Chapter 2 Mie Theory: A Review

Thomas Wriedt

Abstract In optical particle characterisation and aerosol science today light scattering simulations are regarded as an indispensable tool to develop new particle characterisation techniques or in solving inverse light scattering problems. Mie scattering and related computational methods have evolved rapidly during the past decade such that scattering computations for spherical scatterers a few order of magnitudes larger, than the incident wavelength can be easily performed. This significant progress has resulted from rapid advances in computational algorithms developed in this field and from improved computer hardware. In this chapter the history and a review of the recent progress of Mie scattering and Mie-related light scattering theories and available computational programs is presented. We will focus on Mie scattering theories but as there is much overlap to related scattering theories they will also be mentioned where appropriate. Short outlines of the various methods are given. This review is of course biased by my interest in optical particle characterisation and my daily reading.

2.1 Introduction

When Gustav Mie wrote his classic paper on light scattering by dielectric absorbing spherical particles in 1908 he was interested in explaining the colourful effects connected with colloidal Gold solutions. Nowadays, the interest in Mie's theory is much broader. Interests range from areas in physics problems involving interstellar dust, near-field optics and plasmonics to engineering subjects like optical particle characterisation. Mie theory is still being applied in many areas because scattering particles or objects are often homogeneous isotropic spheres or can be approximated in such a way that Mie's theory is applicable.

T. Wriedt (🖂)

Institut für Werkstofftechnik, Badgasteiner Str., 328359 Bremen, Germany e-mail: thw@iwt.uni-bremen.de

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On the 100th anniversary of Mie's theory a number of review papers, special papers and conference proceedings were published [1-10] commemorating his 1908th paper.

In this chapter I would like to review the history and the state of the art in Mie scattering as it developed over the previous decades. I will give a short description of the various extensions to Mie scattering available and provide information about computation programs making reference to review papers where available. For more profound reviews the interested reader is referred to the cited review articles.

2.2 Nonspherical Particles

In this review I am concerned with spherical scattering particles. Nevertheless, to guide the reader interested in the broader aspects of light scattering I will also briefly consider nonspherical particles in this section.

A number of light scattering theories also suitable for nonspherical particles have been developed, all having their pros and cons. Extensive overviews of available theories have been published by Wriedt [11], Kahnert [12] and more recently by Veronis and Fan [13]. A review of this subject with emphasis on colloid science has been written by Niklasson and Vargas [14]. A paper by Zhao et al. [15] provides an overview of the methods that are currently being used to study the electromagnetics of silver and gold nanoparticles. Of historic interest might be the critical review by Bouwkamp [16] who presents the progress in classical diffraction theory up to 1954. In this paper both scalar and electromagnetic problems are discussed. This report may also serve as an introduction to general diffraction theory. Interesting reviews on related subjects of nanooptics and metamaterials have recently been published by Myroshnychenko et al. [17] and by Veselago et al. [18].

2.3 History of Mie's Theory

In 1908, Gustav Mie published his famous paper on simulation of the colour effects connected with colloidal Gold particles [19]. In this paper he gave a first outline of how to compute light scattering by small spherical particles using Maxwell's electromagnetic theory. With his first computations he managed to explain the colour of gold colloids changing with diameter of the Gold spheres, which was later interpreted in terms of surface plasmon resonances. First computations of scattering diagrams for larger spheres of diameters up to 3.2λ are presented by *Richard Gans* (1880–1954) [20] and *Hans Blumer* [21] in 1925. The early study of scattering by a sphere is traced by *Nelson A. Logan* [22], who comments on Blumer's results, that he missed the regular undulations in the scattering diagram because of numerical mistakes. This paper is interesting reading for all interested in the history of light scattering.

Electromagnetic scattering by a homogeneous, isotropic sphere is commonly referred to as Mie theory, although *Gustav Mie* (1868–1957) was not the first to formulate this electromagnetic scattering problem. Before him *Alfred Clebsch* (1833–72), solving the elastic point source scattering problem of a perfectly rigid sphere using potential functions [23], and *Ludvig Lorenz* (1829–91) [24, 25] contributed to this problem. In 1909, *Peter Debye* (1884–1966) considered the related problem of radiation pressure on a spherical particle [26] utilising two scalar potential functions like Mie. Therefore, plane wave scattering by a homogeneous isotropic sphere is also referred to as Lorenz-Mie theory [27], or even Lorenz-Mie-Debye theory [28]. The incorrect name Lorentz-Mie theory is also quite commonly used (e.g. in Burlak [29]). *Milton Kerker* (1920) provides an extensive postscript on the history of scattering by a sphere in his book [30].

In 1890, Danish physics *Ludvig Lorenz* published essentially the same calculation on the scattering of radiation by spheres [24]. This paper was not much noticed at the time because it was written in Danish and it remained hardly known even after it had been translated to French [25]. Also, Lorenz did not connect his derivation with the Maxwells theory of electromagnetics [31, 32]. For information about Ludvig Lorenz, see the article by *Helge Kragh* [33] who outlines his career and his contributions to optical theory.

Cardona and Marx [34] commented that Mie's 1908 paper was almost ignored until about 1945 but its importance rose with increasing interest in colloids starting from the 1950s such that hundred years after publication the paper is still much cited [35] with currently 291 citations a year according to the *Web of Science. Google* currently gives 4,064 citations and the *Web of Science* 4,958. The paper is called Dornröschen (Sleeping Beauty) by the researchers at Information Retrieval Services of Max Planck Society [36] because of its low recognition considering the number of citations during the first years after its publication. But in the 1930s, contemporary scientists acknowledged the importance of his contribution. In a special issue devoted to Mie's 70th birthday *Ilse Fränz-Gotthold* and *Max von Laue* [37] dedicate their paper to "*Gustav Mie* whom physics owes the mathematical treatment of diffraction by a sphere".

Apparently one of the first English language versions of Mie theory was published by *Harry Bateman* (1882–1946) [38]. Mie's original paper was translated into the English language as late as 1976 by the Royal Aircraft Establishment in the UK [39] and 2 years later by Sandia Laboratories in US [40]. Recently, a Spanish translation of the original paper became available [41] and Chinese, Hebrew and Italian translations are on the way [42]. For information about typographical errors in the original paper please refer to the Mie Translation Project [42]. Those typographical errors have been corrected in the Spanish version of the paper [41].

Early citations of Mie's theory make reference to the classical textbook on electromagnetic theory by *Julius Adams Stratton* (1901–1994) [43]. In outlining the theory, Stratton made use of so-called vector spherical wave functions (VSWF) as first introduced by *William Webster Hansen* (1909–1949) [44]. Later references were made to the classic optics book by *Max Born* (1882–1970) and *Emil Wolf* (1922) [45] who used the Debye potential in their derivation. *Hendrik Christoffel van de Hulst* (1918–2000) [46] and Bohren and Hufman [47] follow the Stratton approach.

An up-to-date version of the derivation of Mie's theories has been published in Appendix H of the recent book by Le Ru and Etchegin [48] and in a book chapter by Enguehard [49]. Both provide an outline on how to solve the electromagnetic scattering problem in the case of a spherical particle using Mie's theory which give the most useful mathematical expressions of Mie theory and its derivatives and also information about implementation.

2.4 Mie Algorithms

Understandably, prior to the development of electronic computers in the middle of the last century there were not many papers written on computing scattering problems using Mie's theory since the computational labour involved in evaluating functions such as Riccati-Bessel functions was quite extreme.

Even with the rise of the computer it took some time before stable algorithms were developed. Gradually, several generally reliable and stable scattering programs were published. Early well-known algorithms were published by Giese [50] and Dave [51]. In a report Cantrell [52] reviews the different numerical methods for the accurate calculation of spherical Bessel functions as needed in Mie's theory. Deirmendjann [53] presents computational results of scattering parameters of polydispersions in a number of tables, produced by application of the Mie theory. According to Cantrell [52], Deirmendjian et al. [54] appear to have been the first to calculate the logarithmic derivative of the Riccati-Bessel function to evaluate the Mie coefficients. Dave [51] improved upon the approach of Deirmendjian et al. by applying downward recursion to the correct calculation of logarithmic derivative of the Riccati-Bessel function. The IBM report by Dave from 1968 [51] was still sent out on request in the 1990s.

Apparently at that time there was also independent research in this field such that one can find papers not often cited such as Metz and Dettmar [55]. With multiple databases and easy Internet search available today, the existence of other early and at that time available Fortran program can be confirmed such as for example the program by Maguire [56].

Nowadays, a number of efficient algorithms and Fortran programs are available. A major step was the program *MIEV0* written by Wiscombe [57, 58], which is based on Lentz's continued-fraction method for the calculation of spherical Bessel functions [59]. The program is well-tested and widely used. The Supermidi program by Gréhan and Gouesbet [60] is also based on Lentz's algorithm. The authors give numerical results over a wide range of size parameters and refractive indices. The advantage of Lentz's method is that errors do not accumulate as can occur with the use of faster recurrence relation methods [61].

It has been demonstrated that Mie's theory can now be successfully applied up to size parameters of 10.000 [62–64]. Recently, Gogoi et al. [65] presented a new

efficient and reliable computer program written in the C programming language to compute the scattering matrix elements.

2.5 Spheres in an Absorbing Medium

Originally, the Mie theory was restricted to a nonabsorbing ambient medium although some real-world applications require that the absorbing surrounding media be accounted for in the theory. This is a topic in colloid science and computer graphics.

Apparently one of the first derivation of the Lorenz-Mie theory for a scattering sphere immersed in an absorbing host medium is presented by Mundy et al. [66] and by Bohren and Gilra [67]. Similar extension to the Mie theory was studied by Quinten and Rostalski [68], Sudiarta [69] and Frisvad et al. [70]. It was found that the absorption of the ambient medium can alter the scattering efficiency and the scattering pattern of a sphere. The effect on the absorption efficiency is much less. To extend such theories for light scattering by coated sphere immersed in an absorbing medium is a small step [71].

2.6 Coated Spheres

As it is easy to consider spherical scatterers there are many extensions of the Mie theory covering different aspects. A theory for a coated dielectric sphere was first published by Aden and Kerker [72]. The Fortran code BART by Arturo Quirantes [73] is based on the Aden-Kerker theory to calculate light-scattering properties for coated spherical particles. In the program polydispersity is included for either core, coating or entire particle.

A basic Fortan (BHCOAT) code is printed in the appendix of the book by Bohren and Huffman [47]. An advanced algorithm is given by Toon and Ackerman [74]. An algorithm for a sphere having two coatings has been presented by Kaiser and Schweiger [75]. These theories have also been extended to spherical particles consisting of multiple layers by Li Kai [76]. Another algorithm for plane wave and shaped beam scattering by a multilayered sphere has been published by Wu et al. [77]. Even in recent times, improved algorithms have been published on this subject [78].

2.7 Distorted Spheres

To compute scattering by a slightly distorted sphere Martin [79, 80] developed a first-order perturbation theory. He derives formulae bearing close resemblance to the zero-order ones encountered in Mie scattering theory, expressing the perturbation

applied to the surface of the sphere in angular functions identical to those used in the spherical harmonic expansion. The approximation is that the particle be smooth and not deviate far from sphericality.

2.8 Magnetic Spheres

With growing interest in magnetic nanostructures there is also interest in Mie scattering of magnetic spheres. A Mie theory allowing for magnetic media where the media properties includes a nonzero permeability μ has been developed early by Kerker et al. [81, 82]

A Fortran code for spherical scatterers with both a complex permittivity and a complex permeability is listed in a report by Milham [83]. Tarento et al. [84] considered Mie scattering of magnetic spheres extending the classical Mie scattering approach to a media where the dielectric constant is no more a real number but a tensor with a gyrotropic form. A usable code for scattering by a sphere having a different magnetic permeability than the surrounding is included in the Matlab program by *Christian Mätzler* [85].

2.9 Chiral and Anisotropic Spheres

During the previous decades, much attention has been focused on the light scattering interaction between chiral and anisotropic particles and electromagnetic waves, as a result of numerous applications in the electromagnetic scattering and antenna theory. The historical background, and a general description, of the subject of electromagnetic chirality and its applications can be found in the books by Lakhtakia and Varadan [86] and Weiglhofer and Lakhtakia [87]. A isotropic chiral medium or an optical active medium is rotationally symmetric but not mirror symmetric. Only circularly polarised plane waves can propagate in the chiral medium without a change in their state of polarisation.

A scattering sphere can also be chiral. The extension of Mie's theory to an optically active sphere was published by Bohren [88] and later extended to a sphere with a chiral shell [89]. Bohren devised a transformation to decompose the problem such that he could consider two independent modes of propagation in the chiral medium, namely left- and right-circularly polarised waves. In the limit of no chirality the solution is identical to the Mie solution.

Theories and programs for such types of scatterers have been published by Bohren in his thesis for a chiral sphere [90].

Using the Bohren decomposition Hinders and Rhodes [91] investigate the problem of scattering by chiral spheres embedded in a chiral host medium.

As colour pigments and crystals are often anisotropic there is some interest to extend Mie's theory to such kind of scattering particles. Stout et al. [92] established

a vector spherical harmonic expansion of the electromagnetic field propagating inside an arbitrary anisotropic medium to solve this problem. A similar problem of a uniaxial anisotropic sphere was considered by Geng et al. [93] to find the coefficients of the scattered field. Droplets of liquid crystals may be considered as spherical particles with radial anisotropy. This scattering problem is discussed by Qiu et al. [94] using an extension of Mie theory.

2.10 Scattering by a Short Pulse

The history of the investigation of time domain scattering by a sphere, given an incident short pulse, can be traced back at least to Kennaugh [95]. The interest was to investigate short-pulse radar systems for target discrimination. The incident pulse is expanded in a Fourier series. For each wavelength in the Fourier series Mie scattering is computed.

Ito et al. [96] analyse the transient responses of a perfectly conducting sphere. For numerical calculation a Laplace transform algorithm is used. This method was later extended to a dielectric sphere [97] to analyse the multiple reflections within a sphere. Bech et al. [98] provided an extension by way of the Fourier-Lorenz-Mie-Theory (FLMT) [99], which permits the scattering of a laser beam and the separation of individual scattered light orders using the Debye series expansion to compute scattering by a femtosecond Laser pulse to determine the particle diameter from the time differences between the scattered light orders of the Debye series. The Debye series expansion is analogous to a multiple internal reflection treatment such that it is similar to geometrical optics where each term has a clear physical interpretation such as diffraction, reflection, refraction and higher order refractions.

2.11 Nanosized Spheres

With a nanosized nobel metal particle of size lower than about 20 nm, various modifications, extensions and corrections to Mie's original theory are needed to take into account that "sharp" boundary conditions do not hold in the nanoscale [100]. In his recent survey paper [101] Kreibig lists among others the following supplementary models to the Mie theory, i.e. non plane-wave incident field, non step-like boundary condition and a particle size-dependent dielectric function. Applying these extensions help to explain measured absorption spectra of Ag nanoparticles and plasmon polaritons.

2.12 Gaussian Beam Scattering

The traditional Lorenz-Mie theory describes the scattering by a spherical homogeneous dielectric particles illuminated by an incident plane wave. However, in many applications such as optical particle sizers, confocal microscopes, optical trapping and optical manipulation scattering by a focused laser beam is quite often of interest. In his recent book Quinten [102] refers to Möglich [103] who in 1933 derived expression for the expansion coefficients of the field in the focal point of a lens system to compute scattering in the Rayleigh approximation.

There are different concepts available to handle the problem of laser beam scattering. With a point matching approach you just need an analytical description of the incident field at the matching points on the particle surface. This method which is also suitable for a spherical scatterer has been implemented in the Multiple Multipole Program (MMP) by Evers et al. [104]. But in this review we are concerned with the Mie theory and within this theory various beam expansion methods have been developed.

A laser beam with Gaussian intensity distribution can be expanded into spherical vector wave functions or into a spectrum of plane waves [105]. The Generalised Lorenz Mie Theory (GLMT) developed by *Gérard Gouesbet* and co-workers is based on the first approach computing beam shape coefficients. It has recently been reviewed by Gouesbet [106]. Plane wave expansion is used by Albrecht et al. [99] and it is integrated into the Null-Field Methods with Discrete Sources (NFM-DS) developed by Doicu and co-workers [107]. Doicu et al. [105] give quantitative comparison of the localised approximation method and the plane wave spectrum method for the beam shape coefficients of an off-axis Gaussian beam. Usually the plane wave expansion method is considered computationally inefficient compared to the GLMT method [108].

Since its foundation at the end of the 1970s *Gérard Gouesbet* and his co-worker *Gérard Gréhand* developed the Generalised Lorenz-Mie Theory (GLMT). Initially the theory only included a single spherical scatterer but the theory was later extended to aggregates of spheres [109], coated spheres [110], a sphere with an eccentrically located spherical inclusion [111] and pulsed Laser scattering [112]. Based on the Davis formulation of the Gaussian beam [113] Gouesbet and co-workers developed a theory to expand the beam into vector spherical wave functions which is compatible with the Lorenz-Mie Theory. In the first implementation the expansion was restricted to on-axis spheres. This theory was later extended to an arbitrarily positioned sphere. Parallel to this development the localised approximation was investigated to reduce the computational demand in computing the beam shape coefficients. Since 1998 the Livre GMTL, fully outlining the GLMT theory and providing printouts of Fortran programs, is available via the Internet [114]. This year Gouesbet and Gréhan published a revised version with the Springer publisher [106].

Moore et al. [115] developed an alternate generalisation of the Lorenz-Mie theory wherein the incident fields are complex focus fields which are nonparaxial generalisations of Gaussian beams. This approach results in an easily calculable closed form

for the coefficients in the multipolar expansion of the incident field that results from a beam passing through a high numerical aperture lens system.

2.13 Near Fields

With the recent rise of plasmonics there seems to be an increasing interest in computing the near field or the internal field by scattering particles. There is especially interest in morphological resonances and in plasmon resonances. There are not many programs available which focus on near field computation. Most programs consider the far field approximation of the radiating spherical vector wave functions to compute scattering patterns in the far field. The T-Matrix programs on the disk accompanying the book by Barber and Hill [116] allow for the simulation of the internal and external near field intensity distribution by a scattering sphere.

Near field and internal field computations of a spherical particle in a Gaussian laser beam can be done using the Windows program GLMT Champ Internes by *Loic Mees* [117].

To compute near fields by a number of scattering spheres you can use the extension of *Yu-lin Xu's GMM* program by *Moritz Ringer*. He extended GMM while working on his PhD thesis [118]. His Fortran program GMM-Field allows for the computation of the near field. GMM-Dip gives the near field with a dipole as the incident field. Apparently *Giovanni Pellegrini* did a similar extension of the GMM program in this PhD thesis [119]. A paper on parallising multiple scattering and near field computation by coated spheres was recently published by Boyde et al. [120].

The LightScatPro Matlab program by *Sylvain Lecler* used for his thesis [121] is also suitable for near field computation for light scattering by a number of spheres.

2.14 Longitudal Modes

Basically, in the Mie theory, transverse wave modes are dominant. However, there is the question about what the theory would look like if there were also longitudinal modes created inside the scattering sphere.

Ruppin [122] extended Mie theory to the case of small metal spheres whose material sustains the propagation of longitudinal waves. This theory is also outlined in the book by Borghese et al. [123]. Ruppin demonstrated that a slight shift of the surface plasmon peak towards higher frequencies would occur. According to Quinten in his recent book [102], all effects connected with longitudal modes have not yet been identified experimentally. Travis and Guck [124] recently revisited the Mie theory and also include longitudinal vector spherical wavefunctions in the expansion of the internal field. The authors argue that in the optical wavelength range the longitudinal wavenumber is almost purely imaginary such that for particles larger than about 2 nm

the longitudinal plasma modes are evanescent and the normal Mie approximation is acceptable.

2.15 Aggregates of Spheres

Scattering by an aggregate or cluster of spheres will be considered in this section. There is a recent extensive review on this topic by Okada [125] giving a timeline of the development in the field since the 1960s. Multiple scattering by a number of spheres dates at least as far back as Trinks [126], who used multipole expansions combined with the translation addition theorem for spherical vector wave functions to express the scattered fields of all other spheres at the origin of a sphere.

Levine et al. [127] extended the work of Trinks by considering two Rayleigh particles, arbitrarily positioned in relation to the incident plane wave. Lenine et al. also made use of Debye scalar potentials as did Trinks. In the following years various rigorous methods extending the Mie theory were developed. Bruning and Lo [128, 129] presented the first solution for two spheres using recursive relations for the translation coefficients.

Later, Fuller et al. [130] considered the two-sphere problem using the order-of-scattering approach, a chain of spheres [131] and an arbitrary cluster of spheres [132].

Next, two well-known rigorous methods were developed to simulate the light scattering by an aggregate of spheres, Mackowski [133] and Mackowski and Mishchenko [134] developed the multiple scattering T-matrix algorithm and the generalised multisphere Mie-solution (GMM) method developed by Xu [135, 136]. Today, there are efficient Fortran programs made available by Mackowski [134] and Yu-lin Xu [135].

These multiple scattering programs are commonly used to study the scattering and absorption properties of soot aggregates [137].

The theory has recently been extended to clusters of rotationally symmetric particles [138] and arbitrary shaped particles [6] using the T-Matrix method.

2.16 Parallelisation

Another current issue is the parallelisation of executing programs. Various methods such as Open Multiple-Processing (OpenMP) and Message Passing Interface (MPI) are available. Within the T-Matrix methods the NFM-DS has recently been parallelised [139]. With the T-Matrix method the computational demand lies mostly in the need to compute the surface integrals. This can of course be easily done by dividing the surface of the scatterer into different sections and then computing the integral of this sections using a separate parallel thread. Mackowski et al. [140] recently implemented parallelisation of a multiple scattering program. A paper on parallizing multiple scattering by coated spheres was published by Boyde et al. [120].

2.17 Further Topics

Not all extensions of the Mie theory can be extensively covered in this chapter. Therefore, in this section some interesting topics not treated above will be briefly mentioned.

Travis and Guck revised the Mie theory [124] using a modern T-matrix formalism and discuss inclusion of longitudinal components of the dielectric permittivity tensor.

Tagviashvili [141] considered the classical Mie theory for electromagnetic radiation scattering by homogeneous spherical particles in the dielectric constant (ε) \rightarrow 0 limit and TE field resonances in the visible spectrum are demonstrated.

With Mie scattering morphological resonances show up. This can be used to determine the diameter of a spherical droplet to a high precision. Ward et al. [142] used a white light LED for illumination to study the broadband Mie backscattering from optically levitated aerosol droplets to observe the morphological Mie resonances simultaneously across a spectral range from 480 to 700 nm. Correlating the measured resonances to the mode order and mode number using Mie theory the droplet size can be determined with an accuracy of ± 2 nm.

As the scattering of a plane electromagnetic wave by a dielectric sphere is considered a canonical problem, Mie's theory is still widely used as a standard reference to validate methods intended for more complex scattering problems [143, 144]. For example, Khoury et al. [145] compare COMSOL's finite element method (FEM) algorithm with the Mie theory for solving the electromagnetic fields in the vicinity of a silica–silver core–shell nanoparticle. It is demonstrated that the COMSOL FEM algorithm also generates accurate solutions of the near field. Takano and Liou [146] developed a geometrical optics ray-tracing program to compute scattering for concentrically stratified spheres and in the validation section show that it produces the same general scattering features as the "exact" Lorenz–Mie theory for a size parameter of 600.

2.18 Further Reading

There are various topics not considered in this review. For these topics I suggest some further reading. For the basics on the Mie theory readers may refer to the classical books by Stratton [43], van de Hulst [46] (available as a budget Dover edition), Born and Wolf [45], Kerker [30] and Bohren and Huffman [47]. For a more recent and extensive discussion on the topic refer to Grandy [27]. Morphological resonances in Mie scattering are extensively covered in the book by Davis and Schweiger [28].

Scattering particles are commonly positioned on a plane interface and particle– surface scattering interaction will have to be considered in the corresponding extension of Mie theory. This is for example a problem when simulation particle surface scanners detect particle conterminants on wafers. For these who are interested in such kinds of problems there are methods based on the T-matrix method taking account of the plane surface. Such methods are fully outlined in the books by Doicu et al. [147] and Borghese et al. [123]. There is a section on supported nanoparticles in the recent book by Quinten [102]. For those interested in plasmonics and the optics of nanosized noble metalparticles, Quinten's book gives an overview of analytical and numerical models for the optical response of nanoparticles and nanoparticle systems. Nanooptics is the topic of the book by Novotny and Hecht [148] who also care for the topic of particles on surfaces in an extensive way.

2.19 Available Programs

Those looking for computational programs to compute Mie scattering or to solve related scattering problems there are various web sites available which provide information about these topics or give links to available computer programs. First of all there is the portal *ScattPort* [149] which is intended to be a Light Scattering Information Portal for the light scattering community. The basic concept of this information portal includes features such as database of available computer programs and up-to-date information related to the subject of light scattering, e.g. conference announcements, available jobs, new books, etc. Many of the listed programs are based on Mie theory or are extensions of Mie theory. Further information about the history and concept of the portal is presented by Hellmers and Wriedt [150].

SCATTERLIB by Flatau [151] is another web site with an emphasis to list open access computational programs suitable to compute light scattering by particles. In the list Mie theory has been implemented in various traditional programming languages originating in Fortran, but are also available in Pascal, C++ and Java. It has also been programmed in computer algebra systems such as Maple and Mathematica. Additionally, it is available in numerical mathematical systems such as IDL and Matlab [149] and 3 years ago the Mie theory has even been programmed on a Java enabled Mobile Phone using a Matlab clone [152].

2.20 Sample Simulation Results

To graphically demonstrate the differences of various kinds of extensions of the Mie's theory we next plot some scattering diagrams. All programs used are available from *ScattPort* [149]. As basic parameters for this comparison, we choose a particle diameter of d = 700 nm and an incident wavelength of $\lambda = 500$ nm. Figure 2.1 shows the scattering pattern of a dielectric sphere with a refractive index of n = 1.5 calculated using the Mie theory. Both p- and s-polarisation are plotted. The next figures demonstrate the variation in the scattering pattern with change in the properties of the scattering sphere. Even a small amount of absorption gives a change in the scattering pattern as seen from Fig. 2.2. Also, a coating with a shell having a slightly lower refractive index gives another scattering diagram (Fig. 2.3). The next

Fig. 2.1 Scattering pattern of a homogeneous nonabsorbing sphere d = 700 nm, $\lambda = 500$ nm, n = 1.5

Fig. 2.2 Scattering pattern of a homogeneous absorbing sphere d = 700 nm, $\lambda = 500 \text{ nm}$, n = 1.5 + i 0.1





scattering pattern (Fig. 2.4) is for a sphere possessing a refractive index gradient gradient with n = 1.33 at the centre of the sphere and n = 1.5 at the boundary of the sphere. This gradient is approximated by 50 steps. With a chiral or optically active sphere there are also great differences in the scattering pattern (Fig. 2.5).

If the sphere is positioned in a highly focused laser beam with Gaussian intensity distribution pronounced differences to the first scattering diagram show up (Fig. 2.6). A slightly perturbed sphere gives also only slight perturbation in the scattering diagram (Fig. 2.7). With an unisotropic particle having three different refractive indices in the three cartesian coordinates the scattering pattern is no longer rotationally symmetric (Fig. 2.8).

Fig. 2.4 Scattering pattern of a sphere possessing a refractive index gradient d = 700 nm, $\lambda = 500$ nm, gradient n = 1.33-1.5

Fig. 2.5 Scattering pattern of a homogeneous chiral sphere d = 700 nm. $\lambda = 500 \text{ nm}$, n = 1.5, kb=0.1

Fig. 2.6 Scattering pattern of a homogeneous sphere in a Gaussian laser beam d = 700 nm, $\lambda = 500$ nm, beam waist diameter = 500 nm, n = 1.5

Fig. 2.7 Scattering pattern of a homogeneous slighly rough sphere beam d = 700 nm, $\lambda =$ 500 nm, epsilon (perturbation) = 0.2, n = 1.5



Fig. 2.8 Scattering pattern of an unisotropic sphere beam d= 700 nm, λ = 500 nm, n_x = 1.2, n_y = 1.3, n_z = 1.5



2.21 Conclusion

What is the current state of Mie's theory? It seems to be as lively as ever. It is continuously used for code validation. Wherever particles can be considered spherical, Mie scattering is applicable. It is applied everyday in diffraction-based instruments to characterise particles. To this day, new approaches in computing Mie scattering are developed and the methods are continuously extended to cover related scattering problems such as coated spheres.

It is not only used for educating students and the validation of more advanced theories but also it is the basis of radiative transfer, Lidar and optical particle characterisation. Even today there is still progress in programming and new programs which are based on Mie theory or which extend Mie theory in some respect show up every year.

In this chapter an overview of the progress in developing light scattering programs suitable for Mie-related scattering problems has been given. A short description of each technique has been presented and suitable references have been provided such that the reader can find more detailed information about the various methods and sources of computer programs.

The state of the art in numerical light scattering modelling is progressing rapidly especially with fast advancing research fields such as nanophotonics and near-field optics. With almost all concepts there was much progress in the recent years.

The recent advances in computer hardware and the development of fast algorithms with reduced computational demands and memory requirements have made the exact numerical solution of the problem of scattering from large scattering particles highly feasible. Today, scattering by spherical particles of realistic sizes can be computed in an efficient way. Especially, the number of open source programs and development projects is increasing continuously.

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