EXTINCTION AND ABSORPTION EFFICIENCY FACTORS OF A FINITE-LENGTH CYLINDER IN THE DISCRETE DIPOLE AND WENTZEL-KRAMERS-BRILLOUIN APPROXIMATIONS

K. A. Shapovalov
Department of Medical and Biological Physics,
Krasnoyarsk State Medical University named after Prof. V.F.Voino-Yasenetsky,
Krasnoyarsk, 660022, Russia

ABSTRACT
The values of light scattering extinction and absorption efficiency factors of an optically “soft” \( n-\chi_\mu<1 \), where \( \chi_\mu = n + i\mu \) is the relative refractive index of the cylinder) finite-length circular cylinder irradiated by linear polarized light in the direction at any angle to the cylinder symmetry axis are compared in the Wentzel-Kramers-Brillouin (WKB) approximation and in the Discrete Dipole Approximation (DDA). The amended expressions of light scattering extinction and absorption efficiency factors in the WKB approximation for an optically “soft” finite-length circular cylinder are presented. The differences between parallel and perpendicular polarizations of light scattering extinction and absorption efficiency factors for a finite-length circular cylinder are calculated in the WKB approximation and in the DDA. As a result of the minimal error of comparison of light scattering extinction and absorption efficiency factors in the WKB approximation and in the DDA is equal about 10%. The correctness of the new revised formulas for light scattering extinction and absorption efficiency in the WKB approximation of a finite-length circular cylinder in the vector form is validated numerically.

Key words: Light Scattering, Efficiency Factors, The Discrete Dipole Approximation, The Wentzel-Kramers-Brillouin Approximation.

http://www.iaeme.com/ijciet/issues.asp?JType=IJCIET&VType=9&IType=8
1. INTRODUCTION

1.1. Importance of the problem
The modern studies of light scattering by non-spherical particles comprised of natural and artificial aerosols, hydrosols, macromolecules, and biological-particle suspensions are very important for atmospheric and oceanic monitoring, colloid chemistry, biomedical optics and other fields [4, 7, 21, 22].

The light scattering technique is nondestructive and useful diagnostic tool for atmospheric and astrophysical particles, which are not easily accessible [17, 21]. Besides, many essential instruments based on this technique have been developed for routine measurements in industry and medicine [4, 10, 15].

1.2. Framework of the problem
Many biological and aerosol particles of great interest in nature are such that their refractive index $m$, relative to the surrounding medium is sufficiently close to unity [17]. The particles satisfying the condition $|m-1|<<1$ (where $m=n+i\chi$ is its relative refractive index) are generally termed as optically “soft” particles. Alternatively, the assumption of “soft” particles suggests that the refraction and reflection of the ray passing through the particle are negligible and that the absorption is not very strong. Moreover, we will consider only elastic and single light scattering in this paper [8].

If light scattering particles are optically “soft” then the Rayleigh–Gans–Debye (RGD) [16, 18, 19], Anomalous Diffraction (AD) [20, 21], or Wentzel–Kramers–Brillouin (WKB) approximations can be applied [2, 6, 7, 9].

The RGD approximation (known as the first Born approximation in quantum mechanics) is valid when the phase shift $\Delta$ is much smaller compared with unity $\Delta<<1$, where we use so-called “phase shift” of central ray $\Delta = 2\pi a \text{Im}(\chi)$, where $a$ is the longest dimension through the particle, $k = 2\pi/\lambda$ is the wavenumber, $\lambda$ is the wavelength in a medium with dispersion). An extensive study of the range of the RGD approximation’s validity has been made by Kerker [8]. The RGD approximation assumes that each volume element of a scatterer gives Rayleigh scattering, that it does so independently of the other volume elements, and that the waves scattered in a given direction by all these elements interfere because of the different positions of the volume elements in space.

The AD approximation of van de Hulst [21] is valid when the phase shift $\Delta$ is greater compared with unity $\Delta>1$. The main premise of the AD approximation is that the extinction of light by a particle is primarily the result of the interference between the rays that pass through the particle with those that do not pass through it [20]. The AD approximation can calculate the scattering and absorption cross-sections. However, it cannot be used to calculate phase functions.

Note that the wide range of validity of the WKB approximation is included ranges of validity of both the RGD and the AD approximations [7].

There have been some attempts to apply the WKB and RGD approximations to a particle of completely arbitrary shape and size, but none of these has been truly satisfactory [11, 12], because of it leads us to a numerical solution by means of Fourier and Laplace transformations. The analytical expressions are preferred by reason of they have more precise results and can serve as a basis for rigorous solution. See also the discussion about advantages of analytical approximate solutions over numerical solution in the book of Sharma and Somerford [17].
The formulas for light scattering extinction and absorption efficiency factors of a finite-length cylinder with polarization in the WKB approximation are obtained earlier by author [14]. Comparing with rigorous solution for an infinitely long cylinder [14], such expressions for light scattering extinction and absorption efficiency factors in the WKB approximation for a finite cylinder of large length have been checked.

1.3. The purpose of research
The final check of accuracy of expressions for light scattering extinction and absorption efficiency factors in the WKB approximation of a finite-length cylinder can be estimated by comparing the results with their counterparts simulated from other exact methods for a finite-length cylinder. In this study, we select the Discrete-Dipole Approximation (DDA) [5] as a reference test method and use the Amsterdam DDA (ADDA) code developed by Yurkin and Hoekstra [23].

Now the aim of this paper is a further comparison of light scattering extinction and absorption efficiency factors of a finite-length cylinder (not very large length) in the WKB approximation and in the DDA or the ADDA.

2. METHOD

2.1. The Discrete-Dipole Approximation
The DDA is a strictly numerical approximation. The modern DDA, including retardation effects, was proposed by Purcell and Pennypacker [13], who used it to study interstellar dust grains. The DDA has been applied to a broad range of problems, including interstellar dust grains, ice crystals in the atmosphere of the Earth, interplanetary dust, human blood cells, surface of semiconductors, gold nanoparticles and their aggregates, and more [3, 5]. The main physical idea behind DDA is to approximate a target volume of particle by an array of polarizable points or small cubical sub-volumes, termed “dipoles” [5]. The numerical accuracy of the DDA method depends on the number of dipoles used to represent the geometry of the particle. The DDA method is essentially an “exact” method as it directly solves the equations in the context of electrodynamics, and can be employed as a reference to test the accuracy of results computed from the WKB approximation. In this work we have employed the Amsterdam DDA program (ADDA ver. 1.3b4) developed by Yurkin and Hoekstra [23] for “benchmark” simulations. The ADDA is a C implementation of the DDA.

2.2. Light scattering amplitude in the WKB approximation
Let the symmetry axis of a static homogeneous cylinder of height $H$ and radius $a$ be aligned with the $Z$ axis and a plane electromagnetic wave be incident in the $ZOY$ plane of the Cartesian coordinate system at the angle $\theta_i$ to the $Z$ axis (see Figure 1):

$$E_i(r) = e_i \cdot \exp[i k (y \sin \theta_i + z \cos \theta_i)],$$

where $k$ is the wavenumber and the unit vector $e_i$ is aligned to the polarization of an incident plane electromagnetic wave.
Figure 1 Geometry of light scattering by a circular cylinder of radius \( a \) and height \( H \), where \( \mathbf{i} \) is the unit vector in the incident direction of light.

In the WKB approximation, rectilinear propagation of the incident wave in the scattering object is also assumed, as with the RGD approximation, but in addition a change of phase of the wave is allowed, in proportion to the degree of penetration into the object [9]. This leads to an increase of the particle size region in calculations of the angular intensity, but usually only for small angles. We use integral representation of the light scattering amplitude in the WKB approximation [7]:

\[
f(\mathbf{s},\mathbf{i}) = \frac{k^2}{4\pi} \left[ -\mathbf{s} \times (\mathbf{s} \times \mathbf{e}) \right] \left( (m^2 - 1)T(m, \theta) \right) \exp \left[ ik \left( (m - 1)(\mathbf{r} \cdot \mathbf{i} - \xi) + \mathbf{r}(\mathbf{i} - \mathbf{s}) \right) \right] dV,
\]

where the unit vectors \( \mathbf{s} \) and \( \mathbf{i} \) are aligned with the light scattering and propagation directions, respectively, \( \xi \) is the input coordinate on the particle surface for the wave passing through the point \( \mathbf{r} \), \( T = T(m, \theta) \) is the Fresnel transmission coefficient, where \( T(m, \pi/2) = 2/(m + 1) \), and \( \mathbf{r} \) is the radius-vector of a point inside the particle.

2.3. Light scattering efficiency factors in the WKB approximation

According to the optical theorem [7], the so-called extinction efficiency factor \( Q_e \), i.e., the extinction cross-section \( \sigma_e \) per unit area \( S \) of particle projection onto the plane perpendicular to the beam axis, is

\[
Q_e = \frac{\sigma_e}{S} = \frac{4\pi}{k} \frac{S}{S} \text{Im}(f(\mathbf{i}, \mathbf{i})) \cdot \mathbf{e}_i
\]

Thus, substitution of light scattering amplitude (2) into equation (3) yields us the light scattering extinction efficiency factor.

3. RESULTS

3.1. The amended form of light scattering efficiency factors in the WKB approximation

It should be noted inaccuracy in the equations for light scattering efficiency factors in the WKB approximation, published earlier [14].
The light scattering extinction efficiency factor by a finite-length circular cylinder in the WKB approximation for the polarizations parallel (∥) and perpendicular (⊥) to the plane ZOY (see Figure 1) has the new amended form after author’s correction:

\[
Q_{\parallel,\perp} = \frac{1}{S} \left[ \frac{\text{Im}[ (m+1)(f1+f2) ]}{\text{Im}[ (m+1)(f3+f4) ]} \right] \quad \text{for} \quad 0 \leq \theta_i < \arctg \left( \frac{D}{H} \right),
\]

\[
\frac{2 \sqrt{1-x^2}}{1-x^2+\sqrt{m^2-x^2}},
\]

Where the Fresnel coefficients are

\[
T1_{\parallel,\perp} = T3_{\perp,\parallel} (m, \cos \theta_i), \quad T2_{\parallel,\perp} = T3_{\parallel,\perp} (m, \sin \theta_i),
\]

\[
T3_{\perp,\perp} (m, x) = \frac{2 \sqrt{1-x^2}}{1-x^2+\sqrt{m^2-x^2}};
\]

\[
f1 = T1_{\parallel,\perp} iS_1 Rq(i\Delta_H), \quad f2 = T2_{\parallel,\perp} i \left[ S_1 Rq(i\Delta_H) + \left( \pi S_2 - S_1 \right) Rp(i\Delta_H) \right],
\]

\[
f3 = i 4 (m+1) S_2 \int_0^1 T3_{\parallel,\perp} (m, x) \sqrt{1-x^2} Rq \left( i \Delta_D \sqrt{1-x^2} \right) dx,
\]

\[
f4 = i \left( \frac{m+1}{2} \right) T3_{\parallel,\perp} (m, x) Rp \left( i \Delta_D \sqrt{1-x^2} \right) \left[ S_1 - 4 S_2 \sqrt{1-x^2} \right] dx,
\]

\[
R_p(x) = 1 - \exp(x), \quad R_q(x) = \frac{R_p(x)}{x} + 1, \quad \Delta_D = k D (m-1)/\sin \theta_i, \quad \Delta_H = k H (m-1)/\cos \theta_i.
\]

\[
S_1 = DH \sin \theta_i, \quad S_2 = a^2 \cos \theta_i, \quad S = S_1 + \pi S_2, \quad D = 2a.
\]

Then, in the scalar form (when \( T1_{\parallel,\perp} = T2_{\parallel,\perp} = T3_{\parallel,\perp} = 2/(m+1) \)) we have [14]:

\[
f3 = 2 \pi S_2 \left[ \frac{2 H_1(\Delta_D)}{\Delta_D} + i \left( 1 - \frac{2 J_1(\Delta_D)}{\Delta_D} \right) \right],
\]

\[
f4 = \pi S_2 \left[ \frac{2 H_1(\Delta_D)}{\Delta_D} - 2 H_0(\Delta_D) + i \left[ J_0(\Delta_D) - J_2(\Delta_D) - 1 \right] \right] + \frac{S_1}{2} \left( J_1(\Delta_D) + i H_1(\Delta_D) \right),
\]

where \( H_0(x), H_1(x), J_0(x), J_1(x), J_2(x) \) are Struve and Bessel functions of the first kind [1].

The amended absorption efficiency factor \( Q_a \) for a homogeneous finite-length cylinder in the WKB approximation is

\[
Q_{\parallel,\perp} = \frac{n}{S} \left\{ \begin{array}{ll} 
Q_1 + Q_2 & \text{for} \quad 0 \leq \theta_i < \arctg \left( \frac{D}{H} \right), \\
Q_3 + Q_4 & \text{for} \quad \arctg \left( \frac{D}{H} \right) \leq \theta_i \leq \pi/2,
\end{array} \right.
\]

Where
In the scalar form, it follows from equation (6) expressions for \( Q_3, Q_4 \) only in terms of modified Bessel and Struve functions of the first kind [14]. We have to summarize the main distinctions of new revised equations in the WKB approximation. It's concerned the duplicate usage of the Fresnel coefficients in [14] and author has been corrected these mistakes here in the amended equations (4), (6). The equations for light scattering extinction and absorption efficiency factors of a homogeneous finite-length cylinder in the WKB approximation in the scalar form is not changed.

3.2. Numerical Results

The comparison of the ADDA and the WKB approximation is realized for finite-length cylinders with \( kR=2, kH=4, 6, 8, 20 \) and refractive index \( m=1.1+i 0.01 \). The computer graphs of values of light-scattering extinction and absorption efficiency factors of parallel polarization \( Q_{\parallel\parallel} \), \( Q_{\parallel\perp} \) vs phase shift \( \Delta \) by finite-length cylinder with \( kR=2, kH=4 \) and infinitely long cylinder (see algorithm of rigorous solution in [4]) for angles of incidence \( \theta_i=2\frac{\pi}{3}, \frac{\pi}{2} \) are shown in Figure 2. Figure 2 (see (b), (c)) indicates that values of extinction efficiency factors \( Q_e \) in the scalar form of the WKB approximation are lower than values of extinction efficiency factors of parallel polarization \( Q_{\parallel\parallel} \) in the WKB approximation. Obviously, it should be noted that the dependences of light scattering extinction and absorption efficiency factors vs phase shift \( \Delta \) by an infinitely long cylinder and a finite-length cylinder in the WKB approximation are similar only for angle of incidence \( \theta_i=\frac{\pi}{2} \) (see Figure 2 (c), (f)) and strong differed for other angles.
Figure 2. Extinction and absorption efficiency factors of parallel polarization $Q_{e\parallel}, Q_{a\parallel}$ vs. phase shift $\Delta$ in the DDA, the WKB approximation by finite-length cylinder with $kR=2$, $kH=4$ and infinitely long cylinder (rigorous solution) for incident angles $\theta_i = 0$: (a),(d); $\theta_i = \frac{\pi}{3}$: (b),(e); $\theta_i = \frac{\pi}{2}$: (c), (f).

Figure 3. The difference between parallel and perpendicular polarization of extinction and absorption efficiency factors $Q_{e\parallel}-Q_{e\perp}, Q_{a\parallel}-Q_{a\perp}$ vs. phase shift $\Delta$ in the DDA, the WKB approximation by finite-length cylinder with $kR=2$, $kH=4$ and infinitely long cylinder (rigorous solution) for incident angles $\theta_i = \frac{\pi}{3}$: (a), (b); $\theta_i = \frac{\pi}{2}$: (c), (d).
The absolute values of light scattering extinction and absorption efficiency factors of perpendicular polarization are differed from parallel polarization insignificantly (from 1 to 5%) and fully coincided for the angle $\theta = 0$ (see also Figure 3). Therefore, further the differences between parallel and perpendicular polarizations of light scattering extinction and absorption efficiency factors are calculated in the WKB approximation and in the DDA.

The differences between parallel and perpendicular polarizations of light scattering extinction and absorption efficiency factors $Q_{e||} - Q_{e\perp}$, $Q_{a||} - Q_{a\perp}$ vs phase shift $\Delta$ are shown in Figure 3 for infinitely long cylinder and finite cylinder with $kR=2$, $kH=4$ in the WKB approximation and in the DDA. The minimal and maximal errors for this comparison were equal about 10% and 25% respectively. It should be noted that a maximal error had been found only in the extrema of light scattering extinction and absorption efficiencies.

When the phase shift is greater compared with unity $\Delta > 1$ one can observe (see Figure 3) that a behavior of the difference between parallel and perpendicular polarizations of light scattering extinction and absorption efficiency factors $Q_{e||} - Q_{e\perp}$, $Q_{a||} - Q_{a\perp}$ for an infinitely long cylinder is similar to a finite-length cylinder.

4. DISCUSSION

After additional careful check we are corrected the formulas for light scattering extinction and absorption efficiency factors in the WKB approximation by a finite-length circular cylinder in the vector form (see equations (4), (6)). Evidently, revised expressions of light scattering extinction and absorption efficiency factors in the WKB approximation for an optically “soft” finite-length circular cylinder are improved quality and application’s possibilities of the WKB approximation.

Earlier Klett and Sutherland [9] have been proved analytically that the expressions for light scattering extinction efficiency factor in the scalar form of the WKB approximation and in the AD approximation are identical for non-absorbing arbitrary-shape homogeneous particles. Then author is proved analytically this identity of the extinction efficiency factor in the scalar form of the WKB and in the AD approximations for absorbing arbitrary-shape homogeneous particles with an accuracy of up to the sign of $\chi$ in [14].

In consequence of all formulas in the AD approximation give us almost ready expression of the imaginary part of light scattering amplitude in the WKB approximation in the scalar form. It is important to note for further discussion that we can get from the AD approximation only the imaginary part, not real part of light scattering amplitude in the scalar form.

However, the author is not accepted wrong assertions appearing in the book of Wax and Backman [22] that the AD and the WKB approximations are fully equivalent each other and differed only by names. Such inadequate comparison [22] of the WKB and the AD approximations is depreciated all possibilities of the WKB approximation. Then we elucidate our critical standpoint on such comparison of the WKB and the AD approximations. The main imperfection of the RGD and AD approximations consists of their scalar nature and ignoring the wave polarization. Hence the WKB approximation has another important advantage over scalar AD, RGD approximations, except more wide range of validity, because the WKB approximation provide us description of the polarization of light scattering characteristics. Notice too that it is impossible to calculate directly differential light scattering characteristics, such as the phase function for any particles in the AD approximation, in contrast to the WKB approximation, where we can do it directly.

Thus, we are proved and confirmed superiority and advantage of the vector form’s WKB approximation over the scalar AD approximation in this paper not only by numerical calculations once more.
Extinction and Absorption Efficiency Factors of A Finite-Length Cylinder In The Discrete Dipole and Wentzel-Kramers-Brillouin Approximations

Nevertheless, author have to admit that the quality of such description of polarization of light scattering extinction and absorption efficiency factors in the WKB approximation is not so best when the phase shift $\Delta$ is smaller compared with ten (see Figure 3).

5. CONCLUSIONS

Thus, the values of light scattering extinction and absorption efficiency factors in the WKB approximation and in the DDA for a finite-length homogeneous cylinder are compared. The careful numerical check in comparison with the DDA allows us to find inaccuracy in the equations for light scattering efficiency factors in the WKB approximation. Then new revised expressions of light scattering extinction and absorption efficiency factors in the WKB approximation for an optically “soft” finite-length circular cylinder are presented. The differences between parallel and perpendicular polarizations of light scattering extinction and absorption efficiency factors by a finite-length circular cylinder are computed in the WKB approximation and in the DDA. The minimal and maximal errors for this comparison were equal about 10% and 25% respectively. The maximal error had been found only in the extrema of light scattering extinction and absorption efficiencies. In summary, the amended formulas in the WKB approximation for the vector form of light scattering extinction and absorption efficiency factors by an optically “soft” homogeneous finite-length circular cylinder are verified numerically.

Further, the expressions of light scattering extinction and absorption efficiency factors in the WKB approximation may be generalized for an inhomogeneous or structured “soft” finite-length cylinder too. Over a long-term perspective the new expressions of light scattering extinction and absorption efficiency factors in the WKB approximation may be obtained in the vector form (not only in the scalar form as well-known expressions) for some simple shapes of light scattering particle, such as spheroid, parallelepipeds, prism etc.

REFERENCES


