Improvements to the Chebyshev Expansion of Attenuation Correction Factors for Cylindrical Samples

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Abstract

The accuracy of the Chebyshev expansion coefficients used for the calculation of attenuation correction factors for cylindrical samples has been improved. An increased order of expansion allows the method to be useful over a greater range of attenuation. It is shown that many of these coefficients are exactly zero, others are rational numbers, and others are rational fractions of $\pi^{-1}$. The assumptions of Sears [J. Appl. Cryst. (1984), 17, 226-230] in his asymptotic expression of the attenuation correction factor are also examined.

1. Introduction

Carpenter (1969) (referred to hereafter as paper I) has shown that the attenuation factor for scattering of X-rays and neutrons in cylindrical samples can be expressed for all scattering angles in terms of a Fourier cosine series. Sears (1984) has also calculated these factors by numerical integration and has given tables (Sears, 1983) of values with an accuracy of $10^{-4}$. The accuracy of these values has been verified at scattering angles of 0 and $\pi$ for which a single-quadrature formula can be found (Sears, 1975). Sears has also given an approximate analytic expression for the correction factor which is adequate for most cases of neutron diffraction and inelastic scattering. This asymptotic expression can be expressed approximately in terms of the first two Chebyshev expansion coefficients. Sears justifies this procedure because Carpenter's least-squares-adjusted values of the expansion coefficients are very small beyond the second term. We reexamine this expansion and find that many of these small terms are in fact zero. We also find other interesting properties for these expansion coefficients. With more-accurate values for the expansion coefficients, the limited range of applicability of the Chebyshev expansion method can be extended to greater values of attenuation and with increased accuracy.

2. Attenuation correction

We readdress the problem of computing the attenuation correction factor for X-rays or neutrons in cylindrical samples. We assume that the cylinder is bathed uniformly by the incident radiation, which is attenuated as it travels a distance $l$ to the point of scattering, and the emerging radiation is similarly attenuated travelling a distance $l'$. If the sample is viewed uniformly by the detector, the attenuation correction factor is given by $\langle\exp(-\mu l)\exp(-\mu' l')\rangle$, where the brackets $\langle\cdots\rangle$ denote an average over all points within the volume exposed to the incident beam, and where $\mu$ and $\mu'$ are the absorption coefficients for the incident and scattered radiation. For clarity, we take the case for elastic scattering ($\mu = \mu'$), even though the Chebyshev expansion method is probably more important for the computation of attenuation factors in neutron inelastic scattering, for which other methods may not be valid.

Various tables of values for the attenuation factor, $A(\theta)$, have been given (Weber, 1967; Rouse, Cooper, York & Chakera, 1970; International Tables for X-ray Crystallography, 1985) for cylindrical samples in which the scattering plane is perpendicular to the cylinder axis, and for limited ranges of $\mu R$. $R$ is the cylinder radius and $\theta$ is the scattering angle. Modern data-analysis methods make direct calculation of the attenuation correction preferable to table interpolation. Rouse et al. (1970) have given analytic expressions which may be used for calculating approximate attenuation correction factors with limited accuracy. For cylindrical samples these are given by

$$A(\theta) = \exp\left\{-\sum_{i=1}^{2} [a_i + b_i \sin^2(\theta/2)](\mu R)^i\right\}, \quad (1)$$

where the accuracy is $<0.0035$. Table 1 gives the values for the coefficients $a_i$ and $b_i$. Hewat (1979) has noted the advantages of this form of the attenuation correction for the refinement of neutron powder
Table 1. Values of the constants to be used for equation (1)

<table>
<thead>
<tr>
<th>Value</th>
<th>Least-squares adjusted values</th>
<th>Asymptotic values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_1$</td>
<td>1.7133</td>
<td>2$a_1 = 1.6977$</td>
</tr>
<tr>
<td>$b_1$</td>
<td>-0.0368</td>
<td>0</td>
</tr>
<tr>
<td>$a_2$</td>
<td>-0.0927</td>
<td>$2a_2^2 = -0.0590$</td>
</tr>
<tr>
<td>$b_2$</td>
<td>-0.3750</td>
<td>-1/2</td>
</tr>
</tbody>
</table>

Diffraction data. For example, $k = \exp[-a_1 \mu R - a_2 (\mu R)^2]$ gives a scaling factor, and $\Delta B = \lambda [b_1 \mu R - b_2 (\mu R)^2]$ gives an overall Debye–Waller factor.

Higher accuracy may be achieved either by a Fourier expansion (paper I) or by a 15th-degree Gauss product formula (Stroud, 1971). The latter method computes the attenuation using the expression

$$A(\theta) = \frac{1}{2} \sum_{n=1}^{16} \sum_{m=1}^{4} b_n \exp\{- 2 \[\mu \left[1 - \rho_n \sin^2(m \pi/8)\right]^{1/2} - \rho_n \cos(m \pi/8)\] + \mu \left[1 - \rho_n \sin^2((\pi - \theta) - m \pi/8)\right]^{1/2} - \rho_n \cos((\pi - \theta) - m \pi/8)\}.$$  

(2)

Table 2 gives the values of the constants $b_n$ and $\rho_n$ to be used with this formula. The Fourier expansion requires the minimum of computation time by using Chebyshev polynomials in $\cos \theta$. The attenuation correction factor is given by

$$A(\theta) = (\pi R^2) \int_{\theta = 0}^{\pi} \exp(-\mu l) \exp(-\mu l') \rho \rho' d\rho d\rho'$$

$$= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{(-\mu R)^m (-\mu R')^n}{m!n!}$$

$$\times \sum_{s=0}^{\infty} c_s(m,n) \cos(s \theta),$$  

(3)

with the summations extending over a range dependent on the required accuracy. Carpenter has given the coefficients $c_s(m,n)$ for $(m + n) \leq 5$, which limits the range of applicability. We give an improvement to the Chebyshev expansion method in this paper, by computing the coefficients $c_s(m,n)$ to greater accuracy and determining which values are truly zero, and by extending the range over which the coefficients are computed. This increases the range of attenuation for which the technique is valid.

Sears (1984) has calculated attenuation factors for scattering of X-rays and neutrons in cylindrical samples by numerical integration and has given tables (Sears, 1983) of values with an accuracy of $10^{-4}$. The accuracy of these values has been verified at scattering angles of 0 and $\pi$ for which a single-quadrature formula can be found (Sears, 1975). Sears has also given an approximate analytic expression which for elastic scattering reduces to

$$A(\theta) = \exp(-2a_1 \mu R)[1 + 4b_1 (\mu R)^2 - \frac{1}{2}(\mu R)^2 \cos^2(\theta/2)],$$

(4)

where $a_1 = 8/3\pi = 0.8488$ and $b_1 = (1 - a_1^2)/2 = 0.1397$. This expression has been derived on the basis of knowing the exact expression at scattering angles of 0 and $\pi$, and justified since it can be expressed using only the first two coefficients in the Chebyshev expansion for intermediate scattering angles. This seems reasonable since the convergence of this expansion is much more rapid than for other expansions. Assuming that (4) has the leading terms of the Rouse formulism, Sears has given asymptotic values of the constants $a_1$ and $b_1$ (see Table 1) to be used in equation (1) of Rouse et al. The Sears values give far smaller errors in $A$ than the interpolation formula of Rouse et al. for $\mu R < 0.2$.

3. Chebyshev Expansion

Carpenter (1969) has given in paper I a method of calculating the value of $A$ for any value of $\theta$ and $\mu R$, by expanding the exponentials in terms of a power series, and expressing the resulting simplified integrals in terms of Chebyshev expansions. The attenuation correction factor is given by

$$A(\theta) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{(-\mu R)^m + n}{m!n!} Z_{mn}(\theta),$$

(5)

where the functions $Z_{mn}(\theta)$ are given by

$$Z_{mn}(\theta) = \sum_{s=0}^{\infty} c_s(m,n) \cos(s \theta),$$

(6)

and the terms $c_s(m,n)$ are the Chebyshev expansion coefficients of the simplified integrals. Carpenter calculated values of $Z_{mn}(\theta)$ directly by expanding in terms of a Fourier cosine series and determined the coefficients $c_s(m,n)$ by least-squares fitting. In prac-
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Carpenter considers the case of inelastic neutron scattering by cylindrical samples for which the attenuation coefficients for the incident and emergent radiations are different. This general method of computing attenuation correction factors can be extended (Mildner, Carpenter & Pelizzari, 1974; referred to hereafter as paper II) to cases in which the scattering plane is not perpendicular to the cylinder axis.

This expansion is an absolutely convergent series, and in practice we may compute all terms up to $(m + n) = N$ for the determination of $A$. Therefore the error (precision) is less than the $(N + 1)$th-order term, so that for all $\theta$ the error is less than $(2\mu R)^{N+1}Z_{0,N+1}/(N+1)!$. Values of $A$ obtained by this method for $N = 5$ have been shown to be in reasonable agreement with those found in International Tables for X-ray Crystallography for $\mu R < 0.6$, beyond which the calculated values diverge dramatically.

In paper II we have extended this range by expressing the attenuation correction as the product of an approximate correction factor and a series expansion that corrects this approximate factor. This procedure gives reasonable approximations for $A$ for values of $\mu R < 2.0$. Some average distance $l$ is chosen as typical of the distances $l$ and $l'$ (see below), so that the attenuation correction factor is now given by

$$A(\theta) = \exp(-2\mu l) \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{(-\mu R)^{m+n}}{m!n!} Y_{mn}(\theta),$$

where the functions $Y_{mn}(\theta)$ are given by

$$Y_{mn}(\theta) = \sum_{i=0}^{m} \sum_{j=0}^{n} \left( \begin{array}{c} m \\ i \end{array} \right) \left( \begin{array}{c} n \\ j \end{array} \right) (-l/R)^{m+n-i-j}Z_i(\theta),$$

the terms $\left( \begin{array}{c} m \\ i \end{array} \right)$ are the binomial coefficients and the functions $Z_i(\theta)$ are as before.

These expansions also give an alternating convergent series, and computing all terms for which $(m + n) < N$ gives an error (precision) to the determination of $A$ which is less than the $(N + 1)$th-order term. This can be shown to be given by

$$\exp(-2\mu l) \frac{(2\mu R)^{N+1}}{(N+1)!} \sum_{j=0}^{N+1} \left( \begin{array}{c} N+1 \\ j \end{array} \right) (-l/R)^{N+1-j}Z_j.$$
P is the \( p \) integral given by

\[
P = \int_0^1 \rho \, d\rho \, (-1)^{n-j+k+l} (2+m-i+2k+n-j+2l)^{-1},
\]

(12)

and \( \Xi \) is the \( \xi \) integral given by

\[
\Xi = \pi^{-1} \int_0^{2\pi} \cos(\xi)^{m-i} \sin(\xi)^{(p-q)} \, d\xi \times (\sin(\xi)^{2k+2l+(p-q)}) \, d\xi,
\]

(13)

which is non-zero only if the exponents of \( \cos \xi \) and \( \sin \xi \) are both even. The coefficients \( \binom{i/2}{k} \) are given by \( \frac{(i/2)!}{k!(i/2-k)!} \). Hence for even \( i \) these are the binomial coefficients and are 0 for \( k > i/2 \), and for odd \( i \) the coefficients exist for all values of \( k \). The coefficients are unity for \( k = 0 \) (for non-zero \( i \)), and zero for \( i = 0 \) and \( k = 0 \).

The powers of \( \cos \theta \) and \( \sin \theta \) may be expressed in terms of \( \cos(s\theta) \) using the Chebyshev polynomials. Hence the coefficients \( c_s(m,n) \) may be determined by comparison of (6) with the results of the computation of \( Z_m(\theta) \) in (11) in terms of \( \cos(s\theta) \). Earlier, Carpenter (1969) has commented that the smaller coefficients in his table for \( (m+n) < 5 \) are probably insignificant. Indeed, we find that many of the smaller Chebyshev expansion coefficients obtained for \( Z_m(\theta) \) in paper I are in fact zero, and some others are rational numbers. For example, it can be seen from (13) that \( p-q \) must be even for non-zero contributions, and from (11) that for even values of \( j \) the maximum exponent of \( \cos \theta \) is \( n \). Hence we find for all \( m \) that \( c_s(m,n) = 0 \) when \( s = n+2, n+4 \) etc. Since \( c_s(m,n) = c_s(n,m) \), this implies further zeros when \( m \) is even and \( n \) is odd, and vice versa. The coefficients \( c_s(m,n) \) are rational numbers when \( s, m \) and \( n \) all have the same parity, since both \( i \) and \( j \) must be even for non-zero contributions, so that the sums on \( k \) and \( l \) are finite and each term is a rational fraction. In all other cases, the non-zero coefficients \( c_s(m,n) \) are irrational numbers and their computed accuracy is determined by the upper limit of the slowly converging infinite sums on \( k \) and \( l \) in (11).

The numerical accuracy of the coefficients determined using the power-series expansion is limited. As an alternative, the expansion coefficients may be projected out by noting that

\[
\int_{-\pi}^{\pi} Z_{s\theta}(\theta) \cos t \theta \, d\theta = \sum_{s=0}^{\infty} c_s(m,n) \int_{-\pi}^{\pi} \cos s \theta \cos t \theta \, d\theta
\]

\[
= \begin{cases} 
\pi c_s(m,n) & t \neq 0 \\
2\pi c_s(m,n) & t = 0.
\end{cases}
\]

(14)

This method requires the evaluation of integrals given by (9). For \( s > 0 \), the Chebyshev expansion coefficients are given by

\[
c_s(m,n) = \pi^{-2} \int_0^1 \rho \, d\rho \int_0^{2\pi} \rho \cos \xi \cos s \theta \, d\theta \times (1 - \rho^2 \sin^2 \xi)^{1/2} \]

\[
+ \frac{1}{2\rho^2} \sin^2 \xi - \rho \cos(\xi + \theta) \]

\[
+ [1 - \rho^2 \sin^2(\xi + \theta)]^{1/2} \pi \]

\[
s > 0.
\]

(15)

These integrals may be evaluated numerically using a power-series expansion for the complete elliptical integrals. (It has been useful in the case of the lower-order coefficients to note that the integrals are \( \rho \) moments of combinations of complete integrals of the first and second kinds, which are expressible in terms of infinite summations.) When \( s \) has the same parity as \( m \) (or \( n \)), the \( \xi \) (or \( \psi \)) integral in (16) gives an expression involving \( \pi \) multiplied by a polynomial in \( \rho \). This gives rise to the general properties of the Chebyshev expansion coefficients given in the Appendix. This method can be used for the lower-order coefficients, and has served as a check on the power-series expansion [(11)].

We give the values of the coefficients \( c_s(m,n) \) for \( (m+n) < 10 \) in Table 3 with an accuracy of at least \( 10^{-4} \), and of \( 10^{-6} \) for the lower-order coefficients. A large number of the coefficients are zero. Those coefficients which can be expressed as rational fractions of \( \pi^{-1} \) have been computed directly and are given with an accuracy of \( 10^{-7} \). About 30% of the coefficients are irrational numbers and require evaluation with some degree of precision. A few lower-order irrational coefficients have been determined numerically using elliptical integrals with an accuracy of \( 10^{-7} \). While we have established by the elliptical integral technique those coefficients \( c_s(m,n) \) which are rational numbers, we have not been able to deduce a generally useful formula to predict those coefficients. Some coefficients with irrational values can be expressed as rational fractions of \( \pi^{-1} \), in the same way as \( c_0(m,0) = Z_{0m, m} \).
Table 3. Chebyshev expansion coefficients for the calculation of $Z_{m,n}(\theta)$

Coefficients $c_{m,n}$ for $s$ up to 9 and $m + n \leq 10$.

<table>
<thead>
<tr>
<th>$s$</th>
<th>$c_{(1,1)}$</th>
<th>$c_{(1,2)} = c_{(2,1)}$</th>
<th>$c_{(1,3)} = c_{(3,1)}$</th>
<th>$c_{(1,4)} = c_{(4,1)}$</th>
<th>$c_{(1,5)} = c_{(5,1)}$</th>
<th>$c_{(1,6)} = c_{(6,1)}$</th>
<th>$c_{(1,7)} = c_{(7,1)}$</th>
<th>$c_{(1,8)} = c_{(8,1)}$</th>
<th>$c_{(1,9)} = c_{(9,1)}$</th>
<th>$c_{(2,2)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.7302420</td>
<td>0.8488264</td>
<td>1.1390928</td>
<td>1.6410643</td>
<td>2.5089764</td>
<td>3.9870587</td>
<td>6.524778</td>
<td>10.9132508</td>
<td>18.598772</td>
<td>1.0</td>
</tr>
<tr>
<td>1</td>
<td>-0.25</td>
<td>-0.4527074</td>
<td>-0.75</td>
<td>-1.2417117</td>
<td>-2.0833333</td>
<td>-3.5477477</td>
<td>-6.125</td>
<td>-10.7029696</td>
<td>-18.9</td>
<td>-0.821191</td>
</tr>
<tr>
<td>2</td>
<td>0.0194715</td>
<td>0.0565884</td>
<td>0.118072</td>
<td>0.2263537</td>
<td>0.419067</td>
<td>0.7712938</td>
<td>1.408755</td>
<td>2.5871535</td>
<td>4.735539</td>
<td>0.1666667</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>0.000229</td>
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<td>-0.0048504</td>
<td>-0.012138</td>
<td>0.0011549</td>
<td>0.0003274</td>
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<td>0.0000030</td>
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<td>0</td>
</tr>
<tr>
<td>6</td>
<td>0.000012</td>
<td>0</td>
<td>-0.000025</td>
<td>0</td>
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<td>0</td>
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<td>7</td>
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<td>0</td>
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<tr>
<td>8</td>
<td>0.000001</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Where coefficients may be expressed as rational fractions of $\pi^{-1}$, their values have been given to seven decimal places. Those coefficients marked * have been evaluated numerically using complete elliptical integrals.

Values of $Z_{m,n}(\theta)$ which are constant: $Z_{00} = 1; Z_{01} = 8/3\pi; Z_{02} = 1; Z_{03} = 64/15\pi; Z_{04} = 2; Z_{05} = 1024/105\pi; Z_{06} = 5; Z_{07} = 8192/315\pi; Z_{08} = 14; Z_{09} = 262144/3465\pi; Z_{010} = 42$. 

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Table 4. Values of $\mu R$ below which the calculations of $A$ using the Chebyshev expansion of Carpenter (1969) for $(m + n) \leq 5$ and $(m + n) \leq 7$ for different scattering angles $\theta$ are within 2% and 3% of the values quoted in International Tables for X-ray Crystallography.

$A(1)$ is the value calculated using the Chebyshev expansion and $A(I)$ is the value given in International Tables for X-ray Crystallography.

The precision of the computations is less than 2% for $\mu R < 0.6$ for $(m + n) \leq 5$ and for $\mu R < 0.84$ for $(m + n) \leq 7$.

<table>
<thead>
<tr>
<th>$\theta$</th>
<th>$(m + n) \leq 5$</th>
<th>$(m + n) \leq 7$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$\mu R &lt; 0.70$</td>
<td>$\mu R &lt; 1.00$</td>
</tr>
<tr>
<td>60</td>
<td>0.68</td>
<td>0.99</td>
</tr>
<tr>
<td>90</td>
<td>0.63</td>
<td>0.90</td>
</tr>
<tr>
<td>120</td>
<td>0.56</td>
<td>0.82</td>
</tr>
<tr>
<td>180</td>
<td>0.53</td>
<td>0.74</td>
</tr>
</tbody>
</table>

odd. We have found these by the elliptical integral technique, though again we have not been able to find a simple general rule.

Some useful properties of the functions $Z_{mn}(\theta)$ are given in paper I. We can formulate useful sum rules for the Chebyshev expansion coefficients by considering two special cases. For the scattering angle $\theta = \pi$, the distances $l$ and $l'$ are equal which leads to the identity $Z_{mn}(\pi) = Z_{0(m+n)}$, and to the sum rule

$$
\sum_{s=0}^{\infty} (-1)^s c_s(m,n) = Z_{0(m+n)}.
$$

(17)

For the scattering angle $\theta = 0$, $l/R + l'/R = 2 \times (1 - \rho^2 \sin^2 \theta)^{1/2}$, so that (9) is integrable. It can be shown that this leads to the sum rule

$$
\sum_{s=0}^{\infty} c_s(m,n) = Z_{0(m+n)} / \binom{m+n}{m}.
$$

(18)

We find that these sum rules are obeyed very well for the coefficients that we have computed. Further details are found in the Appendix.

Results using this enlarged table of Chebyshev coefficients show that for $(m + n) \leq 7$ the straightforward expansion is now adequate for $\mu R < 0.9$ (slightly lower for larger scattering angles), as opposed to $\mu R < 0.6$ for $(m + n) \leq 5$. The computations again diverge dramatically from those found in International Tables for X-ray Crystallography for larger values of $\mu R$ (a consequence of the truncation of the expansion). These results are illustrated in Table 4. The Chebyshev expansion for $(m + n) \leq 9$ is sufficiently accurate for $\mu R < 1.0$ (which is the usual range for neutron diffraction).

Extra precision may be obtained by using the Chebyshev expansion as a correction to an approximation to $A$, as in paper II, though it is less easy to express these results. The accuracy of computing an attenuation correction factor depends on the ratio $l/R$, the best value of which varies with the scattering angle $\theta$, especially for large values of the attenuation coefficient $\mu$. The results are reasonable for $\mu R < 2.5$ for $(m + n) \leq 7$, as opposed to $\mu R < 2.0$ for $(m + n) \leq 5$, when $l/R$ is set equal to unity. For large attenuation coefficients and large scattering angles $(\theta - \pi)$, the best value of $l/R$ is smaller as expected. We find that the Sears formulism has in effect taken out an approximate factor, $\exp(-2\mu l/R)$, which is equivalent to $\exp(-2\mu l)$, such that $l/R = a = 0.8488$, which is certainly in the region of the best $l/R$ for all scattering angles $\theta$ (see paper II).

5. Asymptotic approximation

Sears has shown that his asymptotic expression can be expressed approximately in terms of Carpenter's Chebyshev expansion coefficients by

$$
A(\theta) = 1 - 8/3\pi(2\mu R) + (\mu R)^2[1 + Z_{11}(\theta)],
$$

(19)

where

$$
Z_{11}(\theta) = \begin{cases} 
1/2 & \theta = 0 \\
1 & \theta = \pi.
\end{cases}
$$

$Z_{11}(\theta)$ is an even function of $\theta$ and may be expanded in terms of a Fourier cosine series

$$
Z_{11}(\theta) = \sum_{s=0}^{\infty} c_s(1,1) \cos(s\theta)
$$

(20)

as in (6). Sears has shown that the exact values for $A$ at $\theta = 0$ and $\pi$ produces the following sum rules:

$$
\sum_{s=0}^{\infty} c_s(1,1) = 1/2 \quad \theta = 0
$$

$$
\sum_{s=0}^{\infty} (-1)^s c_s(1,1) = 1 \quad \theta = \pi.
$$

(21)

These are consistent with the more-general sum rules for all $m, n$ given by (17) and (18). Sears keeps only the first two values of $s$, and assumes effectively, therefore, that $c_0(1,1) = 3/4$, $c_1(1,1) = -1/4$ and $c_s(1,1) = 0$ for $s \geq 2$. From these two coefficients he obtains values for the constants to be used in the formula of Rouse et al. [equation (1) and see Table 1].
Comparison of values of $c_s(1,1)$ used by Sears and the coefficients both found by least-squares adjustment by Carpenter and by direct expansion and/or the elliptical integral technique in the present work are given in Table 3. We find that $c_s(1,1) = 0$ for odd $s > 1$ anyway, so that $c_s(1,1) = -1/4$ exactly. We find that $c_0(1,1) = 0.7302420$ by the projection technique [equation (14)], so that $c_0(1,1) = 3/4$ is a reasonable approximation (Sears, 1984). We also find that $c_0(1,1) = 0.0194715$, rather than zero.

The advantage of using the Chebyshev expansion is that the convergence is much quicker than for other expansions. In practice, however, only the sum of the even $s$ coefficients $c_s(1,1)$ is equal to $3/4$. $Z_{11}(\theta)$ is really given by

$$Z_{11}(\theta) = \sum_{s=0}^{\infty} c_s(1,1) \cos(s\theta)$$

$$= -\frac{1}{2} \cos \theta + \sum_{\text{even } s} c_s(1,1) \cos(s\theta).$$

By assuming that this last term may be approximated by $3/4$, Sears has determined

$$A(\theta) = 1 - \frac{3}{4} \pi(2\mu R) + 2(\mu R)^2 - \frac{1}{4}(\mu R)^2 \cos^2(\theta/2).$$

If we take the actual expansion coefficients for $Z_{11}(\theta)$ given in Table 3, and expand (21) in terms of powers of $\cos^2(\theta/2)$, we may obtain modified asymptotic values for the formula of Rouse et al. [11], but the values do not give as good an approximation to the attenuation as those of Sears.

6. Concluding remarks

The attenuation correction factor $A(\theta)$ for all scattering angles $\theta$ can be expressed in terms of a cosine series of functions $Z_{mn}(\theta)$, which are independent of scattering angle $\theta$ for $m$ or $n$ equal to zero, using Chebyshev expansion coefficients $c_s(m,n)$, as outlined by Carpenter. Sears has shown for scattering angles $\theta = 0$ and $\pi$ that these factors can be determined explicitly, so that the summation of the coefficients $c_s(m,n)$ for odd and even $s$ can be determined for all $m, n$.

We have computed values of $c_s(m,n)$ to six decimal places for all $m, n$ for $(m + n) \leq 10$, and for $s$ between 0 and 9, and shown that many of these coefficients are identically equal to zero. The values of $c_s(1,1)$ for $s > 1$ are found to be very small, which justifies Sears’ neglect of these terms in his approximation. (Though small, the neglected even terms are in fact non-zero.)

We have found some interesting properties of these expansion coefficients; the summation of coefficients $c_s(m,n)$ may be expressed in terms of fractions of $Z_{0(m+n)}$, also the difference between the summation of the coefficients $c_s(m,n)$ for even $s$ and the summation of $c_s(m,n)$ for odd $s$ is given exactly by $Z_{0(m+n)}$. These sum laws provide a check on the accuracy of the computation of the coefficients. We find that the sum laws for our computed coefficients are obeyed very well. When both $m$ and $n$ are even (odd), these summations are rational numbers, and the coefficients themselves are also rational numbers for even (odd) $s$. When $m$ and $n$ are mixed indices, these summations are rational fractions of $\pi^{-1}$, and the coefficients themselves are also rational fractions of $\pi^{-1}$ for all $s$.

With the corrected values of the expansion coefficients and the extension of the range over which they are tabulated, the result provides for calculations of the attenuation correction to within 2% for $\mu R < 1$, and for all scattering angles. If an angular-independent approximation to the attenuation correction is assumed {such as $\exp[-(\mu + \mu')l]$ where $l = (\pi/4)R$, the half mean chord, or even $l = R$}, and the Chebyshev expansion technique is applied as a refinement to that approximation, then the calculations of the attenuation corrections are valid for $\mu R < 2.5$, a range far beyond that generally useful for neutron scattering.

APPENDIX

Properties of Chebyshev expansion coefficients

We have computed values of the Chebyshev expansion coefficients $c_s(m,n)$ to six decimal places for all $m, n$ for $(m + n) \leq 10$, and for $s$ between 0 and 9. We find the following general properties for these coefficients.

If $m$ and $n$ are both even (or both odd), the only non-zero coefficients for even (odd) values of $s$ exist for all $s$ up to a maximum of the lesser of $m$ and $n$; these non-zero coefficients are rational numbers (these are given in Table 5). Coefficients for odd (even) values of $s$ are irrational.

If $m$ and $n$ are of mixed parity, the only non-zero coefficients for even (odd) values of $s$ exist for all $s$ up to a maximum of the even (odd) value of $m$ or $n$;
all these non-zero coefficients may be expressed as rational fractions of $\pi^{-1}$ (these are given in Table 7).

If either $m$ or $n$ is 0, the only non-zero coefficient is for $s = 0$; that is, $Z_{m0}$ is a constant and independent of $\theta$.

In effect, this means that the coefficient $c_s(m,n)$ is zero for values of $s$ where:

1. both $m$ and $n$ are even (odd), and $s$ is even (odd) and greater than the lesser of $m$ and $n$;
2. either $m$ or $n$ is even (odd), and $s$ is even (odd) and greater than $m$ or $n$.

We find the following sum rules for the Chebyshev expansion coefficients $c_s(m,n)$:

For any given values of $m$ and $n$, the sum of the coefficients is equal to $Z_{\theta(m+n)}$ divided by $\binom{m+n}{m}$; that is

$$\sum_{s=0}^{\infty} c_s(m,n) = Z_{\theta(m+n)} \binom{m+n}{m}. \quad (A1)$$

For any given values of $m$ and $n$, the difference between the sum of the coefficients for even values of $s$ and the sum of the coefficients for odd values of $s$ is exactly equal to $Z_{\theta(m+n)}$; that is,

$$\sum_{s=0}^{\infty} (-1)^s c_s(m,n) = Z_{\theta(m+n)}. \quad (A2)$$

We find that the sum laws are obeyed exactly for $m$ and $n$ having mixed parity since each coefficient is known exactly (all are rational fractions of $\pi^{-1}$). The coefficients for $m$ and $n$ with the same parity evaluated using infinite sums also obey the sum laws remarkably well.

For $m$ and $n$, the coefficients are known exactly, but the degree of accuracy for coefficients with $s$ having the opposite parity to $m$ and $n$ decreases with increasing values of $(m+n)$. On the other hand, their importance to the computation of the attenuation correction factor is modified by the inverse of $m!n!$ [see (3)].

Those coefficients which are rational or irrational numbers may be deduced from inspection of (16). If $s$ and $m$ have the same parity, the $\theta$ integral may be evaluated as $\pi$ multiplied by a finite polynomial in $\rho$.

If $s$ and $m$ have opposite parity, the $\theta$ integral may be evaluated as finite polynomials in $\rho$ multiplied by elliptical integrals of the first and second kind, and similarly for the $\psi$ integral. The $\rho$ integral of the elliptical integrals can be evaluated as the sum of rational numbers. Hence the evaluation of $c_s(m,n)$ by (16) gives the following results:

1. If $m$ and $n$ have similar parities to $s$, $c_s(m,n)$ is a rational number (see Table 6).
2. If $m$ and $n$ have similar parities, but opposite to $s$, $c_s(m,n)$ is an irrational number.
3. If $m$ and $n$ have opposite parities, $c_s(m,n)$ is a rational number multiplied by $\pi^{-1}$, for all $s$ (see Table 7).

We have found from the evaluation of (16) the following general relationship between certain coefficients:

$$c_s(m,s+2) = (s+2)c_s(m,s), \quad \text{for all } s \geq 1, \text{ and for all } m$$

(A3)
though for $s = 0$, we note that $c_0(m, 2) = c_0(m, 0) = Z_{0m}$ for all $m$. This relationship together with the sum rules allows the evaluation of all coefficients which are either rational numbers or rational fractions of $\pi^{-1}$ from the computation of a smaller set.

Carpenter (1969) has given the formula for $Z_{0n}$

$$Z_{0n} = 2^{n+1} \Gamma [(n+1)/2] / \pi^{1/2} \Gamma (n/2 + 1).$$

(A44)

If $n$ is even, we have

$$Z_{0n} = \prod_k [2(2k-1)/(k+1)] Z_{00},$$

(A5)

which reduces to

$$\left( \frac{n}{n/2} \right) / (n/2 + 1).$$

Hence the values of the function $Z_{0n}$, where $n$ is even, form the series given by the Catalan numbers, 1, 2, 5, 14, 42, 132, 429, .... On the other hand, if $n$ is odd, we have

$$Z_{0n} = \prod_k [2(2k-1)/(2k + 1)] Z_{01},$$

(A6)

which reduces to $Z_{0n} = 8^{n+1}/[(n+1)!/(n/2)!] \pi$.

We have deduced from the sum rules further relationships between successive coefficients given in Tables 6 and 7. The ratio of every other constant coefficient $c_0(0, n) = Z_{0n}$ is given by

$$\frac{Z_{0(n+2)}}{Z_{0n}} = \frac{4(n+1)}{(n+4)}.$$

(A7)

valid for all $n$. The coefficients $c_1(1, n) = -Z_{0(n+1)n} \times [2(n+1)]^{-1}$, so that the relationship

$$\frac{c_1(1, n+2)}{c_1(1, n)} = \frac{4(n+1)(n+2)^2}{n(n+3)(n+5)}$$

(A8)

holds for all $n \geq 1$. Also the coefficients $c_2(2, n) = Z_{0(n+2)} / [2(n^2 + 3n + 4)/[2(n+1)(n+2)] - Z_{0n0}$, so that the relationship

$$\frac{c_2(2, n+2)}{c_2(2, n)} = \frac{4(n+1)(n+2)^3}{n^2(n+4)(n+6)}$$

(A9)

holds for all $n \geq 2$. There does not appear, however, to be a more general formula.

References


