Spectral decomposition for the optical response of cylinder chains

Andreas J Reuben

Department of Applied Physics, University of Technology, Sydney, PO Box 123, Broadway, New South Wales, Australia

Abstract.   We obtain the complete modal decomposition for the response to a constant electric field of both finite and infinite chains of circular cylinders of arbitrary refractive index. A by-product of the technique in the infinite case is a simple expression relating the position of the leading resonance with the cylinder spacing.

1. Introduction

The determination of the optical response of heterogeneous media to electromagnetic waves in the long-wavelength limit is a longstanding problem. The standard averaging methods used initially were based on formulations such as those of Maxwell–Garnett [1], Lorentz–Lorenz [2, 3] or Bruggeman, all of which are essentially dipole theories. Interest has come to centre on the question of the importance of long-range interactions for both ordered and disordered particulate arrays as well as on the effect of close approach between individual particles. It has become clear that even in the long-wavelength or quasi-static case the detailed microgeometry of such composite structures must be taken into account [4]. In a landmark paper, Rayleigh [5] investigated the limits of applicability of the Lorentz–Lorenz formula and in so doing developed a classic approach to the problem of determining the effective dielectric function of a two-component composite with cylindrical inclusions.

In the wake of recent experimental work [6], much attention has come to focus on the optical and transport properties as well as the band structure of systems containing metallic inclusions [7–12]. Useful new insights into the behaviour of these composite structures have been gained through such studies. One approach, using the 'Bloch wave' method, has been successfully used to examine energy losses in colloidal metals with structure on the nanometre scale [13]. This work has indicated that in the case of cylindrical and spherical inclusions, the loss spectrum depends only on basic geometric parameters such as inter-particle separation. A significant finding of this study is that in these materials the nanostructure can be replaced by an inhomogeneous effective medium and that the effective medium concept works well in this instance. In a further study Pitarke *et al* [14] evaluate the effective long-wavelength dielectric response for a regular array of metallic cylinders using previously developed photonic band structure calculations [15, 16]. They find that Maxwell–Garnett results work well if the centre-to-centre separation between neighbouring cylinders is at least twice the cylinder diameter.

In an extension of the Rayleigh method Fu *et al* [17] studied interfacial polarization for a dielectric system of spherical particles subject to a low-frequency potential. In this case it is

found that for spherically symmetric two-particle distributions all multipole moments *except* dipoles are zero and that within the mean-field approximation the Maxwell–Garnett result is rigorous. However, they find that for clustered inclusions and particle chaining there can be large deviations from the Maxwell–Garnett formula due to the presence of strong multipolar effects. For spherical metal particles in an insulating host the absorption peak is found to be both greatly increased in intensity and significantly red-shifted [18], a finding which is in line with earlier reports that unusually large far-infrared absorption of some heterogeneous systems is attributable to clustering effects [19]. A drawback of the technique developed by Fu and co-workers is that for large numbers of closely spaced particles, very large matrices must be employed to obtain satisfactory convergence.

There is no doubt that the availability of high-speed computers has now made the unwieldy calculations required by several recent approaches much less of a problem. It would nonetheless be worthwhile developing simpler models leading to the generation of smaller matrices and thus to the possibility of obtaining analytic results which could be of use in the fitting of observed data. With this in mind we now address the problem of determining the quasi-static dielectric response of a two-component composite consisting of either a finite or an infinite chain of cylinders of one material embedded in a matrix made of a second material. The cylinders will be considered to be of infinite length and so the problem becomes one of solving the Laplace equation in two dimensions. We shall use combinations of appropriate coordinate frames and then write down the series expansions for the harmonic potentials in terms of the corresponding variables. Once this is done, the imposition of the relevant boundary conditions at each cylinder surface leads naturally to an explicit spectral decomposition for the polarization response.

If the relative dielectric function for our two-component system is given by ϵ then we show that the coefficients in the series expansion for the induced potential satisfy the following equation:

$$(\nu \boldsymbol{I} + \boldsymbol{S}) \cdot \boldsymbol{A} = \boldsymbol{K} \qquad \nu = \frac{1 + \epsilon}{1 - \epsilon} \tag{1}$$

where $\boldsymbol{A}$ is the sought-after vector of potential coefficients, $\boldsymbol{I}$ is the unit matrix, $\boldsymbol{K}$ is a constant vector and $\boldsymbol{S}$ is the *structure matrix* which only depends on the sizes and spatial disposition of the cylinders. We then diagonalize the matrix $\boldsymbol{S}$, find the $1/r$ coefficient of the far-field expansion for the induced potential and thus determine the polarizability. This leads to the following expression for the effective response [20]:

$$\langle \chi \rangle = \sum_n \frac{g_n'}{\nu + t_n} \tag{2}$$

where the t_i are the eigenvalues of the structure matrix $\boldsymbol{S}$. We thus arrive at the *Bergman spectral representation* [21] for the response in terms of the so-called spectral weights g_n and depolarization factors L_n:

$$\langle \chi \rangle = \sum_n \frac{g_n}{\chi^{-1} + L_n} \qquad \chi = \epsilon - 1 \tag{3}$$

where

$$g_n = \tfrac{1}{2} g_n' \qquad L_n = \tfrac{1}{2}(1 - t_n).$$

Since its advent, the spectral formulation (3) for the average dielectric response of a two-component system has attracted a lot of attention [22, 23] and been usefully extended [24].

The quasi-static absorption response for infinite chains of metallic cylinders at optical and infrared frequencies has been examined previously [25], however, the full normal-mode

Bergman decomposition for such chains has not been presented so far. In their work Kempe *et al* [25] use a rapidly convergent technique based on a periodic conformal transformation. Their matrix equation for the polarization is found by satisfying the boundary conditions in terms of polar coordinates on one cylinder and then determining the coefficients in the series expansion for the induced potential by means of a Fourier decomposition. The built-in translational symmetry guarantees that this matching procedure is automatically achieved for all cylinder surfaces in the chain. The three-dimensional analogue of this method has been successfully applied to the response problem of an infinite chain of identical metallic spheres [26] by means of hypercomplex variable theory [27]. At close approach the cylinder and sphere chains exhibit qualitatively similar responses but both the red shift and absorption strength are greater in the cylinder case.

This paper completes and extends the two-dimensional cylinder chain work initiated by Kempe *et al*. We consider both finite and infinite chains. In the former case we adopt a recently developed method involving combinations of coordinate frames [20]. In the latter case we employ a completely new approach which provides a remarkably concise and elegant solution for the response. Cylinder chain structures are of particular interest because of the large infrared absorption peak. Kempe *et al* make the plausible suggestion that this peak is essentially the spectral weight of the fundamental mode, that is, the $n = 1$ term in (3). In this paper we show that this is in fact the case and that for chains of aluminium cylinders containing at least four cylinders most of the spectral weight is in the fundamental mode which is strongly red-shifted and intense. For both the finite and infinite cases we shall obtain the elements of S in analytic form and, in the case of the uniformly spaced infinite chain, use this to obtain a simple closed expression for the leading eigenvalue (and thus the leading depolarization mode L_1) as a function of the cylinder spacing. This result will be of particular relevance in the fitting and interpretation of optical data for composites known to contain chain-like clusters of metallic inclusions.

2. Governing equations

The approach employed here to find the spectral decomposition (3) for cylinder chains is an interesting extension of methods presented previously [20, 28]. As in these earlier studies we adopt the complex variable formalism to construct appropriate conformally determined coordinate frames whose contour lines include the circular cylinder boundaries. The present technique has several unexpected advantages, the most noteworthy being that the elements of the structure matrix can be determined exactly in closed form. We shall exemplify the method by first considering finite chains containing an even number of cylinders and then in the following section move on to a consideration of the infinite chain.

We shall consider applied fields of unit strength acting along the chain axis. At all cylinder boundaries the following matching conditions must be satisfied by the inner ($(\phi^{(in)})$), outer ($(\phi^{(out)})$), and applied ($(\phi^{(app)})$) potentials:

$$\phi^{(app)} + \phi^{(out)} = \phi^{(in)} \tag{4a}$$

$$\frac{\partial \phi^{(app)}}{\partial n} + \frac{\partial \phi^{(out)}}{\partial n} = \epsilon \frac{\partial \phi^{(in)}}{\partial n}. \tag{4b}$$

If we introduce the complex variable $z = x + iy$ then an applied field of unit strength acting along the chain (x) axis will have a potential given by the real part of

$$\phi^{(app)} = z.$$

The strategy which we adopt to solve the Laplace equation is based on a well-established sequence of steps [20]. The most important elements of this approach are the following two
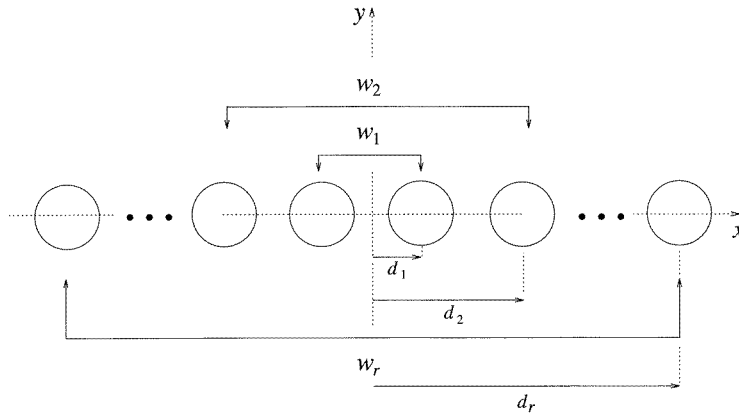
Finite Chain with $2r$ Unit Cylinders

Figure 1. A chain of $2r$ circular unit cylinders centred along the x-axis at the points $\pm d_i$, $i = 1, \ldots, r$. The bipolar coordinate frames w_i corresponding to cylinder pair i are indicated.

results: first, that the Laplace equation remains invariant under a conformal transformation of the variables and, second, that linear combinations of harmonic functions which vanish at infinity are also harmonic functions vanishing at infinity. We shall apply these two key observations in the following solution of the response problem for finite chains.

3. The finite chain

We shall restrict attention to fields acting along the chain axis as this is the case giving rise to the red shift in the response. The solution for a transverse field will follow trivially from the longitudinal solution through an application of Keller's reciprocal theorem [29]. For simplicity we shall only consider chains containing an even number of equally sized cylinders. It is a simple matter to modify the technique to chains containing an odd number of differently sized circular cylinders. We shall therefore consider chains containing $2r$ non-intersecting circular cylinders of unit radius. The geometrical arrangement is displayed in figure 1.

We shall view the chain as being composed of a sequence of nested cylinder pairs emanating from the chain centre at $z = 0$. In this scheme the 'first' cylinder pair is the innermost one centred at the points $\pm d_1$, the 'second' pair is centred at the points $\pm d_2$, and so on. Each of the r cylinder pairs is allocated its own 'local' bipolar frame. So, the bipolar frame corresponding to the ith cylinder pair will be given by w_i where [28]:

$$w_i = u_i + i v_i = \frac{1}{2a_i} \log\left(\frac{z + a_i}{z - a_i}\right) \qquad a_i = \sqrt{d_i^2 - 1}. \tag{5}$$

The boundary of the right-hand unit cylinder of pair i is given by

$$u_{i,0} = \frac{1}{2a_i} \log\left(a_i + \sqrt{1 + a_i^2}\right). \tag{6}$$

The local outer potential for cylinder pair i will be the real part of

$$\phi_i^{(\text{out})}(w_i) = \sum_{n=1}^{\infty} A_n^{(i)} \sinh(2a_i n w_i) \tag{7}$$

and the corresponding potential within the right-hand member of pair i will be the real part of

$$\phi_i^{(\text{in})}(w_i) = \sum_{n=1}^{\infty} B_n^{(i)} e^{-2a_i n w_i}. \tag{8}$$

Each cylinder pair will contribute its 'own' outer potential to the total outer potential which will be denoted by Φ_r. We thus have

$$\Phi_r(z) = \sum_{i=1}^{r} \phi_i(w_i). \tag{9}$$

The series expansion for the potential of the applied field in terms of the variables of frame w_i will be given by the real part of

$$z = a_i \left(\frac{1 + e^{-2a_i w_i}}{1 - e^{-2a_i w_i}} \right) = 2a_i \sum_{n=1}^{\infty} e^{-2na_i w_i} \tag{10}$$

to within a constant term. The expansion (10) tells us that the eigenfunctions for the cylinder pair i are the exponentials

$$e^{-2a_i k w_i}. \tag{11}$$

The total response potential Φ_r is now matched across the boundary of the right-hand cylinder of each pair in succession according to (4) in such a way that when matching across the boundary of cylinder pair i all variables are expressed in terms of the eigenfunctions (11) of that pair. In this way we shall obtain $2r$ equations for the set of $2r$ unknown coefficients $A_n^{(i)}$ and $B_n^{(i)}$, $i = 1, \ldots, r$. We then eliminate the $B_n^{(i)}$ and obtain a matrix equation of the form (1) for the desired outer coefficients $A_n^{(i)}$.

We now consider the matching procedure on cylinder pair i. To do this we must be able to expand the outer potentials for cylinder pair j ($j \neq i$), namely the $\sinh 2a_j n w_j$, in terms of the eigenfunctions (11) in a series which is convergent on the boundary of the right-hand cylinder of pair i. Eliminating z between the expressions (5) for w_i and w_j and then defining

$$\mu_{ij} = \frac{a_i + a_j}{a_i - a_j}$$

we obtain the following [30]:

$$e^{\pm 2a_j n w_j} = \mu_{ij}^{\pm n} \left(\frac{1 + \mu_{ij}^{\mp 1} e^{-2a_i w_i}}{1 + \mu_{ij}^{\pm 1} e^{-2a_i w_i}} \right)^n = \sum_{k=1}^{\infty} R_{n,k}^{\pm}(i, j) e^{-2a_i k w_i}$$

for

$$|\mu_{ij} e^{-2a_i w_i}| < 1 \tag{12}$$

where

$$R_{n,k}^{\pm}(i, j) = n \mu_{ij}^{\pm(n+k)} (1 + \mu_{ij}^{\mp 2})(-1)^k F_{2,1}(1 - n, 1 - k, 2, 1 + \mu_{ij}^{\mp 2}).$$

On the boundary of the right-hand cylinder of pair i we have, using (6), that

$$\rho_i = |e^{-2a_i w_{i,0}}| = e^{-2a_i u_{i,0}} = \left(a_i + \sqrt{1 + a_i^2} \right)^{-1}$$

from which it is easy to show that the convergence condition (12) is satisfied for non-intersecting cylinders whenever $i \neq j$. We therefore obtain

$$\sinh 2a_j n w_j = \sum_{k=0}^{\infty} \tilde{R}_{n,k}(i, j) e^{-2a_i k w_i}$$

where

$$\tilde{R}_{n,k}(i, j) = \tfrac{1}{2}(R_{n,k}^+(i, j) - R_{n,k}^-(i, j)).$$

Substituting $\phi_i^{(out)}$ from (7), $\phi_i^{(in)}$ from (8) and the applied potential from (10) into the boundary conditions (4) leads to two linear equations in $\cos 2a_i n v_i$ connecting the $A_n^{(i)}$ and the $B_n^{(i)}$. Dropping the summation over n and eliminating the $B_n^{(i)}$ produces the following equation for the coefficients $A_n^{(i)}$ of cylinder pair i:

$$A_n^{(i)}(v + \rho_i^{2n}) + \sum_{\substack{j=1 \\ j \neq i}}^{r} \sum_{k=1}^{\infty} S_{n,k}(i, j)A_k^{(j)} = 4a_i \rho_i^{2n} \tag{13}$$

where we have substituted for $u_{i,0}$ from (6) and defined

$$S_{n,k}(i, j) = -2\rho_i^{2n} \tilde{R}_{k,n}(i, j).$$

We thus have r equations of the form (13) each corresponding to the matching of the total outer potential Φ_r with each of the $\phi_i^{(in)}$ across the right-hand cylinders of pairs i, $i = 1, \ldots, r$. Each of the equations (13), truncated to order N, can be written in matrix form as

$$(v\boldsymbol{I}_N + \boldsymbol{P}_N^{(i)}) \cdot \boldsymbol{A}_N^{(i)} + \sum_{j \neq i} \boldsymbol{S}_N(i, j) \cdot \boldsymbol{A}_N^{(j)} = \boldsymbol{K}_n^{(i)} \tag{14}$$

where $\boldsymbol{S}_N(i, j)$ is the matrix of elements $S_{n,k}(i, j)$, $1 \leqslant n \leqslant N$, $1 \leqslant k \leqslant N$ and

$$\boldsymbol{P}_N^{(i)} = \begin{pmatrix} \rho_i^2 & 0 & \cdots & 0 \\ 0 & \rho_i^4 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \rho_i^{2N} \end{pmatrix} \qquad \boldsymbol{K}_N^{(i)} = 4a_i \begin{pmatrix} \rho_i^2 \\ \rho_i^4 \\ \vdots \\ \rho_i^{2N} \end{pmatrix}.$$

Now, putting the equations (14) for all $1 \leqslant i \leqslant r$ together and defining

$$\boldsymbol{A} = \begin{pmatrix} \boldsymbol{A}_N^{(1)} \\ \vdots \\ \boldsymbol{A}_N^{(r)} \end{pmatrix} \qquad \boldsymbol{K} = \begin{pmatrix} \boldsymbol{K}_N^{(1)} \\ \vdots \\ \boldsymbol{K}_N^{(r)} \end{pmatrix}$$

we obtain the system (1) of rN equations where the $rN \times rN$ structure matrix is given by

$$\boldsymbol{S} = \begin{pmatrix} \boldsymbol{P}_N^{(1)} & \boldsymbol{S}_N(1, 2) & \cdots & \boldsymbol{S}_N(1, r) \\ \boldsymbol{S}_N(2, 1) & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \boldsymbol{S}_N(r-1, r) \\ \boldsymbol{S}_N(r, 1) & \cdots & \boldsymbol{S}_N(r, r-1) & \boldsymbol{P}_N^{(r)} \end{pmatrix}. \tag{15}$$

We obtain the polarizability by determining the z^{-1} term in the far-field expansion of the outer potential (9). This is given by [28]

$$\langle \chi \rangle_r = \frac{4}{r} \sum_{i=1}^{r} \sum_{n=1}^{N} n a_i A_n^{(i)}. \tag{16}$$

We now diagonalize the structure matrix (15), solve for A and then substitute into (16) to obtain the weights g_n corresponding to the eigenvalues t_n of the matrix (15). We obtain decomposition (3) with

$$g_n = \frac{2}{r} \sum_{p=1}^{rN} \sum_{q=1}^{rN} a_{\lceil n/N \rceil} \left(n - N \left\lfloor \frac{n-1}{N} \right\rfloor \right) U_{pn} \bar{U}_{nq} K_q \qquad L_n = \tfrac{1}{2}(1 - t_n) \qquad (17)$$

for $n = 1, \ldots, rN$, where the U_{ij} and $\bar{U}_{ij}$ are the elements of the matrices U and U^{-1}, respectively, which diagonalize the matrix S defined by (15) and the t_n are the eigenvalues of S.

The results (17) are valid for any set of $2r$ non-intersecting co-axial unit cylinders with centres $\pm d_i$, $i = 1, \ldots, r$. It is a routine matter to obtain the response for chains containing an odd number of cylinders. In this case we would place the middle cylinder at the origin of coordinates and assign it a polar frame. The remaining cylinders will form pairs on the left and right of this central cylinder and to these we would assign bipolar frames in the manner outlined above.

4. The infinite chain

We begin here by reviewing the problem encountered when a single coordinate frame is used to represent the contours of each cylinder within an infinitely long chain of such cylinders. This chain frame was obtained by situating sources and sinks along the horizontal axis. The problem here occurred when one wanted to consider closely spaced cylinders. In this instance the contours lost their circular shape and became more and more elongated as the inter-cylinder spacing decreased [28]. This difficulty was overcome in the Kempe *et al* [25] study of the infinite chain problem by means of a semi-numerical matching of boundary conditions on a single cylinder. Here we take a completely new approach which leads to a concise solution permitting explicit determination of the elements of the structure matrix in a very simple closed form. As each element of the structure matrix can be determined exactly, the only approximation occurs via truncation. This will enable us to achieve excellent convergence.

For simplicity we will again illustrate the technique in the case of a chain of equally spaced unit cylinders. We begin by placing the origin of coordinates at the centre of a cylinder, the zeroth cylinder, say. To each cylinder in the chain we allocate a corresponding polar frame centred at the relevant cylinder's centre. If the cylinder centres are at the points $z = 2ma$, $m \in \mathbf{Z}$, then these polar frames will be given by

$$w_m = \log(z - 2ma) \qquad a > 1.$$

Consider now the central cell to which is associated the coordinate frame w_0. The outer potential for this cylinder will be the real part of

$$\phi_0^{\text{(out)}} = \sum_{n=1}^{\infty} A_n^{(0)} e^{-(2n-1)w_0} = \sum_{n=1}^{\infty} \frac{A_n^{(0)}}{z^{2n-1}}$$

while its interior potential will be the real part of

$$\phi_0^{\text{(in)}} = \sum_{n=1}^{\infty} B_n^{(0)} e^{(2n-1)w_0} = \sum_{n=1}^{\infty} B_n^{(0)} z^{2n-1}. \qquad (18)$$

Analogously, the outer potential corresponding to the cylinder centred at the point $z = 2ma$ will be the real part of

$$\phi_m^{\text{(out)}} = \sum_{n=1}^{\infty} A_n^{(m)} e^{-(2n-1)w_m} = \sum_{n=1}^{\infty} \frac{A_n^{(m)}}{(z - 2ma)^{2n-1}}. \qquad (19)$$

Now, just as in the case of the finite chains, we take the total outer potential, Φ_∞, to be the sum of all the local outer potentials $\phi_m^{(\text{out})}$, $m \in \mathbf{Z}$. However, since each cylinder in an evenly spaced infinite chain of identical cylinders which will behave identically, we have

$$A_n^{(m)} = A_n \qquad B_n^{(m)} = B_n \qquad m \in \mathbb{Z}. \tag{20}$$

Thus the total outer potential 'seen' by the cylinder centred at the origin $z = 0$ will be the real part of

$$\Phi_\infty(z) = \sum_{m=-\infty}^{\infty} \phi_m^{(\text{out})} = \sum_{n=1}^{\infty} A_n \left(\frac{1}{z^{2n-1}} + \underbrace{\sum_{m \neq 0} \frac{1}{(z - 2ma)^{2n-1}}}_{M_n(z,\,a)} \right). \tag{21}$$

The key to the solution is to obtain an appropriate form for the series $M_n(z, a)$. Using the result [31]

$$\sum_{r=0}^{\infty} \frac{1}{(z+r)^s} = \frac{1}{\Gamma(s)} \int_0^\infty \frac{t^{s-1} e^{-tz}}{1 - e^{-t}} \, dt \qquad \text{Re } s > 1$$

we obtain the following:

$$M_n(z, a) = \frac{-2}{(2a)^{2n-1}(2n-1)!} \int_0^\infty \frac{t^{2n-2}}{e^t - 1} \sinh\left(\frac{tz}{2a}\right) dt. \tag{22}$$

Expanding the integrand in (22) in positive powers of z leads to

$$M_n(z, a) = \sum_{k=1}^{\infty} C_{n,k}(a) z^{2k-1} \tag{23}$$

where

$$C_{n,k}(a) = -\frac{2}{(2a)^{2n+2k-2}} \binom{2n + 2k - 3}{2k - 1} \zeta(2n + 2k - 2) \tag{24}$$

where we have used the following definition for the Riemann zeta function [32]:

$$\zeta(s) = \frac{1}{\Gamma(s)} \int_0^\infty \frac{t^{s-1}}{e^t - 1} \, dt \qquad \text{Re } s > 1.$$

We now match boundary conditions on the central cylinder. The relevant inner and outer potentials are, by (18), (20), (21) and (23), just

$$\phi^{(\text{in})} = \sum_{n=1}^{\infty} B_n z^{2n-1} \qquad \Phi_\infty(z) = \sum_{n=1}^{\infty} A_n \left(\frac{1}{z^{2n-1}} + \sum_{k=1}^{\infty} C_{n,k}(a) z^{2k-1} \right) \tag{25}$$

with

$$\phi^{(\text{app})} = z. \tag{26}$$

Substituting the expressions (25) and (26) into the boundary conditions (4) and working in polar coordinates (r, θ) we obtain two linear equations in $\cos n\theta$ connecting the A_n and the B_n. Dropping the summation over n and eliminating the B_n leads to the form (1) for the A_n where the elements S_{ij} and K_i of the structure matrix S and the constant vector K, respectively, are given by

$$S_{ij} = C_{i,j}(a) \qquad K_i = \delta_{i1}. \tag{27}$$

The polarizability of the central cylinder is found from the $1/z$ coefficient of $\phi^{(\text{out})}$ and so

$$\langle \chi \rangle_\infty = A_1.$$

We now diagonalize S and solve for A in order to determine A_1. In this way we obtain the decomposition (3) with

$$g_n = U_{1n}\bar{U}_{n1} \qquad L_n = \tfrac{1}{2}(1 - t_n) \tag{28}$$

for $n = 1, \ldots, N$, where the U_{ij} and $\bar{U}_{ij}$ are the elements of the matrices U and U^{-1}, respectively, which diagonalize the matrix S defined in (27) and the t_n are the eigenvalues of this matrix.

It is important to note that although the spectral weights and depolarization factors for a given geometry are unique, the values of the terms in (1) are not. In other words, different solution methods will generally lead to different structure matrices and thus to different rates of convergence in numerical calculations. With this in mind, and for the purposes of comparison, the matrix equations of Kempe *et al* have been recast into the form (1) and the resulting structure matrix S' determined. A numerical examination of S' shows that it contains the structure matrix S defined by (27) as a sub-matrix. In particular, we find that the individual elements of these two matrices are related by

$$S_{ij} = S'_{2i-1,2j-1}$$

and that

$$t_1(N) = t'_1(2N) \tag{29}$$

where $t_1(N)$ and $t'_1(N)$ denote the respective first eigenvalues of the truncated structure matrices S_N and S'_N as functions of the truncation order N. Relation (29) shows that for numerical calculations the solution for the infinite chain presented in this section converges twice as rapidly as that of Kempe *et al* .

5. Application

We have used the results of sections 3 and 4 to obtain some sample responses as functions of wavelength for aluminium cylinders in air. Uniformly spaced chains are considered in which the centre-to-centre spacing is 2.1 units (for the finite chains: $d_i = (2i - 1)d$ with $d = 1.05$; for the infinite chain: $a = 1.05$). We have used equations (2), (17) and (28) to calculate the imaginary part of the polarizability for cylinder chains containing four, twenty and an infinite number of cylinders. These plots as functions of wavelength are displayed in figure 2. In each case the field acts along the chain axis. The wavelength dependencies of the complex dielectric constants for metallic aluminium are obtained from tabulated values [33]. In each case the contributions of the first couple of resonances were examined separately and it was seen that the red-shifted peak was almost entirely the contribution of the fundamental mode ($n = 1$). Therefore, if we could obtain a simple enough expression for the first eigenvalue in terms of the spacing parameter a, then it would be possible to use experimentally determined response curves to reliably calculate the spacing parameters for thin films containing cylinder chain structures. We now deduce an expression for this first eigenvalue using the expression (24) for the elements of the structure matrix of the infinite chain.

We begin by noting that for even integers the Riemann zeta function can be written in terms of Bernoulli numbers, B_n, in the following way [32]:

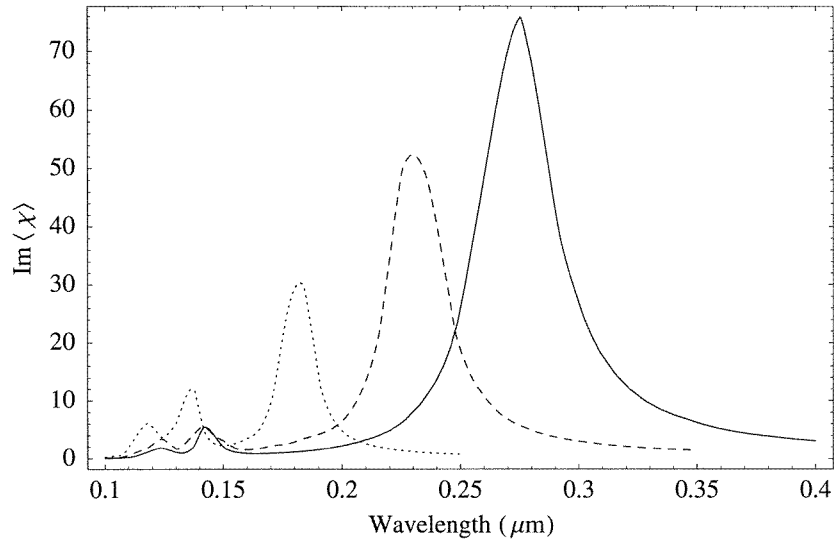$$\zeta(2n) = \frac{(2\pi)^{2n}}{2(2n)!}|B_{2n}| \qquad n = 1, 2, \ldots$$

Figure 2. Plots of the imaginary part of the response as a function of wavelength for chains of aluminium cylinders in air. The centre-to-centre separation between cylinders is 2.1 units in each case. The responses for two finite chains are displayed, one containing four cylinders (shown dotted) the other containing 20 cylinders (shown dashed), together with the response for the infinite chain (shown solid).

thus yielding the following expression for the elements of the structure matrix:

$$S_{ij} = -\frac{|B_{2i+2j-2}|\bar{a}^{2-2i-2j}}{(2i+2j-2)(2j-1)!(2i-2)!} \tag{30}$$

where

$$\bar{a} = a/\pi.$$

The infinite chain structure matrix truncated to order two is

$$S_2 = -\begin{pmatrix} \dfrac{1}{12\bar{a}^2} & \dfrac{1}{240\bar{a}^4} \\[2mm] \dfrac{1}{720\bar{a}^4} & \dfrac{1}{3024\bar{a}^6} \end{pmatrix}$$

where we have substituted the values for the Bernoulli numbers B_2, B_4 and B_6 [32] into (30). Calculation of the larger of the two eigenvalues of S_2 provides the following approximate formula for the first eigenvalue:

$$t_1(a) \approx \frac{5(1 + 252\bar{a}^4) + \sqrt{25 - 7308\bar{a}^4 + 1587\,600\bar{a}^8}}{30\,240\bar{a}^6}. \tag{31}$$

As can be seen from figure 3 the approximate expression (31) for the first eigenvalue compares well with the exact value over the whole range of values of the spacing parameter a. For very close approach between the cylinders ($a \to 1$), the approximation (31) is in error by about only 8.5%.

We now relate the value for t_1 to the wavelength at which the leading resonance occurs. For the purpose of illustration we consider metal cylinders *in vacuo* and let $\epsilon = \epsilon' + i\epsilon''$. If we realize the denominator in expression (2) for the response then we see that the value of ϵ' at the nth resonance for longitudinal applied fields will be given by [28]:

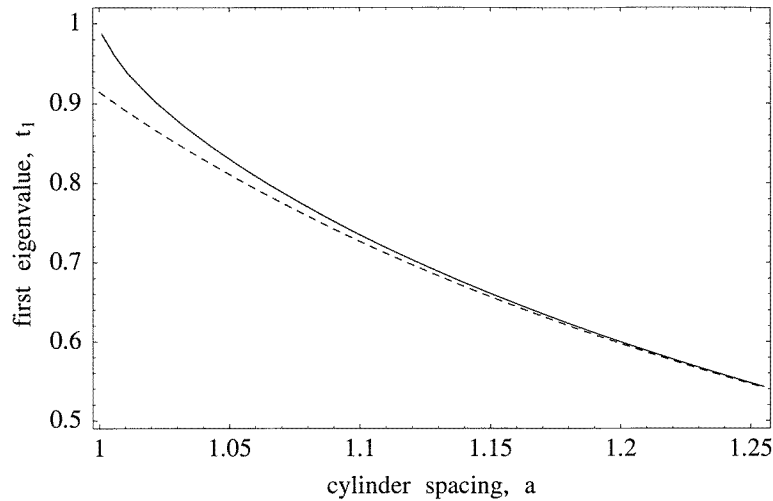$$\epsilon'_n = \frac{t_n + 1}{t_n - 1}. \tag{32}$$

Figure 3. A graph showing the value of the first eigenvalue t_1 of the structure matrix S as a function of the separation parameter a for the infinite chain. The solid curve represents the exact value of t_1 calculated directly from the truncated structure matrix S_N. The dashed curve is a plot of the approximation (31) for t_1.

Hence, by (32), for the uniformly spaced infinite chain the wavelength, λ_c, at which the leading resonance occurs, will satisfy

$$\epsilon'(\lambda_c) = \frac{t_1(a) + 1}{t_1(a) - 1}. \tag{33}$$

Substituting expression (31) for $t_1(a)$ into (33) then gives a simple relationship between λ_c and the chain parameter a.

6. Conclusion

In this paper we have successfully solved the electrostatic response problem for cylinder chains containing either a finite or an infinite number of circular cylinders and obtained spectral decompositions for their responses. The interesting aspect of this physical problem is the existence of a largely isolated first resonance corresponding to the first eigenvalue of the structure matrix. The method used to obtain the response for chains of infinite extent has enabled an accurate expression to be obtained for this eigenvalue in terms of the inter-cylinder spacing. This is of obvious benefit for those wishing to obtain geometrical parameters from optical data.

The work presented here can be extended in two different ways. The generalization of the technique of section 4 to two-dimensional chains and arrays of elliptical cylinders has recently been completed. A report on this work, couched in terms of the traditional Rayleigh approach, will appear shortly [34]. Work is also under way on the response problem for finite chains and clusters of spheres based on a combination of the superposition technique outlined in section 3 and the hypercomplex variable formalism cited earlier.

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