Scattering of elastic waves by periodic arrays of spherical bodies

I. E. Psarobas* and N. Stefanou
Section of Solid State Physics, University of Athens, Panepistimioupolis, GR-157 84 Athens, Greece

A. Modinos
Department of Physics, National Technical University of Athens, Zografou Campus, GR-157 73 Athens, Greece
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We develop a formalism for the calculation of the frequency band structure of a phononic crystal consisting of nonoverlapping elastic spheres, characterized by Lamé coefficients which may be complex and frequency dependent, arranged periodically in a host medium with different mass density and Lamé coefficients. We view the crystal as a sequence of planes of spheres, parallel to and having the two-dimensional periodicity of a given crystallographic plane, and obtain the complex band structure of the infinite crystal associated with this plane. The method allows one to calculate, also, the transmission, reflection, and absorption coefficients for an elastic wave (longitudinal or transverse) incident, at any angle, on a slab of the crystal of finite thickness. We demonstrate the efficiency of the method by applying it to a specific example.

I. INTRODUCTION

The elastic properties of a locally homogeneous and isotropic composite material are characterized by a mass density ρ and Lamé coefficients λ and μ which vary in space.[1] The composite materials we shall be concerned with in this paper consist of homogeneous particles (solid or fluid inclusions the dimensions of which must be large enough in order for a macroscopic description of their elastic properties to be valid) distributed periodically in a host medium characterized by different mass density and Lamé coefficients. We assume, throughout this paper, that the particles do not overlap with each other (cermet topology[2]). The alternative case, when the particles connect with each other to form a continuous network is also interesting but will not concern us here. When identical particles are distributed periodically in a host medium, the composite material may be referred to as a phononic crystal. In this case the mass density and the Lamé coefficients vary periodically in space:

$$\rho(\mathbf{r}+\mathbf{R}_n)=\rho(\mathbf{r}), \quad \mu(\mathbf{r}+\mathbf{R}_n)=\mu(\mathbf{r}), \quad \lambda(\mathbf{r}+\mathbf{R}_n)=\lambda(\mathbf{r}), \tag{1.1}$$

where $\{\mathbf{R}_n\}$ denotes a Bravais lattice.

In recent years there has been a growing interest in the study of phononic crystals which is inspired to a large degree by corresponding work in photonic crystals.[3,4] These are composite materials with a dielectric function which varies periodically in space. A typical example: identical particles, large enough to be describable by a macroscopic dielectric function, are arranged periodically in a host material with a different dielectric function. Photonic crystals have many interesting properties both in relation to basic physics and technological applications. In particular, the existence of absolute frequency gaps (photonic gaps) in certain such crystals, i.e., regions of frequency over which electromagnetic (EM) waves can not exist within the crystal, has attracted a lot of attention, mainly because of promising applications in optoelectronics, as pointed out initially by Yablonovich.[5] In principle, one can design a perfect mirror, nonabsorbing over a selected region of frequency (corresponding to a photonic gap), a nonabsorbing resonance cavity, etc.[6] A number of theoretical calculations predict the existence of such gaps for appropriately designed photonic crystals, but so far only crystals which exhibit gaps up to the infrared region have been constructed.[7] However, progress to higher frequencies is expected in the near future. In relation to basic physics, photonic crystals are interesting in a number of ways.[8] For example, they can be the starting point in a process of gradual introduction of disorder and a study of consequent phenomena, including Anderson localization.[9]

Now, phononic crystals have properties which mirror those of photonic crystals and corresponding applications too.[10–19] With an appropriate choice of the parameters involved one may obtain phononic crystals with absolute frequency gaps (phononic gaps) in selected regions of frequency. An elastic wave, whose frequency lies within an absolute gap of a phononic crystal, will be completely reflected by it; from which follows the possibility of constructing nonabsorbing mirrors of elastic waves and vibration-free cavities which might be very useful in high-precision mechanical systems operating in a given frequency range. And in relation to basic physics, one can use elastic waves to study phenomena such as those associated with disorder,[20] in more or less the same manner as with EM waves.

There are, however, some essential differences between EM and elastic waves and this means that the normal modes of the elastic field in a phononic crystal are in some ways quite different from those of the EM field in a photonic crystal. In a homogeneous isotropic medium the elastic waves can, in general, be purely longitudinal [in which case the displacement vector $\mathbf{u}(\mathbf{r})$ satisfies the condition $\nabla\times\mathbf{u}=0$] or purely transverse (in which case $\nabla\cdot\mathbf{u}=0$). In a phononic crystal this is no longer the case and a normal mode usually has a longitudinal and a transverse component. One expects that because of this coupling between longitudinal and transverse waves, it will be more difficult to obtain absolute frequency gaps in a phononic crystal. We recall that the normal modes of the EM field in a photonic crystal are exclusively transverse. On the other hand there are, in general, more parameters relevant to the determination of phononic gaps than there are in the determination of photonic gaps. In the case of a binary system (consisting of material 2 distributed in material 1) we have for photonic crystals two independent parameters: the ratio of the dielectric functions of the two materials ϵ_2/ϵ_1; and the fractional volume occupied by material 2, to be denoted by f. For phononic crystals there are five independent parameters: μ_2/μ_1, λ_2/λ_1, ρ_2/ρ_1, μ_2/λ_1 and f; where ρ_j, λ_j, μ_j denote the mass density, and the Lamé coefficients of material $j=1,2$.

We have, so far, implicitly assumed that the Lamé coefficients describing the constituent materials of the phononic crystals are all different from zero, real quantities, and constant (independent of the frequency). But this is not always the case. The phononic crystal may consist, for example, of solid particles (material 2) arranged periodically (at least approximately) in a liquid (material 1). If the liquid is a normal fluid, like water, $\mu_1=0$ and the transverse sound in the liquid is suppressed. This, however, is not the case for a viscous fluid. The role of shear viscosity in phononic crystals has been pointed out by Sprik and Wegdam.[13] Shear viscosity is equally important in phononic crystals consisting of liquid particles in a solid host background (liquid-containing porous solids[21–24]). Colloidal suspensions of solid spheres in a liquid, also, have interesting acoustic properties.[25] Finally, it may be of some interest to consider composite materials consisting of two liquids (e.g., drops of oil in water) although in this case a periodic arrangement of the drops can only be a rough approximation to the real system. It appears that acoustic gaps are easily obtained in three-dimensional (3D) fluid-fluid composites, when $\mu_1=\mu_2=0$.[11]

The few calculations published so far relating to 3D phononic crystals deal, almost exclusively, with the frequency band structure of these crystals, which is obtained via a plane-wave expansion of the displacement field.[10–13] On the other hand, a lot of theoretical and experimental work has been done on systems with two-dimensional (2D) periodicity, with translational invariance along the third dimension. A typical example of such systems consists of a set of long identical cylinders parallel to the z direction, crossing the xy plane at the sites of a 2D lattice. By considering waves propagating normal to the cylinders, the problem is reduced to two dimensions.[14–19] The above investigations have shown that phononic gaps are possible in both 2D and 3D systems.

Although knowing the frequency band structure of a phononic crystal is very useful, more is required for a full interpretation and analysis of the experimental data. In an experiment one usually measures the reflection and/or transmission coefficients of an acoustic/elastic wave incident on a slab of the phononic crystal, and consequently theory should be able to provide reliable estimates of these, the experimentally measured quantities, as well. The so-called on-shell methods developed in relation to photonic crystals can do exactly that, besides an accurate evaluation of the frequency band structure.[26–28] In these methods one determines for a given frequency ω and a given reduced wave vector, $\mathbf{k}_\parallel$, parallel to a given crystallographic plane of the crystal, the Bloch-wave solutions of the elastic field of the infinite crystal; these consist of propagating and evanescent waves. The propagating waves constitute the normal modes of the infinite phononic crystal. The evanescent waves do not represent real waves, they are mathematical entities which enter directly or indirectly (depending on the method of calculation) into the evaluation of the reflection and transmission coefficients of a wave, with given ω and $\mathbf{k}_\parallel$, incident on a slab of the crystal parallel to the given crystallographic plane. On-shell methods have certain advantages over the plane-wave method, even if one is only interested in the frequency band structure and the corresponding normal modes of vibration of the infinite phononic crystal. In an on-shell method one can easily allow the Lamé coefficients of any of the constituent materials of the crystal to depend on the frequency, as is necessary in some cases, without any difficulty, which is not the case with the plane-wave method. And, as a rule, on-shell methods are computationally more efficient.[26,29]

The on-shell method we describe in the present paper is analogous to that which some of us have developed for photonic crystals.[27] It applies to systems which consist of nonoverlapping spherical particles arranged periodically in a host medium characterized by different mass density and Lamé coefficients. Sections II to VI are devoted to the development of the formalism.[30] In Sec. VII we demonstrate the applicability of the method on a specific system: an fcc crystal of silica spheres in ice. Finally the last section concludes this article.

II. MULTIPOLE EXPANSION OF THE ELASTIC FIELD

The displacement vector $\mathbf{U}(\mathbf{r},t)$, in a homogeneous elastic medium of mass density ρ and Lamé coefficients λ, μ, satisfies the equation[1]

$$(\lambda+2\mu)\nabla(\nabla\cdot\mathbf{U})-\mu\nabla\times(\nabla\times\mathbf{U})-\rho\partial_t^2\mathbf{U}=0. \quad (2.1)$$

In the case of a harmonic elastic wave of angular frequency ω, we have

$$\mathbf{U}(\mathbf{r},t)=\mathrm{Re}[\mathbf{u}(\mathbf{r})\exp(-i\,\omega t)], \quad (2.2)$$

and Eq. (2.1) reduces to the following time-independent form:

$$(\lambda+2\mu)\nabla(\nabla\cdot\mathbf{u})-\mu\nabla\times(\nabla\times\mathbf{u})+\rho\omega^2\mathbf{u}=0. \quad (2.3)$$

We note that for ordinary elastic media the Lamé coefficients are real numbers. Media where loss is possible, assuming the time dependence given in Eq. (2.2), are described by complex Lamé coefficients:[31]

$$\lambda=\lambda_e-i\omega\lambda_v, \quad \mu=\mu_e-i\omega\mu_v. \quad (2.4)$$

The most general solution of Eq. (2.3) consists of two elastic waves which propagate independently. These are: a longitudinal (irrotational) wave, which satisfies the equations

$$\nabla^2\mathbf{u}+q_l^2\mathbf{u}=0, \quad \nabla\times\mathbf{u}=0, \quad (2.5)$$

where $q_l=\omega/c_l$, $c_l=\sqrt{(\lambda+2\mu)/\rho}$ being the speed of propagation of this wave; and a transverse (divergenceless) wave, which satisfies the equations

$$\nabla^2\mathbf{u}+q_t^2\mathbf{u}=0, \quad \nabla\cdot\mathbf{u}=0, \quad (2.6)$$

where $q_t = \omega / c_t$, $c_t = \sqrt{\mu/\rho}$ being the speed of propagation of this wave.

In the present paper we shall use, besides the more familiar solutions of Eqs. (2.5) and (2.6) representing longitudinal and transverse plane elastic waves [see Eq. (3.1) below], the so-called spherical-wave solutions of these equations. A complete set of spherical-wave solutions of Eq. (2.5), known as irrotational vector wave functions, is given by[32]

$$\mathbf{u}_{lm}^{L}(\mathbf{r}) = \frac{1}{q_l} \nabla [f_l(q_l r) Y_l^m(\hat{\mathbf{r}})], \tag{2.7a}$$

where f_l may be any linear combination of the spherical Bessel function, j_l, and the spherical Hankel function, h_l^+. $Y_l^m(\hat{\mathbf{r}})$ are the usual spherical harmonics, with $\hat{\mathbf{r}}$ denoting the angular variables (θ, ϕ) of $\mathbf{r}$ in a system of spherical coordinates.

A complete set of spherical-wave solutions of Eq. (2.6) is given by[32]

$$\mathbf{u}_{lm}^{M}(\mathbf{r}) = f_l(q_t r) \mathbf{X}_{lm}(\hat{\mathbf{r}}) \tag{2.7b}$$

and

$$\mathbf{u}_{lm}^{N}(\mathbf{r}) = \frac{i}{q_t} \nabla \times f_l(q_t r) \mathbf{X}_{lm}(\hat{\mathbf{r}}), \tag{2.7c}$$

which are also known as solenoidal vector wave functions. The vector spherical harmonics, denoted by $\mathbf{X}_{lm}(\hat{\mathbf{r}})$, are defined by

$$\sqrt{l(l+1)}\mathbf{X}_{lm}(\hat{\mathbf{r}}) = \mathbf{L} Y_l^m(\hat{\mathbf{r}}) \equiv -i \mathbf{r} \times \nabla Y_l^m(\hat{\mathbf{r}}). \tag{2.8a}$$

By definition $\mathbf{X}_{00}(\hat{\mathbf{r}}) = 0$; for $l \geqslant 1$ we have

$$\begin{aligned}\sqrt{l(l+1)}\mathbf{X}_{lm}(\hat{\mathbf{r}}) = {} & [\alpha_l^{-m} \cos\theta e^{i\phi} Y_l^{m-1}(\hat{\mathbf{r}}) - m \sin\theta Y_l^m(\hat{\mathbf{r}}) \\ & + \alpha_l^m \cos\theta e^{-i\phi} Y_l^{m+1}(\hat{\mathbf{r}})]\hat{\mathbf{e}}_\theta \\ & + i[\alpha_l^{-m} e^{i\phi} Y_l^{m-1}(\hat{\mathbf{r}}) \\ & - \alpha_l^m e^{-i\phi} Y_l^{m+1}(\hat{\mathbf{r}})]\hat{\mathbf{e}}_\phi,\end{aligned} \tag{2.8b}$$

where

$$\alpha_l^m = \frac{1}{2}[(l-m)(l+m+1)]^{1/2}, \tag{2.8c}$$

and $\hat{\mathbf{e}}_\theta$, $\hat{\mathbf{e}}_\phi$, are the usual polar and azimuthal unit vectors, respectively, in the chosen system of spherical coordinates.

The most general displacement field can be written as a linear sum of the spherical waves given by Eqs. (2.7a)–(2.7c), as follows:

$$\begin{aligned}\mathbf{u}(\mathbf{r}) = \sum_{lm} \Big\{ & a_{lm}^M f_l(q_t r) \mathbf{X}_{lm}(\hat{\mathbf{r}}) + a_{lm}^N \frac{i}{q_t} \nabla \times f_l(q_t r) \mathbf{X}_{lm}(\hat{\mathbf{r}}) \\ & + a_{lm}^L \frac{1}{q_l} \nabla [f_l(q_l r) Y_l^m(\hat{\mathbf{r}})] \Big\},\end{aligned} \tag{2.9}$$

where a_{lm}^P, $P = M, N, L$, are coefficients to be determined.

III. SCATTERING OF A PLANE WAVE BY A SPHERE

A plane elastic wave, of wave vector $\mathbf{q}$, propagating in a homogeneous elastic medium has the form

$$\mathbf{u}_{\text{in}}(\mathbf{r}) = \mathbf{u}_0(\mathbf{q}) \exp(i \mathbf{q} \cdot \mathbf{r}), \tag{3.1}$$

with $\mathbf{u}_0(\mathbf{q}) = u_0(\mathbf{q}) \hat{\mathbf{e}}$, where u_0 denotes the magnitude and $\hat{\mathbf{e}}$, a unit vector, the polarization of the displacement field. In the case of a longitudinal plane wave we can write $\mathbf{q} = q_l \hat{\mathbf{e}}_q$ and $\hat{\mathbf{e}} = \hat{\mathbf{e}}_q$. Since the plane wave is finite everywhere, its multipole expansion into spherical waves, according to Eq. (2.7a), involves only the radial functions $j_l(q_l r)$; we have

$$\mathbf{u}_{\text{in}}(\mathbf{r}) = \sum_{lm} a_{lm}^{0L} \frac{1}{q_l} \nabla [j_l(q_l r) Y_l^m(\hat{\mathbf{r}})]. \tag{3.2}$$

One can easily show that the coefficients a_{lm}^{0L} are given by

$$a_{lm}^{0L} = \mathbf{A}_{lm}^{0L}(\hat{\mathbf{q}}) \cdot \mathbf{u}_0(\mathbf{q}), \tag{3.3}$$

where

$$\mathbf{A}_{lm}^{0L}(\hat{\mathbf{q}}) = 4\pi i^{l+1} (-1)^{m+1} Y_l^{-m}(\hat{\mathbf{q}}) \hat{\mathbf{e}}_q. \tag{3.4}$$

In the case of a transverse plane wave we have $\mathbf{q} = q_t \hat{\mathbf{e}}_q$ and $\hat{\mathbf{e}} \perp \hat{\mathbf{e}}_q$. Such a wave can be written as a linear sum of the spherical waves given by Eqs. (2.7b) and (2.7c), and again involves only the radial functions $j_l(q_t r)$; we have

$$\mathbf{u}_{\text{in}}(\mathbf{r}) = \sum_{lm} \left\{ a_{lm}^{0M} j_l(q_t r) \mathbf{X}_{lm}(\hat{\mathbf{r}}) + a_{lm}^{0N} \frac{i}{q_t} \nabla \times j_l(q_t r) \mathbf{X}_{lm}(\hat{\mathbf{r}}) \right\}. \tag{3.5}$$

The coefficients a_{lm}^{0P}, with $P = M, N$, can be written as

$$a_{lm}^{0P} = \mathbf{A}_{lm}^{0P}(\hat{\mathbf{q}}) \cdot \mathbf{u}_0(\mathbf{q}), \tag{3.6}$$

where

$$\begin{aligned}\mathbf{A}_{lm}^{0M}(\hat{\mathbf{q}}) = \frac{4\pi i^l (-1)^{m+1}}{\sqrt{l(l+1)}} \{ & [\alpha_l^m \cos\theta e^{i\phi} Y_l^{-m-1}(\hat{\mathbf{q}}) + m \sin\theta Y_l^{-m}(\hat{\mathbf{q}}) + \alpha_l^{-m} \cos\theta e^{-i\phi} Y_l^{-m+1}(\hat{\mathbf{q}})]\hat{\mathbf{e}}_\theta \\ & + i[\alpha_l^m e^{i\phi} Y_l^{-m-1}(\hat{\mathbf{q}}) - \alpha_l^{-m} e^{-i\phi} Y_l^{-m+1}(\hat{\mathbf{q}})]\hat{\mathbf{e}}_\phi \},\end{aligned} \tag{3.7}$$

and

$$\mathbf{A}_{lm}^{0N}(\hat{\mathbf{q}})=\frac{4\pi i^{l}(-1)^{m+1}}{\sqrt{l(l+1)}}\{i[\alpha_l^m e^{i\phi}Y_l^{-m-1}(\hat{\mathbf{q}})-\alpha_l^{-m}e^{-i\phi}Y_l^{-m+1}(\hat{\mathbf{q}})]\hat{\mathbf{e}}_\theta-[\alpha_l^m\cos\theta e^{i\phi}Y_l^{-m-1}(\hat{\mathbf{q}})$$
$$+m\sin\theta Y_l^{-m}(\hat{\mathbf{q}})+\alpha_l^{-m}\cos\theta e^{-i\phi}Y_l^{-m+1}(\hat{\mathbf{q}})]\hat{\mathbf{e}}_\phi\}, \tag{3.8}$$

where θ and ϕ denote the angular variables of $\mathbf{q}$ in the chosen system of spherical coordinates.

We now consider a sphere of radius S, centered at the origin of coordinates. We assume that the sphere, which has a uniform mass density ρ_s, is embedded in a homogeneous medium of mass density ρ; the wave numbers of the elastic waves in the sphere ($q_{s\nu}$) and in the host medium (q_ν), where $\nu=l$ or t, are also different. When a plane wave is incident on the sphere, it is scattered by it, so that the wave field outside the sphere consists of the incident wave and a scattered wave. Since the scattered wave is outgoing at infinity, its expansion in spherical waves is given by Eq. (2.9) with $f_l=h_l^+$, which has the asymptotic form appropriate to an outgoing spherical wave: $h_l^+(qr)\approx(-i)^l\exp(iqr)/iqr$ as $r\to\infty$. We have

$$\mathbf{u}_{\mathrm{sc}}(\mathbf{r})=\sum_{lm}\left\{a_{lm}^{+M}h_l^+(q_tr)\mathbf{X}_{lm}(\hat{\mathbf{r}})+a_{lm}^{+N}\frac{i}{q_t}\nabla\times h_l^+(q_tr)\mathbf{X}_{lm}(\hat{\mathbf{r}})+a_{lm}^{+L}\frac{1}{q_l}\nabla[h_l^+(q_lr)Y_l^m(\hat{\mathbf{r}})]\right\}. \tag{3.9}$$

The wave field inside the sphere is given by Eq. (2.9) with $f_l=j_l$, since it must be finite at the origin; we have

$$\mathbf{u}_I(\mathbf{r})=\sum_{lm}\left\{a_{lm}^{IM}j_l(q_{st}r)\mathbf{X}_{lm}(\hat{\mathbf{r}})+a_{lm}^{IN}\frac{i}{q_{st}}\nabla\times j_l(q_{st}r)\mathbf{X}_{lm}(\hat{\mathbf{r}})+a_{lm}^{IL}\frac{1}{q_{sl}}\nabla[j_l(q_{sl}r)Y_l^m(\hat{\mathbf{r}})]\right\}. \tag{3.10}$$

The coefficients a_{lm}^{+P}, a_{lm}^{IP}, $P=M,N,L$, in Eqs. (3.9) and (3.10) are determined by the requirement of continuity of the displacement vector, $\mathbf{u}(\mathbf{r})$, and of the surface traction, $\tau(\mathbf{r})\equiv\overline{\sigma}(\mathbf{r})\cdot\hat{\mathbf{r}}$, at the surface of the sphere; $\overline{\sigma}(\mathbf{r})$ denotes the stress tensor. The components of the surface traction are given by (see, e.g., Ref. 1)

$$\tau_r=\lambda\nabla\cdot\mathbf{u}+2\mu\partial_r u_r, \tag{3.11a}$$

$$\tau_\theta=\mu\left[\frac{1}{r}\partial_\theta u_r+\partial_r u_\theta-\frac{u_\theta}{r}\right], \tag{3.11b}$$

$$\tau_\phi=\mu\left[\frac{1}{r\sin\theta}\partial_\phi u_r+\partial_r u_\phi-\frac{u_\phi}{r}\right]. \tag{3.11c}$$

The continuity of u_r, u_θ, u_ϕ, τ_r, τ_θ, τ_ϕ at the surface of the sphere allows us to determine uniquely the coefficients a_{lm}^{+P} $(P=M,N,L)$ of the scattered wave, given by Eq. (3.9), and the coefficients a_{lm}^{IP} of the wave inside the sphere, given by Eq. (3.10), in terms of the known coefficients a_{lm}^{0P} of the incident wave, given by Eqs. (3.2) or (3.5). After some lengthy but straightforward algebra one obtains (see, e.g., Ref. 31)

$$a_{lm}^{+P}=\sum_{P'l'm'}T_{lm;l'm'}^{PP'}a_{l'm'}^{0P'}. \tag{3.12}$$

Explicit expressions for the nonzero elements of the $\mathbf{T}$ matrix in the case of a solid scatterer in a solid host are given in Appendix A. Similar expressions for the cases involving a liquid scatterer or host can be found in Ref. 31.

IV. SCATTERING BY A PLANE OF SPHERES

We consider a plane of spheres at $z=0$: an array of spheres centered on the sites of a 2D lattice specified by

$$\mathbf{R}_n=n_1\mathbf{a}_1+n_2\mathbf{a}_2, \tag{4.1}$$

where $\mathbf{a}_1$ and $\mathbf{a}_2$ are primitive vectors in the xy plane and $n_1,n_2=0,\pm1,\pm2,\pm3,\ldots$.

The corresponding 2D reciprocal lattice is obtained in the usual manner[33,34] as follows:

$$\mathbf{g}=m_1\mathbf{b}_1+m_2\mathbf{b}_2, \tag{4.2}$$

where $m_1,m_2=0,\pm1,\pm2,\pm3,\ldots$ and $\mathbf{b}_1,\mathbf{b}_2$ are defined by

$$\mathbf{b}_i\cdot\mathbf{a}_j=2\pi\delta_{ij}. \tag{4.3}$$

We now assume that a plane wave (it can be longitudinal or transverse) is incident on the plane of spheres. We write the displacement vector $\mathbf{u}_{\mathrm{in}}(\mathbf{r})$ corresponding to it as follows:

$$\mathbf{u}_{\mathrm{in}}^{s'}(\mathbf{r})=\sum_{i'}[u_{\mathrm{in}}]_{\mathbf{g}'i'}^{s'}\exp(i\mathbf{K}_{\mathbf{g}'\nu'}^{s'}\cdot\mathbf{r})\hat{\mathbf{e}}_{i'}, \tag{4.4}$$

where $s'=+(-)$ corresponds to a wave incident on the plane of spheres from the left (right); ν' specifies the polarization of the incident wave: $q_{\nu'}=q_l=\omega/c_l$ for a longitudinal wave and $q_{\nu'}=q_t=\omega/c_t$ for a transverse wave;

$$\mathbf{K}_{\mathbf{g}'\nu'}^{\pm}\equiv\mathbf{k}_\parallel+\mathbf{g}'\pm[q_{\nu'}^2-(\mathbf{k}_\parallel+\mathbf{g}')^2]^{1/2}\hat{\mathbf{e}}_z, \tag{4.5}$$

where $\hat{\mathbf{e}}_z$ is the unit vector along the z axis, and we have written the component of the incident wave vector parallel to the plane of spheres as the sum of a reduced wave vector $\mathbf{k}_\parallel$, which lies in the surface Brillouin zone (SBZ) of the given lattice, and an appropriate reciprocal-lattice vector $\mathbf{g}'$. This is always possible and it facilitates the subsequent calculation. For $\nu'=l$, $i'=1$ denotes the only nonzero component of the displacement vector, $\hat{\mathbf{e}}_1$ being the radial unit vector along the direction of $\mathbf{K}_{\mathbf{g}'l}^{s'}$. For $\nu'=t$, $i'=2,3$ denote the only nonzero components of the displacement vector; $\hat{\mathbf{e}}_2,\hat{\mathbf{e}}_3$ being the polar and azimuthal unit vectors, respectively, which are perpendicular to $\mathbf{K}_{\mathbf{g}'t}^{s'}$. In the same manner [as in Eq. (4.5)] we define, for given $\mathbf{k}_\parallel$, ω, a wave vector $\mathbf{K}_{\mathbf{g}\nu}^{s}$ and the corresponding $\hat{\mathbf{e}}_i$ for any $\mathbf{g}$ and any ν. We remember that the $i=1$ component of the displacement vector is always associated with a longitudinal plane wave ($\nu=l$), and that the $i=2,3$ components of the displacement vector are always associated with a transverse plane wave ($\nu=t$), so that the character (longitudinal or transverse) of a given plane wave is automatically determined by the non-vanishing components of the displacement vector associated with it, and need not be stated explicitly in every case. When $(\mathbf{k}_\parallel+\mathbf{g})^2>q_\nu^2$ the corresponding wave decays to the right for $s=+$, and to the left for $s=-$; and the corresponding unit vectors $\hat{\mathbf{e}}_i$ become complex. Indeed, the unit vectors $\hat{\mathbf{e}}_i$ are defined in a Cartesian system of coordinates as follows:

$$\hat{\mathbf{e}}_1=\hat{\mathbf{e}}_x\sin\theta\cos\phi+\hat{\mathbf{e}}_y\sin\theta\sin\phi+\hat{\mathbf{e}}_z\cos\theta, \tag{4.6a}$$

where θ and ϕ denote the angular variables of $\mathbf{K}^s_{\mathbf{g}l}$, and

$$\hat{\mathbf{e}}_2=\hat{\mathbf{e}}_x\cos\theta\cos\phi+\hat{\mathbf{e}}_y\cos\theta\sin\phi-\hat{\mathbf{e}}_z\sin\theta, \tag{4.6b}$$

$$\hat{\mathbf{e}}_3=-\hat{\mathbf{e}}_x\sin\phi+\hat{\mathbf{e}}_y\cos\phi, \tag{4.6c}$$

where θ and ϕ here denote the angular variables of $\mathbf{K}^s_{\mathbf{g}t}$. We note that the z component of $\mathbf{K}^s_{\mathbf{g}\nu}$ (denoted by $K^s_{\mathbf{g}\nu z}$) is real if $(\mathbf{k}_\parallel+\mathbf{g})^2<q_\nu^2$ and imaginary if $(\mathbf{k}_\parallel+\mathbf{g})^2>q_\nu^2$. In the latter case, $\cos\theta_{\mathbf{K}^s_{\mathbf{g}\nu}}$ in Eqs. (4.6a) and (4.6b) is replaced by $K^s_{\mathbf{g}\nu z}/q_\nu$ and $\sin\theta_{\mathbf{K}^s_{\mathbf{g}\nu}}$ by $|\mathbf{k}_\parallel+\mathbf{g}|/q_\nu$, so that $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$ become complex.

Because of the 2D periodicity of the structure under consideration, the wave scattered from it, when the wave given by Eq. (4.4) is incident upon it, has the form

$$\begin{aligned}\mathbf{u}_{\mathrm{sc}}(\mathbf{r})=\sum_{lm}\Big\{&b^{+M}_{lm}\sum_{\mathbf{R}_n}\exp(i\mathbf{k}_\parallel\cdot\mathbf{R}_n)h_l^+(q_tr_n)\mathbf{X}_{lm}(\hat{\mathbf{r}}_n)\\&+b^{+N}_{lm}\frac{i}{q_t}\nabla\times\sum_{\mathbf{R}_n}\exp(i\mathbf{k}_\parallel\cdot\mathbf{R}_n)h_l^+(q_tr_n)\mathbf{X}_{lm}(\hat{\mathbf{r}}_n)\\&+b^{+L}_{lm}\frac{1}{q_l}\nabla\sum_{\mathbf{R}_n}\exp(i\mathbf{k}_\parallel\cdot\mathbf{R}_n)h_l^+(q_lr_n)Y_l^m(\hat{\mathbf{r}}_n)\Big\},\end{aligned} \tag{4.7}$$

where $\mathbf{r}_n=\mathbf{r}-\mathbf{R}_n$. We note that $\exp[i(\mathbf{k}_\parallel+\mathbf{g})\cdot\mathbf{R}_n]=\exp(i\mathbf{k}_\parallel\cdot\mathbf{R}_n)$ because of Eq. (4.3). Equation (4.7) tells us that the scattered wave is a sum of outgoing spherical waves centered on the spheres of the plane, and that the wave scattered from the sphere at $\mathbf{R}_n$ differs from that scattered from the sphere at the origin ($\mathbf{R}_n=\mathbf{0}$) only by the phase factor $\exp(i\mathbf{k}_\parallel\cdot\mathbf{R}_n)$. We note the presence in the scattered wavefield of both longitudinal and transverse waves even when the incident wave is purely longitudinal or purely transverse.

The coefficients b^{+P}_{lm} which determine the scattered wave from the sphere at the origin are determined from the *total* incident wave on that sphere, which consists of the incident plane wave and the sum of the waves scattered from all the other spheres in the plane. The latter, denoted by $\mathbf{u}'_{\mathrm{sc}}(\mathbf{r})$, is obtained from $\mathbf{u}_{\mathrm{sc}}(\mathbf{r})$ by the removal of the term corresponding to $\mathbf{R}_n=\mathbf{0}$ in Eq. (4.7). $\mathbf{u}'_{\mathrm{sc}}(\mathbf{r})$ can be expanded into spherical waves about the origin as follows:

$$\begin{aligned}\mathbf{u}'_{\mathrm{sc}}(\mathbf{r})=\sum_{lm}\Big\{&b'^{M}_{lm}j_l(q_tr)\mathbf{X}_{lm}(\hat{\mathbf{r}})+b'^{N}_{lm}\frac{i}{q_t}\nabla\times j_l(q_tr)\mathbf{X}_{lm}(\hat{\mathbf{r}})\\&+b'^{L}_{lm}\frac{1}{q_l}\nabla[j_l(q_lr)Y_l^m(\hat{\mathbf{r}})]\Big\}.\end{aligned} \tag{4.8}$$

It can be shown (see Appendix B) that

$$b'^{P}_{lm}=\sum_{P'l'm'}\Omega^{PP'}_{lm;l'm'}b^{+P'}_{l'm'}. \tag{4.9}$$

It is worth noting that the matrix elements of $\boldsymbol{\Omega}$ depend on the geometry (4.1) of the plane and, through q_ν, on the frequency, the mass density and the Lamé coefficients of the medium surrounding the spheres of the plane; they depend also on the reduced wave vector $\mathbf{k}_\parallel$ of the incident wave; but they do not depend on the scattering properties of the individual sphere.

The coefficients b^{+P}_{lm}, which describe the scattered wave from the sphere at the origin of the coordinates, are given by

$$b^{+P}_{lm}=\sum_{P'l'm'}T^{PP'}_{lm;l'm'}(a^{0P'}_{l'm'}+b'^{P'}_{l'm'}). \tag{4.10}$$

The coefficients on the right-hand side of Eq. (4.10) describe the total wave incident on the sphere at the origin of coordinates; a^{0P}_{lm} derive from the incident plane wave given by Eq. (4.4) via Eqs. (3.3) and (3.6), and b'^{P}_{lm} from the field defined by Eq. (4.8). Combining Eqs. (4.9) and (4.10), we obtain

$$\begin{aligned}&\sum_{P'l'm'}\Big[\delta_{PP'}\delta_{ll'}\delta_{mm'}-\sum_{P''l''m''}T^{PP''}_{lm;l''m''}\Omega^{P''P'}_{l''m'';l'm'}\Big]b^{+P'}_{l'm'}\\&\quad=\sum_{P'l'm'}T^{PP'}_{lm;l'm'}a^{0P'}_{l'm'}.\end{aligned} \tag{4.11}$$

Equation (4.11) determines the coefficients b^{+P}_{lm} of the wave scattered from the plane of spheres, given by Eq. (4.7), in terms of the coefficients a^{0P}_{lm} of the incident wave. According to Eqs. (3.3) and (3.6), we write the coefficients a^{0P}_{lm} of the incident plane wave, defined by Eq. (4.4), in the form

$$a^{0P}_{lm}=\sum_{i'}A^{0P}_{lm;i'}(\hat{\mathbf{K}}^{s'}_{\mathbf{g}'\nu'})[u_{\mathrm{in}}]^{s'}_{\mathbf{g}'i'}, \tag{4.12}$$

where $\mathbf{A}^{0P}_{lm}$ are given by Eqs. (3.4), (3.7), and (3.8). Due to the linearity of Eqs. (4.11), the coefficients b^{+P}_{lm} can be written as follows:

$$b^{+P}_{lm}=\sum_{i'}B^{+P}_{lm;i'}(\mathbf{K}^{s'}_{\mathbf{g}'\nu'})[u_{\mathrm{in}}]^{s'}_{\mathbf{g}'i'}, \tag{4.13}$$

so that the system of Eqs. (4.11) reduces to

$$\sum_{P'l'm'}\left[\delta_{PP'}\delta_{ll'}\delta_{mm'}-\sum_{P''l''m''}T^{PP''}_{lm;l''m''}\Omega^{P''P'}_{l''m'';l'm'}\right]\times B^{+P'}_{l'm';i'}(\mathbf{K}^{s'}_{\mathbf{g}'\nu'})=\sum_{P'l'm'}T^{PP'}_{lm;l'm'}A^{0P'}_{l'm';i'}(\hat{\mathbf{K}}^{s'}_{\mathbf{g}'\nu'}). \tag{4.14}$$

We remember that i', s', and $\mathbf{g}'$ are parameter values characterizing the incident wave (we remember also that ν' is determined by i': $\nu'=l$ for $i'=1$ and $\nu'=t$ for $i'=2,3$). Equations (4.14) [or, equivalently, Eqs. (4.11)] constitute a system of infinitely many linear equations. It is solved by introducing an angular momentum cutoff, $l_{\max}$, truncating all angular momentum expansions to $l_{\max}$, thus reducing the dimension of the system to $3l_{\max}^2+6l_{\max}+1$. Moreover, by using the properties of the matrix elements $\Omega^{PP'}_{lm;l'm'}$ given by Eqs. (B11) of Appendix B, this system can be reduced to two independent systems of $(3l_{\max}^2+5l_{\max})/2$ and $(3l_{\max}^2+7l_{\max}+2)/2$ linear equations, respectively.

Finally, the scattered wave given by Eq. (4.7) can be expressed as a sum of plane waves using the following identity:

$$\sum_{\mathbf{R}_n}\exp(i\mathbf{k}_{\|}\cdot\mathbf{R}_n)h_l^+(q_\nu r_n)Y_l^m(\hat{\mathbf{r}}_n)=\sum_{\mathbf{g}}\frac{2\pi(-i)^l}{q_\nu A_0 K^+_{\mathbf{g}\nu z}}Y_l^m(\hat{\mathbf{K}}^\pm_{\mathbf{g}\nu})\exp(i\mathbf{K}^\pm_{\mathbf{g}\nu}\cdot\mathbf{r}), \tag{4.15}$$

where A_0 denotes the area of the unit cell of the lattice given by Eq. (4.1). The plus (minus) sign on $\mathbf{K}_{\mathbf{g}\nu}$ must be used for $z>0$ $(z<0)$. We note that $K^\pm_{\mathbf{g}\nu z}$ can be real or imaginary. In the latter case $\cos\theta_{\mathbf{K}^\pm_{\mathbf{g}\nu}}$ in the standard formulas for $Y_l^m(\hat{\mathbf{K}}^\pm_{\mathbf{g}\nu})$ is replaced by $K^\pm_{\mathbf{g}\nu z}/q_\nu$ [see text following Eq. (4.6c)].

Using Eq. (4.15) we can expand the scattered wave into a series of longitudinal and transverse plane waves, as follows:

$$\mathbf{u}^s_{\rm sc}(\mathbf{r})=\sum_{\mathbf{g}}\sum_{Plm}b^{+P}_{lm}\mathbf{\Delta}^P_{lm}(\mathbf{K}^s_{\mathbf{g}\nu})\exp(i\mathbf{K}^s_{\mathbf{g}\nu}\cdot\mathbf{r}), \tag{4.16}$$

where

$$\mathbf{\Delta}^L_{lm}(\mathbf{K}^s_{\mathbf{g}l})=\frac{2\pi(-i)^{l-1}}{q_l A_0 K^+_{\mathbf{g}lz}}Y_l^m(\hat{\mathbf{K}}^s_{\mathbf{g}l})\hat{\mathbf{e}}_1, \tag{4.17a}$$

$$\mathbf{\Delta}^M_{lm}(\mathbf{K}^s_{\mathbf{g}t})=\frac{2\pi(-i)^l}{q_t A_0 K^+_{\mathbf{g}tz}\sqrt{l(l+1)}}\{[\alpha_l^{-m}\cos\theta e^{i\phi}Y_l^{m-1}(\hat{\mathbf{K}}^s_{\mathbf{g}t})-m\sin\theta Y_l^m(\hat{\mathbf{K}}^s_{\mathbf{g}t})+\alpha_l^m\cos\theta e^{-i\phi}Y_l^{m+1}(\hat{\mathbf{K}}^s_{\mathbf{g}t})]\hat{\mathbf{e}}_2 + i[\alpha_l^{-m}e^{i\phi}Y_l^{m-1}(\hat{\mathbf{K}}^s_{\mathbf{g}t})-\alpha_l^m e^{-i\phi}Y_l^{m+1}(\hat{\mathbf{K}}^s_{\mathbf{g}t})]\hat{\mathbf{e}}_3\}, \tag{4.17b}$$

$$\mathbf{\Delta}^N_{lm}(\mathbf{K}^s_{\mathbf{g}t})=\frac{2\pi(-i)^l}{q_t A_0 K^+_{\mathbf{g}tz}\sqrt{l(l+1)}}\{i[\alpha_l^{-m}e^{i\phi}Y_l^{m-1}(\hat{\mathbf{K}}^s_{\mathbf{g}t})-\alpha_l^m e^{-i\phi}Y_l^{m+1}(\hat{\mathbf{K}}^s_{\mathbf{g}t})]\hat{\mathbf{e}}_2-[\alpha_l^{-m}\cos\theta e^{i\phi}Y_l^{m-1}(\hat{\mathbf{K}}^s_{\mathbf{g}t})-m\sin\theta Y_l^m(\hat{\mathbf{K}}^s_{\mathbf{g}t}) + \alpha_l^m\cos\theta e^{-i\phi}Y_l^{m+1}(\hat{\mathbf{K}}^s_{\mathbf{g}t})]\hat{\mathbf{e}}_3\}, \tag{4.17c}$$

with θ and ϕ denoting the angular variables of $\mathbf{K}^s_{\mathbf{g}t}$. Substituting b^{+P}_{lm} from Eq. (4.13) into Eq. (4.16) we obtain

$$\mathbf{u}^s_{\rm sc}(\mathbf{r})=\sum_{\mathbf{g}i}[u_{\rm sc}]^s_{\mathbf{g}i}\exp(i\mathbf{K}^s_{\mathbf{g}\nu}\cdot\mathbf{r})\hat{\mathbf{e}}_i, \tag{4.18}$$

with

$$[u_{\rm sc}]^s_{\mathbf{g}i}=\sum_{i'}\sum_{Plm}\Delta^P_{lm;i}(\mathbf{K}^s_{\mathbf{g}\nu})B^{+P}_{lm;i'}(\mathbf{K}^{s'}_{\mathbf{g}'\nu'})[u_{\rm in}]^{s'}_{\mathbf{g}'i'}, \tag{4.19}$$

where the superscript $s=+(-)$ holds for $z>0$ $(z<0)$. We note that the $\mathbf{K}^s_{\mathbf{g}\nu}$ in Eq. (4.18) have the same frequency ω (the same wave number q_ν) and the same reduced wave vector $\mathbf{k}_{\|}$ as the incident wave. We remember that for $i=1$, $\nu=l$ and, for a given $\mathbf{g}$, $\hat{\mathbf{e}}_1$ is the radial unit vector along the direction of $\mathbf{K}^s_{\mathbf{g}l}$. Similarly, for $i=2,3$, $\nu=t$ and, for given $\mathbf{g}$, $\hat{\mathbf{e}}_2,\hat{\mathbf{e}}_3$ are the polar and azimuthal unit vectors, respectively, which are orthogonal to $\mathbf{K}^s_{\mathbf{g}t}$. Equation (4.18) tells us that the scattered wave consists, in general, of a number of diffracted beams, of the same ω and $\mathbf{k}_{\|}$, corresponding to different $\mathbf{g}$ vectors and polarization modes (longitudinal or transverse). We note, however, that only beams for which $K^s_{\mathbf{g}\nu z}$ is real constitute propagating waves. The coefficients in Eq. (4.18), given by Eq. (4.19), are functions of the $B^{+P}_{lm;i'}(\mathbf{K}^{s'}_{\mathbf{g}'\nu'})$ coefficients and through them depend on the incident plane wave. These coefficients are to be evaluated for an incident longitudinal $(i'=1)$ or transverse $(i'=2,3)$ plane wave, with a wave vector $\mathbf{K}^{s'}_{\mathbf{g}'\nu'}$ given by Eq. (4.5), incident from the left $(s'=+)$ or from the right $(s'=-)$, with a displacement vector along the i'th direction of magnitude equal to unity. In other words, $B^{+P}_{lm;i'}(\mathbf{K}^{s'}_{\mathbf{g}'\nu'})$ are calculated from Eq. (4.14), substituting $A^{0P}_{lm;i'}(\hat{\mathbf{K}}^{s'}_{\mathbf{g}'\nu'})$, given by Eqs. (3.4), (3.7), and (3.8), on the right-hand side of this

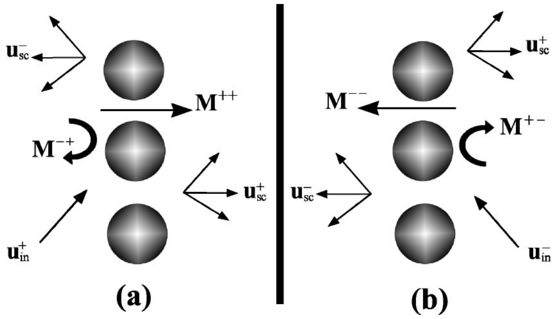

FIG. 1. Scattering of a plane elastic wave by a plane of spheres: (a) the wave is incident from the left; (b) the wave is incident from the right.

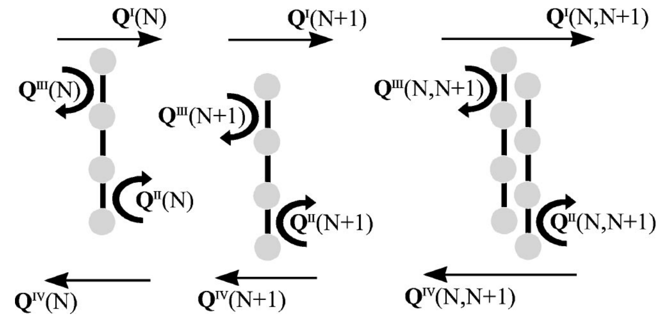

FIG. 2. The **Q** matrices for two successive layers are obtained from those of the individual layers.

equation. Obviously, when $i'=1$, only the coefficients $A^{0L}_{lm;i'}(\hat{\mathbf{K}}^{s'}_{\mathbf{g}'l})$ are nonzero, and when $i'=2,3$ only $A^{0M}_{lm;i'}(\hat{\mathbf{K}}^{s'}_{\mathbf{g}'t})$ and $A^{0N}_{lm;i'}(\hat{\mathbf{K}}^{s'}_{\mathbf{g}'t})$ are nonzero.

Let us for the sake of clarity assume that a plane wave given by Eq. (4.4) is incident on the plane of spheres from the left as in Fig. 1(a). Then the transmitted wave (incident +scattered) on the right of the plane of spheres can be written as

$$\mathbf{u}^{+}_{\mathrm{tr}}(\mathbf{r})=\sum_{\mathbf{g}i}[u_{\mathrm{tr}}]^{+}_{\mathbf{g}i}\exp(i\mathbf{K}^{+}_{\mathbf{g}\nu}\cdot\mathbf{r})\hat{\mathbf{e}}_i,\quad z>0, \tag{4.20}$$

with

$$[u_{\mathrm{tr}}]^{+}_{\mathbf{g}i}=[u_{\mathrm{in}}]^{+}_{\mathbf{g}'i}\delta_{\mathbf{gg}'}+[u_{\mathrm{sc}}]^{+}_{\mathbf{g}i}=\sum_{i'}M^{++}_{\mathbf{g}i;\mathbf{g}'i'}[u_{\mathrm{in}}]^{+}_{\mathbf{g}'i'}, \tag{4.21}$$

and the reflected wave as

$$\mathbf{u}^{-}_{\mathrm{rf}}(\mathbf{r})=\sum_{\mathbf{g}i}[u_{\mathrm{rf}}]^{-}_{\mathbf{g}i}\exp(i\mathbf{K}^{-}_{\mathbf{g}\nu}\cdot\mathbf{r})\hat{\mathbf{e}}_i,\quad z<0, \tag{4.22}$$

with

$$[u_{\mathrm{rf}}]^{-}_{\mathbf{g}i}=[u_{\mathrm{sc}}]^{-}_{\mathbf{g}i}=\sum_{i'}M^{-+}_{\mathbf{g}i;\mathbf{g}'i'}[u_{\mathrm{in}}]^{+}_{\mathbf{g}'i'}. \tag{4.23}$$

Equations (4.19), (4.21) and (4.23) define the transmission (M^{++}) and reflection (M^{-+}) matrix elements for a plane wave incident on the plane of spheres from the left. Similarly, we can define the transmission matrix elements $M^{--}_{\mathbf{g}i;\mathbf{g}'i'}$ and the reflection matrix elements $M^{+-}_{\mathbf{g}i;\mathbf{g}'i'}$ for a plane wave incident on the plane of spheres from the right [see Fig. 1(b)]. We obtain

$$M^{ss'}_{\mathbf{g}i;\mathbf{g}'i'}=\delta_{ss'}\delta_{\mathbf{gg}'}\delta_{ii'}+\sum_{Plm}\Delta^{P}_{lm;i}(\mathbf{K}^{s}_{\mathbf{g}\nu})B^{+P}_{lm;i'}(\mathbf{K}^{s'}_{\mathbf{g}'\nu'}). \tag{4.24}$$

One can show that the above matrix elements obey the following symmetry relations:

$$M^{-s-s'}_{\mathbf{g}i;\mathbf{g}'i'}=(-1)^{i+i'}M^{ss'}_{\mathbf{g}i;\mathbf{g}'i'}. \tag{4.25}$$

V. SCATTERING BY A SLAB

In what follows we need to evaluate the scattering properties of a slab which by definition consists of a number of layers (planes of spheres). For this purpose it is convenient to express the plane waves on the left of a given plane of spheres with respect to an origin, $\mathbf{A}_l$, on the left of the plane at $-\mathbf{d}_l$ from its center, and the plane waves on the right of this plane with respect to an origin, $\mathbf{A}_r$, on the right of the plane at $\mathbf{d}_r$ from its center, i.e., a wave on the left of the plane will be written as $\Sigma_{\mathbf{g}i}u^{s}_{\mathbf{g}i}\exp[i\mathbf{K}^{s}_{\mathbf{g}\nu}\cdot(\mathbf{r}-\mathbf{A}_l)]\hat{\mathbf{e}}_i$ and a wave on the right of the plane will be written as $\Sigma_{\mathbf{g}i}u^{s}_{\mathbf{g}i}\exp[i\mathbf{K}^{s}_{\mathbf{g}\nu}\cdot(\mathbf{r}-\mathbf{A}_r)]\hat{\mathbf{e}}_i$. The relationships between the amplitudes of the incident and of the reflected and transmitted waves, when these are expressed with respect to the above origins, follow directly from the corresponding equations of Sec. IV. Accordingly, the amplitudes of these waves are related through the **Q**-matrix elements given below:

$$Q^{\mathrm{I}}_{\mathbf{g}i;\mathbf{g}'i'}=M^{++}_{\mathbf{g}i;\mathbf{g}'i'}\exp[i(\mathbf{K}^{+}_{\mathbf{g}\nu}\cdot\mathbf{d}_r+\mathbf{K}^{+}_{\mathbf{g}'\nu'}\cdot\mathbf{d}_l)],$$

$$Q^{\mathrm{II}}_{\mathbf{g}i;\mathbf{g}'i'}=M^{+-}_{\mathbf{g}i;\mathbf{g}'i'}\exp[i(\mathbf{K}^{+}_{\mathbf{g}\nu}\cdot\mathbf{d}_r-\mathbf{K}^{-}_{\mathbf{g}'\nu'}\cdot\mathbf{d}_r)],$$

$$Q^{\mathrm{III}}_{\mathbf{g}i;\mathbf{g}'i'}=M^{-+}_{\mathbf{g}i;\mathbf{g}'i'}\exp[-i(\mathbf{K}^{-}_{\mathbf{g}\nu}\cdot\mathbf{d}_l-\mathbf{K}^{+}_{\mathbf{g}'\nu'}\cdot\mathbf{d}_l)],$$

$$Q^{\mathrm{IV}}_{\mathbf{g}i;\mathbf{g}'i'}=M^{--}_{\mathbf{g}i;\mathbf{g}'i'}\exp[-i(\mathbf{K}^{-}_{\mathbf{g}\nu}\cdot\mathbf{d}_l+\mathbf{K}^{-}_{\mathbf{g}'\nu'}\cdot\mathbf{d}_r)], \tag{5.1}$$

whose physical meaning is made obvious by their one-to-one correspondence with the **M**-matrix elements of Sec. IV. From this point on, we shall write the above matrices in compact form as $\mathbf{Q}^{\mathrm{I}}$, $\mathbf{Q}^{\mathrm{II}}$, $\mathbf{Q}^{\mathrm{III}}$ and $\mathbf{Q}^{\mathrm{IV}}$.

We obtain the transmission and reflection matrices for a pair of two successive layers, N and $N+1$, to be denoted by $\mathbf{Q}(N,N+1)$, by combining the matrices $\mathbf{Q}(N)$ and $\mathbf{Q}(N+1)$ of the two layers, as shown schematically in Fig. 2. One can easily show that

$$\mathbf{Q}^{\mathrm{I}}(N,N+1)=\mathbf{Q}^{\mathrm{I}}(N+1)[\mathbf{I}-\mathbf{Q}^{\mathrm{II}}(N)\mathbf{Q}^{\mathrm{III}}(N+1)]^{-1}\mathbf{Q}^{\mathrm{I}}(N),$$

$$\mathbf{Q}^{\mathrm{II}}(N,N+1)=\mathbf{Q}^{\mathrm{II}}(N+1)+\mathbf{Q}^{\mathrm{I}}(N+1)\mathbf{Q}^{\mathrm{II}}(N)\times[\mathbf{I}-\mathbf{Q}^{\mathrm{III}}(N+1)\mathbf{Q}^{\mathrm{II}}(N)]^{-1}\mathbf{Q}^{\mathrm{IV}}(N+1),$$

$$\mathbf{Q}^{\mathrm{III}}(N,N+1)=\mathbf{Q}^{\mathrm{III}}(N)+\mathbf{Q}^{\mathrm{IV}}(N)\mathbf{Q}^{\mathrm{III}}(N+1)\times[\mathbf{I}-\mathbf{Q}^{\mathrm{II}}(N)\mathbf{Q}^{\mathrm{III}}(N+1)]^{-1}\mathbf{Q}^{\mathrm{I}}(N),$$

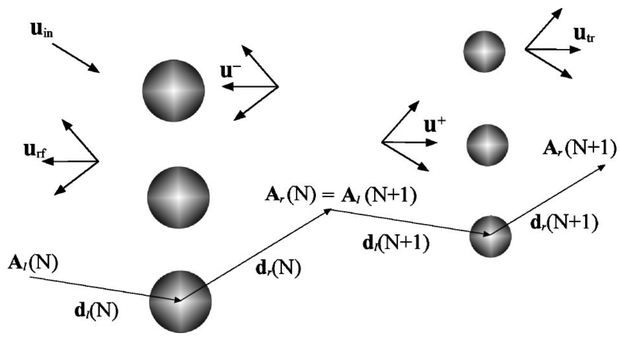

FIG. 3. Putting together a pair of planes of spheres.

$$\mathbf{Q}^{\mathrm{IV}}(N,N+1)=\mathbf{Q}^{\mathrm{IV}}(N)[\mathbf{I}-\mathbf{Q}^{\mathrm{III}}(N+1)\times\mathbf{Q}^{\mathrm{II}}(N)]^{-1}\mathbf{Q}^{\mathrm{IV}}(N+1). \tag{5.2}$$

For example, knowing that

$$[\mathbf{I}-\mathbf{Q}^{\mathrm{II}}(N)\mathbf{Q}^{\mathrm{III}}(N+1)]^{-1}=\mathbf{I}+\mathbf{Q}^{\mathrm{II}}(N)\mathbf{Q}^{\mathrm{III}}(N+1)+\mathbf{Q}^{\mathrm{II}}(N)\mathbf{Q}^{\mathrm{III}}(N+1)\times\mathbf{Q}^{\mathrm{II}}(N)\mathbf{Q}^{\mathrm{III}}(N+1)+\cdots, \tag{5.3}$$

we can write the first of Eqs. (5.2) as follows:

$$\mathbf{Q}^{\mathrm{I}}(N,N+1)=\mathbf{Q}^{\mathrm{I}}(N+1)\mathbf{Q}^{\mathrm{I}}(N)+\mathbf{Q}^{\mathrm{I}}(N+1)\mathbf{Q}^{\mathrm{II}}(N)\times\mathbf{Q}^{\mathrm{III}}(N+1)\mathbf{Q}^{\mathrm{I}}(N)+\mathbf{Q}^{\mathrm{I}}(N+1)\mathbf{Q}^{\mathrm{II}}(N)\times\mathbf{Q}^{\mathrm{III}}(N+1)\mathbf{Q}^{\mathrm{II}}(N)\mathbf{Q}^{\mathrm{III}}(N+1)\mathbf{Q}^{\mathrm{I}}(N)+\cdots. \tag{5.4}$$

The meaning of the terms is obvious. The first term signifies transmission through the Nth layer, followed by transmission through the $(N+1)$th layer. The second term signifies transmission through the Nth layer, followed by reflection by the $(N+1)$th layer, followed by reflection by the Nth layer, followed by transmission through the $(N+1)$th layer. The third and higher terms can be interpreted in the same way: a wave incident from the left on the pair of layers will be multiply reflected, any number of times, between the layers before exiting the pair by transmission through the second layer. In similar fashion one can understand the remaining Eqs. (5.2). All matrices refer of course to the same ω and $\mathbf{k}_\parallel$. We remember that the waves on the left (right) of the pair of layers are referred to an origin at $-\mathbf{d}_l(N)$ $[+\mathbf{d}_r(N+1)]$ from the center of the Nth $[(N+1)$th$]$ layer. The choice of $\mathbf{d}_l(N)$ and $\mathbf{d}_r(N)$ is to some degree arbitrary, but it must be such that $\mathbf{A}_r(N)$ coincides with $\mathbf{A}_l(N+1)$, in accordance with the definition of these quantities (see Fig. 3).

It is obvious that by the same process we can obtain the transmission and reflection matrices of three layers, by combining those of the pair of layers with those of the third layer; and that we can in similar fashion obtain the transmission and reflection matrices for a slab consisting of any finite number of layers. In particular, having calculated the $\mathbf{Q}$-matrix elements of a single layer, we can obtain those of a slab of $N_{\max}=2^M$ identical layers by a doubling-layer scheme as follows: we calculate the $\mathbf{Q}$-matrix elements of two consecutive layers in the manner described above, then, using as units the $\mathbf{Q}$-matrix elements of a pair of layers, we obtain those of four consecutive layers, and in this way, by doubling the number of layers at each stage, we obtain the $\mathbf{Q}$-matrix elements of the slab.

In summary, for a plane wave of polarization ν', $\sum_i[u_{\mathrm{in}}]^+_{\mathbf{g}'i}\exp[i\mathbf{K}^+_{\mathbf{g}'\nu'}\cdot(\mathbf{r}-\mathbf{A}_L)]\hat{\mathbf{e}}_i$, incident on the slab from the left, we finally obtain a reflected wave $\sum_{\mathbf{g}i}[u_{\mathrm{rf}}]^-_{\mathbf{g}i}\exp[i\mathbf{K}^-_{\mathbf{g}\nu}\cdot(\mathbf{r}-\mathbf{A}_L)]\hat{\mathbf{e}}_i$ on the left of the slab and a transmitted wave $\sum_{\mathbf{g}i}[u_{\mathrm{tr}}]^+_{\mathbf{g}i}\exp[i\mathbf{K}^+_{\mathbf{g}\nu}\cdot(\mathbf{r}-\mathbf{A}_R)]\hat{\mathbf{e}}_i$ on the right of the slab, where $\mathbf{A}_L$ $(\mathbf{A}_R)$ is the appropriate origin on the left (right) of the slab. We have

$$[u_{\mathrm{tr}}]^+_{\mathbf{g}i}=\sum_{i'}Q^{\mathrm{I}}_{\mathbf{g}i;\mathbf{g}'i'}[u_{\mathrm{in}}]^+_{\mathbf{g}'i'}, \tag{5.5}$$

$$[u_{\mathrm{rf}}]^-_{\mathbf{g}i}=\sum_{i'}Q^{\mathrm{III}}_{\mathbf{g}i;\mathbf{g}'i'}[u_{\mathrm{in}}]^+_{\mathbf{g}'i'}, \tag{5.6}$$

where the $\mathbf{Q}$-matrix elements are those of the slab. In the present formulation of the problem we assume that the host material between the spheres extends to the left and right of the slab to infinity. However, the extension of the formalism to deal with different materials on the left and right sides of the slab can be easily effected by treating the interfaces as scattering elements described by appropriate $\mathbf{Q}$ matrices, as in the case of photonic crystals.[27]

A transmitted beam (a plane wave with a real $K^+_{\mathbf{g}\nu z}$ component of the corresponding wave vector) carries with it an energy flux density which, averaged over a time period $T=2\pi/\omega$, gives (a formal proof of this formula can be obtained by applying the standard definition of the Poynting vector $\mathbf{P}$ for elastic waves, $P_i=-\sigma_{ik}\dot{u}_k$, to a plane wave[35])

$$\mathbf{P}^{\mathrm{tr}}_{\mathbf{g}\nu}=\frac{1}{2}\rho\omega c_\nu^2\left\{\sum_i [u_{\mathrm{tr}}]^+_{\mathbf{g}i}([u_{\mathrm{tr}}]^+_{\mathbf{g}i})^*\right\}\mathbf{K}^+_{\mathbf{g}\nu}. \tag{5.7}$$

We recall that for a longitudinal wave $(\nu=l)$ $i=1$, while for a transverse wave $(\nu=t)$ $i=2,3$; and * denotes, as usual, complex conjugation. We note that the quantity in braces in Eq. (5.7) gives the square of the amplitude of the displacement associated with the given plane wave. The transmitted energy per unit area of the slab per unit time, associated with the $\mathbf{g},\nu$ beam, is given by the magnitude of the z component, $|P^{\mathrm{tr}}_{\mathbf{g}\nu z}|$, of $\mathbf{P}^{\mathrm{tr}}_{\mathbf{g}\nu}$. A similar formula gives the energy flux associated with any of the propagating reflected beams, or with the incident wave. For the reflected beams we have

$$\mathbf{P}^{\mathrm{rf}}_{\mathbf{g}\nu}=\frac{1}{2}\rho\omega c_\nu^2\left\{\sum_i [u_{\mathrm{rf}}]^-_{\mathbf{g}i}([u_{\mathrm{rf}}]^-_{\mathbf{g}i})^*\right\}\mathbf{K}^-_{\mathbf{g}\nu}. \tag{5.8}$$

And for the incident wave (of given $\mathbf{k}_\parallel+\mathbf{g}'$ and polarized along the i' direction) we obtain

$$\mathbf{P}^{\mathrm{in}}_{\mathbf{g}'i'}=\frac{1}{2}\rho\omega c_{\nu'}^2\{[u_{\mathrm{in}}]^+_{\mathbf{g}'i'}([u_{\mathrm{in}}]^+_{\mathbf{g}'i'})^*\}\mathbf{K}^+_{\mathbf{g}'\nu'}. \tag{5.9}$$

The reflected energy per unit area of the slab per unit time associated with the $\mathbf{g},\nu$ reflected beam is given by the magnitude of the z component, $|P^{\mathrm{rf}}_{\mathbf{g}\nu z}|$, of $\mathbf{P}^{\mathrm{rf}}_{\mathbf{g}\nu}$ and the incident energy per unit area of the slab per unit time is given by the magnitude of the z component, $|P^{\mathrm{in}}_{\mathbf{g}'i'z}|$, of $\mathbf{P}^{\mathrm{in}}_{\mathbf{g}'i'}$. By definition the reflectance is given by

$$\mathcal{R}(\omega,\mathbf{k}_\parallel+\mathbf{g}',i')=\frac{\sum_{\mathbf{g}\nu}|P^{\rm rf}_{\mathbf{g}\nu z}|}{|P^{\rm in}_{\mathbf{g}'i'z}|}=\frac{\sum_{\mathbf{g}i}c_\nu^2[u_{\rm rf}]^-_{\mathbf{g}i}([u_{\rm rf}]^-_{\mathbf{g}i})^*K^+_{\mathbf{g}\nu z}}{c_{\nu'}^2[u_{\rm in}]^+_{\mathbf{g}'i'}([u_{\rm in}]^+_{\mathbf{g}'i'})^*K^+_{\mathbf{g}'\nu' z}},\tag{5.10}$$

and the transmittance by

$$\mathcal{T}(\omega,\mathbf{k}_\parallel+\mathbf{g}',i')=\frac{\sum_{\mathbf{g}\nu}|P^{\rm tr}_{\mathbf{g}\nu z}|}{|P^{\rm in}_{\mathbf{g}'i'z}|}=\frac{\sum_{\mathbf{g}i}c_\nu^2[u_{\rm tr}]^+_{\mathbf{g}i}([u_{\rm tr}]^+_{\mathbf{g}i})^*K^+_{\mathbf{g}\nu z}}{c_{\nu'}^2[u_{\rm in}]^+_{\mathbf{g}'i'}([u_{\rm in}]^+_{\mathbf{g}'i'})^*K^+_{\mathbf{g}'\nu' z}},\tag{5.11}$$

where we have denoted explicitly the dependence of these coefficients on the incident parameters. As long as there are no energy losses in the slab, we have

$$\mathcal{T}+\mathcal{R}=1.\tag{5.12}$$

VI. THE COMPLEX BAND STRUCTURE

We view the infinite crystal as a sequence of identical layers parallel to the xy plane, extending over all space (from $z\to-\infty$ to $z\to+\infty$). If Eq. (4.1) is the 2D space lattice for the layer, and $\mathbf{a}_3$ is a vector which takes us from a point in the Nth layer to an equivalent point in the $(N+1)$th layer, then $\{\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3\}$ is a set of primitive vectors for the crystal.

In the region between the Nth and the $(N+1)$th layers the wavefield, of given ω and $\mathbf{k}_\parallel$, has the form

$$\mathbf{u}(\mathbf{r})=\sum_{\mathbf{g}i}\{u^+_{\mathbf{g}i}(N)\exp[i\mathbf{K}^+_{\mathbf{g}\nu}\cdot(\mathbf{r}-\mathbf{A}_r(N))]+u^-_{\mathbf{g}i}(N)\exp[i\mathbf{K}^-_{\mathbf{g}\nu}\cdot(\mathbf{r}-\mathbf{A}_r(N))]\}\hat{\mathbf{e}}_i.\tag{6.1}$$

The coefficients $u^s_{\mathbf{g}i}(N)$ are related to the $u^s_{\mathbf{g}i}(N+1)$ coefficients through the scattering properties of the Nth layer. We have

$$u^-_{\mathbf{g}i}(N)=\sum_{\mathbf{g}'i'}Q^{\rm IV}_{\mathbf{g}i;\mathbf{g}'i'}u^-_{\mathbf{g}'i'}(N+1)+\sum_{\mathbf{g}'i'}Q^{\rm III}_{\mathbf{g}i;\mathbf{g}'i'}u^+_{\mathbf{g}'i'}(N),$$

$$u^+_{\mathbf{g}i}(N+1)=\sum_{\mathbf{g}'i'}Q^{\rm I}_{\mathbf{g}i;\mathbf{g}'i'}u^+_{\mathbf{g}'i'}(N)+\sum_{\mathbf{g}'i'}Q^{\rm II}_{\mathbf{g}i;\mathbf{g}'i'}u^-_{\mathbf{g}'i'}(N+1),\tag{6.2}$$

where $\mathbf{Q}$ are the transmission/reflection matrices of the layer.

A generalized Bloch wave, by definition, has the property

$$u^s_{\mathbf{g}i}(N+1)=\exp(i\mathbf{k}\cdot\mathbf{a}_3)u^s_{\mathbf{g}i}(N),\tag{6.3}$$

with

$$\mathbf{k}=(\mathbf{k}_\parallel,k_z(\omega,\mathbf{k}_\parallel)),\tag{6.4}$$

where k_z is, for a given $\mathbf{k}_\parallel$, a function of ω, to be determined.

We choose the reduced $\mathbf{k}$ zone of reciprocal space as follows: $(\mathbf{k}_\parallel,k_z)$ where $\mathbf{k}_\parallel=(k_x,k_y)$ extends over the SBZ of the given crystallographic plane, and $-|\mathbf{b}_3|/2<k_z\leqslant|\mathbf{b}_3|/2$, where $\mathbf{b}_3\equiv 2\pi\mathbf{a}_1\times\mathbf{a}_2/\mathbf{a}_1\cdot(\mathbf{a}_2\times\mathbf{a}_3)=\hat{\mathbf{e}}_z 2\pi/a_{3z}$. The periodicity of the frequency band structure parallel to the xy plane follows from Eq. (6.1); for replacing $\mathbf{k}_\parallel$ by $\mathbf{k}_\parallel+\mathbf{g}$ in this equation renames the coefficients without changing the form of the wave function. Also, because the eigenvalues of Eq. (6.5) below are of the form $\exp(i\mathbf{k}\cdot\mathbf{a}_3)$, values of k_z differing by an integral multiple of $|\mathbf{b}_3|$ correspond to the same Bloch wave; which establishes the periodicity of the band structure normal to the xy plane. Substituting Eq. (6.3) into Eq. (6.2) we obtain, after some algebra (see Appendix C), the following system of equations:

$$\begin{pmatrix}\mathbf{Q}^{\rm I} & \mathbf{Q}^{\rm II}\\ -[\mathbf{Q}^{\rm IV}]^{-1}\mathbf{Q}^{\rm III}\mathbf{Q}^{\rm I} & [\mathbf{Q}^{\rm IV}]^{-1}[\mathbf{I}-\mathbf{Q}^{\rm III}\mathbf{Q}^{\rm II}]\end{pmatrix}\begin{pmatrix}\mathbf{u}^+(N)\\ \mathbf{u}^-(N+1)\end{pmatrix}=\exp(i\mathbf{k}\cdot\mathbf{a}_3)\begin{pmatrix}\mathbf{u}^+(N)\\ \mathbf{u}^-(N+1)\end{pmatrix},\tag{6.5}$$

where $\mathbf{u}^\pm$ are column matrices with elements: $u^\pm_{\mathbf{g}_1 1}$, $u^\pm_{\mathbf{g}_1 2}$, $u^\pm_{\mathbf{g}_1 3}$, $u^\pm_{\mathbf{g}_2 1}$, $u^\pm_{\mathbf{g}_2 2}$, $u^\pm_{\mathbf{g}_2 3}$, $u^\pm_{\mathbf{g}_3 1}$, ... In practice we keep $g_{\max}$ $\mathbf{g}$ vectors (those of the smallest magnitude) in which case $\mathbf{u}^\pm$ are column matrices with $3g_{\max}$ elements. The enumeration of the $\mathbf{g}$ vectors implied in the above definition of $\mathbf{u}^\pm$ is of course the same with the one implied in relation to the $\mathbf{Q}$ matrices, each of which has $3g_{\max}\times 3g_{\max}$ elements; $\mathbf{I}$ is the $3g_{\max}\times 3g_{\max}$ unit matrix. For given $\mathbf{k}_\parallel$ and ω, we obtain $6g_{\max}$ eigenvalues of k_z from the eigenvalues of the $6g_{\max}\times 6g_{\max}$ matrix on the left-hand side of Eq. (6.5). The eigenvalues $k_z(\omega;\mathbf{k}_\parallel)$, looked upon as functions of real ω, define, for each $\mathbf{k}_\parallel$, $6g_{\max}$ lines in the complex k_z space. Taken together they constitute the complex band structure of the infinite crystal associated with the given crystallographic plane. A line of given $\mathbf{k}_\parallel$ may be real (in the sense that k_z is real) over certain frequency regions, and be complex (in the sense that k_z is complex) for ω outside these regions. It turns out that for given $\mathbf{k}_\parallel$ and ω, out of the $6g_{\max}$ eigenvalues of $k_z(\omega;\mathbf{k}_\parallel)$ none or, at best, a few are real; the eigensolutions of Eq. (6.5) corresponding to them, represent propagating modes of the elastic field in the given infinite crystal. The remaining eigenvalues of $k_z(\omega;\mathbf{k}_\parallel)$ are complex and the corresponding eigensolutions represent evanescent waves. These have an amplitude which increases exponentially in the positive or negative z direction and, unlike the propagating waves, do not exist as physical entities in the infinite crystal. However, they are an essential part of the physical solutions of the elastic field in a semi-infinite crystal (extending from $z\to-\infty$ to $z=0$) or in a slab of finite thickness. A region of frequency where propagating waves do not exist for given $\mathbf{k}_\parallel$ constitutes a frequency gap of the elastic field for the given $\mathbf{k}_\parallel$. If over a frequency region no propagating wave exists whatever the value of $\mathbf{k}_\parallel$, then this region constitutes an (absolute) frequency gap.

Finally, it is worth noting that, when there is a plane of mirror symmetry associated with the surface under consider-

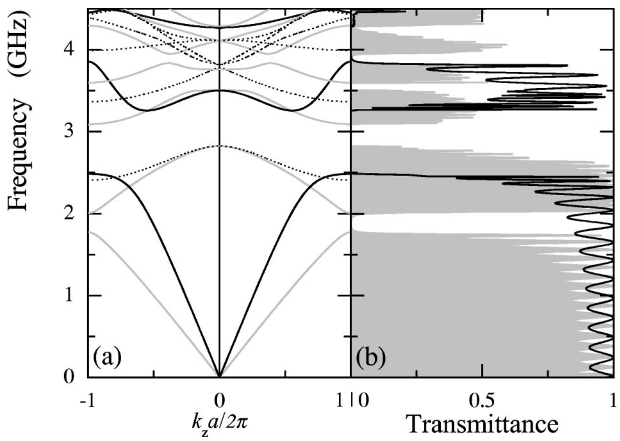

FIG. 4. The phononic band structure at the center of the SBZ of a (001) surface of an fcc crystal of silica spheres in ice (a); and the corresponding transmittance curve of a slab of 16 layers parallel to the same surface (b). The lattice constant is 1 μm and the radius of the spheres is 0.25 μm. In (a) the black lines represent longitudinal modes (in the sense defined in the text), the grey lines transverse modes, and the dotted lines are deaf bands. Correspondingly in (b) the solid line shows the transmittance for longitudinal incident elastic waves; and the shaded curve that for transverse incident waves.

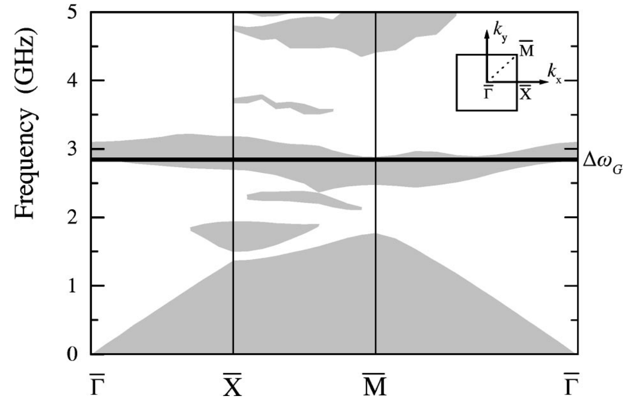

FIG. 5. Projection of the frequency band structure on the SBZ of the (001) surface of the fcc phononic crystal described in the caption of Fig. 4. The shaded areas show the frequency gaps in the considered frequency region. The inset shows the SBZ of the (001) surface.

ation, the eigensolutions (Bloch waves) of Eq. (6.5) appear in pairs: $k_z(\omega;\mathbf{k}_\parallel)$ and $-k_z(\omega;\mathbf{k}_\parallel)$.

VII. AN EXAMPLE

We demonstrate the applicability of our method by applying it to a specific example, which has also been considered by Sprik and Wegdam:[13] a system of silica spheres of radius $S=0.25$ μm centered on the sites of an fcc lattice with a lattice constant of 1 μm; the host material being ice. The relevant parameters are, for silica: $\rho=2200$ kg m^{-3}, $c_l=5970$ m s^{-1}, $c_t=3760$ m s^{-1}, and for ice (at $-16\,°$C): $\rho=940$ kg m^{-3}, $c_l=3830$ m s^{-1}, $c_t=1840$ m s^{-1}. We view the crystal as a succcession of planes of spheres parallel to the (001) direction of the fcc lattice. Figure 4 shows the frequency band structure normal to the (001) plane ($\mathbf{k}_\parallel=\mathbf{0}$) and the corresponding transmission spectrum for both longitudinal and transverse waves incident normally on a slab of the above crystal consisting of 16 layers.

To begin with, we compare the band structure normal to the (001) plane with the results of Sprik and Wegdam[13] obtained by the plane-wave method (using 343 plane waves) with an accuracy, as stated by the above authors, of a few percent. Our results obtained with an angular momentum cutoff $l_{\max}=4$ and 13 $\mathbf{g}$ vectors are converged within an accuracy of 10^{-3}, and they agree with those of Sprik and Wegdam[13] within the stated accuracy of their results. Furthermore, the evaluation of the transmission coefficient, easily obtainable by our method but not possible by the plane-wave method, confirms the validity of the band-structure calculation. The transmittance curves are shown in Fig. 4 by the shaded curve for the transverse waves and by the solid line for the longitudinal waves. The oscillations in the transmittance curves are due to multiple reflections at the edges of the slab (Fabry-Pérot like oscillations). As expected, for frequencies within a gap the corresponding transmission coefficient vanishes.

The eigenmodes of the phononic crystal are strictly speaking always hybrid, having a longitudinal and a transverse component. However, along symmetry directions the following situation may arise. We consider for simplicity the normal modes corresponding to $\mathbf{k}_\parallel=\mathbf{0}$ (the direction normal to the surface). In this case the component of the field associated with the $\mathbf{g}=\mathbf{0}$ beam is either longitudinal or transverse; the field associated with the $\mathbf{g}\neq\mathbf{0}$ components need not be of the same type. However, only the $\mathbf{g}=\mathbf{0}$ component couples to the external field (incident, reflected and transmitted waves), if $(\mathbf{k}_\parallel+\mathbf{g})^2>q_\nu^2$ for $\mathbf{g}\neq\mathbf{0}$. Therefore an incident longitudinal or transverse wave will excite a mode (or modes) in the interior of the crystal with a $\mathbf{g}=\mathbf{0}$ component of the same type. As long as the amplitude of the $\mathbf{g}=\mathbf{0}$ component of these modes is much greater than those of the $\mathbf{g}\neq\mathbf{0}$ components, which is the case in the example we have considered, the transmitted and reflected waves will be of the same type as the incident wave, but this need not be the case in general. Our results shown in Fig. 4 are termed longitudinal or transverse in the above sense. For waves incident at an angle on the surface of the slab ($\mathbf{k}_\parallel\neq\mathbf{0}$) the above distinction between longitudinal and transverse waves no longer applies (the $\mathbf{g}=\mathbf{0}$ component of the elastic field inside the crystal is a hybrid one) and therefore an incident wave of a specific type (longitudinal or transverse) will give rise to reflected and transmitted waves of a mixed type.

In Fig. 5 we show the projection of the frequency band structure on the SBZ of the (001) plane along its symmetry lines. This is obtained, for a given $\mathbf{k}_\parallel$, as follows: the regions of ω for which there are no propagating states in the infinite crystal [the corresponding values of all $k_z(\omega,\mathbf{k}_\parallel)$ are complex] are shown shaded, against the white areas which correspond to regions over which propagating states do exist [for a given ω there is at least one solution corresponding to $k_z(\omega,\mathbf{k}_\parallel)$ real]. We note the existence of a narrow absolute gap, denoted by $\Delta\omega_G$, extending from 2.82 GHz to 2.89 GHz. An absolute gap at approximately the same frequency and of approximately the same width was found by Sprik and Wegdam.[13]

A considerable number of bands of longitudinal and transverse waves exist above the absolute gap (see Fig. 4). Below this gap we have two bands of transverse waves, which are doubly degenerate, extending from 0 GHz to 1.77 GHz and from 2.01 GHz to 2.82 GHz, with a gap in between. On the other hand, a nondegenerate band of longitudinal waves extends from 0 GHz to 2.48 GHz. In addition to these bands, we find a nondegenerate band, extending from 2.40 GHz to 2.82 GHz, for which the $\mathbf{g}=\mathbf{0}$ component of the corresponding eigenmodes of the elastic field vanishes. Because the $\mathbf{g}=\mathbf{0}$ beam is the only one which matches (couples with) a propagating wave outside the crystal, an internal mode with a vanishing $\mathbf{g}=\mathbf{0}$ component is not excited by the incident wave. Therefore, if this were the only band over the stated frequency region, the wave would be totally reflected. However, in our example transmission through the slab in the frequency range of this deaf band occurs, because other bands with nonvanishing $\mathbf{g}=\mathbf{0}$ components exist in the same frequency region. We note that analogous deaf bands are known to exist in photonic crystals.[36]

The long wavelength limit ($k_z \to 0$) is represented by the linear segments of the dispersion curves, the slopes of which determine the propagation velocities of longitudinal and transverse waves ($\overline{c_l}=3893$ m s^{-1},$\overline{c_t}=2033$ m s^{-1}) in a corresponding effective medium.

VIII. CONCLUSION

We have shown that for a system of nonoverlapping elastic spheres arranged periodically in a host medium of different elastic coefficients one can, using the formalism of the present paper, calculate accurately and efficiently the phonon spectrum of the infinite crystal and, also, the transmission, reflection, and absorption coefficients of elastic waves incident on a slab of the material of finite thickness.

APPENDIX A

The nonzero elements of the $\mathbf{T}$ matrix for a solid sphere in a solid host are

$$T^{MM}_{lm;l'm'}=\frac{(\rho_s z_t^2/\rho x_t^2) j_l(z_t)[x_t j_l'(x_t)-j_l(x_t)]-j_l(x_t)[z_t j_l'(z_t)-j_l(z_t)]}{j_l(x_t)[z_t h_l^{+\prime}(z_t)-h_l^+(z_t)]-(\rho_s z_t^2/\rho x_t^2) h_l^+(z_t)[x_t j_l'(x_t)-j_l(x_t)]}\delta_{ll'}\delta_{mm'}, \quad l,l'\geqslant 1,$$

$$T^{NN}_{lm;l'm'}=\frac{W_l^{NN}}{D_l}\delta_{ll'}\delta_{mm'}, \quad l,l'\geqslant 1,$$

$$T^{NL}_{lm;l'm'}=(z_t/z_l)\frac{W_l^{NL}\sqrt{l(l+1)}}{D_l}\delta_{ll'}\delta_{mm'}, \quad l\geqslant 1, \quad l'\geqslant 0,$$

$$T^{LN}_{lm;l'm'}=(z_l/z_t)\frac{W_l^{LN}}{D_l\sqrt{l(l+1)}}\delta_{ll'}\delta_{mm'}, \quad l\geqslant 0, \quad l'\geqslant 1,$$

$$T^{LL}_{lm;l'm'}=\frac{W_l^{LL}}{D_l}\delta_{ll'}\delta_{mm'}, \quad l,l'\geqslant 0, \tag{A1}$$

with $z_\nu=Sq_\nu$, $x_\nu=Sq_{s\nu}$ and $\nu=l,t$. The elements of the 4×4 determinant D_l are given by

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

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

$$d_{31}=[l(l+1)-z_t^2/2-1]h_l^+(z_t)-z_t h_l^{+\prime}(z_t),$$

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

$$d_{12}=h_l^+(z_l),$$

$$d_{22}=z_l h_l^{+\prime}(z_l),$$

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

$$d_{42}=[l(l+1)-z_t^2/2]h_l^+(z_l)-2z_l h_l^{+\prime}(z_l), \tag{A2}$$

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

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

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

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

$$d_{14}=j_l(x_l),$$

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

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

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

where j_l' and $h_l^{+\prime}$ denote the first derivatives of the spherical Bessel and Hankel functions, respectively. $W_l^{PP'}$ are given by the following determinants:

$$W_l^{NN}=-\begin{vmatrix} d_1^N & d_{12} & d_{13} & d_{14} \\ d_2^N & d_{22} & d_{23} & d_{24} \\ d_3^N & d_{32} & d_{33} & d_{34} \\ d_4^N & d_{42} & d_{43} & d_{44} \end{vmatrix},$$

$$W_l^{NL}=\begin{vmatrix} d_1^L & d_{12} & d_{13} & d_{14}\\ d_2^L & d_{22} & d_{23} & d_{24}\\ d_3^L & d_{32} & d_{33} & d_{34}\\ d_4^L & d_{42} & d_{43} & d_{44}\end{vmatrix},$$

$$W_l^{LN}=\begin{vmatrix} d_{11} & d_1^N & d_{13} & d_{14}\\ d_{21} & d_2^N & d_{23} & d_{24}\\ d_{31} & d_3^N & d_{33} & d_{34}\\ d_{41} & d_4^N & d_{43} & d_{44}\end{vmatrix},$$

$$W_l^{LL}=-\begin{vmatrix} d_{11} & d_1^L & d_{13} & d_{14}\\ d_{21} & d_2^L & d_{23} & d_{24}\\ d_{31} & d_3^L & d_{33} & d_{34}\\ d_{41} & d_4^L & d_{43} & d_{44}\end{vmatrix}, \tag{A3}$$

where

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

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

$$d_3^N=[l(l+1)-z_t^2/2-1]j_l(z_t)-z_t j_l'(z_t),$$

$$d_4^N=l(l+1)[z_t j_l'(z_t)-j_l(z_t)], \tag{A4}$$

and

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

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

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

$$d_4^L=[l(l+1)-z_t^2/2]j_l(z_l)-2z_l j_l'(z_l). \tag{A5}$$

APPENDIX B

A longitudinal (transverse) spherical wave about $\mathbf{R}_n\neq\mathbf{0}$ remains a longitudinal (transverse) wave when expanded about the origin of coordinates $(\mathbf{R}_n=\mathbf{0})$, and therefore the matrix elements of $\boldsymbol{\Omega}$ defined by Eq. (4.9) are obtained independently for longitudinal and transverse waves.

For the transverse waves the evaluation of these elements proceeds as in the case of the electromagnetic (EM) field described in Ref. 37. We note that the M transverse elastic wave corresponds to the H component of the electric field of the EM wave and the N transverse elastic wave corresponds to the E component of the electric field of the EM wave [compare Eqs. (15) and (16) of Ref. 37 with Eqs. (4.7) and (4.8) of the present article]. Therefore, the $\Omega^{PP'}$-matrix elements with $P=M,N$ and $P'=M,N$ can be taken directly from Ref. 37. Taking into account the fact that the expansion coefficients in Eq. (4.7) above and those in Eq. (15) of Ref. 37 are multiplied by different constants, one readily obtains

$$\Omega^{MM}_{lm;l'm'}=\frac{2\alpha_l^{-m}\alpha_{l'}^{-m'}Z^{lm-1}_{l'm'-1}(q_t)+mm'Z^{lm}_{l'm'}(q_t)+2\alpha_l^{m}\alpha_{l'}^{m'}Z^{lm+1}_{l'm'+1}(q_t)}{[l(l+1)l'(l'+1)]^{1/2}},\quad l,l'\geqslant 1,$$

$$\Omega^{NN}_{lm;l'm'}=\Omega^{MM}_{lm;l'm'},\quad l,l'\geqslant 1, \tag{B1}$$

$$\begin{aligned}\Omega^{MN}_{lm;l'm'}=-\Omega^{NM}_{lm;l'm'}=&(2l+1)[l(l+1)l'(l'+1)]^{-1/2}\times\{(8\pi/3)^{1/2}(-1)^m\alpha_{l'}^{m'}Z^{l-1m+1}_{l'm'+1}(q_t)B_{l-1,m+1}(1,\\&-1;lm)-(8\pi/3)^{1/2}(-1)^m\alpha_{l'}^{-m'}Z^{l-1m-1}_{l'm'-1}(q_t)B_{l-1,m-1}(1,1;lm)\\&+m'Z^{l-1m}_{l'm'}(q_t)[(l+m)(l-m)/(2l-1)(2l+1)]^{1/2}\},\quad l,l'\geqslant 1,\end{aligned} \tag{B2}$$

where

$$Z^{l'm'}_{lm}(q_t)\equiv\sum_{\mathbf{R}_n\neq\mathbf{0}}\exp(i\mathbf{k}_\parallel\cdot\mathbf{R}_n)G_{lm;l'm'}(-\mathbf{R}_n;q_t), \tag{B3}$$

$$G_{lm;l''m''}(-\mathbf{R}_n;q_t)\equiv 4\pi\sum_{l'm'}(-1)^{(l-l'-l'')/2}(-1)^{m'+m''}B_{lm}(l'm';l''m'')h^+_{l'}(q_tR_n)Y_{l'}^{-m'}(-\hat{\mathbf{R}}_n), \tag{B4}$$

$$B_{lm}(l'm';l''m'')\equiv\int d\hat{\mathbf{r}}Y_l^m(\hat{\mathbf{r}})Y_{l'}^{m'}(\hat{\mathbf{r}})Y_{l''}^{-m''}(\hat{\mathbf{r}}). \tag{B5}$$

The expression for Ω^{MN} can be simplified further by the evaluation of the B_{lm} coefficients defined by Eq. (B5). Using standard formulas (see, e.g., Ref. 38) one finally obtains

$$\Omega^{MN}_{lm;l'm'}=(2l+1)\frac{-2\alpha_{l'}^{-m'}\gamma_l^{m}Z^{l-1m-1}_{l'm'-1}(q_t)+m'\zeta_l^mZ^{l-1m}_{l'm'}(q_t)+2\alpha_{l'}^{m'}\gamma_l^{-m}Z^{l-1m+1}_{l'm'+1}(q_t)}{[l(l+1)l'(l'+1)]^{1/2}},\quad l,l'\geqslant 1,$$

$$\Omega^{NM}_{lm;l'm'}=-\Omega^{MN}_{lm;l'm'},\quad l,l'\geqslant 1, \tag{B6}$$

where

$$\gamma_l^m = \frac{1}{2}[(l+m)(l+m-1)]^{1/2}/[(2l-1)(2l+1)]^{1/2},$$

$$\zeta_l^m = [(l+m)(l-m)]^{1/2}/[(2l-1)(2l+1)]^{1/2}. \tag{B7}$$

The derivation of the above formulas is based on the following relation:[37]

$$h_l^+(qr_n)Y_l^m(\hat{\mathbf{r}}_n) = \sum_{l'm'} G_{lm;l'm'}(-\mathbf{R}_n;q)j_{l'}(qr)Y_{l'}^{m'}(\hat{\mathbf{r}}), \tag{B8}$$

which expresses a scalar spherical wave about $\mathbf{R}_n \neq \mathbf{0}$, as a sum of spherical waves about the origin $(\mathbf{R}_n = \mathbf{0})$. The longitudinal wave, described by the third term of Eq. (4.7), is obtained by multiplying Eq. (B8) with $\exp(i\mathbf{k}_\parallel \cdot \mathbf{R}_n)$ and summing over all $\mathbf{R}_n \neq \mathbf{0}$, which immediately tells us that

$$\Omega_{lm;l'm'}^{LL} = Z_{l'm'}^{lm}(q_l), \quad l,l' \geqslant 0. \tag{B9}$$

The evaluation of the matrices $\mathbf{\Omega}$ involves the evaluation of the matrix $\mathbf{Z}$ which is a well known quantity in the theory of low-energy electron diffraction (LEED) and a computer program for its evaluation is already available in the literature.[33] Further calculation is made simpler by the following property of $Z_{lm}^{l'm'}(q_\nu)$:[33]

$$Z_{lm}^{l'm'}(q_\nu) = 0, \quad \text{unless} \quad l+m+l'+m': \quad \text{even}. \tag{B10}$$

It follows from Eq. (B10) that

$$\Omega_{lm;l'm'}^{MM} = \Omega_{lm;l'm'}^{NN} = \Omega_{lm;l'm'}^{LL} = 0, \quad \text{unless} \quad l+m+l'+m': \quad \text{even},$$

$$\Omega_{lm;l'm'}^{MN} = \Omega_{lm;l'm'}^{NM} = 0, \quad \text{unless} \quad l+m+l'+m': \quad \text{odd}. \tag{B11}$$

APPENDIX C

Equation (6.5), initially derived by McRae for the case of electron scattering by atomic layers[39] can be proven as follows. We replace the quantities on the left of Eqs. (6.2) with the aid of Eq. (6.3) to obtain

$$\exp(i\mathbf{k}\cdot\mathbf{a}_3)\begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{Q}^{\mathrm{III}} & \mathbf{Q}^{\mathrm{IV}} \end{pmatrix}\begin{pmatrix} \mathbf{u}^+(N) \\ \mathbf{u}^-(N+1) \end{pmatrix} = \begin{pmatrix} \mathbf{Q}^{\mathrm{I}} & \mathbf{Q}^{\mathrm{II}} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}\begin{pmatrix} \mathbf{u}^+(N) \\ \mathbf{u}^-(N+1) \end{pmatrix}. \tag{C1}$$

The inverse of the matrix on the left of Eq. (C1) is given by

$$\begin{pmatrix} \mathbf{I} & \mathbf{0} \\ -[\mathbf{Q}^{\mathrm{IV}}]^{-1}\mathbf{Q}^{\mathrm{III}} & [\mathbf{Q}^{\mathrm{IV}}]^{-1} \end{pmatrix}. \tag{C2}$$

Multiplying both sides of Eq. (C1) with the above matrix we obtain Eq. (6.5).

*Also at Department of Physics, National Technical University of Athens, Zografou Campus, GR-157 73, Athens, Greece.

[1] L. D. Landau and E. M. Lifshitz, *Theory of Elasticity*, 3rd ed. (Butterworth-Heinemann Ltd., Oxford, 1986).

[2] W. Lamb, D.M. Wood, and N.W. Ashcroft, Phys. Rev. B **21**, 2248 (1980).

[3] J. D. Joannopoulos, R. D. Meade, and J. N. Winn, *Photonic Crystals* (Princeton University Press, Princeton, NJ, 1995).

[4] *Photonic Band Gap Materials*, edited by C. M. Soukoulis (Kluwer Academic, Dordrecht, 1996).

[5] E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987); E. Yablonovitch and T.J. Gmitter, **63**, 1950 (1989).

[6] E. Yablonovitch, J. Phys.: Condens. Matter **5**, 2443 (1993); T.F. Krauss and R.M. De La Rue, Prog. Quantum Electron. **23**, 51 (1999).

[7] B.G. Levi, Phys. Today **52** (1), 17 (1999).

[8] S. John, Phys. Today **44** (5), 32 (1991).

[9] *Scattering and Localization of Classical Waves in Random Media*, edited by P. Sheng (World Scientific, Singapore, 1990).

[10] E.N. Economou and M. Sigalas, J. Acoust. Soc. Am. **95**, 1734 (1994); M. Kafesaki, M.M. Sigalas, and E.N. Economou, Solid State Commun. **96**, 285 (1995).

[11] M.S. Kushwaha and B. Djafari-Rouhani, J. Appl. Phys. **80**, 3191 (1996); M.S. Kushwaha and P. Halevi, J. Acoust. Soc. Am. **101**, 619 (1997).

[12] M.S. Kushwaha, B. Djafari-Rouhani, L. Dobrzynski, and J.O. Vasseur, Eur. Phys. J. B **3**, 155 (1998).

[13] R. Sprik and G.H. Wegdam, Solid State Commun. **106**, 77 (1998).

[14] M.S. Kushwaha, P. Halevi, L. Dobrzynski, and B. Djafari-Rouhani, Phys. Rev. Lett. **71**, 2022 (1993); M.S. Kushwaha, P. Halevi, G. Martínez, L. Dobrzynski, and B. Djafari-Rouhani, Phys. Rev. B **49**, 2313 (1994); M.M. Sigalas and E.N. Economou, Phys. Rev. Lett. **75**, 3580 (1995); M.S. Kushwaha, P. Halevi, L. Dobrzynski, and B. Djafari-Rouhani, *ibid.* **75**, 3581 (1995).

[15] M.S. Kushwaha and P. Halevi, Appl. Phys. Lett. **64**, 1085 (1994); **69**, 31 (1996); M.S. Kushwaha, *ibid.* **70**, 3218 (1997).

[16] M. Sigalas and E.N. Economou, Solid State Commun. **86**, 141 (1993); J. Appl. Phys. **75**, 2845 (1994); Europhys. Lett. **36**, 241 (1996); M.M. Sigalas, J. Acoust. Soc. Am. **101**, 1256 (1997); J. Appl. Phys. **84**, 3026 (1998).

[17] J.O. Vasseur, B. Djafari-Rouhani, L. Dobrzynski, M.S. Kush-

waha, and P. Halevi, J. Phys.: Condens. Matter **6**, 8759 (1994); J.O. Vasseur, B. Djafari-Rouhani, L. Dobrzynski, and P.A. Deymier, *ibid.* **9**, 7327 (1997); J.O. Vasseur, P.A. Deymier, G. Frantziskonis, G. Hong, B. Djafari-Rouhani, and L. Dobrzynski, *ibid.* **10**, 6051 (1998).

[18] R. Mártinez-Sala, J. Sancho, J.V. Sánchez, V. Gómez, J. Llinares, and F. Meseguer, Nature (London) **378**, 241 (1995); J.V. Sánchez-Pérez, D. Caballero, R. Mártinez-Sala, C. Rubio, J. Sánchez-Dehesa, F. Meseguer, J. Llinares, and F. Gálvez, Phys. Rev. Lett. **80**, 5325 (1998); F. Meseguer, M. Holgado, D. Caballero, N. Benaches, J. Sánchez-Dehesa, C. López, and J. Llinares, Phys. Rev. B **59**, 12 169 (1999).

[19] F.R. Montero de Espinosa, E. Jiménez, and M. Torres, Phys. Rev. Lett. **80**, 1208 (1998); M. Torres, F.R. Montero de Espinosa, D. García-Pablos, and N. García, *ibid.* **82**, 3054 (1999).

[20] R.L. Weaver, Wave Motion **12**, 129 (1990); Phys. Rev. B **47**, 1077 (1993); L. Ye, G. Cody, M. Zhou, P. Sheng, and A.N. Norris, Phys. Rev. Lett. **69**, 3080 (1992).

[21] M.A. Biot, J. Appl. Phys. **33**, 1482 (1961); K. Attenborough, Phys. Rep. **82**, 179 (1982).

[22] L.M. Schwartz and D.L. Johnson, Phys. Rev. B **30**, 4302 (1984); D.L. Johnson, T.J. Ploma, and H. Kojima, J. Appl. Phys. **76**, 115 (1994).

[23] J.A. Marqusee and J.M. Deutch, J. Chem. Phys. **75**, 5239 (1981).

[24] D.L. Johnson, J. Chem. Phys. **77**, 1531 (1983).

[25] J. Liu, L. Ye, D.A. Weitz, and P. Sheng, Phys. Rev. Lett. **65**, 2602 (1990); X. Jing, P. Sheng, and M. Zhou, *ibid.* **66**, 1240 (1991); X. Jing, P. Sheng, and M. Zhou, Phys. Rev. A **46**, 6513 (1992).

[26] J.B. Pendry and A. MacKinnon, Phys. Rev. Lett. **69**, 2772 (1992); J.B. Pendry, J. Mod. Opt. **41**, 209 (1994).

[27] N. Stefanou, V. Karathanos, and A. Modinos, J. Phys.: Condens. Matter **4**, 7389 (1992); N. Stefanou, V. Yannopapas, and A. Modinos, Comput. Phys. Commun. **113**, 49 (1998).

[28] K. Ohtaka, Phys. Rev. B **19**, 5057 (1979); K. Ohtaka and Y. Tanabe, J. Phys. Soc. Jpn. **65**, 2276 (1996).

[29] Y. Qiu, K.M. Leung, L. Carin, and D. Kralj, J. Appl. Phys. **77**, 3631 (1995).

[30] The reader who is not familiar with on-shell methods may find it easier to follow the formalism of the present paper if he familiarizes himself with the concepts and methodology of these methods as applied to the simpler problem of electron scattering in crystals (see, e.g., Chaps. 3 and 4 of Ref. 34).

[31] D. Brill and G. Gaunaurd, J. Acoust. Soc. Am. **81**, 1 (1987).

[32] W. C. Chew, *Waves and Fields in Inhomogeneous Media* (Van Nostrant Reinhold, New York, 1990).

[33] J. B. Pendry, *Low Energy Electron Diffraction* (Academic Press, London, 1974).

[34] A. Modinos, *Field, Thermionic and Secondary Electron Emission Spectroscopy* (Plenum Press, New York, 1984).

[35] B. A. Auld, *Acoustic Fields and Waves in Solids* (Wiley, New York, 1973), Vol. I.

[36] V. Karathanos, J. Mod. Opt. **45**, 1751 (1998).

[37] A. Modinos, Physica A **141**, 575 (1987).

[38] M. E. Rose, *Elementary Theory of Angular Momentum* (Wiley, New York, 1957).

[39] E.G. McRae, Surf. Sci. **11**, 479 (1968); **11**, 492 (1968).