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The scattering properties of anisotropic dielectric spheres on electromagnetic waves

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Abstract

The scattering coefficients of spheres with dielectric anisotropy are calculated analytically in this paper using the perturbation method. It is found that the different modes of vector spherical harmonics and polarizations are coupled together in the scattering coefficients (*c*-matrix) in contrast to the isotropic case where all modes are decoupled from each other. The generalized *c*-matrix is then incorporated into our codes for a vector wave multiple scattering program; the preliminary results on face centred cubic structure show that dielectric anisotropy reduces the symmetry of the scattering *c*-matrix and removes the degeneracy in photonic band structures composed of isotropic dielectric spheres.

1. Introduction

Photonic crystals are periodically modulated dielectric structures, which can be made either by a periodic arrangement of one dielectric material embedded in another or by removing material to create a periodic formation of voids in bulk materials [1–3]. Recently, new techniques such as self-assembly of colloid particles from solvent to form artificial opal and inverse opal brought us a step closer to realizing photonic band gaps at optical wavelengths [4–6]. The propagation of electromagnetic waves in synthetic photonic crystals is very similar to electron propagation in a natural crystal. By the Bloch theorem, the propagation modes of photons form a band structure. If an absolute band gap exists in the photonic band structures, the absolute gap prohibits the spontaneous emission of electromagnetic waves within the frequency range of the gap, leading to many plausible industrial and commercial applications in advanced optical devices. Examples of such applications are frequency selective reflectors, optical polarizers, band filters, and low threshold micro-cavity lasers [7, 8].

To date, the most popular method for calculating photonic band structures is the plane wave method [9–11]. The finite difference time domain method [12–14], widely used in the engineering community, has proved useful in some situations. These methods work well for

photonic crystals made of dielectric components but the convergence becomes problematic when the photonic crystals carry metallic components [12, 15]. Dispersion also presents a significant challenge for these formalisms. If there are metallic components inside photonic crystals, there are necessarily very rapid changes in the electromagnetic fields near the interfaces between the metallic components and the embedded medium. To describe such a rapid change of field, one has to use a very large number of plane waves or use a very fine mesh of points to achieve an accurate solution, making these methods impractical. Formalisms such as the multiple scattering and Korringa–Kohn–Rostoker (KKR) methods [16, 17] that take into account the proper boundary condition of the interface are more desirable. In the multiple scattering method [16–18], the whole crystal is treated as an assembly of scattering centres and its scattering properties are taken as sums over individual scatterers. Once the scattering properties (the c -matrix) of the individual scatterers are known, the scattered wave of the whole crystal can be constructed from these matrices, and so can the band structures of the photonic crystals.

In contrast with the plane wave expansion method where the expansion is carried out in reciprocal space, the multiple scattering method expands locally in real space around each scattering centre. Therefore, it offers higher numerical accuracy and demands less computer time, and high quality results can be obtained on a Pentium PC. The multiple scattering method was originally developed for electronic band structures [16–18] where electrons are described by the scale wavefunction. The extension of the KKR method to the case of electromagnetic waves was first formulated by Ohtaka and Tanabe [19, 20] who set up the foundation for the mathematical formalism. A very useful extension to the slab geometry was made by Modinos [21] and Stefanou and Modinos [22–24]. They used the layer doubling scheme to calculate the transmission and reflection spectra of electromagnetic waves from a slab of photonic crystal; their program codes not only yield the complex photonic band structures, but also yield results that can be compared directly with experimental measurements. More recently, vector wave KKR methods were also derived and implemented by other groups [25–28] from different points of view. We have also written a general computer code for implementing the vector wave multiple scattering method for photonic band structures in three dimensional photonic crystals [28], and the code is very efficient and much faster than the finite difference time domain method as long as we are concerned with spherical scatterers. Comparison with the finite difference time domain method shows that solutions are already convergent at an angular momentum $l = 5$ for photonic crystals made of metal spheres if the filling ratio of the metal spheres is not too large [12].

Previous vector wave multiple scattering methods concentrate on spherical objects, where the scattering c -matrix can be calculated analytically; thus the effect of the scattering centres can be included in the boundary condition. For nonspherical objects or spheres with dielectric anisotropy, the exact analytic forms of the scattering c -matrices are not available. As photonic crystals containing spherical objects have been thoroughly investigated and the existence of photonic band gaps is only found in the diamond structure and the inverse opal face centred cubic structure if dielectric materials are considered [6, 10, 29], it is worthwhile to extend the vector wave multiple scattering method to the situation with anisotropic objects. In fact, studies have been carried out before on both shape anisotropy and dielectric anisotropy within the framework of the plane wave expansion and the finite difference time domain method [13, 30–33]. However, one has to use a very large number of plane waves or use a very fine mesh of points to achieve an accurate solution. In this paper, the general scattering c -matrix of spheres with an arbitrary dielectric tensor is calculated perturbatively up to its first order terms and the results have been used to calculate the photonic band structure of a periodic array of spheres with dielectric anisotropy. Unlike the case for isotropic dielectric spheres, the different

vector spherical harmonics and polarizations are coupled together in the scattering c -matrix if the spheres have dielectric anisotropy. The symmetry reduction in the scattering c -matrix removes the degeneracy in the photonic band structure of isotropic spheres.

The rest of the paper is organized as follows. In section 2, the scattering problem for spheres with dielectric isotropy is briefly reviewed, various eigensolutions are defined and the scattering c -matrix is calculated. In section 3, using the perturbation approximation the first order correction to the eigensolutions of the isotropic medium is calculated analytically for a medium with dielectric anisotropy. The corrected eigensolutions are then substituted into the boundary condition to obtain the scattering c -matrix for the general dielectric tensor. Remarks on and discussions of the derivation are given in section 4. As an illustration of the influence of dielectric anisotropy, an example of photonic band structure for face centred cubic crystal is demonstrated and compared with that of isotropic dielectric material. Section 5 gives our conclusions.

2. Eigensolutions and the scattering c -matrix in the isotropic case

In the vector wave multiple scattering method, the formulism includes two independent parts: the structural factor of a given crystal and the scattering properties of the scatterers. To extend the multiple scattering method to spheres with dielectric anisotropy, the scattering coefficients (c -matrix) have to be provided. Usually, the scattering c -matrix can be obtained by matching the amplitudes of electromagnetic modes inside and outside of a sphere. Since the exact eigensolutions for an electromagnetic wave in the presence of dielectric anisotropy are not available in spherical coordinates, a perturbation method has to be adopted to calculate the approximate eigensolutions. To start with, let us first consider an isotropic dielectric sphere with radius a and dielectric constant ϵ embedded in vacuum. The magnetic permeability is set as $\mu = 1$ so nonmagnetic dielectric material is considered. Note that for an embedding medium other than vacuum, a scaling law can be used to extract the corresponding scattering c -matrix. The electromagnetic wave in a homogeneous medium is described by the following wave equation:

$$\nabla \times [\nabla \times \mathbf{E}(\mathbf{r})] - \kappa^2 \epsilon \mathbf{E}(\mathbf{r}) = 0, \quad (1)$$

where $\kappa = \omega/c$; ω and c are the frequency and light velocity in vacuum, respectively. The eigensolutions of the above equation can be solved analytically in spherical coordinates and four types of vector spherical harmonics are given by [34]

$$\mathbf{J}_{l,m}^{(m)}(n\kappa\mathbf{r}) = j_l(n\kappa r) \mathbf{X}_{l,m}^m(\hat{\mathbf{r}}); \quad (2a)$$

$$\mathbf{N}_{l,m}^{(m)}(n\kappa\mathbf{r}) = n_l(n\kappa r) \mathbf{X}_{l,m}^m(\hat{\mathbf{r}}); \quad (2b)$$

$$\mathbf{J}_{l,m}^{(e)}(n\kappa\mathbf{r}) = -\frac{i}{n\kappa} \nabla \times \mathbf{J}_{l,m}^{(m)}(n\kappa\mathbf{r}); \quad (2c)$$

$$\mathbf{N}_{l,m}^{(e)}(n\kappa\mathbf{r}) = -\frac{i}{n\kappa} \nabla \times \mathbf{N}_{l,m}^{(m)}(n\kappa\mathbf{r}). \quad (2d)$$

Here $n = \sqrt{\epsilon}$, $j_l(n\kappa r)$ and $n_l(n\kappa r)$ are the spherical Bessel and Neumann functions. $\vec{\mathbf{X}}_{l,m}^{(m)}(\hat{\mathbf{r}})$ is one of the three polarization vectors for mode (l, m) [34] listed below:

$$\mathbf{X}_{l,m}^{(m)}(\hat{\mathbf{r}}) = -\frac{i}{\sqrt{l(l+1)}} \hat{\mathbf{r}} \times \nabla Y_{l,m}(\hat{\mathbf{r}}); \quad (3a)$$

$$\mathbf{X}_{l,m}^{(e)}(\hat{\mathbf{r}}) = \frac{1}{\sqrt{l(l+1)}} r \nabla Y_{l,m}(\hat{\mathbf{r}}); \quad (3b)$$

$$\mathbf{X}_{l,m}^{(o)}(\hat{\mathbf{r}}) = \hat{\mathbf{r}} Y_{l,m}(\hat{\mathbf{r}}) \quad (3c)$$

with $\mathbf{X}_{l,m}^{(m)}(\hat{\mathbf{r}})$ and $\mathbf{X}_{l,m}^{(e)}(\hat{\mathbf{r}})$ for the two transverse modes, and $\mathbf{X}_{l,m}^{(o)}(\hat{\mathbf{r}})$ for the longitudinal mode. $Y_{l,m}(\hat{r})$ are the scalar spherical harmonics [34]. All three modes satisfy the mutual orthogonality and normalization condition $\langle \mathbf{X}_{l,m}^{(\sigma)} | \mathbf{X}_{l',m'}^{(\sigma')} \rangle = \delta_{l,l'} \delta_{m,m'} \delta_{\sigma,\sigma'}$. The general eigensolutions of equation (2) are valid both for an isotropic dielectric medium ($n = \sqrt{\epsilon}$) and for vacuum ($n = 1$).

In dealing with the scattering problem, one can either compute the scattering t -matrix or the scattering coefficients (c -matrix). They are equivalent to each other and have the relationship $t = -ic/(1 + ic)$. However, because the c -matrix is a Hermitian matrix in the absence of dissipation it is more suitable for perturbation calculation [35]. For a given (l, m) mode with polarization σ ($\sigma = m$ or e), the electric and magnetic fields of the incident wave are

$$\mathbf{E}_{\text{inc}}(\mathbf{r}) = a_{l,m}^{(m)} \mathbf{J}_{l,m}^{(m)}(\kappa \mathbf{r}) + a_{l,m}^{(e)} \mathbf{J}_{l,m}^{(e)}(\kappa \mathbf{r}), \quad (4a)$$

$$\mathbf{H}_{\text{inc}}(\mathbf{r}) = a_{l,m}^{(m)} \mathbf{J}_{l,m}^{(e)}(\kappa \mathbf{r}) - a_{l,m}^{(e)} \mathbf{J}_{l,m}^{(m)}(\kappa \mathbf{r}). \quad (4b)$$

The corresponding fields induced inside the dielectric sphere can be written as

$$\mathbf{E}_{\text{ins}}(\mathbf{r}) = b_{l,m;l,m}^{(mm)0} \mathbf{J}_{l,m}^{(m)}(n\kappa \mathbf{r}) + b_{l,m;l,m}^{(ee)0} \mathbf{J}_{l,m}^{(e)}(n\kappa \mathbf{r}), \quad (5a)$$

$$\mathbf{H}_{\text{ins}}(\mathbf{r}) = n[b_{l,m;l,m}^{(mm)0} \mathbf{J}_{l,m}^{(e)}(n\kappa \mathbf{r}) - b_{l,m;l,m}^{(ee)0} \mathbf{J}_{l,m}^{(m)}(n\kappa \mathbf{r})] \quad (5b)$$

and the fields scattered off the sphere are given by

$$\mathbf{E}_{\text{scat}}(\mathbf{r}) = s_{l,m;l,m}^{(mm)0} \mathbf{N}_{l,m}^{(m)}(\kappa \mathbf{r}) + s_{l,m;l,m}^{(ee)0} \mathbf{N}_{l,m}^{(e)}(\kappa \mathbf{r}), \quad (6a)$$

$$\mathbf{H}_{\text{scat}}(\mathbf{r}) = s_{l,m;l,m}^{(mm)0} \mathbf{N}_{l,m}^{(e)}(\kappa \mathbf{r}) - s_{l,m;l,m}^{(ee)0} \mathbf{N}_{l,m}^{(m)}(\kappa \mathbf{r}). \quad (6b)$$

For the scattering scenario given above, the total electromagnetic waves inside and outside of the sphere can be constructed. Together with the requirement that tangential components of both electric and magnetic fields have to be continuous across the spherical surface, this yields the scattering coefficient c -matrix for the isotropic dielectric sphere [36]:

$$c_{l,m;l,m}^{(mm)0} = \frac{s_{l,m;l,m}^{(mm)0}}{a_{l,m}^{(m)}} = (-1) \frac{\psi_l(n\kappa a) \psi_l'(\kappa a) - n \psi_l'(\kappa a) \psi_l(n\kappa a)}{\psi_l(n\kappa a) \psi_l'(\kappa a) - n \psi_l'(\kappa a) \psi_l(n\kappa a)}, \quad (7a)$$

$$c_{l,m;l,m}^{(ee)0} = \frac{s_{l,m;l,m}^{(ee)0}}{a_{l,m}^{(e)}} = (-1) \frac{n \psi_l(n\kappa a) \psi_l'(\kappa a) - \psi_l'(\kappa a) \psi_l(n\kappa a)}{n \psi_l(n\kappa a) \psi_l'(\kappa a) - \psi_l'(\kappa a) \psi_l(n\kappa a)}. \quad (7b)$$

Note that $\psi_l(x) = x j_l(x)$ and $\varphi_l(x) = x n_l(x)$ are the so-called Ricatti Bessel and Ricatti Neumann functions; the prime on a function denotes the derivative with respect to its variable, a is the radius of the sphere. From the above expressions, one notices that the scattering c -matrix is a diagonal matrix if the sphere is composed of an isotropic dielectric medium. Also the scattering c -matrix is independent of the azimuthal quantum number m .

3. Approximate eigensolutions and the scattering c -matrix in the anisotropic case

Knowing the scattering property of an isotropic dielectric sphere paves the way to the more complex situation of a sphere with dielectric anisotropy. In this case, the general dielectric tensor ϵ can be expressed as

$$\epsilon = \epsilon + \epsilon_1 = (1/3) \text{Tr}(\epsilon) + \begin{pmatrix} \epsilon_{11} & 0 & 0 \\ 0 & \epsilon_{22} & 0 \\ 0 & 0 & \epsilon_{33} \end{pmatrix}. \quad (8)$$

Here ϵ and ϵ_1 are the isotropic and the anisotropic components, respectively. ϵ_1 is assumed to be small with respect to ϵ so that the perturbation method can be applied.

In order to study the scattering property of spheres with dielectric anisotropy, the first step is to calculate the approximate eigensolutions of electromagnetic wave in such an anisotropic dielectric medium. Since ϵ_1 is a small parameter, the electromagnetic fields can be expanded in power series. Substituting the power series into the Maxwell equation and keeping the terms up to the first order, the electromagnetic wave equation becomes

$$\nabla \times [\nabla \times \mathbf{E}_0(\mathbf{r})] - \kappa^2 \epsilon \mathbf{E}_0(\mathbf{r}) = 0, \quad (9a)$$

$$\nabla \times [\nabla \times \mathbf{E}_1(\mathbf{r})] - \kappa^2 \epsilon \mathbf{E}_1(\mathbf{r}) = \kappa^2 \epsilon_1 \cdot \mathbf{E}_0(\mathbf{r}). \quad (9b)$$

$\mathbf{E}_0(\mathbf{r})$ and $\mathbf{E}_1(\mathbf{r})$ are the zeroth and first order components, respectively. Obviously, $\mathbf{E}_0(\mathbf{r})$ satisfies the same equation as for the isotropic dielectric medium with dielectric constant ϵ ; its eigensolutions are the vector spherical harmonics $\mathbf{J}_{l,m}^{(m)}(n\kappa\mathbf{r})$ and $\mathbf{J}_{l,m}^{(e)}(n\kappa\mathbf{r})$.

To find the corrections $\mathbf{J}_{l,m}^{(\sigma)1}(n\kappa\mathbf{r})$ to the zeroth order eigensolutions $\mathbf{J}_{l,m}^{(\sigma)}(n\kappa\mathbf{r})$, it is convenient to introduce the dyadic Green function $\mathbf{d}_0(\mathbf{r} - \mathbf{r}')$ in a homogeneous isotropic medium,

$$\nabla \times [\nabla \times \mathbf{d}_0(\mathbf{r} - \mathbf{r}')] - \kappa^2 \epsilon \mathbf{d}_0(\mathbf{r} - \mathbf{r}') = \delta(r - r') \mathbf{I}. \quad (10)$$

Here, ϵ is the isotropic part of the dielectric tensor and \mathbf{I} is the unit matrix. For infinite space, the dyadic Green function has the form

$$\mathbf{d}_0(\mathbf{r} - \mathbf{r}') = \left[\mathbf{I} + \frac{1}{\kappa^2 \epsilon} \nabla \nabla \right] \frac{\cos(n\kappa|\mathbf{r} - \mathbf{r}'|)}{4\pi|\mathbf{r} - \mathbf{r}'|}. \quad (11)$$

Using the dyadic Green function, the correction to a given mode reads

$$\mathbf{J}_{l,m}^{(\sigma)1}(n\kappa\mathbf{r}) = \int d^3\mathbf{r}' \mathbf{d}_0(\mathbf{r} - \mathbf{r}') \cdot \kappa^2 \epsilon_1 \cdot \mathbf{J}_{l,m}^{(\sigma)}(\mathbf{r}'). \quad (12)$$

To facilitate the derivation, the dyadic Green function [35, 37, 38] and $\epsilon_1 \cdot \mathbf{J}_{l,m}^{(\sigma)}(n\kappa\mathbf{r})$ are both expanded below using the vector spherical harmonics:

$$\begin{aligned} \mathbf{d}_0(\mathbf{r} - \mathbf{r}') = & -\frac{\hat{r}\hat{r}}{\kappa^2 \epsilon} \delta(r - r') - n\kappa \sum_{l,m,\sigma}^{\sigma=m,e} [\mathbf{J}_{l,m}^{(\sigma)}(n\kappa\mathbf{r}) \mathbf{N}_{l,m}^{(\sigma)*}(n\kappa\mathbf{r}') \Theta(r' - r) \\ & + \mathbf{N}_{l,m}^{(\sigma)}(n\kappa\mathbf{r}) \mathbf{J}_{l,m}^{(\sigma)*}(n\kappa\mathbf{r}') \Theta(r - r')], \end{aligned} \quad (13)$$

$$\begin{aligned} \epsilon_1 \cdot \mathbf{J}_{l,m}^{(m)}(\mathbf{r}) = & j_l(n\kappa r) \sum_{\mu=0,\pm 2} \left[A_{l,m;l,m-\mu}^{(mm)} \mathbf{X}_{l,m-\mu}^{(m)}(\hat{\mathbf{r}}) \right. \\ & \left. + \sum_{\lambda=\pm 1} (B_{l,m;l-\lambda,m-\mu}^{(me)} \mathbf{X}_{l-\lambda,m-\mu}^{(e)}(\hat{\mathbf{r}}) + C_{l,m;l-\lambda,m-\mu}^{(mo)} \mathbf{X}_{l-\lambda,m-\mu}^{(o)}(\hat{\mathbf{r}})) \right], \end{aligned} \quad (14a)$$

$$\begin{aligned} \epsilon_1 \cdot \mathbf{J}_{l,m}^{(e)}(\mathbf{r}) = & \sqrt{\frac{l+1}{2l+1}} j_{l-1}(n\kappa r) \sum_{\mu=0,\pm 2} \left[A_{l,m;l-1,m-\mu}^{(em)-} \mathbf{X}_{l-1,m-\mu}^{(m)}(\hat{\mathbf{r}}) \right. \\ & \left. + \sum_{\lambda=\pm 1} (B_{l,m;l-1-\lambda,m-\mu}^{(ee)-} \mathbf{X}_{l-1-\lambda,m-\mu}^{(e)}(\hat{\mathbf{r}}) + C_{l,m;l-1-\lambda,m-\mu}^{(eo)-} \mathbf{X}_{l-1-\lambda,m-\mu}^{(o)}(\hat{\mathbf{r}})) \right] \\ & - \sqrt{\frac{l}{2l+1}} j_{l+1}(n\kappa r) \sum_{\mu=0,\pm 2} \left[A_{l,m;l+1,m-\mu}^{(em)+} \mathbf{X}_{l+1,m-\mu}^{(m)}(\hat{\mathbf{r}}) \right. \\ & \left. + \sum_{\lambda=\pm 1} (B_{l,m;l+1-\lambda,m-\mu}^{(ee)+} \mathbf{X}_{l+1-\lambda,m-\mu}^{(e)}(\hat{\mathbf{r}}) + C_{l,m;l+1-\lambda,m-\mu}^{(eo)+} \mathbf{X}_{l+1-\lambda,m-\mu}^{(o)}(\hat{\mathbf{r}})) \right]. \end{aligned} \quad (14b)$$

$\Theta(r)$ in equation (13) is the usual Heaviside step function. The derivations of parameters $A_{l,m;l,m-\mu}^{(mm)}$, $B_{l,m;l-\lambda,m-\mu}^{(me)}$, $C_{l,m;l-\lambda,m-\mu}^{(mo)}$, $A_{l,m;l+1,m-\mu}^{(em)+}$, $B_{l,m;l+1-\lambda,m-\mu}^{(ee)+}$, $C_{l,m;l+1-\lambda,m-\mu}^{(eo)+}$,

$A_{l,m;l-1,m-\mu}^{(em)-}$, $B_{l,m;l-1-\lambda,m-\mu}^{(ee)-}$ and $C_{l,m;l-1-\lambda,m-\mu}^{(eo)-}$ are straightforward, but tedious. Their detailed expression is left to appendix A. After substituting equations (13), (14) into equation (12), the corrections to the zeroth order eigensolutions $\mathbf{J}_{l,m}^{(\sigma)}(n\kappa\mathbf{r})$ are given by

$$\begin{aligned} \mathbf{J}_{l,m}^{(m)1}(n\kappa\mathbf{r}) = & -\frac{1}{\epsilon} j_l(n\kappa r) \sum_{\substack{\lambda=\pm 1 \\ \mu=0,\pm 2}} C_{l,m;l-\lambda,m-\mu}^{(mo)} \mathbf{X}_{l-\lambda,m-\mu}^{(o)}(\hat{\mathbf{r}}) \\ & - n\kappa^3 \sum_{\mu=0,\pm 2} [F_{l,m;l,m-\mu}^{(mm)}(r) \mathbf{J}_{l,m-\mu}^{(m)}(n\kappa\mathbf{r}) + G_{l,m;l,m-\mu}^{(mm)}(r) \mathbf{N}_{l,m-\mu}^{(m)}(n\kappa\mathbf{r})] \\ & - n\kappa^3 \sum_{\substack{\lambda=\pm 1 \\ \mu=0,\pm 2}} [F_{l,m;l-\lambda,m-\mu}^{(me)}(r) \mathbf{J}_{l-\lambda,m-\mu}^{(e)}(n\kappa\mathbf{r}) \\ & + G_{l,m;l-\lambda,m-\mu}^{(me)}(r) \mathbf{N}_{l-\lambda,m-\mu}^{(e)}(n\kappa\mathbf{r})], \end{aligned} \quad (15a)$$

$$\begin{aligned} \mathbf{J}_{l,m}^{(e)1}(n\kappa\mathbf{r}) = & \sqrt{\frac{l+1}{2l+1}} \left\{ -\frac{1}{\epsilon} j_{l-1}(n\kappa r) \sum_{\substack{\lambda=\pm 1 \\ \mu=0,\pm 2}} C_{l,m;l-1-\lambda,m-\mu}^{(eo)-} \mathbf{X}_{l-1-\lambda,m-\mu}^{(o)}(\hat{\mathbf{r}}) \right. \\ & - n\kappa^3 \sum_{\mu=0,\pm 2} [F_{l,m;l-1,m-\mu}^{(em)-}(r) \mathbf{J}_{l-1,m-\mu}^{(m)}(n\kappa\mathbf{r}) + G_{l,m;l-1,m-\mu}^{(em)-}(r) \mathbf{N}_{l-1,m-\mu}^{(m)}(n\kappa\mathbf{r})] \\ & - n\kappa^3 \sum_{\substack{\lambda=\pm 1 \\ \mu=0,\pm 2}} [F_{l,m;l-1-\lambda,m-\mu}^{(ee)-}(r) \mathbf{J}_{l-1-\lambda,m-\mu}^{(e)}(n\kappa\mathbf{r}) \\ & + G_{l,m;l-1-\lambda,m-\mu}^{(ee)-}(r) \mathbf{N}_{l-1-\lambda,m-\mu}^{(e)}(n\kappa\mathbf{r})] \left. \right\} \\ & - \sqrt{\frac{l}{2l+1}} \left\{ -\frac{1}{\epsilon} j_{l+1}(n\kappa r) \sum_{\substack{\lambda=\pm 1 \\ \mu=0,\pm 2}} C_{l,m;l+1-\lambda,m-\mu}^{(eo)+} \mathbf{X}_{l+1-\lambda,m-\mu}^{(o)}(\hat{\mathbf{r}}) \right. \\ & - n\kappa^3 \sum_{\mu=0,\pm 2} [F_{l,m;l+1,m-\mu}^{(em)+}(r) \mathbf{J}_{l+1,m-\mu}^{(m)}(n\kappa\mathbf{r}) + G_{l,m;l+1,m-\mu}^{(em)+}(r) \mathbf{N}_{l+1,m-\mu}^{(m)}(n\kappa\mathbf{r})] \\ & - n\kappa^3 \sum_{\substack{\lambda=\pm 1 \\ \mu=0,\pm 2}} [F_{l,m;l+1-\lambda,m-\mu}^{(ee)+}(r) \mathbf{J}_{l+1-\lambda,m-\mu}^{(e)}(n\kappa\mathbf{r}) \\ & + G_{l,m;l+1-\lambda,m-\mu}^{(ee)+}(r) \mathbf{N}_{l+1-\lambda,m-\mu}^{(e)}(n\kappa\mathbf{r})] \left. \right\}. \end{aligned} \quad (15b)$$

The functions F and G involve integrations between the coupled modes and their detailed analytic expressions are included in appendix B.

Once the approximate form for the eigensolutions in the anisotropic dielectric medium is known, it is relatively easy to obtain the corresponding scattering c -matrix. The procedure is quite similar to the dielectric isotropic case, except that the eigensolutions $\mathbf{J}_{l,m}^{(\sigma)}(n\kappa\mathbf{r})$ in an isotropic dielectric medium have to be replaced by $\mathbf{J}_{l,m}^{(\sigma)}(n\kappa\mathbf{r}) + \mathbf{J}_{l,m}^{(\sigma)1}(n\kappa\mathbf{r})$ in an anisotropic dielectric medium. Because of the coupling effect among different (l, m) as well as (σ) modes, the scattering c -matrix has to be computed separately for each individual (σ) mode.

Case 1: the (m) mode.

The incident electromagnetic wave takes the $(l, m, (m))$ mode:

$$\mathbf{E}_{\text{inc}}(\mathbf{r}) = a_{l,m}^{(m)} \mathbf{J}_{l,m}^{(m)}(\kappa\mathbf{r}), \quad (16a)$$

$$\mathbf{H}_{\text{inc}}(\mathbf{r}) = a_{l,m}^{(m)} \mathbf{J}_{l,m}^{(e)}(\kappa\mathbf{r}); \quad (16b)$$

the electromagnetic waves induced inside the dielectric sphere can be, up to first order, written as

$$\mathbf{E}_{\text{ins}}(\mathbf{r}) = b_{l,m;l,m}^{(mm)0} [\mathbf{J}_{l,m}^{(m)}(n\kappa\mathbf{r}) + \mathbf{J}_{l,m}^{(m)1}(n\kappa\mathbf{r})] + \sum_{l',m'} [b_{l,m;l',m'}^{(mm)1} \mathbf{J}_{l',m'}^{(m)}(n\kappa\mathbf{r}) + b_{l,m;l',m'}^{(me)1} \mathbf{J}_{l',m'}^{(e)}(n\kappa\mathbf{r})], \quad (17a)$$

$$\mathbf{H}_{\text{ins}}(\mathbf{r}) = b_{l,m;l,m}^{(mm)0} [n\mathbf{J}_{l,m}^{(e)}(n\kappa\mathbf{r}) + (1/i\kappa)\nabla \times \mathbf{J}_{l,m}^{(m)1}(n\kappa\mathbf{r})] + \sum_{l',m'} [nb_{l,m;l',m'}^{(mm)1} \mathbf{J}_{l',m'}^{(e)}(n\kappa\mathbf{r}) - nb_{l,m;l',m'}^{(me)1} \mathbf{J}_{l',m'}^{(m)}(n\kappa\mathbf{r})]. \quad (17b)$$

The corresponding electromagnetic wave scattered off the sphere is given by

$$\mathbf{E}_{\text{scat}}(\mathbf{r}) = s_{l,m;l,m}^{(mm)0} \mathbf{N}_{l,m}^{(m)}(\kappa\mathbf{r}) + \sum_{l',m'} [s_{l,m;l',m'}^{(mm)1} \mathbf{N}_{l',m'}^{(m)}(\kappa\mathbf{r}) + s_{l,m;l',m'}^{(me)1} \mathbf{N}_{l',m'}^{(e)}(\kappa\mathbf{r})], \quad (18a)$$

$$\mathbf{H}_{\text{scat}}(\mathbf{r}) = s_{l,m;l,m}^{(mm)0} \mathbf{N}_{l,m}^{(e)}(\kappa\mathbf{r}) + \sum_{l',m'} [s_{l,m;l',m'}^{(mm)1} \mathbf{N}_{l',m'}^{(e)}(\kappa\mathbf{r}) - s_{l,m;l',m'}^{(me)1} \mathbf{N}_{l',m'}^{(m)}(\kappa\mathbf{r})]. \quad (18b)$$

Here $b_{l,m;l',m'}^{(\sigma\sigma')1}$ and $s_{l,m;l',m'}^{(\sigma\sigma')1}$ are the first order corrections to the amplitudes $b_{l,m;l,m}^{(mm)0}$ and $s_{l,m;l,m}^{(mm)0}$. All the scattering coefficients $s_{l,m;l',m'}^{(\sigma\sigma')1}$ can be obtained in terms of the incident amplitude $a_{l,m}^{(m)}$ if the boundary conditions are imposed on tangential components of electric and magnetic fields; this yields the first order terms of the scattering c -matrix for the m mode in the presence of dielectric anisotropy:

$$c_{l,m;l,m-\mu}^{(mm)1} = \frac{s_{l,m;l,m-\mu}^{(mm)1}}{a_{l,m}^{(m)}} = -G_{l,m;l,m-\mu}^{(mm)}(a) \times \frac{b_{l,m;l,m}^{(mm)0}}{a_{l,m}^{(m)}} n\kappa^3 \frac{\psi_l(n\kappa a)\phi_l'(n\kappa a) - \psi_l'(n\kappa a)\phi_l(n\kappa a)}{\psi_l(n\kappa a)\phi_l'(\kappa a) - n\psi_l'(n\kappa a)\phi_l(\kappa a)}, \quad (19a)$$

$$c_{l,m;l\pm 1,m-\mu}^{(me)1} = \frac{s_{l,m;l\pm 1,m-\mu}^{(me)1}}{a_{l,m}^{(m)}} = -G_{l,m;l\pm 1,m-\mu}^{(me)}(a) \times \frac{b_{l,m;l,m}^{(mm)0}}{a_{l,m}^{(m)}} n\kappa^3 \frac{\psi_{l\pm 1}(n\kappa a)\phi_{l\pm 1}'(n\kappa a) - \psi_{l\pm 1}'(n\kappa a)\phi_{l\pm 1}(n\kappa a)}{n\psi_{l\pm 1}(n\kappa a)\phi_{l\pm 1}'(\kappa a) - \psi_{l\pm 1}'(n\kappa a)\phi_{l\pm 1}(\kappa a)}. \quad (19b)$$

$b_{l,m;l,m}^{(mm)0}/a_{l,m}^{(m)} = n[\psi_l(\kappa a)\phi_l'(\kappa a) - \psi_l'(\kappa a)\phi_l(\kappa a)]/[\psi_l(n\kappa a)\phi_l'(n\kappa a) - n\psi_l'(n\kappa a)\phi_l(n\kappa a)]$ stands for the zeroth order amplitude of the (m) mode inside the sphere.

Case 2: the (e) mode.

The incident electromagnetic wave takes the $(l, m, (e))$ mode:

$$\mathbf{E}_{\text{inc}}(\mathbf{r}) = a_{l,m}^{(e)} \mathbf{J}_{l,m}^{(e)}(\kappa\mathbf{r}), \quad (20a)$$

$$\mathbf{H}_{\text{inc}}(\mathbf{r}) = -a_{l,m}^{(e)} \mathbf{J}_{l,m}^{(m)}(\kappa\mathbf{r}); \quad (20b)$$

the electromagnetic wave inside the dielectric sphere can be written as

$$\mathbf{E}_{\text{ins}}(\mathbf{r}) = b_{l,m;l,m}^{(ee)0} [\mathbf{J}_{l,m}^{(e)}(n\kappa\mathbf{r}) + \mathbf{J}_{l,m}^{(e)1}(n\kappa\mathbf{r})] + \sum_{l',m'} [b_{l,m;l',m'}^{(em)1} \mathbf{J}_{l',m'}^{(m)}(n\kappa\mathbf{r}) + b_{l,m;l',m'}^{(ee)1} \mathbf{J}_{l',m'}^{(e)}(n\kappa\mathbf{r})], \quad (21a)$$

$$\mathbf{H}_{\text{ins}}(\mathbf{r}) = b_{l,m;l,m}^{(ee)0} [-n\mathbf{J}_{l,m}^{(m)}(n\kappa\mathbf{r}) + (1/i\kappa)\nabla \times \mathbf{J}_{l,m}^{(e)1}(n\kappa\mathbf{r})] + \sum_{l',m'} [nb_{l,m;l',m'}^{(em)1} \mathbf{J}_{l',m'}^{(e)}(n\kappa\mathbf{r}) - nb_{l,m;l',m'}^{(ee)1} \mathbf{J}_{l',m'}^{(m)}(n\kappa\mathbf{r})], \quad (21b)$$

and the corresponding electromagnetic wave scattered off the sphere is given by

$$\mathbf{E}_{\text{scat}}(\mathbf{r}) = s_{l,m;l,m}^{(ee)0} \mathbf{N}_{l,m}^{(e)}(\boldsymbol{\kappa}\mathbf{r}) + \sum_{l',m'} [s_{l,m;l',m'}^{(em)1} \mathbf{N}_{l',m'}^{(m)}(\boldsymbol{\kappa}\mathbf{r}) + s_{l,m;l',m'}^{(ee)1} \mathbf{N}_{l',m'}^{(e)}(\boldsymbol{\kappa}\mathbf{r})] \quad (22a)$$

$$\mathbf{H}_{\text{scat}}(\mathbf{r}) = -s_{l,m;l,m}^{(ee)0} \mathbf{N}_{l,m}^{(m)}(\boldsymbol{\kappa}\mathbf{r}) + \sum_{l',m'} [s_{l,m;l',m'}^{(em)1} \mathbf{N}_{l',m'}^{(e)}(\boldsymbol{\kappa}\mathbf{r}) - s_{l,m;l',m'}^{(ee)1} \mathbf{N}_{l',m'}^{(m)}(\boldsymbol{\kappa}\mathbf{r})]. \quad (22b)$$

The first order terms of the scattering c -matrix for the (e) mode are

$$c_{l,m;l-1,m-\mu}^{(em)1} = \frac{s_{l,m;l-1,m-\mu}^{(em)1}}{a_{l,m}^{(e)}} = -\sqrt{\frac{l+1}{2l+1}} G_{l,m;l-1,m-\mu}^{(em)-}(a) \\ \times \frac{b_{l,m;l,m}^{(ee)0}}{a_{l,m}^{(e)}} n\kappa^3 \frac{\psi_{l-1}(n\kappa a)\phi'_{l-1}(n\kappa a) - \psi'_{l-1}(n\kappa a)\phi_{l-1}(n\kappa a)}{\psi_{l-1}(n\kappa a)\phi'_{l-1}(\kappa a) - n\psi'_{l-1}(n\kappa a)\phi_{l-1}(\kappa a)}, \quad (23a)$$

$$c_{l,m;l+1,m-\mu}^{(em)1} = \frac{s_{l,m;l+1,m-\mu}^{(em)1}}{a_{l,m}^{(e)}} = \sqrt{\frac{l}{2l+1}} G_{l,m;l+1,m-\mu}^{(em)+}(a) \\ \times \frac{b_{l,m;l,m}^{(ee)0}}{a_{l,m}^{(e)}} n\kappa^3 \frac{\psi_{l+1}(n\kappa a)\phi'_{l+1}(n\kappa a) - \psi'_{l+1}(n\kappa a)\phi_{l+1}(n\kappa a)}{\psi_{l+1}(n\kappa a)\phi'_{l+1}(\kappa a) - n\psi'_{l+1}(n\kappa a)\phi_{l+1}(\kappa a)}, \quad (23b)$$

$$c_{l,m;l-2,m-\mu}^{(ee)1} = \frac{s_{l,m;l-2,m-\mu}^{(ee)1}}{a_{l,m}^{(e)}} = -\sqrt{\frac{l+1}{2l+1}} G_{l,m;l-2,m-\mu}^{(ee)-}(a) \\ \times \frac{b_{l,m;l,m}^{(ee)0}}{a_{l,m}^{(e)}} n\kappa^3 \frac{\psi_{l-2}(n\kappa a)\phi'_{l-2}(n\kappa a) - \psi'_{l-2}(n\kappa a)\phi_{l-2}(n\kappa a)}{n\psi_{l-2}(n\kappa a)\phi'_{l-2}(\kappa a) - \psi'_{l-2}(n\kappa a)\phi_{l-2}(\kappa a)}, \quad (23c)$$

$$c_{l,m;l+2,m-\mu}^{(ee)1} = \frac{s_{l,m;l+2,m-\mu}^{(ee)1}}{a_{l,m}^{(e)}} = \sqrt{\frac{l}{2l+1}} G_{l,m;l+2,m-\mu}^{(ee)+}(a) \\ \times \frac{b_{l,m;l,m}^{(ee)0}}{a_{l,m}^{(e)}} n\kappa^3 \frac{\psi_{l+2}(n\kappa a)\phi'_{l+2}(n\kappa a) - \psi'_{l+2}(n\kappa a)\phi_{l+2}(n\kappa a)}{n\psi_{l+2}(n\kappa a)\phi'_{l+2}(\kappa a) - \psi'_{l+2}(n\kappa a)\phi_{l+2}(\kappa a)}, \quad (23d)$$

$$c_{l,m;l,m-\mu}^{(ee)1} = \frac{s_{l,m;l,m-\mu}^{(ee)1}}{a_{l,m}^{(e)}} = -\left[\sqrt{\frac{l+1}{2l+1}} G_{l,m;l,m-\mu}^{(ee)-}(a) - \sqrt{\frac{l}{2l+1}} G_{l,m;l,m-\mu}^{(ee)+}(a) \right] \\ \times \frac{b_{l,m;l,m}^{(ee)0}}{a_{l,m}^{(e)}} n\kappa^3 \frac{\psi_l(n\kappa a)\phi'_l(n\kappa a) - \psi'_l(n\kappa a)\phi_l(n\kappa a)}{n\psi_l(n\kappa a)\phi'_l(\kappa a) - \psi'_l(n\kappa a)\phi_l(\kappa a)}. \quad (23e)$$

$b_{l,m;l,m}^{(ee)0}/a_{l,m}^{(e)} = n[\psi_l(\kappa a)\phi'_l(\kappa a) - \psi'_l(\kappa a)\phi_l(\kappa a)]/[n\psi_l(n\kappa a)\phi'_l(\kappa a) - \psi'_l(n\kappa a)\phi_l(\kappa a)]$ is the zeroth order amplitude of the (e) mode inside the sphere.

4. Remarks on and discussion of the derivation

Generally speaking, the scattering c -matrix can be obtained either by solving a differential equation for eigensolutions for the single dielectric sphere and imposing the scattering boundary condition or by solving the exact Lippmann–Schwinger integral equation by using an iteration scheme. The second scheme is straightforward, but involves a large number of numerical integrations in three dimensions for different modes and for different frequencies. It yields the scattering t -matrix directly, and the scattering c -matrix required by the multiple scattering method has to be deduced from the relation $t = -ic/(1 + ic)$. Since accurate three dimensional integrations are usually very computationally intensive, the second scheme is

more suitable for nonspherical objects where analytical calculation is difficult to implement. For spherical objects with dielectric anisotropy, we adopt the first scheme since imposing the spherical boundary condition together with using the approximate eigensolutions inside the spheres can save a lot of computational time.

To carry out the perturbation calculation on the scattering properties of spherical objects with dielectric anisotropy, the complete orthogonal base vectors can be chosen as either $(\mathbf{J}_{l,m}^{(\sigma)}(n\kappa\mathbf{r}), \mathbf{H}_{l,m}^{(\sigma)}(n\kappa\mathbf{r}))$ or $(\mathbf{J}_{l,m}^{(\sigma)}(n\kappa\mathbf{r}), \mathbf{N}_{l,m}^{(\sigma)}(n\kappa\mathbf{r}))$; they yield either the scattering t -matrix or the scattering c -matrix. Our detailed analyses show that the c -matrix has a nice Hermitian property in the absence of dielectric dissipation, and perturbation calculation on the c -matrix always conserves this physical requirement while perturbation calculation on the scattering t -matrix does not guarantee that the extracted c -matrix satisfies the Hermitian property although the exact t -matrix does yield a Hermitian c -matrix [35]. This is why we choose the c -matrix instead of the t -matrix for carrying out the perturbation.

We should emphasize that although our calculation on the scattering c -matrix is of first order in terms of ϵ_1 , the corresponding contribution to the scattering t -matrix is not of first order; instead, the multiple scattering effects depicted in the Lippmann–Schwinger integral equation are partly taken into account for an infinite series of diagrams involving the zeroth and first order scattering coefficients $c_{l,m;l,m}^{(\sigma\sigma')0}$ and $c_{l,m;l,m}^{(\sigma\sigma')1}$. Another point worth mentioning is that our perturbation calculation is carried out with respect to the isotropic part ϵ of the dielectric sphere, not with respect to the embedded medium (vacuum in our case). Thus the true small parameter with which we expand the eigensolutions is ϵ_1/ϵ instead of ϵ_1 ; this improves the accuracy of our perturbation results.

In the derivation presented in section 3, one notices that although both F and G functions appear in the corrections to the zeroth order eigensolutions, only G functions contribute to the scattering c -matrix. In fact, the effect of F functions is to renormalize the coefficients of the first order corrections $b_{l,m;l',m'}^{(\sigma\sigma')1}$ inside the dielectric sphere, and the total scattering solution inside the sphere is uniquely determined.

The scattering c -matrix presented in equations (19) and (23) reveals the following important information; unlike the isotropic dielectric medium case where the scattering c -matrix conserves the angular momentum between the incident and outgoing waves, the anisotropic nature of the dielectric medium generally mixes the neighbouring angular momentum states.

- (1) For an (m) mode incident electromagnetic wave, the scattered (m) mode electromagnetic wave has the same angular quantum number l , but the scattered (e) mode electromagnetic wave has the angular quantum number $l \pm 1$.
- (2) For an (e) mode incident electromagnetic wave, the scattered (m) mode electromagnetic wave has the angular quantum number $l \pm 1$, but the scattered (e) mode electromagnetic wave has the angular quantum numbers $l, l \pm 2$.

The scattered wave generally has the azimuthal quantum numbers $m, m \pm 2$. Therefore, the diagonal structure of the scattering c -matrix in an isotropic dielectric medium becomes a diagonal stripe structure in the anisotropic dielectric medium. This causes a reduction in symmetry of the scattering c -matrix and removes the degeneracy in the photonic band structure of isotropic spheres.

As an example, let us consider a face centred cubic crystal. Such a photonic crystal can be made using self-assembly of dielectric ellipsoids. To achieve a parallel orientation of dielectric ellipsoids, application of an external electric field is thus required during the self-assembly process so that the principal axis with the largest component of the dielectric constant aligns along the external electric field direction. Once the crystal structure is formed,

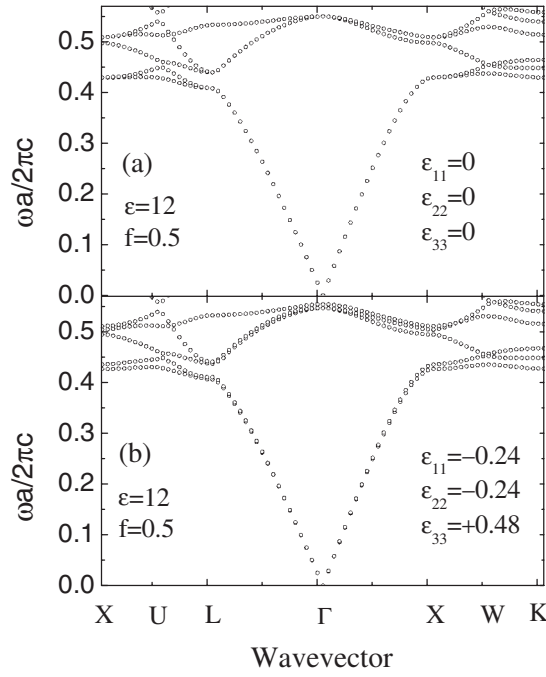


Figure 1. The photonic band structures of face centred cubic crystal composed of dielectric spheres embedded in vacuum; the filling ratio $f = 0.5$ and the maximum angular momentum $l_{\max} = 5$. The dielectric tensors are (a) $\epsilon = 12$ for isotropic dielectric spheres; (b) $\epsilon = 12$ plus $\epsilon_{11} = -0.24$, $\epsilon_{22} = -0.24$ and $\epsilon_{33} = +0.48$ for anisotropic dielectric spheres.

it remains there since the van der Waals interaction is minimized for ideal periodic structure. The scattering coefficients $c(\psi, \theta, \varphi)$ in general Cartesian coordinates can be obtained easily once the scattering coefficients c on the principal axes are known; they are related to each other by $c(\psi, \theta, \varphi) = R^+(\psi, \theta, \varphi)cR(\psi, \theta, \varphi)$, where R is the rotation matrix and ψ, θ, φ specify the angles of the new Cartesian coordinates. For simplicity, we assume that the principal axes of dielectric ellipsoids align along the axes of the crystal lattice. We have computed the photonic band structure with dielectric anisotropy and compared with that of the isotropic case; the result is presented in figure 1 for face centred cubic crystal. The material parameters used are: $\epsilon = 12$ for isotropic dielectric spheres; $\epsilon_{11} = -0.24$, $\epsilon_{22} = -0.24$ and $\epsilon_{33} = +0.48$ for spheres with dielectric anisotropy in addition to the isotropic part $\epsilon = 12$; the embedded medium is assumed to be vacuum and the filling ratios of the dielectric spheres for both cases are $f = 0.5$. As can be seen from figure 1, the photonic band structures are quite similar for small anisotropy—clear evidence for the dielectric anisotropy removing some of the degeneracies in the band dispersions. The possibility of optimizing the photonic band gap using dielectric anisotropy is an interesting topic which is worth pursuing.

5. Conclusions

In this paper, we have studied the scattering properties of spheres with dielectric anisotropy within the framework of the perturbation method. The calculation is carried out on the scattering c -matrix since its Hermitian property is conserved during such iterative procedures. The example of the photonic band structure of a face centred cubic crystal shows that dielectric

anisotropy reduces the symmetry of the scattering c -matrix, which causes band splittings. Further work is needed to explore whether dielectric anisotropy can help to create absolute band gaps for crystal structures where dielectric isotropy does not.

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Appendix A. Expansion of the dielectric tensor

$$A_{l,m;l,m-2}^{(mm)} = \frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \frac{1}{l(l+1)} \sqrt{(l+m)(l+m-1)(l-m+1)(l-m+2)}, \quad (\text{A.1})$$

$$A_{l,m;l,m}^{(mm)} = \left[\frac{1}{2}(\epsilon_{11} + \epsilon_{22})(l^2 + l - m^2) + \epsilon_{33}m^2 \right] \frac{1}{l(l+1)}, \quad (\text{A.2})$$

$$A_{l,m;l,m+2}^{(mm)} = \frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \frac{1}{l(l+1)} \sqrt{(l-m)(l-m-1)(l+m+1)(l+m+2)}, \quad (\text{A.3})$$

$$A_{l,m;l-1,m-2}^{(em)-} = -\frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \frac{1}{l} \sqrt{\frac{(l+m)(l+m-1)(l+m-2)(l-m+1)}{(l-1)(2l-1)}}, \quad (\text{A.4})$$

$$A_{l,m;l-1,m}^{(em)-} = \left[-\frac{1}{2}(\epsilon_{11} + \epsilon_{22}) + \epsilon_{33} \right] \frac{m}{l} \sqrt{\frac{(l+m)(l-m)}{(l-1)(2l-1)}}, \quad (\text{A.5})$$

$$A_{l,m;l-1,m+2}^{(em)-} = \frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \frac{1}{l} \sqrt{\frac{(l-m)(l-m-1)(l-m-2)(l+m+1)}{(l-1)(2l-1)}}, \quad (\text{A.6})$$

$$A_{l,m;l+1,m-2}^{(em)+} = -\frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \frac{1}{l+1} \sqrt{\frac{(l+m)(l-m+1)(l-m+2)(l-m+3)}{(l+2)(2l+3)}}, \quad (\text{A.7})$$

$$A_{l,m;l+1,m}^{(em)+} = -\left[-\frac{1}{2}(\epsilon_{11} + \epsilon_{22}) + \epsilon_{33} \right] \frac{m}{l+1} \sqrt{\frac{(l+m+1)(l-m+1)}{(l+2)(2l+3)}}, \quad (\text{A.8})$$

$$A_{l,m;l+1,m+2}^{(em)+} = \frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \frac{1}{l+1} \sqrt{\frac{(l-m)(l+m+1)(l+m+2)(l+m+3)}{(l+2)(2l+3)}}, \quad (\text{A.9})$$

$$B_{l,m;l-1,m-2}^{(me)} = \frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \frac{1}{l} \sqrt{\frac{(l-1)(l+m)(l+m-1)(l+m-2)(l-m+1)}{(l+1)(2l-1)(2l+1)}}, \quad (\text{A.10})$$

$$B_{l,m;l-1,m}^{(me)} = -\left[-\frac{1}{2}(\epsilon_{11} + \epsilon_{22}) + \epsilon_{33} \right] \frac{m}{l} \sqrt{\frac{(l-1)(l-m)(l+m)}{(l+1)(2l-1)(2l+1)}}, \quad (\text{A.11})$$

$$B_{l,m;l-1,m+2}^{(me)} = -\frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \frac{1}{l} \sqrt{\frac{(l-1)(l-m)(l-m-1)(l-m-2)(l+m+1)}{(l+1)(2l-1)(2l+1)}}, \quad (\text{A.12})$$

$$B_{l,m;l+1,m-2}^{(me)} = \frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \frac{1}{l+1} \sqrt{\frac{(l+2)(l+m)(l-m+1)(l-m+2)(l-m+3)}{l(2l+1)(2l+3)}}, \quad (\text{A.13})$$

$$B_{l,m;l+1,m}^{(me)} = \left[-\frac{1}{2}(\epsilon_{11} + \epsilon_{22}) + \epsilon_{33} \right] \frac{m}{l+1} \sqrt{\frac{(l+2)(l+m+1)(l-m+1)}{l(2l+1)(2l+3)}}, \quad (\text{A.14})$$

$$B_{l,m;l+1,m+2}^{(me)} = -\frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \frac{1}{l+1} \sqrt{\frac{(l+2)(l-m)(l+m+1)(l+m+2)(l+m+3)}{l(2l+1)(2l+3)}}, \quad (\text{A.15})$$

$$B_{l,m;l-2,m-2}^{(ee)-} = -\frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \times \frac{1}{2l-1} \sqrt{\frac{(l-2)(l+m)(l+m-1)(l+m-2)(l+m-3)}{l(l-1)(2l-3)}}, \quad (\text{A.16})$$

$$B_{l,m;l-2,m}^{(ee)-} = -\left[-\frac{1}{2}(\epsilon_{11} + \epsilon_{22}) + \epsilon_{33} \right] \times \frac{1}{2l-1} \sqrt{\frac{(l-2)(l-m)(l-m-1)(l+m-1)(l+m)}{l(l-1)(2l-3)}}, \quad (\text{A.17})$$

$$B_{l,m;l-2,m+2}^{(ee)-} = -\frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \times \frac{1}{2l-1} \sqrt{\frac{(l-2)(l-m)(l-m-1)(l-m-2)(l-m-3)}{l(l-1)(2l-3)}}, \quad (\text{A.18})$$

$$B_{l,m;l,m-2}^{(ee)-} = -\frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \times \frac{1}{l(2l-1)} \sqrt{\frac{(l+1)(l+m)(l+m-1)(l-m+1)(l-m+2)}{2l+1}}, \quad (\text{A.19})$$

$$B_{l,m;l,m}^{(ee)-} = \left[\frac{1}{2}(\epsilon_{11} + \epsilon_{22})(l^2 - l + m^2) + \epsilon_{33}(l^2 - m^2) \right] \frac{1}{l(2l-1)} \sqrt{\frac{l+1}{2l+1}}, \quad (\text{A.20})$$

$$B_{l,m;l,m+2}^{(ee)-} = -\frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \times \frac{1}{l(2l-1)} \sqrt{\frac{(l+1)(l-m)(l-m-1)(l+m+1)(l+m+2)}{2l+1}}, \quad (\text{A.21})$$

$$B_{l,m;l,m-2}^{(ee)+} = -\frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \times \frac{1}{(l+1)(2l+3)} \sqrt{\frac{l(l+m)(l+m-1)(l-m+1)(l-m+2)}{2l+1}}, \quad (\text{A.22})$$

$$B_{l,m;l,m}^{(ee)+} = \left[\frac{1}{2}(\epsilon_{11} + \epsilon_{22})(l^2 + 3l + m^2 + 2) + \epsilon_{33}(l+m+1)(l-m+1) \right] \times \frac{1}{(l+1)(2l+3)} \sqrt{\frac{l}{2l+1}}, \quad (\text{A.23})$$

$$B_{l,m;l,m+2}^{(ee)+} = -\frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \times \frac{1}{(l+1)(2l+3)} \sqrt{\frac{l(l-m)(l-m-1)(l+m+1)(l+m+2)}{2l+1}}, \quad (\text{A.24})$$

$$B_{l,m;l+2,m-2}^{(ee)+} = -\frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \times \frac{1}{2l+3} \sqrt{\frac{(l+3)(l-m+1)(l-m+2)(l-m+3)(l-m+4)}{(l+1)(l+2)(2l+5)}}, \quad (\text{A.25})$$

$$B_{l,m;l+2,m}^{(ee)+} = -\left[-\frac{1}{2}(\epsilon_{11} + \epsilon_{22}) + \epsilon_{33}\right] \times \frac{1}{2l+3} \sqrt{\frac{(l+3)(l-m+1)(l-m+2)(l+m+1)(l+m+2)}{(l+1)(l+2)(2l+5)}}, \quad (\text{A.26})$$

$$B_{l,m;l+2,m+2}^{(ee)+} = -\frac{1}{4}(\epsilon_{11} - \epsilon_{22}) \times \frac{1}{2l+3} \sqrt{\frac{(l+3)(l+m+1)(l+m+2)(l+m+3)(l+m+4)}{(l+1)(l+2)(2l+5)}}, \quad (\text{A.27})$$

$$C_{l,m;l-1,m-\mu}^{(mo)} = -\sqrt{\frac{l}{l-1}} B_{l,m;l-1,m-\mu}^{(me)}, \quad (\text{A.28})$$

$$C_{l,m;l+1,m-\mu}^{(mo)} = \sqrt{\frac{l+1}{l+2}} B_{l,m;l+1,m-\mu}^{(me)}, \quad (\text{A.29})$$

$$C_{l,m;l-2,m-\mu}^{(eo)-} = -\sqrt{\frac{l-1}{l-2}} B_{l,m;l-2,m-\mu}^{(ee)-}, \quad (\text{A.30})$$

$$C_{l,m;l,m-\mu}^{(eo)-} = \sqrt{\frac{l}{l+1}} B_{l,m;l,m-\mu}^{(ee)-}, \quad (\text{A.31})$$

$$C_{l,m;l,m-\mu}^{(eo)+} = -\sqrt{\frac{l+1}{l}} B_{l,m;l,m-\mu}^{(ee)+}, \quad (\text{A.32})$$

$$C_{l,m;l+2,m-\mu}^{(eo)+} = \sqrt{\frac{l+2}{l+3}} B_{l,m;l+2,m-\mu}^{(ee)+}. \quad (\text{A.33})$$

Appendix B. The functions F and G

$$G_{l,m;l,m-\mu}^{(mm)}(r) = A_{l,m;l,m-\mu}^{(mm)} \frac{1}{n^3 \kappa^3} \int_0^{n\kappa r} dx \psi_l(x) \psi_l(x), \quad (\text{B.1})$$

$$G_{l,m;l-1,m-\mu}^{(em)-}(r) = A_{l,m;l-1,m-\mu}^{(em)-} \frac{1}{n^3 \kappa^3} \int_0^{n\kappa r} dx \psi_{l-1}(x) \psi_{l-1}(x), \quad (\text{B.2})$$

$$G_{l,m;l+1,m-\mu}^{(em)+}(r) = A_{l,m;l+1,m-\mu}^{(em)+} \frac{1}{n^3 \kappa^3} \int_0^{n\kappa r} dx \psi_{l+1}(x) \psi_{l+1}(x), \quad (\text{B.3})$$

$$G_{l,m;l-1,m-\mu}^{(me)}(r) = -B_{l,m;l-1,m-\mu}^{(me)} \frac{1}{n^3 \kappa^3} \int_0^{n\kappa r} dx \psi_l(x) \psi_l(x), \quad (\text{B.4})$$

$$G_{l,m;l+1,m-\mu}^{(me)}(r) = B_{l,m;l+1,m-\mu}^{(me)} \frac{1}{n^3 \kappa^3} \int_0^{n\kappa r} dx \psi_l(x) \psi_l(x), \quad (\text{B.5})$$

$$G_{l,m;l-2,m-\mu}^{(ee)-}(r) = -B_{l,m;l-2,m-\mu}^{(ee)-} \frac{1}{n^3 \kappa^3} \int_0^{n\kappa r} dx \psi_{l-1}(x) \psi_{l-1}(x), \quad (\text{B.6})$$

$$G_{l,m;l,m-\mu}^{(ee)-}(r) = B_{l,m;l,m-\mu}^{(ee)-} \frac{1}{n^3 \kappa^3} \int_0^{n\kappa r} dx \psi_{l-1}(x) \psi_{l-1}(x), \quad (\text{B.7})$$

$$G_{l,m;l,m-\mu}^{(ee)+}(r) = -B_{l,m;l,m-\mu}^{(ee)+} \frac{1}{n^3 \kappa^3} \int_0^{n\kappa r} dx \psi_{l+1}(x) \psi_{l+1}(x), \quad (\text{B.8})$$

$$G_{l,m;l+2,m-\mu}^{(ee)+}(r) = B_{l,m;l+2,m-\mu}^{(ee)+} \frac{1}{n^3 \kappa^3} \int_0^{n\kappa r} dx \psi_{l+1}(x) \psi_{l+1}(x), \quad (\text{B.9})$$

$$F_{l,m;l,m-\mu}^{(mm)}(r) = A_{l,m;l,m-\mu}^{(mm)} \frac{1}{n^3 \kappa^3} \int_{n\kappa r}^{\infty} dx \psi_l(x) \varphi_l(x), \quad (\text{B.10})$$

$$F_{l,m;l-1,m-\mu}^{(em)-}(r) = A_{l,m;l-1,m-\mu}^{(em)-} \frac{1}{n^3 \kappa^3} \int_{n\kappa r}^{\infty} dx \psi_{l-1}(x) \varphi_{l-1}(x), \quad (\text{B.11})$$

$$F_{l,m;l+1,m-\mu}^{(em)+}(r) = A_{l,m;l+1,m-\mu}^{(em)+} \frac{1}{n^3 \kappa^3} \int_{n\kappa r}^{\infty} dx \psi_{l+1}(x) \varphi_{l+1}(x), \quad (\text{B.12})$$

$$F_{l,m;l-1,m-\mu}^{(me)}(r) = -B_{l,m;l-1,m-\mu}^{(me)} \frac{1}{n^3 \kappa^3} \int_{n\kappa r}^{\infty} dx \psi_l(x) \varphi_l(x), \quad (\text{B.13})$$

$$F_{l,m;l+1,m-\mu}^{(me)}(r) = B_{l,m;l+1,m-\mu}^{(me)} \frac{1}{n^3 \kappa^3} \int_{n\kappa r}^{\infty} dx \psi_l(x) \varphi_l(x), \quad (\text{B.14})$$

$$F_{l,m;l-2,m-\mu}^{(ee)-}(r) = -B_{l,m;l-2,m-\mu}^{(ee)-} \frac{1}{n^3 \kappa^3} \int_{n\kappa r}^{\infty} dx \psi_{l-1}(x) \varphi_{l-1}(x), \quad (\text{B.15})$$

$$F_{l,m;l,m-\mu}^{(ee)-}(r) = B_{l,m;l,m-\mu}^{(ee)-} \frac{1}{n^3 \kappa^3} \int_{n\kappa r}^{\infty} dx \psi_{l-1}(x) \varphi_{l-1}(x), \quad (\text{B.16})$$

$$F_{l,m;l,m-\mu}^{(ee)+}(r) = -B_{l,m;l,m-\mu}^{(ee)+} \frac{1}{n^3 \kappa^3} \int_{n\kappa r}^{\infty} dx \psi_{l+1}(x) \varphi_{l+1}(x), \quad (\text{B.17})$$

$$F_{l,m;l+2,m-\mu}^{(ee)+}(r) = B_{l,m;l+2,m-\mu}^{(ee)+} \frac{1}{n^3 \kappa^3} \int_{n\kappa r}^{\infty} dx \psi_{l+1}(x) \varphi_{l+1}(x). \quad (\text{B.18})$$

References

- [1] Yablonoitch E 1987 *Phys. Rev. Lett.* **58** 2059
- [2] Yablonoitch E, Gmitter T J and Bhat R 1988 *Phys. Rev. Lett.* **61** 2546
- [3] Yablonoitch E and Gmitter T J 1989 *Phys. Rev. Lett.* **63** 1950
- [4] Tarhan I I and Watson G H 1996 *Phys. Rev. Lett.* **76** 315
- [5] Vos W L *et al* 1996 *Phys. Rev. B* **53** 16231
- [6] John S 1987 *Phys. Rev. Lett.* **58** 2486
Busch K and John S 1998 *Phys. Rev. E* **58** 3896
- [7] Wang T, Moll N, Cho K and Joannopoulos J D 1999 *Phys. Rev. Lett.* **82** 3304
- [8] Szymanska M H, Hughes A F and Pike E R 1999 *Phys. Rev. Lett.* **83** 69
- [9] Zhang Z and Satpathy S 1990 *Phys. Rev. Lett.* **65** 2650
- [10] Ho K M, Chan C T and Soukoulis C M 1990 *Phys. Rev. Lett.* **65** 3152
Sigalas M M, Soukoulis C M, Chan C T and Ho K M 1994 *Phys. Rev. B* **49** 11080
- [11] Meade R D, Rappe A M, Brommer K D, Joannopoulos J D and Alerhand O L 1993 *Phys. Rev. B* **48** 8434
- [12] Fan S, Villeneuve P R and Joannopoulos J D 1996 *Phys. Rev. B* **54** 11245
- [13] Chan Y S, Chan C T and Liu Z Y 1998 *Phys. Rev. Lett.* **80** 956
- [14] Ward A J and Pendry J B 1998 *Phys. Rev. B* **58** 7252
- [15] Kuzmiak V and Maradudin A A 1997 *Phys. Rev. B* **55** 7427
- [16] Korringa J 1947 *Physica* **13** 392
- [17] Kohn W and Rostoker N 1954 *Phys. Rev.* **94** 1111
- [18] Beeby J L 1964 *Proc. R. Soc. A* **279** 82
- [19] Ohtaka K 1979 *Phys. Rev. B* **19** 5057
Ohtaka K 1980 *J. Phys. C: Solid State Phys.* **13** 667
- [20] Ohtaka K and Tanabe Y 1996 *J. Phys. Soc. Japan* **65** 2265
Ohtaka K and Tanabe Y 1996 *J. Phys. Soc. Japan* **65** 2670
Ohtaka K and Tanabe Y 1996 *J. Phys. Soc. Japan* **65** 2276
Ohtaka K, Ueta T and Tanabe Y 1996 *J. Phys. Soc. Japan* **65** 3068
- [21] Modinos A 1987 *Physica A* **141** 575
- [22] Stefanou N and Modinos A 1991 *J. Phys.: Condens. Matter* **3** 8135
- [23] Stefanou N, Karathanos V and Modinos A 1992 *J. Phys.: Condens. Matter* **4** 7389
- [24] Stefanou N, Yannopoulos V and Modinos A 1998 *Comput. Phys. Commun.* **113** 49
- [25] Wang X D, Zhang X-G, Yu Q L and Harmon B N 1993 *Phys. Rev. B* **47** 4161

-
- [26] Moroz A 1995 *Phys. Rev. B* **51** 2068
Moroz A 1994 *J. Phys.: Condens. Matter* **6** 171
- [27] Tayeb G and Maystre D 1997 *J. Opt. Soc. Am. A* **14** 3323
- [28] Zhang W, Lei X Y, Wang Z L, Zheng D G, Tam W Y, Chan C T and Sheng P 2000 *Phys. Lett.* **84** 2853
- [29] Moroz A 2002 *Phys. Rev. B* **66** 115109
- [30] Li Z Y, Gu B Y and Yang G Z 1998 *Phys. Rev. Lett.* **81** 2574
- [31] Li Z Y, Gu B Y and Yang G Z 1999 *Eur. Phys. J. B* **11** 65
- [32] Li Z Y, Wang J and Gu B Y 1998 *Phys. Rev. B* **58** 3721
- [33] Li Z Y, Lin L L, Gu B Y and Yang G Z 2000 *Physica B* **279** 159
- [34] Jackson J D 1962 *Classical Electrodynamics* 2nd edn (New York: Wiley)
- [35] Williams A R and van Morgan J W 1974 *J. Phys. C: Solid State Phys.* **7** 37
- [36] Bohren G F and Huffman D R 1983 *Absorption and Scattering of Light by Small Particles* (New York: Wiley)
- [37] Tai C-T 1994 *Dyadic Green's Functions in Electromagnetic Theory* (Piscataway, NJ: IEEE) (equations (10)–(24))
- [38] Butler W H, Gonis A and Zhang X G 1993 *Phys. Rev. B* **48** 2118