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Power Series Expansion of the Mie Scattering Phase Function*

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Abstract

We develop power series expansions for both the Mie theory scattering amplitudes and the scattering phase matrix elements in terms of the variable $s = \sin^2\frac{1}{2}\theta$, where θ is the scattering angle. It is easily seen that s is the natural variable for such expansions. These expansions should prove particularly useful whenever the forward diffraction peak, rather than the entire phase function, is of primary interest. Possible applications include the analysis of solar aureole data and the modelling of laser beam propagation in fogs and dust clouds.

1. Mie Scattering

The scattering of an electromagnetic wave by small particles is usually characterized by four scattering amplitudes S_1, S_2, S_3 and S_4, which may be defined by (van de Hulst 1957; Liou 1980)

$$\begin{pmatrix} E_l^{\mathrm{s}} \\ E_{\mathrm{r}}^{\mathrm{s}} \end{pmatrix} = \frac{\exp(-\mathrm{i}\,kr+\mathrm{i}\,kz)}{\mathrm{i}\,kr}\begin{pmatrix} S_2 & S_3 \\ S_4 & S_1 \end{pmatrix}\begin{pmatrix} E_l^{\mathrm{i}} \\ E_{\mathrm{r}}^{\mathrm{i}} \end{pmatrix}, \tag{1}$$

where the subscripts l and r denote the field components parallel and perpendicular respectively to the scattering plane, and the superscripts i and s denote incident and scattered waves respectively. Note carefully that the presence of the imaginary i factor in the denominator effectively exchanges the roles of real and imaginary parts of these amplitudes, by comparison with the usual quantum mechanical definitions.

Clearly, in the case of spherical particles (the subject of Mie theory), symmetry requires that

$$S_3 = S_4 = 0. \tag{2}$$

For a spherical particle of complex index of refraction m and size parameter $x = kr = 2\pi r/\lambda$, Mie theory gives (Stratton 1941; van de Hulst 1957; Deirmendjian 1969; Liou 1980)

$$S_1(\theta) = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)}\{a_n\,\pi_n(\cos\theta) + b_n\,\pi_n(\cos\theta)\}, \tag{3a}$$

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$$S_2(\theta) = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)}\{a_n \tau_n(\cos\theta) + b_n \pi_n(\cos\theta)\}, \tag{3b}$$

where

$$\pi_n(\cos\theta) = \frac{\mathrm{P}_n^1(\cos\theta)}{\sin\theta}, \qquad \tau_n(\cos\theta) = \frac{\mathrm{d}}{\mathrm{d}\theta}\mathrm{P}_n^1(\cos\theta), \tag{4a, b}$$

and a_n and b_n are complex functions of x and m, but not θ.

Of more direct interest is the scattered intensity and polarization, usually expressed via the Stokes parameters:

$$\begin{bmatrix} I^{\mathrm{s}} \\ Q^{\mathrm{s}} \\ U^{\mathrm{s}} \\ V^{\mathrm{s}} \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} & 0 & 0 \\ M_{12} & M_{11} & 0 & 0 \\ 0 & 0 & M_{33} & -M_{34} \\ 0 & 0 & M_{34} & M_{33} \end{bmatrix} \begin{bmatrix} I^{\mathrm{i}} \\ Q^{\mathrm{i}} \\ U^{\mathrm{i}} \\ V^{\mathrm{i}} \end{bmatrix}, \tag{5}$$

where

$$M_{11} = (S_1 S_1^* + S_2 S_2^*)/2k^2r^2, \qquad M_{12} = (S_2 S_2^* - S_1 S_1^*)/2k^2r^2, \tag{6a, b}$$

$$M_{33} = (S_2 S_1^* + S_1 S_2^*)/2k^2r^2, \qquad M_{34} = \mathrm{i}(S_2 S_1^* - S_1 S_2^*)/2k^2r^2. \tag{6c, d}$$

The scattering cross section is given by

$$\begin{aligned} \sigma_{\mathrm{s}} &= \frac{\pi}{k_2}\int_0^{\pi} (S_1 S_1^* + S_2 S_2^*)\sin\theta \, \mathrm{d}\theta \\ &= 2\pi r^2 \int_0^{\pi} M_{11} \sin\theta \, \mathrm{d}\theta, \end{aligned} \tag{7}$$

and the normalized phase function by

$$\mathrm{P}(\theta) = r^2 M_{11}(\theta)/\sigma_{\mathrm{s}}, \tag{8}$$

so that

$$\int_0^{2\pi}\int_0^{\pi} \mathrm{P}(\theta)\sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi = 1. \tag{8'}$$

Finally for completeness we may note that the extinction (total) cross section may be obtained from the optical theorem:

$$\sigma_{\mathrm{e}} = 4\pi k^{-2}\,\mathrm{Re}\, S(0), \tag{9}$$

where

$$S(0) = S_1(0) = S_2(0) = \tfrac{1}{2}\sum_{n=1}^{\infty} (2n+1)(a_n + b_n). \tag{10}$$

2. Power Series Expansion

We start by defining the variables

$$\mu = \cos\theta, \tag{11}$$

$$s = \sin^2\tfrac{1}{2}\theta = \tfrac{1}{2}(1-\mu). \tag{12}$$

The first step is to expand π_n and τ_n in terms of s. Noting that

$$\mathrm{P}_n(\theta) = F(n+1, -n; 1; s), \tag{13}$$

where F is the standard hypergeometric function (Spiegel 1968), and that

$$\pi_n(\theta) = (\mathrm{d}/\mathrm{d}\mu)\mathrm{P}_n(\theta) = \tfrac{1}{2}n(n+1)\,F(n+2, -n+1; 2; s), \tag{14}$$

we readily obtain

$$\pi_n(s) = \sum_{i=0}^{n-1} (-1)^i C_n^i s^i, \tag{15}$$

where

$$C_n^i = \frac{(n+i+1)!}{2(n-i-1)!(i+1)!i!}. \tag{16}$$

Similarly, noting that

$$\tau_n(s) = n(1-2s)\pi_n(s) - (n+1)\pi_{n-1}(s), \tag{17}$$

we readily obtain

$$\tau_n(s) = \sum_{i=0}^{n} (-1)^i D_n^i s^i, \tag{18}$$

where

$$\begin{aligned} D_n^i &= \frac{\{n(n+1)(2i+1) - i(i+1)\}(n+i)!}{2(n-i)!(i+1)!i!} \\ &= \frac{(n-i)(n+i+1) + 2in(n+1)}{(n-i)(n+i+1)} C_n^i. \end{aligned} \tag{19}$$

The power series expansions for S_1 and S_2 may now be obtained by substituting equations (15) and (18) into (3):

$$S_1 = \sum_{j=0}^{\infty} (-1)^j \alpha_j s^j, \qquad S_2 = \sum_{j=0}^{\infty} (-1)^j \beta_j s^j, \tag{20a, b}$$

where

$$\alpha_j = \sum_{n=j+1}^{\infty} \frac{2n+1}{n(n+1)} (a_n C_n^j + b_n D_n^j) + \frac{(2j+1)!}{(j+1)!(j-1)!} b_j, \tag{21a}$$

$$\beta_j = \sum_{n=j+1}^{\infty} \frac{2n+1}{n(n+1)} (a_n D_n^j + b_n C_n^j) + \frac{(2j+1)!}{(j+1)!(j-1)!} a_j. \tag{21b}$$

If the main purpose of the calculation is to evaluate, say, $\mathrm{P}(\theta)$ for small θ, then the evaluation of the α_j and β_j coefficients should suffice, and P can be calculated via equations (6a) and (8). There are occasions, however, in which the intensity (or the elements of the Stokes vector) is required. This may determined from

$$i_1 \equiv S_1 S_1^* = \sum_{i=0}^{\infty} (-1)^i A_i^1 s^i, \qquad i_2 \equiv S_2 S_2^* = \sum_{i=0}^{\infty} (-1)^i A_i^2 s^i, \tag{22a, b}$$

$$i_3 \equiv S_2 S_1^* = \sum_{i=0}^{\infty} (-1)^i A_i^3 s^i, \qquad i_4 \equiv S_1 S_2^* = \sum_{i=0}^{\infty} (-1)^i A_i^4 s^i, \tag{22c, d}$$

where

$$A_i^1 = \sum_{j=0}^{i} \alpha_j \alpha_{i-j}^*, \qquad A_i^2 = \sum_{j=0}^{i} \beta_j \beta_{i-j}^*, \tag{23a, b}$$

$$A_i^3 = \sum_{j=0}^{i} \beta_j \alpha_{i-j}^*, \qquad A_i^4 = \sum_{j=0}^{i} \alpha_j \beta_{i-j}^*. \tag{23c, d}$$

3. Connection with Legendre Expansion

The most usual expansion for a function of $\cos\theta$ between 0 and π is in terms of Legendre polynomials. This procedure is often used when scattering functions are required for radiative transfer calculations (Chu and Churchill 1955; Chandrasekhar 1960; Dave 1970; Herman and Browning 1975). Due to the relation between s and μ (for example equation 12), the expansion of any function of θ in terms of Legendre polynomials can be converted into a power series in s, and vice versa. Thus, for arbitrary $f(\theta)$, we define

$$f(\theta) = \sum_{n=0}^{\infty} \omega_n \mathrm{P}_n(\mu), \tag{24}$$

where

$$\omega_n = (n+\tfrac{1}{2}) \int_{-1}^{1} f(\mu) \mathrm{P}_n(\mu)\, \mathrm{d}\mu, \tag{24$'$}$$

and $\mathrm{P}_n(\mu)$ is the Legendre polynomial of order n.

This same arbitrary function may also be expanded in terms of s:

$$f(\theta) = \sum_{i=0}^{\infty} (-1)^i A_i s^i. \tag{25}$$

Inserting equation (25) in (24′), we find

$$\begin{aligned}\omega_n &= (n+\tfrac{1}{2}) \sum_{i=0}^{\infty} (-1)^i A_i \int_0^1 s^i F(-n; n+1; 1; s)\, 2\, \mathrm{d}s \\ &= (-1)^n (2n+1) \sum_{i=m}^{\infty} (-1)^i A_i \frac{i!}{(i-n)!} \frac{i!}{(n+i+1)!},\end{aligned} \tag{26}$$

where the integral has been performed using equation (7.512.2) of Gradshteyn and Ryzhik (1965).

Conversion in the other direction is easily accomplished by expanding P_n in equation (24) as a hypergeometric function in s, giving

$$f(\theta) = \sum_{n=0}^{\infty} \omega_n \sum_{i=0}^{n} (-1)^i \frac{(n+i)!}{(n-i)!\,i!\,i!} s^i, \tag{27a}$$

so that

$$A_i = \frac{1}{(i!)^2} \sum_{n=i}^{\infty} \frac{(n+i)!}{(n-i)!} \omega_n. \tag{27b}$$

4. Applications

The power series expansion cannot be recommended for the complete reconstruction of the various scattering functions for all sized spheres, as the expansion coefficients soon become so large that the least significant figure carried by the computer is larger in magnitude than the actual result being calculated. (However, it should be pointed out that the A coefficients are essentially the squares of the α and β coefficients, so it is clearly more accurate to use the latter to first compute S_1 and S_2, and use them to compute the various scattering functions.) For such purposes, the Legendre expansion is clearly superior.

The series expansion should prove most useful whenever details of the forward peak are required, as in this case only comparatively few coefficients will be required. (Note, however, that the usual complement of a_n and b_n coefficients will still need to be computed, i.e. about $x+10$, where x is the size parameter. In most foreseeable applications, these would have to be computed anyway in order to calculate the extinction and/or scattering efficiency factors.) Among the uses for which this expansion should prove appropriate, we shall examine three.

In the small-angle scattering approximation to the propagation of a narrow laser beam in a medium such as a fog or dust cloud (Box and Deepak 1981), it is common to employ simple analytic models of the forward diffraction peak, rather than exact Mie theory. Two such model phase functions are the gaussian

$$P(\psi) = \alpha^2 \exp(-\alpha^2\psi^2)/\pi, \tag{28}$$

and the binomial

$$P(\psi) = \mu\alpha^2(1+\alpha^2\psi^2)^{-\mu-1}/\pi. \tag{29}$$

In both these expressions, ψ may be variously interpreted as θ, $\sin\theta$, $2\sin\frac{1}{2}\theta$ etc., and α and μ are adjustable parameters. By expanding either equation (28) or (29) in a Taylor series, and comparing the leading terms with the first few terms of the power series expansion of the appropriate Mie theory phase function, it should be possible to select optimum values for α and μ, and also to gain a feel for the appropriateness of the approximate phase function employed.

One of the methods of remotely sensing the optical properties of atmospheric aerosols is to make narrow band measurements of the scattered sunlight in the region of the solar aureole (Deirmendjian 1969; Green *et al.* 1971). This involves scattering angles of up to roughly 20°. This data is then analysed via one of the standard methods for inverting the resulting Fredholm integral equation (Twomey 1977; Deepak *et al.* 1982). Since all these methods have a number of problems associated with them, particularly regarding their stability, it may prove advantageous to convert the measured data into a set of power series expansion coefficients, and perform an inversion on them.

Measurements of optical extinction due to scattering particles are subject to a number of errors (Shaw 1976), including the fact that some of the scattered light is inevitably received by the detector (Deepak and Box 1978; Box and Deepak 1979). For optically thin media, a single-scattering correction procedure has been developed (Deepak and Box 1978) which involves integrating the phase function of the scattering particles over the solid angle subtended by the detector. In general, this should be small, so that it should be possible to perform such integrals analytically if the power series expansion coefficients are available.

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