Numerical techniques for shaped beam scattering by large and absorbing particle using variable separation methods

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Abstract

Shaped beam scattering and numerical computations are two very active domains of research in light interaction with particles. The shaped beams may invoke special effects when interacting with particles which are essence of many applications. The variable separation methods, typically the Generalized Lorenz-Mie theory, solve the problem rigorously, but the numerical evaluation of relevant physical quantities is always a challenge for practical applications. To deal with these difficulties it is often necessary to combine physical understandings, mathematical skills and algorithmic faculties. Sophisticated techniques will be presented to solve numerical problems arising in the calculation of the scattering and absorption properties, the internal and near fields, the radiation pressure and torque exerted on very large and strong absorbing particles illuminated by circular and elliptical Gaussian beams, Bessel and Doughnut beams. Software integrating these experiences on the prediction of all the physical quantities of any shaped beam by a homogeneous or stratified sphere will be presented.

1 Introduction

Numerical computation occupies today a crucial place in the scientific research and its role is even primordial for many theoretical researches and their applications. It permits, and it is often the only means, to reveal physical laws and to discover new phenomena of the nature based on the developed theories. The applications of new theories depend also much on our capacity to realize the reliable "computation" in a reasonable time.

In the point view of scientific research, especially in the field we are concerned, the numerical computations may be classified into two categories: a). discretising the equations, i.e. Maxwell equations, governing the physical phenomena and solving the problem numerically, such as the T-matrix, the discrete dipole approximation (DDA), the finite element method (FEM), the finite-difference time-domain method (FDTD), the method of moment (MoM); b). resolving the equations to obtain "analytical expressions" and then calculating the physical quantities numerically, such as the variable separation method in the light scattering. The first is usually more flexible but needs great computer resource. The latter is often considered to be rigorous and easier, but the reality is not always the case. Furthermore, the complexity of the problem, i.e. the

particle shape, inhomogeneity, etc., are also limited due to the availability of mathematical tools. The numerical techniques attract much attention in the first category but less for the second. However, the numerical problem in the second category is neither much easier, nor less important. It is true that the boom in the computer technology in the last centuries provides formidable facility for scientific research, but the development of stable and reliable algorithms remains still a challenge in the field of the light interaction with particles and its applications.

The simplest case in this field is the scattering of the plane wave by a homogeneous sphere. Theory has been established more than a century [1,2] but the first practical algorithm is known [3-5] in 1980's. The physical mysteries behind this simplest model are extremely rich and attract the attention of a great number of researchers [6-8]. The scattering of the plane wave by a circular infinite cylinder is similar [9]. These are the two only cases we can calculate for a particle almost as large as we want and they are served as reference to valid the results of theoretical/numerical results for other theories or for other particles. Nevertheless, all the "numerical" problems are not resolved for the simplest particles [10]. When the particle is neither spherical nor circular infinite cylindrical, an analytical solution is possible if its shape corresponds to a mathematical coordinate system, but the numerical problem is often difficulty.

The invention of the laser provides a revolutionary development in the optics, certainly also for the light scattering by small particles and its applications to the optical metrology in the fluid mechanics [11,12], the environmental control [13] as well as in the optical manipulation of micro- and nanoparticle in life science and in material research (see [14-16] and references therein). At the same time, it provides a means to reveal particular phenomena which cannot be observed when a particle is illuminated homogeneously (plane wave). To describe the scattering of a laser beam or other inhomogeneous wave (e.g. evanescent wave) by a particle the shape of the beam are described by the beam shape coefficients (BSC). The most successful theory lies in the framework of the classical Lorenz-Mie theory, so called Generalized Lorenz-Mie Theories (GLMT). Many authors have contributed in different manners to these theories. A general description of these theories will be given with emphasis on the

numerical techniques in the evaluation of the beam shape coefficients.

The rest of the paper will be organized in four sections. The theoretical framework of the variable separation method will be first described in Section 2. Sections 3 and 4 are devoted respectively to the numerical techniques for the evaluation of the scattering coefficients and the beam shape coefficients. The special problems encountered in the calculation of the physical quantities by combining the above mentioned two kinds of coefficients will dealt with in Section 5.

2 Theoretical framework of variable separation method

The variable separation method is based on the fact that the wave functions of three variables $\psi(x_1, x_2, x_3)$ can be, in general, expressed as a product of the functions of one variable $X_1(x_1)$, $X_2(x_2)$ and $X_3(x_3)$, where x_1, x_2 and x_3 are the spatial coordinates. Each of the three functions satisfies a differential equation and they are related by two indices (n, m), discrete or continuous. The incident wave, the scattered waves as well as the waves in the particle are expanded in the eigen functions of $X_i(x_i)$. The expansion coefficients depend therefore on the properties of the particle and the shape of the incident beam. In general case, the coefficients depending on the particle's properties, called hereafter as scattering coefficients, are independent of the beam parameters, and in the counterpart, the beam shape coefficients should not contain any particle's properties. The fundamentals of the theories can be found in the monographs [17-20].

3 Scattering coefficients

The scattering coefficients are function of the particle properties, such as the size, the refractive index and the morphology parameters (e.g. aspect ratio for spheroidal, ellipsoidal sphere, or elliptical cylinder).

For a spherical particle (homogeneous or stratified), we need two series of coefficients a_n and b_n for the external field and two series coefficients c_n and d_n for the internal field [14,15]. Here, only one expansion index n is necessary because of the symmetry of the problem, and it extends theoretical from 0 to infinity. In practice, for the calculation of the scattering diagram or integral quantities such as the cross sections, the radiation pressure and torque, the summation on n is truncated to

$$n_{stop} = x + 4.05 x^{1/3} + 2 \qquad (1)$$

where $x = 2\pi a / \lambda$ is the particle size parameter with a the particle radius and λ the wavelength. This criterion has been proposed by Wiscombe [4] and largely used in the Mie calculation [15]. It is in fact because the spherical Bessel function involved in the scattering coefficients decreases rapidly to less than 10^{-8} when n exceeds n_{stop}. If more precision (e.g. double or quadruple precision for example) is needed more terms should be taken in the calculation.

The scattering coefficients of a homogeneous sphere are expressed simply as function of Riccati-Bessel functions and we can calculate for very large and absorbing particles. Nevertheless, if we want to isolate different mode by using the Debye theory, the problem becomes more delicate since both the first and the second Hankel functions are involved [10].

The scattering coefficients of a stratified sphere are formulated in determinant by Kerker [17] and those for a coated sphere are coded by Bohren [19]. But to simulate a temperature/refractive index gradient, many layers are needed; the algorithm in matrix form [17] is limited in number of layers N_l and size. Li et al have proposed to calculate the coefficients by the ratios of the Bessel function between successive layers [21], the performance was still not sufficient to reply the real demand. Wu et al [22] then proposed to calculate the logarithmic derivatives of the Bessel function. This algorithm is proved to be very stable. With some improvement [23], we can calculate for a very large particle of many layers, $x \cdot N_l > 10^8$ on a personal computer. And this number is limited only by the computer resources. However, the attention must be paid to the fact that if eq. (1) is applied, the results may be erroneous. The summation number should calculated according to the product of the refractive index and the size parameters of all layers by

$$n_{stop} = \max(| m_j x_j | + 4.05 | m_j x_j |^{1/3}) + 16 \qquad (2)$$

Furthermore, some astuteness is also necessary to avoid the numerical problem when two successive layers have the (quasi)equal refractive index [24]. This algorithm has also been applied to the scattering of shaped beam [25]

The scattering of the plane wave by an infinite circular cylinder is similar to a spherical particle. But four series of coefficients are necessary for the external field and four series of coefficients for the internal field because of the cross polarization in the case of oblique incidence [19]. The numerical techniques are similar to the spherical particle. Here another numerical problem may occur when the incident angle tends to zero; this is inevitable case for the scattering of a shaped beam by using the plane wave expansion [26,27] and the asymptotic expression for the Bessel functions are used [28]. The Debye theory for a stratified circular cylinder at oblique incident is much more complicated. Li et al proposed a very intelligent schema [29].

If the particle is neither a sphere nor a circular infinite cylinder, the problem becomes much more complicated. Even though the solution of variable separation method is still possible for particles of simple shape (spheroid, elliptical infinite cylinder, ellipsoid, etc.), the calculable particle size is seriously limited. The scattering of the plane wave or a shaped beam by a homogeneous or stratified, isotropic or anisotropic spheroidal particle are well documented [30-41]. Much effort has also devoted to the numerical calculation, the calculable size parameter can be as big as 650, same order as the capacity of pure numerical methods [42].

The scattering of elliptical infinite cylinder has been extensively studied by Yeh[43], Gouesbet et al [34-46]. But the numerical calculation is still more difficulty for two reasons: the first is due to difficulty in the calculation of the Mathieu functions for large argument which limit the size parameter and the other is the evaluation of the scattered wave in far zone for shaped beam scattering (see section 5).

4 Beam shape coefficients in different coordinate systems

When the spatial variation of the beam on the particle is not negligible, the incident wave can no longer be considered as the plane wave and it is taken into account by the so-called the beam shape coefficients.

In fact, in the variable separation methods, the plane wave is also expanded as partial waves, but the expansion coefficients are only function of the summation indices. For all shaped beam, the BSC depend not only on the geometry of the beam, i.e. the form, the waist radius, the polarization state, the axicon, the mode, etc., but also the position of the beam and the coordinate system in which the BSC are calculated. However they must be independent of the particle properties. The particle size, for example, must not intervene in the BSC calculation. The BSC are usually series of two indices which can be both discrete as in the spherical or ellipsoidal coordinate system, or one discrete and the other continuous as in the case of the infinite cylinder.

4.1 BSC in spherical coodinate system

This is the case the most studied and well developed (see [20, 47] and references therein). It is also the basis for the scattering of shaped beam by a spheroidal particle.

Two series of BSC are necessary to describe an arbitrarily shaped beam in spherical coordinate system. We find different definitions in the literature [48-51] and they are proved equivalent [52]. The definitions in the GLMT noted by $g_{n,TM}^m$ and $g_{n,TE}^m$ have a clear physical signification and are the most used. They are calculated respectively by the radial components of electric and magnetic fields. Theoretically, they are defined by the double or triple integrations. The double integration form for $g_{n,TM}^m$ is given by [20,50,51]

$$g_{n,TM}^m = \frac{kri^{n+1}}{4\pi j_n(kr)} \int_0^{2\pi} \int_0^{\pi} \frac{E_r(r,\theta,\phi)}{E_0} P_n^{|m|}(\cos\theta)e^{-im\phi} \sin\theta\, d\theta\, d\phi \quad (2)$$

We observe that the coefficients depend explicitely on the coordinate r but it should not. In fact, if the electromagnetic field satisfies strictly the Maxwell equations, the BSC calculated by eq. (2) are independent of r as we can demonstrate theoretically for the plane wave [52]. However, Analytical expressions of shaped beams often do not satisfy strictly the Maxwell equations [53], for example the Gaussian beam [54,55]. Fortunitely, this dependence is weak for well defined beam. It may also be eliminated by the integration on r [51-53]. In the point view of numerical calculation, the precision and the performance of the algorithm for the evaluation of the

integration in eq. (2) depend much on the choice of the value r. Ren et al [51,52] have shown that the best choice is $kr=n+1/2$ because the oscillation of the integral kernal as function of θ is the weakest so the integration covegres the most rapidly[52].

It is worth to note that for any given BSC, the reconstructed field satisfies perfactly the Maxwell equation and any means to calculate the BSC are just to find the BSC which are the most faithful to the given analytical field expression. Four methods have been developed for the evaluation of the BSC in the spherical coordinate system: i). integration, ii). Localized Approximation, iii). Finite series iv). Standard beam.

The integration method is issued directely from the definition of the BSC, it is rigorous, flexible and ued as reference to evaluate the other methods but it is the most costly in term of the computer resources and time.

The localized approximation (LA) is not rigorously established but the precision is usually sufficient. Therefore, it is the most used in the practical calculation, especilly for Gaussian beam [38]. It is based on the localization principle [18]: the spherical wave component n corresponds to the ray arriving at a distance $r=(n+1/2)/k$ (k being the wave number) from z axis. The procedure of the LA consists of replacing the coodinate r by $(n+1/2)/k$ and θ by $\pi/2$. The BSC are the expansion cofficients of the incident wave as function of $e^{im\phi}$ ajusted with a prefactor Z_n^m [56]. The original version is for circular Gaussian beam in infinite series and has been largely used in the calculation of the scattering of the shaped beam [57]. Ren et al have extended it to the elliptical Gaussian beam [58]. However, when n is large, the series are not numerically stable because of limit of the precision [52]. Doicu et al [59] have demonstrated by the addition theorem that the BSC can be expressed as the cylindrical Bessel function. In fact if we compare the infinite series of the BSC and the definition of the Bessel function [60], it is easy to observe that the two terms in the infinite series of the BSC are just two Bessel function. This can be proved more easily by the localized approximation in integral form given by [61]

$$g_{n,TM}^m = \frac{Z_n^m}{2\pi E_0} \int_0^{2\pi} E_r(kr = n+1/2, \theta = \pi/2, \phi)e^{-im\phi} d\phi \quad (3)$$

called therefore as the integral localized approximation (ILA). This combined the advantage of the flexibility of integration method and the rapidity of the localized appximaation. ILA can be applied directly to evaluate the BSC of any collimated beam propagating along z axis. The BSC of the fifth order Gaussian beam are with eleven terms of Bessel function [62]. The BSC of the Bessel beam [8] and the doughnut beam[63] can also be obtained easily.

Theoretically, the index n goes from 0 to infinity and m from $-n$ to $+n$. But in the numerical calculation they are truncted according to both the particle size and the beam parameters.

The finite series [52,64] and the standard beam [20,47] have also developed for different orders of Gaussian beam. However, the finite series becomes very rapidely

unstable for large index n so it is raely used in the beam scattering.

4.2 BSC in other coodinate system

The BSC in spheroidal coordinate can be obtained from the BSC in spherical coodinate system by using the relation between the spheroidal vector wave functions and the spherical vector wave functions [33,37-39].

In the plane wave expansion method, the BSC in cylindrical coordinate system $I_{m,TM}(\gamma)$ and $I_{m,TE}(\gamma)$ are defined respectively by the z components of the electric and magnetic fields in the similar way as the BSC in the spherical coordinates. For example, $I_{m,TM}(\gamma)$ reads as [26]

$$I_{m,TM}(\gamma) = \frac{i^m}{4\pi^2 J_m(R)} \int_0^{2\pi} e^{-im\phi} \int_{-\infty}^{\infty} \frac{E_z(Z,R,\phi)}{E_0} e^{-i\gamma Z} dZ d\phi \qquad (4)$$

with $Z = kz$ and $R = k\rho(1-\gamma^2)$. But the expansion index γ is continuous which can be understood as the cosine of the incident angle of the plane wave component. So in the expansion of a wave by these coefficients in the framework of GLMT [26], the integration over γ goes from –1 to 1 while Lock extended this integration from -∞ to ∞ [27]. Ren et al have introduced also the localized approximation to evaluate the BSC [26,64,65]. This localized approximation for cylindrical coordinate system has later been applied to the BSC in the elliptical coordinate system for arbitrary shaped beam [44-46].

5 Calculation of physical quantities and general ramarks

In principle, once we possess the scattering coefficients and the BSC we can calculate all the physical quantities, such as the cross scattering section, the radiation pressure forces and torques, the scattering diagram (or scattering matrix), the internal field, and the external field in near or far zone. However, certain caution should be paid to the combination of the coefficients, especially the choice of the limits in the truncation of the summation indices. If they are not sufficient the results are not correct if they are too big, we will encounter the problem of overflow or underflow. This choice depends not only the properties of the particles, the beam shape and its position, but also the physical quantity to be calculated

The integral quantities are often expressed as the summation product of the scattering coefficients and the BSC, the truncation terms are to be examined according to their product. The scattering diagram needs also the angular functions, their variation as function of the summation index is essential for the determination of the number of terms. In the calculation of the internal and near fields, we need to calculate the internal coefficients (e.g. c_n and d_n for spherical particle) and Bessel/Hankel functions with the position as argument. Each term is therefore the product of four factors and it's their combination weight in the summation.

In the case of shaped beam illumination, the scattered field of an infinite cylinder is neither spherical nor cylindrical; there is no asymptotic expression for the scattered wave in far zone. So *stricto sensu* to obtain the scattered wave at a distance ρ for the cylinder, the Bessel functions with arguments $k\rho$ must be calculated [26]. Lock [27] has used a method of stationary phase to evaluate the intensity in far zone and given the physical interpretation of the results, but no numerical results are shown. So this is still an open problem.

To conclude, some general remarks may be made for the numerical calculation light interaction with particle:
1) The results of the special functions are to be checked by comparing with standard tools. Codes found on internet, even in the literature or routines of standard libraries may be incorrect or imprecise, especially in the extreme case (usually for very large or very small argument). It is suggested to compare with the results of Maple or Mathematica at least for some special cases since it standard mathematical tools, the precision of the results is ensured and we can calculate with any precision we want.
2) Before implementation of an algorithm, it is worth to study the properties of the function to be calculated, for example, the kernel of the integration for the calculation of the BSC for a given beam, then to choose adequate parameters and integration procedure.
3) If possible, avoid series form which are often unstable or reformulate the mathematical expressions to improve the convergence of the series.
4) Try to understand the physical significance of the parameters to help its choice. For example, in the point of view of localization, the index n in the spherical BSC stands for a ray at distance $r=(n+1/2)/k$, the summation terms should be increased if the beam is far off axis. The index m stands for the azimuth component and the summation terms must be adjusted according to the symmetry of the problem. It may take only ±1 for the plane wave until 30 or 50 for an off-axis Gaussian bean, or even bigger if the dissymmetry of the problem is important.
5) In case of underflow or overflow, try to store the exponent to a variable and then count it in the final calculation.

Software **ABSphere** with friendly graphical interface has been developed for the calculation of all physical quantities of the scattering of any shaped beam by a spherical particle [67,68]. It is available by request to the author.

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7 References

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