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Zero slopes of the scattering function and scattering matrix for strict forward and backward scattering by mirror symmetric collections of randomly oriented particles

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ABSTRACT

Single scattering of light by a finite mirror symmetric collection of independently scattering randomly oriented particles is considered as observed in the far-field. It is shown that the slopes of the scattering function and all other elements of the scattering matrix are functions of the scattering angle that tend to zero when the direction of the scattered light tends to the strict forward or backward direction. This result is obtained by introducing an extended scattering matrix, based on symmetry arguments. The theory is illustrated and clarified by practical examples of scattering functions and scattering matrices. Various applications are also considered.

1. Introduction

In theoretical and experimental studies of light scattering by particles a key role is played by the scattering matrix. This 4×4 matrix determines the four Stokes parameters of singly scattered light traveling in a certain direction for a given beam of polarized incident light [1–4]. The scattering matrix depends in general on a polar angle, θ, in the closed range $[0, \pi]$, and an azimuth angle, ϕ, in the closed range $[0, 2\pi]$, where $\theta = 0$ for strict forward scattering and $\theta = \pi$ for strict backward scattering. In this paper we only consider single scattering by finite mirror symmetric collections of randomly oriented particles. The particles scatter light independently and a detector is located in the far-field. Such collections are frequently met in theoretical and numerical work on light scattering. In practice they are often very suitable approximations. Due to rotational symmetry of the collections there is no dependence on azimuth and the scattering matrix can be written as $\boldsymbol{F}(\theta)$.

The first element of $\boldsymbol{F}(\theta)$ is the scattering function $F(\theta)$. This scalar function is the only element we need when polarization is ignored. In general it has several interesting features like maxima and minima [1–5]. The features near strict forward and backward scattering are, however, difficult to uncover by experimental means [6]. Furthermore, in results of numerical computations the behavior of $F(\theta)$ when θ tends to zero or π is often not clearly shown, due to the use of an insufficient number of values for the scattering angle (i.e. the mess is too coarse). This happens in particular for the strong forward peak of the scattering function produced by large particles. Similar problems near strict forward and backward scattering occur for some other elements of the scattering matrix.

In this paper we study the behavior of all elements of the scattering matrix when the scattering angle tends to zero or π. In Section 2 the form of the scattering matrix, $\boldsymbol{F}(\theta)$, is discussed and the extended scattering matrix, $\boldsymbol{G}(\theta)$, is introduced. It is shown that all elements of $\boldsymbol{G}(\theta)$ have a

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horizontal tangent if θ is zero or π. For this reason the slopes of all elements of $\boldsymbol{F}(\theta)$ tend to zero when θ tends to zero or π. This also holds for a number of combinations of such elements, as proven in Section 3. The next section is devoted to examples that clarify and corroborate the theory expounded in the preceding sections. Various applications of the main results of the theory are discussed in Section 5. Appendix A is devoted to derivatives of electric fields, Stokes parameters and elements of the extended scattering matrix. In Appendix B some general properties of polynomials are employed to show that all generalized spherical functions have finite derivatives with respect to x and θ, where $x=\cos(\theta)$.

2. Scattering in a plane

Suppose a finite collection of independently scattering particles at the origin, O, of a Cartesian coordinate system is illuminated by a beam of light and provides beams of singly scattered light in all directions in three dimensional space. A detector is located at a far-field observation point. Fig. 1 shows the situation for a direction of the scattered light with polar angle θ. We use Stokes parameters I, Q, U and V to describe the intensity (or flux) and state of polarization of a beam of quasi-monochromatic light and make these parameters elements of a column vector, $\boldsymbol{I}=[I,Q,U,V]^t$, called the Stokes vector, where the superscript t stands for transpose [1,4]. Here I is positive and not smaller than the absolute value of any of the other Stokes parameters. The reference plane for the Stokes parameters is the plane of scattering, i.e. the plane defined by the directions of the incident and scattered light beams.

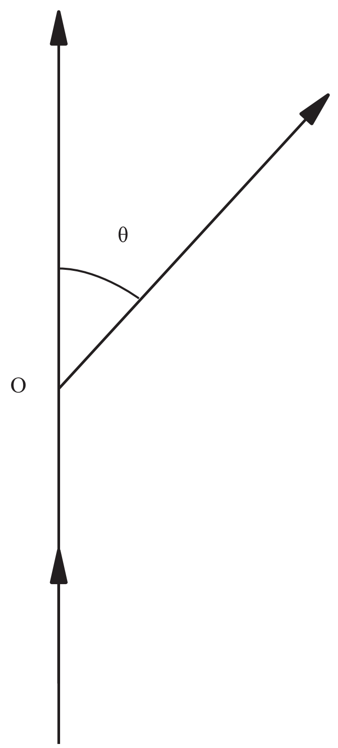

Fig. 1. Light scattering by a collection of particles at a point O in a direction making an angle θ with the direction of the incident light.

We can now write

$$\boldsymbol{I}^s(\theta)=c\boldsymbol{F}(\theta)\boldsymbol{I}^i(0), \tag{1}$$

where $\boldsymbol{I}^i(0)$ and $\boldsymbol{I}^s(\theta)$ are the Stokes vectors of the incident and scattered light beams, respectively, c is a positive constant that does not depend on θ and $\boldsymbol{F}(\theta)$ is the 4 by 4 scattering matrix. It is important to note that the angle θ in Eq. (1) is restricted to the range $0\le\theta\le\pi$. For an arbitrary collection of particles the Stokes vector of the scattered light and the scattering matrix may not only depend on θ, but also on an azimuthal angle, as far as directions are concerned. However, this is not the case in this paper, since we only consider mirror symmetric collections of randomly oriented particles. Therefore, the scattering matrix is of the form:

$$\boldsymbol{F}(\theta)=\begin{pmatrix} F_{11}(\theta) & F_{12}(\theta) & 0 & 0 \\ F_{12}(\theta) & F_{22}(\theta) & 0 & 0 \\ 0 & 0 & F_{33}(\theta) & F_{34}(\theta) \\ 0 & 0 & -F_{34}(\theta) & F_{44}(\theta) \end{pmatrix}, \tag{2}$$

where $F_{ij}(\theta)$ stands for the element in the i-th row and j-th column of $\boldsymbol{F}(\theta)$. Among the collections included are [1] the following:

(i) randomly oriented particles with a plane of symmetry, like spheres, bi-spheres, spheroids, cylinders, cubes, etc.,
(ii) randomly oriented particles with their mirror particles in equal numbers, like right-handed screws and left-handed screws,
(iii) randomly oriented particles that are so small compared to the wavelength that Rayleigh scattering is sufficiently accurate, like molecules for visible incident light.

The positive element $F_{11}(\theta)$ is the scattering function and can also be written as $F(\theta)$. The absolute value of each other element is smaller than or equal to $F_{11}(\theta)$. The relations $F_{21}(\theta)=F_{12}(\theta)$ and $F_{43}(\theta)=-F_{34}(\theta)$ are due to reciprocity. The fact that the eight elements of the 2×2 matrices in the lower left and upper right corners are identically equal to zero is due to mirror symmetry with respect to the scattering plane. This was briefly mentioned by Hovenier in 1969 [7] and treated more extensively in [4].

To study the behavior of the scattering matrix when θ tends to zero or π we will now extend the range of θ by measuring θ clockwise from the forward scattering direction in the range $[0,2\pi]$, which is equivalent to measuring θ anti-clockwise from the forward scattering direction in the range $[0,-2\pi]$. This is shown in Fig. 2 where we have $0\le\theta\le\pi$ in S_1, i.e. the right half-plane (as in Fig. 1) and $-\pi\le\theta\le0$ in S_2, i.e. the left half-plane. For strict forward scattering $\theta=0$ and for strict backward scattering $\theta=\pm\pi$. The directions given by θ and $-\theta$ of the scattered beam are symmetric with respect to the strict forward as well as strict backward scattering directions. We have thus combined two half-planes into one complete plane. We can now write instead of Eq. (1):

$$\boldsymbol{I}^s(\theta)=c\boldsymbol{G}(\theta)\boldsymbol{I}^i(0), \tag{3}$$

where $-\pi\le\theta\le\pi$. We use $G_{ij}(\theta)$ to denote the element in the i-th row and j-th column of $\boldsymbol{G}(\theta)$. For a fixed beam of

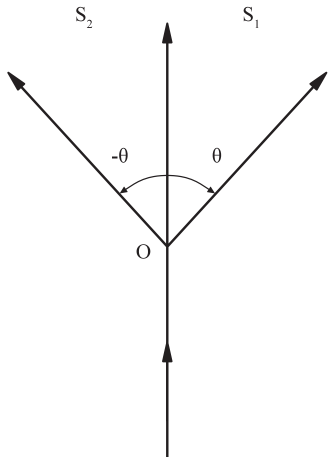

Fig. 2. Light scattering by a collection of particles at a point O in two directions lying in one plane which is composed of two half-planes, S_1 and S_2. The two directions of the scattered light are mirror symmetric with respect to the directions given by $\theta=0$ and $\theta=\pi$ or $-\pi$.

incident light the rotational symmetry of the collection of particles entails

$$\boldsymbol{I}^s(\theta)=\boldsymbol{I}^s(-\theta) \tag{4}$$

which gives, according to Eq. (3),

$$\boldsymbol{G}(-\theta)=\boldsymbol{G}(\theta). \tag{5}$$

To determine $\boldsymbol{G}(\theta)$ from $\boldsymbol{F}(\theta)$ we can use that they are equal for $0\le\theta\le\pi$, while Eq. (5) can be employed for $-\pi\le\theta\le 0$. We call $\boldsymbol{F}(\theta)$ the scattering matrix and $\boldsymbol{G}(\theta)$ the extended scattering matrix. Their one–one elements are called the scattering function and the extended scattering function. It is clear from Eqs. (4) and (5) that the elements of $\boldsymbol{I}^s(\theta)$ and $\boldsymbol{G}(\theta)$ are even functions of θ. Certain properties of electromagnetic fields make it possible to show that all elements of $\boldsymbol{I}^s(\theta)$ and $\boldsymbol{G}(\theta)$ are continuous functions with continuous derivatives (see Appendix A). So in particular the first derivative of these functions exists and is continuous.

Let us now discuss some general properties of (single-valued) even functions of a single real variable. Clearly, the curve representing an even function $y(\theta)$ in a Cartesian coordinate system is mirror symmetric about the vertical axis, which means that the curve remains unchanged after mirroring about the vertical axis. Furthermore, we have the following theorems:

1. The sum of two even functions is even.
2. The product of two even functions is even.
3. The ratio of two even functions is even, if the denominator is not identically zero.
4. The composition of a function with an even function is even.
5. The first derivative of an even function is an odd function, if this derivative exists.

The first four theorems follow directly from the definition of an even function. The fifth theorem is readily found from the definition of the first derivative of a function, since the mirror image with respect to the vertical axis of a small change Δy equals Δy, but the mirror image of the corresponding $\Delta\theta$ is $-\Delta\theta$.

Hence, any even function of θ times an element of $\boldsymbol{G}(\theta)$ is even and the natural (base e), as well as the Briggsian (base 10), logarithm of an element of $\boldsymbol{G}(\theta)$ is even. These corollaries are important for making plots. The fifth theorem means that if $\boldsymbol{G}'(\theta)$ is the first derivative of $\boldsymbol{G}(\theta)$, we have

$$\boldsymbol{G}'(\theta)=-\boldsymbol{G}'(-\theta). \tag{6}$$

By letting θ tend to zero in this equation we find

$$\boldsymbol{G}'(0)=-\boldsymbol{G}'(0), \tag{7}$$

yielding

$$\boldsymbol{G}'(0)=\boldsymbol{O}, \tag{8}$$

where $\boldsymbol{O}$ stands for a matrix having only zero elements. The directions of the scattered beams given by θ and $-\theta$ coincide in this case and form the strict forward scattering direction. Consequently, in a Cartesian coordinate system each element of $\boldsymbol{G}(\theta)$ has a horizontal tangent (i.e. parallel to the θ-axis) at $\theta=0$. Or in other words, the slope of the tangent is zero for $\theta=0$, which means there is a maximum or minimum there, unless the function is constant in a range with $\theta=0$ as an interior point. This is illustrated by means of an example in the range $[-\pi,\pi]$ of Fig. 3. We see that the tangents of the function in a point and its mirror point have opposite slopes. If we move both points to $\theta=0$ the tangents tend to a horizontal tangent at $\theta=0$. This provides a geometrical explanation of Eq. (8). It should be noted that an element of $\boldsymbol{G}(\theta)$ cannot have a point of inflection at $\theta=0$ with a horizontal tangent, since in that case the element would not be symmetric about the vertical axis.

To explore the situation near the back scattering direction we will now extend the range of theta even further. The directions given by $\theta=\pi$ and $\theta=-\pi$ coincide and form the strict backward scattering direction (see Fig. 2). Note that, e.g., $\theta=\pi+\pi/6$ is the same direction as $\theta=-\pi+\pi/6$. More generally, the directions represented by $\theta=\pi$ and $\theta=\pi\pm 2\pi$ are the same. Therefore, all elements of $\boldsymbol{G}(\theta)$ are periodic functions with period 2π. Because of the symmetry with respect to the backward

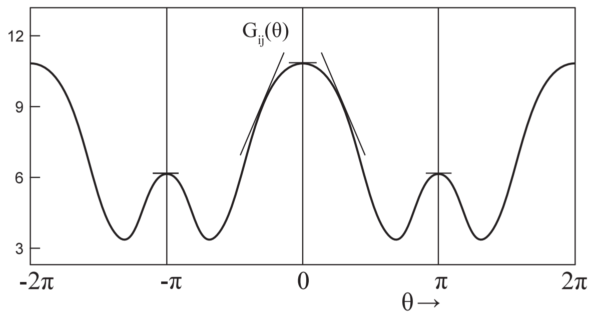

Fig. 3. Example of an element $G_{ij}(\theta)$. This function is mirror symmetric about the vertical through $\theta=0$, but the slopes at points that are mirror symmetric have opposite signs since the tangents at such points are also mirror symmetric with respect to the vertical through $\theta=0$. Similar situations exist for $\theta=\pm\pi$. Furthermore, $G_{ij}(\theta)$ is a periodic function with period 2π. Clearly, these properties are independent of the normalization of $G_{ij}(\theta)$.

scattering direction $\boldsymbol{G}(\theta)$ is symmetric with respect to $\theta=\pi$ and $\theta=-\pi$ (see Fig. 3). Letting θ tend to π in Eq. (6) yields

$$\boldsymbol{G}'(\pi)=-\boldsymbol{G}'(-\pi). \tag{9}$$

But $\boldsymbol{G}'(\theta)$ is periodic with period 2π, since $\boldsymbol{G}(\theta)$ has this periodicity. So we have

$$\boldsymbol{G}'(-\pi)=\boldsymbol{G}'(\pi). \tag{10}$$

It follows from Eqs. (9) and (10) that

$$\boldsymbol{G}'(\pi)=\boldsymbol{O}. \tag{11}$$

Because of symmetry with respect to the vertical through π this point cannot be a point of inflection with a horizontal tangent. So all elements of $\boldsymbol{G}(\theta)$ have a horizontal tangent, not only at $\theta=0$, but also at $\theta=\pi$, which means there is a maximum or minimum at these points, unless the function is constant in a range containing such a point as an interior point. In Fig. 3 we see the situation around the strict backward scattering direction. It is clear that the tangents at two points that are symmetric with respect to π have opposite slopes and coincide when both points are moved to $\theta=\pi$. This explains Eq. (11).

In case the scattering matrix is of the form given by Eq. (2) it is customary in the literature to restrict the treatment of a scattering problem in the scattering plane to a half-plane in which θ runs from zero (strict forward scattering) to π (strict backward scattering), with both end points included (see Eqs. (1) and (2)). Eq. (8) shows that at $\theta=0$ the left-hand and right-hand derivatives of $G_{ij}(\theta)$ are equal and both are zero. Since at $\theta=0$ the right-hand derivative of $G_{ij}(\theta)$ is the same as the right-hand derivative of $F_{ij}(\theta)$ we can conclude that the right-hand derivative of $F_{ij}(\theta)$ is zero at $\theta=0$. Similarly, Eq. (11) shows that the left-hand derivative of $F_{ij}(\theta)$ is zero for $\theta=\pi$. We have thus shown that the slope of (the graph of) $F_{ij}(\theta)$ tends to zero when θ tends to zero or π, or in other words, the tangents tend to become parallel to the θ-axis if θ tends to zero or π. This result has been obtained by considering scattering in the complete scattering plane, instead of only in a half-plane. So, the behavior of $\boldsymbol{F}(\theta)$ near the borders, i.e. near $\theta=0$ and $\theta=\pi$, can be better understood by looking across the borders. Evidently, this is independent of the normalization of the scattering matrix. It should be mentioned [3,4] that for $\theta=0$ we have $F_{22}=F_{33}$ and $F_{12}=F_{34}=0$, while for $\theta=\pi$ we have $F_{22}=-F_{33}$, $F_{12}=F_{34}=0$ and $F_{44}=F_{11}-2F_{22}$.

3. Combinations

Combinations of elements of the scattering matrix frequently occur in the literature. To deal with them we can use the general rules that the sum, difference, product and ratio of differentiable functions are differentiable, provided no vanishing denominator occurs. For the same kind of combinations the same rules hold for the continuity of continuous functions and the periodicity of periodic functions having the same period. In addition we can employ the rules for combinations of even and odd functions given earlier. In graphs and tables one often considers ratios of the elements of the scattering matrix like $F_{11}(\theta)/F_{11}(\theta_c)$, where θ_c is a fixed angle, and other elements divided by $F_{11}(\theta)$, which is larger than zero. Because of our results for $\boldsymbol{G}(\theta)$ and the rules given above it is clear that the right-hand derivatives at $\theta=0$ and the left-hand derivatives at $\theta=\pi$ are zero for such combinations. If the Briggsian logarithm (indicated as log) of an even positive function $f(\theta)$ with continuous derivative is plotted in the range $-\pi\le\theta\le\pi$ one finds for the derivative $\log e(1/f(\theta))(df(\theta)/d\theta)$, which is also zero at 0 and π. So in all these plots the slopes tend to zero when θ tends to zero or π.

According to Eq. (3) all four elements of the Stokes vector of the scattered light $\boldsymbol{I}^s(\theta)$ are, for a fixed beam of incident light, a sum of a constant times an element of $\boldsymbol{G}(\theta)$. So the derivatives of all elements of $\boldsymbol{I}^s(\theta)$ are continuous and vanish at $\theta=0$ and $\theta=\pi$. If we only consider $0\le\theta\le\pi$ we find zero slopes for all elements of $\boldsymbol{I}^s(\theta)$ in the limits of θ tending to zero or π.

Combinations of Stokes parameters are also frequently used like

(a) the relative intensity:

$$I_r(\theta)=\frac{I(\theta)}{I(\theta_c)}, \tag{12}$$

where θ_c is a fixed angle, e.g., 30°,

(b) the degree of linear polarization (in case U vanishes):

$$p_s(\theta)=-\frac{Q(\theta)}{I(\theta)}, \tag{13}$$

(c) the degree of circular polarization:

$$p_c(\theta)=\frac{V(\theta)}{I(\theta)}. \tag{14}$$

For the same reasons as given above for the elements of the scattering matrix, the slopes of the curves in these three combinations must also tend to zero when θ approaches zero or π.

4. Examples

As a first example we consider the case of Rayleigh scattering for particles with isotropic polarizability, as the limiting case for very small particles [1]. To determine $\boldsymbol{G}(\theta)$ from $\boldsymbol{F}(\theta)$ we use that they are equal for $0\le\theta\le\pi$, while Eq. (5) can be employed for $-\pi\le\theta\le0$. This gives

$$G_{11}(\theta)=\tfrac{3}{4}\left(1+\cos^2\theta\right). \tag{15}$$

So the expression at the right-hand side of this equation is the same as for $F_{11}(\theta)$ in the range $0\le\theta\le\pi$, but is valid for $G_{11}(\theta)$ in the range $-\pi\le\theta\le\pi$. It is also periodic with period 2π. The derivative of $G_{11}(\theta)$ is the odd function:

$$G_{11}'(\theta)=-\tfrac{3}{4}\sin(2\theta), \tag{16}$$

which is continuous and vanishes at $\theta=0$ and $\theta=\pi$. In the same way $\boldsymbol{F}(\theta)$ provides the other non-zero elements of $\boldsymbol{G}(\theta)$, namely $G_{22}(\theta)=G_{11}(\theta)$, $G_{12}(\theta)=-\frac{3}{4}\sin^2(\theta)$ and $G_{33}(\theta)=G_{44}(\theta)=\frac{3}{2}\cos\theta$. These are all even functions, with continuous derivatives which are zero at $\theta=0$ and $\theta=\pi$. Consequently, all elements of the scattering matrix for this case, as functions of the scattering angle, tend to have zero slopes when θ approaches zero or π. This concludes our first example.

A very useful general example is provided by a scattering matrix of the form given by Eq. (2) with elements that can be written as the sum of $N+1$ generalized spherical functions $P^l_{mn}(x)$ with $x=\cos\theta$ [4]. Using the equality of $\boldsymbol{G}(\theta)$ and $\boldsymbol{F}(\theta)$ for $0\le\theta\le\pi$ as well as Eq. (5) we can now write the elements of $\mathbf{G}(\theta)$ as follows:

$$G_{11}(\theta)=\sum_{k=0}^{N}\alpha_1^k P_{00}^k(x)=\sum_{k=0}^{N}\alpha_1^k P_k(x) \tag{17}$$

$$G_{22}(\theta)=\frac{1}{2}\sum_{k=2}^{N}\alpha_2^k\left\{P_{22}^k(x)+P_{2-2}^k(x)\right\}+\alpha_3^k\left\{P_{22}^k(x)-P_{2-2}^k(x)\right\} \tag{18}$$

$$G_{33}(\theta)=\frac{1}{2}\sum_{k=2}^{N}\alpha_2^k\left\{P_{22}^k(x)-P_{2-2}^k(x)\right\}+\alpha_3^k\left\{\left(P_{22}^k(x)+P_{2-2}^k(x)\right\}\right. \tag{19}$$

$$G_{44}(\theta)=\sum_{k=0}^{N}\alpha_4^k P_{00}^k(x)=\sum_{k=0}^{N}\alpha_4^k P_k(x) \tag{20}$$

$$G_{12}(\theta)=\sum_{k=2}^{N}\beta_1^k P_{02}^k(x)=-\sum_{k=2}^{N}\sqrt{\frac{(k-2)!}{(k+2)!}}\beta_1^k P_k^2(x) \tag{21}$$

$$G_{34}(\theta)=\sum_{k=2}^{N}\beta_2^k P_{02}^k(x)=-\sum_{k=2}^{N}\sqrt{\frac{(k-2)!}{(k+2)!}}\beta_2^k P_k^2(x). \tag{22}$$

In these equations $P_k(x)=P_{00}^k(x)$ are Legendre polynomials. The functions $P_k^2(x)$ are associated Legendre functions. It is shown in Appendix B that the functions $P_k^2(x)$, $P_{22}^k(x)$ and $P_{2-2}^k(x)$ are polynomials of x if $k\ge 2$, and consequently have finite continuous derivatives with respect to x. Clearly all elements of $\boldsymbol{G}(\theta)$ are even functions of θ. Using the chain rule of differential calculus and the fact that the derivative of $\cos\theta$ is $-\sin\theta$ we find that all six matrix elements occurring in Eqs. (17)–(22) have finite continuous derivatives with respect to θ, which vanish for $\theta=0$ and $\theta=\pi$. Consequently, all elements of the scattering matrix for this case, as functions of the scattering angle, tend to have zero slopes when θ approaches zero or π. In many studies of light scattering polarization is ignored and the scattering function is written as a sum of Legendre polynomials. Eqs. (18)–(22) can then be ignored and it follows from Eq. (17) that the slopes of the scattering function as a function of θ tend to zero when θ tends to zero or π.

5. Applications

In the preceding sections we have shown that in certain cases the slopes of the elements of the scattering matrix, as functions of θ, tend to zero when the scattering angle tends to zero or π. Some applications of this result will be discussed in this section. They pertain to single scattering by finite mirror symmetric collections of independently scattering particles in random orientation, as observed in the far-field. We mention the following:

(i) Numerical computations of scattering matrices using Mie theory, the T-matrix method, DDA, and other methods [8–13] should always be checked. This is especially important for the strong forward scattering peak of the scattering function (and of some other elements of the scattering matrix) exhibited by relatively large particles. Furthermore, the scattered light near $\theta=\pi$ is often much weaker than at smaller scattering angles, which is a disadvantage for the accuracy of Monte Carlo calculations. In both cases it may help to know that the derivatives of the functions must tend to zero when θ approaches 0 or π.

(ii) A large variety of approximate scattering functions (and some other elements of the scattering matrix) exist in the form of formulae with several constants [4,14] and references therein. It is of course desirable that the derivatives of such functions with respect to θ tend to zero on approaching strict forward and backward scattering. This is in order for the very popular Henyey–Greenstein function. In this case we have (see Eq. (5))

$$G_{11}(\theta)=\frac{1-g^2}{(1+g^2-2g\cos\theta)^{3/2}}, \tag{23}$$

where the asymmetry parameter g is a constant in the range $(-1,1)$. Differentiation gives

$$G'_{11}(\theta)=\frac{3g(g^2-1)\sin\theta}{(1+g^2-2g\cos\theta)^{5/2}}, \tag{24}$$

which is zero at $\theta=0$ and $\theta=\pi$. So the derivatives of a Henyey–Greenstein scattering function in the range $0\le\theta\le\pi$ tend to zero on approaching strict forward and backward scattering and, evidently, the same is true for a sum of Henyey–Greenstein scattering functions. However when, for example [14], a function is defined as

$$h(\theta)=t\exp(-s\theta), \tag{25}$$

where t and s are non-zero constants, and this would be chosen as an approximate scattering function we would have for the derivative in the range $0<\theta<\pi$

$$h'(\theta)=-ts\exp(-s\theta), \tag{26}$$

which does not tend to zero when θ tends to zero or π. So this approximate scattering function does not have the proper behavior near strict forward and backward scattering.

(iii) For particles large compared to the wavelength a strong forward peak occurs in the scattering function and some other elements of the scattering matrix. If θ tends to zero the slope of the scattering function may then rather abruptly tend to zero in a small region near $\theta=0$. It should be realized that in such cases significant inaccuracies may occur in numerical calculations, unless a very fine mesh of values of θ is used near the strict forward scattering direction.

(iv) Experimental determinations of elements of the scattering matrix as functions of the scattering angle are usually restricted to a range with a lower bound of 3°–5° and an upper bound of about 175°. Therefore, extrapolations are needed to obtain data for the entire range $0 \le \theta \le \pi$. This is important for studies of single light scattering and indispensable for investigations involving multiple light scattering when these are based on an experimental scattering matrix. Several methods for such extrapolations have been reported [15–18]. We can now make use of the fact that for each element of the scattering matrix the right-hand derivative at $\theta = 0$ and the left-hand derivative at $\theta = \pi$ must both vanish. This can be illustrated as follows. Let $f(\theta)$ be an element of the scattering matrix $\boldsymbol{F}(\theta)$ with $0 \le \theta \le \pi$. Suppose $f_1 = f(\theta_1)$ and $f_2 = f(\theta_2)$ are known, with θ_2 larger than θ_1, while both angles are somewhat larger than zero. To make interpolations and extrapolations in the range $0 \le \theta \le \theta_2$ we can use, e.g., the quadratic polynomial:

$$f(\theta) = a_0 + a_2\theta^2. \tag{27}$$

The linear term in this equation is absent because the right-hand derivative of $f(\theta)$ must be zero if $\theta = 0$. We can now determine the coefficients a_0 and a_2 from f_1 and f_2 in the usual way, i.e. by solving two linear equations with two unknowns. The result is

$$a_0 = f_1 - \frac{(f_1 - f_2)\theta_1^2}{\theta_1^2 - \theta_2^2} \tag{28}$$

and

$$a_2 = \frac{f_1 - f_2}{\theta_1^2 - \theta_2^2}. \tag{29}$$

In this way we find approximate values for $f(\theta)$ in the whole range $0 \le \theta \le \theta_2$ and in particular $f(0) = a_0$, from only two experimental values. It should be noted that we made no assumptions about the size, shape, structure and composition of the particles.

In experimental determinations of scattering matrices one often measures [6] $F_{11}(\theta)/F_{11}(\theta_c)$, $F_{22}(\theta)/F_{11}(\theta)$, $F_{33}(\theta)/F_{11}(\theta)$, $F_{44}(\theta)/F_{11}(\theta)$, $-F_{12}(\theta)/F_{11}(\theta)$ and $F_{34}(\theta)/F_{11}(\theta)$ in the range $0 < \theta_{min} \le \theta \le \theta_{max} < \pi$, where θ_c is a fixed angle, e.g., 30° and $F_{11}(\theta)$ is larger than zero. As mentioned in Section 3 these ratios also have vanishing right-hand derivatives at $\theta = 0$ and vanishing left-hand derivatives at $\theta = \pi$. This can be used for interpolation and extrapolation to $\theta = 0$ and $\theta = \pi$.

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Appendix A

In this appendix we consider derivatives of, consecutively, electric fields, Stokes parameters and elements of the extended scattering matrix. It is generally assumed, either explicitly [19] or implicitly, that electromagnetic field vectors are finite throughout the entire field and are continuous functions of position and time with continuous derivatives of all orders at every point in whose neighborhood the physical properties of the medium are continuous. In this paper we can go further than this general assumption because we deal with single scattering by a finite scattering object with a far-field observation point. This makes it possible to use an expression for the scattered electric field [20] that shows this field behaves as a single outgoing wave. Recently, Dr. M.I. Mishchenko informed us that this expression can be differentiated with respect to the position of the observation point, as many times as desired. It should be noted that if the derivative of order n of a function exists, the derivative of order $n-1$ is continuous, so that e.g the first order derivative is a continuous derivative if the second order derivative exists.

Using polar coordinates r, θ and ϕ for the points in the space outside the collection of particles it is clear now that the components of the electric field that are combined to define the Stokes parameters of the scattered beam of light considered in Section 2 are continuous functions of θ with continuous derivatives. It follows that the same is true for the Stokes parameters of this beam [2].

If we now choose the Stokes vectors $(1,0,0,0)$, $(1,1/2,1/2,0)$ and $(1,0,0,1/2)$, in that order, for the incident beam we obtain from Eq. (3), respectively, the Stokes vectors $c(G_{11},G_{12},0,0)$, $c(G_{11}+G_{12}/2, G_{12}+G_{22}/2, G_{33}/2, -G_{34}/2)$ and $c(G_{11},G_{12},G_{34}/2,G_{44}/2)$ for the scattered beam. It is then readily seen by using the rules for sums and differences of continuous and differentiable functions that all elements of $\boldsymbol{G}(\theta)$ are continuous functions of θ with continuous derivatives.

Appendix B

In this appendix we use some properties of polynomials to show that all functions of x occurring in Eqs. (17)–(22) have continuous finite derivatives with respect to x. A real-valued polynomial function of a real variable x can be written as

$$j(x) = e_0 + e_1x + e_2x^2 + \ldots + e_nx^n, \tag{B.1}$$

where n is a non-negative integer and $e_0, e_1, e_2, \ldots, e_n$ are real constant coefficients. The expression on the right-hand side of Eq. (B.1) is called a polynomial. A single constant, including zero, is also a polynomial. We mention the following properties of polynomials. The sum, difference and product of two polynomials is also a polynomial. Any derivative with respect to x of a polynomial function is finite as well as continuous and is also a polynomial function.

Legendre polynomials occur in Eqs. (17) and (20). So the right-hand sides of these equations have finite continuous derivatives with respect to x.

Associated Legendre functions are present in Eqs. (21) and (22). It is well-known that not all associated Legendre functions are polynomials. However, we have [21]

$$P_k^2(x) = \left(1-x^2\right)\frac{d^2P_k(x)}{dx^2}, \tag{B.2}$$

and this product of polynomials is a polynomial for every value of k. Therefore, the right-hand sides of Eqs. (21) and (22) have finite continuous derivatives with respect to x.

Eqs. (18) and (19) contain the more complicated functions $P^k_{22}(x)$ and $P^k_{2-2}(x)$. To show that these functions are also polynomial functions we use the recurrence relation [4]

$$k\sqrt{(k+1)^2-n^2}\sqrt{(k+1)^2-m^2}P^{k+1}_{mn}(x) + (k+1)\sqrt{k^2-n^2}\sqrt{k^2-m^2}P^{k-1}_{mn}(x) = (2k+1)\{k(k+1)x-mn\}P^k_{mn}(x), \tag{B.3}$$

starting with

$$P^2_{22}(x)=\tfrac{1}{4}\left(1+2x+x^2\right) \tag{B.4}$$

and

$$P^3_{22}(x)=\tfrac{1}{4}\left(-2-x+4x^2+3x^3\right). \tag{B.5}$$

Eqs. (B.4) and (B.5) follow directly from the definition of generalized spherical functions [4]. Using the recurrence relation (B.3) and the polynomial functions given by Eqs. (B.4) and (B.5) we readily find that $P^k_{22}(x)$ is a polynomial function for every value of $k \geq 2$. Similarly, we find that $P^k_{2-2}(x)$ is a polynomial function for every value of $k \geq 2$. Hence, the right-hand sides of Eqs. (18) and (19) have finite continuous derivatives with respect to x. This concludes our proof that all functions of x occurring in Eqs. (17)–(22) have finite continuous derivatives with respect to x.

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