Coherent backscattering effects with Discrete Dipole Approximation method

Antti Penttilä[1] and Kari Lumme[1]

[1]Observatory, P.O. box 14, FIN-00014 University of Helsinki, Finland
fax: +358 9 1912 2952, e-mail: Antti.I.Penttila@helsinki.fi

Abstract

We use the Discrete Dipole Approximation method to simulate light scattering from a dense cloud of wavelength-sized spherical particles. We will mimic the set-up that was used in recent articles from Mishchenko et al.[1, 2] where the superposition T-matrix method was used to simulate the scattering characteristics. We will show that the same demonstration of the evolution of the coherent backscattering phenomena can be produced with the Discrete Dipole Approximation.

1 Introduction

The coherent backscattering (CB) or the weak localization effect of electromagnetic waves has been studied both theoretically and with laboratory experiments, and recently also by numerical simulations[1, 2, and the references therin]. Mishchenko et al.[1, 2] have used the superposition T-matrix method to study the scattering characteristics from a dense cloud of wavelength-sized uniform spheres. They were able to simulate scattering from systems with up to 240 spheres. Mishchenko et al. make the (probably legitimate) claim, that they were able to show the evolution of the CB effect directly for the first time.

The superposition T-matrix method has some practical limitations in its convergence and the size of the system in [1, 2] is the largest that can be computed with current implementations and computing resources. On the other hand, the Discrete Dipole Approximation (DDA) method, among some other methods, can also be used to compute scattering from a cloud of spheres. Currently, there is only one implementation of the DDA as far as we know, the "Amsterdam DDA" (ADDA) code[3], that can handle as large systems as in the experiment by Mishchenko et al. The reason for this is that the ADDA can be run in parallel computing clusters where the system matrix in DDA can be divided among the operating memory banks of different processors. The other DDA codes suffer from the limitation of the available operating memory in single processor environments.

In this article we will show that the DDA approach can produce the same results as the superposition T-matrix implementations with the same set-up as in [1, 2]. The idea behind this is that once the applicability of the DDA is verified in this case, it can be used in larger or more complicated problems when studying the CB. The T-matrix approach is limited to solids with rotational symmetries, while the DDA can be used with arbitrary geometry. In the future it could be studied, e.g., if the CB effect needs a cloud of separated constituents, or could it also be produced by e.g. a large single random and porous particle.

2 Numerical results

We will mimick the set-up in [1, 2] and place either 80 or 160 spheres with size parameter $kr = 4$ randomly inside a large sphere with size $kR = 40$, where r and R are the radii of the small and large spheres and k is the wave number $k = 2\pi/\lambda$. The refractive index of the particles is 1.32.

This experiment uses just one realization of the random particle positions. With T-matrix method the scattering is averaged over all orientations of the system, thus producing different 'views' to the system. The

DDA method is not capable to produce exact orientation averaging, but the DDA computations can be run with different target orientations and then averaged, producing an estimate of random orientation scattering.

Currently, we have computed 22 different orientation directions placed systematically in spherical coordinates (θ, ϕ). In the DDA method the different rotations of the scattering plane in some orientation direction (θ_i, ϕ_i) are cheap to compute and we have used 256 different planes, making a total of 22x256=5632 orientations. Because one of the rotational angles is so overrepresented in the orientation averaging, the deviation in the random orientation estimate is larger than in the case of more balanced systematic sampling over the rotation angles.

The results of the simulations are presented in Figs. 1 and 2. In Fig. 1 are the scattering characteristics for both the 80- and 160-sphere systems computed with both the T-matrix and the DDA method. The elements of the Mueller matrix are labeled with $a_1, \ldots, a_4$ for diagonal elements and with b_1 for element $(1, 2)$ and $(2, 1)$ and with b_2 for element $(3, 4)$ and $-(4, 3)$. Different combinations of these elements are presented, e.g. intensity a_1 in subfigs. (a) and (e), and linear polarization $-b_1/a_1$ in subfigs. (d) and (l).

3 Conclusions

Mishchenko et al.[1, 2] analyze the behavior of the different scattering characteristics of the sphere clusters in question. Most obvious signs of the coherent backscattering phenomena in these clusters are seen in the peaks in the backscattering region in intensity (Fig. 1(e)) and in different polarizations states in Figs. 1(f)-(k). It is clear that the DDA method produces the same effects and is therefore well applicable in CB studies. The errors due to the limited number of orientations, as seen in Fig. 2 are still large, but will decrease as more orientations are computed.

The CPU times needed for the DDA computations are much larger than for the T-matrix method. Roughly estimated CPU-time for the T-matrix solution of the 80-sphere problem is $\sim$ 100 CPU-hours[2] with a modern PC. CPU-time for one orientation (with 256 scattering planes) with the ADDA code was $\sim$ 70 CPU-h. For 22 orientations it was roughly 1500 CPU-h, and at least twice this much orientations would be needed for the result to fit better to the exact results from the T-matrix method. Nevertheless, the available computing resources grow rapidly and the flexibility of the DDA method with arbitrary geometry does make the DDA approach very advantageous.

Acknowledgments

I would like to thank M. Mishchenko for providing me the data from the T-matrix simulations.

References

[1] M.I. Mishchenko and L. Liu. Weak localization of electromagnetic waves by densely packed many-particle groups: Exact 3d results. JQSRT, doi:10.1016/j.jqsrt.2007.01.039, 2007.

[2] M.I. Mishchenko, L. Liu, D.W. Mackowski, B. Cairns, and G. Videen. Multiple scattering by random particulate media: exact 3d results. Optics Express, in press, 2007.

[3] M.A. Yurkin, V.P. Maltsev, and A.G. Hoekstra. The discrete dipole approximation for simulation of light scattering by particles much larger than the wavelength. JQSRT, doi:10.1016/j.jqsrt.2007.01.033, 2007.

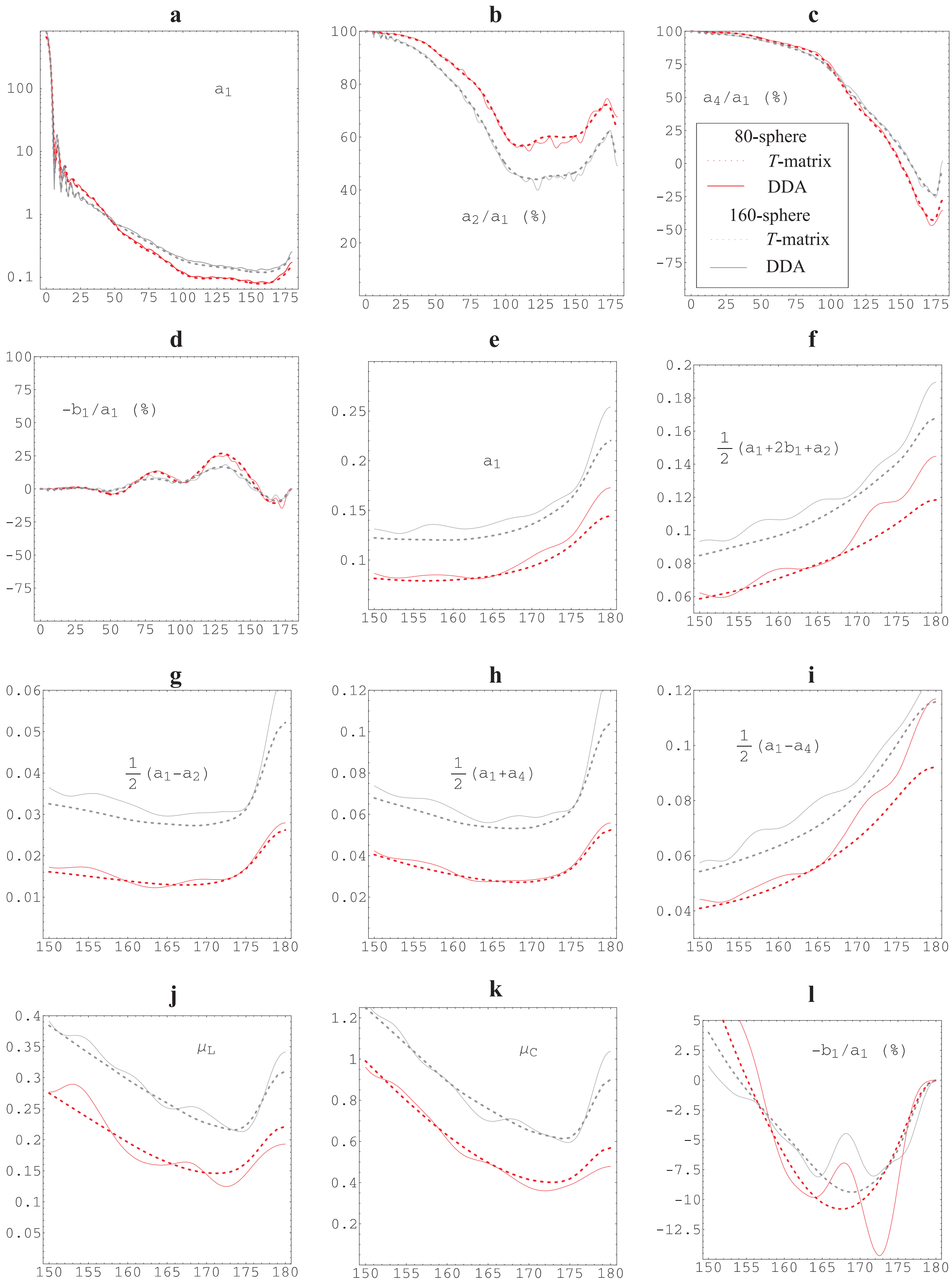

Figure 1: Different scattering characteristics for both the 80- and 160-sphere systems computed with the T-matrix or the DDA method as a function of the scattering angle.

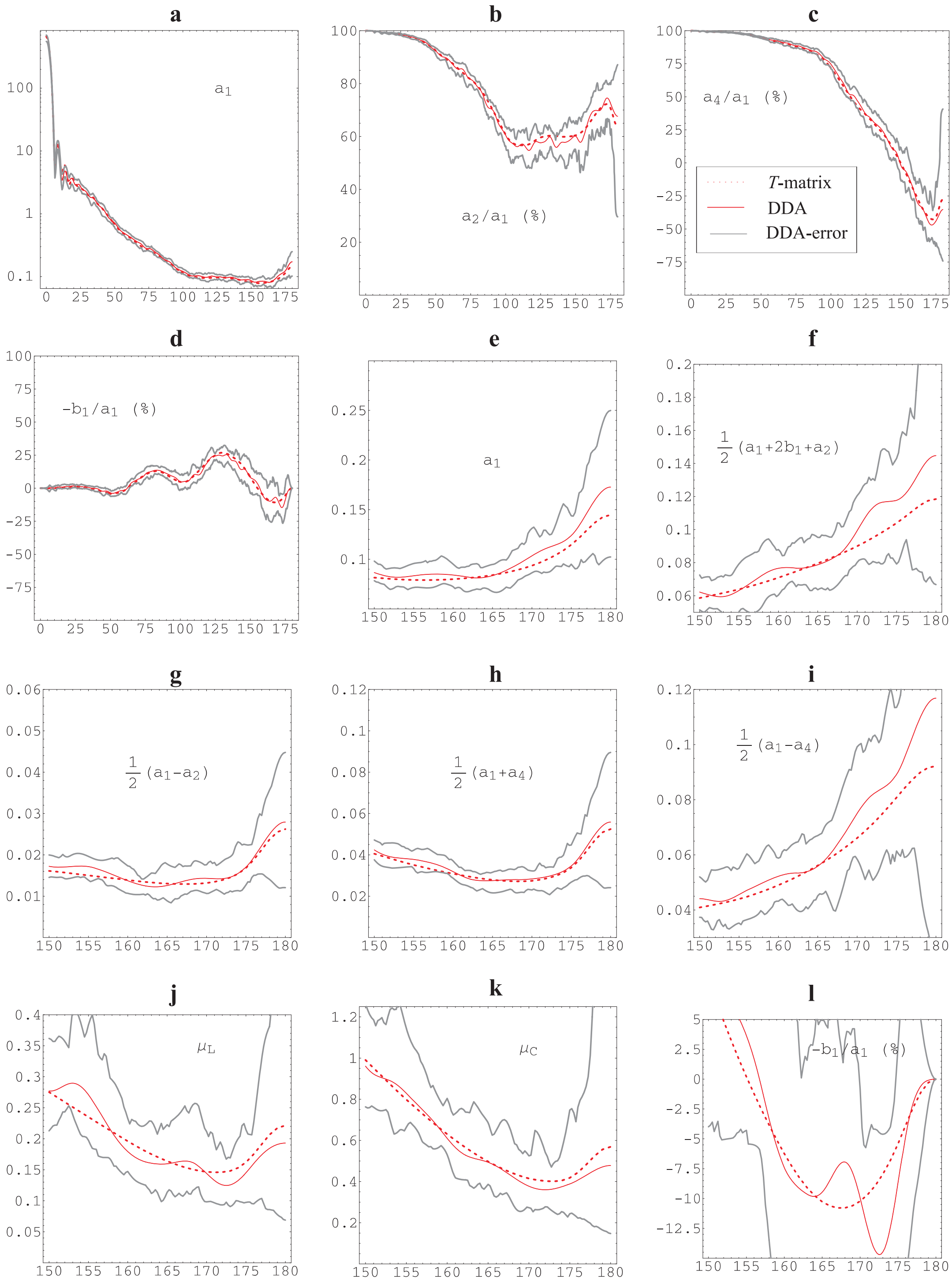

Figure 2: Scattering characteristics for the 80-sphere system and a typical error of the DDA orientation averaging. The lower and upper error lines are the 4th smallest and largest values in the 22 orientations at that scattering angle. This non-parametric error estimate encloses 64 % of the observations. The widely used mean-±-σ -error encloses 68 % of obervations, but it is symmetric while the errors in e.g. backscattering region in subfigs. (g) and (h) are not.