Coefficients of the Legendre and Fourier Series for the Scattering Functions of Spherical Particles

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Results of computations are presented to show the variations of coefficients of four different Legendre series, one for each of the four scattering functions needed in describing directional dependence of the radiation scattered by a sphere. Values of the size parameter (x) covered for this purpose vary from 0.01 to 100.0. An adequate representation of the entire scattering function vs scattering angle curve is obtained after making use of about $2x + 10$ terms of the series. It is shown that a section of a scattering function vs scattering angle curve can be adequately represented by a fourier series with less than $2x + 10$ terms. The exact number of terms required for this purpose depends upon values of the size parameter and refractive index, as well as upon the values of the scattering angles defining the section under study. Necessary expressions for coefficients of such fourier series are derived with the help of the addition theorem of spherical harmonics.

I. Introduction

Currently, values of four scattering functions describing the characteristics of electromagnetic radiation scattered by a sphere are usually computed from the expressions for the same as derived by Mie.[1–5] However, these scattering functions show strong variations with scattering angle (Θ) when the radius (r) of the sphere is large compared to the wavelength (λ) under investigation. In fact, for a sphere with size parameter $x(= 2\pi r/\lambda)$, a scattering function vs Θ curve shows about x number of maxima and minima as Θ is varied from 0° to 180°. For several applications, it is desirable to evaluate the field of the scattered radiation at about $10x$ positions in the scattering angle.[6,7] Furthermore, when one is interested in scattering characteristics of spherical polydispersions, it is necessary to compute these scattering functions for several hundred values of x for good reliability.[8,9] Even with modern digital computers, experience has shown that such computational tasks can be very tedious and time consuming.

Following Mie,[1] one first evaluates two complex quantities [$S_1(x,m,\Theta)$ and $S_2(x,m,\Theta)$], where m is the refractive index of the material of the sphere with respect to its surroundings. Values of the four scattering functions [$M_2(x,m,\Theta)$, $M_1(x,m,\Theta)$, $S_{21}(x,m,\Theta)$, and $D_{21}(x,m,\Theta)$] are then obtained by combining these quantities.[2] The expressions for S_1 and S_2 contain functions $\pi_n(\cos\Theta)$ and $\tau_n(\cos\Theta)$, which are expressible in terms of the first and second derivatives of the ordinary Legendre functions, and hence produce the strong directional dependence. Hartel[10] first suggested that the expressions for these scattering functions could be simplified by the repeated use of recurrent relationships between the derivatives and products of Legendre functions.[11] This would yield for each of these functions a series whose terms are the ordinary Legendre polynomials weighted by coefficients depending upon m and x only. Chandrasekhar[12] showed that a solution of the equation of transfer in the nth approximation for a general phase function can be obtained by expressing the phase function in the form of such Legendre series. Legendre series expressions for all four scattering functions were first derived by Sekera.[13] Later, Chu and Churchill[14] independently obtained similar expressions for the scalar phase function and published values of the coefficients of its Legendre series for some selected values of x.[15] It was observed that such Legendre representation of the scattering functions of a sphere requires about $2x + 10$ number of terms, while the quantities S_1 and S_2 are fully represented by about $x + 10$ number of terms only. Fraser[16] used a modified Legendre series method for a limited study aimed at evaluating the characteristics of the radiation scattered by spherical polydispersions. Further progress in this direction has been hampered because of the need to include a very large number of terms before meaningful results can be arrived at.

The purpose of this paper is twofold: (1) to discuss some of the computational results for the coefficients of Legendre series representing scattering functions for spheres with size parameter up to 100; and (2) to show that for cases where only a section of the entire scatter-

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Received 27 October 1969.

ing function vs Θ curve is required, equally reliable values can be obtained by including fewer terms. Such cases are encountered very frequently during multiple-scattering calculations.[17]

II. Coefficients of the Legendre Series

Necessary Expressions

As mentioned earlier, Sekera[13] has expressed the four scattering functions in the form of Legendre series. In what follows, his final results are reproduced after some minor changes for conformity with current notation, and for adaptability to automatic computations. The first scattering function appearing in Van de Hulst's transformation matrix (Ref. 2, Sec. 5.14) is $M_2(x,m,\Theta)$, which is given by

$$M_2(x,m,\Theta) = \sum_{k=1}^{\infty} L_k^{(1)}(x,m)P_{k-1}(\cos\Theta). \tag{1}$$

Similar expressions for the remaining three elements, viz., $M_1(x,m,\Theta)$, $S_{21}(x,m,\Theta)$, and $D_{21}(x,m,\Theta)$, can be obtained after substituting $j = 2$, 3, and 4, respectively, in $L_k^{(j)}(x,m)$.

The Legendre coefficients $L_k^{(j)}(x,m)$ are given by

$$L_k^{(1)}(x,m) = (k - 0.5) \sum_{m=k'}^{\infty} a_m^{(k-1)} \sum_{i=0}^{k'} b_i^{(k-1)}\Delta_{i,k} \times \mathrm{Re}[D_p(x,m)D_q^*(x,m)], \tag{2}$$

$$L_k^{(2)}(x,m) = (k - 0.5) \sum_{m=k'}^{\infty} a_m^{(k-1)} \sum_{i=0}^{k'} b_i^{(k-1)}\Delta_{i,k} \times \mathrm{Re}[C_p(x,m)C_q^*(x,m)], \tag{3}$$

$$L_k^{(3)}(x,m) = (0.5k - 0.25) \sum_{m=k'}^{\infty} a_m^{(k-1)} \sum_{i=0}^{k'} b_i^{(k-1)}\Delta_{i,k} \times \mathrm{Re}[C_p(x,m)D_q^*(x,m) + C_p^*(x,m)D_q(x,m)], \tag{4}$$

and

$$L_k^{(4)}(x,m) = (0.5k - 0.25) \sum_{m=k'}^{\infty} a_m^{(k-1)} \sum_{i=0}^{k'} b_i^{(k-1)}\Delta_{i,k} \times \mathrm{Im}[C_p(x,m)D_q^*(x,m) - C_p^*(x,m)D_q(x,m)]. \tag{5}$$

The superscript asterisk (*) represents the complex conjugate of the corresponding function. The symbols Re[ ] and Im[ ] imply the real and imaginary part, respectively, of the complex quantity within the enclosed brackets.

$$k' = \begin{cases} (k-1)/2 & \text{for odd } k, \\ (k-2)/2 & \text{for even } k. \end{cases} \tag{6}$$

$$\Delta_{i,k} = \begin{cases} 1 & \text{for } i = 0, \text{ odd } k, \\ 2 & \text{for } i > 0, \text{ odd } k, \\ 2 & \text{for } i \geq 0, \text{ even } k. \end{cases} \tag{7}$$

The subscripts p and q are given by $p = m - i + 1$ and $q = m + i + 1 + \delta$, where $\delta = 0$ for odd values of k, and $\delta = 1$ for even values of k.

For odd values of $k > 1$, the quantities $a_m^{(k-1)}$ and $b_i^{(k-1)}$ are first obtained after using the following recurrence relationships for a value of $m = k'$, and of $i = 0$, respectively:

$$a_{(k-1)/2}^{(k-1)} = \frac{4(k-1)(k-2)}{(2k-1)(2k-3)} a_{(k-3)/2}^{(k-3)}, \tag{8}$$

and

$$b_0^{(k-1)} = \left(\frac{k-2}{k-1}\right)^2 b_0^{(k-3)}. \tag{9}$$

For $k = 1$, $a_0^{(0)} = 2$ and $b_0^{(0)} = 1$. Then for $m > k'$, $a_m^{(k-1)}$ is obtained from the following recurrence relationship:

$$a_m^{(k-1)} = \frac{(2m-k)(2m+k-1)}{(2m+k)(2m-k+1)} a_{m-1}^{(k-1)}, \tag{10}$$

and for $i > 0$, $b_i^{(k-1)}$ is given by

$$b_i^{(k-1)} = \frac{(k-2i+1)(k+2i-2)}{(k-2i)(k+2i-1)} b_{i-1}^{(k-1)}. \tag{11}$$

For even values of $k > 2$, the quantities $a_m^{(k-1)}$ and $b_i^{(k-1)}$ are first computed using the following recurrence relationships for a value of $m = k'$ and $i = 0$, respectively:

$$a_{(k-2)/2}^{(k-1)} = \frac{4(k-1)(k-2)}{(2k-1)(2k-3)} a_{(k-4)/2}^{(k-3)}, \tag{12}$$

and

$$b_0^{(k-1)} = \frac{(k-1)(k-3)}{k(k-2)} b_0^{(k-3)}. \tag{13}$$

For $k = 2$, $a_0^{(1)} = \frac{4}{3}$ and $b_0^{(1)} = \frac{1}{2}$. Then for $m > k'$, $a_m^{(k-1)}$ is obtained after making use of the following recurrence relationship:

$$a_m^{(k-1)} = \frac{(2m-k+1)(2m+k)}{(2m+k+1)(2m-k+2)} a_{m-1}^{(k-1)}, \tag{14}$$

and for $i > 0$, $b_i^{(k-1)}$ is obtained from

$$b_i^{(k-1)} = \frac{(2i+k-1)(2i-k)}{(2i-k+1)(2i+k)} b_{i-1}^{(k-1)}. \tag{15}$$

Finally, the complex functions $C_k(x,m)$ and $D_k(x,m)$ [where k here stands for p or q in Eqs. (2)–(5)] are computed from the values of the complex Mie amplitudes $a_n(x,m)$ and $b_n(x,m)$ (Refs. 4 and 7) by means of the following formulas:

$$C_k(x,m) = (1/k)(2k-1)(k-1)b_{k-1}(x,m) + (2k-1)\sum_{i=1}^{\infty} \{[p^{-1} + (p+1)^{-1}]a_p(x,m) - [(p+1)^{-1} + (p+2)^{-1}]b_{p+1}(x,m)\}, \tag{16}$$

and

$$D_k(x,m) = (1/k)(2k-1)(k-1)a_{k-1}(x,m) + (2k-1)\sum_{i=1}^{\infty} \{[p^{-1} + (p+1)^{-1}]b_p(x,m) - [(p+1)^{-1} + (p+2)^{-1}]a_{p+1}(x,m)\}, \tag{17}$$

where for Eqs. (16) and (17), $p = k + 2i - 2$. Evidently, $a_0(x,m) = b_0(x,m) = 0$.

Variations of the Legendre Coefficients with Size Parameter

The values of the Legendre coefficients $L_k^{(j)}(x,m)$ were computed for several values of x and $m = 1.342$ using an IBM System/360 Model 91 computer and double precision arithmetic. Starting with a value of x and m, the CPU time required for computations of all coefficients for $x = 10$ and 100 was about 0.1 sec and 16 sec, respectively. Values of the scattering functions M_2, M_1, S_{21}, and D_{21} as obtained from the use of Eq. (1), and from the values of $S_1(x,m,\Theta)$ and $S_2(x,m,\Theta)$, were found to agree up to five significant figures for several test cases for which some manual checks were performed. In what follows, we shall refer to the normalized coefficients given by

$$\Lambda_k^{(j)}(x,m) = [4/Q_s(x,m)x^2]L_k^{(j)}(x,m), \qquad (18)$$

where $Q_s(x,m)$ is the so-called efficiency factor for scattering.[2]

The values of the first five normalized coefficients for $j = 1$ and for $x = 0.01$, 0.1, and 1.0 are given in Table I. For $x = 0.01$ and 0.1, values of these coefficients corresponding to $k = 1$ and 3 are exactly the same as those predicted by Rayleigh's law of scattering. As x increases from 0.1 to 1.0, values of these two coefficients show a small but significant increase. On the other hand, values of the remaining three coefficients ($k = 2$, 4, and 5) which vanish in the Rayleigh limit, show a very rapid increase with x. Similar trends were also seen in the values of these coefficients for $j = 2$ and 3, except that now the only nonvanishing coefficients in the Rayleigh limit are $\Lambda_1^{(2)}(x,m)$ and $\Lambda_2^{(3)}(x,m)$, with each having a value of 1.5. For $j = 4$, the highest absolute values of the normalized Legendre coefficients are 4.3×10^{-13}, 4.3×10^{-8}, and 3.2×10^{-3} for $x = 0.01$, 0.1, and 1.0, respectively. These variations imply that significant deviations in the polarization characteristics from the Rayleigh case become evident when $x \sim 0.1$. However, even a sphere with size parameter of the order of unity would exhibit extremely weak elliptical polarization, if any.

Values of the first 35 normalized Legendre coefficients for $j = 1$ through 4 are presented in Table II for a sphere with size parameter $x = 10$ and $m = 1.342$. The main purpose of this table is to provide the reader with at least one complete set of values which he can use for independent checking of his computer program. Except for round-off errors, all the values are expected to be correct up to five significant places. It should be added that scattering functions for various values of Θ should be computed from values which carry all significant figures available inside the computer. From Table II, it can be seen that the series for each of the scattering functions can be terminated after about 30 terms, i.e., the upper limit for summation in Eq. (1) is not infinity but N, where $N \doteqdot 2x + 10$.

In Fig. 1, we have presented variations of the absolute values of the Legendre coefficients of the series for the scattering function $M_2(x,m,\Theta)$ as a function of k, for three different values of x, viz., 20, 50, and 100.

Table I. Values of the First Five Normalized Coefficients of Legendre Series for the Scattering Function M_2 (x,m,Θ); $m = 1.342$

k	$\Lambda_k^{(1)}$ (0.01, m)	$\Lambda_k^{(1)}$ (0.1, m)	$\Lambda_k^{(1)}$ (1.0, m)
1	5.0000 (−01)[a]	5.0000 (−1)	5.1269 (−1)
2	4.3767 (−05)	4.3749 (−3)	4.4557 (−1)
3	1.0000	1.0000	1.0371
4	2.3029 (−05)	2.3012 (−3)	2.2534 (−1)
5	1.2627 (−10)	1.2608 (−6)	2.1224 (−2)

[a] The number in the parenthesis represents the power of 10 by which the preceding number is to be multiplied, e.g., 5.0 (−01) = 5.0×10^{-1}. If there is no parentheses after the number, the power of 10 is equal to zero.

Only a few of the coefficients assume negative values, e.g., for $x = 50$, the coefficients $\Lambda_k^{(1)}(x,m)$ are negative for $k = 104$, 105, 106, and 110 only. For these three values of x, $\Lambda_1^{(1)}(x,m)$ is very close to unity, and again the series can be terminated when $N \doteqdot 2x + 10$. The curves of $|\Lambda_k^{(1)}(x,m)|$ vs subscript k are fairly smooth except for $n > 2x$, where the slope is very steep. For clarity of the diagrams, a few alternate values are omitted in the region where there is very little difference between two successive values. The variations of $|\Lambda_k^{(2)}(x,m)|$ and $|\Lambda_k^{(3)}(x,m)|$ as functions of k were also found to show similar trends.

The variations in $|\Lambda_k^{(4)}(x,m)|$ as a function of k are very erratic, and as such their graphical presentation poses some problem. Some of the possible confusion is avoided by plotting absolute values of these coefficients vs k in two different sets; the upper curves in Figs. 2 and 3 represent variations in $|\Lambda_k^{(4)}(x,m)|$ vs k for even values of k, while the lower curves are for odd values of k. In Fig. 2, results of computation are presented for $x =$

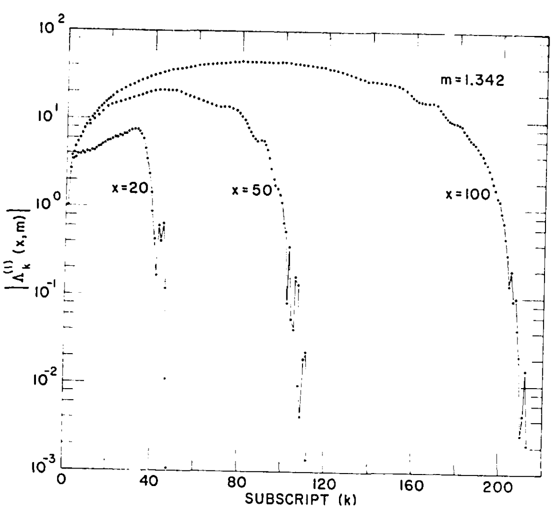

Fig. 1. Variations of the absolute values of normalized coefficients of the Legendre series for the scattering function $M_2(x,m,\Theta)$ as a function of subscript k of the coefficient.

Table II. **Values of the Normalized Coefficients of the Legendre Series for Scattering Functions of a Sphere;** $x = 10.0$, $m = 1.342$

k	$\Lambda_k^{(1)}(x,m)$	$\Lambda_k^{(2)}(x,m)$	$\Lambda_k^{(3)}(x,m)$	$\Lambda_k^{(4)}(x,m)$
1	1.0645	9.3551 (−1)	9.0259 (−1)	−1.0109 (−1)
2	2.1853	1.9286	2.0843	4.4926 (−2)
3	2.7321	2.7926	2.6642	−9.0608 (−2)
4	2.5467	2.4535	2.4983	2.9276 (−2)
5	2.2937	2.3913	2.3778	1.3266 (−1)
6	2.1454	2.2061	2.0681	4.6171 (−2)
7	2.0520	2.0194	2.1048	2.9736 (−1)
8	2.1552	2.0738	2.0710	1.6766 (−1)
9	2.3562	2.1007	2.2183	2.9973 (−1)
10	2.5434	2.3038	2.4925	2.8820 (−1)
11	2.9173	2.4815	2.6113	2.7102 (−1)
12	3.1462	2.7860	3.1150	3.5453 (−1)
13	3.4761	3.1150	3.2254	2.8577 (−1)
14	3.8971	3.5953	3.8084	3.1660 (−1)
15	3.9568	3.9086	4.0649	3.7816 (−1)
16	4.4225	4.7123	4.4791	6.1476 (−2)
17	4.1765	4.5631	4.5421	2.5024 (−1)
18	3.8141	5.0155	4.5404	−3.7044 (−1)
19	3.0307	4.0056	3.5374	−7.8945 (−1)
20	2.2171	2.5007	2.4057	−8.7630 (−1)
21	1.4823	1.3086	1.1182	−9.0760 (−1)
22	3.4957 (−1)	−1.2688 (−1)	1.0509 (−1)	−5.4768 (−2)
23	1.4843 (−1)	7.2065 (−2)	9.5872 (−2)	−2.4685 (−2)
24	4.5331 (−2)	2.0767 (−2)	2.9265 (−2)	−7.0836 (−3)
25	1.1477 (−2)	4.5711 (−3)	7.0955 (−3)	−1.4658 (−3)
26	2.5031 (−3)	8.4961 (−4)	1.4629 (−3)	−2.4298 (−4)
27	4.8173 (−4)	1.3824 (−4)	2.6389 (−4)	−3.3629 (−5)
28	8.3323 (−5)	2.0143 (−5)	4.2478 (−5)	−3.9757 (−6)
29	1.3134 (−5)	2.6727 (−6)	6.1969 (−6)	−4.0650 (−7)
30	1.9069 (−6)	3.2724 (−7)	8.2970 (−7)	−3.5526 (−8)
31	2.5508 (−7)	3.7323 (−8)	1.0310 (−7)	−1.3215 (−9)
32	3.0920 (−8)	3.7615 (−9)	1.1234 (−8)	−1.1240 (−11)
33	3.4798 (−9)	3.5833 (−10)	1.1529 (−9)	−5.5487 (−14)
34	3.5894 (−10)	3.1542 (−11)	1.0902 (−10)	1.8598 (−15)
35	3.3466 (−11)	2.5254 (−12)	9.3547 (−12)	6.5504 (−17)

20 and 50, while those in Fig. 3 are for $x = 100$. Unlike the values of the coefficients for the other three scattering functions, several values of $\Lambda_k^{(4)}(x,m)$ carry a negative sign. It is interesting to note that the Legendre coefficients for this fourth scattering function attain their highest values when $k \sim 2x$; it is not so for the other three cases (e.g., Fig. 1).

To determine the scattering properties of a unit volume of spherical polydispersions, it is necessary to integrate the unnormalized Legendre coefficients over the size-distribution. For this purpose, it is desirable to study, in some detail, variations of $L_k^{(j)}(x,m)$ as a function of x. In Fig. 4, values of $L_1^{(j)}(x,m)/x^2$ and $Q_s(x,m)$ are plotted as a function of size parameter in the range $x = 10.00\ (0.05)\ 15.00$. Variations in $Q_s(x,m)$ as a function of x (lowermost curve) are identical to those presented on a much more extensive scale by Penndorf.[18] A more detailed discussion of these variations can be found in Ref. 2 (Secs. 11.22, 13.42, and 17.26). It will suffice to state here that this curve shows a periodicity of about 0.8 in x superimposed over another variation having much greater periodicity and

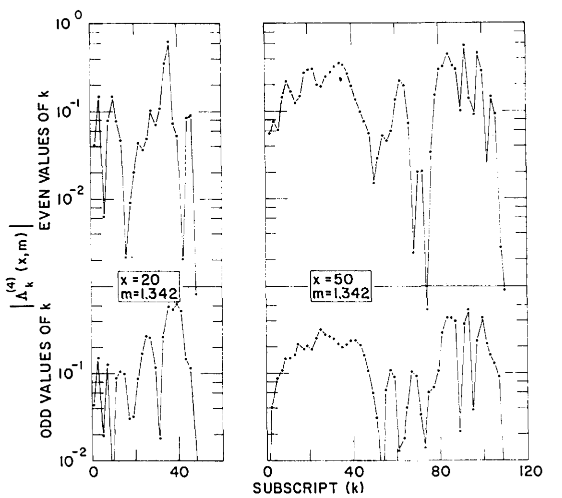

Fig. 2. Variations of the absolute values of normalized coefficients of the Legendre series for the scattering function $D_{21}(x, m, \Theta)$ as a function of subscript k of the coefficient. For clarity, coefficients with odd and even values of k are plotted separately.

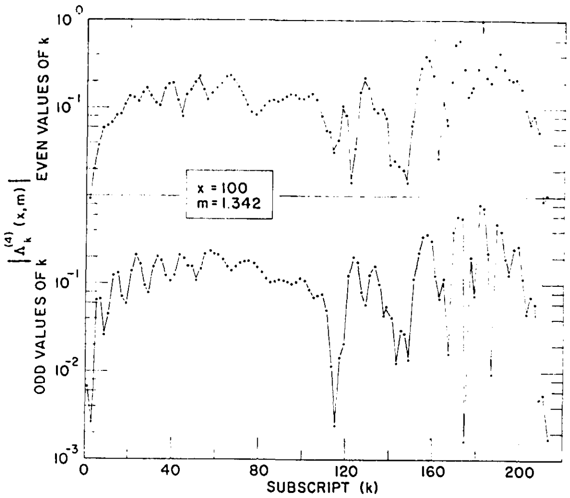

Fig. 3. Same as Fig. 2.

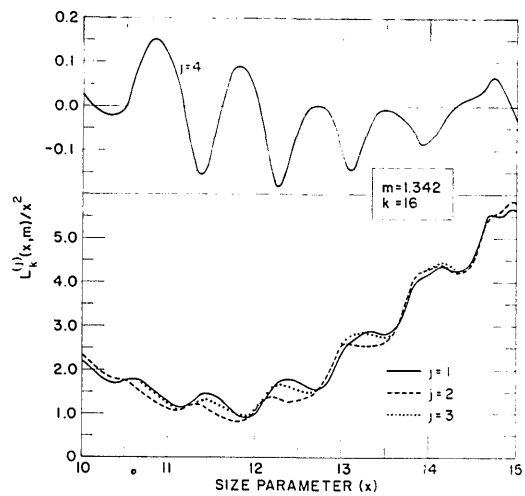

Fig. 5. Same as Fig. 4, but for $k = 16$.

amplitude. The curves of the coefficients for the first three scattering functions ($j = 1$, 2, and 3) show variations similar to those for $Q_s(x,m)$ except that now their values increase much more rapidly with size parameter for $x > 12.5$. The presence of some additional minor disturbance is also noticeable on $L_1^{(3)}(x,m)/x^2$ vs x curve (dotted curve). The function $L_1^{(4)}(x,m)/x^2$ is negative for all values of x of interest to us in this discussion (topmost curve). The maxima and minima are much sharper compared with those for other cases discussed above. Besides, one now observes several additional maxima and minima for $13.0 \leq x \leq 15.0$. Similar results for $L^{(j)}{}_{16}(x,m)/x^2$ corresponding to $j = 1$ through 4 are presented in Fig. 5. For the fourth scattering function $D_{21}(x,m,\Theta)$, these coefficients exhibit a positive sign at several places.

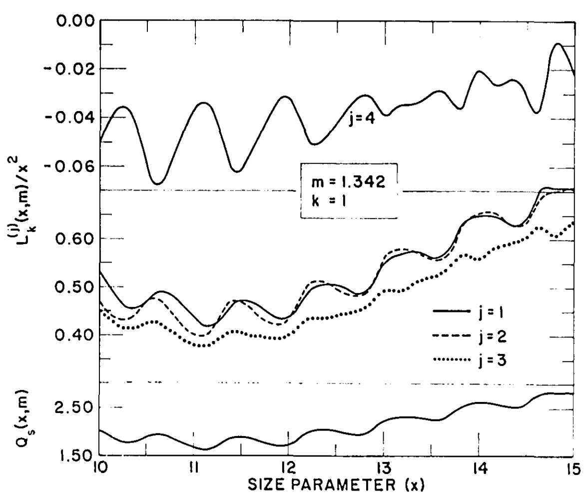

Fig. 4. Variations of the coefficients of the Legendre series for four different scattering functions ($j = 1$ through 4) as a function of size parameter of the sphere, $k = 1$.

Values of $L^{(j)}{}_{26}(x,m)$ show about a four orders-of-magnitude increase as x is increased from 10 to 15. Furthermore, for each of the four cases ($j = 1$ through 4), we find that some values of these functions are negative. Therefore, in Figs. 6 and 7 we have plotted as a function of x, absolute values of $L^{(j)}{}_{26}(x,m)/x^2$ on a semilogarithmic scale. The Legendre coefficients of the series for $M_2(x,m,\Theta)$ (solid curve in Fig. 6) are positive and increase by about two orders of magnitude as x increases from 10 to 11.5. A further small increase in x results in a very rapid decrease. The values of $L^{(1)}{}_{26}(x,m)$ at $x = 11.90$, 11.95, and 12.00 are negative. Another small increase in x by 0.05 results in a change of sign, and the function increases by three orders of magnitude as x is increased from 12.05 to 12.50. Further increase in x results in relatively very small changes. The curve of $|L^{(2)}{}_{26}(x,m)|/x^2$ vs x (broken curve in Fig. 6) also exhibits somewhat similar variations except that the range of its negative values now extends from $x = 11.50$ to $x = 12.05$. It is interesting to note that the sum of $L^{(1)}{}_{26}(x,m)$ and $L^{(2)}{}_{26}(x,m)$, which would represent the value of the 26th coefficient of the series for the normalized phase function, attains negative values for values of x between 11.65 and 12.05. Lone appearances of a few negative values in the tables of Clark, Chu, and Churchill[15] are thus understandable. The variations in $|L^{(3)}{}_{26}(x,m)|/x^2$ as a function of x (solid curve, Fig. 7) are also similar to those for the other two functions ($j = 1$ and 2) described above. This function is, in general, positive except for $11.65 \leq x \leq 11.95$. As was the case for $k = 1$ and 16, the variations in $L^{(4)}{}_{26}(x,m)$ as a function of x show very sharp maxima and minima. As before, this function is, in general, negative except for $11.65 \leq x \leq 12.20$, $x = 12.95$, and $14.05 \leq x \leq 14.55$.

From the discussion of the results for several representative cases given above, it is clear that reliable values of the Legendre coefficients of the series representing scattering functions of spherical polydispersions can be obtained only after integrating with a fine incre-

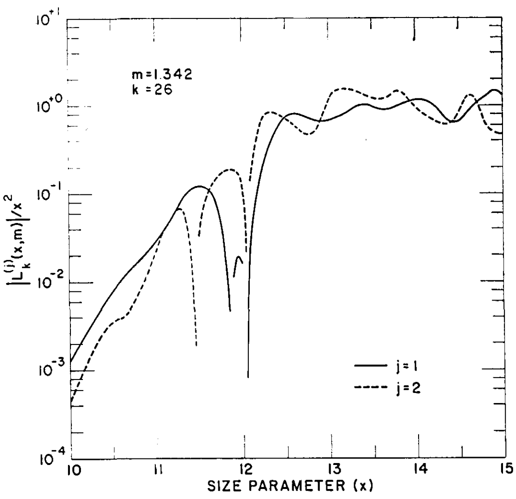

Fig. 6. Same as Fig. 4, but for $j = 1, 2$, and $k = 26$.

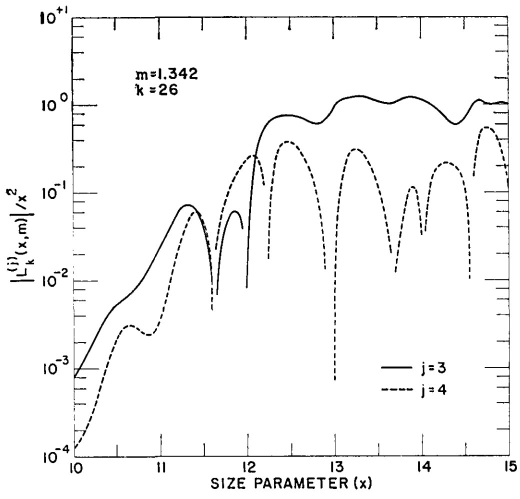

Fig. 7. Same as Fig. 4, but for $j = 3, 4$, and $k = 26$.

ment in x over the entire range. If the integration interval is narrow, it appears that one would require an integration increment of about 0.01 or even less for obtaining reliable values of the fourth scattering function $D_{21}(x,m,\Theta)$. However, for atmospheric problems where rather wide size distribution functions are encountered,[5] an increment of about 0.2 in x should be sufficient for most purposes.[9]

III. Coefficients of Fourier Series

Necessary Expressions

For multiple-scattering calculations, it is convenient to transfer the reference system from the plane of scattering to two vertical planes containing the direction of incidence, or that of scattering. Let θ and θ' be, respectively, the angles which the directions of incidence and scattering make with local zenith, and φ and φ' be their azimuths referred to an arbitrary vertical plane. Denoting $\mu = \cos\theta$ and $\mu' = \cos\theta'$, we have for the scattering angle Θ

$$\cos\Theta = \mu\mu' + (1 - \mu^2)^{\frac{1}{2}}(1 - \mu'^2)^{\frac{1}{2}} \cos(\varphi' - \varphi). \quad (19)$$

Expanding the Legendre polynomials [Eq. (1)] for the argument $\cos\Theta$ by the addition theorem of spherical harmonics (Ref. 12, Sec. 48), we have

$$\frac{4}{x^2 Q_s(x,m)} M_2(x,m,\Theta) = \sum_{k=1}^{N} \Lambda_k^{(1)}(x,m) \sum_{n=1}^{k} (2 - \delta_{1n}) \times \frac{(k-n)!}{(k+n-2)!} P_{k-1}^{n-1}(\mu) P_{k-1}^{n-1}(\mu') \cos(n-1)(\varphi' - \varphi), \quad (20)$$

where δ_{1n} is the Kronecker delta function given by $\delta_{1n} = 1$ when $n = 1$ and otherwise zero, and the $P_k^n(\mu)$ are the associated Legendre functions of degree k and order n. The summation limit is lowered from infinity to N following the results presented in Sec. II above. Inverting the order of summation on the right-hand side of Eq. (20), we have

$$\frac{1}{x^2 Q_s(x,m)} M_2(x,m,\Theta) = \sum_{n=1}^{N} F_n^{(1)}(x,m,\mu',\mu) \cos(n-1)(\varphi' - \varphi), \quad (21)$$

where

$$F_n^{(1)}(x,m,\mu',\mu) = (2 - \delta_{1n}) \sum_{k=n}^{N} \Lambda_k^{(1)}(x,m) Y_{k-1}^{n-1}(\mu) Y_{k-1}^{n-1}(\mu'). \quad (22)$$

Equations identical to (20), (21), and (22) can be written down for the other three scattering functions by making appropriate changes in the superscript of $\Lambda_k^{(j)}$ and $F_n^{(j)}$. The renormalized associated Legendre functions appearing in Eq. (22) are given by

$$Y_{k-1}^{n-1}(\mu) = [(k-n)!/(k+n-2)!]^{\frac{1}{2}} P_{k-1}^{n-1}(\mu). \quad (23)$$

This renormalization is advisable because for large values of k and n, the numerical factor $(k - n)!/(k + n - 2)!$ approaches zero very rapidly, while the corresponding associated Legendre functions attain very large values. Computations of these renormalized functions [Eq. (23)] pose some minor problems which are discussed elsewhere.[19]

For very small particles (Rayleigh scattering), the following expressions for the six nonvanishing coefficients of the fourier series can be obtained after substitution of the expression for $\cos\Theta$ [Eq. (19)] in the expression for the phase matrix for Rayleigh scattering (Ref. 12, p. 37):

$$F_1^{(1)}(x,m,\mu',\mu) = \tfrac{3}{4}(1 - \mu^2 - \mu'^2 + 3\mu^2\mu'^2), \quad (24)$$

$$F_2^{(1)}(x,m,\mu',\mu) = 3\mu\mu'(1 - \mu^2)^{\frac{1}{2}}(1 - \mu'^2)^{\frac{1}{2}}, \quad (25)$$

$$F_3^{(1)}(x,m,\mu',\mu) = \tfrac{3}{4}(1 - \mu^2)(1 - \mu'^2), \quad (26)$$

$$F_1^{(2)}(x,m,\mu',\mu) = 3/2, \quad (27)$$

$$F_1^{(3)}(x,m,\mu',\mu) = \tfrac{3}{2}\mu\mu', \quad (28)$$

and

$$F_2^{(3)}(x,m,\mu',\mu) = \frac{3}{2}(1 - \mu^2)^{\frac{1}{2}}(1 - \mu'^2)^{\frac{1}{2}}. \quad (29)$$

Table III. Values of $F_n^{(1)}(x,m,\mu',\mu)$ for a Few Selected Values of μ'; $x = 10.0$, $m = 1.342$, $\mu = 0.0$

n	$\mu' = \cos 10°$	$\mu' = \cos 30°$	$\mu' = \cos 50°$	$\mu' = \cos 70°$	$\mu' = \cos 90°$
1	2.0907 (−01)	3.3096 (−01)	6.6961 (−01)	1.3142	3.2897
2	4.5249 (−02)	2.6843 (−01)	8.0138 (−01)	2.0044	5.8812
3	−5.4385 (−02)	1.1697 (−01)	5.7854 (−01)	1.5084	5.2537
4	5.1981 (−02)	5.5943 (−02)	2.6323 (−01)	9.3576 (−1)	4.4934
5	2.7793 (−02)	2.1202 (−03)	1.6559 (−01)	5.2051 (−1)	3.9230
6	−1.1307 (−02)	2.6341 (−02)	3.8726 (−02)	2.8169 (−1)	3.5697
7	−3.5766 (−03)	−5.8576 (−03)	2.3252 (−02)	8.4788 (−2)	3.3050
8	9.5099 (−04)	7.8603 (−03)	−4.9093 (−02)	−3.1264 (−2)	3.1581
9	2.2385 (−04)	3.0818 (−02)	−5.0069 (−02)	−1.0552 (−1)	3.0507
10	−4.0067 (−05)	−4.2322 (−02)	−7.6546 (−02)	−2.3122 (−1)	2.9468
11	−7.8530 (−06)	−2.9079 (−02)	−6.5303 (−02)	−2.2998 (−1)	2.8587
12	9.4096 (−07)	2.1328 (−02)	−5.0866 (−02)	−3.7047 (−1)	2.7589
13	1.6304 (−07)	1.0994 (−02)	−7.8184 (−03)	−3.1891 (−1)	2.5997
14	−1.2774 (−08)	−4.3674 (−03)	−8.6115 (−03)	−3.7280 (−1)	2.5051
15	−2.0120 (−09)	−2.0076 (−03)	−1.1672 (−02)	−2.9478 (−1)	2.2414
16	9.9630 (−11)	4.2701 (−04)	5.1686 (−02)	−1.9189 (−1)	2.0696
17	1.4065 (−11)	1.8425 (−04)	3.1464 (−02)	−8.8012 (−2)	1.7402
18	−4.3836 (−13)	−1.9455 (−05)	−1.6651 (−02)	1.4685 (−2)	1.3664
19	−4.7748 (−14)	−7.6247 (−06)	−1.0440 (−02)	3.7958 (−2)	1.0059
20	1.2755 (−15)	4.0059 (−07)	9.6949 (−04)	1.2373 (−1)	6.1834 (−1)
21	4.4328 (−17)	7.3321 (−08)	7.0878 (−04)	8.6092 (−2)	3.9090 (−1)
22	−4.0331 (−18)	−1.2211 (−08)	3.4031 (−05)	1.6949 (−2)	9.1213 (−2)
23	−2.3747 (−20)	8.4767 (−10)	4.1930 (−05)	7.5101 (−3)	3.6892 (−2)
24	5.3215 (−21)	3.5734 (−10)	1.2702 (−05)	2.2149 (−3)	1.0902 (−2)
25	4.2733 (−22)	6.3490 (−11)	2.7864 (−06)	5.3111 (−4)	2.6850 (−3)
26	2.1317 (−23)	8.2559 (−12)	4.9833 (−07)	1.0870 (−4)	5.7139 (−4)
27	8.3048 (−25)	8.8035 (−13)	7.6418 (−08)	1.9535 (−5)	1.0753 (−4)
28	2.7288 (−26)	8.0988 (−14)	1.0354 (−08)	3.1462 (−6)	1.8215 (−5)
29	8.0002 (−28)	6.6859 (−15)	1.2692 (−09)	4.6126 (−7)	2.8151 (−6)
30	2.1641 (−29)	5.0887 (−16)	1.4336 (−10)	6.2327 (−8)	4.0105 (−7)

Results of Computation

Values of $F_n^{(j)}(x,m,\mu',\mu)$ were computed as a function of n for several combinations of x, μ', and μ, and for all four values of j. We shall limit our discussion to selected numerical results for three values of x only, viz., 0.01, 10.0, and 100.0. For $x = 0.01$, computed values of the fourier coefficients were found to agree up to five significant figures with those obtained from Eqs. (24) to (29).

Values of $F_n^{(1)}(10.0,\ 1.342,\ \mu',\ 0.0)$ for $n = 1(1)30$ are given in tabulated form (Table III) primarily for assisting the reader to obtain independent checks of his computer program. Because of the nature of the renormalized associated Legendre functions [Eq. (23)], the absolute value of $F_n^{(1)}$ decreases much more rapidly with increase of n as μ' changes from 0.0 to 1.0 (or from 0.0 to -1.0, a range for which no numerical results are given). For example, for $\mu' = \cos 10°$, absolute values of the function with subscript $n \geq 11$ are less than one-ten thousandth of the highest value which is the very first value in this case. This trend is still better understood by appealing to Eq. (19), from which it can be seen that for the case $\mu' = \cos 10°$, $\mu = \cos 90°$, we are dealing with only a section of the $M_2(x,m,\Theta)$ vs Θ curve. This section is bounded by $\Theta_1 = 80°$ and $\Theta_2 = 100°$, where the function does not exhibit very strong variations. Hence it should be possible to reproduce this part of the function with a number of terms much less than $N \doteqdot 2x + 10$. Thus, Eq. (21) can be rewritten by replacing the fixed upper limit N of the series by a variable upper limit $N(\mu',\mu)$. It is evident that among other parameters, values of $N(\mu',\mu)$ will also depend upon the criterion used for terminating the series.

In what follows, we shall define $N(\mu',\mu)$ as that value of the subscript n such that all $|F_n^{(j)}(x,m,\mu',\mu)|$ with $n > N(\mu',\mu)$ are less than 10^{-4} times the maximum value of $|F_n^{(j)}(x,m,\mu',\mu)|$. For a given set of parameters, $N(\mu',\mu)$ can vary slightly as j is increased from 1 through 4. In that case, the maximum of four values will be taken. With this criterion, for $x = 10.0$, $m = 1.342$, and $\mu = 0.0$, $N(\mu',\mu) = 1, 10, 15, 19, 21, 23, 24, 25, 26$, and 26 for values of $\cos^{-1}\mu'$ given by $\theta' = 0°(10°)90°$, respectively. For $\mu \neq 0$, values of $N(\mu',\mu)$ are even less than those given above. From Table III, it can be seen that the shape of the $N(\mu',\mu)$ vs μ' curve is not very sensitive to the numerical factor in the criterion.

Absolute values of the coefficients $F_n^{(1)}$ (100.0, 1.342, μ', 0.0) of the fourier series for the normalized scattering function $M_2(x,m,\Theta)$ are plotted in Fig. 8 for three values of μ' for which $\theta' = 10°$, 50°, and 90°. The case $\mu = 0.0$, $\mu' = 0.0$ corresponds to representing the entire scattering function curve ($\Theta = 0°$ to $180°$) by a fourier series. On comparison with the corresponding curve in Fig. 1, it can be seen that the Legendre coefficient vs its subscript k curve shows a broad maximum at $k \doteqdot 90$, while the fourier coefficient vs n curve shows a maximum at $n = 2$. However, N, the maximum of terms necessary for achieving a desired accuracy, is about the same for both cases. In general, values of $|F_n^{(1)}(x,m,\mu',\mu)|$ decrease as θ' is decreased from 90° to 10°. However, variations in this quantity with n are very strong when $\theta' \neq 90°$. Hence, a part of the numerical results (between $n = 7$ and 50) are not plotted for $\theta' = 50°$ to avoid confusion. It can be seen from Fig. 8 that the variable upper limit $N(\mu',\mu)$, mentioned earlier, decreases rapidly with θ'.

Further details about variations in $N(\mu',\mu)$ as a function of θ' and θ can be found in Table IV where these quantities are tabulated for $x = 100.0$ at $\theta' = 0°(10°)$ 180° and for $\theta = 30°$, 60°, and 90°. Because of the nature of high order associated Legendre polynomials, $N(\mu',\mu) = 1$ whenever μ' or $\mu = \pm 1$, i.e., θ or $\theta' = 0°$ or 180°. For $\theta = 30°$, a plot of $N(\mu',\mu)$ vs θ' would show a strong increase from 1 to about 80 as θ' is increased from 0° to 20°, and a broad maximum (a plateau with $N(\mu',\mu) \doteqdot 117$) between 30° and 150°. A further increase in θ' results in a rapid decrease. Similar trends can also be found for the other two cases for which similar numerical results are presented in Table IV. However, the value of $N(\mu',\mu)$ near the plateau is approximately 190 and 217 for $\theta = 60°$ and 90°, respectively. Similar trends were also observed for other values of x for which computations were performed.

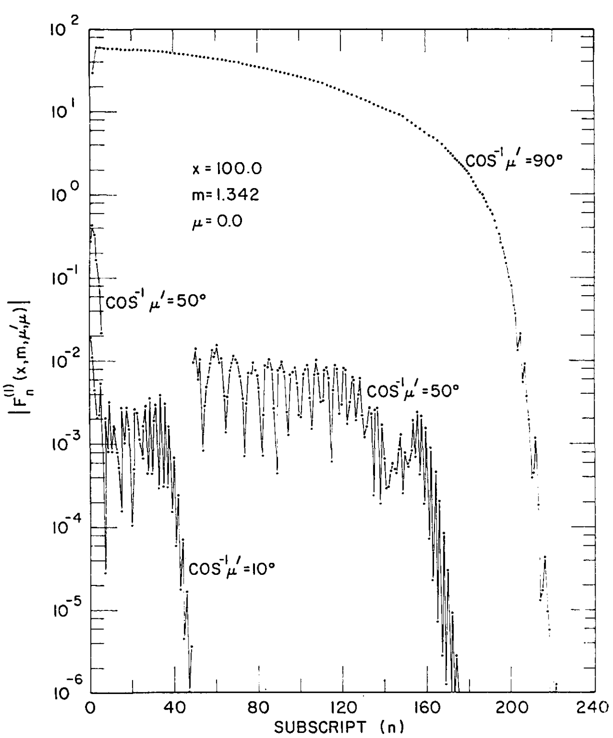

Fig. 8. Variations of the absolute values of coefficients $F_n^{(1)}(x, m, \mu', \mu)$ of the fourier series for the scattering function $M_2(x, m, \Theta)$ as a function of subscript n; $x = 100$, $m = 1.342$, $\theta = 90°$, $\theta' = 10°$, 50°, and 90°.

Table IV. Values of $N(\mu' = \cos\theta', \mu = \cos\theta)$ for Three Different Values of θ; $x = 100.0$, $m = 1.342$

θ'/θ	30°	60°	90°
0	1	1	1
10	45	47	48
20	83	82	84
30	111	115	117
40	117	144	150
50	116	171	170
60	117	190	190
70	115	190	206
80	117	192	215
90	118	189	217
100	117	190	215
110	118	193	206
120	118	190	190
130	118	173	170
140	118	148	150
150	113	118	117
160	84	83	84
170	47	47	48
180	1	1	1

IV. Conclusion

In the foregoing sections, we have shown that reliable values of the directional scattering properties of a sphere can also be obtained with the help of modified Mie expressions[13] where each of the four scattering functions is expressed in the form of a Legendre or fourier series. The task of computing coefficients of these series and of computing values of scattering functions therefrom is usually much more tedious than that of doing the same using the well-known Mie method currently employed by other investigators. In fact, experience has shown that the difference in computational time for identical tasks using these two methods, though negligible for small values of size parameter ($x \sim 1$), increases very rapidly thereafter. Thus, the alternate method described in this paper would be unattractive when one is interested in computing scattering functions for a few values of scattering angle. The advantages of using this alternate method become apparent when one faces the problem of obtaining a very fine picture of the directional dependence of scattering characteristics for spherical polydispersions encountered in the atmosphere.[9] From the results presented here (Figs. 4–7), one cannot categorically state that width of integration increment for obtaining equally reliable results will be the same for these two methods. If a somewhat coarser integration increment can be used, the present method would be still more attractive for extensive calculations.

One important finding of the present study is that a section of the scattering function versus scattering angle curve can be fully represented by a fourier series whose upper limit depends upon the boundary of the section under study. If this section is a small part of the entire curve, this limit is much less than the maximum possible value, which is approximately equal to $2x + 10$. If this finding can be successfully used in multiple-scattering calculations, one can simplify the computational task considerably. Some work in this direction has been carried out, and preliminary results of this investigation can be found in a recent report.[17]

Some relief in computational time may be obtained if a recurrence relationship can be set up for computations of C_k and D_k directly from x and m instead of making use of Eqs. (16) and (17). If it should be possible to obtain recurrence formulas which can be used for computations of $L_k^{(j)}(x,m)$ directly from x and m, the computational task might become very light indeed. Further work aimed at obtaining such recurrence relationships is very desirable.

I would like to express my sincere thanks to my colleague, B. H. Armstrong and to R. S. Fraser of TRW systems for a careful reading of the original manuscript and for their very helpful comments.

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Spectral Line Shapes Symposium

A Symposium on Spectral Line Shapes will take place during the Second Annual Meeting of the Division of Electron and Atomic Physics of the American Physical Society, to be held on 23–25 November 1970 at the Pacific Science Center in Seattle, Washington. This Symposium is a successor to Gordon Conferences on the same subject held in the past and will be organized by **Marshall Lapp** (General Electric Research and Development Center) and **Earl Smith** (National Bureau of Standards). The deadline for contributed papers will be the middle of September in order to ensure publication of the abstracts in the **Bulletin of the American Physical Society.** A limited number of postdeadline papers will be accepted if time is available. Three copies of each abstract should be sent to Dr. Smith at Plasma Physics Section (271.06), National Bureau of Standards, Boulder, Colorado 80302. Abstracts should conform to the format suggested in the **Bulletin.** Further information concerning this DEAP meeting will appear in the **Bulletin.**