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On the validity of the anomalous diffraction theory to light scattering by cubes

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Abstract

The extinction and absorption efficiencies of a cube at light incidence normal to its four-fold symmetry axis are calculated using the anomalous diffraction theory (ADT). The results are compared with those based on the discrete dipole approximation (DDA). It is shown that for certain cases of the orientation of a cube relative to the direction of the incident light the extinction efficiency calculated using DDA and ADT do not agree. However, the ADT-based absorption efficiencies for the cases studied are dependent on a particle volume and exhibit smaller errors. Hence the validity of the ADT for cubes is not as good as for spheres.

1. Introduction

Nonspherical particles are common in nature. Examples are hexagonal ice crystals, interstellar dust and aerosols. Light scattering by irregular particles is of importance e.g. in the remote sensing of cirrus clouds [1] and in studying of their influence on climate and climate feedback [2]. It is also important in studying the influence of the aerosol shape to Earth's global albedo [3] and in estimating the microphysical properties of interstellar dust [4,5]. The exact solutions of Maxwell equations are known for several simple shapes [6,7] (spheres, infinitely long cylinders, and spheroids) only. Thus, there is a need to resort to numerical procedures such as the discrete dipole approximation [8]. The DDA is a flexible and general technique for calculating the scattering and absorption characteristics of arbitrarily shaped particles but it requires rather large computer storage and CPU time [9,10]. One of the most frequently used approximate methods is the anomalous diffraction theory [6] (because of its simplicity) which can be applied in case of optically soft particles ($|m-1| \ll 1$ where $m = m_{re} + i m_{im}$ is the refractive index of a particle) large compared to the wavelength λ of the incident radiation. The validity of the ADT was tested for spheres and infinite circular cylinders by comparing the results for extinction and absorption efficiencies with those obtained from the exact solution of Maxwell's equations [6,11–14]. Other shapes were

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studied including: cube for particular orientations relative to the direction of the incident light [15,16], hexagon in arbitrary orientation [17], arbitrarily oriented thin disc and ellipsoid of revolution [18], and prismatic columns perpendicular to the incident radiation [19,20].

In this paper we discuss comparisons between rigorous and approximate methods for cubes.

2. Discrete dipole approximation

The DDA replaces the solid particle with an array of N point dipoles occupying positions on a cubic lattice (see Fig. 1) [8–10]. The lattice spacing d has to be small compared to the wavelength of the incident radiation. Each dipole i is characterized by an oscillating polarization $\boldsymbol{P}_i$,

$$\boldsymbol{P}_1 = \alpha_i \boldsymbol{E}_i \tag{1}$$

in response to the total electric field $\boldsymbol{E}_i$ at its position; $\boldsymbol{E}_i$ is the sum of the incident plane wave and the electric fields from all of the other dipoles in the array and α_i is the ith dipole polarizability.

The scattering problem can be compactly written as

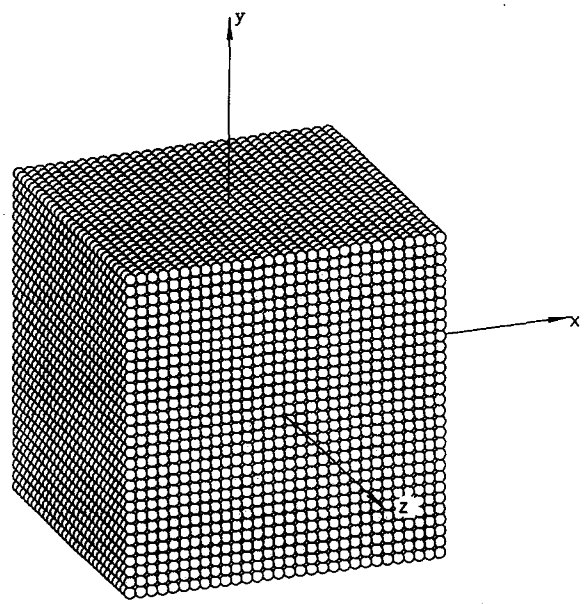

Fig. 1. Pseudocube composed of 30×30×30 dipoles on cubical lattice.

$$\tilde{A}\tilde{P} = \tilde{E}_{\mathrm{inc}}, \tag{2}$$

where $\tilde{A}$ is a $3N \times 3N$ symmetric complex matrix depending on the particle shape, dielectric properties and the ratio of the interdipole distance to the incident wavelength, $\tilde{P}$ is a $3N$ dimensional unknown vector of dipole polarizations and $\tilde{E}_{\mathrm{inc}}$ is a $3N$ dimensional vector of the incident electric field. The prescription for the polarizabilities, the lattice dispersion relation (LDR), follows recent work of Draine and Goodman [21]. The conjugate gradient (CG) algorithm together with the fast Fourier transform (FFT) method is used to solve Eq. (2) [9,10]. Once the polarization of every dipole in an array is found the scattering and absorptive properties of the particle approximated by this array of dipoles can be calculated [9].

3. Anomalous diffraction theory – basic concepts

As it was pointed out in Sect. 1 the anomalous diffraction theory of van de Hulst [6] is being actively developed. The method is simple and was validated for a large range of sizes for spheres and cylinders [6,11–14]. However, the polarization effects cannot be treated within the ADT and it is unknown if extrapolations based on the comparisons with the exact solution for spheres and cylinders hold universally for other shapes.

Efficiencies in the ADT can be calculated by the two-dimensional integral. It can be shown [18,20] that the extinction efficiency is given by

$$Q_{\mathrm{ext}} = \frac{2}{P}\int [1-\exp(-r)\cos(\rho)]\,\mathrm{d}P, \tag{3}$$

and the absorption efficiency is

$$Q_{\mathrm{abs}} = \frac{1}{P}\int [1-\exp(-2r)]\,\mathrm{d}P, \tag{4}$$

where

$$\rho = kl\,(m_{\mathrm{re}}-1), \tag{5}$$

$$r = klm_{\mathrm{im}}, \tag{6}$$

l is the distance the light travels inside the particle, k is the wavenumber ($k=2\pi/\lambda$) and P is the projected area of a particle on the plane perpendicular to the

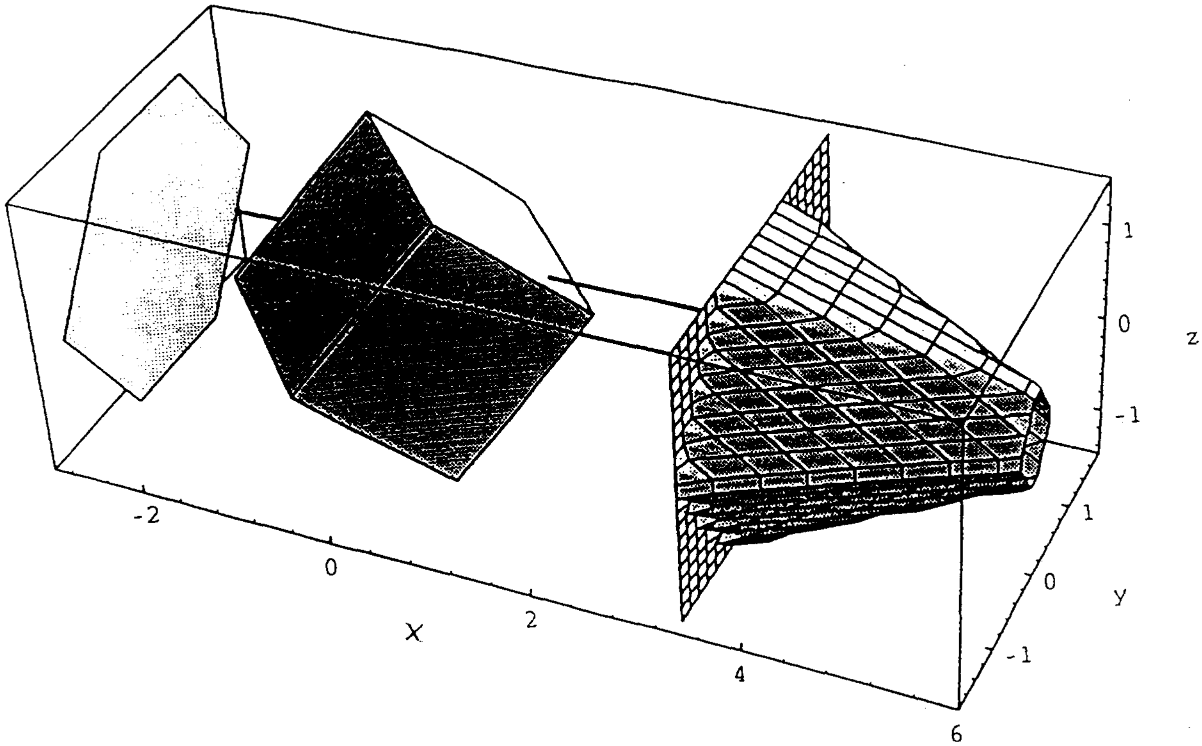

Fig. 2. Cube in arbitrary orientation. The shadow of a cube is presented. It is obtained by projecting vertices and calculating their convex hull. The distances inside a cube are also shown.

direction of the electromagnetic wave. The solution of Eqs. (3) and (4) depends on a distance l which the light passes through the particle. For most shapes it can be done analytically but due to the complexity of the results the studies are often limited to "easy" orientations of the particle relative to the direction of light [15,19,20]. In the next section we present a new and fast algorithm based on the ray-tracing method valid for convex particles in arbitrary orientation.

4. The ray-tracing scheme

To get the distance l needed to calculate the phase shifts (5) and (6) we use a ray–convex polyhedron algorithm [22]. This requires defining a target by its vertices. Such assumption is not limiting: cube, prisms, and polygonal approximations to spheres and cylinders can be defined by a linked list of vertices.

A particle is defined by a vertices of polyhedron. Thus, for example, a cube is defined by eight vertices. The vertices are used in connectivity list which gives a set of co-planar faces (polygons) defining the object. Thus, a cube would have six such faces. A target can be arbitrarily rotated. After defining the object we project its vertices on a plane and we calculate the convex hull of projected vertices [23,24]. We also define a rectangular grid encompassing the convex hull. For each line intersecting the rectangular grid and parallel to the light propagation we calculate the distance l inside the polyhedron using the ray–polyhedron intersection algorithm [22] (see Fig. 2). In this way we obtain a distance array for arbitrary orientation of an object. The validity of this algorithm was established by implementing it and comparing the results with the analytical ones.

5. Results

We present the DDA and ADT calculations for extinction and absorption efficiencies of a cube at light incidence normal to the four-fold symmetry axis of a cube. A cube is assumed to be rotated around y-axis

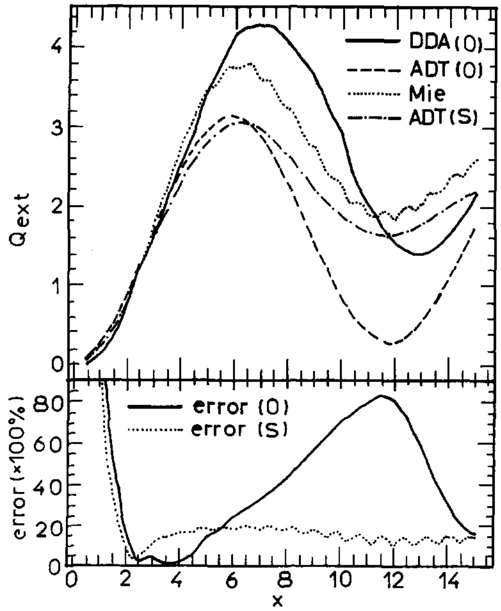

Fig. 3. Extinction efficiency of a cube at face incidence ($\theta=0$) calculated using DDA (DDA(0)) and ADT (ADT(0)) together with extinction efficiency of a sphere calculated using Mie theory and ADT (ADT(S)). Refractive index of particles $m=1.33+0.01i$. Error $(0)=|Q_{ext}(ADT(0))/Q_{ext}(DDA(0))-1|$, error $(S)=|Q_{ext}(ADT(S))/Q_{ext}(Mie)-1|$.

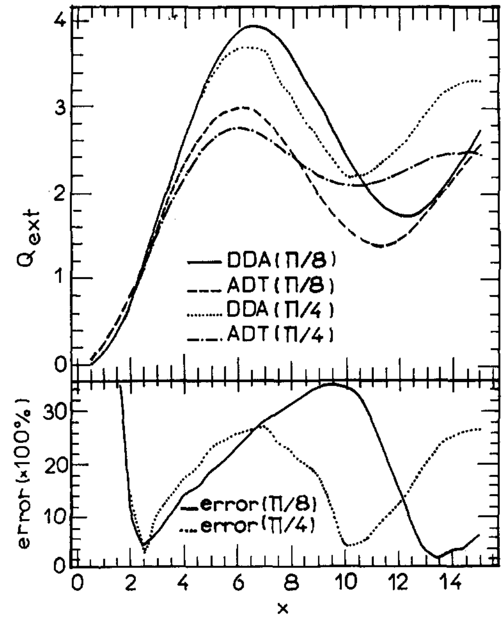

Fig. 4. Extinction efficiency of a cube at middle incidence ($\theta=\pi/8$) and at edge incidence ($\theta=\pi/4$) calculated using DDA (DDA(θ)) and ADT (ADT(θ)) ($\theta=\pi/8, \pi/4$). Refractive index of particles $m=1.33+0.01i$. Error $(\theta)=|Q_{ext}(ADT(\theta))/Q_{ext}(DDA(\theta))-1|$.

by an angle θ; the $\theta=0$ case is presented in Fig. 1 where the direction of the incident light (x-direction) is normal to one of the faces of a cube. Three different orientations of a cube relative to the incoming light have been considered: face incidence ($\theta=0$), middle incidence ($\theta=\pi/8$) and edge incidence ($\theta=\pi/4$). The efficiencies of extinction and absorption are normalized to the projected area of a sphere of radius a_{eff} and of a volume equal to a volume of a cube. Calculations are performed in the range $x=0.5$–15 of size parameters where $x=2\pi a_{eff}/\lambda$. The ADT is not nominally valid for small size parameters x and we ignore this range in our discussion. The efficiencies are calculated for refractive index $m=1.33+0.01i$, $m=1.2+0.01i$ and $m=1.33$. The resolution of the cubic lattice was varied to keep the dipole-size related parameter $|m|kd$ in the 0.6–1.1 range and computational time manageable [21]. Thus, for $x=0.5$–5 we used a $16\times16\times16$ lattice, for $x=5.5$–10 we used a $25\times25\times25$ lattice and for $x=10.5$–15 we used a $30\times30\times30$ lattice. Thus, the amount of dipoles used was varied between $N=4096$

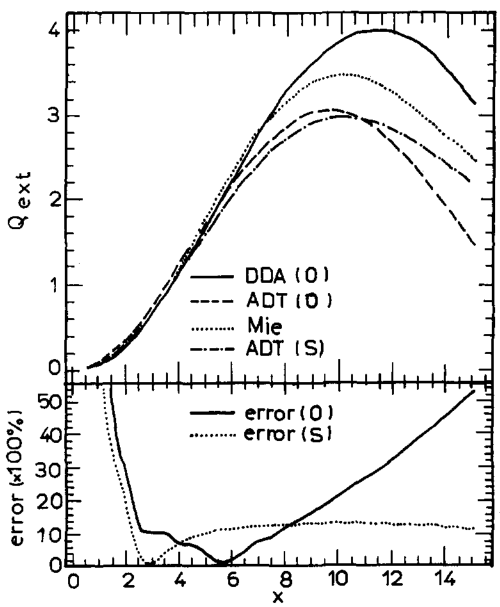

Fig. 5. Same as Fig. 3, but for $m=1.2+0.01i$.

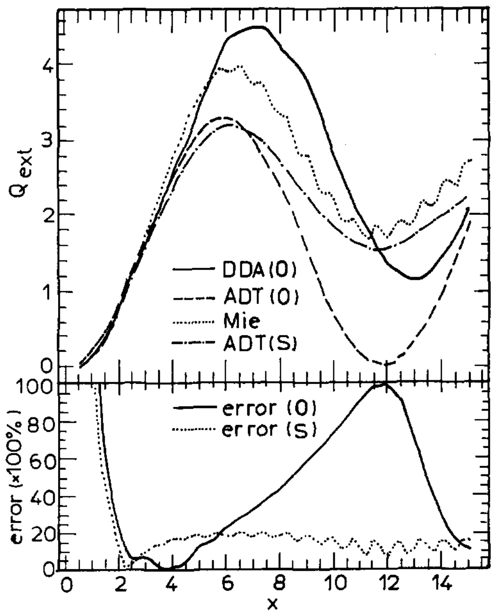

Fig. 6. Same as Fig. 3, but for $m = 1.33$.

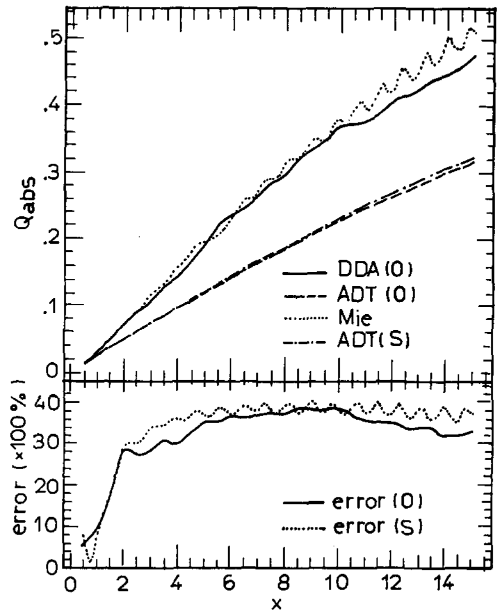

Fig. 8. Same as Fig. 3, but for absorption efficiency.

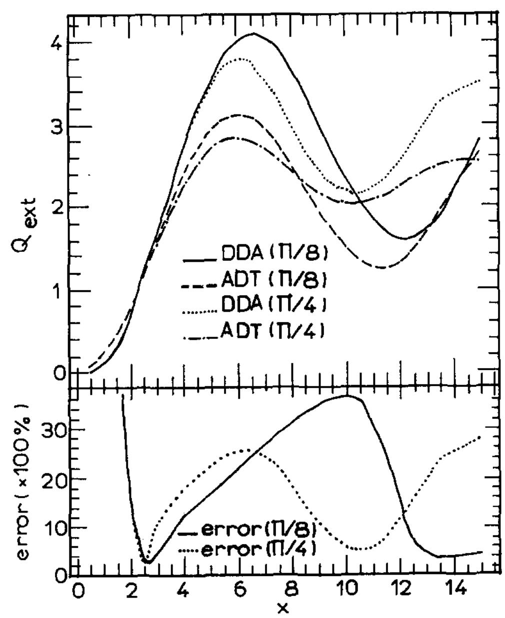

Fig. 7. Same as Fig. 4, but for $m = 1.33$.

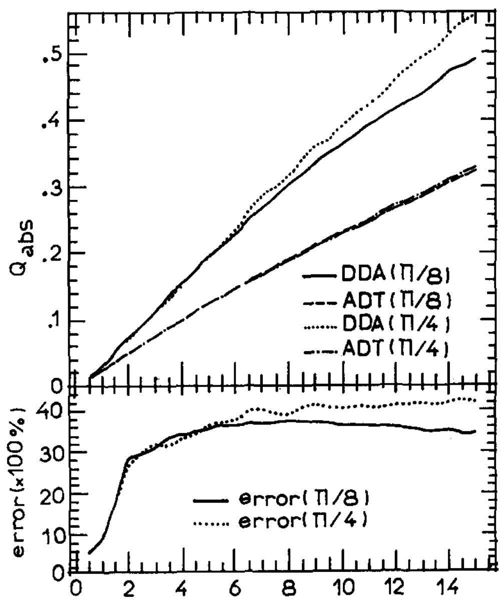

Fig. 9. Same as Fig. 4, but for absorption efficiency.

and $N = 27000$. The fractional error convergence criterion for the conjugate gradient solver was set in the 10^{-5}–10^{-3} range. Less precision was requested for larger size parameters to reduce computer time.

The extinction efficiencies of a cube calculated using DDA and ADT methods as a function of the size parameter x are presented in Figs. 3–7. Figs. 3, 5 and 6 present also Mie solution versus ADT comparisons of extinction for spheres. The relative error in Q_{ext} is shown. The results for the edge incidence of light

($\theta=\pi/4$) for $m=1.33+0.01i$ and $m=1.33$, presented in Figs. 4 and 7, respectively show fairly good agreement between the two methods. The error is similar to that between exact solution for spheres and the ADT in this size parameter range (see Figs. 3 and 6) and is less than 30%. Surprisingly, the $\theta=\pi/8$ case (Figs. 4 and 7) shows much larger deviations between DDA and ADT. The error exceeds 30% and the ADT curve is shifted relative to the DDA curve (the ADT maximum for both $m=1.33+0.01i$ and $m=1.33$ is shifted by $\Delta x \simeq 0.5$ in comparison to the DDA). The most pronounced disagreement for both refractive indexes appears for face incidence case (Figs. 3, 6). The shift of $\Delta x \simeq 1$ is observed and the errors are larger in comparison to the edge and the middle incidence cases. For the $m=1.33$ case the error reaches 100%. For face incidence case and $m=1.2+0.01i$ a shift between both curves is even larger and reaches $\Delta x \simeq 2$ (Fig. 5). The error there exceeds 50% for $x=15$.

Figs. 8 and 9 show absorption efficiencies for the three orientations of a cube relative to the incident light and for $m=1.33+0.01i$. A qualitative behavior is similar to that for Mie versus ADT for spheres. Absorption seems to be independent in this size range of a particle shape. This result agrees with the result of the semiempirical theory of Pollack and Cuzzi [3] who notice that for $2m_i x<1$ the absorption depends on the particle volume and not on its shape. Thus, the absorption for optically soft cubes in the size range studied can be approximated by the ADT. Additional empirical corrections are needed, defined in a similar way to corrections for spheres [12]. Such semiempirical corrections for extinction and scattering efficiencies are more difficult to establish due to the sensitivity of these efficiencies to the shape of a particle.

6. Conclusions

In this paper we compare efficiencies for light scattering on cubes using rigorous and approximate methods. We show that extinction efficiencies do not agree for certain cases of light incidence. We conclude that the ADT cannot be used as a rule for scattering by arbitrary shaped particles without verification with rigorous methods.

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