of the reaction operator in the L representation from Eq. (25),

$$i\frac{c_\nu^3}{\omega}T_{\mathrm{LL}'} = \mathcal{K}_{\mathrm{LL}'} + \sum_{\mathrm{L}''} \mathcal{K}_{\mathrm{LL}''}T_{\mathrm{L}''\mathrm{L}'}. \tag{54}$$

In a similar manner we define a wave which is irregular at the origin and matches continuously an outgoing spherical wave of given L outside the sphere. For this purpose, we write the displacement field outside the sphere as $\sum_{\mathrm{L}} c_{\mathrm{L}}^0 \mathbf{H}_{\mathrm{L}}(\mathbf{r})$ and inside the sphere as $\sum_{\mathrm{L}}[c_{\mathrm{L}}^I \mathbf{J}_{\mathrm{L}}^s(\mathbf{r}) + c_{\mathrm{L}}^{I+}\mathbf{H}_{\mathrm{L}}^s(\mathbf{r})]$, where $\mathbf{H}_{\mathrm{L}}^s(\mathbf{r})$ is given by Eqs. (36), (37), and (38) with $q=\omega/c_{sl}$ if $P=L$, and $q=\omega/c_{st}$ if $P=M,N$, and $f_l=h_l^+$. Imposing the appropriate boundary conditions we obtain a system of linear equations, the solution of which gives us c_{L}^I, c_{L}^{I+} in terms of c_{L}^0, as follows (see Appendix A):

$$c_{\mathrm{L}}^{I+} = \sum_{\mathrm{L}'} Q_{\mathrm{LL}'}c_{\mathrm{L}'}^0, \quad c_{\mathrm{L}}^I = \sum_{\mathrm{L}'} P_{\mathrm{LL}'}c_{\mathrm{L}'}^0, \tag{55}$$

where the matrices $\mathbf{Q}$, $\mathbf{P}$ are diagonal in angular momentum (lm) and have nonzero elements for $PP' = MM,NN,NL,LN$ and $l\geqslant 1$, and for $PP'=LL$ and $l\geqslant 0$, as can be seen from Eqs. (A5) and (A6). Therefore the dimensionless eigenfunction of $\mathbf{\Lambda}(\mathbf{r})$, corresponding to such a spherical wave, of given L, takes the form

$$\begin{aligned}\mathbf{I}_{\mathrm{L}}(\mathbf{r}) &= \mathbf{H}_{\mathrm{L}}(\mathbf{r})\Theta(r-S) + \sqrt{\rho_s/\rho}\sum_{\mathrm{L}'}[P_{\mathrm{L}'\mathrm{L}}\mathbf{J}_{\mathrm{L}'}^s(\mathbf{r}) \\ &\quad + Q_{\mathrm{L}'\mathrm{L}}\mathbf{H}_{\mathrm{L}'}^s(\mathbf{r})]\Theta(S-r).\end{aligned} \tag{56}$$

Obviously, the irregular spherical waves defined above do not represent physical solutions of the elastic field; but using them we can write down the Green's function of the given system (a homogeneous sphere in a homogeneous host medium) as follows

$$\begin{aligned}G_{ii'}^{(s)}(\mathbf{r},\mathbf{r}') &= -i\sum_{\mathrm{L}} \frac{\omega}{c_\nu^3}[R_{\mathrm{L};i}(\mathbf{r})\overline{I_{\mathrm{L};i'}}(\mathbf{r}')\Theta(r'-r) \\ &\quad + I_{\mathrm{L};i}(\mathbf{r})\overline{R_{\mathrm{L};i'}}(\mathbf{r}')\Theta(r-r')].\end{aligned} \tag{57}$$

Indeed, one can verify by straightforward algebra that the above satisfies Eq. (13) for the case under consideration and the correct boundary conditions [the same as for $g_{ii'}(\mathbf{r},\mathbf{r}')$ of Eq. (47)]. To do so one needs to remember that $g_{ii'}(\mathbf{r},\mathbf{r}')$ of Eq. (47) satisfies Eq. (13) for the homogeneous medium and use the following properties:

$$c_\nu^3 T_{\mathrm{LL}'} = c_{\nu'}^3 T_{\mathrm{L}'\mathrm{L}}, \tag{58}$$

$$\sum_{\mathrm{L}} c_\nu^{-3}C_{\mathrm{L}'\mathrm{L}}Q_{\mathrm{L}''\mathrm{L}} = \sum_{\mathrm{L}} c_\nu^{-3}Q_{\mathrm{L}'\mathrm{L}}C_{\mathrm{L}''\mathrm{L}} = c_{s\nu'}^{-3}\frac{\rho}{\rho_s}\delta_{\mathrm{L}'\mathrm{L}''}, \tag{59}$$

$$\sum_{\mathrm{L}} c_\nu^{-3}C_{\mathrm{L}'\mathrm{L}}P_{\mathrm{L}''\mathrm{L}} = \sum_{\mathrm{L}} c_\nu^{-3}P_{\mathrm{L}'\mathrm{L}}C_{\mathrm{L}''\mathrm{L}}, \tag{60}$$

which can be shown by solving Eqs. (A1), (A2), (A5), and (A6).

It should be pointed out that, unlike the displacement field, the eigenfunctions $\mathbf{R}_{\mathrm{L}}(\mathbf{r})$, $\mathbf{I}_{\mathrm{L}}(\mathbf{r})$, given by Eqs. (49) and (56), respectively, and the Green's function, given by Eq. (57), are discontinuous functions at the surface of the sphere, because of the discontinuity of the mass density of the system.

The difference in the number of states up to a frequency ω between the given system (a homogeneous spherical scatterer in a homogeneous host medium) and the homogeneous host medium can be evaluated using Eq. (32) in the L representation and Eqs. (52) and (53). We obtain

$$\Delta N(\omega)=\frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}\ln[\mathbf{I}+\mathbf{T}]_{\{\mathrm{L}\}},\tag{61}$$

where {L} denotes matrices in L space: **I** is the unit matrix and the matrix elements of **T** are obtained from Eq. (48) or Eq. (51). We note that the trace of the logarithm of a square matrix is equal to the logarithm of the determinant of this matrix.

V. ARRAYS OF SPHERES

We shall now consider a system of nonoverlapping homogeneous spherical scatterers centered at sites $\mathbf{R}_n$ in a homogeneous host medium. We note that an outgoing vector spherical wave about $\mathbf{R}_{n'}$ can be expanded into a sum of regular vector spherical waves about $\mathbf{R}_n$ as follows:

$$\mathbf{H}_{\mathrm{L}'}(\mathbf{r}-\mathbf{R}_{n'})=\sum_{\mathrm{L}}\Omega^{nn'}_{\mathrm{LL}'}\mathbf{J}_{\mathrm{L}}(\mathbf{r}-\mathbf{R}_n).\tag{62}$$

Explicit expressions for $\Omega^{nn'}_{\mathrm{LL}'}$, the so-called free-space (which here means the homogeneous host medium) propagator functions, are given in Appendix B. It follows that an outgoing elastic wave about $\mathbf{R}_{n'}$, $\Sigma_{\mathrm{L}'}b^{+n'}_{\mathrm{L}'}\mathbf{H}_{\mathrm{L}'}(\mathbf{r}-\mathbf{R}_{n'})$, can be written as an incoming wave about $\mathbf{R}_n$, $\Sigma_{\mathrm{L}}b'^{n}_{\mathrm{L}}(n')\mathbf{J}_{\mathrm{L}}(\mathbf{r}-\mathbf{R}_n)$, where

$$b'^{n}_{\mathrm{L}}(n')=\sum_{\mathrm{L}'}\Omega^{nn'}_{\mathrm{LL}'}b^{+n'}_{\mathrm{L}'}.\tag{63}$$

The wave scattered from the sphere at $\mathbf{R}_n$ is determined by the total wave incident on this sphere; therefore

$$b^{+n}_{\mathrm{L}}=\sum_{\mathrm{L}'}T^{n}_{\mathrm{LL}'}\left[a^{0n}_{\mathrm{L}'}+\sum_{n'\neq n}b'^{n}_{\mathrm{L}'}(n')\right],\tag{64}$$

where $T^{n}_{\mathrm{LL}'}$ are the elements of the scattering matrix [see Eqs. (48)] for the sphere at $\mathbf{R}_n$, and $a^{0n}_{\mathrm{L}'}$ are the coefficients in the multiple expansion about $\mathbf{R}_n$ of an external incident wave. From Eqs. (63) and (64) we obtain

$$\sum_{n'\mathrm{L}'}\left[\delta_{nn'}\delta_{\mathrm{LL}'}-\sum_{\mathrm{L}''}T^{n}_{\mathrm{LL}''}\Omega^{nn'}_{\mathrm{L}''\mathrm{L}'}\right]b^{+n'}_{\mathrm{L}'}=\sum_{\mathrm{L}'}T^{n}_{\mathrm{LL}'}a^{0n}_{\mathrm{L}'}.\tag{65}$$

We now turn to the evaluation of the Green's function for the array of spheres. Starting from Eq. (47) and using Eq. (62), we obtain the following site-centered expansion for the Green's function of a homogeneous medium:

$$g_{ii'}(\mathbf{R}_n+\mathbf{r}_n,\mathbf{R}_{n'}+\mathbf{r}'_{n'})=g_{ii'}(\mathbf{r}_n,\mathbf{r}'_{n'})\delta_{nn'}+\sum_{\mathrm{LL}'}\overline{J}_{\mathrm{L};i}(\mathbf{r}_n)\times\left[\frac{-i\omega}{c_\nu^3}\Omega^{n'n}_{\mathrm{L}'\mathrm{L}}\right]J_{\mathrm{L}';i'}(\mathbf{r}'_{n'}),\tag{66}$$

where $g_{ii'}(\mathbf{r}_n,\mathbf{r}'_{n'})$ is given by Eq. (47), and $\mathbf{r}_n=\mathbf{r}-\mathbf{R}_n$, $\mathbf{r}'_{n'}=\mathbf{r}'-\mathbf{R}_{n'}$ are restricted within nonoverlapping space-filling cells (about $\mathbf{R}_n$, $\mathbf{R}_{n'}$, respectively).[1] Using these site-centered position vectors, Eq. (13) takes the form

$$\sum_{i}[\omega^2\delta_{i''i}-\Lambda_{i''i}(\mathbf{R}_n+\mathbf{r}_n)]G_{ii'}(\mathbf{R}_n+\mathbf{r}_n,\mathbf{R}_{n'}+\mathbf{r}'_{n'})=\delta_{i''i'}\delta(\mathbf{r}_n-\mathbf{r}'_{n'})\delta_{nn'}.\tag{67}$$

For $n\neq n'$, the source term vanishes and the Green's function can be expanded into regular spherical wave solutions $\mathbf{R}^{n}_{\mathrm{L}}(\mathbf{r}_n)$ and $\mathbf{R}^{n'}_{\mathrm{L}'}(\mathbf{r}'_{n'})$, corresponding to the scattering spheres at sites $\mathbf{R}_n$, $\mathbf{R}_{n'}$, respectively. For $n=n'$, the source term in Eq. (67) no longer vanishes and one expects a term which should be the Green's function $G^{(s)n}_{ii'}$ given by Eq. (57), for the nth sphere embedded in the homogeneous host medium. Therefore, we seek the Green's function of the assembly of spheres in the following form [similar to Eq. (66)]:

$$G_{ii'}(\mathbf{R}_n+\mathbf{r}_n,\mathbf{R}_{n'}+\mathbf{r}'_{n'})=G^{(s)n}_{ii'}(\mathbf{r}_n,\mathbf{r}'_{n'})\delta_{nn'}+\sum_{\mathrm{LL}'}\overline{R}^{n}_{\mathrm{L};i}(\mathbf{r}_n)\times\left[\frac{-i\omega}{c_\nu^3}D^{n'n}_{\mathrm{L}'\mathrm{L}}\right]R^{n'}_{\mathrm{L}';i'}(\mathbf{r}'_{n'}).\tag{68}$$

The matrix elements $D^{nn'}_{\mathrm{LL}'}$ entering in Eq. (68) can be determined from the first of Eqs. (23), considering the homogeneous host medium as the reference system. We obtain

$$\begin{aligned}G_{ii'}(\mathbf{R}_n+\mathbf{r}_n,\mathbf{R}_{n'}+\mathbf{r}'_{n'})&=g_{ii'}(\mathbf{R}_n+\mathbf{r}_n,\mathbf{R}_{n'}+\mathbf{r}'_{n'})\\&\quad+\sum_{n''}\int d^3r''_{n''}\sum_{kk'}g_{ik}(\mathbf{R}_n+\mathbf{r}_n,\mathbf{R}_{n''}+\mathbf{r}''_{n''})\\&\quad\times\Gamma^{n''}_{kk'}(\mathbf{r}''_{n''})G_{k'i'}(\mathbf{R}_{n''}+\mathbf{r}''_{n''},\mathbf{R}_{n'}+\mathbf{r}'_{n'}),\end{aligned}\tag{69}$$

where $\Gamma^{n}_{ii'}(\mathbf{r}_n)=\Gamma_{ii'}(\mathbf{R}_n+\mathbf{r}_n)$. Substituting Eqs. (66) and (68) in Eq. (69) we obtain after some straightforward calculation

$$D^{nn'}_{\mathrm{LL}'}=\Omega^{nn'}_{\mathrm{LL}'}+\sum_{n''}\sum_{\mathrm{L}''\mathrm{L}'''}D^{nn''}_{\mathrm{LL}''}T^{n''}_{\mathrm{L}''\mathrm{L}'''}\Omega^{n''n'}_{\mathrm{L}'''\mathrm{L}'},\tag{70}$$

where $T^{n}_{\mathrm{LL}'}$ are the elements of the scattering matrix of the nth sphere. Formal iteration of Eq. (70) gives

$$D^{nn'}_{\mathrm{LL}'}=\Omega^{nn'}_{\mathrm{LL}'}+\sum_{n''}\sum_{\mathrm{L}''\mathrm{L}'''}\Omega^{nn''}_{\mathrm{LL}''}T^{n''}_{\mathrm{L}''\mathrm{L}'''}\Omega^{n''n'}_{\mathrm{L}'''\mathrm{L}'}+\cdots,\tag{71}$$

which shows [we remember the definition of $\Omega^{nn'}_{\mathrm{LL}'}$ by Eqs. (62) and (63)] that $D^{nn'}_{\mathrm{LL}'}$ are propagator functions which give the coefficients in a L expansion of the wave incident on the sphere at $\mathbf{R}_n$, due to an outgoing wave from the sphere at $\mathbf{R}_{n'}$, which reaches $\mathbf{R}_n$ directly or after scattering any number of times by any number of spheres (including those at $\mathbf{R}_n$ and $\mathbf{R}_{n'}$).

We note in passing a generalization of Eq. (70) which might be useful in some cases. We can treat the scattering at $\mathbf{R}_n$ in two stages. The first-stage scattering is described by $T^{\;n}_{0\mathrm{LL}'}$, which correspond to arbitrarily defined spheres centered at the sites $\mathbf{R}_n$ (reference scatterers), and the second-stage scattering by $\Delta T^n_{\mathrm{LL}'} = T^n_{\mathrm{LL}'} - T^{\;n}_{0\mathrm{LL}'}$. We obtain

$$D^{nn'}_{\mathrm{LL}'} = D^{\;nn'}_{0\mathrm{LL}'} + \sum_{n''} \sum_{\mathrm{L''L'''}} D^{nn''}_{\mathrm{LL''}} \Delta T^{n''}_{\mathrm{L''L'''}} D^{\;n''n'}_{0\mathrm{L'''L}'}, \tag{72}$$

where $D^{\;nn'}_{0\mathrm{LL}'}$ are the solution of Eq. (70) when $T^n_{\mathrm{LL}'} = T^{\;n}_{0\mathrm{LL}'}$.

Let us now consider a periodic structure specified by Bravais lattice vectors $\mathbf{R}_\lambda$ and nonprimitive translation vectors $\mathbf{t}_\alpha$ denoting the positions of the spheres (if there are more than one) within the unit cell; in this case the site index n stands for the composite index $\lambda\alpha$. We begin with the normal modes of the crystal. They are obtained by putting the external incident wave equal to zero in Eq. (65); because they satisfy Bloch's theorem: $b^{+\lambda'\alpha'}_{\mathrm{L}'} = \exp[i\mathbf{k}\cdot(\mathbf{R}_{\lambda'} - \mathbf{R}_\lambda)] b^{+\lambda\alpha'}_{\mathrm{L}'}$, we obtain the following secular equation:

$$\det\left[\delta_{\alpha\alpha'} \delta_{\mathrm{LL}'} - \sum_{\mathrm{L}''} T^{\alpha}_{\mathrm{LL}''} \Omega^{\alpha\alpha'}_{\mathrm{L''L}'}(\mathbf{k}) \right] = 0, \tag{73}$$

where

$$\Omega^{\alpha\alpha'}_{\mathrm{LL}'}(\mathbf{k}) = \sum_{\lambda'} \Omega^{nn'}_{\mathrm{LL}'} \exp[-i\mathbf{k}\cdot(\mathbf{R}_\lambda - \mathbf{R}_{\lambda'})], \tag{74}$$

which does not depend on λ and

$$\Omega^{nn'}_{\mathrm{LL}'} = \frac{1}{\upsilon}\int_{BZ} d^3k \exp[i\mathbf{k}\cdot(\mathbf{R}_\lambda - \mathbf{R}_{\lambda'})] \Omega^{\alpha\alpha'}_{\mathrm{LL}'}(\mathbf{k}), \tag{75}$$

υ being the volume of the first Brillouin zone (BZ). Both $T^{\alpha}_{\mathrm{LL}'}$ and $\Omega^{\alpha\alpha'}_{\mathrm{LL}'}(\mathbf{k})$ in Eq. (73) are functions of the frequency of the wave, but the $T^{\alpha}_{\mathrm{LL}'}$ depend only on the properties of a single scatterer, whereas $\Omega^{\alpha\alpha'}_{\mathrm{LL}'}(\mathbf{k})$ depend only on the geometry and we refer to them as the structure constants, adopting the terminology introduced by Korringa, Kohn, and Rostoker[15] in relation to calculations of the electronic band structure of periodic solids. The calculation of the structure constants, which needs to be done only once for a given lattice, usually requires Ewald-summation techniques.[16] We note also that though Eq. (73) as written involves infinite-dimensional matrices, in actual calculations it is sufficient to truncate the angular momentum index l to some relatively small number $l_{\max}$.

We now turn to the evaluation of the Green's function given by Eq. (68). For a periodic arrangement of spheres, the evaluation of $D^{nn'}_{\mathrm{LL}'}$ through Eq. (70) can be achieved by a lattice Fourier transform as follows. We can write

$$D^{nn'}_{\mathrm{LL}'} = \frac{1}{\upsilon}\int_{BZ} d^3k \exp[i\mathbf{k}\cdot(\mathbf{R}_\lambda - \mathbf{R}_{\lambda'})] D^{\alpha\alpha'}_{\mathrm{LL}'}(\mathbf{k}), \tag{76}$$

with

$$D^{\alpha\alpha'}_{\mathrm{LL}'}(\mathbf{k}) = \sum_{\lambda'} D^{nn'}_{\mathrm{LL}'} \exp[-i\mathbf{k}\cdot(\mathbf{R}_\lambda - \mathbf{R}_{\lambda'})]. \tag{77}$$

If we multiply Eq. (70) by $\exp[-i\mathbf{k}\cdot(\mathbf{R}_\lambda - \mathbf{R}_{\lambda'})]$, take the sum over $\mathbf{R}_{\lambda'}$ (note that for a periodic structure the scattering matrix does not depend on the primitive cell λ), and use Eqs. (74) and (77) we obtain

$$D^{\alpha\alpha'}_{\mathrm{LL}'}(\mathbf{k}) = \Omega^{\alpha\alpha'}_{\mathrm{LL}'}(\mathbf{k}) + \sum_{\alpha''} \sum_{\mathrm{L''L'''}} D^{\alpha\alpha''}_{\mathrm{LL''}}(\mathbf{k}) T^{\alpha''}_{\mathrm{L''L'''}} \Omega^{\alpha''\alpha'}_{\mathrm{L'''L}'}(\mathbf{k}). \tag{78}$$

Substitution of $D^{\alpha\alpha'}_{\mathrm{LL}'}(\mathbf{k})$, obtained from Eq. (78), into Eq. (76) gives $D^{nn'}_{\mathrm{LL}'}$. We should point out that the numerical integration over the BZ requires a very dense mesh of $\mathbf{k}$ points due to singularities in $D^{\alpha\alpha'}_{\mathrm{LL}'}(\mathbf{k})$.[17,18]

A calculation of $D^{nn'}_{\mathrm{LL}'}$ directly from Eq. (70) involves, as a rule, a summation over a large number of lattice sites because the free-space propagator functions $\Omega^{nn'}_{\mathrm{LL}'}$ decay slowly with the distance $|\mathbf{R}_n - \mathbf{R}_{n'}|$. But there are exceptions to this rule. For example, the lattice sum in Eq. (70) may be rapidly convergent in the case of a phononic crystal which possesses an absolute frequency gap because in this case the propagator functions $D^{nn'}_{\mathrm{LL}'}$ decay exponentially with distance at frequencies which lie within the gap, and then the direct evaluation of $D^{nn'}_{\mathrm{LL}'}$ from Eq. (70) is to be preferred.

Multiple scattering theory is perhaps particularly useful when dealing with defects and disorder. For the description of point defects at a finite number of sites, one needs to calculate the propagator functions $D^{nn'}_{\mathrm{LL}'}$ of the system with the defects. This can be done in real space, using Eq. (72) by considering the periodic crystal (without any defect) as the reference system. In this case, the sum over n'' in Eq. (72) is restricted to those sites at which there are defects; only there $\Delta T^n_{\mathrm{LL}'} = T^n_{\mathrm{LL}'} - T^{\;n}_{0\mathrm{LL}'}$ is not zero. An approximate treatment of disorder is also possible within the framework of the virtual-crystal, the average-T-matrix, or the coherent-potential approximations.[1]

We conclude this section with a derivation of a formula for $\Delta N(\omega)$, the difference in the number of states up to a frequency ω between the assembly of spheres and the homogeneous host medium. Using Eq. (32) in the L representation, we can write

$$\Delta N(\omega) = \frac{1}{\pi} \mathrm{Im\,Tr\,ln}[\mathbf{I} + \mathbf{T}^{\mathrm{tot}}]_{\{\mathrm{L}\}}, \tag{79}$$

which has the form of Eq. (61), but of course here $\mathbf{T}^{\mathrm{tot}}$ is the scattering matrix for the assembly of spheres. It can be shown that Eq. (79) takes the form (see Appendix C)

$$\Delta N(\omega) = \frac{1}{\pi} \mathrm{Im\,Tr\,ln}[\mathbf{I} + \mathbf{T}]_{\{n\mathrm{L}\}} - \frac{1}{\pi} \mathrm{Im\,Tr\,ln}[\mathbf{I} - \mathbf{T}\boldsymbol{\Omega}]_{\{n\mathrm{L}\}}, \tag{80}$$

where $T^{nn'}_{\mathrm{LL}'}=\delta_{nn'}T^{n}_{\mathrm{LL}'}$, $\mathbf{\Omega}$ is the matrix defined by Eqs. (62), (63), and $\{n\mathrm{L}\}$ denotes matrices in nL space.

We can find the difference in the number of states up to a frequency ω, $\Delta N_0(\omega)$, between the given assembly of spheres and an arbitrary reference system of spheres characterized by $T^{n}_{0\mathrm{LL}'}$, by applying Eq. (80) to the two systems and using Eqs. (70) and (72). We obtain

$$\Delta N_0(\omega)=\frac{1}{\pi}\mathrm{Im\,Tr}\ln[\mathbf{I}+\mathbf{T}]_{\{n\mathrm{L}\}}-\frac{1}{\pi}\mathrm{Im\,Tr}\ln[\mathbf{I}+\mathbf{T}_0]_{\{n\mathrm{L}\}}-\frac{1}{\pi}\mathrm{Im\,Tr}\ln[\mathbf{I}-\Delta\mathbf{T}\mathbf{D}_0]_{\{n\mathrm{L}\}}. \tag{81}$$

Let us apply the above to a periodic structure as defined in the text following Eq. (72). Obviously, $T^{nn'}_{\mathrm{LL}'}=\delta_{nn'}T^{\alpha}_{\mathrm{LL}'}$. Using Eq. (75), one can show that

$$\{[\mathbf{T}\mathbf{\Omega}]^{\kappa}\}^{nn'}_{\mathrm{LL}'}=\frac{1}{v}\int_{BZ}d^3k\,\exp[i\mathbf{k}\cdot(\mathbf{R}_\lambda-\mathbf{R}_{\lambda'})]\times\{[\mathbf{T}\mathbf{\Omega}(\mathbf{k})]^{\kappa}\}^{\alpha\alpha'}_{\mathrm{LL}'},\quad \kappa=1,2,3,\ldots \tag{82}$$

and with the help of the power series expansion of the logarithm of a square matrix, that

$$\{\ln[\mathbf{I}-\mathbf{T}\mathbf{\Omega}]\}^{nn'}_{\mathrm{LL}'}=\frac{1}{v}\int_{BZ}d^3k\,\exp[i\mathbf{k}\cdot(\mathbf{R}_\lambda-\mathbf{R}_{\lambda'})]\times\{\ln[\mathbf{I}-\mathbf{T}\mathbf{\Omega}(\mathbf{k})]\}^{\alpha\alpha'}_{\mathrm{LL}'}. \tag{83}$$

Substituting Eq. (83) in Eq. (80), we obtain

$$\Delta N(\omega)=\frac{N}{v}\int_{BZ}d^3k\,\Delta N(\mathbf{k};\omega), \tag{84}$$

where N is the number of unit cells of the crystal and

$$\Delta N(\mathbf{k};\omega)=\frac{1}{\pi}\mathrm{Im\,Tr}\ln[\mathbf{I}+\mathbf{T}]_{\{\alpha\mathrm{L}\}}-\frac{1}{\pi}\mathrm{Im\,Tr}\ln[\mathbf{I}-\mathbf{T}\mathbf{\Omega}(\mathbf{k})]_{\{\alpha\mathrm{L}\}}. \tag{85}$$

We should note that Eqs. (84) and (85) are valid for crystals of any dimensions, provided that $\mathbf{k}$ is taken in the proper BZ.

VI. THE GREEN'S FUNCTION OF A SLAB

In the previous sections we dealt with an infinite phononic crystal. In reality we are dealing with slabs of phononic crystals. A slab consists of a number of layers: a succession of planes of spheres parallel to a given crystallographic plane. If the slab is sufficiently thick the local density of states within the slab (a few layers away from either surface) will be practically the same with that of the infinite crystal. However, the situation may be very different at the surface layers of the slab, especially if surface states of the elastic field (these extend to infinity parallel to the surface, but decay exponentially on either side of it) exist in the given frequency region. Of course, the infinite-crystal approximation cannot be used for thin slabs of one or two planes of spheres.

In this section we shall obtain the Green's function for a slab (a layered structure). We shall derive formulas which permit the calculation of the local density of states at the surface of the slab and in the host region between consecutive planes of spheres, and formulas for the integrated $\mathbf{k}_{\|}$-resolved density of states of the slab. The method is similar to the one described in Ref. 19 for the corresponding electronic problem.

The slab we consider consists of a number of parallel planes of nonoverlapping spheres (layers), perpendicular to the z axis, with the same 2D periodicity in the xy plane. The spheres are centered on the sites $\mathbf{R}_\lambda+\mathbf{t}_\alpha$; here $\{\mathbf{R}_\lambda\}$ is a 2D Bravais lattice and $\mathbf{t}_\alpha$ denote the positions of the spheres (if there are more than one) within the 2D unit cell. The 2D reciprocal vectors $\mathbf{g}$, and the surface Brillouin zone (SBZ) corresponding to this lattice are defined in the usual manner.[10] Because of the 2D periodicity of the system, the eigenmodes of the elastic wave field in the host region between two consecutive layers are sums of plane waves with wave vectors $\mathbf{q}=(\mathbf{k}_{\|}+\mathbf{g},q_z)$, of the same reduced wave vector $\mathbf{k}_{\|}$ (which lies in the SBZ). Accordingly, we write the Green's function [Eq. (35)] of a homogeneous medium, at a given frequency ω, as follows:

$$g_{ii'}(\mathbf{r},\mathbf{r}')=\frac{1}{(2\pi)^3}\sum_{\mathrm{p}\mathbf{g}}\frac{1}{c_\nu^2}\int\int_{SBZ}d^2k_{\|}\times\exp[i(\mathbf{k}_{\|}+\mathbf{g})\cdot(\mathbf{r}_{\|}-\mathbf{r}'_{\|})]\times\int_{-\infty}^{\infty}dq_z\frac{\exp[iq_z(z-z')]e_{\mathrm{p};i}(\mathbf{q})e_{\mathrm{p};i'}(\mathbf{q})}{(\omega/c_\nu)^2-[(\mathbf{k}_{\|}+\mathbf{g})^2+q_z^2]}, \tag{86}$$

where for p$=1$, $c_\nu=c_l$ and for p$=2,3$, $c_\nu=c_t$. In what follows, we write the wave vector of a plane wave of given $\mathbf{q}_{\|}=\mathbf{k}_{\|}+\mathbf{g}$ and given $q_\nu=\omega/c_\nu$ as $\mathbf{K}^{\pm}_{\mathbf{g}\nu}=(\mathbf{k}_{\|}+\mathbf{g},\pm[q_\nu^2-(\mathbf{k}_{\|}+\mathbf{g})^2]^{1/2})$. We note that when $q_\nu^2<(\mathbf{k}_{\|}+\mathbf{g})^2$, the above defines a decaying wave; the positive (negative) sign corresponds to a wave propagating or decaying to the right (left). Evaluating the q_z integral in Eq. (86) by contour integration, we obtain

$$g_{ii'}(\mathbf{r},\mathbf{r}')=\frac{-i}{8\pi^2}\int\int_{SBZ}d^2k_{\|}\sum_{\mathrm{p}\mathbf{g}}\frac{1}{c_\nu^2K^{+}_{\mathbf{g}\nu;z}}\times\{\exp[i\mathbf{K}^{+}_{\mathbf{g}\nu}\cdot(\mathbf{r}-\mathbf{r}')]\times e_{\mathrm{p};i}(\mathbf{K}^{+}_{\mathbf{g}\nu})e_{\mathrm{p};i'}(\mathbf{K}^{+}_{\mathbf{g}\nu})\Theta(z-z')+\exp[i\mathbf{K}^{-}_{\mathbf{g}\nu}\cdot(\mathbf{r}-\mathbf{r}')]e_{\mathrm{p};i}(\mathbf{K}^{-}_{\mathbf{g}\nu})e_{\mathrm{p};i'}(\mathbf{K}^{-}_{\mathbf{g}\nu})\times\Theta(z'-z)\}. \tag{87}$$

We wish to calculate the Green's function $G_{ii'}(\mathbf{r},\mathbf{r}')$ of a slab, consisting of a number of planes of spheres, in the host region between two consecutive planes. We put $\mathbf{r}=\mathbf{r}'$, since it is $G_{ii'}(\mathbf{r},\mathbf{r})$ which provides the local density of states according to Eq. (15). Using Eq. (87) in the Lippmann-Schwinger equation [the second of Eqs. (23)], we obtain

$$G_{ii'}(\mathbf{r},\mathbf{r})=g_{ii'}(\mathbf{r},\mathbf{r})+\frac{-i}{8\pi^2}\int\int_{SBZ}d^2k_{\|}\sum_{\mathrm{pg}}\frac{1}{c_\nu^2K^+_{\mathbf{g}\nu;z}}\{\mathrm{v}^+_{\mathrm{p}\mathbf{gk}_{\|};i}(\mathbf{r})\times\exp[-i\mathbf{K}^+_{\mathbf{g}\nu}\cdot\mathbf{r}]e_{\mathrm{p};i'}(\mathbf{K}^+_{\mathbf{g}\nu})+\mathrm{v}^-_{\mathrm{p}\mathbf{gk}_{\|};i}(\mathbf{r})\times\exp[-i\mathbf{K}^-_{\mathbf{g}\nu}\cdot\mathbf{r}]e_{\mathrm{p};i'}(\mathbf{K}^-_{\mathbf{g}\nu})\},\tag{88}$$

where

$$\mathrm{v}^+_{\mathrm{p}\mathbf{gk}_{\|};i}(\mathbf{r})=\sum_{j,j'}\int\int d^3r_1d^3r_2g_{ij}(\mathbf{r},\mathbf{r}_1)\mathcal{T}_{jj'}(\mathbf{r}_1,\mathbf{r}_2)\times\exp[i\mathbf{K}^+_{\mathbf{g}\nu}\cdot\mathbf{r}_2]e_{\mathrm{p};j'}(\mathbf{K}^+_{\mathbf{g}\nu})\Theta(z_2-z),$$

$$\mathrm{v}^-_{\mathrm{p}\mathbf{gk}_{\|};i}(\mathbf{r})=\sum_{j,j'}\int\int d^3r_1d^3r_2g_{ij}(\mathbf{r},\mathbf{r}_1)\mathcal{T}_{jj'}(\mathbf{r}_1,\mathbf{r}_2)\times\exp[i\mathbf{K}^-_{\mathbf{g}\nu}\cdot\mathbf{r}_2]e_{\mathrm{p};j'}(\mathbf{K}^-_{\mathbf{g}\nu})\Theta(z-z_2).\tag{89}$$

$\mathcal{T}_{jj'}(\mathbf{r}_1,\mathbf{r}_2)$ is the on-shell scattering transition matrix for the given slab, relative to the homogeneous host medium. According to Eq. (22), we can write

$$\hat{\mathcal{T}}=\hat{\Gamma}+\hat{\Gamma}\hat{g}\hat{\Gamma}+\hat{\Gamma}\hat{g}\hat{\Gamma}\hat{g}\hat{\Gamma}+\cdots=\hat{\Gamma}+\hat{\Gamma}\hat{g}\hat{\mathcal{T}}.\tag{90}$$

By splitting $\hat{\Gamma}$ into two independent contributions, $\hat{\Gamma}_1$ and $\hat{\Gamma}_2$ ($\hat{\Gamma}=\hat{\Gamma}_1+\hat{\Gamma}_2$), where $\Gamma_{1jj'}(\mathbf{r}_2)$ vanishes for $z_2>z$ and $\Gamma_{2jj'}(\mathbf{r}_2)$ vanishes for $z_2<z$, we can write

$$\hat{\mathcal{T}}=\hat{\mathcal{T}}^++\hat{\mathcal{T}}^-,\tag{91}$$

where

$$\hat{\mathcal{T}}^+=\hat{\Gamma}_2+\hat{\Gamma}\hat{g}\hat{\Gamma}_2+\hat{\Gamma}\hat{g}\hat{\Gamma}\hat{g}\hat{\Gamma}_2+\cdots=\hat{\Gamma}_2+\hat{\Gamma}\hat{g}\hat{\mathcal{T}}^+\tag{92}$$

and

$$\hat{\mathcal{T}}^-=\hat{\Gamma}_1+\hat{\Gamma}\hat{g}\hat{\Gamma}_1+\hat{\Gamma}\hat{g}\hat{\Gamma}\hat{g}\hat{\Gamma}_1+\cdots=\hat{\Gamma}_1+\hat{\Gamma}\hat{g}\hat{\mathcal{T}}^-.\tag{93}$$

It then follows that $\mathcal{T}_{jj'}(\mathbf{r}_1,\mathbf{r}_2)\Theta(z_2-z)$ is to be identified with $\mathcal{T}^+(\mathbf{r}_1,\mathbf{r}_2)$ and $\mathcal{T}_{jj'}(\mathbf{r}_1,\mathbf{r}_2)\Theta(z-z_2)$ with $\mathcal{T}^-(\mathbf{r}_1,\mathbf{r}_2)$.

We now introduce the on-shell scattering transition operator $\hat{\mathcal{T}}_1$ which takes into account all scattering from the left of $\mathbf{r}$. This includes scattering by the planes of spheres to the left of $\mathbf{r}$, as well as the scattering at the interface of the slab with the medium that lies to the left of the slab. We have

$$\hat{\mathcal{T}}_1=\hat{\Gamma}_1+\hat{\Gamma}_1\hat{g}\hat{\Gamma}_1+\hat{\Gamma}_1\hat{g}\hat{\Gamma}_1\hat{g}\hat{\Gamma}_1+\cdots=\hat{\Gamma}_1+\hat{\Gamma}_1\hat{g}\hat{\mathcal{T}}_1.\tag{94}$$

Obviously, $\mathcal{T}_{1jj'}(\mathbf{r}_1,\mathbf{r}_2)$ is not zero only if $z_1,z_2<z$. We define a matrix $\mathbf{Q}_1^{\mathrm{II}}$ at $\mathbf{r}$ describing the reflection from the left of $\mathbf{r}$, as follows:

$$\sum_{\mathrm{p}'\mathbf{g}'}\mathbf{Q}^{\mathrm{II}}_{1\,\mathrm{p}'\mathbf{g}';\mathrm{pg}}\exp[i\mathbf{K}^+_{\mathbf{g}'\nu'}\cdot\mathbf{r}]e_{\mathrm{p}';i}(\mathbf{K}^+_{\mathbf{g}'\nu'})=\sum_{j,j'}\int\int d^3r_1d^3r_2g_{ij}(\mathbf{r},\mathbf{r}_1)\mathcal{T}_{1jj'}(\mathbf{r}_1,\mathbf{r}_2)\times\exp[i\mathbf{K}^-_{\mathbf{g}\nu}\cdot\mathbf{r}_2]e_{\mathrm{p};j'}(\mathbf{K}^-_{\mathbf{g}\nu}).\tag{95}$$

Similarly, we define $\hat{\mathcal{T}}_2$ which takes into account all scattering from the right of $\mathbf{r}$. We have

$$\hat{\mathcal{T}}_2=\hat{\Gamma}_2+\hat{\Gamma}_2\hat{g}\hat{\Gamma}_2+\hat{\Gamma}_2\hat{g}\hat{\Gamma}_2\hat{g}\hat{\Gamma}_2+\cdots=\hat{\Gamma}_2+\hat{\Gamma}_2\hat{g}\hat{\mathcal{T}}_2.\tag{96}$$

Obviously, $\mathcal{T}_{2jj'}(\mathbf{r}_1,\mathbf{r}_2)$ is not zero only if $z_1,z_2>z$. We define a matrix $\mathbf{Q}_2^{\mathrm{III}}$ at $\mathbf{r}$ describing the reflection from the right of $\mathbf{r}$, as follows:

$$\sum_{\mathrm{p}'\mathbf{g}'}\mathbf{Q}^{\mathrm{III}}_{2\,\mathrm{p}'\mathbf{g}';\mathrm{pg}}\exp[i\mathbf{K}^-_{\mathbf{g}'\nu'}\cdot\mathbf{r}]e_{\mathrm{p}';i}(\mathbf{K}^-_{\mathbf{g}'\nu'})=\sum_{j,j'}\int\int d^3r_1d^3r_2g_{ij}(\mathbf{r},\mathbf{r}_1)\mathcal{T}_{2jj'}(\mathbf{r}_1,\mathbf{r}_2)\times\exp[i\mathbf{K}^+_{\mathbf{g}\nu}\cdot\mathbf{r}_2]e_{\mathrm{p};j'}(\mathbf{K}^+_{\mathbf{g}\nu}).\tag{97}$$

The matrices $\mathbf{Q}_1^{\mathrm{II}}$ and $\mathbf{Q}_2^{\mathrm{III}}$, which are functions of $\mathbf{k}_{\|}$, ω and depend on $\mathbf{r}$, can be obtained from the matrices which describe the scattering by individual layers and by the interfaces of the slab with the media surrounding it (if these are different from the host medium in the slab) in the manner described in Ref. 10, and we need not say anything more about that aspect of the problem here. Clearly, $\mathcal{T}_{1jj'}(\mathbf{r}_1,\mathbf{r}_2)$ and $\mathcal{T}_{2jj'}(\mathbf{r}_1,\mathbf{r}_2)$ depend on $\mathbf{r}$. Only in the case of an infinitely thick slab (infinite crystal) these matrices become independent of $\mathbf{r}$.

Using Eqs. (92), (93), (94), and (96), one can easily verify that

$$\hat{\mathcal{T}}^+=\hat{\mathcal{T}}_2+\hat{\mathcal{T}}_1\hat{g}\hat{\mathcal{T}}_2+\hat{\mathcal{T}}_2\hat{g}\hat{\mathcal{T}}_1\hat{g}\hat{\mathcal{T}}_2+\cdots\tag{98}$$

and

$$\hat{\mathcal{T}}^-=\hat{\mathcal{T}}_1+\hat{\mathcal{T}}_2\hat{g}\hat{\mathcal{T}}_1+\hat{\mathcal{T}}_1\hat{g}\hat{\mathcal{T}}_2\hat{g}\hat{\mathcal{T}}_1+\cdots.\tag{99}$$

According to the Lippmann-Schwinger equation [Eq. (20)], $\mathbf{v}^{\pm}_{\mathrm{p}\mathbf{gk}_{\|}}(\mathbf{r})$, given by Eqs. (89), are the waves produced at $\mathbf{r}$ by the multiple scattering (multiple reflections to all orders) from the left and right of $\mathbf{r}$, described by Eqs. (98) and (99), originating from incident plane waves of polarization $\hat{\boldsymbol{e}}_{\mathrm{p}}$ and wave vectors $\mathbf{K}^{\pm}_{\mathbf{g}\nu}$, respectively. Summing up the infinite series resulting from the different reflection sequences involved, we obtain

$$
\begin{aligned}
\mathrm{v}^{+}_{\mathrm{p}\mathbf{g}\mathbf{k}_{\|};i}(\mathbf{r}) = \sum_{\mathrm{p}'\mathbf{g}'} \{ & [\mathbf{Q}_1^{\mathrm{II}}\mathbf{Q}_2^{\mathrm{III}} + \mathbf{Q}_1^{\mathrm{II}}\mathbf{Q}_2^{\mathrm{III}}\mathbf{Q}_1^{\mathrm{II}}\mathbf{Q}_2^{\mathrm{III}} + \cdots]_{\mathrm{p}'\mathbf{g}';\mathrm{p}\mathbf{g}} \\
& \times \exp[i\mathbf{K}^{+}_{\mathbf{g}'\nu'}\cdot\mathbf{r}] e_{\mathrm{p}';i}(\mathbf{K}^{+}_{\mathbf{g}'\nu'}) \\
& + [\mathbf{Q}_2^{\mathrm{III}} + \mathbf{Q}_2^{\mathrm{III}}\mathbf{Q}_1^{\mathrm{II}}\mathbf{Q}_2^{\mathrm{III}} + \cdots]_{\mathrm{p}'\mathbf{g}';\mathrm{p}\mathbf{g}} \\
& \times \exp[i\mathbf{K}^{-}_{\mathbf{g}'\nu'}\cdot\mathbf{r}] e_{\mathrm{p}';i}(\mathbf{K}^{-}_{\mathbf{g}'\nu'}) \} \\
= \sum_{\mathrm{p}'\mathbf{g}'} \{ & [\mathbf{Q}_1^{\mathrm{II}}\mathbf{Q}_2^{\mathrm{III}}(\mathbf{I} - \mathbf{Q}_1^{\mathrm{II}}\mathbf{Q}_2^{\mathrm{III}})^{-1}]_{\mathrm{p}'\mathbf{g}';\mathrm{p}\mathbf{g}} \\
& \times \exp[i\mathbf{K}^{+}_{\mathbf{g}'\nu'}\cdot\mathbf{r}] e_{\mathrm{p}';i}(\mathbf{K}^{+}_{\mathbf{g}'\nu'}) \\
& + [\mathbf{Q}_2^{\mathrm{III}}(\mathbf{I} - \mathbf{Q}_1^{\mathrm{II}}\mathbf{Q}_2^{\mathrm{III}})^{-1}]_{\mathrm{p}'\mathbf{g}';\mathrm{p}\mathbf{g}} \\
& \times \exp[i\mathbf{K}^{-}_{\mathbf{g}'\nu'}\cdot\mathbf{r}] e_{\mathrm{p}';i}(\mathbf{K}^{-}_{\mathbf{g}'\nu'}) \},
\end{aligned} \tag{100}
$$

and

$$
\begin{aligned}
\mathrm{v}^{-}_{\mathrm{p}\mathbf{g}\mathbf{k}_{\|};i}(\mathbf{r}) = \sum_{\mathrm{p}'\mathbf{g}'} \{ & [\mathbf{Q}_1^{\mathrm{II}} + \mathbf{Q}_1^{\mathrm{II}}\mathbf{Q}_2^{\mathrm{III}}\mathbf{Q}_1^{\mathrm{II}} + \cdots]_{\mathrm{p}'\mathbf{g}';\mathrm{p}\mathbf{g}} \\
& \times \exp[i\mathbf{K}^{+}_{\mathbf{g}'\nu'}\cdot\mathbf{r}] e_{\mathrm{p}';i}(\mathbf{K}^{+}_{\mathbf{g}'\nu'}) \\
& + [\mathbf{Q}_2^{\mathrm{III}}\mathbf{Q}_1^{\mathrm{II}} + \mathbf{Q}_2^{\mathrm{III}}\mathbf{Q}_1^{\mathrm{II}}\mathbf{Q}_2^{\mathrm{III}}\mathbf{Q}_1^{\mathrm{II}} + \cdots]_{\mathrm{p}'\mathbf{g}';\mathrm{p}\mathbf{g}} \\
& \times \exp[i\mathbf{K}^{-}_{\mathbf{g}'\nu'}\cdot\mathbf{r}] e_{\mathrm{p}';i}(\mathbf{K}^{-}_{\mathbf{g}'\nu'}) \} \\
= \sum_{\mathrm{p}'\mathbf{g}'} \{ & [\mathbf{Q}_1^{\mathrm{II}}(\mathbf{I} - \mathbf{Q}_2^{\mathrm{III}}\mathbf{Q}_1^{\mathrm{II}})^{-1}]_{\mathrm{p}'\mathbf{g}';\mathrm{p}\mathbf{g}} \\
& \times \exp[i\mathbf{K}^{+}_{\mathbf{g}'\nu'}\cdot\mathbf{r}] e_{\mathrm{p}';i}(\mathbf{K}^{+}_{\mathbf{g}'\nu'}) \\
& + [\mathbf{Q}_2^{\mathrm{III}}\mathbf{Q}_1^{\mathrm{II}}(\mathbf{I} - \mathbf{Q}_2^{\mathrm{III}}\mathbf{Q}_1^{\mathrm{II}})^{-1}]_{\mathrm{p}'\mathbf{g}';\mathrm{p}\mathbf{g}} \\
& \times \exp[i\mathbf{K}^{-}_{\mathbf{g}'\nu'}\cdot\mathbf{r}] e_{\mathrm{p}';i}(\mathbf{K}^{-}_{\mathbf{g}'\nu'}) \}.
\end{aligned} \tag{101}
$$

Substituting Eqs. (100) and (101) into Eq. (88), we obtain an expression for the Green's function of the slab at a point $\mathbf{r}$, in the host region between two consecutive layers, in terms of the above reflection matrices of the two parts of the slab on the left and on the right of $\mathbf{r}$. Similarly we obtain the Green's function at the surfaces of the slab.

Finally, we evaluate the difference in the number of states up to a given frequency ω, between a slab of finite thickness and a homogeneous medium identical with that which surrounds the slab (we assume that to be the same to the left and to the right of the slab), from Eq. (32). In this case, it is convenient to work in $s\mathrm{p}\mathbf{g}\mathbf{k}_{\|}$ representation ($s=\pm$), in which the on-shell scattering transition operator is diagonal in $\mathbf{k}_{\|}$. We obtain

$$
\Delta N(\omega) = \frac{N}{A}\int\int_{SBZ} d^2k_{\|}\Delta N(\mathbf{k}_{\|};\omega), \tag{102}
$$

where A is the area of the *SBZ*, N is the number of surface unit cells of the slab, and

$$
\Delta N(\mathbf{k}_{\|};\omega) = \frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}\,\ln[\mathbf{I} + \mathbf{T}(\mathbf{k}_{\|})]_{\{s\mathrm{p}\mathbf{g}\}}, \tag{103}
$$

$\{s\mathrm{p}\mathbf{g}\}$ denoting matrices in $s\mathrm{p}\mathbf{g}$ space. Explicit expressions for the matrix elements $T^{ss'}_{\mathrm{p}\mathbf{g};\mathrm{p}'\mathbf{g}'}(\mathbf{k}_{\|})$ can be obtained by comparing the expressions for the waves scattered by the slab (the transmitted and reflected waves), given by the Lippmann-Schwinger equation [Eq. (20) taken together with the formulas of this section], with those obtained by a direct calculation of the reflection and transmission matrices, $\mathbf{Q}^{\mathrm{I}}$, $\mathbf{Q}^{\mathrm{II}}$, $\mathbf{Q}^{\mathrm{III}}$, and $\mathbf{Q}^{\mathrm{IV}}$, of the slab, as defined in Ref. 10. We obtain

$$
\begin{aligned}
T^{++}_{\mathrm{p}\mathbf{g};\mathrm{p}'\mathbf{g}'}(\mathbf{k}_{\|}) &= \exp[i(\mathbf{K}^{+}_{\mathbf{g}'\nu'}\cdot\mathbf{A}_1 - \mathbf{K}^{+}_{\mathbf{g}\nu}\cdot\mathbf{A}_2)]Q^{\mathrm{I}}_{\mathrm{p}\mathbf{g};\mathrm{p}'\mathbf{g}'} \\
&\quad - \delta_{\mathrm{p}\mathrm{p}'}\delta_{\mathbf{g}\mathbf{g}'}, \\
T^{+-}_{\mathrm{p}\mathbf{g};\mathrm{p}'\mathbf{g}'}(\mathbf{k}_{\|}) &= \exp[i(\mathbf{K}^{-}_{\mathbf{g}'\nu'}\cdot\mathbf{A}_2 - \mathbf{K}^{+}_{\mathbf{g}\nu}\cdot\mathbf{A}_2)]Q^{\mathrm{II}}_{\mathrm{p}\mathbf{g};\mathrm{p}'\mathbf{g}'}, \\
T^{-+}_{\mathrm{p}\mathbf{g};\mathrm{p}'\mathbf{g}'}(\mathbf{k}_{\|}) &= \exp[i(\mathbf{K}^{+}_{\mathbf{g}'\nu'}\cdot\mathbf{A}_1 - \mathbf{K}^{-}_{\mathbf{g}\nu}\cdot\mathbf{A}_1)]Q^{\mathrm{III}}_{\mathrm{p}\mathbf{g};\mathrm{p}'\mathbf{g}'}, \\
T^{--}_{\mathrm{p}\mathbf{g};\mathrm{p}'\mathbf{g}'}(\mathbf{k}_{\|}) &= \exp[i(\mathbf{K}^{-}_{\mathbf{g}'\nu'}\cdot\mathbf{A}_2 - \mathbf{K}^{-}_{\mathbf{g}\nu}\cdot\mathbf{A}_1)]Q^{\mathrm{IV}}_{\mathrm{p}\mathbf{g};\mathrm{p}'\mathbf{g}'} \\
&\quad - \delta_{\mathrm{p}\mathrm{p}'}\delta_{\mathbf{g}\mathbf{g}'}.
\end{aligned} \tag{104}
$$

The phase factors in Eqs. (104) arise from the need to refer the scattered waves to a common origin, while $\mathbf{Q}^{\mathrm{I}}$, $\mathbf{Q}^{\mathrm{II}}$, $\mathbf{Q}^{\mathrm{III}}$, $\mathbf{Q}^{\mathrm{IV}}$ in Ref. 10 were obtained with the waves on the left of the slab referred to an origin $\mathbf{A}_1$ and the waves to the right of the slab to an origin $\mathbf{A}_2$.

VII. AN EXAMPLE

We demonstrate the applicability of our formalism by applying it to a specific example:[20] a thin slab of steel spheres ($\rho_s=7800$ kg/m^3,$c_{sl}=5940$ m/sec,$c_{st}=3200$ m/sec) embedded in a polyester matrix ($\rho=1220$ kg/m^3,$c_l=2490$ m/sec,$c_t=1180$ m/sec) extending over all space. The radius of the spheres is $S=0.585$ mm. We consider two cases.

In the first case the slab consists of just one plane of spheres (layer) centered at the sites of a 2D lattice, a square array in the xy plane, defined by the primitive vectors $\mathbf{a}_1=a_0(1,0,0)$ and $\mathbf{a}_2=a_0(0,1,0)$ with $a_0=3.95$ mm. We calculated $\Delta n(\mathbf{k}_{\|};\omega)$, the difference between the $\mathbf{k}_{\|}$-resolved density of states of this system and that of polyester, for $\mathbf{k}_{\|}=\mathbf{0}$. We did this by numerical differentiation of the corresponding difference in the number of states up to a frequency ω, $\Delta N(\mathbf{0};\omega)$, evaluated in the angular-momentum representation [Eq. (85)] and independently in the plane-wave representation [Eq. (103)]. The results obtained in the two representations are practically identical; they are shown in Fig. 1(a). $\Delta n(\mathbf{0};\omega)$ is characterized by the presence of two resonance peaks centered at $\omega_{\mathrm{I}}a_0/c_l=2.62$ and at $\omega_{\mathrm{II}}a_0/c_l=2.79$ which imply the existence of virtual bound states (resonances) of the elastic field at these frequencies. In each case the displacement field peaks about the plane of spheres falling to a much lower value away from it. The low-frequency resonance corresponds to a longitudinal virtual bound state which is nondegenerate: integrated over the frequency region of this resonance, $\Delta n(\mathbf{0};\omega)$ gives approximately 1. This resonance is responsible for the dip in the

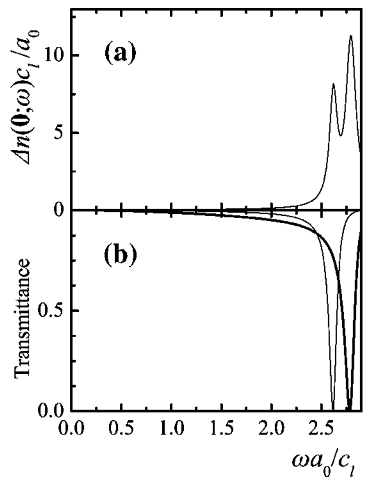

FIG. 1. (a) The change in the $\mathbf{k}_{\|}$-resolved density of states of a polyester matrix due to the presence of a square array ($a_0 = 3.95$ mm) of steel spheres ($S = 0.585$ mm), for $\mathbf{k}_{\|} = \mathbf{0}$. (b) The transmission coefficient of a longitudinal (thin line) and a transverse (thick line) elastic wave incident normally on the plane of spheres.

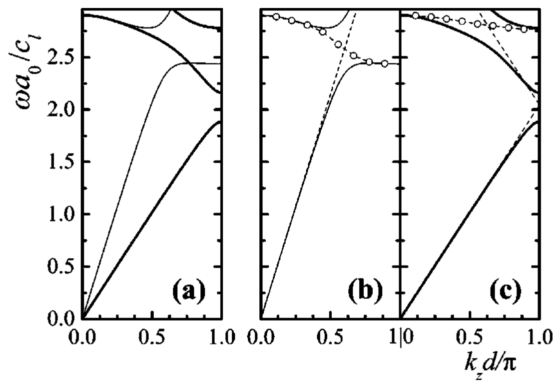

FIG. 3. The phononic frequency band structure of an infinite fcc crystal $[\mathbf{a}_1 = a_0(1,0,0,), \mathbf{a}_2 = a_0(0,1,0,), \mathbf{a}_3 = a_0(1/2,1/2,\sqrt{2}/2,), a_0 = 3.95$ mm$]$ of steel spheres ($S = 0.585$ mm) normal to the (001) surface. The thin (thick) solid lines represent longitudinal (transverse) bands. In (b) and (c) the dashed lines with the open circles are the unhybridized bands of resonant modes and the straight dashed lines the unhybridized effective-medium bands.

transmission of longitudinal waves at $\omega = \omega_{\mathrm{I}}$ [thin line of Fig. 1(b)]. The high-frequency resonance corresponds to a transverse virtual bound state which is doubly degenerate: integrated over the frequency region of this resonance, $\Delta n(\mathbf{0};\omega)$ gives approximately 2. This resonance is responsible for the dip in the transmission of transverse waves at $\omega = \omega_{\mathrm{II}}$ [thick line of Fig. 1(b)].

In the second case the slab consists of two layers (the same as in the first case) separated by a translation vector $\mathbf{a}_3 = a_0(1/2,1/2,\sqrt{2}/2)$. The results for $\Delta n(\mathbf{0};\omega)$ for this slab, calculated on the basis of Eq. (103), are shown by the solid line in Fig. 2. By comparing with $\Delta n(\mathbf{0};\omega)$ for the single layer (dashed line in Fig. 2) we deduce the following. The longitudinal virtual bound states of the two layers interacting with each other give rise to two coupled resonant modes, one at $\omega a_0/c_l = 2.51$ and one at $\omega a_0/c_l \cong 2.80$. The coupling between the transverse virtual bound states of the two layers is apparently much weaker and the resulting coupled modes (two doubly degenerate resonant modes) lie at about the same frequency $\omega a_0/c_l \cong 2.80$. Therefore, $\Delta n(\mathbf{0};\omega)$ (given by the solid line in Fig. 2) integrated over the region of the low-frequency resonance gives approximately 1, and when integrated over the region of the high-frequency resonance gives approximately 5.

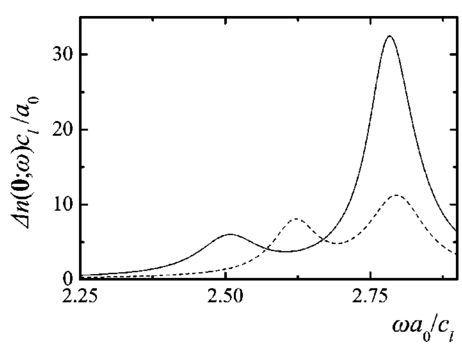

FIG. 2. The change in the $\mathbf{k}_{\|}$-resolved density of states of a polyester matrix due to the presence of a thin slab consisting of two identical square arrays $[\mathbf{a}_1 = a_0(1,0,0,), \mathbf{a}_2 = a_0(0,1,0,), a_0 = 3.95$ mm$]$ of steel spheres ($S = 0.585$ mm), separated by a translation $\mathbf{a}_3 = a_0(1/2,1/2,\sqrt{2}/2,)$, for $\mathbf{k}_{\|} = \mathbf{0}$ (solid line). The corresponding quantity for a single plane of spheres [the same as in Fig. 1(a)] is shown by a dashed line for comparison.

Finally, it is worth commenting on the role of the abovementioned resonances (virtual bound states of the elastic field about individual planes) in the formation of the frequency band structure of the infinite (fcc) crystal, made up by an infinite sequence of such layers each displaced relative to the one preceding it by $\mathbf{a}_3 = a_0(1/2,1/2,\sqrt{2}/2)$. This is best done by reference to Fig. 3. The frequency band structure of the (infinite) phononic crystal for $\mathbf{k}_{\|} = \mathbf{0}$ is shown in Fig. 3(a), calculated using the method of Ref. 10. The longitudinal bands, represented by the thin lines arise as follows. In a homogeneous effective medium (the host medium modified to some degree by the spherical scatterers) one obtains a band, the dashed straight line in Fig. 3(b), with a slope defined by the longitudinal velocity $\overline{c_l}$. We obtain $\overline{c_l} = 2406$ m/sec from the slope of the exact curve in the limit $\omega \to 0$ and $\overline{c_l} = 2408$ m/sec from the effective medium theory.[21] The band described by the open circles in the same figure arises from the resonant modes of the individual planes when the interaction between them has taken place. We have determined this band by calculating the transmission coefficient of longitudinal waves incident normally on a slab consisting of eight layers (a slab sufficiently thick as evidenced by the results of our calculation). One clearly sees, in this case, superimposed on an otherwise smooth curve, sharp dips in the transmittance, similar to those in Fig. 1(b), at frequencies ω_i, $i = 1,2,\ldots,8$ with which we associate values of k_z given by $k_{z;i} = \pi i/(N+1)d$ where $d = a_0\sqrt{2}/2$ is the thickness of one layer and N is the number of layers in the slab ($N = 8$ in the present case). The open circles in Fig.

3(b) are the points $(\omega_i, k_{z;i})$, $i=1,2,\ldots,8$ obtained in this manner, and define the band of resonant modes in question. The two unhybridized bands shown in Fig. 3(b), the effective-medium band (dashed straight line) and the band of resonant modes (open circles), interact at the point in the (ω, k_z) space where the two meet, opening up a hybridization gap there, but away from the crossing point the exact bands [solid lines in Fig. 3(b)] are determined by one or the other of the unhybridized bands over the frequency region shown here.

A similar analysis applies to the transverse bands, as shown in Fig. 3(c). We see again that where the dashed straight line representing the transverse band in the effective medium meets the transverse band of resonant modes (open circles) the two interact leading to the separate hybridized bands (exact bands) shown by the solid lines in Fig. 3(c). We note, again, that the exact bands are determined by one or the other of the unhybridized bands, except about the region where the latter bands cross each other. In the present case there is also a Bragg gap opening up about $\omega a_0/c_l=2.04$, but the physics behind this is well known and we need not say anything about it here. When comparing Fig. 3(b) with Fig. 3(c) it is worth noting that the width of the transverse band of resonant modes is considerably smaller than that of the corresponding longitudinal one. It is also worth noting that in the transverse bands one does not obtain, as in the case of the longitudinal bands, a frequency gap as a result of the above-mentioned hybridization. Clearly, the appearance of a hybridization gap depends on the detailed shape of the unhybridized bands. In particular, the slope of the effective-medium band, the exact shape of the band of resonant modes, and the requirement that the unhybridized bands should converge to the above away from the crossing point decide at the end whether a frequency gap arises as a result of the hybridization.

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APPENDIX A

We consider the case of a solid homogeneous sphere of radius S in a solid homogeneous host medium. The displacement vector and the surface traction, associated with an elastic field in this system, must be continuous everywhere and, therefore, at the surface of the sphere.[10] The continuity of the above at the surface of the sphere constitutes the appropriate boundary conditions of the given problem. Assuming a regular at the origin wave field, which has the form $\Sigma_{\mathrm{L}} a^I_{\mathrm{L}} \mathbf{J}^s_{\mathrm{L}}(\mathbf{r})$ inside the sphere and $\Sigma_{\mathrm{L}}[a^0_{\mathrm{L}}\mathbf{J}_{\mathrm{L}}(\mathbf{r}) + a^+_{\mathrm{L}}\mathbf{H}_{\mathrm{L}}(\mathbf{r})]$ outside of it (see Sec. IV), and imposing the above boundary conditions, we obtain the following systems of linear equations

$$\begin{pmatrix} \frac{d_{11}}{z_t} & \frac{-\sqrt{l(l+1)}d_{12}}{z_l} & \frac{-d_{13}}{x_t} & \frac{\sqrt{l(l+1)}d_{14}}{x_l} \\ \frac{d_{21}}{z_t} & \frac{-\sqrt{l(l+1)}d_{22}}{z_l} & \frac{-d_{23}}{x_t} & \frac{\sqrt{l(l+1)}d_{24}}{x_l} \\ \frac{d_{31}}{z_t} & \frac{-\sqrt{l(l+1)}d_{32}}{z_l} & \frac{-d_{33}}{x_t} & \frac{\sqrt{l(l+1)}d_{34}}{x_l} \\ \frac{d_{41}}{z_t} & \frac{-\sqrt{l(l+1)}d_{42}}{z_l} & \frac{-d_{43}}{x_t} & \frac{\sqrt{l(l+1)}d_{44}}{x_l} \end{pmatrix} \begin{pmatrix} a^+_{Nlm} \\ a^+_{Llm} \\ a^I_{Nlm} \\ a^I_{Llm} \end{pmatrix} = \begin{pmatrix} -\frac{d^N_1}{z_t}a^0_{Nlm} + \frac{\sqrt{l(l+1)}d^L_1}{z_l}a^0_{Llm} \\ -\frac{d^N_2}{z_t}a^0_{Nlm} + \frac{\sqrt{l(l+1)}d^L_2}{z_l}a^0_{Llm} \\ -\frac{d^N_3}{z_t}a^0_{Nlm} + \frac{\sqrt{l(l+1)}d^L_3}{z_l}a^0_{Llm} \\ -\frac{d^N_4}{z_t}a^0_{Nlm} + \frac{\sqrt{l(l+1)}d^L_4}{z_l}a^0_{Llm} \end{pmatrix}, \tag{A1}$$

$$\begin{pmatrix} -d_{21} & d_{23} \\ -d_{41} & d_{43} \end{pmatrix} \begin{pmatrix} a^+_{Mlm} \\ a^I_{Mlm} \end{pmatrix} = \begin{pmatrix} d^N_2 a^0_{Mlm} \\ d^N_4 a^0_{Mlm} \end{pmatrix}, \tag{A2}$$

where

$$d_{11}=z_t h^{+\prime}_l(z_t)+h^+_l(z_t),$$

$$d_{21}=l(l+1)h^+_l(z_t),$$

$$d_{31}=\left[l(l+1)-\frac{z_t^2}{2}-1\right]h^+_l(z_t)-z_t h^{+\prime}_l(z_t),$$

$$d_{41}=l(l+1)[z_t h^{+\prime}_l(z_t)-h^+_l(z_t)],$$

$$d_{12}=h^+_l(z_l), \quad d_{22}=z_l h^{+\prime}_l(z_l),$$

$$d_{32}=z_l h^{+\prime}_l(z_l)-h^+_l(z_l),$$

$$d_{42}=\left[l(l+1)-\frac{z_t^2}{2}\right]h^+_l(z_l)-2z_l h^{+\prime}_l(z_l),$$

$$d_{13}=x_t j_l{}'(x_t)+j_l(x_t),$$

$$d_{23}=l(l+1)j_l(x_t),$$

$$d_{33}=\frac{\rho_s}{\rho}\left(\frac{z_t}{x_t}\right)^2\left\{\left[l(l+1)-\frac{x_t^2}{2}-1\right]j_l(x_t)-x_t j_l{}'(x_t)\right\},$$

$$d_{43}=\frac{\rho_s}{\rho}\left(\frac{z_t}{x_t}\right)^2 l(l+1)[x_t j_l{}'(x_t)-j_l(x_t)],$$

$$d_{14}=j_l(x_l),\quad d_{24}=x_l j_l{}'(x_l),$$

$$d_{34}=\frac{\rho_s}{\rho}\left(\frac{z_t}{x_t}\right)^2[x_l j_l{}'(x_l)-j_l(x_l)],$$

$$d_{44}=\frac{\rho_s}{\rho}\left(\frac{z_t}{x_t}\right)^2\left\{\left[l(l+1)-\frac{x_t^2}{2}\right]j_l(x_l)-2x_l j_l{}'(x_l)\right\}, \tag{A3}$$

and

$$d_1^N=z_t j_l{}'(z_t)+j_l(z_t),$$

$$d_2^N=l(l+1)j_l(z_t),$$

$$d_3^N=\left[l(l+1)-\frac{z_t^2}{2}-1\right]j_l(z_t)-z_t j_l{}'(z_t),$$

$$d_4^N=l(l+1)[z_t j_l{}'(z_t)-j_l(z_t)],$$

$$d_1^L=j_l(z_l),$$

$$d_2^L=z_l j_l{}'(z_l),$$

$$d_3^L=z_l j_l{}'(z_l)-j_l(z_l),$$

$$d_4^L=\left[l(l+1)-\frac{z_t^2}{2}\right]j_l(z_l)-2z_l j_l{}'(z_l), \tag{A4}$$

with $z_\nu=\omega S/c_\nu$ and $x_\nu=\omega S/c_{s\nu}$.

Similarly, for the irregular at the origin wave field which has the form $\Sigma_{\mathrm{L}}[c_{\mathrm{L}}^I\mathbf{J}_{\mathrm{L}}^s(\mathbf{r})+c_{\mathrm{L}}^{I+}\mathbf{H}_{\mathrm{L}}^s(\mathbf{r})]$ inside the sphere and $\Sigma_{\mathrm{L}}c_{\mathrm{L}}^0\mathbf{H}_{\mathrm{L}}(\mathbf{r})$ outside of it, we obtain

$$\begin{pmatrix} \frac{w_{11}}{x_t} & \frac{-\sqrt{l(l+1)}w_{12}}{x_l} & \frac{-d_{13}}{x_t} & \frac{\sqrt{l(l+1)}d_{14}}{x_l} \\ \frac{w_{21}}{x_t} & \frac{-\sqrt{l(l+1)}w_{22}}{x_l} & \frac{-d_{23}}{x_t} & \frac{\sqrt{l(l+1)}d_{24}}{x_l} \\ \frac{w_{31}}{x_t} & \frac{-\sqrt{l(l+1)}w_{32}}{x_l} & \frac{-d_{33}}{x_t} & \frac{\sqrt{l(l+1)}d_{34}}{x_l} \\ \frac{w_{41}}{x_t} & \frac{-\sqrt{l(l+1)}w_{42}}{x_l} & \frac{-d_{43}}{x_t} & \frac{\sqrt{l(l+1)}d_{44}}{x_l} \end{pmatrix}\begin{pmatrix} c_{Nlm}^{I+} \\ c_{Llm}^{I+} \\ c_{Nlm}^{I} \\ c_{Llm}^{I} \end{pmatrix}$$

$$=\begin{pmatrix} -\frac{w_1^N}{z_t}c_{Nlm}^0+\frac{\sqrt{l(l+1)}w_1^L}{z_l}c_{Llm}^0 \\ -\frac{w_2^N}{z_t}c_{Nlm}^0+\frac{\sqrt{l(l+1)}w_2^L}{z_l}c_{Llm}^0 \\ -\frac{w_3^N}{z_t}c_{Nlm}^0+\frac{\sqrt{l(l+1)}w_3^L}{z_l}c_{Llm}^0 \\ -\frac{w_4^N}{z_t}c_{Nlm}^0+\frac{\sqrt{l(l+1)}w_4^L}{z_l}c_{Llm}^0 \end{pmatrix}, \tag{A5}$$

$$\begin{pmatrix} -w_{21} & d_{23} \\ -w_{41} & d_{43} \end{pmatrix}\begin{pmatrix} c_{Mlm}^{I+} \\ c_{Mlm}^{I} \end{pmatrix}=\begin{pmatrix} w_2^N c_{Mlm}^0 \\ w_4^N c_{Mlm}^0 \end{pmatrix}, \tag{A6}$$

where

$$w_{11}=-x_t h_l^+{}'(x_t)-h_l^+(x_t),$$

$$w_{21}=-l(l+1)h_l^+(x_t),$$

$$w_{31}=-\frac{\rho_s}{\rho}\left(\frac{z_t}{x_t}\right)^2\left\{\left[l(l+1)-\frac{x_t^2}{2}-1\right]h_l^+(x_t)-x_t h_l^+{}'(x_t)\right\},$$

$$w_{41}=-\frac{\rho_s}{\rho}\left(\frac{z_t}{x_t}\right)^2 l(l+1)[x_t h_l^+{}'(x_t)-h_l^+(x_t)],$$

$$w_{12}=-h_l^+(x_l),\quad w_{22}=-x_l h_l^+{}'(x_l),$$

$$w_{32}=-\frac{\rho_s}{\rho}\left(\frac{z_t}{x_t}\right)^2[x_l h_l^+{}'(x_l)-h_l^+(x_l)],$$

$$w_{42}=-\frac{\rho_s}{\rho}\left(\frac{z_t}{x_t}\right)^2\left\{\left[l(l+1)-\frac{x_t^2}{2}\right]h_l^+(x_l)-2x_l h_l^+{}'(x_l)\right\}, \tag{A7}$$

and

$$w_1^N=z_t h_l^+{}'(z_t)+h_l^+(z_t),$$

$$w_2^N=l(l+1)h_l^+(z_t),$$

$$w_3^N=\left[l(l+1)-\frac{z_t^2}{2}-1\right]h_l^+(z_t)-z_t h_l^+{}'(z_t),$$

$$w_4^N=l(l+1)[z_t h_l^+{}'(z_t)-h_l^+(z_t)],$$

$$w_1^L=h_l^+(z_l),\quad w_2^L=z_l h_l^+{}'(z_l),$$

$$w_3^L=[z_l h_l^+{}'(z_l)-h_l^+(z_l)],$$

$$w_4^L=\left[l(l+1)-\frac{z_t^2}{2}\right]h_l^+(z_l)-2z_l h_l^+{}'(z_l). \tag{A8}$$

Equations similar to the above can be derived for any other combination of solid or fluid sphere in a solid or fluid homogeneous host medium.

APPENDIX B

Using the following mathematical identities[22]

$$\exp[i\mathbf{q}\cdot\mathbf{r}]=4\pi\sum_{lm} i^l j_l(qr)Y_l^m(\hat{\mathbf{r}})Y_l^{m}{}^*(\hat{\mathbf{q}}), \tag{B1}$$

$$\frac{\exp[iq|\mathbf{r}-\mathbf{r}'|]}{|\mathbf{r}-\mathbf{r}'|}=4\pi iq\sum_{lm} j_l(qr_<)h_l^+(qr_>)Y_l^m(\hat{\mathbf{r}})Y_l^{m}{}^*(\hat{\mathbf{r}}'), \tag{B2}$$

one can express scalar spherical waves, regular or irregular, about $\mathbf{R}_{n'}$ in terms of such waves about $\mathbf{R}_n$ as follows:

$$h^+_{l'}(qr_{n'})Y^{m'}_{l'}(\hat{\mathbf{r}}_{n'})=\sum_{lm} G_{l'm';lm}(\mathbf{R}_{nn'};q)j_l(qr_n)Y^m_l(\hat{\mathbf{r}}_n),\quad r_n<R_{nn'}, \tag{B3}$$

$$j_{l'}(qr_{n'})Y^{m'}_{l'}(\hat{\mathbf{r}}_{n'})=\sum_{lm} \xi_{l'm';lm}(\mathbf{R}_{nn'};q)j_l(qr_n)Y^m_l(\hat{\mathbf{r}}_n), \tag{B4}$$

$$h^+_{l'}(qr_{n'})Y^{m'}_{l'}(\hat{\mathbf{r}}_{n'})=\sum_{lm} \xi_{l'm';lm}(\mathbf{R}_{nn'};q)h^+_l(qr_n)Y^m_l(\hat{\mathbf{r}}_n),\quad r_n>R_{nn'} \tag{B5}$$

where $\mathbf{R}_{nn'}=\mathbf{R}_n-\mathbf{R}_{n'}$, $\mathbf{r}_{n'}=\mathbf{r}-\mathbf{R}_{n'}$, and $\mathbf{r}_n=\mathbf{r}-\mathbf{R}_n$. The coefficients $G_{lm;l'm'}$ and $\xi_{lm;l'm'}$ in the above expressions are given by

$$G_{lm;l'm'}(\mathbf{R}_{nn'};q)=4\pi\sum_{l''m''}(-1)^{(l-l'-l'')/2}(-1)^{m'+m''}\times B_{lm}(l''m'';l'm')h^+_{l''}(qR_{nn'})\times Y^{-m''}_{l''}(\hat{\boldsymbol{R}}_{nn'}), \tag{B6}$$

and

$$\xi_{lm;l'm'}(\mathbf{R}_{nn'};q)=4\pi\sum_{l''m''}(-1)^{(-l+l'+l'')/2}(-1)^{m'+m''}\times B_{lm}(l''m'';l'm')j_{l''}(qR_{nn'})\times Y^{-m''}_{l''}(\hat{\boldsymbol{R}}_{nn'}) \tag{B7}$$

with

$$B_{lm}(l''m'';l'm')=\int d\hat{\mathbf{r}}Y^m_l(\hat{\mathbf{r}})Y^{-m'}_{l'}(\hat{\mathbf{r}})Y^{m''}_{l''}(\hat{\mathbf{r}}). \tag{B8}$$

Starting from Eqs. (B3), (B4), and (B5) and proceeding as described in Ref. 10, we obtain the following expressions relating the corresponding vector spherical waves referred to an origin at $\mathbf{R}_{n'}$ with those referred to an origin at $\mathbf{R}_n$:

$$\mathbf{H}_{\mathrm{L}'}(\mathbf{r}_{n'})=\sum_{\mathrm{L}}\Omega^{nn'}_{\mathrm{LL}'}\mathbf{J}_{\mathrm{L}}(\mathbf{r}_n),\quad r_n<R_{nn'}, \tag{B9}$$

$$\mathbf{J}_{\mathrm{L}'}(\mathbf{r}_{n'})=\sum_{\mathrm{L}}\Xi^{nn'}_{\mathrm{LL}'}\mathbf{J}_{\mathrm{L}}(\mathbf{r}_n), \tag{B10}$$

$$\mathbf{H}_{\mathrm{L}'}(\mathbf{r}_{n'})=\sum_{\mathrm{L}}\Xi^{nn'}_{\mathrm{LL}'}\mathbf{H}_{\mathrm{L}}(\mathbf{r}_n),\quad r_n>R_{nn'}. \tag{B11}$$

The nonzero matrix elements $\Omega^{nn'}_{\mathrm{LL}'}$ and $\Xi^{nn'}_{\mathrm{LL}'}$, $\mathrm{L}=Plm$, are

$$\begin{aligned}\Omega^{nn'}_{Mlm;Ml'm'}&=\Omega^{nn'}_{Nlm;Nl'm'}\\&=[l(l+1)l'(l'+1)]^{-1/2}\\&\quad\times[2\alpha^{-m}_l\alpha^{-m'}_{l'}G_{l'm'-1;lm-1}(\mathbf{R}_{nn'};q_t)\\&\quad+mm'G_{l'm';lm}(\mathbf{R}_{nn'};q_t)\\&\quad+2\alpha^m_l\alpha^{m'}_{l'}G_{l'm'+1;lm+1}(\mathbf{R}_{nn'};q_t)],\\&\quad l,l'\geqslant 1,\end{aligned} \tag{B12}$$

$$\begin{aligned}\Omega^{nn'}_{Mlm;Nl'm'}&=-\Omega^{nn'}_{Nlm;Ml'm'}\\&=(2l+1)[l(l+1)l'(l'+1)]^{-1/2}\\&\quad\times[-2\alpha^{-m'}_{l'}\gamma^m_lG_{l'm'-1;l-1m-1}(\mathbf{R}_{nn'};q_t)\\&\quad+m'\zeta^m_lG_{l'm';l-1m}(\mathbf{R}_{nn'};q_t)\\&\quad+2\alpha^{m'}_{l'}\gamma^{-m}_lG_{l'm'+1;l-1m+1}(\mathbf{R}_{nn'};q_t)],\\&\quad l,l'\geqslant 1,\end{aligned} \tag{B13}$$

$$\Omega^{nn'}_{Llm;Ll'm'}=G_{l'm';lm}(\mathbf{R}_{nn'};q_l),\quad l,l'\geqslant 0, \tag{B14}$$

and

$$\begin{aligned}\Xi^{nn'}_{Mlm;Ml'm'}&=\Xi^{nn'}_{Nlm;Nl'm'}\\&=[l(l+1)l'(l'+1)]^{-1/2}\\&\quad\times[2\alpha^{-m}_l\alpha^{-m'}_{l'}\xi_{l'm'-1;lm-1}(\mathbf{R}_{nn'};q_t)\\&\quad+mm'\xi_{l'm';lm}(\mathbf{R}_{nn'};q_t)\\&\quad+2\alpha^m_l\alpha^{m'}_{l'}\xi_{l'm'+1;lm+1}(\mathbf{R}_{nn'};q_t)],\\&\quad l,l'\geqslant 1,\end{aligned} \tag{B15}$$

$$\begin{aligned}\Xi^{nn'}_{Mlm;Nl'm'}&=-\Xi^{nn'}_{Nlm;Ml'm'}\\&=(2l+1)[l(l+1)l'(l'+1)]^{-1/2}\\&\quad\times[-2\alpha^{-m'}_{l'}\gamma^m_l\xi_{l'm'-1;l-1m-1}(\mathbf{R}_{nn'};q_t)\\&\quad+m'\zeta^m_l\xi_{l'm';l-1m}(\mathbf{R}_{nn'};q_t)\\&\quad+2\alpha^{m'}_{l'}\gamma^{-m}_l\xi_{l'm'+1;l-1m+1}(\mathbf{R}_{nn'};q_t)],\\&\quad l,l'\geqslant 1,\end{aligned} \tag{B16}$$

$$\Xi^{nn'}_{Llm;Ll'm'}=\xi_{l'm';lm}(\mathbf{R}_{nn'};q_l),\quad l,l'\geqslant 0, \tag{B17}$$

where α^m_l is given by Eq. (40) and

$$\gamma^m_l=\tfrac{1}{2}[(l+m)(l+m-1)]^{1/2}/[(2l-1)(2l+1)]^{1/2},$$

$$\zeta^m_l=[(l+m)(l-m)]^{1/2}/[(2l-1)(2l+1)]^{1/2}. \tag{B18}$$

We note that for $n=n'$, by definition, $\Omega^{nn'}_{\mathrm{LL}'}=0$ and $\Xi^{nn'}_{\mathrm{LL}'}=\delta_{\mathrm{LL}'}$. A useful property of $\Xi^{nn'}_{\mathrm{LL}'}$ resulting from Eq. (B10) is

$$\sum_{\mathrm{L}''} \Xi^{nn''}_{\mathrm{LL}''}\Xi^{n''n'}_{\mathrm{L}''\mathrm{L}'}=\Xi^{nn'}_{\mathrm{LL}'}. \tag{B19}$$

Finally, it can be shown that

$$\Omega^{nn'}_{Plm;P'l'm'}=(-1)^{m+m'}\Omega^{n'n}_{Pl'-m';P'l-m}, \tag{B20}$$

and that $\boldsymbol{\Xi}$ is a Hermitian matrix

$$\Xi^{nn'}_{Plm;P'l'm'}=\Xi^{n'n*}_{P'l'm';Plm}. \tag{B21}$$

It is also worth noting that $\Phi^{nn'}_{\mathrm{LL}'}$ defined by

$$i\Phi^{nn'}_{\mathrm{LL}'}=\Omega^{nn'}_{\mathrm{LL}'}-\Xi^{nn'}_{\mathrm{LL}'}+\delta_{\mathrm{LL}'}\delta_{nn'} \tag{B22}$$

express an (irregular) vector spherical wave $\mathbf{N}_{\mathrm{L}'}(\mathbf{r}_{n'})=-i[\mathbf{H}_{\mathrm{L}'}(\mathbf{r}_{n'})-\mathbf{J}_{\mathrm{L}'}(\mathbf{r}_{n'})]$ about $\mathbf{R}_{n'}$ [this is given by Eqs. (36), (37), and (38) with $q=\omega/c_l$ if $P=L$ and $q=\omega/c_t$ if $P=M,N$, and $f_l=n_l$, the spherical Neumann function] in terms of regular vector spherical waves, $\mathbf{J}_{\mathrm{L}}(\mathbf{r}_n)$, about another site $\mathbf{R}_n$. By definition, $\Phi^{nn'}_{\mathrm{LL}'}=0$ for $n=n'$. It can be shown that $\boldsymbol{\Phi}$ is a Hermitian matrix

$$\Phi^{nn'}_{Plm;P'l'm'}=\Phi^{n'n*}_{P'l'm';Plm}. \tag{B23}$$

APPENDIX C

In order to find an explicit expression for the matrix elements of $\mathbf{T}^{\mathrm{tot}}$, entering in Eq. (79), we write the wave incident on and the wave scattered by the assembly of spheres, at a given frequency ω, as $\sum_{\mathrm{L_I}} a^0_{\mathrm{L_I}}\mathbf{J}_{\mathrm{L_I}}(\mathbf{r})$ and $\sum_{\mathrm{L_O}} a^+_{\mathrm{L_O}}\mathbf{H}_{\mathrm{L_O}}(\mathbf{r})$, respectively. Here $\mathbf{r}$ refers to one given origin of coordinates which we can assume to be at the center of a large sphere containing the entire assembly. We write, as in the first of Eqs. (48),

$$a^+_{\mathrm{L_O}}=\sum_{\mathrm{L_I}} T^{\mathrm{tot}}_{\mathrm{L_OL_I}}a^0_{\mathrm{L_I}}. \tag{C1}$$

An explicit expression for $T^{\mathrm{tot}}_{\mathrm{L_OL_I}}$ is obtained as follows. We write the wave incident on and the wave scattered by the assembly of spheres as sums of spherical waves about the centers of the individual spheres: $\sum_{\mathrm{L_I}} a^0_{\mathrm{L_I}}\mathbf{J}_{\mathrm{L_I}}(\mathbf{r})=\sum_{\mathrm{L}'} b^{0n'}_{\mathrm{L}'}\mathbf{J}_{\mathrm{L}'}(\mathbf{r}_{n'})$ and $\sum_{\mathrm{L_O}} a^+_{\mathrm{L_O}}\mathbf{H}_{\mathrm{L_O}}(\mathbf{r})=\sum_{n\mathrm{L}} b^{+n}_{\mathrm{L}}\mathbf{H}_{\mathrm{L}}(\mathbf{r}_n)$, respectively. Then, using Eqs. (B10) and (B11) of Appendix B, one can write

$$b^{0n'}_{\mathrm{L}'}=\sum_{\mathrm{L_I}} \Xi^{n'0}_{\mathrm{L}'\mathrm{L_I}}a^0_{\mathrm{L_I}} \tag{C2}$$

and

$$a^+_{\mathrm{L_O}}=\sum_{n\mathrm{L}} \Xi^{0n}_{\mathrm{L_OL}}b^{+n}_{\mathrm{L}}. \tag{C3}$$

An incident wave can be scattered out of the assembly after a single scattering by any one sphere, or after scattering any number of times by any number of spheres. Mathematically, this means that

$$\begin{aligned} b^{+n}_{\mathrm{L}}&=\sum_{n'\mathrm{L}'} [\mathbf{T}+\mathbf{T}\boldsymbol{\Omega}\mathbf{T}+\mathbf{T}\boldsymbol{\Omega}\mathbf{T}\boldsymbol{\Omega}\mathbf{T}+\cdots]^{nn'}_{\mathrm{LL}'}b^{0n'}_{\mathrm{L}'}\\ &=\sum_{n'\mathrm{L}'} \{[\mathbf{I}-\mathbf{T}\boldsymbol{\Omega}]^{-1}\mathbf{T}\}^{nn'}_{\mathrm{LL}'}b^{0n'}_{\mathrm{L}'}, \end{aligned} \tag{C4}$$

where $T^{nn'}_{\mathrm{LL}'}=\delta_{nn'}T^n_{\mathrm{LL}'}$ and $\boldsymbol{\Omega}$ is the matrix defined by Eqs. (62) and (63). Using Eqs. (C1)–(C4) we obtain

$$T^{\mathrm{tot}}_{\mathrm{L_OL_I}}=\sum_{n\mathrm{L},n'\mathrm{L}'} \Xi^{0n}_{\mathrm{L_OL}}\{[\mathbf{I}-\mathbf{T}\boldsymbol{\Omega}]^{-1}\mathbf{T}\}^{nn'}_{\mathrm{LL}'}\Xi^{n'0}_{\mathrm{L}'\mathrm{L_I}}. \tag{C5}$$

Substituting Eq. (C5) into Eq. (79), and using the identity

$$\mathrm{Tr}\ln[\mathbf{I}+\mathbf{AB}]=\mathrm{Tr}\ln[\mathbf{I}+\mathbf{BA}], \tag{C6}$$

where $\mathbf{A}$, $\mathbf{B}$ are in general nonsquare matrices of dimensions $N_1\times N_2$, $N_2\times N_1$, respectively, together with Eq. (B19), we obtain

$$\begin{aligned} \Delta N(\omega)&=\frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}\ln\{\mathbf{I}+\mathbf{T}\boldsymbol{\Xi}[\mathbf{I}-\mathbf{T}\boldsymbol{\Omega}]^{-1}\}_{\{n\mathrm{L}\}}\\ &=\frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}\ln[\mathbf{I}+\mathbf{T}]_{\{n\mathrm{L}\}}-\frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}\ln[\mathbf{I}-\mathbf{T}\boldsymbol{\Omega}]_{\{n\mathrm{L}\}}\\ &\quad+\frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}\ln\{[\mathbf{I}+\mathbf{T}]^{-1}[\mathbf{I}-\mathbf{T}(\boldsymbol{\Omega}-\boldsymbol{\Xi})]\}_{\{n\mathrm{L}\}}, \end{aligned} \tag{C7}$$

where $\{n\mathrm{L}\}$ denotes matrices in $n\mathrm{L}$ space. We shall now demonstrate that the last term in Eq. (C7) vanishes. Defining $B^{nn'}_{\mathrm{LL}'}=(c^3_\nu/\omega)\delta_{nn'}\delta_{\mathrm{LL}'}$ we have $[\mathbf{I}+\mathbf{T}]^{-1}[\mathbf{I}-\mathbf{T}(\boldsymbol{\Omega}-\boldsymbol{\Xi})]=\mathbf{I}-\mathbf{B}^{-1}\boldsymbol{\mathcal{K}}\boldsymbol{\Phi}$, where $\boldsymbol{\mathcal{K}}$ is defined by $\mathcal{K}^{nn'}_{\mathrm{LL}'}=\mathcal{K}^{n}_{\mathrm{LL}'}\delta_{nn'}$, with the elements $\mathcal{K}^n_{\mathrm{LL}'}$ of the reaction matrix of the nth sphere given by Eq. (54), and $\boldsymbol{\Phi}$ is given by Eq. (B22). $\boldsymbol{\mathcal{K}}$ and $\boldsymbol{\Phi}$ are Hermitian matrices. Using Eq. (C6) and the fact that $\mathbf{B}^{-1}\boldsymbol{\Phi}=\boldsymbol{\Phi}\mathbf{B}^{-1}$, one can easily show that $\mathrm{Tr}\{\ln[\mathbf{I}-\mathbf{B}^{-1}\boldsymbol{\mathcal{K}}\boldsymbol{\Phi}]\}^\dagger=\mathrm{Tr}\{\ln[\mathbf{I}-\mathbf{B}^{-1}\boldsymbol{\mathcal{K}}\boldsymbol{\Phi}]\}$, from which follows directly that $\mathrm{Im}\,\mathrm{Tr}\{\ln[\mathbf{I}-\mathbf{B}^{-1}\boldsymbol{\mathcal{K}}\boldsymbol{\Phi}]\}=0$. Therefore, Eq. (C7) gives

$$\Delta N(\omega)=\frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}\ln[\mathbf{I}+\mathbf{T}]_{\{n\mathrm{L}\}}-\frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}\ln[\mathbf{I}-\mathbf{T}\boldsymbol{\Omega}]_{\{n\mathrm{L}\}}. \tag{C8}$$

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