Calculation of the Radiation forces on each dipole in the discrete dipole approximation

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Abstract

The theory of the Discrete Dipole Approximation (DDA) for light scattering is extended to allow for the calculation of radiation forces on each dipole in the DDA model. Starting with the theory of Draine and Weingartner (Astrophys. J. **470**, 551-565, 1996) we derive an expression for the radiation force on each dipole. We test the theory on spheres, by comparing the resulting accumulated radiation forces with Mie theory. The accuracy for the total radiation pressure cross section is comparable to that obtained for extinction cross sections calculated with DDA, i.e. in the order of a few percent.

1 Introduction

Radiation force plays an important role in many scientific disciplines. Trapping and manipulation of small particles, or even trapping and cooling of single molecules and atoms are but a few of many fascinating examples. Also in the realm of astrophysics the radiation force plays an important role. In collaboration with the Astronomical Institute "Anton Pannekoek" of the University of Amsterdam we investigate radiation forces on dust particles in circumstellar disks. The total radiation pressure on the dust particles is not the only important effect. It is suspected that in the detailed process of formation of dust particles in a circumstellar disk, i.e. co-agulation of small grains into dust particles [1], radiation forces could play an important role [2]. In order to study the importance of radiation forces on the formation of dust particles knowledge of the total radiation pressure on the particle is therefore not enough. It is also necessary to know the radiation forces acting on *each* constituent grain that make up the dust particle. This notion triggered us to develop a method to calculate radiation forces in the Discrete Dipole Approximation (DDA) of light scattering. The radiation pressure cross section C_{pr} is

$$C_{pr} = C_{ext} - gC_{sca}, \tag{1}$$

with C_{ext} the extinction cross section, C_{sca} the scattering cross section and g the asymmetry parameter. This expression holds for any small particle illuminated by a beam of light. [3]

Independently, Draine and Weingartner [4] and Kimura and Mann [5] included the possibility to calculate radiation pressure into DDA by integrating the momentum carried by the scattered radiation over the total space angle. Draine and Weingartner started with the DDA equations and a general expression for the force on a dipole in an electromagnetic field. Next, they derived a formal expression for the force on each dipole in the DDA. This formal expression was not further elaborated, but by invoking some straightforward argument Eq. (1) was again recovered. The radiation forces where subsequently obtained by calculating gC_{sca} by an integration of the scattered fields. We take the work of Draine and Weingartner as a starting point, and derive expressions for the radiation force on each dipole in the DDA. We test our procedure by calculating the radiation force on a sphere, and compare DDA results with exact Mie calculations.

2 Theory of Radiation Force in DDA

This section will provide a summary of the theory. All details will be published elsewhere [6]. Following Draine and Weingartner, [4] the averaged total radiation force on a particle can be expressed as

$$\langle \mathbf{F}_{rad} \rangle = \langle \mathbf{F}_{inc} \rangle + \langle \mathbf{F}_{sca} \rangle = \sum_{i=1}^{N} \langle \mathbf{F}_{inc,i} \rangle + \sum_{i=1}^{N} \langle \mathbf{F}_{sca,i} \rangle , \tag{2}$$

$$\langle \mathbf{F}_{inc,i} \rangle = \frac{1}{2} \mathrm{Re}\Big((\mathbf{p}_{i,0}^{*} \cdot \nabla_i)(\mathbf{E}_{inc,0} e^{i\mathbf{k}\cdot\mathbf{r}_i}) + ik\mathbf{p}_{i,0}^{*} \times (\hat{\mathbf{k}} \times \mathbf{E}_{inc,0} e^{i\mathbf{k}\cdot\mathbf{r}_i}) \Big), \tag{3}$$

$$\langle \mathbf{F}_{sca,i} \rangle = \sum_{j \neq i} \frac{1}{2} \mathrm{Re}\Big((\mathbf{p}_{i,0}^{*} \cdot \nabla_i)\mathbf{E}_{ij} + ik\mathbf{p}_{i,0}^{*} \times \mathbf{B}_{ij} \Big). \tag{4}$$

The total force is divided into a part due to the incoming plane wave and a part due to the fields radiated by all dipoles. The index i and j denote a dipole, N is the total number of dipoles, $\mathbf{p}$ is the dipole moment, $\mathbf{E}$ and $\mathbf{B}$ the electric- and magnetic fields, and $\mathbf{k}$ the wave vector. For the details we refer to [4] and [6]. Evaluating Eq. (3) results in

$$\langle \mathbf{F}_{inc,i} \rangle = \frac{1}{2} \mathrm{Re}\Big(i\mathbf{k}(\mathbf{p}_{i,0}^{*} \cdot \mathbf{E}_{inc,0}) \exp(i\mathbf{k} \cdot \mathbf{r}_i) \Big). \tag{5}$$

By applying the expression for the extinction coefficient in the DDA as obtained from the optical theorem [7] the final expression for $\langle \mathbf{F}_{inc} \rangle$ becomes

$$\langle \mathbf{F}_{inc} \rangle = \frac{1}{8\pi} C_{ext} \left| \mathbf{E}_{inc,0} \right|^2 \hat{\mathbf{k}} . \tag{6}$$

$\langle \mathbf{F}_{inc} \rangle$ can be interpreted as the average rate with which momentum is removed from the incident beam. This force is in the direction of the incident beam. The next step is to calculate $\langle \mathbf{F}_{sca} \rangle$ from Eq. (2) and (4). This was however not done by Draine and Weingartner, because it would lead to summations involving $N(N\text{-}1)$ terms, which could be computationally prohibitive. [4] They did however suggest that this operation count could be reduced to O($N\log N$) by using FFT techniques. Below we will show explicit expressions for $\langle \mathbf{F}_{sca} \rangle$, but first we show how Draine and Weingartner proceeded.

By invoking momentum conservation it is easy to show that the net rate of momentum transported to infinity by the scattered field, denoted by $\langle \mathbf{F}_{out} \rangle$ must be equal to $-\langle \mathbf{F}_{sca} \rangle$. Draine and Weingartner show that

$$\langle \mathbf{F}_{out} \rangle = \frac{k^4}{8\pi} \int d\Omega \hat{\mathbf{n}} \left| \sum_{i=1}^{N} \big(\mathbf{p}_{i,0} - \hat{\mathbf{n}}(\hat{\mathbf{n}} \cdot \mathbf{p}_{i,0}) \big) e^{-ik\hat{\mathbf{n}}\cdot\mathbf{r}_i} \right|^2 , \tag{7}$$

with $\hat{\mathbf{n}}$ the direction vector on the unit sphere. We will now demonstrate how to calculate $\langle \mathbf{F}_{sca} \rangle$ directly from the dipole moments. First, we note that $\mathbf{E}_{ij}$ and $\mathbf{B}_{ij}$ in Eq. (4) are expressed as

$$\mathbf{E}_{ij} = e^{ikr_{ij}} \left[\left(\frac{k^2}{r_{ij}} + \frac{ik}{r_{ij}^2} - \frac{1}{r_{ij}^3} \right) \mathbf{p}_{j,0} + \left(-\frac{k^2}{r_{ij}} - \frac{3ik}{r_{ij}^2} + \frac{3}{r_{ij}^3} \right) \hat{\mathbf{n}}_{ij} (\hat{\mathbf{n}}_{ij} \cdot \mathbf{p}_{j,0}) \right] . \tag{8}$$

$$\mathbf{B}_{ij} = \sum_{j \neq i} k^2 \frac{e^{ikr_{ij}}}{r_{ij}^2} (\mathbf{r}_{ij} \times \mathbf{p}_{j,0}) \left(1 - \frac{1}{ikr_{ij}}\right) . \tag{9}$$

To calculate $\langle \mathbf{F}_{sca,i} \rangle$ from Eq. (4) we need to evaluate $(\mathbf{p}_i^{*} \cdot \nabla_i)\mathbf{E}_{ij}$. From Eq. (8) it is clear that this boils down to four non-trivial differentiations. In Ref. [6] these calculations are performed. The magnetic term in Eq. (4) is straightforward. Combining everything gives the final result.

$$< \mathbf{F}_{sca,i} > = \sum_{j \neq i} \frac{1}{2} \mathrm{Re}(\mathbf{F}_{ij}) , \tag{10}$$

$$\mathbf{F}_{ij} = e^{ikr_{ij}}\Big[\big((\mathbf{p}_{i,0}^{*}\cdot\mathbf{p}_{j,0})\hat{\mathbf{n}}_{ij} + \mathbf{p}_{i,0}^{*}(\hat{\mathbf{n}}_{ij}\cdot\mathbf{p}_{j,0}) + (\mathbf{p}_{i,0}^{*}\cdot\hat{\mathbf{n}}_{ij})\mathbf{p}_{j,0} - 5(\mathbf{p}_{i,0}^{*}\cdot\hat{\mathbf{n}}_{ij})\hat{\mathbf{n}}_{ij}(\hat{\mathbf{n}}_{ij}\cdot\mathbf{p}_{j,0})\big)\Big(-\frac{k^2}{r_{ij}^2} - \frac{3ik}{r_{ij}^3} + \frac{3}{r_{ij}^4}\Big) + \big((\mathbf{p}_{i,0}^{*}\cdot\mathbf{p}_{j,0})\hat{\mathbf{n}}_{ij} - (\mathbf{p}_{i,0}^{*}\cdot\hat{\mathbf{n}}_{ij})\hat{\mathbf{n}}_{ij}(\hat{\mathbf{n}}_{ij}\cdot\mathbf{p}_{j,0})\big)\Big(\frac{ik^3}{r_{ij}} - \frac{k^2}{r_{ij}^2}\Big)\Big], \quad (11)$$

where $\hat{\mathbf{n}}_{ij} = \mathbf{r}_{ij}/r_{ij}$. Eqs. (10) and (11) provide the force on each dipole due to the field radiated from all other dipoles. Together with Eq. (5) the total radiation force $\langle\mathbf{F}_i\rangle$ on each dipole is obtained. These equations are applied in the next section. The calculation of the forces can be formulated as a discrete convolution, thus allowing O(*N*log*N*) calculation of the forces. [6]

3 Tests on Spheres

As a test case we study the radiation force on a sphere. Using Mie theory and the DDA, the total radiation force on the sphere is calculated. In the case of DDA simulations we calculate $\langle\mathbf{F}_{sca}\rangle$ directly from the dipole polarizabilities and also by integration of the scattered field, i.e. by applying Eq. (7). In the later case a two-dimensional version of the Romberg integration method is applied. [8] For the DDA simulations we apply our parallel fast DDA method. [9,10] We have carried out a very large number of tests. Here we show a small subset, details can be found elsewhere. [6, 11]

Fig. 1 shows the forces on each dipole for a x = 2.5 sphere with m = 1.05, 1.33 + 0.01i, and 1.14 + 0.38i respectively. In these figures half of the sphere is removed. The incident light travels from right to left and was polarized in the y-direction. The first two spheres seem to be 'pulled' into the positive z-direction by forces that are largest in the back (left side) of the sphere. In case of a large absorption the largest forces are in front of the sphere, and it seems to be pushed into the positive z-direction. Clearly there is a close connection between the forces on the dipoles and the internal field in the particle. In a previous paper we investigated the internal fields in VIEF, a method closely related to DDA. [12] In that paper we noticed the clear distinction between the internal fields for particles with and without a large absorption, which correlates to the forces as depicted in Fig. 1.

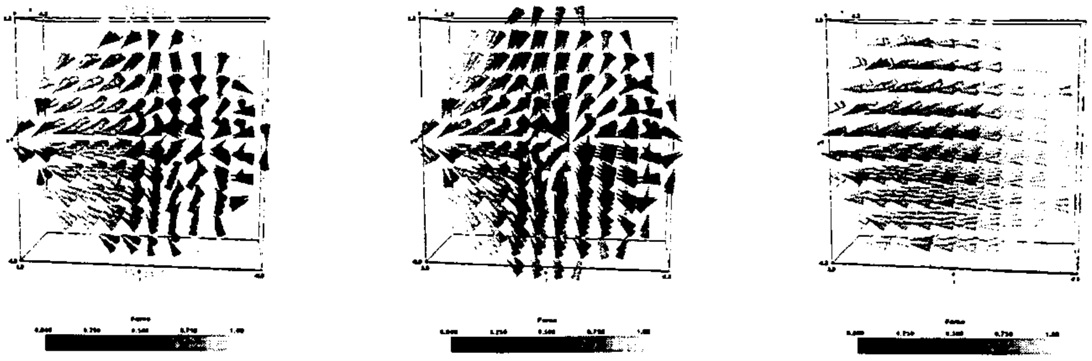

Figure 1: The total radiation force on each dipole for a sphere with x = 2.5 and m = 1.05 (left), 1.33 + 0.01i (middle) and 1.14 + 0.38i (right). The incident light travels from right to left. The maximum force is scaled to 1. Only one half of the sphere is shown.

We also calculated gC_{sca} and C_{pr}, using Mie theory, direct calculations of the forces per dipole, and from integration of the scattered field (data not shown). In all cases that we considered the direct calculation of the force and subsequent summation leads to the same numerical results as integration of the scattered fields. For a sphere with incident radiation in the z-direction, the x- and y-components of the radiation force are exactly zero. The direct calculation of the forces indeed results in very small x- and y-

components. The direct method results in almost all cases in x- and y-components in the order of 10^{-6} to 10^{-8} times the z-component. This very small remaining fraction is attributed to round-off errors in the numerical calculations. The integration of the scattered fields shows somewhat different results. The y-component is also very small, comparable to the direct method. However, the x-component (i.e. perpendicular to the polarization of the incident field) the integration results in small, as compared to the z-component, but finite values. Increasing the accuracy of the Romberg integration did not remove these finite values. Finally, in all cases considered the relative error in the radiation pressure coefficient as obtained with DDA is comparable (i.e. of the same order) as the relative error in the extinction coefficient.

4 Conclusions

We presented theoretical expressions to calculate the radiation force on each dipole in the DDA. This allows not only to calculate radiation pressure on arbitrarily shaped particles, but also to calculate the radiation forces inside arbitrarily shaped particles. The resulting relative errors in the radiation pressure coefficients as obtained by DDA has the same order of magnitude, i.e. in the order 1 %, as the relative error in the extinction coefficient.

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