Scattering coefficients for a multilayered sphere: analytic expressions and algorithms

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A calculational procedure for obtaining the complete set of scattering coefficients for a multilayered sphere is proposed. The procedure is based on the utilization of a prescription which relates the coefficients for an r-layered sphere to those for an (r-1)-layered sphere. The prescription is derived directly from the determinantal form of the scattering amplitudes for a multilayered sphere. The complete set of coefficients considered includes the coefficients required to describe the fields within the various regions of the multilayered sphere.

I. Introduction

Chylek and Bhandari¹ recently considered the case of light scattering by a double-layered sphere in connection with the study of the absorption of visible light by a water droplet contaminated with graphitic carbon (soot). Within this double-layered sphere model, the soot forms a thin concentric shell inside the water droplet. It is a case intermediate between the soot existing as the core and the soot forming a shell on the outside of the water droplet. During the course of the calculation, the present author observed serious numerical inaccuracies in the calculation of the absorption cross section when the particle size was large compared to the wavelength of light. In the past several authors²⁻⁶ reported similar problems in the use of analytic expressions for the homogeneous sphere and the single-layered sphere. In the case of the homogeneous sphere, the technique of employing logarithmic derivatives² has proved to be very successful in resolving the numerical problems. Recently, Toon and Ackerman⁶ recast the conventional analytic expressions for the single-layered sphere in a form amenable to accurate calculations by using logarithmic derivatives, suitable ratios, and products of Ricatti-Bessel functions. It is the primary objective of this paper to propose a calculational procedure for a multilayered sphere with an arbitrary number of layers on top of the core. The calculational procedure is based on a prescription which

relates the scattering coefficients for an r-layered sphere to those for an (r-1)-layered sphere. This prescription, in effect, permits us to obtain the complete analytic expressions for an r-layered sphere, starting from the standard Mie coefficients for a homogeneous sphere. The set of coefficients we give also includes those which determine the fields within the various regions of the multilayered sphere.

Recursive methods for multilayered nonplanar configurations have been considered in the past.^{7,8} For example, in connection with his study of the multilayered sphere, Wait used an iterative method based on an analogy with transmission lines connected in tandem. The method we provide here utilizes a prescription which is derived directly from an examination of the determinantal form of the scattering amplitudes.9 This prescription is finally recast into a form which vields, directly through the iterative procedure, suitable calculational forms for the scattering coefficients. We have successfully applied the resulting algorithm to the study of scattering by a water droplet containing a concentric shell of carbon within it (a case of two layers on top of a core). In another piece of work¹⁰ the author has discussed in detail the case of scattering by such a sphere in the limit that the inner shell (which is carbon in the foregoing case of water droplet) is very thin. In addition, he has worked out the cases of the outer shell being very thin or the core being very tiny in the scattering of light by a single-layered sphere. 11 Such limiting cases, it is shown, provide a good test of the calculational procedure outlined in this paper.

II. Scattering Coefficients

Following van de Hulst's treatment¹² of light scattering by a homogeneous sphere, one can write for each region j of the (r-1)-layered sphere (Fig. 1):

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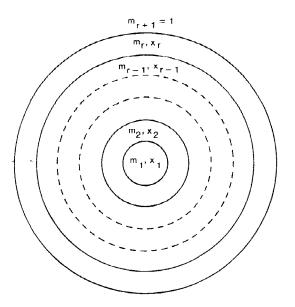


Fig. 1. Multilayered sphere which scatters an incident plane wave. m_i , x_i are the refractive index and the size parameter for the *i*th region.

$$u^{(r,j)} = (-1)^{r-j} \exp(i\omega t) \cos\phi \sum_{n=1}^{\infty} m_j (-i)^n \frac{2n+1}{n(n+1)} P_n^1(\cos\theta)$$

$$\times \{ [a_n^{(r,j)} - \delta_{j,r+1}] j_n(m_j x) - c_n^{(r,j)} n_n(m_j x) \}, \qquad (1a)$$

$$v^{(r,j)} = (-1)^{r-j} \exp(i\omega t) \sin\phi \sum_{n=1}^{\infty} m_j (-i)^n \frac{2n+1}{n(n+1)} P_n^1(\cos\theta)$$

$$\times \{ [b_n^{(r,j)} - \delta_{j,r+1}] j_n(m_j x) - d_n^{(r,j)} n_n(m_j x) \}$$

$$(1 \le j \le r+1). \qquad (1b)$$

 m_j denotes the refractive index of the material in the jth region. In what follows, we assume $m_j=1$ whenever j corresponds to the region outside the sphere. In the case considered here, the value of j for this region is r+1 (see Fig. 1). The size parameters are $x_i=2\pi r_i/\lambda$, where r_i are the various radii and λ the wavelength of the plane wave incident on the sphere. The spherical Bessel functions j_n and n_n can have complex arguments by virtue of the general complex nature of refractive index. $\mathbf{x}=2\pi R/\lambda$, where \mathbf{R} is the radial distance. The spherical polar angles θ and ϕ give the direction of the scattered light with respect to the incident beam. The functions $u^{(r,j)}$ and $v^{(r,j)}$ satisfy the scalar wave equation. \mathbf{R}

Coefficients $a_n^{(r,j)}$, $c_n^{(r,j)}$, $b_n^{(r,j)}$, and $d_n^{(r,j)}$ are initially unknown with the exceptions $c_n^{(r,1)} = d_n^{(r,1)} = 0$ (inside the core) and $c_n^{(r,r+1)} = ia_n^{(r,r+1)}$, $d_n^{(r,r+1)} = ib_n^{(r,r+1)}$ (outside the sphere). The latter are required to ensure the outgoing nature of the scattered spherical wave at $r \to \infty$. The scattering amplitudes $a_n^{(r,r+1)}$ and $b_n^{(r,r+1)}$ determine the various cross sections in the following way:

$$\sigma_{\text{ext}} = \frac{\lambda^2}{2\pi} \sum_{n=1}^{\infty} (2n+1) \operatorname{Re} \left[a_n^{(r,r+1)} + b_n^{(r,r+1)} \right], \tag{2a}$$

$$\sigma_{\rm sc} = \frac{\lambda^2}{2\pi} \sum_{n=1}^{\infty} (2n+1) [|a_n^{(r,r+1)}|^2 + |b_n^{(r,r+1)}|^2], \tag{2b}$$

$$\sigma_{abs} = \sigma_{ext} - \sigma_{sc} = \frac{\lambda^2}{2\pi} \sum_{n=1}^{\infty} (2n+1) \{ \text{Re}[a_n^{(r,r+1)} + b_n^{(r,r+1)}] - |a_n^{(r,r+1)}|^2 - |b_n^{(r,r+1)}|^2 \}.$$
 (2c)

Application of the boundary conditions, namely, the matching of H_{θ} , H_{ϕ} , E_{θ} , and E_{ϕ} (the tangential components) at the interfaces of the different regions (see Fig. 1), results in two sets of 2r simultaneous equations. One set, associated with the u functions [Eq. (1a)], involves the 2r variables $a_n^{(r,j)}$ and $c_n^{(r,j)}$ ($j \neq 1$ and $j \neq r+1$), while the other, associated with the v functions [Eq. (1b)], connects $b_n^{(r,j)}$ and $d_n^{(r,j)}$ ($j \neq 1$ and $j \neq r+1$), 2r in number. Solution of these simultaneous equations for the coefficients leads to expressions which are ratios of $2r \times 2r$ determinants in each case. For example, the scattering coefficient $a_n^{(r,r+1)}$ can be expressed as

$$a_n^{(r,r+1)} = N^{(r,r+1)}/D^{(r,r+1)},\tag{3}$$

where

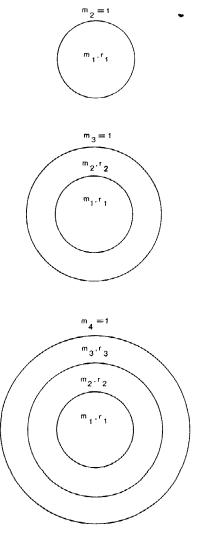


Fig. 2. Homogeneous sphere, a single-layered sphere, and a double-layered sphere.

$N^{(r,r+1)} =$	$ \begin{vmatrix} m_{r+1}\psi_n(m_{r+1}x_r) \\ \psi'_n(m_{r+1}x_r) \\ 0 \\ 0 \\ 0 \\ \vdots \end{vmatrix} $	$m_r \psi_n(m_r x_r)$ $\psi_n(m_r x_r)$ $m_r \psi_n(m_r x_{r-1})$ $\psi_n(m_r x_{r-1})$ 0 0 :	$m_r \chi_n(m_r x_r)$ $\chi_n(m_r x_r)$ $m_r \chi_n(m_r x_{r-1})$ $\chi_n(m_r x_{r-1})$ 0 0	0 0 $m_{r-1}\psi_n(m_{r-1}x_{r-1})$ $\psi'_n(m_{r-1}x_{r-1})$ $m_{r-1}\psi_n(m_{r-1}x_{r-2})$ $\psi'_n(m_{r-1}x_{r-2})$ 0	$0 0 m_{r-1}\chi_n(m_{r-1}x_{r-1}) \chi'_n(m_{r-1}x_{r-1}) m_{r-1}\chi_n(m_{r-1}x_{r-2}) \chi'_n(m_{r-1}x_{r-2}) 0$	00 00 00 00 0	- (4)
	:	:	:	0	0	:	i
	1:	:	:	:	:	$m_1\psi_n(m_1x_1)$	ı
	0	0	0	0	0	$\psi_n(m_1x_1)$	

 $\psi_n(z)=zj_n(z)$ and $\chi_n(z)=-zn_n(z)$ are known as Ricatti-Bessel functions. $D^{(r,r+1)}$ in Eq. (3) obtains from $N^{(r,r+1)}$ by the replacement of $\psi_n(m_{r+1}x_r)$ and $\psi_n(m_{r+1}x_r)$ with $\zeta_n(m_{r+1}x_r)$ and $\zeta_n(m_{r+1}x_r)$, respectively. $\zeta_n(z)=\psi_n(z)+i\chi_n(z)$. The prime denotes the derivative of the function with respect to its argument. The foregoing determinants are like the determinants given by Kerker¹³ for $a_n^{(r,r+1)}$. However, our purpose here is to formulate a procedure which generates the complex analytic expression for $a_n^{(r,r+1)}$ from the knowledge of Mie coefficients only. As we shall see, this process also leads to expressions which are utilized in expressing the coefficients for the fields within the sphere.

If now another shell is added to the sphere of Fig. 1, the sphere becomes r layered. The numerator $N^{(r+1,r+2)}$ in the scattering amplitude $a_n^{(r+1,r+2)}$ is now a $(2r+2) \times (2r+2)$ determinant given by

	$m_{r+2}\psi_n(m_{r+2}x_{r+1})$	$m_{r+1}\psi_n(m_{r+1}x_{r+1})$	$m_{r+1}\chi_n(m_{r+1}x_{r+1})$	0	0	00	
	$\psi_n(m_{r+2}x_{r+1})$	$\psi_n(m_{r+1}x_{r+1})$	$\chi_n(m_{r+1}x_{r+1})$	0	0	00	
	0	$m_{r+1}\psi_n(m_{r+1}x_r)$	$m_{r+1}\chi_n(m_{r+1}x_r)$	$m_r\psi_n(m_rx_r)$	$m_r \chi_n(m_r x_r)$	00	
	0	$\psi_n(m_{r+1}x_r)$	$\chi_n(m_{r+1}x_r)$	$\psi'_n(m_rx_r)$	$\chi_n'(m_r x_r)$	00	
$N^{(r+1,r+2)} =$	0	0	0	$m_r \psi_n (m_r x_{r-1})$	$m_r \chi_n (m_r x_{r-1})$	0	• (5)
	0 .	0	0	$\psi'_n(m_rx_{r-1})$	$\chi_n'(m_r x_{r-1})$	0	
	:	:	:	0	0	:	
	;	;	:	:	:	$m_1\psi_n(m_1x_1)$	
	0	0	0	0	0	$\psi_n(m_1x_1)$	

According to our earlier assumption $m_{r+2} = 1$ here and $m_{r+1} \neq 1$ now. One notes here that the deletion of the top two rows and the first and third columns of $N^{(r+1,r+2)}$ yields the $N^{(r,r+1)}$ determinant of Eq. (4). To express the $N^{(r+1,r+2)}$ determinant in terms of the $N^{(r,r+1)}$ determinant we rewrite the former as the sum of two $(2r+2\times 2r+2)$ determinants by splitting its third column in the following way:

[Only the third column of each determinant (resulting from the split) is shown. The rest of the columns are precisely those of the determinant shown in Eq. (5).] After interchanging columns 2 and 3 in the second determinant, the above expression takes the form

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	[
	$m_{r+2}\psi_n(m_{r+2}x_{r+1})$	$m_{r+1}\psi_n(m_{r+1}x_{r+1})$	0	00	
	$ \psi_n(m_{r+2}x_{r+1}) $	$\psi'_n(m_{r+1}x_{r+1})$	0	00	
	0	$m_{r+1}\psi_n(m_{r+1}x_r)$	$m_{r+1}\chi_n(m_{r+1}x_r)$	$m_r \psi_n(m_r x_r) \dots 0$	
$N^{(r+1,r+2)} =$	0	$\psi_n'(m_{r+1}x_r)$	$\chi'_n(m_{r+1}x_r)$	$\psi'_n(m_rx_r) \ldots 0$	
	0	0	0	$m_r\psi_n(m_rx_{r-1})$.0	
	11	1	0	$\psi'_n(m_rx_{r-1}) \ldots 0$,	
		ĺ	0	0 :	
	1 1		:	: $m_1\psi_n(m_1x_1)$	
•	lò	0	_ 0	0 $\psi_n(m_1x_1)$	
		, ,			(7)
	$m_{r+2}\psi_n(m_{r+2}x_{r+1})$	$m_{r+1}\chi_n(m_{r+1}x_{r+1})$	$m_{r+1}\psi_n(m_{r+1}x_{r+1})$	0	
	$\psi_n(m_{r+2}x_{r+1})$	$\chi_n(m_{r+1}x_{r+1})$	$\psi_n(m_{r+1}x_{r+1})$	00	
	0	0	$m_{r+1}\psi_n(m_{r+1}x_r)$	$m_r\psi_n(m_rx_r)\ldots 0$	
	0	0	$\psi_n(m_{r+1}x_r)$	$\psi_n'(m_r x_r) \ldots 0$	
	1 1		0	$m_r \psi_n(m_r x_{r-1}) \cdot 0$	
	.	1	0	$\psi'_n(m_rx_{r-1}) \ldots 0$	
		1		0 111	
	 	•	i		
	1 i	İ	li	$m_1\psi_n(m_1x_1)$	
	Ö	Ò	0	$0 \ldots \psi_n(m_1x_1)$	
	•				

Each of these determinants is a product of the (2×2) and the $(2r \times 2r)$ determinants shown in the boxes. The (2×2) determinant in the first of the above two determinants is the numerator obtained in the case of scattering by a homogeneous sphere with refractive index m_{r+1} and size parameter x_{r+1} (remember $m_{r+2} = 1$). Henceforth, we will denote it by n_H . On the other hand, the $(2r \times 2r)$ determinant indicated by the box in the second $(2r + 2 \times 2r + 2)$ determinant of Eq. (7) is nothing but $N^{(r,r+1)}$ [see Eq. (4)] with $m_{r+1} \neq 1$. This we will denote by $N^{(r,r+1)}_m$. Thus

$$N^{(r+1,r+2)} = n_H \tilde{N}_m^{(r,r+1)} - \tilde{n}_H N_m^{(r,r+1)}, \tag{8}$$

where

$$\begin{split} n_{H} &= n_{H}(m_{r+2}, m_{r+1}, x_{r+1}) \\ &= m_{r+2} \psi_{n}(m_{r+2} x_{r+1}) \psi_{n}'(m_{r+1} x_{r+1}) \\ &- m_{r+1} \psi_{n}'(m_{r+2} x_{r+1}) \psi_{n}(m_{r+1} x_{r+1}), \quad m_{r+2} = 1, \end{split} \tag{8a}$$

$$\tilde{n}_H = m_{r+2}\psi_n(m_{r+2}x_{r+1})\chi'_n(m_{r+1}x_{r+1}) - m_{r+1}\psi'_n(m_{r+2}x_{r+1})\chi_n(m_{r+1}x_{r+1}), \quad m_{r+2} = 1,$$
 (8b)

$$\tilde{N}_{m}^{(r,r+1)} = N_{m}^{(r,r+1)},\tag{8c}$$

with
$$\psi_n(m_{r+1}x_r), \psi_n(m_{r+1}x_r)$$
 replaced by $\chi_n(m_{r+1}x_r), \chi_n'(m_{r+1}x_r)$, respectively.

Equation (8), which relates $N^{(r+1,r+2)}$ to $N_n^{(r,r+1)}$, is the general prescription for building analytical expressions for a multilayered sphere, starting with the homogeneous sphere. When r=1 (homogeneous sphere, see Fig. 2)

$$\begin{split} N^{(r,r+1)} &= N^{(1,2)} = n_H(m_2,m_1,x_1) = m_2 \psi_n(m_2 x_1) \psi_n'(m_1 x_1) \\ &- m_1 \psi_n'(m_2 x_1) \psi_n(m_1 x_1) = W_1(m_2 = 1). \end{split} \tag{9a}$$

For r = 2 (single-layered sphere, see Fig. 2),

$$N^{(r,r+1)} = N^{(2,3)} = n_H(m_3, m_2, x_2) \bar{N}_m^{(1,2)} - \tilde{n}_H(m_3, m_2, x_2) N_m^{(1,2)} = W_2 W_6 - W_7 W_1,$$
 (9b)

whe**r**e

$$\begin{split} W_7 &= m_3 \psi_n(m_3 x_2) \chi_n'(m_2 x_2) - m_2 \psi_n'(m_3 x_2) \chi_n(m_2 x_2), \\ W_6 &= m_2 \chi_n(m_2 x_1) \psi_n'(m_1 x_1) - m_1 \chi_n'(m_2 x_1) \psi_n(m_1 x_1), \end{split}$$

$$W_2 = m_3 \psi_n(m_3 x_2) \psi'_n(m_2 x_2) - m_2 \psi'_n(m_3 x_2) \psi_n(m_2 x_2),$$

$$(m_3 = 1).$$

and W_1 is the same as in Eq. (9a) except that $m_2 \neq 1$. For r = 3 (double-layered case, see Fig. 2),

$$\begin{split} N^{(r,r+1)} &= N^{(3,4)} = n_H(m_4, m_3, x_3) \bar{N}^{(2,3)} \\ &- \bar{n}_H(m_4, m_3, x_3) N_m^{(2,3)} \\ &= W_3(W_5 W_6 - W_8 W_1) - W_4(W_2 W_6 - W_7 W_1), \end{split} \tag{9c}$$

where

$$\begin{split} W_3 &= m_4 \psi_n(m_4 x_3) \psi_n'(m_3 x_3) - m_3 \psi_n'(m_4 x_3) \psi_n(m_3 x_3), \\ W_4 &= m_4 \psi_n(m_4 x_3) \chi_n'(m_3 x_3) - m_3 \psi_n'(m_4 x_3) \chi_n(m_3 x_3), \\ W_5 &= m_3 \chi_n(m_3 x_2) \psi_n'(m_2 x_2) - m_2 \chi_n'(m_3 x_2) \psi_n(m_2 x_2), \\ W_8 &= m_3 \chi_n(m_3 x_2) \chi_n'(m_2 x_2) - m_2 \chi_n'(m_3 x_2) \chi_n(m_2 x_2), \\ & \cdot \qquad (m_4 = 1) \end{split}$$

and W_6 , W_7 , W_2 , W_1 are the same as in Eq. (9b) except that $m_3 \neq 1$. $N^{(r,r+1)}$ for higher values of r can be similarly generated. The function $D^{(r,r+1)}$ in general is obtained from $N^{(r,r+1)}$ by replacing $\psi_n(m_{r+1}x_r)$ and its derivative with $\zeta_n(m_{r+1}x_r)$ and its derivative. The scattering coefficient $a_n^{(r,r+1)}$ is thus analytically expressed through Eq. (3) without having to deal directly with the $(2r \times 2r)$ determinant of Eq. (4). In fact, it may not be inconceivable to write a computer program which generates the scattering coefficient $a_n^{(r,r+1)}$ using the foregoing procedure for an arbitrary value of r and subsequently computes it. For more on the computational aspect, see Sec. III.

In an identical fashion, one expresses the coefficients $a_n^{(r,i)}$ $(i=1,\ldots r)$ and $c_n^{(r,i)}$ $(i=2,\ldots r)$ which are needed to describe the fields within the sphere. For example,

$$a_n^{(r,r)} = N^{(r,r)}/D^{(r,r+1)},$$
 (10)

where

$m_r \chi_n(m_r x_r)$	0	00	
$\chi_n(m_r x_r)$	0	00	
$m_r \chi_n(m_r x_{r-1})$	$m_{r-1}\psi_n(m_{r-1}x_{r-1})$	$m_{r-1}\chi_n(m_{r-1}x_{r-1})\ldots 0$	
$\chi_n(m_r x_{r-1})$	$\psi_n(m_{r-1}x_{r-1})$	$\chi'_n(m_{r-1}x_{r-1})$	
0	$m_{r-1}\psi_n(m_{r-1}x_{r-2})$	$m_{r-1}\chi_n(m_{r-1}x_{r-2})\ldots 0$	
0	$\psi_n'(m_{r-1}x_{r-2})$	$\chi_n'(m_{r-1}x_{r-2})\cdot\ldots\ldots 0$	
	0	0 :	
11		$\left \dots \dots m_1 \psi_n(m_1 x_1) \right $	
0	0	$0 \ldots \psi_n(m_1x_1)$	

[Compare the above with $N^{(r,r+1)}$ in Eq. (4) and $D^{(r,r+1)}$. $N^{(r,r)}$ is the product of the determinants corresponding to the matrices shown in the boxes. The (2×2) determinant yields i since $m_{r+1} = 1$. The other determinant is nothing but $\tilde{N}_{m}^{(r-1,r)}$. Thus

$$N^{(r,r)} = (i)\tilde{N}_m^{(r-1,r)}/D^{(r,r+1)}. \tag{12}$$

Through similar considerations, one finds that in general

$$a_n^{(r,j)} = \frac{(-1)^{r-j} (m_1 m_2 \dots m_r) (i) \tilde{N}_m^{(j-1,j)}}{(m_1 m_2 \dots m_j) D^{(r,r+1)}} \qquad (1 \le j \le r). \quad (13)$$

Similarly,

$$c_n^{(r,j)} = \frac{(-1)^{r-j-1}(m_1m_2\dots m_r)(i)N_m^{(j-1,j)}}{(m_1m_2\dots m_j)D^{(r,r+1)}} \qquad (2 \le j \le r), (14)$$

$$c_n^{(r,1)} = 0, \text{ as pointed out earlier.}$$

 $N_m^{(j-1j)}$ and $\tilde{N}_m^{(j-1j)}$ are defined in Eq. (8c) and the preceding paragraph. $\tilde{N}_m^{(0,1)}=1$.

Equations (9a)–(9c) are expressions involving 2×2 determinants such as W_1, W_2 , etc. If the refractive indices appearing as factors in the 2 terms of each of these determinants are interchanged, expressions defining $a_n^{(r,r+1)}$ automatically become expressions for $b_n^{(r,r+1)} = 1, \ldots r + 1$). As an example,

$$b_n^{(2,3)} = N^{(2,3)}/D^{(2,3)},$$
 (15)

where

$$N^{(2,3)} = W_2 W_6 - W_7 W_1 \tag{16}$$

as in Eq. (9b), but with W_1 , W_7 , W_6 , and W_2 defined in the following way:

$$\begin{split} W_1 &= m_1 \psi_n(m_2 x_1) \psi_n'(m_1 x_1) - m_2 \psi_n'(m_2 x_1) \psi_n(m_1 x_1), \\ W_7 &= m_2 \psi_n(m_3 x_2) \chi_n'(m_2 x_2) - m_3 \psi_n'(m_3 x_2) \chi_n(m_2 x_2), \\ W_6 &= m_1 \chi_n(m_2 x_1) \psi_n'(m_1 x_1) - m_2 \chi_n'(m_2 x_1) \psi_n(m_1 x_1), \\ W_2 &= m_2 \psi_n(m_3 x_2) \psi_n'(m_2 x_2) - m_3 \psi_n'(m_3 x_2) \psi_n(m_2 x_2), \end{split}$$

Compare this set of W functions with the set in Eq. (9b). Similarly, the coefficients $b_n^{(r,j)}$ and $d_n^{(r,j)}$ are derived from $a_n^{(r,j)}$ and $c_n^{(r,j)}$ of Eqs. (13) and (14), respec-

For completeness, we point out that the scattering coefficients for any multilayered sphere must reduce to those for a multilayered sphere with a smaller number of layers in suitable conditions. As an illustration, one notes that a double-layered sphere (see Fig. 2) reduces

to a homogeneous sphere under the following sets of limits:

(11)

	Homogeneous sphere with Refractive		
Limits	Radius	index	
(i) $m_1 = m_2 = m_3 = m$	r_3	m	
(ii) $m_1 = m_2 = m$, $m_3 = 1$	r_2	m	
(iii) $m_2 = m_3 = 1$	r_1	m_1	
(iv) $r_1 = r_2 = r_3 = R$	R	m_1	
(v) $r_1 = r_2 = 0$	r_3	m_3	
(vi) $r_1 = 0$, $r_2 = r_3 = R$	R	m_2	

We have checked our expressions for $N^{(3,4)}$ under the aforementioned limits, and they do reduce to the Mie coefficients. In cases (i)-(iv), we performed the check initially by examining directly the determinant $N^{(3,4)}$ under the limits. By cleverly shifting the columns around and performing subtraction operation involving columns, the original 6 × 6 determinant was shown to reduce to a block diagonal form which was then expressed as a product of three 2×2 determinants, two of which were always the Wronskians between the χ and the ψ functions, while the third corresponded to the numerator of the Mie coefficient. In a similar way, $D^{(3,4)}$ was shown to reduce to a block diagonal form. The ratio $N^{(3,4)}/D^{(3,4)}$ then equaled the Mie coefficient $a_n^{(1,2)}$ as expected. The manner in which the check for cases (v) and (vi) was performed is illustrated easily by considering the limiting case $r_1 \rightarrow 0$ in the case of a single-layered sphere. For a single-layered case, the numerator is (with $m_3 = 1$)

$$N^{(2,3)} = \begin{pmatrix} \psi_n(x_2) & m_2\psi_n(m_2x_2) & m_2\chi_n(m_2x_2) & 0 \\ \psi_n'(x_2) & \psi_n'(m_2x_2) & \chi_n'(m_2x_2) & 0 \\ 0 & m_2\psi_n(m_2x_1) & m_2\chi_n(m_2x_1) & m_1\psi_n(m_1x_1) \\ 0 & \psi_n'(m_2x_1) & \chi_n'(m_2x_1) & \psi_n'(m_1x_1) \end{pmatrix}.$$

$$\lim_{x_1 \to 0} N^{(2,3)} = \begin{vmatrix} \psi_n(x_2) & m_2 \psi_n(m_2 x_2) \\ \psi'_n(x_2) & \psi'_n(m_2 x_2) \end{vmatrix} \quad \begin{vmatrix} m_2 \chi_n(m_2 x_1) & m_1 \psi_n(m_2 x_1) \\ \chi'_n(m_2 x_1) & \psi'_n(m_2 x_1) \end{vmatrix} .$$

This reduction is made possible by the fact that $\lim_{x_1\to 0}$ $\psi_n(m_2x_1) \to 0$, $\lim_{x_1 \to 0} \psi'_n(m_2x_1) \to 0$. Similarly,

$$D^{(2,3)} = \begin{vmatrix} \zeta_n(x_2) & m_2 \psi_n(m_2 x_2) \\ \zeta_n(x_2) & \psi_n'(m_2 x_2) \end{vmatrix} \quad \begin{vmatrix} m_2 \chi_n(m_2 x_1) & m_1 \psi_n(m_1 x_1) \\ \chi_n'(m_2 x_1) & \psi_n'(m_1 x_1) \end{vmatrix} \; .$$

The ratio $N^{(2,3)}/D^{(2,3)}$ in the aforementioned limit then equals $a_n^{(1,2)}$. Similar mathematical manipulations show that the other coefficients in the foregoing example, $a_n^{(3,3)}, a_n^{(3,2)}, a_n^{(3,1)}, b_n^{(3,4)}, b_n^{(3,3)}, b_n^{(3,2)}, b_n^{(3,1)}, c_n^{(3,2)}, \text{etc., ap-}$ propriately reduce.

III. Alternative Forms for Scattering Amplitudes: $a_n^{(r,r+1)}$ and $b_n^{(r,r+1)}$

In connection with the computation of various cross sections for the homogeneous and the single-layered sphere, it has been noted in the past²⁻⁶ that inaccuracies can arise if the scattering amplitudes are calculated directly from the analytic expressions of the type given in the preceding section. It has been further pointed out that the use of logarithmic derivatives,2 suitable ratios, and products of Ricatti-Bessel functions⁶ smooths out such problems. In what follows, we formulate a procedure for the caculation of scattering amplitudes for the general case of a multilayered sphere in a numerically stable manner. As we shall see, our procedure involves logarithmic derivatives and only two types of ratio of Ricatti-Bessel functions.

We proceed by first noting that $a_n^{(r,r+1)}$ in Eq. (3) remains unaltered if the functions χ_n and χ'_n appearing in the determinants $N^{(r,r+1)}$ [see Eq. (4)] and $D^{(r,r+1)}$ are replaced by the corresponding functions ζ_n and ζ_n' . Thus all the subsequent expressions are still valid provided, whenever χ_n appears, it is understood that ζ_n replaces it and similarly for the derivative of χ_n . Not to complicate matters unnecessarily, we will retain the notation hitherto used for the determinants. With the above changes incorporated, we now rewrite $N^{(r+1,r+2)}$

$$N^{(r+1,r+2)} = \psi_n(m_{r+2}x_{r+1})\psi_n(m_{r+1}x_{r+1})\zeta_n(m_{r+1}x_r)\psi_n(m_rx_r) \\ \times \zeta_n(m_rx_{r-1}) \dots \zeta_n(m_2x_1)\psi_n(m_1x_1) \\ \times N_R^{(r+1,r+2)}, \tag{17}$$

where $N_R^{(r+1,r+2)}$ is a reduced $(2r+2\times 2r+2)$ determinant, obtained from the $N^{(r+1,r+2)}$ determinant by dividing each column of the latter by the corresponding factor in front of $N_R^{(r+1,r+2)}$. For example, the first column of $N_R^{(r+1,r+2)}$ = the first column of $\hat{N}^{(r+1,r+2)}$ divided by $\psi_n(m_{r+2}x_{r+1})$, and so on. Likewise, we reexpress n_H , given in Eq. (8a), as

$$n_{H} = \psi_{n}(m_{r+2}x_{r+1})\psi_{n}(m_{r+1}x_{r+1})$$

$$\times [m_{r+2}\psi'_{n}(m_{r+1}x_{r+1})/\psi_{n}(m_{r+1}x_{r+1})$$

$$- m_{r+1}\psi'_{n}(m_{r+2}x_{r+1})/\psi_{n}(m_{r+2}x_{r+1})].$$
(18a)

Furthermore.

$$\bar{N}_{m}^{(r,r+1)} = \zeta_{n}(m_{r+1}x_{r})\psi_{n}(m_{r}x_{r})\zeta_{n}(m_{r}x_{r-1})\psi_{n}(m_{r-1}x_{r-1}) \dots \zeta_{n}(m_{2}x_{1})\psi_{n}(m_{1}x_{1})\bar{N}_{m_{R}}^{(r,r+1)},$$
(18b)

where $\tilde{N}_{mR}^{(r,r+1)}$ is a reduced $(2r \times 2r)$ determinant related to $\tilde{N}_{m}^{(r,r+1)}$ in the same manner as $N_{R}^{(r+1,r+2)}$ to $N^{(r+1,r+2)}$ in Eq. (17). Similarly,

$$\tilde{n}_{H} = \psi_{n}(m_{r+2}x_{r+1})\zeta_{n}(m_{r+1}x_{r}) \left[m_{r+2} \frac{\zeta_{n}(m_{r+1}x_{r+1})}{\zeta_{n}(m_{r+1}x_{r+1})} \frac{\zeta_{n}(m_{r+1}x_{r+1})}{\zeta_{n}(m_{r+1}x_{r})} - m_{r+1} \frac{\overline{\zeta}_{n}(m_{r+1}x_{r+1})}{\zeta_{n}(m_{r+1}x_{r})} \frac{\psi_{n}'(m_{r+2}x_{r+1})}{\psi_{n}(m_{r+2}x_{r+1})} \right].$$
(18c)

Also

$$N_{m}^{(r,r+1)} = \psi_{n}(m_{r+1}x_{r})\psi_{n}(m_{r}x_{r})\zeta_{n}(m_{r}x_{r-1})\dots\zeta_{n}(m_{2}x_{1}) \times \psi_{n}(m_{1}x_{1})N_{mR}^{(r,r+1)} = \psi_{n}(m_{r+1}x_{r+1})\psi_{n}(m_{r}x_{r})\zeta_{n}(m_{r}x_{r-1})\dots\zeta_{n}(m_{2}x_{1}) \times \psi_{n}(m_{1}x_{1}) \left[\frac{\psi_{n}(m_{r+1}x_{r})}{\psi_{n}(m_{r+1}x_{r+1})} \right] N_{mR}^{(r,r+1)}.$$
(18d)

Substitution of Eqs. (17)-(18d) into Eq. (8) yields

$$N_{R}^{(r+1,r+2)} = \left[n_{HR} \bar{N}_{mR}^{(r,r+1)} - \frac{\zeta_{n}(m_{r+1}x_{r+1})}{\zeta_{n}(m_{r+1}x_{r})} \frac{\psi_{n}(m_{r+1}x_{r})}{\psi_{n}(m_{r+1}x_{r+1})} \bar{n}_{HR} N_{mR}^{(r,r+1)} \right], \quad (19)$$

where

$$n_{HR} = m_{r+2} \frac{\psi'_n(m_{r+1}x_{r+1})}{\psi_n(m_{r+1}x_{r+1})} - m_{r+1} \frac{\psi'_n(m_{r+2}x_{r+1})}{\psi_n(m_{r+2}x_{r+1})}, \qquad (20a)$$

$$\tilde{n}_{HR} = m_{r+2} \frac{\zeta'_n(m_{r+1}x_{r+1})}{\zeta_n(m_{r+1}x_{r+1})} - m_{r+1} \frac{\psi'_n(m_{r+2}x_{r+1})}{\psi_n(m_{r+2}x_{r+1})}. \qquad (20b)$$

$$\tilde{n}_{HR} = m_{r+2} \frac{\zeta_n(m_{r+1}x_{r+1})}{\zeta_n(m_{r+1}x_{r+1})} - m_{r+1} \frac{\psi_n(m_{r+2}x_{r+1})}{\psi_n(m_{r+2}x_{r+1})}.$$
 (20b)

Writing

$$D^{(r+1,r+2)} = \zeta_n(m_{r+2}x_{r+1})\psi_n(m_{r+1}x_{r+1}) \times \zeta_n(m_{r+1}x_r) \dots \zeta_n(m_{2}x_1)\psi_n(m_{1}x_1)D_R^{(r+1,r+2)}, \quad (21)$$

one obtains

$$a_n^{(r+1,r+2)} = N^{(r+1,r+2)}/D^{(r+1,r+2)}$$

$$= \frac{\psi_n(m_{r+2}x_{r+1})}{\zeta_n(m_{r+2}x_{r+1})} N_R^{(r+1,r+2)}/D_R^{(r+1,r+2)}.$$
(22)

Equation (19) in conjunction with Eqs. (20a) and (20b) is the starting point for building up analytic expressions for $N_R^{(r+1,r+2)}$ [and also for $D_R^{(r+1,r+2)}$]. One begins with the case r = 1 corresponding to a homogeneous sphere, for which one has

$$N_R^{(1,2)} = n_{HR} = m_2 \frac{\psi_n'(m_1 x_1)}{\psi_n(m_1 x_1)} - m_1 \frac{\psi_n'(m_2 x_1)}{\psi_n(m_2 x_1)}. \tag{23}$$

Because of the involvement of Eqs. (19)–(20b), the final analytic expression consists of logarithmic derivatives of the Ricatti-Bessel functions ψ_n and ζ_n and ratios of the type shown in Eq. (19). It is the particular forms of these ratios which motivated the factorizations given in Eqs. (17)-(18d). For these forms, the ratios have the useful property of boundedness which is discussed below. Appropriate recursion relations determine these ratios as well as the logarithmic derivatives. For example, the logarithmic derivatives of the ψ_n function, represented below by $A_n(z) = \psi'_n(z)/\psi_n(z)$, are calculated by the downward recurrence14:

$$A_{n-1}(z) = n/z - 1/[A_n(z) + n/z]$$
 (24)

with

$$A_N(z) = 0.0 + i0.0, \qquad N > n_{\text{max}},$$
 (24a)

where n_{max} is the cutoff in the series expansion of the cross sections defined in Eqs. (2a)-(2c). The logarithmic derivative of the ζ_n function, denoted by $F_n(z)$, is calculated by the upward recurrence^{14,6}:

$$F_n(z) = -n/z + 1/[n/z - F_{n-1}(z)], \qquad (25)$$

with

$$F_o(z) = -i. (25a)$$

The ratios of the type $\psi_n(m_ix_j)/\psi_n(m_ix_{j+1})$ are calculated in the following manner⁶:

$$\frac{\psi_n(m_ix_j)}{\psi_n(m_ix_{j+1})} = \frac{\psi_{n-1}(m_ix_j)}{\psi_{n-1}(m_ix_{j+1})} \left(\frac{x_j}{x_{j+1}}\right) \frac{\left[m_ix_{j+1}A_n(m_ix_{j+1}) + n\right]}{\left[m_ix_jA_n(m_ix_j) + n\right]},$$
(26)

with the starting ratio

$$\frac{\psi_o(m_i x_j)}{\psi_o(m_i x_{j+1})}$$

being bounded since $x_j < x_{j+1}$ and the imaginary part of m_i is always negative. If $m_i x_j = a_1 - ib_1$ and $m_i x_{j+1} = a_2 - ib_2$, the ratio can be expressed as

$$\frac{\psi_o(m_i x_j)}{\psi_o(m_i x_{j+1})} = \frac{\exp(ia_1) - \exp(-ia_1) \exp(-2b_1)}{\exp(ia_2) - \exp(-ia_2) \exp(-2b_2)} \exp(b_1 - b_2),$$
(27)

which is bounded as $b_1 < b_2$. One sees directly from the expansion for $\psi_n(z)$ that the ratio $\psi_n(m_ix_j)/\psi_n(m_ix_{j+1})$ in Eq. (19) approaches zero as $(x_j/x_{j+1})^n$ when $n \to \infty$. Similarly, we find that the ratios of the type $\zeta_n(m_ix_{j+1})/\zeta_n(m_ix_j)$ encountered in the evaluation of the scattering amplitudes can be calculated as follows:

$$\frac{\zeta_n(m_i x_{j+1})}{\zeta_n(m_i x_j)} = \frac{\zeta_{n-1}(m_i x_{j+1})}{\zeta_{n-1}(m_i x_j)} \left(\frac{x_j}{x_{j+1}}\right) \left[\frac{n - x_{j+1} F_{n-1}(m_i x_{j+1})}{n - x_j F_{n-1}(m_i x_j)}\right] \cdot (28)$$

This relation is derived using the recursion relation

$$\zeta_n(z) = (n/z)\zeta_{n-1}(z) - \zeta'_{n-1}(z). \tag{29}$$

If $m_i x_{i+1} = a_2 - ib_2$ and $m_i x_i = a_1 - ib_1$,

$$\zeta_o(m_i x_{j+1})/\zeta_o(m_i x_j) = \exp[-i(a_2 - a_1)] \exp[(b_1 - b_2)], \quad (30)$$

which is bounded since $b_2 > b_1$. One also notes that, as $n \to \infty$, the ratio on the left-hand side of Eq. (28) must go to zero as $(x_j/x_{j+1})^n$.

We wish to remark here that the finiteness of the logarithmic derivative of $\zeta_n(z)$ for z=0 as well as the bounded nature of the ratio in Eq. (28) prompted us to recast the analytic expressions in terms of the ψ_n and the ζ_n functions as explained earlier in the second paragraph of this section. As before, the denominator $D_R^{(r+1,r+2)}$ in Eq. (22) (corresponding to r layers and a core) is obtained from the numerator $N_R^{(r+1,r+2)}$ by the replacement of $\psi_n(m_{r+2}x_{r+1})$ and its derivative in the latter with $\zeta_n(m_{r+2}x_{r+1})$ and its derivative. Moreover, if the positions of m_{r+2} and m_{r+1} are interchanged in Eqs. (20a) and (20b), the same procedure yields $N^{(r+1,r+2)}$ and $D^{(r+1,r+2)}$ for the scattering amplitude $b_n^{(r+1,r+2)}$.

Below we give expressions for $N_R^{(r,r+1)}$ for a few values of r:

(i) r = 1

$$N_R^{(1,2)} = G_1 \qquad (m_2 = 1);$$
 (31a)

(ii) r = 2

$$N_R^{(2,3)} = G_2 G_6 - S_n Q_n G_7 G_1 \qquad (m_3 = 1); \tag{31b} \label{eq:31b}$$

(iii) r = 3

$$N_R^{(3,4)} = G_3(G_5G_6 - S_nQ_nG_8G_1) - R_nP_nG_4(G_2G_6 - S_nQ_nG_7G_1)$$

$$(m_4 = 1). \quad (31c)$$

where

$$G_{1} = m_{2}A_{n}(z_{1}) - m_{1}A_{n}(z_{2}),$$

$$G_{2} = m_{3}A_{n}(z_{3}) - m_{2}A_{n}(z_{4}),$$

$$G_{6} = m_{2}A_{n}(z_{1}) - m_{1}F_{n}(z_{2}),$$

$$G_{7} = m_{3}F_{n}(z_{3}) - m_{2}A_{n}(z_{4}),$$

$$G_{3} = m_{4}A_{n}(z_{5}) - m_{3}A_{n}(z_{6}),$$

$$G_{5} = m_{3}A_{n}(z_{3}) - m_{2}F_{n}(z_{4}),$$

$$G_{8} = m_{3}F_{n}(z_{3}) - m_{2}F_{n}(z_{4}),$$

$$G_{4} = m_{4}F_{n}(z_{5}) - m_{3}A_{n}(z_{6}),$$

$$(31d)$$

$$z_1 = m_1 x_1, \quad z_2 = m_2 x_1, \quad z_3 = m_2 x_2,$$

$$z_4 = m_3 x_2, \quad z_5 = m_3 x_3, \quad z_6 = m_4 x_3,$$
 (31e)

$$A_n(z_i) = \psi'_n(z_i)/\psi_n(z_i), \quad F_n(z_i) = \zeta'_n(z_i)/\zeta_n(z_i),$$
 (31f)

$$S_n = \zeta_n(z_3)/\zeta_n(z_2), \quad R_n = \zeta_n(z_5)/\zeta_n(z_4),$$
 (31g)

$$Q_n = \psi_n(z_2)/\psi_n(z_3), \quad P_n = \psi_n(z_4)/\psi_n(z_5).$$
 (31h)

Note that the form for $a_n^{(2,3)}$ [and similarly $b_n^{(2,3)}$] we obtain by using Eq. (31b) is different from that employed by Toon and Ackerman⁶ in their calculation for a single-layered sphere. They do not utilize explicitly the ratio S_n given in Eq. (31g), although the ratios Q_n [Eq. (31h)] and the logarithmic derivatives are used. Presence of ratios such as S_n [see Eq. (28)] is a characteristic of our analytic expressions for the scattering amplitudes in general. It may also be mentioned that ratios such as S_n and Q_n and similarly R_n and P_n [see Eqs. (31b) and (31c) come as products. When n is large compared to the size parameters in questions, such products approach zero rapidly. For example, the product S_nQ_n in Eq. (31b) behaves as $(x_1/x_2)^{2n+1}$ when $n \gg x_2$. This has the consequence that for such large values of n, $a_n^{(2,3)}$, given by Eq. (31b) and with $S_nQ_n \cong 0$, reduces to $a_n^{(1,2)}$ corresponding to a homogeneous sphere with parameters m_2, x_2 . In the event that $x_1 \ll$ x_2 (tiny core), the product $S_nQ_n \sim (x_1)^{2n+1}$ for $n \gg x_1$ (a less stringent condition than before), and the amplitude $a_n^{(2,3)}$ in this case also would be essentially given by $a_n^{(1,2)}$ corresponding to the parameters m_2, x_2 . Anyway, in the limit $x_1 \rightarrow 0$, it is clear that the single-layered sphere of Eq. (31b) reduces to the foregoing homogeneous sphere. The same arguments apply to the amplitude $b_n^{(2,3)}$. A similar analysis applied to the double-layered sphere [Eq. (31c)] yields expressions for a single-layered sphere and a homogeneous sphere under appropriate limits.

Although this section has focused on the alternative forms for the scattering amplitudes, similar forms for the remaining scattering coefficients, Eqs. (13) and (14), can also be given.

Before we conclude, we wish to add a note of caution. The calculational procedure can fail if one of the logarithmic derivatives or the ratios involving the ψ_n function becomes very large. This will occur whenever the argument of the ψ_n function is real and very near a zero of the ψ_n function. In addition, since the ratio involving the ψ_n functions is derived from the starting ratio ψ_o $(m_i x_j)/\psi_o(m_i x_{j+1})$ [see Eq. (26)], it will blow up when-

ever $\psi_o(m_i x_{j+1}) = \sin(m_i x_{j+1}) = 0$, i.e., whenever $m_i x_{j+1} = m\pi$, where m is an integer. Thus whenever one of the above undesirable conditions is obeyed, extra checks must be performed to ensure the numerical stability of the calculational procedure.

IV. Conclusion

We have provided a complete set of scattering coefficients for a multilayered sphere. The set includes coefficients needed to describe the fields within the various regions of the sphere. The analytic expressions are derived directly from the Mie coefficients using a prescription which relates the coefficients for an rlayered sphere to those for an (r-1)-layered sphere. This procedure has the advantage that the handling of cumbersome determinants $[(2r \times 2r)]$ when the number of layers is r-1], which normally occur in the expressions, is circumvented. We have further recast the analytic expressions for the scattering amplitudes into a form which we believe should yield numerically stable and accurate results. We have applied this calculational procedure to the calculation of scattering by a double-layered sphere without any problems.^{1,10} It is worth remarking again that, based on our calculational procedure, a computer program for the scattering of a sphere with an arbitrary number of layers is not inconceivable.

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References

- P. Chylek and R. Bhandari, "Specific Absorption of Graphitic Carbon within a Double-Layered Sphere," Appl. Opt., submitted.
- A. L. Aden, "Electromagnetic Scattering from Spheres with Sizes Comparable to the Wavelength," J. Appl. Phys. 22, 601 (1951).
- 3. J. V. Dave, "Subroutines for Computing the Parameters of the Electromagnetic Radiation Scattered by a Sphere," Report 320-3237, IBM Scientific Center, Palo Alto, Calif. (1968).
- J. V. Dave, "Scattering of Visible Light by Large Water Spheres," Appl. Opt. 8, 155 (1969).
- G. A. Kattawar and D. A. Hood, "Electromagnetic Scattering from a Spherical Polydispersion of Coated Spheres," Appl. Opt. 15, 1996 (1976).
- O. B. Toon and T. P. Ackerman, "Algorithms for the Calculation of Scattering by Stratified Spheres," Appl. Opt. 20, 3657 (1981).
- J. R. Wait, "Electromagnetic Scattering from a Radially Inhomogeneous Sphere," Appl. Sci. Res. Sect. B 10, 441 (1963).
- H. E. Bussey and J. H. Richmond, "Scattering by a Lossy Dielectric Circular Cylindrical Multilayer, Numerical Values," IEEE Trans. Antennas Propag. AP-23, 723 (1975).
- 9. Reference 7 (and also Ref. 8) came to the author's attention after the work reported in this paper had been carried out. The prescription for the multilayered sphere, as given in Ref. 7, is not in a form suitable for numerical calculation, but it can be transformed into a calculational form along lines similar to ours.
- R. Bhandari, "Scattering by a Double-Layered Sphere in the Limit of a Thin Inner Shell," Appl. Opt., to be submitted.
- R. Bhandari, "Tiny Core or Thin Layer as a Perturbation in Scattering by a Single-Layered Sphere," J. Opt. Soc. Am. A, submitted.
- H. C. van de Hulst, Light Scattering by Small Particles (Dover, New York, 1981).
- 13. M. Kerker, The Scattering of Light and Other Electromagnetic Radiation (Academic, New York, 1969).
- G. W. Kattawar and G. N. Plass, "Electromagnetic Scattering from Absorbing Spheres," Appl. Opt. 6, 1377 (1967).