Propagation of electromagnetic waves in periodic lattices of spheres: Green's function and lattice sums

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(Received 16 August 1994)

We have recently exhibited expressions for Green's functions for dynamic scattering problems for gratings and two-dimensional arrays, expressed in terms of lattice sums. We have also discussed efficient techniques to evaluate these sums and how their use in Green's function forms leads naturally to Rayleigh identities for scattering problems. These Rayleigh identities express connections between regular parts of wave solutions near a particular scatterer and irregular parts of the solution summed over all other scatterers in a system. Here we discuss these ideas and techniques in the context of the problem of the scattering of a scalar wave by a regular lattice of spheres. We discuss expressions for lattice sums which can be integrated arbitrarily-many times to accelerate convergence, a computationally efficient Green's function form, and the appropriate Rayleigh identity for the problem. We also discuss the long-wavelength limit and obtain the Maxwell-Garnett formula for lattices of perfectly conducting spheres.

PACS number(s): 03.50.De, 41.20.Jb, 71.25.Cx

I. INTRODUCTION

Recently, it has been proved, both theoretically and experimentally, that periodic dielectric structures in one, two, or three dimensions exhibit photonic band gaps [1,2]. In such structures, called "dielectric crystals," new types of electron-photon interactions appear leading to a specific behavior of light.

The most widely used theoretical approach in calculating the photonic band structures relies on the treatment of the full vector Maxwell equations by means of Bloch expansions [3–5]. In this method, the coefficients of the series expansions are the solutions of a homogeneous linear system of equations. At the same time, from the secular equation associated with this system, one obtains the wave numbers of the propagating modes. The effective dielectric constant of the composite is obtained as the long-wavelength (or quasistatic) limit of the photonic band structure problem [6]. Due to the fact that the Bloch expansions converge slowly, this method requires a large number of terms in the series in order to obtain accurate numerical results. This also requires the evaluation of large determinants by complicated and time consuming numerical algorithms.

The Korringa-Kohn-Rostoker (KKR) method [7–9] is a classical technique for the solution of the Schrödinger equation in periodic lattices of atoms. The KKR method, as developed by Korringa [7], was explicitly inspired by a formulation due to Lord Rayleigh [10] for the solution of electrostatic problems involving lattices of spheres or arrays of cylinders. The work in this paper represents the continuation of a series of papers which have extended Rayleigh's technique from static to dynamic problems, for both singly [11,12] and doubly periodic [13,14] systems. We now turn to triply periodic scattering systems and exhibit what may be regarded as either the generalization of the KKR method to photonics, called for by Lamb *et al.* [15] and Moroz [16], or as a further development in our generalizations of the Rayleigh method.

In order to illustrate the method, we restrict our considerations to the propagation of an electromagnetic wave through a periodic lattice of perfectly conducting spheres embedded in an isotropic homogeneous host medium. In this case we may use the scalar wave equation. First, we present the spatial form and the spectral domain form of the Green's function. These two forms are related by the Poisson summation formula as generalized to quasiperiodic problems. In this way we obtain dynamic lattice sums which in turn provide us with the Neumann series for the spatial form of the Green's function. Then, by applying the Green's theorem to the pair constituting the Green's function and the general solution of the wave equation, we obtain the dynamic Rayleigh identity in the form of an infinite, linear homogeneous system of equations. The unknowns of this system are the expansion coefficients of the propagating modes, while the zeros of the determinant define the wave numbers of the modes. Finally, we analyze the quasistatic limit of the dynamic Rayleigh identity in the case of a simple cubic lattice. In the first-order approximation, we obtain the usual Maxwell-Garnett formula for a two-phase composite.

The lattice sums involved in our method are represented in terms of absolutely converging series over the reciprocal lattice [14,17]. In contrast to the method used by Ewald [18], these series may be accelerated by successive integrations to any order. By introducing the lattice sums, we obtain a representation of the Green's function in terms of a rapidly convergent Neumann series. In numerical applications, the use of such a representation with fast converging lattice sums leads to a simpler secular equation and consequently to a high efficiency in computing time. This high efficiency is obtained when we need the numerical values of the Green's function or fields at several spatial points. The coefficients of the series expansions for these physical quantities are in essence the lattice sums which, for a given mode in a specified lattice, have to be evaluated once only. Therefore, we need only to evaluate the spatially varying part of a small number of terms in the corresponding Neumann series.

In order to make clear the main parts of our method we have moved most of the mathematical details to appendixes, and refer to results from the Appendixes using bracketed equation numbers.

II. QUASIPERIODIC GREEN'S FUNCTION

We consider the case of a periodic lattice of identical spheres, of radius a, embedded in a homogeneous material. Let $\hat{\mathbf{e}}_1$, $\hat{\mathbf{e}}_2$, and $\hat{\mathbf{e}}_3$ be the three fundamental translation vectors of the lattice. These vectors are not necessarily orthogonal, nor are their lengths necessarily equal. Thus the vectors from the origin of coordinates to the center of the pth sphere are specified by a set of three integers:

$$\mathbf{R}_p = p_1\hat{\mathbf{e}}_1 + p_2\hat{\mathbf{e}}_2 + p_3\hat{\mathbf{e}}_3 \equiv (p_1, p_2, p_3) \quad , \quad p_i \in \mathbb{Z}. \quad (1)$$

We denote by $\mathcal{D}$ the primitive cell of the lattice and by V the volume of $\mathcal{D}$. The primitive cell of the reciprocal lattice is defined by the vectors

$$\hat{\mathbf{u}}_i = \frac{\hat{\mathbf{e}}_j \times \hat{\mathbf{e}}_k}{V}, \quad (i,j,k) = (1,2,3) \quad (2)$$

and the vectors in the reciprocal lattice have the form

$$\mathbf{K}_h = 2\pi(h_1\hat{\mathbf{u}}_1 + h_2\hat{\mathbf{u}}_2 + h_3\hat{\mathbf{u}}_3) \equiv (h_1, h_2, h_3)\,, \quad (3)$$

with $h_i \in \mathbb{Z}$.

The propagation of an electromagnetic wave through the lattice is described by the Maxwell equations. In the case when the host medium is an isotropic homogeneous dielectric in which the electromagnetic wave has the wave number k, the equations for the components of the electric and magnetic fields decouple and each field component satisfies the Helmholtz equation

$$\left(\nabla^2 + k^2\right) f(\mathbf{r}) = 0\,. \quad (4)$$

The solution $f(\mathbf{r})$ has to fulfill the boundary conditions at the surfaces of the spheres and the quasiperiodicity condition

$$f(\mathbf{r} + \mathbf{R}_p) = e^{i\mathbf{k}_i\cdot\mathbf{R}_p} f(\mathbf{r}) \;\; \forall p\,, \quad (5)$$

where $\mathbf{k}_i = (k_i, \theta_i, \varphi_i)$ is the wave vector of the incident radiation (Bloch momentum). The quasiperiodicity condition follows from the Bloch theorem, stating that the field on the pth sphere depends explicitly on the sphere position $(\mathbf{R}_p)$ through the phase factor $\exp(i\mathbf{k}_i \cdot \mathbf{R}_p)$ [19].

The inhomogeneous Helmholtz equation, defining the quasiperiodic Green's function, has the form

$$\left(\nabla_r^2 + k^2\right) G(\mathbf{r};\boldsymbol{\rho}) = -\sum_p \delta(\mathbf{r} - \mathbf{R}_p - \boldsymbol{\rho}) e^{i\mathbf{k}_i\cdot\mathbf{R}_p}, \quad (6)$$

where the Laplacian operator ∇_r^2 acts on the components of the vector $\mathbf{r}$. The solution of this equation is the spatial domain form of the Green's function

$$G(\mathbf{r};\boldsymbol{\rho}) = \frac{1}{4\pi}\sum_p \frac{e^{ik|\mathbf{r}-\mathbf{R}_p-\boldsymbol{\rho}|}}{|\mathbf{r}-\mathbf{R}_p-\boldsymbol{\rho}|} e^{i\mathbf{k}_i\cdot\mathbf{R}_p}. \quad (7)$$

We mention that, in terms of the spherical Bessel functions of the third kind (A3), the Green's function takes the form

$$G(\mathbf{r};\boldsymbol{\rho}) = \frac{ik}{4\pi}\sum_p h_0^{(1)}(k|\mathbf{r}-\mathbf{R}_p-\boldsymbol{\rho}|) e^{i\mathbf{k}_i\cdot\mathbf{R}_p}, \quad (8)$$

which is written in a form similar to the expression of the Green's function for the two-dimensional problem [14].

If we apply on the right-hand side of (6) the Poisson summation formula (as generalized to quasiperiodic problems)

$$\frac{1}{V}\sum_h e^{i\mathbf{Q}_h\cdot\mathbf{r}} = \sum_p \delta(\mathbf{r}-\mathbf{R}_p) e^{i\mathbf{k}_i\cdot\mathbf{R}_p} \quad (9)$$

and expand the Green's function in the Fourier series

$$G(\mathbf{r};\boldsymbol{\rho}) = \sum_h g(\mathbf{Q}_h) e^{i\mathbf{Q}_h\cdot(\mathbf{r}-\boldsymbol{\rho})}\,, \quad (10)$$

where $\mathbf{Q}_h = \mathbf{K}_h + \mathbf{k}_i$, we obtain the spectral domain form of the Green's function

$$G(\mathbf{r};\boldsymbol{\rho}) = \frac{1}{V}\sum_h \frac{e^{i\mathbf{Q}_h\cdot(\mathbf{r}-\boldsymbol{\rho})}}{{Q_h}^2 - k^2}\,. \quad (11)$$

The Green's function, expressed by (7) or (11), is Hermitian:

$$G(\mathbf{r};\boldsymbol{\rho}) = G^*(\boldsymbol{\rho};\mathbf{r})\,, \quad (12)$$

with the asterisk denoting complex conjugation, and satisfies the quasiperiodicity relations

$$G(\mathbf{r}+\mathbf{R}_p;\boldsymbol{\rho}) = e^{i\mathbf{k}_i\cdot\mathbf{R}_p}\, G(\mathbf{r};\boldsymbol{\rho})\,, \quad (13)$$

$$G(\mathbf{r};\boldsymbol{\rho}+\mathbf{R}_p) = e^{-i\mathbf{k}_i\cdot\mathbf{R}_p}\, G(\mathbf{r};\boldsymbol{\rho})\,. \quad (14)$$

Actually, the two forms of the Green's function (7) and (11) are equal [8] and this equality follows from the Poisson summation formula

$$\sum_h \frac{e^{i\mathbf{Q}_h\cdot(\mathbf{r}-\boldsymbol{\rho})}}{{Q_h}^2 - k^2} = \frac{V}{4\pi}\sum_p \frac{e^{ik|\mathbf{r}-\mathbf{R}_p-\boldsymbol{\rho}|}}{|\mathbf{r}-\mathbf{R}_p-\boldsymbol{\rho}|} e^{i\mathbf{k}_i\cdot\mathbf{R}_p}. \quad (15)$$

III. LATTICE SUMS

In this section we will consider the Green's function depending on only one variable $\boldsymbol{\xi} = \mathbf{r} - \boldsymbol{\rho}$, so that (15) may be written in the form

$$\sum_h \frac{e^{i\mathbf{Q}_h\cdot\boldsymbol{\xi}}}{Q_h{}^2 - k^2} = \frac{V}{4\pi}\sum_p \frac{e^{ik|\boldsymbol{\xi}-\mathbf{R}_p|}}{|\boldsymbol{\xi}-\mathbf{R}_p|} e^{i\mathbf{k}_i\cdot\mathbf{R}_p}. \quad (16)$$

We also consider that $\boldsymbol{\xi}$ is restricted to the unit cell centered at the origin of coordinates, so that $\xi < R_p \; \forall p \neq 0$ (see Fig. 1 for the case of a simple cubic lattice and for the definition of angles θ_ξ, φ_ξ, specifying the orientation of $\boldsymbol{\xi}$). We separate the term for $p = 0$ and follow the method from Ref. [14]. Thus we have

$$\frac{e^{ik\xi}}{\xi} + \sum_{p\neq 0} \frac{e^{ik|\boldsymbol{\xi}-\mathbf{R}_p|}}{|\boldsymbol{\xi}-\mathbf{R}_p|} e^{i\mathbf{k}_i\cdot\mathbf{R}_p} = \frac{4\pi}{V}\sum_h \frac{e^{i\mathbf{Q}_h\cdot\boldsymbol{\xi}}}{Q_h{}^2 - k^2}. \quad (17)$$

Then we expand the terms of the series on the left-hand side and the exponentials on the right-hand side, according to the relations (A12) and (A9), respectively,

$$\frac{1}{4\pi}\frac{e^{ik\xi}}{\xi} + ik\sum_{\ell,m} j_\ell(k\xi) Y_{\ell m}(\theta_\xi,\varphi_\xi) \times \left[\sum_{p\neq 0} h_\ell^{(1)}(kR_p) Y^*_{\ell m}(\theta_p,\varphi_p) e^{i\mathbf{k}_i\cdot\mathbf{R}_p}\right] = \frac{4\pi}{V}\sum_{\ell,m} i^\ell Y_{\ell m}(\theta_\xi,\varphi_\xi)\left[\sum_h \frac{j_\ell(Q_h\xi)}{Q_h^2 - k^2} Y^*_{\ell m}(\theta_h,\varphi_h)\right].$$

Finally, by multiplying both sides by $Y^*_{\ell m}(\theta_\xi,\varphi_\xi)$ and integrating over the directions of $\boldsymbol{\xi}$, we obtain

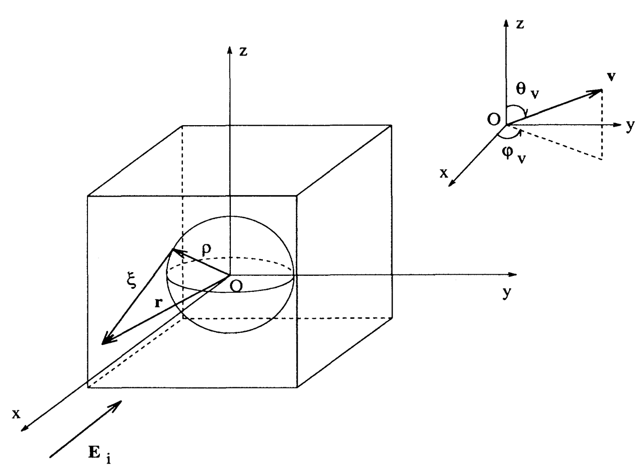

FIG. 1. The unit cell for a simple cubic lattice of spheres. The inset shows the declination (θ_v) and the azimuthal (φ_v) angles, which define the direction of the arbitrary vector $\mathbf{v} = (v, \theta_v, \varphi_v)$.

$$\frac{ik}{\sqrt{4\pi}} h_0^{(1)}(k\xi)\delta_{\ell,0}\delta_{m,0} + ikj_\ell(k\xi)S_{\ell m} = \frac{4\pi}{V} i^\ell \sum_h \frac{j_\ell(Q_h\xi)}{Q_h{}^2 - k^2} Y^*_{\ell m}(\theta_h,\varphi_h),$$

where we have identified the dynamic lattice sums

$$S_{\ell m} = \sum_{p\neq 0} h_\ell^{(1)}(kR_p) Y^*_{\ell m}(\theta_p,\varphi_p)\, e^{i\mathbf{k}_i\cdot\mathbf{R}_p} \quad (18)$$

and $h_\ell^{(1)}(z)$ are spherical Bessel functions of the third kind (A3).

In this way we have obtained the representation of the lattice sums in terms of series over the reciprocal lattice

$$S_{\ell m} j_\ell(k\xi) = -\frac{1}{\sqrt{4\pi}} h_0^{(1)}(k\xi)\delta_{\ell,0}\delta_{m,0} - \frac{4\pi}{kV} i^{\ell+1} \sum_h \frac{j_\ell(Q_h\xi)}{Q_h{}^2 - k^2} Y^*_{\ell m}(\theta_h,\varphi_h). \quad (19)$$

We may also define $S_{\ell m} = S^j_{\ell m} + iS^y_{\ell m}$, where

$$S^j_{\ell m} = \sum_{p\neq 0} j_\ell(kR_p) Y^*_{\ell m}(\theta_p,\varphi_p)\, e^{i\mathbf{k}_i\cdot\mathbf{R}_p}, \quad (20)$$

$$S^y_{\ell m} = \sum_{p\neq 0} y_\ell(kR_p) Y^*_{\ell m}(\theta_p,\varphi_p)\, e^{i\mathbf{k}_i\cdot\mathbf{R}_p}. \quad (21)$$

As in the two-dimensional case, we may evaluate exactly the lattice sums $S^j_{\ell m}$. Starting with the Poisson summation formula

$$\sum_p e^{i\mathbf{R}_p\cdot\mathbf{s}} = \frac{4\pi}{V}\sum_h \delta(\mathbf{s} - \mathbf{K}_h) \quad (22)$$

and choosing $\mathbf{s} = \mathbf{k} + \mathbf{k}_i$, under the assumption that $\mathbf{s} \neq \mathbf{K}_h \; \forall h$, we obtain

$$\sum_p e^{i\mathbf{R}_p\cdot(\mathbf{k}+\mathbf{k}_i)} = 0. \quad (23)$$

Here $\mathbf{k}$ is an arbitrary wave vector. Then we separate the term for $p = 0$ and expand $\exp(i\mathbf{k}\cdot\mathbf{R_p})$ according to (A9),

$$\sum_{\ell m} i^\ell S^j_{\ell m} Y_{\ell m}(\theta_k,\varphi_k) = -\frac{1}{4\pi} = -\frac{1}{\sqrt{4\pi}} Y_{00}(\theta_k,\varphi_k). \quad (24)$$

Integration over the directions of $\mathbf{k}$ and use of the orthogonality relation (A14) gives

$$S^j_{\ell m} = -\frac{1}{\sqrt{4\pi}}\delta_{\ell,0}\delta_{m,0}. \quad (25)$$

By substituting (25) in (19) we obtain the representation of the nontrivial lattice sums (21)

$$S^y_{\ell m} j_\ell(k\xi) = -\frac{1}{\sqrt{4\pi}} y_0(k\xi)\delta_{\ell,0}\delta_{m,0} - \frac{4\pi}{kV} i^\ell \sum_h \frac{j_\ell(Q_h\xi)}{Q_h{}^2 - k^2} Y^*_{\ell m}(\theta_h,\varphi_h). \quad (26)$$

For fixed k, ℓ, m, Eq. (26) is true independent of ξ and provides us with an identity relating sums of spherical Bessel functions. The vector $\boldsymbol{\xi}$ has always to be confined within the unit cell. Therefore, in numerical applications, we set $\xi = \min\{|\hat{\mathbf{e}}_k|\}$.

For large arguments, the spherical Bessel functions of the first kind have the principal asymptotic form [20]

$$j_\ell(z) \sim \frac{1}{z}\cos(z - \ell\pi/2 - \pi/2)$$

and so the series of moduli, associated with the series in (26), diverge logarithmically. Hence, in the representation (26) all the lattice sums $S^y_{\ell m}$ converge conditionally. Following the method for series acceleration, from Ref. [14], we may express the lattice sums $S^y_{\ell m}$ in terms of absolutely converging series. Thus we multiply both sides in (26) by $\xi^{\ell+2}$ and integrate over ξ from 0 to η, where $\eta \leq 1$. The integrals may be expressed in the closed forms [20]

$$\int_0^\eta \xi^{\ell+2} j_\ell(a\xi)d\xi = \eta^{\ell+2}\frac{j_{\ell+1}(a\eta)}{a}, \quad (27)$$

$$\int_0^\eta \xi^{\ell+2} y_\ell(a\xi)d\xi = \eta^{\ell+2}\frac{y_{\ell+1}(a\eta)}{a} + \frac{2^{\ell+1}\Gamma(\ell+3/2)}{a^{\ell+3}\sqrt{\pi}} \quad (28)$$

for $\ell \geq 0$. Then we change η into ξ and repeat the same procedure, this time multiplying both sides of the equation by $\xi^{\ell+3}$. After q steps, we obtain

$$S^y_{\ell m} j_{\ell+q}(k\xi) = -\frac{1}{\sqrt{4\pi}}\left[y_q(k\xi) + w_q(k\xi)\right]\delta_{\ell,0}\delta_{m,0} - \frac{4\pi}{kV} i^\ell \sum_h \left(\frac{k}{Q_h}\right)^q \frac{j_{\ell+q}(Q_h\xi)}{Q_h{}^2 - k^2} \times Y^*_{\ell m}(\theta_h, \varphi_h), \quad (29)$$

where

$$w_q(k\xi) = \frac{1}{2\sqrt{\pi}}\sum_{p=0}^{q-1}\frac{\Gamma(q-p+1/2)}{p!}\left(\frac{2}{k\xi}\right)^{q-2p+1}.$$

Now, for all $q \geq 1$, the series in (29) converge absolutely. At the same time, by increasing the value of q we make the series in (29) converge more rapidly. This is an important feature in numerical computations. As in the case of two-dimensional lattice sums, too large values of q lead to an instability of the numerical algorithm [14]. In particular, for small k we have to use small values for q (for instance, 2 or 3) and replace the term $y_q(k\xi)+w_q(k\xi)$ by the convergent part from the series expansion of $y_q(z)$ [21],

$$y_q(k\xi) + w_q(k\xi) = \frac{\sqrt{\pi}}{2}\sum_{p=q}^{\infty}\frac{(-1)^{p-q}}{p!\Gamma(p-q+1/2)}\left(\frac{k\xi}{2}\right)^{2p-q-1}.$$

We mention that (29) may be used for $m \geq 0$. The lattice sums with $m < 0$ are given by the equation

$$S^y_{\ell,-m} = (-1)^\ell S^{y*}_{\ell m}, \quad (30)$$

which follows directly from the definition (21).

In Fig. 2 we compare the convergence of the lattice sum S^y_{20} with the number of terms involved in summation over

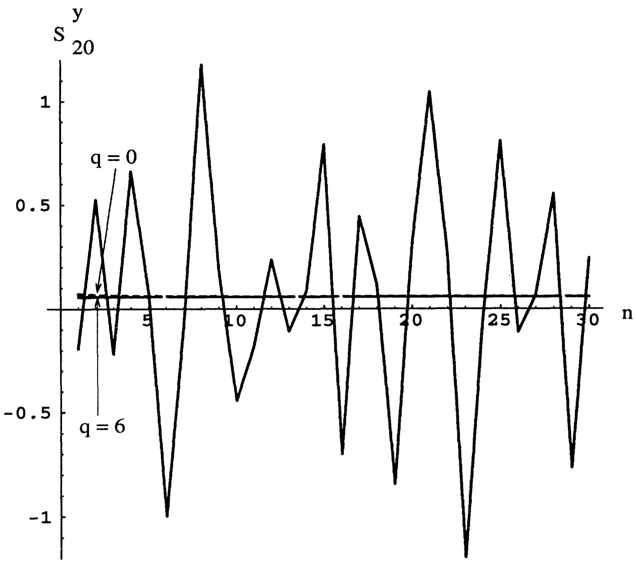

FIG. 2. The dynamic lattice sum S^y_{20} for $\mathbf{k}_i = (1.2, 0, 0.5)$ and $k = 2.3$. The solid curve represents S^y_{20} as given by the sum (21) over the direct lattice with $p_{1,2,3} \in [-n, n]$, while the dashed curves represent S^y_{20} as given by the sum (29) over the reciprocal lattice with $h_{1,2,3} \in [-n, n]$ and $\xi = 1$, for different orders of series acceleration q.

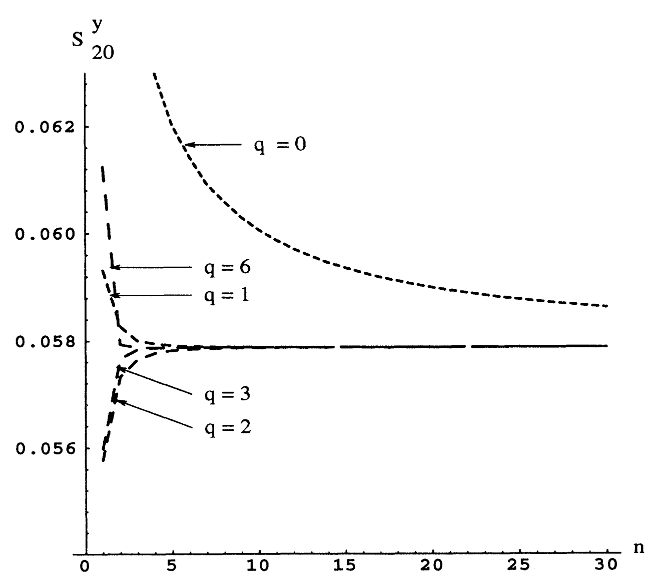

FIG. 3. The dynamic lattice sum S^y_{20} as given by the sum (29) over the reciprocal lattice with $h_{1,2,3} \in [-n, n]$ and $\xi = 1$, for different orders of series acceleration q. Also, $\mathbf{k}_i = (1.2, 0, 0.5)$ and $k = 2.3$.

TABLE I. The numerical values of the lattice sum S_{64}^{y} as a function of k, for $\mathbf{k}_i = (1.2, 0, 0.5)$ and $h_{1,2,3} \in [-30, 30]$, as given by (29), for $q = 0, 1, 3, 6$. The computation time for this table was 429 s (CPU time) for a FORTRAN computer program run on a DEC ALPHA 3000. computer. The number in brackets denotes the power of 10 by which the preceding is to be multiplied.

k	q			
	0	1	3	6
1.0	0.819186411852387[+04]	0.841651684845925[+04]	0.841656244086037[+04]	0.841656012387273[+04]
2.0	0.709019550555784[+02]	0.728436380691055[+02]	0.728440270179216[+02]	0.728440075631804[+02]
3.0	0.487881116948925[+01]	0.501367084205489[+01]	0.501369725187842[+01]	0.501369596654419[+01]
4.0	0.748955049958104[+00]	0.771977146536978[+00]	0.771981505255299[+00]	0.771981301506167[+00]
5.0	−0.488983051569029[+00]	−0.482277566609037[+00]	−0.482276356154453[+00]	−0.482276409668387[+00]
6.0	0.376054591098526[−01]	0.404634033752571[−01]	0.404638861338264[−01]	0.404638663380802[−01]
7.0	0.286510335422465[+00]	0.288176820077083[+00]	0.288177076171283[+00]	0.288177066683895[+00]
8.0	0.810234383167462[+00]	0.811547784925639[+00]	0.811547959731758[+00]	0.811547954103075[+00]
9.0	−0.388981141556492[−01]	−0.374070364938334[−01]	−0.374068825809523[−01]	−0.374068866200560[−01]
10.0	0.568063626017161[+00]	0.571680363085179[+00]	0.571680548800277[+00]	0.571680545314962[+00]

the direct lattice (21) and over the reciprocal lattice (29). Note the oscillatory nature of the direct lattice results, with no evidence of convergence being evident. By contrast, reciprocal lattice results with $q = 0$ and $q = 6$ agree to graphic accuracy from $n \approx 5$ onwards. The numerical values, and those given below, have been calculated in double precision FORTRAN, using double precision routines from AT&T (ftp address netlib.att.com) for Bessel and Γ functions and for associated Legendre functions.

In Fig. 3 we compare the rate of covergence of the reciprocal lattice formula (29) for S_{20}^{y}, for various rates of acceleration. The accelerated forms all agree to graphic accuracy from $n \approx 7$ onwards. A similar comparison is made for S_{64}^{y} in Fig. 4. Note that, as in the case of S_{20}^{y}, the direct lattice summation (21) yields an oscillatory result, which fluctuates about the accelerated reciprocal lattice results.

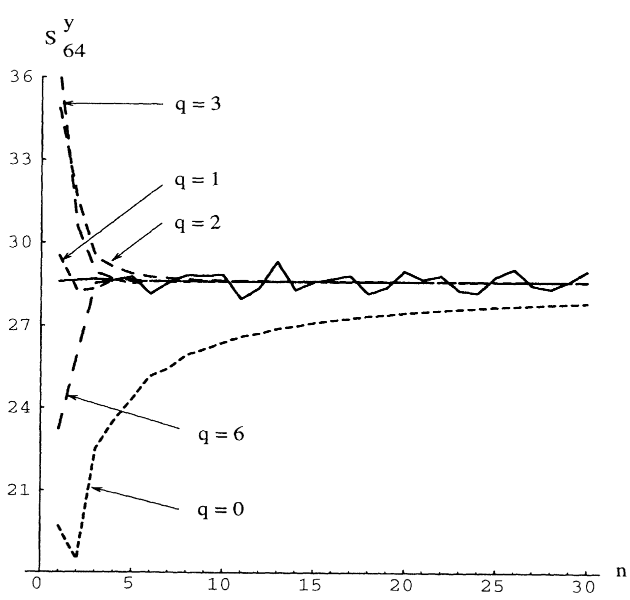

FIG. 4. The dynamic lattice sum S_{64}^{y} for $\mathbf{k}_i = (1.2, 0, 0.5)$ and $k = 2.3$. The solid curve represents S_{64}^{y} as given by the sum (21) over the direct lattice with $p_{1,2,3} \in [-n, n]$, while the dashed curves represent S_{64}^{y} as given by the sum (29) over the reciprocal lattice with $h_{1,2,3} \in [-n, n]$ and $\xi = 1$, for different orders of series acceleration q.

In Table I we provide numerical values for the reciprocal lattice results for S_{64}^{y}. Note that the values for $q = 3, 6$ agree to better than 10^{-6}. As far as we know, no previous values for these lattice sums have been reported. Essentially, the same algorithm was used as that whose results are compared with those of Berman and Greengard [22] for static sums in Appendix C.

In Figs. 5 and 6 we display the behavior of the lattice sums S_{00}^{y} and S_{20}^{y} as functions of k. Note that all lattice sums diverge whenever k is equal to the magnitude of a reciprocal lattice vector $\mathbf{Q}_h$, in agreement with the Bragg condition [19] and Eq. (29). All lattice sums also diverge at the origin ($k = 0$).

IV. NEUMANN SERIES FOR THE GREEN'S FUNCTION

From (7), by means of (A12), we obtain the Green's function as a Neumann series [21] in terms of the spher-

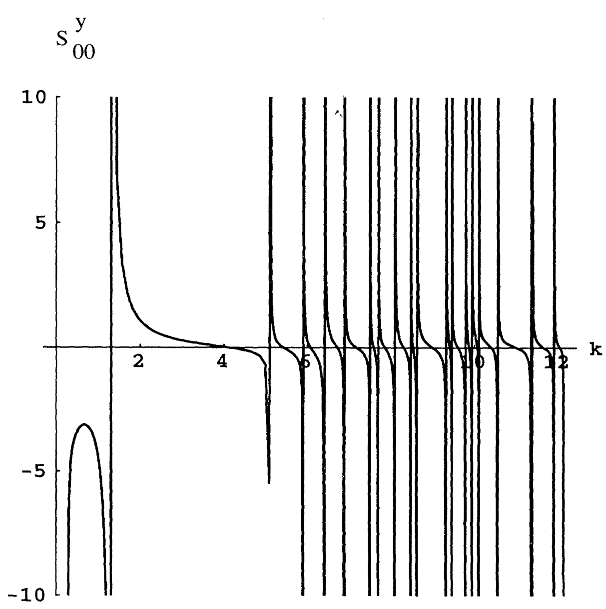

FIG. 5. The lattice sum S_{00}^{y} as a function of k, for $\mathbf{k}_i = (1.2, 0, 0.5)$, $q = 6$, and $h_{1,2,3} \in [-20, 20]$.

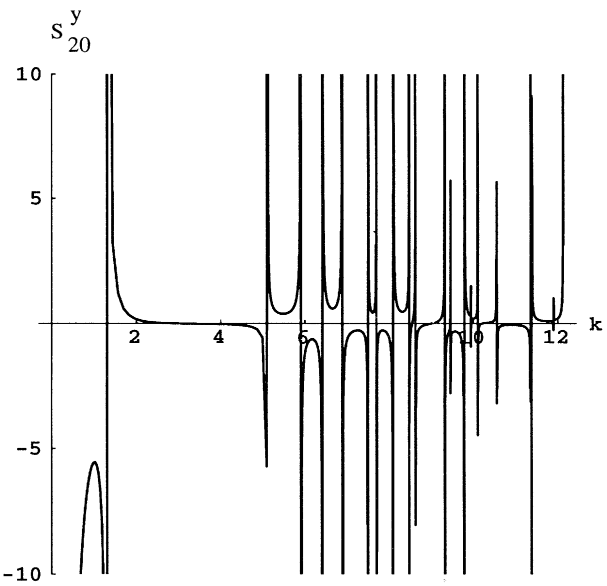

FIG. 6. The lattice sum S^y_{20} as a function of k, for $\mathbf{k}_i = (1.2, 0, 0.5)$, $q = 6$, and $h_{1,2,3} \in [-20, 20]$.

ical Bessel functions of the first kind

$$G(\boldsymbol{\xi}) = \frac{ik}{4\pi} h_0^{(1)}(k\xi) + ik \sum_{\ell m} S_{\ell m} j_\ell(k\xi) Y_{\ell m}(\theta_\xi, \varphi_\xi) \quad (31)$$

and, by substituting (25), we have

$$G(\boldsymbol{\xi}) = -\frac{k}{4\pi} y_0(k\xi) - k \sum_{\ell m} S^y_{\ell m} j_\ell(k\xi) Y_{\ell m}(\theta_\xi, \varphi_\xi). \quad (32)$$

The lattice sums of large order ℓ are well approximated by the nearest-neighbor terms

$$S^{y,\mathrm{NN}}_{\ell m} = \sum_{p \in \mathcal{N}^*} y_\ell(kR_p) Y^*_{\ell m}(\theta_p, \varphi_p) e^{i\mathbf{k}_i \cdot \mathbf{R}_p}.$$

Here $\mathcal{N}^*$ represents the set of triplets $p = (p_1, p_2, p_3)$ indexing the vectors $\mathbf{R}_p$, which point to the nearest neighbors of the sphere centered at the origin

$$\mathcal{N}^* = \{(p_1, p_2, p_3) | p_1, p_2, p_3 \in [-1, 1]\} \setminus \{(0, 0, 0)\}.$$

By means of the nearest-neighbor estimate for the lattice sums, we may apply Kummer's method [20] to accelerate the convergence of the Neumann series in (32),

$$\begin{aligned} G(\boldsymbol{\xi}) = &-\frac{k}{4\pi} y_0(k\xi) \\ &-k \sum_{\ell m} \left(S^y_{\ell m} - S^{y,\mathrm{NN}}_{\ell m} \right) j_\ell(k\xi) Y_{\ell m}(\theta_\xi, \varphi_\xi) \\ &-k \sum_{p \in \mathcal{N}^*} \left[\sum_{\ell m} y_\ell(kR_p) j_\ell(k\xi) Y^*_{\ell m}(\theta_p, \varphi_p) \right. \\ &\left. \times Y_{\ell m}(\theta_\xi, \varphi_\xi) \right] e^{i\mathbf{k}_i \cdot \mathbf{R}_p}. \end{aligned}$$

The asymptotic series has a closed form sum so that we have

$$\begin{aligned} G(\boldsymbol{\xi}) = &-\frac{k}{4\pi} y_0(k\xi) - \frac{k}{4\pi} \sum_{p \in \mathcal{N}^*} y_0(k|\boldsymbol{\xi} - \mathbf{R}_p|) e^{i\mathbf{k}_i \cdot \mathbf{R}_p} \\ &-k \sum_{\ell m} \left(S^y_{\ell m} - S^{y,\mathrm{NN}}_{\ell m} \right) j_\ell(k\xi) Y_{\ell m}(\theta_\xi, \varphi_\xi) \end{aligned}$$

or

$$\begin{aligned} G(\boldsymbol{\xi}) = &-\frac{k}{4\pi} \sum_{p \in \mathcal{N}} y_0(k|\boldsymbol{\xi} - \mathbf{R}_p|) e^{i\mathbf{k}_i \cdot \mathbf{R}_p} \\ &-k \sum_{\ell m} \left(S^y_{\ell m} - S^{y,\mathrm{NN}}_{\ell m} \right) j_\ell(k\xi) Y_{\ell m}(\theta_\xi, \varphi_\xi), \end{aligned}$$

where $\mathcal{N} = \mathcal{N}^* \cup \{(0, 0, 0)\}$. In this way, we obtain rapidly converging series in the representation (32) of the Green's function.

The representations (31) and (32) of the Green's function are valid for $\boldsymbol{\xi}$ restricted to the unit cell centered at the origin of coordinates. We may extend the validity of the series expansions in (31) and (32) to a larger region consisting of nearest-neighbor unit cells, by defining the lattice sums

$$\widetilde{S}_{\ell m} = \sum_{p \notin \mathcal{N}} h_\ell^{(1)}(kR_p) Y^*_{\ell m}(\theta_p, \varphi_p)\, e^{i\mathbf{k}_i \cdot \mathbf{R}_p}. \quad (33)$$

With these modified lattice sums we obtain a representation of the Green's function, consisting of two parts

$$\begin{aligned} G(\boldsymbol{\xi}) = &\frac{ik}{4\pi} \sum_{p \in \mathcal{N}} h_0^{(1)}(k|\boldsymbol{\xi} - \mathbf{R}_p|) e^{i\mathbf{k}_i \cdot \mathbf{R}_p} \\ &+ik \sum_{\ell m} \widetilde{S}_{\ell m} j_\ell(k\xi) Y_{\ell m}(\theta_\xi, \varphi_\xi). \end{aligned} \quad (34)$$

The first part in (34) is related to the cluster formed by the sphere at the origin and its nearest neighbors, while the second part refers to the spheres outside this cluster. Now, the series expansion in the representation (34) of the Green's function is valid in the region formed by the unit cell containing the sphere centered at the origin and the unit cells corresponding to the nearest neighbors of this sphere. This procedure may be continued by considering the set of next-nearest-neighbor spheres, and so on, in order to obtain a representation of the Green's function, in terms of a Neumann series, valid in an arbitrary finite region of the lattice. Of course, continuing this procedure indefinitely returns us the expression (8).

V. RAYLEIGH'S IDENTITY

By means of the addition theorem for scalar waves, we separate the variables $\mathbf{r}$ and $\boldsymbol{\rho}$ in the representation (32) of the Green's function (see Appendix B). Then, within the unit cell, we apply the Green's theorem to the pair constituting the Green's function (B8) and the general solution of the Helmholtz equation (4),

$$f(\mathbf{r}) = \sum_{\ell, m} \left[A_{\ell m} j_\ell(kr) + B_{\ell m} y_\ell(kr) \right] Y_{\ell m}(\theta_r, \varphi_r). \quad (35)$$

Thus we have

$$\int_{\mathcal{D}\setminus\mathcal{S}} \left[f(\boldsymbol{\rho})\nabla_{\rho}{}^2 G(\mathbf{r};\boldsymbol{\rho}) - G(\mathbf{r};\boldsymbol{\rho})\nabla_{\rho}{}^2 f(\boldsymbol{\rho})\right] d\boldsymbol{\rho}$$

$$= \int_{\partial\mathcal{D}\cup\partial\mathcal{S}} \left[f(\boldsymbol{\rho})\frac{\partial G(\mathbf{r};\boldsymbol{\rho})}{\partial \mathbf{n}} - G(\mathbf{r};\boldsymbol{\rho})\frac{\partial f(\boldsymbol{\rho})}{\partial \mathbf{n}}\right] ds. \quad (36)$$

Here $\mathcal{D}$ is the volume of the unit cell (Wigner-Seitz cell) with the boundary $\partial\mathcal{D}$ and $\mathcal{S}$ represents the volume of the sphere with the boundary $\partial\mathcal{S}$, while $\mathcal{D}\setminus\mathcal{S}$ means the unit cell $\mathcal{D}$ excluding the sphere $\mathcal{S}$. The left-hand side of (36) may be evaluated by means of (4) and (6). As $\mathbf{r},\boldsymbol{\rho} \in \mathcal{D}$ we obtain $-f(\mathbf{r})$. On the right-hand side of (36), because of the periodicity of the product Gf, the integral over the cell boundaries ($\partial\mathcal{D}$) vanishes. Hence the only contribution comes from the integral over the surface of the sphere

$$f(\mathbf{r}) = \int \left[f(\boldsymbol{\rho})\frac{\partial G(\mathbf{r};\boldsymbol{\rho})}{\partial \rho} - G(\mathbf{r};\boldsymbol{\rho})\frac{\partial f(\boldsymbol{\rho})}{\partial \rho}\right]_{\rho=a} a^2 d\Omega_{\rho},$$

where a is the radius of the sphere. As an example, in the case of a simple cubic lattice, the layout of the vectors $\mathbf{r}$ and $\boldsymbol{\rho}$ is displayed in Fig. 1.

A straightforward procedure, involving the explicit expressions (35) and (B8) and the Wronskian (A4), leads us to the dynamic Rayleigh identity

$$\sum_{\ell,m} A_{\ell m} j_{\ell}(kr) Y_{\ell m}(\theta_r,\varphi_r)$$

$$= \sum_{\ell' m'} B_{\ell' m'} \sum_{\ell'' m''} \sigma_{\ell'' m'';\ell' m'} j_{\ell''}(kr) Y_{\ell'' m''}(\theta_r,\varphi_r). \quad (37)$$

Physically, this identity has a left-hand side which represents the part of the field component f that is a regular function (i.e., does not diverge) at the origin. The right-hand side expresses this function as a sum of the irregular part of f, summed over all the spheres in the lattice. In other words, the part of f that is regular in the neighborhood of the central sphere must have its sources on all the other spheres in the lattice and the waves emanating from the other spheres are just the irregular part, with an appropriate choice of origin. It is interesting that this is the physical argument that generalizes the reasoning of Lord Rayleigh for static problems. The breakup of f according to regular and irregular parts is preferred; the alternative breakup according to incoming and outgoing waves does not appear to be useful.

By means of the orthogonality of spherical harmonics we obtain from (37) the linear system of equations

$$A_{\ell m} - \sum_{\ell',m'} \sigma_{\ell m;\ell' m'} B_{\ell' m'} = 0\,. \quad (38)$$

The boundary conditions on the surface of the sphere impose a relation between the coefficients $A_{\ell m}$ and $B_{\ell m}$. For scalar boundary value problems such as those involving perfectly conducting spheres, this relation is linear

$$A_{\ell m} = T_{\ell} B_{\ell m} \quad (39)$$

and, from (38), we obtain the homogeneous system

$$\sum_{\ell',m'} \left(T_{\ell}\delta_{\ell\ell'}\delta_{mm'} - \sigma_{\ell m;\ell' m'}\right) B_{\ell' m'} = 0\,. \quad (40)$$

The values k for which the determinant of the system (40) vanishes are the eigenvalues of the Helmholtz equation (4), i.e., the wave numbers of the propagating modes. By solving the system (40) for a wave number we obtain the coefficients for the propagating mode (35).

VI. THE QUASISTATIC LIMIT

The equation

$$\det\left|T_{\ell}\delta_{\ell\ell'}\delta_{mm'} - \sigma_{\ell m;\ell' m'}\right| = 0 \quad (41)$$

also defines the band structure of photons propagating through the lattice. If k is required for a general $\mathbf{k}_i$, which is not invariant under any of the symmetry operations from the lattice symmetry group, we will use the lattice sums defined in (29). If $\mathbf{k}_i$ is invariant under some of the symmetry operations from the lattice symmetry group, we have to analyze in detail the behavior of the lattice sums in such situations.

For any lattice, a point of high symmetry is $\mathbf{k}_i = \mathbf{0}$. In relation to the dispersion curves, in the system k versus $\mathbf{k}_i$, we may distinguish two cases [19]: (i) $\mathbf{k}_i = \mathbf{0}$ and $k \neq 0$ for optical bands and (ii) $\mathbf{k}_i \to \mathbf{0}$ and $k = \alpha k_i$ for the acoustic band. Here, $k_i = |\mathbf{k}_i|$ and α is the effective refractive index of the lattice.

In the first case, the lattice sums (26) are simply changed into the form

$$S^{y}_{\ell m} j_{\ell}(k\xi) = -\frac{1}{\sqrt{4\pi}} y_0(k\xi)\delta_{\ell,0}\delta_{m,0} - \frac{4\pi}{kV} i^{\ell} \sum_{h} \frac{j_{\ell}(K_h\xi)}{K_h{}^2 - k^2} Y^{*}_{\ell m}(\theta'_h,\varphi'_h), \quad (42)$$

with the direction of $\mathbf{K}_h$ being specified by polar angles θ'_h and φ'_h, and further, to the corresponding formula containing accelerated series

$$S^{y}_{\ell m} j_{\ell+q}(k\xi)$$

$$= -\frac{1}{\sqrt{4\pi}} \left[y_q(k\xi) + w_q(k\xi)\right]\delta_{\ell,0}\delta_{m,0} - \frac{4\pi}{kV} i^{\ell} \sum_{h} \left(\frac{k}{K_h}\right)^{q} \frac{j_{\ell+q}(K_h\xi)}{K_h{}^2 - k^2} Y^{*}_{\ell m}(\theta'_h,\varphi'_h), \quad (43)$$

with the same function $w_q(k\xi)$ as in (29). Furthermore, in this case, all the lattice sums are real and

$$S^{y}_{\ell,-m} = (-1)^{\ell} S^{y}_{\ell m}\,.$$

The second case represents the quasistatic limit when the linear system (40) takes the form of Rayleigh's identity for the relevant lattice in an electrostatic field. To illustrate this change of the homogeneous linear system (40) into an inhomogeneous linear system, we consider a simple cubic lattice of spheres. The behavior of the dynamic lattice sums when both k and $\mathbf{k}_i$ tend to zero simultaneously is discussed in Appendix C.

If we assume a Dirichlet problem for the field components $f(\mathbf{r})$ in (35)

$$f(\mathbf{r})|_{\partial S} = 0, \tag{44}$$

then the relations (39) take the form

$$A_{\ell m} = -\frac{y_\ell(ka)}{j_\ell(ka)} B_{\ell m} \tag{45}$$

and (35) may be written in the form

$$f(\mathbf{r}) = -\sum_{\ell m}\left[\frac{j_\ell(kr)}{j_\ell(ka)} - \frac{y_\ell(kr)}{y_\ell(ka)}\right] B_{\ell m} y_\ell(ka) Y_{\ell m}(\theta_r,\varphi_r)$$
$$\sim -\sum_{\ell m}\left[\left(\frac{r}{a}\right)^\ell - \left(\frac{a}{r}\right)^{\ell+1}\right]\widetilde{B}_{\ell m} Y_{\ell m}(\theta_r,\varphi_r). \tag{46}$$

Here (46) represents $f(\mathbf{r})$ in the limit $k \to 0$. To obtain this form we have used the relations (A5) and (A6). At the same time, the coefficients $\widetilde{B}_{\ell m}$ are constants (independent of k) and this suggests that, for small $\mathbf{k}_i$ and $k = \alpha k_i$, the coefficients $B_{\ell m}$ depend on k (or k_i) through the relations

$$B_{\ell m} \sim \frac{\widetilde{B}_{\ell m}}{y_\ell(ka)} \sim -\frac{(\alpha k_i a)^{\ell+1}}{(2\ell-1)!!}\widetilde{B}_{\ell m}. \tag{47}$$

We also have

$$A_{\ell m} \sim -\frac{\widetilde{B}_{\ell m}}{j_\ell(ka)} \sim -\frac{(2\ell+1)!!}{(\alpha k_i a)^\ell}\widetilde{B}_{\ell m}. \tag{48}$$

With these notations, in the first-order approximation, the system (38) reduces to the equation

$$\widetilde{B}_{10}\left[1 - \frac{(\alpha k_i a)^3}{3}\sigma_{10;10}\right] = 0. \tag{49}$$

From (B7) we obtain the expression

$$\sigma_{10;10} = \sqrt{4\pi}\left(S^y_{00} - \frac{2}{\sqrt{5}} S^y_{20}\right). \tag{50}$$

In the quasistatic limit for the lattice sums (C12) and (C14) and by assuming that the Bloch momentum $\mathbf{k}_i$ is oriented parallel to the negative y axis (i.e., $\theta_i = \pi/2$ and $\varphi_i = 3\pi/2$), (50) becomes

$$\sigma_{10;10} \sim \frac{6U^0_2}{(\alpha k_i)^3}. \tag{51}$$

Consequently, we obtain, for Eq. (49),

$$\widetilde{B}_{10}\left(1 - 2a^3 U^0_2\right) = 0. \tag{52}$$

In the direct lattice space, the lattice sums U^m_2 are conditionally convergent. In our example, we are interested in the static lattice sum

$$U^0_2 = \sum_{p\neq 0}\frac{P_2(\cos\theta_p)}{{R_p}^3}. \tag{53}$$

The value of this lattice sum depends on the form of the surface at infinity (Σ_2) which encloses the lattice (see Fig. 7). In Cartesian coordinates, the lattice vectors take the form

$$\mathbf{R}_p = x_p\widehat{\mathbf{x}} + y_p\widehat{\mathbf{y}} + z_p\widehat{\mathbf{z}}, \tag{54}$$

where $\widehat{\mathbf{x}}$, $\widehat{\mathbf{y}}$, and $\widehat{\mathbf{z}}$ are the unit vectors along the axes. Also, in Cartesian coordinates, (53) has the form

$$U^0_2 = \sum_{p\neq 0}\frac{2{x_p}^2 - {y_p}^2 - {z_p}^2}{2{R_p}^5} = \sum_{p\neq 0}\frac{2{x_p}^2 - {s_p}^2}{2({x_p}^2 + {s_p}^2)^{5/2}}, \tag{55}$$

where ${s_p}^2 = {y_p}^2 + {z_p}^2$.

Following the method from Refs. [23,24], we write the series in (53) as a finite sum, containing terms within a large sphere (D_1), excluding the origin O, and an integral over the volume (D_2):

$$U^0_2 = \sum_{\mathbf{R}_p\in(D_1\setminus O)}\frac{2{x_p}^2 - {s_p}^2}{2({x_p}^2 + {s_p}^2)^{5/2}} + \int_{(D_2)}\frac{2x^2 - s^2}{2(x^2+s^2)^{5/2}} N_V\, dV. \tag{56}$$

Here N_V denotes the volume density of lattice points and $N_V = 1/V$ for our simple cubic lattice. Also, for any boundary (Σ_1) of regular shape (e.g., a sphere or a cube with center O) the finite sum in (56) vanishes. Using the Green's theorem together with the relation

$$\frac{2x^2 - s^2}{2(x^2+s^2)^{5/2}} = -\frac{1}{2}\nabla\cdot\left(\frac{\widehat{\mathbf{x}}x}{r^3}\right) \tag{57}$$

we find

$$U^0_2 = -\frac{N_V}{2}\oint_{(\Sigma_1)}\frac{x}{r^3}\widehat{\mathbf{x}}\cdot\mathbf{n}_1 dA_1 - \frac{N_V}{2}\oint_{(\Sigma_2)}\frac{x}{r^3}\widehat{\mathbf{x}}\cdot\mathbf{n}_2 dA_2. \tag{58}$$

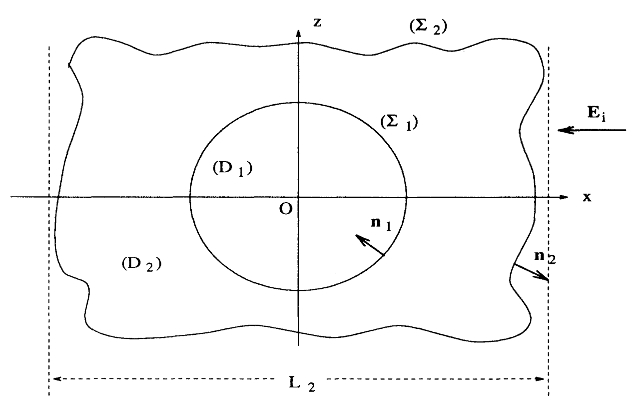

FIG. 7. The volume of integration used in deriving the value of U^0_2. L_2 represents the maximum spatial extension of the lattice.

The first term is simply $2\pi N_V/3$. The second is related to an integral over the surface charge density on the boundary (Σ_2) between the lattice and free space.

Let P denote the polarization or dipole moment per unit volume, where P is independent of position within the lattice. We have

$$P = -4\pi\varepsilon_0 \widetilde{B}_{10} N_V. \tag{59}$$

The second integral in (58) is

$$-\frac{1}{2P}\oint_{(\Sigma_2)} \frac{x}{r^3}\mathbf{P}\cdot\mathbf{n}_2 dA_2 = \frac{2\pi\varepsilon_0 E_P}{P}, \tag{60}$$

where E_P is the x component of the field at O due to the polarization charges on (Σ_2) (for a discussion of these results see, for example, Ref. [25]). Combining (59) and (60), we have

$$U_2^0 = \frac{2}{3}\pi N_V - \frac{1}{2}\frac{E_P}{\widetilde{B}_{1,0}}. \tag{61}$$

By substituting the expression of U_2^0 in (52), we find the inhomogeneous equation

$$\widetilde{B}_{10}(1-p) = -E_P a^3, \tag{62}$$

with $p = 4\pi a^3/(3V)$ the volume fraction occupied by the spheres. The effective dielectric constant of the composite is given by [23,24]

$$\varepsilon^* = 1 - 4\pi\frac{\widetilde{B}_{10}}{E_P}, \tag{63}$$

so that we obtain the Maxwell-Garnett formula for a cubic lattice of perfectly conducting spheres

$$\varepsilon^* = \frac{1+2p}{1-p}. \tag{64}$$

In all these computations, carried out to show how the homogeneous equation (49) is transformed into the inhomogeneous equation (62), the key role is played by the lattice sums S_{00}^y and S_{20}^y (in the dynamic case) and their relation with the lattice sum U_2^0 (in the static case). Apparently, there is a difference between (62) and the corresponding equation for static problems [23,24]

$$\widetilde{B}_{10}(1-p) = -(E_P + E_i)a^3, \tag{65}$$

where E_i represents the applied (static) electric field, while E_P is the depolarization field. The homogeneous equation (49) pertains to modes, which by definition exist without an applied or incident field. Energy is propagating along the y axis and "spreads out" into the x-z plane. The wave emanating from the axis in this plane is reflected back off the discontinuity marking the edge (Σ_2) of the inhomogeneous region containing spheres and this reflected field in the static limit goes over to E_P, the polarization field.

The influence of this polarization field in static problems is governed mathematically by a pair of noncommuting limits ($\mathbf{k}_i \to \mathbf{0}$ and $L_2 \to \infty$; see Fig. 7). Physically, as long as the wavelength of the incident radiation is smaller than the size of the lattice, the fields created by successive regions of opposite charges, associated with $\exp(i\mathbf{k}_i\cdot\mathbf{r})$, cancel between them and $E_P = 0$. When the wavelength of the incident radiation is larger than the size of the lattice, we are in a situation of a lattice placed between the plates of a capacitor in an ac circuit; i.e., at every instant we have a well-defined polarity of the plates and therefore a well-defined depolarization field E_P.

VII. CONCLUSIONS

We have discussed Green's function, lattice sums, and the Rayleigh identity for three-dimensional lattices of spheres, in the context of a scalar wave problem involving Dirichlet boundary conditions on the sphere surfaces. We mention that the representation of lattice sums in terms of absolutely converging series has been achieved. We plan to extend our treatment to the full vector problem, involving the use of Mie theory to match electric and magnetic field components at sphere surfaces. Note that this generalization will not alter the required lattice sums and Green's function. The Rayleigh identity (38) applies unaltered to each Cartesian field component separately. Only Eq. (39) needs to be replaced by a vector equivalent, coupling the tangential components of electric and magnetic fields.

We have obtained the Maxwell-Garnett formula (64) in the quasistatic limit of our dynamic formulas. Lamb *et al.* [15] also treated arrays of spheres in the quasistatic limit and arrived at a generalized Maxwell-Garnett formula. However, their treatment was a vector one and so our scalar validation of the Maxwell-Garnett formula is not in disagreement with their vector modification of it.

ACKNOWLEDGMENTS

This work was undertaken while one of the authors (N.A.N.) was supported by an Australian Research Council Grant. This body also provided computing facilities. The support of the Science Foundation for Physics within the University of Sydney is also acknowledged. R.C.M. acknowledges helpful discussions with Professor L. Greengard.

APPENDIX A: EXPANSIONS IN SPHERICAL BESSEL FUNCTIONS

We use the following definition of the spherical Bessel functions [20]:

$$j_\ell(z) = \sqrt{\frac{\pi}{2z}}\, J_{\ell+1/2}(z)\,, \tag{A1}$$

$$y_\ell(z) = \sqrt{\frac{\pi}{2z}}\, Y_{\ell+1/2}(z)\,, \tag{A2}$$

and

$$h_\ell^{(1)}(z) = j_\ell(z) + iy_\ell(z) = \sqrt{\frac{\pi}{2z}}\, H_{\ell+1/2}^{(1)}(z)\,. \tag{A3}$$

On the right-hand-side of (A1), (A2), and (A3) we have the usual cylindrical Bessel $[J_\nu(z)]$, Neumann $[Y_\nu(z)]$, and Hankel $[H_\nu(z)]$ functions, respectively. The functions $j_\ell(z)$, $y_\ell(z)$, and $h_\ell^{(1)}(z)$ are called *spherical Bessel functions of the first, second,* and *third kind*, respectively.

The Wronskian of the spherical Bessel functions of the first and second kind is

$$W\{j_n(z), y_n(z)\} = j_n(z)y_n'(z) - j_n'(z)y_n(z) = z^{-2}. \tag{A4}$$

For small arguments, the spherical Bessel functions are approximated by the formulas

$$j_n(z) \sim \frac{z^n}{(2n+1)!!}\,, \tag{A5}$$

$$y_n(z) \sim -\frac{(2n-1)!!}{z^{n+1}}\,, \tag{A6}$$

where $(2n+1)!! = (2n+1)(2n-1)\cdots 1$.

From the series expansion

$$e^{iz\cos\theta} = \sum_{\ell=0}^{\infty}(2\ell+1)i^\ell j_\ell(z)P_\ell(\cos\theta) \tag{A7}$$

and the addition theorem for the Legendre polynomials

$$P_\ell(\cos\theta) = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell} Y_{\ell m}(\theta_1,\varphi_1)Y_{\ell m}^*(\theta_2,\varphi_2), \tag{A8}$$

we obtain the expansion of plane waves [20]

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi\sum_{\ell,m} i^\ell j_\ell(kr)Y_{\ell m}(\theta_r,\varphi_r)Y_{\ell m}^*(\theta_k,\varphi_k)\,. \tag{A9}$$

Also, we have [20]

$$\frac{\sin(k\xi)}{k\xi} = \sum_{\ell=0}^{\infty}(2\ell+1)j_\ell(k\rho)j_\ell(kr)P_\ell(\cos\theta), \tag{A10}$$

$$-\frac{\cos(k\xi)}{k\xi} = \sum_{\ell=0}^{\infty}(2\ell+1)j_\ell(k\rho)y_\ell(kr)P_\ell(\cos\theta), \tag{A11}$$

where $\xi = |\mathbf{r}-\boldsymbol{\rho}|$, $\xi^2 = r^2+\rho^2-2r\rho\cos\theta$, and $\rho < r$. From these relations we obtain the expansion of spatial domain Green's function

$$\frac{1}{4\pi}\frac{e^{ik\xi}}{\xi} = ik\sum_{\ell,m} j_\ell(k\rho)\, h_\ell^{(1)}(kr) \times Y_{\ell m}(\theta_r,\varphi_r)Y_{\ell m}^*(\theta_\rho,\varphi_\rho)\,. \tag{A12}$$

For the spherical harmonics we use the definition [26]

$$Y_{\ell m}(\theta,\varphi) = (-1)^m\left[\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}\right]^{1/2} P_\ell^m(\cos\theta)e^{im\varphi},$$

where P_ℓ^m is an associated Legendre function. The spherical harmonics satisfy the relation

$$Y_{\ell,-m}(\theta,\varphi) = (-1)^m Y_{\ell m}^*(\theta,\varphi) \tag{A13}$$

and the orthogonality condition

$$\int Y_{\ell_1 m_1}^*(\theta,\varphi)Y_{\ell_2 m_2}(\theta,\varphi)\,d\Omega = \delta_{\ell_1\ell_2}\,\delta_{m_1 m_2}\,. \tag{A14}$$

The product of two spherical harmonics of equal arguments may be written in the form

$$Y_{\ell_1 m_1}(\theta,\varphi)Y_{\ell_2 m_2}(\theta,\varphi) = \sum_{\ell=|\ell_1-\ell_2|}^{\ell_1+\ell_2}\langle \ell, m_1+m_2|\,\ell_2 m_2\,|\ell_1 m_1\rangle \times Y_{\ell,m_1+m_2}(\theta,\varphi), \tag{A15}$$

where the Gaunt coefficients

$$\langle \ell m|\,\ell_2 m_2\,|\ell_1 m_1\rangle = \int Y_{\ell m}^*(\theta,\varphi)Y_{\ell_2 m_2}(\theta,\varphi)Y_{\ell_1 m_1}(\theta,\varphi)\,d\Omega \tag{A16}$$

may be expressed in terms of vector-coupling (Clebsch-Gordan) coefficients [26]

$$\langle \ell m|\,\ell_2 m_2\,|\ell_1 m_1\rangle = \left[\frac{(2\ell_1+1)(2\ell_2+1)}{4\pi(2\ell+1)}\right]^{1/2} C_{m_1 m_2 m}^{\ell_1\,\ell_2\,\ell}\, C_{0\,0\,0}^{\ell_1\,\ell_2\,\ell}\,. \tag{A17}$$

The Clebsch-Gordan coefficients are nonzero if $m = m_1 + m_2$ and ℓ_1, ℓ_2, ℓ satisfy the triangular condition $|\ell_1-\ell_2| \le \ell \le \ell_1+\ell_2$.

APPENDIX B: SCALAR WAVE ADDITION THEOREM

The spatial domain form of the Green's function (32) is represented by a series expansion in terms of spherical waves

$$\psi_{\ell m}(\boldsymbol{\xi}) = j_\ell(k\xi)Y_{\ell m}(\theta_\xi,\varphi_\xi)\,, \tag{B1}$$

where $\boldsymbol{\xi} = \mathbf{r}-\boldsymbol{\rho}$. In order to separate the variables $\mathbf{r}$ and $\boldsymbol{\rho}$, we follow the method devised by Felderhof and Jones [27]. Thus we expand the terms from the plane wave identity

$$e^{i\mathbf{k}\cdot\boldsymbol{\xi}} = e^{i\mathbf{k}\cdot\mathbf{r}}\,e^{-i\mathbf{k}\cdot\boldsymbol{\rho}}\,, \tag{B2}$$

into series of spherical waves, by means of (A9),

$$\sum_{\ell,m} i^\ell\psi_{\ell m}(\boldsymbol{\xi})Y_{\ell m}^*(\theta_k,\varphi_k) = 4\pi\sum_{\ell_1 m_1}\sum_{\ell_2 m_2} i^{\ell_1-\ell_2} \times\psi_{\ell_1 m_1}(\mathbf{r})Y_{\ell_1 m_1}^*(\theta_k,\varphi_k)\psi_{\ell_2 m_2}^*(\boldsymbol{\rho})Y_{\ell_2 m_2}(\theta_k,\varphi_k). \tag{B3}$$

Multiplying both sides by $Y_{\ell m}(\theta_k, \varphi_k)$ and integrating over the directions of $\mathbf{k}$, we obtain the addition theorem

$$\psi_{\ell m}(\boldsymbol{\xi}) = \sum_{\ell_1 m_1} \sum_{\ell_2 m_2} A^{\ell m}_{\ell_1 m_1;\ell_2 m_2} \psi_{\ell_1 m_1}(\mathbf{r}) \psi^*_{\ell_2 m_2}(\boldsymbol{\rho}), \quad \text{(B4)}$$

where

$$A^{\ell m}_{\ell_1 m_1;\ell_2 m_2} = 4\pi\, i^{\ell_1 - \ell_2 - \ell} \, \langle \ell_1 m_1 | \, \ell_2 m_2 \, | \ell m \rangle \, , \quad \text{(B5)}$$

with the Gaunt coefficients defined in (A17).

By applying the addition theorem (B4) to the series (32) we are led to the following representation of the Green's function:

$$G(\mathbf{r}; \boldsymbol{\rho}) = -\frac{k}{4\pi}\, y_0(k\xi) - k \sum_{\ell m} \sum_{\ell_1 m_1} \sum_{\ell_2 m_2} S^y_{\ell m} A^{\ell, m}_{\ell_1 m_1;\ell_2 m_2} \times \psi_{\ell_1 m_1}(\mathbf{r}) \psi^*_{\ell_2 m_2}(\boldsymbol{\rho}). \quad \text{(B6)}$$

The sum over m is superfluous as the Clebsch-Gordan coefficients in (B5) are nonzero only for $m = m_1 - m_2$. Also, ℓ_1, ℓ_2, and ℓ have to satisfy the triangular condition, so that the series over ℓ is restricted to a finite sum and we may introduce the coefficients

$$\sigma_{\ell_1 m_1;\ell_2 m_2} = \sum_{\ell = |\ell_1 - \ell_2|}^{\ell_1 + \ell_2} S^y_{\ell, m_1 - m_2} \, A^{\ell, m_1 - m_2}_{\ell_1 m_1;\ell_2 m_2} \, . \quad \text{(B7)}$$

Finally, we obtain the spatial domain form of the Green's function with separated variables

$$G(\mathbf{r}; \boldsymbol{\rho}) = -\frac{k}{4\pi}\, y_0(k\xi) - k \sum_{\ell_1 m_1} \sum_{\ell_2 m_2} \sigma_{\ell_1 m_1;\ell_2 m_2} \psi_{\ell_1 m_1}(\mathbf{r}) \psi^*_{\ell_2 m_2}(\boldsymbol{\rho}). \quad \text{(B8)}$$

The first term in (B8) has the form [20]

$$y_0(k\xi) = -\frac{\cos(k\xi)}{k\xi} \, , \quad \text{(B9)}$$

so that, for $\rho < r$, this term has a series expansion of the form (A11).

APPENDIX C: THE LATTICE SUMS IN THE QUASISTATIC LIMIT

The lattice sums $S^y_{\ell m}$, of order $m \geq 0$, are given by the equation

$$S^y_{\ell m} j_\ell(k\xi) = -\frac{1}{\sqrt{4\pi}} y_0(k\xi) \delta_{\ell,0} \delta_{m,0} - \frac{4\pi}{kV} i^\ell \sum_h \frac{j_\ell(Q_h \xi)}{{Q_h}^2 - k^2} Y^*_{\ell m}(\theta_h, \varphi_h). \quad \text{(C1)}$$

For $\ell \geq 3$, in the quasistatic limit, when $k_i = |\mathbf{k}_i|$ is small and $k = \alpha k_i$, we have

$$S^y_{\ell m} j_\ell(k\xi) \sim -\frac{4\pi}{\alpha k_i V} i^\ell \frac{j_\ell(k_i \xi)}{{k_i}^2 (1 - \alpha^2)} Y^*_{\ell m}(\theta_i, \varphi_i) - \frac{4\pi}{\alpha k_i V} i^\ell \sum_{h \neq 0} \frac{j_\ell(K_h \xi)}{{K_h}^2} Y^*_{\ell m}(\theta'_h, \varphi'_h). \quad \text{(C2)}$$

Here θ'_h and φ'_h define the direction of the reciprocal lattice vector $\mathbf{K}_h$.

First, we apply the Poisson summation formula to the series in (C2). In three dimensions, the Poisson summation formula has the standard form

$$\sum_h f(\mathbf{K}_h) = \frac{V}{(2\pi)^3} \sum_p F(\mathbf{R}_p), \quad \text{(C3)}$$

where V is the volume of the primitive cell of the direct lattice and

$$F(\mathbf{R}_p) = \int f(\mathbf{K})\, e^{-i\mathbf{K}\cdot\mathbf{R}_p} \, d\mathbf{K} \, . \quad \text{(C4)}$$

Therefore, we have

$$\begin{aligned} F(\mathbf{R}_p) &= \int \frac{j_\ell(K\xi)}{K^2} Y^*_{\ell m}(\theta_K, \varphi_K) e^{-i\mathbf{K}\cdot\mathbf{R}_p} \, d\mathbf{K} \\ &= \int_0^\infty dK \, j_\ell(K\xi) \int d\Omega_K \, Y^*_{\ell m}(\theta_K, \varphi_K) e^{-i\mathbf{K}\cdot\mathbf{R}_p} \\ &= 4\pi (-i)^\ell \, Y^*_{\ell m}(\theta_p, \varphi_p) \int_0^\infty dK \, j_\ell(K\xi) \, j_\ell(KR_p). \end{aligned}$$

Here we have used the relation

$$j_\ell(KR_p) Y^*_{\ell m}(\theta_p, \varphi_p) = \frac{i^\ell}{4\pi} \int d\Omega_K \, Y^*_{\ell m}(\theta_K, \varphi_K) e^{-i\mathbf{K}\cdot\mathbf{R}_p},$$

which follows from (A9). The integral over K is a special case of the discontinuous Weber-Schafheitlin integral [21]

$$\begin{aligned} \int_0^\infty & dK j_\ell(K\xi) \, j_\ell(KR_p) \\ &= \frac{\pi}{2\sqrt{\xi R_p}} \int_0^\infty dK \, \frac{J_{\ell+1/2}(K\xi) \, J_{\ell+1/2}(KR_p)}{K} \\ &= \frac{\pi}{2(2\ell+1)\sqrt{\xi R_p}} \times \begin{cases} (\xi/R_p)^{\ell+1/2} & \text{if } \xi \leq R_p \\ (R_p/\xi)^{\ell+1/2} & \text{if } \xi \geq R_p. \end{cases} \end{aligned}$$

If $\boldsymbol{\xi}$ is restricted to the unit cell centered at the origin of coordinates (the Wigner-Seitz cell), then $\xi < R_p \ \forall p \neq 0$ and $\xi \geq R_0 = 0$. Consequently, we have

$$F(\mathbf{R}_p) = \frac{2\pi^2}{2\ell+1} (-i)^\ell \frac{\xi^\ell}{{R_p}^{\ell+1}} Y^*_{\ell m}(\theta_p, \varphi_p) \ \ \forall p \neq 0,$$

and $F(\mathbf{R}_0) = 0$.

Now, from (C3), we obtain

$$\sum_h \frac{j_\ell(K_h \xi)}{{K_h}^2} Y^*_{\ell m}(\theta'_h, \varphi'_h) = \frac{V}{4\pi} (-i)^\ell \frac{s_{\ell m}(\xi)}{(2\ell+1)\xi} \, , \quad \text{(C5)}$$

where we have denoted by $s_{\ell m}(\xi)$ the lattice sums

$$s_{\ell m}(\xi) = \sum_{p \neq 0} \left(\frac{\xi}{R_p} \right)^{\ell+1} Y^*_{\ell m}(\theta_p, \varphi_p). \quad \text{(C6)}$$

TABLE II. The static lattice sums U_ℓ^m from (C15), evaluated by means of (C9) with $q = 20$, $h_{1,2,3} \in [-20, 20]$, and $\xi = 1$. The fourth column displays the static lattice sums given by (C6) with $p_{1,2,3} \in [-20, 20]$, while the last column contains numerical values from Ref. [22], obtained by an independent method.

l	m	(C9)	(C6)	[22]
4	0	3.10822668269941	3.10761609357029	3.10822668269940
4	4	1.85752072772944	1.85715583093161	1.85752072772950
6	0	0.57332928943444	0.57332926925510	0.57332928943450
6	4	−1.07260088543324	−1.07260084768101	−1.07260088543320
20	0	2.70422478172723	2.70422478070659	2.70422478070660
20	8	0.73455215840517	0.73455215812998	0.73455215812998
20	16	0.89118810020379	0.89118809986957	0.89118809986958
20	20	1.41533291157431	1.41533291104048	1.41533291104050

With this notation and taking into account the fact that the term for $h = 0$ in (C5) vanishes if $\ell \geq 3$, the series on the right-hand side of (C2) may be written in the form

$$\frac{4\pi}{V} i^\ell \sum_{h\neq 0} \frac{j_\ell(K_h\xi)}{{K_h}^2} Y^*_{\ell m}(\theta'_h, \varphi'_h) = \frac{1}{(2\ell+1)\xi} s_{\ell m}(\xi). \quad \text{(C7)}$$

The lattice sums $s_{\ell m}(\xi)$ are related to the static lattice sums U_ℓ^m [23,24] by means of the formula

$$s_{\ell m}(1) = (-1)^m \left[\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}\right]^{1/2} U_\ell^m. \quad \text{(C8)}$$

The formula (C7) provides us a representation of the static lattice sums by series over the reciprocal lattice. The convergence of these series may be accelerated by multiplying by $\xi^{\ell+2}$ both sides of (C7) and integrating over ξ. The integrals involving the spherical Bessel functions are evaluated by means of (27). Thus, after q successive integrations, we have

$$s_{\ell m}(\xi) = \frac{(2\ell+2q+1)!!}{(2\ell-1)!!} \frac{4\pi\xi^3}{V} i^\ell \times \sum_{h\neq 0} \frac{j_{\ell+q}(K_h\xi)}{(K_h\xi)^{q+2}} Y^*_{\ell m}(\theta'_h, \varphi'_h). \quad \text{(C9)}$$

For $\ell \geq 3$, in the limit $k_i \to 0$, taking into account the behavior of the spherical Bessel functions for small arguments, given by (A5) and (A6), we may express the dynamic lattice sums in the form

$$S^y_{\ell m} \sim -\frac{4\pi}{V} i^\ell \frac{Y^*_{\ell m}(\theta_i, \varphi_i)}{\alpha^{\ell+1}(1-\alpha^2)} \frac{1}{k_i^3} + y_\ell(\alpha k_i \xi) s_{\ell m}(\xi). \quad \text{(C10)}$$

We mention that the second term in (C10) is dominant, being of the order $(1/k_i)^{\ell+1}$.

The lattice sums of order $\ell = 0$ and $\ell = 2$ are special cases and we will analyze them separately. We mention that the lattice sums of order $\ell = 1$ are special cases too, but we will not expand their behavior as these lattice sums are not involved in our considerations concerning the quasistatic limit of the Rayleigh identity. However, the lattice sums of order $\ell = 1$ may be treated in the same way as the lattice sum of order $\ell = 0$.

For $\ell = 0$, $k = \alpha k_i$, and $k_i \sim 0$, the lattice sum S^y_{00} from (C1) may be written in the form

$$S^y_{00} j_0(\alpha k_i \xi) \sim -\frac{1}{\sqrt{4\pi}} y_0(\alpha k_i \xi) - \frac{\sqrt{4\pi}}{V} \frac{j_0(k_i\xi)}{{k_i}^3 \alpha(1-\alpha^2)} - \frac{\sqrt{4\pi}}{\alpha k_i V} \sum_{h\neq 0} \frac{j_0(K_h\xi)}{{K_h}^2}. \quad \text{(C11)}$$

We apply the Cauchy integral test to the series over the reciprocal lattice

$$\int \frac{j_0(K\xi)}{K^2} d\mathbf{K} = \frac{4\pi}{\xi} \int_0^\infty \frac{\sin x}{x} dx = \frac{2\pi^2}{\xi}.$$

Therefore, this series converges for $\xi \neq 0$ and we will denote its value by $\beta_0(\xi)$. Further, we substitute in (C11) the series expansions of $y_0(z)/j_0(z)$ and $1/j_0(z)$, for small arguments

TABLE III. The static lattice sums U_ℓ^m from (C15), evaluated by means of (C9) with $q = 15$, $h_{1,2,3} \in [-30, 30]$, and $\xi = 1$. The fourth column displays the static lattice sums given by (C6) with $p_{1,2,3} \in [-30, 30]$, while the last column contains numerical values from Ref. [22], obtained by an independent method.

l	m	(C9)	(C6)	[22]
4	0	3.10822668269944	3.10795084275112	3.10822668269940
4	4	1.85752072772946	1.85735588183049	1.85752072772950
6	0	0.57332928943446	0.57332928531616	0.57332928943450
6	4	−1.07260088543325	−1.07260087772843	−1.07260088543320
20	0	2.70422478080866	2.70422478070659	2.70422478070660
20	8	0.73455215815726	0.73455215812998	0.73455215812998
20	16	0.89118809990286	0.89118809986957	0.89118809986958
20	20	1.41533291109368	1.41533291104048	1.41533291104050

$$S_{00}^{y} \sim -\frac{1}{\sqrt{4\pi}}\left[-\frac{1}{\alpha k_i\xi}+\frac{\alpha k_i\xi}{3}+\frac{(\alpha k_i\xi)^3}{45}+O(k_i^5)\right] -\frac{\sqrt{4\pi}}{V}\frac{1}{\alpha(1-\alpha^2)}\frac{1}{k_i^3} -\frac{\sqrt{4\pi}}{\alpha V}\left[1+\frac{(\alpha k_i\xi)^2}{6}+O(k_i^4)\right]\frac{1}{k_i}\beta_0(\xi). \quad \text{(C12)}$$

In the case $\ell = 2$, the term for $h = 0$ in (C5) has the form

$$\lim_{k_i\to 0}\lim_{K_h\to 0}\frac{j_2(Q_h\xi)}{{Q_h}^2}Y_{2,m}^{*}(\theta_h,\varphi_h)=\frac{\xi^2}{5!!}Y_{2,m}^{*}(\theta_i,\varphi_i),$$

so that (C5) takes the form

$$\sum_{h\neq 0}\frac{j_2(K_h\xi)}{{K_h}^2}Y_{2,m}^{*}(\theta_h',\varphi_h') = -\frac{\xi^2}{5!!}Y_{2,m}^{*}(\theta_i,\varphi_i) -\frac{V}{4\pi}\frac{s_{2,m}(\xi)}{5\xi}. \quad \text{(C13)}$$

By this method, we obtain

$$S_{2,m}^{y} \sim \frac{4\pi}{V}\frac{Y_{2,m}^{*}(\theta_i,\varphi_i)}{\alpha^3(1-\alpha^2)}\frac{1}{k_i^3}+y_2(\alpha k_i\xi)s_{2,m}(\xi) -\frac{4\pi}{V}\frac{Y_{2,m}^{*}(\theta_i,\varphi_i)}{\alpha^3}\frac{1}{k_i^3} =\frac{4\pi}{V}\frac{Y_{2,m}^{*}(\theta_i,\varphi_i)}{\alpha\,(1-\alpha^2)}\frac{1}{k_i^3}+y_2(\alpha k_i\xi)s_{2,m}(\xi). \quad \text{(C14)}$$

The lattice sums $s_{2,m}$ are related to the static lattice sums U_2^m [23,24] by the general formula (C8).

In Tables II and III we display the numerical results obtained from (C9) for different orders of acceleration q and different number of terms in the series, with $\xi = 1$. These results are compared with numerical values given by (C6) for the same number of terms in the series, also with $\xi = 1$. In order to compare our results with those reported by Berman and Greengard [22] we changed the formula (C8) into

$$s_{\ell m}(1) = \left[\frac{2\ell+1}{4\pi}\right]^{1/2} U_\ell^m . \quad \text{(C15)}$$

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