Optimization of the discrete-dipole approximation for large optically soft particles using the modified Wentzel-Kramers-Brillouin approximation

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We extend the Wentzel-Kramers-Brillouin (WKB) approximation and apply the corresponding approximation of the internal electric field to accelerate the discrete-dipole approximation (DDA). This extension of the WKB, named WKBr, is based on accounting for the ray refraction at the particle boundary, which corrects the part of the errors in the internal fields that scales with the particle size. The tests for large spheres show that using the WKB and, especially, the WKBr as an initial guess of the iterative solver in the DDA significantly accelerates the convergence of the latter.

INTRODUCTION

The DDA solves the direct light scattering problem, i.e. calculates the light scattering pattern (LSP) given the parameters of the particle (scatterer) and the incident wave [1]. The main drawback of this method is the significant computation time. Moreover, a large number of runs with different scatterer parameters are often required to generate a database of LSPs (up to million elements). This database can further be used to solve the inverse light-scattering problem, i.e. to determine the particle parameters from the experimental LSP.

In biological applications one often encounter large optically soft particles, i.e. $|m-1| \ll 1$ and $x \gg 1$, where m is the relative refractive index, $x = kR$ is the size parameter, k is the wave vector, R is the radius of the particle. Therefore, the optimization of the DDA for such particles is a relevant task. The bottleneck of the DDA is solving a system of linear equations (up to a billion unknowns). Such large systems are solved using iterative algorithms, which require a first guess of the electric field inside the scatterer. Using a more accurate guess is expected to lead to a smaller number of iterations and, thus, to accelerate the DDA simulation.

WKB APPROXIMATION WITH REFRACTION

We developed a more accurate approximation of the electric field – WKB with account for the refraction (WKBr). The original WKB takes into account the phase shift of the wave when it passes in a particle with a refractive index different from the host one [2,3]. The WKBr, in addition, takes into account the refraction of rays at the scatterer boundary. While the refraction angle is small for $|m-1| \ll 1$, the corresponding lateral displacement and phase shift can be significant if $x \gg 1$. The additional complication in the case of the WKBr is backtracing from a given point inside a particle to its boundary (refraction point for the incident ray). We developed an algorithm for that based on the fixed-point iteration method [4], and proved it to work robustly in the case of sphere. It also shows that there are regions with different numbers of solutions inside the sphere (neglecting the internal reflections), i.e. shadow region (without solutions) and regions with one and two solutions (rays coming to a given point). These regions are well-known in the geometrical-optics analysis of a sphere – they are related to the Descartes and grazing rays [5,6], e.g., see Fig. 1.

We showed that WKB eliminates the errors of order $x(m-1)$ in the internal field (compared to the incident field), and WKBr further removes all errors of order x (with any dependence on m). In other words, WKBr is obtained from geometric optics (which is exact in the limit $x \to \infty$) in the limit $m \to 1$. Accordingly, the remaining error when using WKBr was of the order of $(m-1)$ (regardless of x) – its elimination would require complete tracing of rays with multiple reflections inside the particle, which we deliberately omitted. We also studied the WKBr approximation through numerical experiments. In particular, we estimated the contribution to the internal-fields error from various factors: rotation and amplitude change of the electric field vector during refraction, addition of electric fields in the region of two solutions, and vanishing of the electric field in the shadow region. This helped to understand which factors should be taken into account in the WKBr for different values of x and m.

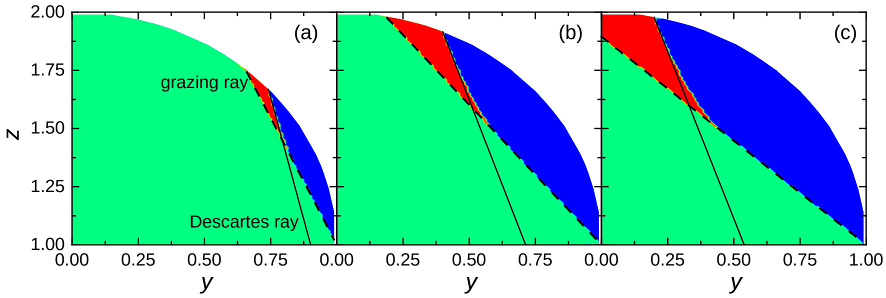

Fig. 1. The number of solutions as a function of the coordinate inside the back hemisphere. Green, red, and blue colors indicate one, two, and no solutions, respectively. Straight and dotted lines correspond to the Descartes and grazing ray, respectively. a) $m = 1.1$, b) $m = 1.3$, c) $m = \sqrt{2}$.

Next, we used the electric field obtained using various approximations as a first guess for the iterative algorithm in the DDA. The ADDA code [7] was used for corresponding numerical tests. We considered the spheres with parameters $x = 50, 250$ and $m = 1.01, 1.05, 1.1$, and show the examples of convergence behavior in Fig. 2 (the residual norm as a function of the iteration number). In all cases, the convergence for WKB and WKBr is faster than that for the standard approaches used in ADDA (zero first guess or that given by the incident field). For the case $x = 50, m = 1.01, 1.05$, there are no differences in the rate of convergence between the WKB and WKBr (similarly at $x = 50, m = 1.01$), while at $m = 1.1$ convergence of the WKBr is slightly faster. In the case of $x = 250$, the acceleration due to the WKBr (in comparison with the WKB) is significant – up to 100 and 1000 iterations for $m = 1.05$ and 1.1, respectively.

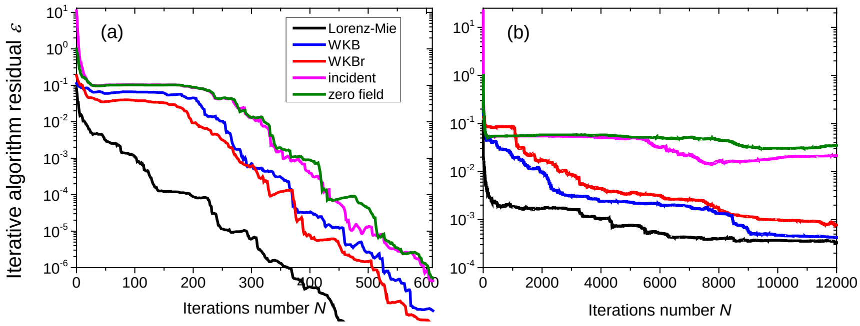

Fig. 2. The residual of the iterative algorithm versus the iteration number for a sphere with size parameter $x = 250$ and relative refractive index: a) $m = 1.05$, b) $m = 1.1$.

CONCLUSIONS

For large optically soft particles both WKB and WKBr approximations (as a first guess of the internal field) result in faster convergence of the iterative algorithm in the DDA. The extra benefit of using WKBr is significant when the phase shift $x|m-1|$ is large – exactly the case, when the validity of the standard WKB is questionable.

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