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Asymptotic solution for an integral appearing in the theory of small-angle X-ray scattering. By K. Šolc,

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The integal corresponding to the smeared intensity scattered by uniform spheres and observed with a slit of infinite height and negligible width, is solved in the form of an asymptotic series. The present result complements Schmidt's solution in the form of a convergent series. The combination of both methods enables a fast and accurate computation of the integral for any value of the argument with no need for tables of Bessel functions and/or numerical integration.

In the theory of small-angle X-ray scattering by uniform spheres one encounters the integral

$$I(x)=\int_0^\infty i(z)\mathrm{d}y \tag{1}$$

where $z=(x^2+y^2)^{1/2}$, and the function $i(z)$ is defined by

$$i(z)=(\sin z-z\cos z)^2/z^6. \tag{2}$$

This integral corresponds to the smeared scattered intensity observed for slits of infinite height and negligible width. It is useful as a test function for collimation-correction programs (Schmidt, 1955) as well as for direct comparison with experimental data on systems containing spherical particles [such as latexes (Bonse & Hart, 1967)]. The integral $I(x)$ can be expressed in terms of the Bessel function $J_0(2x)$, its derivative $J_0'(2x)$ and its integral

$$\bar{J}_0(2x)=\int_0^{2x} J_0(\xi)\mathrm{d}\xi;$$

hence, it is easily accessible in the common range of the variable x (Schmidt, 1955). For high values of the argument x, however, tables of $\bar{J}_0(2x)$ may not be available, and in the absence of other formulas, one would have to resort to numerical integration. In this note, we present an asymptotic solution for $I(x)$ which can be used with good accuracy for $x>6$.

After representing $\sin z$ and $\cos z$ of the integrand by functions of double argument, the integral $I(x)$ can be split in two parts

$$I(x)=I_A(x)+I_B(x) \tag{3}$$

where

$$I_A(x)=\int_x^\infty \frac{(z^2+1)}{2z^5(z^2-x^2)^{1/2}}\,\mathrm{d}z=\frac{\pi}{8x^3}\left(1+\frac{3}{4x^2}\right) \tag{4}$$

$$I_B(x)=\tfrac{1}{2}\int_x^\infty \frac{(z^2-1)\cos(2z)-2z\sin(2z)}{z^5(z^2-x^2)^{1/2}}\,\mathrm{d}z\,. \tag{5}$$

The second integral can be solved by substitution of $z=x(1+2\xi)$. This operation leads to Fourier integrals of the form

$$I_n(x)=\int_0^\infty \frac{\exp(4ix\xi)}{\xi^{1/2}(1+\xi)^{1/2}(1+2\xi)^n}\,\mathrm{d}\xi\,,\quad n=3,4,5\,, \tag{6}$$

which can be expressed as asymptotic series (Erdélyi, 1956)

$$I_n(x)=\tfrac{1}{2}(i/x)^{1/2}\sum_{m=0}^{M-1} i^m X_m(n)+\mathrm{O}(x^{-M})\quad\text{as}\quad |x|\to\infty\,, \tag{7}$$

where

$$X_m(n)=\Gamma(m+\tfrac{1}{2})\,(4x)^{-m}\sum_{l=0}^{m}\binom{-n}{l}\binom{-\frac{1}{2}}{m-l}2^l. \tag{8}$$

The order $\mathrm{O}(x^{-M})$ of the remainder in (7) is applied in the sense defined by Erdélyi (1956), and it does not necessarily imply that the absolute value of the remainder should be of the order of magnitude of x^{-M}. Since the numerical estimate of the remainder does not seem to be trivial, we refrained from this problem.

The sought integral $I_B(x)$ of equation (5) can thus be approximated as

$$\begin{aligned}I_B(x)\simeq{}&2^{-5/2}x^{-7/2}\\&\times\{\cos(2x)\sum_{m=0}[\tau_mX_m(3)\\&-2x^{-1}\sigma_mX_m(4)-x^{-2}\tau_mX_m(5)]\\&-\sin(2x)\sum_{m=0}[\sigma_mX_m(3)+2x^{-1}\tau_mX_m(4)\\&-x^{-2}\sigma_mX_m(5)]\}\end{aligned} \tag{9}$$

where τ_m and σ_m represent the sign sequences

$$\tau_m=(-1)^{[(m+1)/2]},\quad \sigma_m=(-1)^{[m/2]}$$

with $[h]$ denoting the largest integer which is not greater than h. After performing the arithmetic operations indicated in equations (8) and (9) the result reduces to the form

$$\begin{aligned}I_B(x)\simeq{}&I_{B,L}(x)\\={}&-\tfrac{1}{4}x^{-7/2}[\sin(2x-\tfrac{1}{4}\pi)\sum_{k=0}A_{2k}x^{-2k}\\&-\cos(2x-\tfrac{1}{4}\pi)\sum_{k=0}^{[(L-1)/2]}A_{2k+1}x^{-(2k+1)}]\end{aligned} \tag{10}$$

where A_l are constants given in Table 1, and L is the maximum value of the subscripts l employed in the computation.

Table 1. *Constants for the asymptotic expansion* (10)

l	A_l	l	A_l
0	1·7724539	10	$7·5379929\times10^2$
1	−2·1047889	11	$3·9856496\times10^3$
2	$-2·8040774\times10^{-1}$	12	$-2·3038778\times10^4$
3	$1·3695841\times10^{-1}$	13	$-1·4457277\times10^5$
4	$-3·7751798\times10^{-1}$	14	$9·7892716\times10^5$
5	$-9·6817077\times10^{-1}$	15	$7·1148705\times10^6$
6	2·8296517	16	$-5·5250730\times10^7$
7	9·5165418	17	$-4·5656501\times10^8$
8	$-3·6455084\times10^1$	18	$4·0003589\times10^9$
9	$-1·5714058\times10^2$	19	$3·7045300\times10^{10}$

Since the asymptotic series (10) for $I_B(x)$ is not convergent, there exists a certain optimum value of L which gives the best estimate for $I_B(x)$. By analysis of the numerical data, it was found that a good estimate of the maximum error in $I_{B,L}(x)$ is given by the sum of the two immediately following increments

$$\mathrm{err}\,[I_{B,L}(x)]\simeq|I_{B,L+2}(x)-I_{B,L}(x)|\,. \tag{11}$$

Hence, as the best estimate of $I_B(x)$ we took $I_{B,L}(x)$ such that either err $[I_{B,L}(x)] < \varepsilon[I_A(x)+I_{B,L}(x)]$ where ε was some predetermined small number, or err $[I_{B,L}(x)]$ reached a minimum value. With $\varepsilon = 1\times10^{-7}$ the former criterion was effective for $x > 7{\cdot}7$, whereas the latter criterion had to be used in most other cases.*

The results obtained from the asymptotic series in the above manner are surprisingly good. As compared to the converging series calculation, which was performed with relative accuracy better than 3×10^{-7} for $x\le7$, the relative error is smaller than 1×10^{-5} for $x\ge5$ and smaller than 1×10^{-6} for $x\ge6$. The number of series terms A_lx^{-l} in equation (10) required for calculation does not exceed eight for $x\ge10$. The combination of both methods, *i.e.* the converging and asymptotic series expansion, thus enables a fast and accurate calculation of $I(x)$ for any value of the argument with no need for tables of Bessel functions, for interpolation of tabulated values, or for numerical integration. The excellent agreement in the overlapping range indicates that the convergent and asymptotic series calculations are to be preferred to numerical integration. The tables based on the latter method (Anderegg, 1952; Bonse & Hart, 1967) contain errors of up to 1 % and 2·3 % respectively.

* A Fortran subroutine for computing $I(x)$ from the series is available on request.

Table 2. *Values of the reduced integral $I_r(x)$ obtained from the asymptotic expansion formula*

x	$I_r(x)\times10^5$	x	$I_r(x)\times10^5$	x	$I_r(x)\times10^5$
20·0	17·560	30·5	7·3352	40·5	3·3200
20·5	18·880	31·0	7·5750	41·0	2·9251
21·0	22·363	31·5	6·6643	41·5	2·3796
21·5	23·447	32·0	5·2607	42·0	2·0911
22·0	20·413	32·5	4·3966	42·5	2·2116
22·5	15·383	33·0	4·5427	43·0	2·5245
23·0	11·951	33·5	5·2563	43·5	2·6641
23·5	11·919	34·0	5·6574	44·0	2·4498
24·0	14·018	34·5	5·2375	44·5	2·0302
24·5	15·408	35·0	4·2648	45·0	1·7271
25·0	14·300	35·5	3·4743	45·5	1·7376
25·5	11·332	36·0	3·3812	46·0	1·9699
26·0	8·6984	36·5	3·8512	46·5	2·1452
26·5	8·0709	37·0	4·2780	47·0	2·0580
27·0	9·2295	37·5	4·1562	47·5	1·7525
27·5	10·484	38·0	3·5138	48·0	1·4648
28·0	10·302	38·5	2·8393	48·5	1·4009
28·5	8·6010	39·0	2·6127	49·0	1·5557
29·0	6·6479	39·5	2·8849	49·5	1·7326
29·5	5·8055	40·0	3·2697	50·0	1·7307
30·0	6·3456				

Table 2 contains reduced values of the integral, $I_r(x)\equiv 15I(x)/\pi$, for $20\le x\le50$ with x varying in steps of 0·5. For $4\le x\le20$, the asymptotic expansion yields results identical to the five-digit data given in Schmidt's (1955) tables which cover the range of x up to $x=20$. Maxima and minima of $I(x)$ for $x\ge8$ are listed in Table 3. Here again, the asymptotic expansion agrees with Schmidt's (1955) data extending up to $x<20$ (only in two cases there is one-unit difference in the fifth significant digit).

Table 3. *Extrema of $I_r(x)$ obtained from the asymptotic expansion formula*

	Maxima		Minima	
k	x	$I_r(x)\times10^5$	x	$I_r(x)\times10^5$
2	8·6283	383·32	10·675	103·39
3	11·852	144·94	13·821	50·295
4	15·043	69·615	16·964	28·233
5	18·218	38·602	20·105	17·433
6	21·384	23·568	23·246	11·523
7	24·544	15·419	26·386	8·0164
8	27·701	10·627	29·526	5·8034
9	30·855	7·6282	32·666	4·3376
10	34·007	5·6575	35·807	3·3279
11	37·157	4·3098	38·947	2·6096
12	40·306	3·3575	42·087	2·0845
13	43·454	2·6657	45·227	1·6917
14	46·602	2·1513	48·368	1·3919
15	49·748	1·7609	51·508	1·1592
16	52·895	1·4593	54·649	0·97568
17	56·040	1·2227	57·789	0·82905
18	59·186	1·0345	60·930	0·71046
19	62·331	0·88294	64·070	0·61350
20	65·476	0·75954	67·211	0·53345
21	68·620	0·65806	70·352	0·46677
22	71·765	0·57384	73·492	0·41078
23	74·909	0·50338	76·633	0·36342

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