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Dipolar unit size in coupled-dipole calculations of the scattering matrix elements

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The coupled-dipole method is widely used to calculate the light-scattering matrix $S$ from arbitrary particles. An important parameter in the model is the size of the dipolar subunits. Usually a size of $\sim 1/10$ to $\sim 1/20$ of the wavelength of the incident light is sufficient for accurate calculations. However, it was noted that accurate $S_{34}$ calculations require much smaller dipolar subunits. We show that this conclusion is too pessimistic, by examining the sensitivity of the $S_{34}$ elements on surface roughness of spherical particles. Furthermore we give an example of an accurate $S_{34}$ calculation with dipolar subunits as large as $1/10$ of the wavelength.

The coupled-dipole (CD) method, originally formulated by Purcell and Pennypacker,\(^1\) is a powerful method with which to calculate elastic light scattering from arbitrary particles. The CD method divides a particle into small subvolumes, which are assumed to behave as ideal dipoles. The electric field on each dipole, caused by the external field and the field radiated by all other dipoles, is calculated. Next the scattered field is obtained by summation of the fields radiated by all dipoles in the observation points.

By repeating this calculation for a parallel- and a perpendicular-polarized incident electric field, one can compute the complete $(4 \times 4)$ scattering matrix $S$ of the particle. Although the basic concepts of the model are straightforward, the model possesses many parameters that are topics of active research. An example is the choice of the polarizability of the dipolar subunits. Lakhtakia\(^2\) reviewed the CD method.

An important parameter of the CD method is the size of the dipoles. The dipoles are placed on a cubic grid, with grid spacing $d$. The dipoles are therefore assumed to describe the response of a cube with volume $d^3$. The computations of the electric field on the dipoles requires solving a set of $3N$ equations with $3N$ unknowns, where $N$ is the number of dipoles. Therefore it is most advantageous to choose $d$ as large as possible, thus decreasing the total number of dipoles. Therefore it is most advantageous to choose $d$ as large as possible, thus decreasing the number of dipoles. Usually a size of $\sim 1/10$ to $\sim 1/20$ of the wavelength of the incident light is sufficient for accurate calculations. However, it was noted that accurate $S_{34}$ calculations require much smaller dipolar subunits. We show that this conclusion is too pessimistic, by examining the sensitivity of the $S_{34}$ elements on surface roughness of spherical particles. Furthermore we give an example of an accurate $S_{34}$ calculation with dipolar subunits as large as $1/10$ of the wavelength.

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particle with a rough surface. If the same particle is discretized by the use of more dipoles, the surface roughness will be smaller and the particle will be more closely approximated. We investigated the influence of surface roughness on the \( \alpha = 1.55 \) sphere and found that the decrease in surface roughness of the discretized particle as the number of dipoles is increased obscures the conclusions of Singham.

In the CD method we discretize a sphere as follows: place dipoles on grid points with coordinates \((i + 1/2)d, (j + 1/2)d, \) and \((k + 1/2)d\), with \(i, j, k\) integers, demanding that

\[
(i + 1/2)^2 + (j + 1/2)^2 + (k + 1/2)^2 \leq l^2. \tag{1}
\]

The number \(l\) determines the number of dipoles in the discretization; e.g., \(l = 3\) results in \(N = 136\), and \(l = 5\) gives \(N = 552\). The size of the dipoles determines the radius of the simulated sphere, through \(r_{\text{sphere}} = (3N/4\pi)^{1/3}d\) (the equal-volume sphere\(^4\)). The discretized sphere has a radius \(r = r_{\text{sphere}}[1 \pm O(\epsilon)]\), with \(\epsilon\) being a measure of the surface roughness. In our case, the radius is modulated with an amplitude of \(-d/2\); therefore \(\epsilon = 0.5 (3N/4\pi)^{-1/3}\).

Consider a particle with radius

\[
r = r_0[1.0 - (2l)^{-1}\cos(4l\theta)], \tag{2}
\]

with \(\theta\) an azimuthal angle. This is a spherical particle with mean radius \(r_0\) and roughness \(1/(2l)\). If \(l\) is increased, the roughness is decreased, but at the same time the frequency of the modulation is increased (the cosine term). This is what happens when we increase the number of dipoles in the discretization of the sphere by increasing \(l\) in relation (1). Figure 2 shows a cross section of the rough spheres for \(l = 3\) and \(l = 5\).

Note that \((2l)^{-1}\) is approximately equal to the estimated roughness of the discretized sphere. We calculated the \(S_{11}\) and \(S_{34}\) elements of a random distribution of this rough sphere for \(l = 3, l = 5,\) and \(l = 17\) and adjusted \(r_0\) such that the volume of the particle was the same and equal to the test sphere in all cases with \(\alpha = 1.55\). We calculated the scattering properties of this axis-symmetric particle with the T-matrix method, using the computer programs of Barber and Hill.\(^6\) This calculation serves as a model of the surface roughness of the discretized sphere.

Figures 3 and 4 give the results for \(S_{34}\) and \(S_{11}\) for the \(l = 3\) and \(l = 5\) rough spheres, together with Mie calculation for the \(\alpha = 1.55\) sphere. The \(l = 17\) calculation is indistinguishable from the Mie calculation.

The influence of surface roughness is most obvious for the \(S_{34}\) element. The \(S_{11}\) element of the rough sphere deviates slightly from the sphere in the backscattering direction. For \(l = 5\) the results are almost equal to the sphere. The same is true for the \(S_{15}\) and \(S_{35}\) elements (data not shown). However,
the roughness has a much more pronounced effect on the $S_{34}$ element, as seen in Fig. 3. Therefore a coarse discretization of the sphere in the CD method can result in larger errors in the $S_{34}$ element compared with errors in the other scattering matrix elements.

If we compare the calculations on the rough sphere with the CD calculations of Singham (Figs. 1 and 2 in Ref. 3), we see the same trends. For a small number of dipoles (123, comparable with $l = 3$), the $S_{34}$ computation deviates significantly from the exact Mie result in the same way as the rough sphere (see Fig. 3). The $S_{11}$ result of the CD computation already is very good, with only a deviation from the exact Mie result in the backscattering direction. If the number of dipoles is increased in the CD calculation, the $S_{11}$ result is in excellent agreement with the exact Mie calculation. The $S_{34}$ result approaches the exact results, but agreement is far from good.

Surface roughness has a strong effect on the $S_{34}$ element. Therefore, if the CD method is to be used to calculate the $S_{34}$ element of a smooth particle, surface roughness induced by the discretization of the particle must be very small. This is achieved by using a large number of dipolar subunits (large $l$). If the particle is small (e.g., the $a = 1.55$ sphere), relatively small dipolar subunits result. However, for larger particles (see Fig. 1), the subunits can be much larger. In that case, $S_{34}$ calculations with accuracy comparable to $S_{11}$ calculations can be achieved with dipolar subunits with $\lambda/20 \leq d \leq \lambda/10$.

References