Computational Procedures

Computer programmes have been written to simulate light scattering from homogeneous spheres of real refractive index. These programmes allow the computation of four basic representations of scattering :

1. Mie amplitude function $S_p(\vartheta)$
2. Gegenbauer amplitude spectrum $\left(c_n^k\right)_p$
3. Mie irradiance function $\left|S_1(z)\right|^2$
4. Gegenbauer irradiance spectrum $\left(C_l^k\right)_p$

for inner and outer size parameters in the range $0 < \alpha < 1024$ and $0 < \beta \leq 1024$. Such programmes require the accurate generation of Riccati-Bessel functions $\psi_n(\alpha)$, $\psi_n'(\beta)$ and $\chi_n(\alpha)$, $\chi_n'(\beta)$ for orders $n = 0$ to $n > \alpha, \beta$, Gegenbauer polynomials $T_n^k(z)$ for $n = 0$ to $n > \alpha, \beta$ and the decomposition factor ${}^kW_l^{n,m}$ for $0 \leq n, m \leq \alpha, \beta$ and $0 \leq l \leq 2\alpha, 2\beta$.

Bessel Functions

The algorithm used to obtain the two seed values $j_N(z)$ and $j_{N-1}(z)$ is based on Meissels asymptotic approximation of cylindrical Bessel functions for orders greater than the argument [1]. The approximation becomes increasingly accurate for $n \rightarrow \infty$. Meissels formula for half integer order, where $v = n + 1/2$, is given by

$$J_v(z) = \frac{(v\varsigma)^v \exp\left\{v\sqrt{\left(1-\varsigma^2\right)}\right\}\exp\left(-V_v\right)}{e^v\,\Gamma(v+1)\left(1-\varsigma^2\right)^{1/4}\left\{1+\sqrt{\left(1-\varsigma^2\right)}\right\}^v} \qquad 3.0$$

,

where

$$V_v = \frac{1}{24v}\left\{\frac{2+3\varsigma^2}{\left(1-\varsigma^2\right)^{3/2}}-2\right\}-\frac{4\varsigma^2+\varsigma^4}{16v^2\left(1-\varsigma^2\right)^3}$$
$$-\frac{1}{5760v^3}\left\{\frac{16-1512\varsigma^2-3654\varsigma^4-37}{\left(1-\varsigma^2\right)^{3/2}}\right.$$
$$-\frac{32\varsigma^2+288\varsigma^4+232\varsigma^6+13\varsigma^8}{128v^4\left(1-\varsigma^2\right)^6} \qquad 3.1$$

and $\varsigma = z/v$, with the constraint $\varsigma < 1$. To minimise any rounding errors in computing the Gamma function an alternative description was found for $\Gamma(v+1)/(vz)^v$, a simple analysis will show that

$$\frac{\Gamma(v+1)}{(v\varsigma)^v} = \frac{1}{2}\sqrt{\frac{\pi}{v\varsigma}}\prod_{p-1}^{v+1/2}\frac{(2p+1)}{v\varsigma} \qquad 3.2$$

and has a form that lends itself more easily to machine computation.

Gegenbauer Functions

An accurate and fast computational scheme exists for Gegenbauer functions since they are stable under forward recursion. The relationship required for forward recurrence is given by [2]

$$(n+1)T_{n+1}^k(z) = (2k+2n+1)\,z\,T_n^k(z) - (2k+n)\,T_{n-1}^k(z) \qquad 3.3$$

.

Seed values of forward recursion are calculated using

$T_0^k(z) = (2k-1)!! = 1\cdot 1\cdot 3\cdot 5\ldots(2k-1)$ and

$T_1^k(z) = z(2k+1)!! = z\left[1\cdot 3\cdot 5\ldots(2k+1)\right]$.

We judge the accuracy of Gegenbauer recurrence by comparing values of $T_n^k(z)$ when $z=1$ with those calculated directly using the equality

$$T_n^k(1) = \frac{(n+2k)!}{2^k n!\,k!} \qquad 3.4$$

.

An alternative form of this equation is

$$T_n^k(1) = \left\{ \prod_{p=1}^{k} \frac{(n+2k-p+1)}{2} \right\} \left\{ \prod_{p=1}^{k} \frac{(n+2k-p}{p} \right. \quad 3.4$$

,

which is preferred as it is less susceptible to rounding errors. Values computed using Eq. (3.4) are exact and allows forward recurrence to be checked for $z = 1$.

Decomposition Factors

We are principally concerned with first degree Gegenbauer spectra ${}^1W_l^{n,m}$, so only the decomposition factors $k = 1$ will be discussed here for $0 < n, m \le \alpha$. Two basic features of the set of decomposition factors are the large number of such factors and the number of factorials which need to be computed in the evaluation of

$$ {}^1W_l^{n,m} = \frac{1}{4} \frac{(2l+3)}{(l+1)(l+2)} \frac{(s+1)!(s+2)!}{(2s+3)!} \frac{(2a+2)!}{a!(a+1)!} \frac{(2} {b!(\quad 3.5$$

,

where $s = (l+m+n)/2$, $a = (m+n-l)/2$, $b = (l+m-n)/2$ and $c = (l+n-m)/2$. Clearly a strategy is needed which reduces the overall number of mathematical operations that are required.

This is possible by collecting decomposition factors of common l and relating the nearest diagonal and anti-diagonal neighbours by

$$\frac{{}^1W_l^{n+1,m+1}}{{}^1W_l^{n,m}} = \frac{(s+3)}{(2s+5)} \frac{(2a+3)}{(a+1)}; \quad \frac{{}^1W_l^{n-1,m-1}}{{}^1W_l^{n,m}} = \frac{(2s-}{(s+} \quad 3.6a$$

;

and

$$\frac{{}^1W_l^{n+1,m-1}}{{}^1W_l^{n,m}} = \frac{b}{(2b+1)} \frac{(2c+3)}{(c+1)}; \quad \frac{{}^1W_l^{n-1,m+1}}{{}^1W_l^{n,m}} = \frac{(2b-}{(b+} \quad 3.6b$$

.

Other useful relationships are:

$$\frac{{}^1W_{l+2}^{n,m}}{{}^1W_l^{n,m}} = \frac{(l+1)(l+2)}{(l+3)(l+4)} \frac{(2l+7)}{(2l+3)} \frac{(s+3)}{(2s+5)} \frac{a}{(2a+1)} \frac{(2}{(} \quad 3.7a$$

.

$$\frac{{}^{1}W_{l-2}^{n,m}}{{}^{1}W_{l}^{n,m}} = \frac{(l+1)(l+2)}{l(l-1)} \frac{(2l-1)}{(2l+3)} \frac{(2s+3)}{(s+2)} \frac{(2a+3)}{(a+1)} \frac{(2} \quad 3.7b$$

.

In Eqs. (3.6) and (3.7); a, b, c and s are those of ${}^{1}W_{l}^{n,m}$. Eqs. (3.16) and Eqs. (3.17) are the basis of a recurrence scheme for computing all the decomposition factors. The starting point for recurrence of a particular value of l may be

$${}^{1}W_{m}^{0,m} = 1 \quad 3.8a$$

$${}^{1}W_{0}^{n,n} = \frac{3}{2} \frac{(n+1)(n+2)}{(2n+3)} \quad 3.8b$$

$${}^{1}W_{2n}^{n,n} = \frac{(2n)!(2n+1)!\left[(2n+2)!\right]^2}{2\left[(n+1)!\,n!\right]^2 (4n+2)!} \quad 3.8c$$

$${}^{1}W_{1}^{n,n+1} = \frac{5}{2} \frac{(n+1)(n+2)(n+3)}{(2n+3)(2n+5)} \quad 3.8d$$

$${}^{1}W_{2n+1}^{n,n+1} = \frac{(2n+1)!(2n+4)!\left[(2n+2)!\right]^2}{2n!\left[(n+1)!\right]^2 (n+2)!(4n+4)!}, \quad 3.8e$$

whichever is most convenient.

The accuracy of individual decomposition factors may be determined by comparing the factors obtained by recurrence with those given by Eqs. (3.8). A second measure gives the overall accuracy of factors having particular values of m and n by using a sum rule

$$\sum_{l=m-n}^{m+n} {}^{1}W_{l}^{n,m} = T_{n}^{1}(1) \quad 3.9$$

which is shown for $k = 1$ but has been derived for all values of k.

References

1. Watson, G. N. (1944). Meissels first extension of Carlini's formula. A treatise on the Theory of Bessel Functions. Cambridge, University Press: 226-227.
2. Morse, P. M. and H. Feshbach (1953). Boundary conditions and Eigenfunctions. Methods of Theoretical Physics. L. I. Schiff. New York, McGraw-Hill. 1: 781-784.