THE EVALUATION OF A DIFFRACTION INTEGRAL

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1. *Introduction.* In connexion with a study of diffraction phenomena in microscope images (1, 4) it was required to evaluate the integrals

$$C_1 = \frac{1}{2\beta}\int_{-\beta}^{\beta} \cos(x\cos\theta - y\sin\theta)\cos\theta\, d\theta, \quad S_1 = \frac{1}{2\beta}\int_{-\beta}^{\beta} \sin(x\cos\theta - y\sin\theta)\cos\theta\, d\theta \tag{1}$$

and the quantity

$$F(x,y) = C_1\cos x + S_1\sin x \tag{2}$$

for a given value of β (about 0·7 radian) and for values of x and y up to about $x = 60$, $y = 40$. These integrals refer to the diffraction pattern in the space of the image of a line object viewed through an axially symmetrical lens. The variation of $F(x,y)$ with y for given x represents the distribution of amplitude across the diffraction pattern in a plane perpendicular to the axis of the objective, at a distance x (in units of $\lambda/2\pi$) from the focal plane, x and y being both reckoned in object space. The form required for the final results was $F(x,y)$ as a function of y for various, relatively widely spaced, values of x such as $x = 0\,(8)\,64$.

The organization of the numerical work was aimed at producing the results directly in this form, without interpolation; the numerical work itself was carried out on the EDSAC, the automatic calculating machine installed in the Mathematical Laboratory of the University of Cambridge.

2. *Quadrature.* For small values of x and y, evaluation of the integrals (1) by quadrature is quite practicable. The library of subroutines for use with the EDSAC includes several based on the Gauss integration formula, with different numbers of ordinates up to sixteen, and a few tests show over what ranges of x and y adequate accuracy can be obtained by the different formulae, either by a single application, to the whole range $\theta = -\beta$ to β, or by a double application, to the range $\theta = -\beta$ to 0 and to $\theta = 0$ to $+\beta$.

But for larger values of x or y or both, the integrand goes through several oscillations in the range of integration, and it is necessary to subdivide the range of integration further even if a sixteen-point Gauss formula is used in each interval, and the calculation then becomes long. This occurs, for example, for x greater than about 50 on the line $y = 0$, and for y greater than about 30 on the line $x = 30$. This is not surprising, since a sixteen-point Gauss integration formula is only accurate for polynomials of degree 32 or lower, whereas for $\phi \equiv (x\cos\theta - y\sin\theta) = 40$ the main contributions to the Taylor series for $e^{i\phi}$ in the integrand of (1) come from terms which are of degree 40 or thereabouts (and are of the order of 10^{16}), and even the term in ϕ^{100} gives a contribution of order of magnitude 100.

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Hence other methods are desirable for carrying the calculation to the larger values of x and y for which results were required.

3. *Differential equations.* It is convenient to write

$$\phi = x\cos\theta - y\sin\theta, \tag{3}$$

$$C_n = \frac{1}{2\beta}\int_{-\beta}^{\beta} \cos\phi\cos^n\theta\,d\theta, \quad S_n = \frac{1}{2\beta}\int_{-\beta}^{\beta} \sin\phi\cos^n\theta\,d\theta, \tag{4}$$

$$I_n = C_n + iS_n = \frac{1}{2\beta}\int_{-\beta}^{\beta} e^{i\phi}\cos^n\theta\,d\theta \tag{5}$$

(the notation in formula (1) has been chosen consistently with this). Then $\partial I_{n-1}/\partial x = iI_n$, so that in particular

$$C_1 = +\partial S_0/\partial x, \quad S_1 = -\partial C_0/\partial x. \tag{6}$$

It will appear that, if other means than quadrature are used, C_0 and S_0 are simpler to evaluate than C_1 and S_1, and it follows from (6) that any method of evaluating C_0 and S_0 which also provides values of $\partial C_0/\partial x$ and $\partial S_0/\partial x$ will serve for obtaining the results required.

In terms of polar coordinates (r, χ) in the (x, y) plane, I_0 is given by

$$I_0 = \frac{1}{2\beta}\int_{-\beta}^{\beta} \exp\left[ir\cos(\theta+\chi)\right]d\theta = \int_{\chi-\beta}^{\chi+\beta} \exp(ir\cos\gamma)\,d\gamma, \tag{7}$$

and if tables of the 'incomplete Bessel function' $\int_0^z \exp(ir\cos\gamma)\,d\gamma$ were available, they could be used to evaluate I_0. This suggests that it should be possible to find a second-order *ordinary* differential equation for I_0 as a function of r for constant χ, which could then be integrated numerically. Such an equation can be obtained by two differentiations with respect to r followed by an integration by parts with respect to θ, and it would be possible to integrate this equation with respect to x, along lines χ = constant, so as to obtain results at exact values of x without interpolation. But this would not be wholly satisfactory for two reasons. First, it would only give points on the curve of $F(x, y)$ against y at values of y spaced at intervals proportional to x, whereas the lateral scale of the diffraction pattern only increases slightly with x, so that for plotting and drawing the diffraction pattern it would be preferable to have points at the same intervals of y for all x, rather than at intervals proportional to x. And secondly, results were only wanted at wide intervals (4 or 8 units) in x, whereas the integration interval can be at most $\delta x = \frac{1}{8}$, so that the number of values of C_1, S_1 calculated would be much larger (by a factor 64, perhaps) than the number directly used in calculating diffraction patterns by substitution in formula (2).

Results would be obtained directly in the form required if it were possible to find a differential equation for the variation of I_0 with y for x constant. Initial conditions for the solution of this equation, for any value of x, could be obtained by quadrature or from results of integration of the equation for the variation of I_0 with x on $y = 0$ (this equation is the special case $\chi = 0$ of the equation of the variation of I_0 with r on χ = constant). It does not seem obvious that it is possible to find an ordinary differential equation for the variation of I_0 with y at constant x; it might seem that in terms of x and y as independent variables the best that could be expected is a partial

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differential equation. But it turns out to be possible to obtain an equation involving y-derivatives only, as follows.

It is clear that each of the functions I_n satisfies the equation

$$\frac{\partial^2 I_n}{\partial x^2}+\frac{\partial^2 I_n}{\partial y^2}+I_n=0. \tag{8}$$

Further
$$\frac{d}{d\theta}e^{i\phi}=i(-x\sin\theta-y\cos\theta)\,e^{i\phi}$$

and
$$\frac{\partial I_0}{\partial x}=\frac{1}{2\beta}\int_{-\beta}^{\beta}(i\cos\theta)\,e^{i\phi}\,d\theta,\quad \frac{\partial I_0}{\partial y}=\frac{1}{2\beta}\int_{-\beta}^{\beta}(-i\sin\theta)\,e^{i\phi}\,d\theta,$$

so that
$$\begin{aligned}x\frac{\partial I_0}{\partial y}-y\frac{\partial I_0}{\partial x}&=\frac{1}{2\beta}\int_{-\beta}^{\beta}i(-x\sin\theta-y\cos\theta)\,e^{i\phi}\,d\theta\\&=\frac{1}{2\beta}\int_{-\beta}^{\beta}\frac{d}{d\theta}(e^{i\phi})\,d\theta=\frac{1}{2\beta}[e^{i\phi}]_{-\beta}^{\beta}\\&=-(i/\beta)\,e^{ix\cos\beta}\sin(y\sin\beta)=-i\psi_0,\end{aligned} \tag{9}$$

where, for brevity, there has been written

$$\psi_0=(1/\beta)\,e^{ix\cos\beta}\sin(y\sin\beta). \tag{10}$$

Differentiation of (9) with respect to x and with respect to y, and elimination of the term in $\partial^2 I_0/\partial x\,\partial y$ between the two resulting equations, give

$$x^2\frac{\partial^2 I_0}{\partial y^2}-y^2\frac{\partial^2 I_0}{\partial x^2}-x\frac{\partial I_0}{\partial x}+y\frac{\partial I_0}{\partial y}=-i\left(x\frac{\partial\psi_0}{\partial y}+y\frac{\partial\psi_0}{\partial x}\right), \tag{11}$$

which can alternatively be obtained from (9) by operating on both sides with

$$x\frac{\partial}{\partial y}+y\frac{\partial}{\partial x};$$

and equations (8) and (9) can then be used either to eliminate x-derivatives of I_0 from (11) and obtain an equation involving y-derivatives only, or vice versa. Elimination of the x-derivatives gives

$$(x^2+y^2)\frac{\partial^2 I_0}{\partial y^2}-(x^2-y^2)\frac{1}{y}\frac{\partial I_0}{\partial y}+y^2 I_0=i\left[x\left(\frac{\psi_0}{y}-\frac{\partial\psi_0}{\partial y}\right)-y\frac{\partial\psi_0}{\partial x}\right]. \tag{12}$$

Now
$$\frac{\psi_0}{y}-\frac{\partial\psi_0}{\partial y}=\frac{\sin\beta}{\beta}e^{ix\cos\beta}\left[\frac{\sin(y\sin\beta)}{y\sin\beta}-\cos(y\sin\beta)\right],$$

so that if for short we write

$$G(z)=(z^{-1}\sin z-\cos z)/z^2, \tag{13}$$

the right-hand side of equation (12) becomes

$$xy^2\,e^{ix\cos\beta}\frac{\sin\beta}{\beta}\left[\frac{\cos\beta}{x}\frac{\sin(y\sin\beta)}{y\sin\beta}+i\sin^2\beta\,G(y\sin\beta)\right]. \tag{14}$$

The left-hand side of equation (12) can be written in an alternative form so that the equation becomes

$$\begin{aligned}(x^2+y^2)\frac{\partial}{\partial y}\left(\frac{1}{y}\frac{\partial I_0}{\partial y}\right)+y\left[2\left(\frac{1}{y}\frac{\partial I_0}{\partial y}\right)+I_0\right]&=xy\,e^{ix\cos\beta}\frac{\sin\beta}{\beta}\\&\times\left[\frac{\cos\beta}{x}\frac{\sin(y\sin\beta)}{y\sin\beta}+i\sin^2\beta\,G(y\sin\beta)\right].\end{aligned} \tag{15}$$

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This is a convenient form for integration for small values of y, since no division by y is involved; the quantity directly calculated by integration is $\left(\frac{1}{y}\frac{\partial I_0}{\partial y}\right)$, and this is *multiplied* by the small quantity y to give $\partial I_0/\partial y$ which is then integrated to give I_0. The function $G(y \sin\beta)$ can be calculated from its series expansion. From (9) it follows that

$$\left(\frac{1}{y}\frac{\partial I_0}{\partial y}\right)_{y=0} = \frac{1}{x}\left(\frac{\partial I_0}{\partial x} - i\frac{\sin\beta}{\beta}e^{ix\cos\beta}\right), \tag{16}$$

so that the initial values for the integration of equation (15) can be obtained from the solution of the equation for the variation of I_0 with x on $y = 0$.

This equation can be obtained as follows. From equation (14) it follows that, for small y, the right-hand side of (12) is $O(y^2)$ so that

$$\left(\frac{\partial^2 I_0}{\partial y^2}\right)_{y=0} = \left(\frac{1}{y}\frac{\partial I_0}{\partial y}\right)_{y=0},$$

and this is given by (16). Substitution in (8) then gives (for $y = 0$ only)

$$\frac{\partial^2 I_0}{\partial x^2} + \frac{1}{x}\frac{\partial I_0}{\partial x} + I_0 = i\frac{\sin\beta}{\beta x}e^{ix\cos\beta}. \tag{17}$$

The solution of this equation can be evaluated by numerical integration starting from values of I_0 and $\partial I_0/\partial x$ obtained by quadrature for some convenient value of x.

It is possible to obtain equations similar to (15) and (17) for the x- and y-variations if I_1, which is the function directly involved in calculating the results $F(x, y)$ finally required. But the equations for I_1 are considerably more complicated, and since a considerable part of the time of integration is occupied in evaluating the right-hand sides of these equations (which has to be done twice per interval if the standard EDSAC subroutines, based on Gill's version of the Runge-Kutta process (2, 6), are used) it is advisable to use the simpler equations (15) and (17). In the course of integrating equation (16), the quantity $\partial I_0/\partial x = iI_1$ (see (6)) is evaluated in any case; and from the solution of equation (14), I_1 can be obtained by use of the relation (9) as follows:

$$I_1 = -i\frac{\partial I_0}{\partial x} = \frac{\psi_0}{y} - ix\left(\frac{1}{y}\frac{\partial I_0}{\partial y}\right). \tag{18}$$

If intervals $\delta y = \frac{1}{16}$ are used in the integration, and results are required at intervals of $\frac{1}{2}$ in y, formula (18) only has to be evaluated once every 8 intervals of the integration, and so does not add much to the time required for the integration itself.

It is possible to integrate simultaneously the equations for the real and imaginary parts of I_0, so that the evaluation of the final results can be carried out in the course of the solution of the equations; there is no need to print out the results of the integrations and then feed them back into the machine for the evaluation of I_1 and $F(x, y)$.

4. *Notes on the integration.* For the calculations actually carried out numerically, the value $\beta = 0{\cdot}72$ was taken; this is the value for an immersion objective of numerical aperture unity with an immersion oil of refractive index $\mu = 1{\cdot}517$ approximately. An exact value of β was adopted rather than an exact value of μ, as results for an exact value of β are more likely to be useful if a more extensive tabulation is ever required. Only minor alterations in the program tapes would be necessary if numerical results were required for other values of β.

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If results of the required accuracy can be obtained by one or two applications of a Gauss quadrature formula, this provides the quickest way of obtaining them. It will be convenient to use the notation (Qn) for the process of quadrature using a single application of a $2n$-point Gauss formula for the whole range $\theta = -\beta$ to $+\beta$ (Qn happens to be the reference symbol of the corresponding tape in the EDSAC library of sub-routines), and $(Qn)^2$ for the process of using two applications of a $2n$-point Gauss formula, one for the range $\theta = -\beta$ to 0 and the other for the range $\theta = 0$ to $+\beta$.

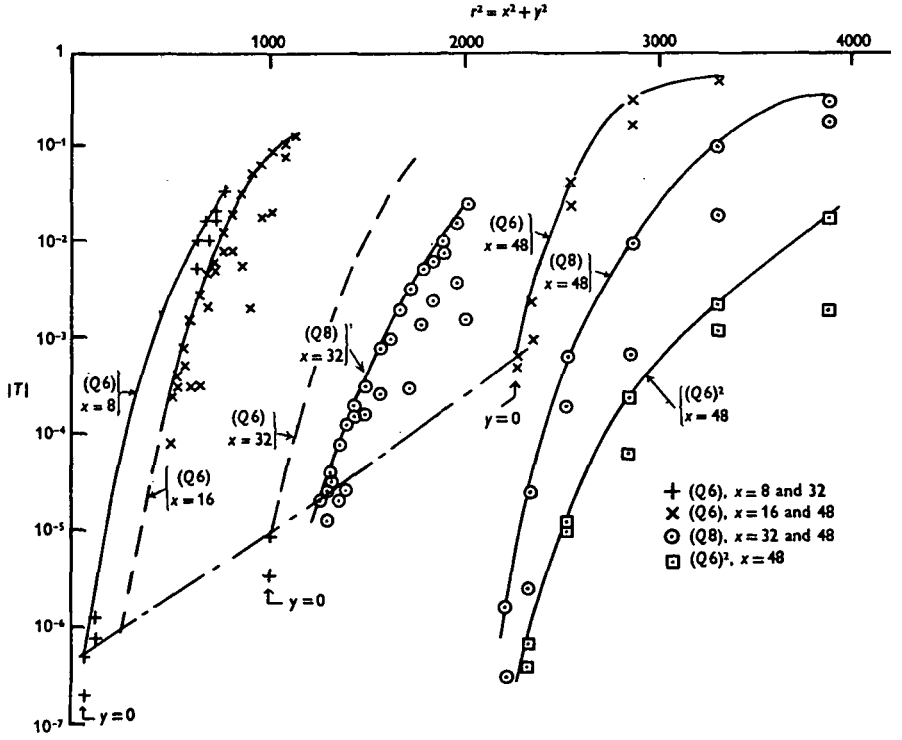


Fig. 1. Truncation errors T in calculation of integrals C_1 and S_1 by different procedures using Gauss integration formulae. The points show $|T|$, on a logarithmic scale, plotted against $r^2 = x^2 + y^2$ for various values of x. The full curves show the trend of the variation of $|T|$ with r for given x; the broken curves are estimated; the dot-and-dash curve (·–·–·) shows the trend of the variation of $|T|$ with r for $y = 0$.

A number of trial quadratures for the integrals I_0 and I_1 were evaluated by the processes $(Q6)$, $(Q8)$, $(Q6)^2$ and $(Q8)^2$, to give an indication of the accuracy attained by these processes in different regions of the (x, y)-plane.

From the integral in the form (7), in polar coordinates (r, χ) in the (x, y) plane, it might be expected that the truncation error of a given integration procedure would depend mainly on r, and that the variation with χ would be small. The actual behaviour is considerably different from this, as illustrated in Fig. 1 which shows the variation of the errors of the processes $(Q6)$ and $(Q8)$ with $r^2 = x^2 + y^2$ for several values of x (the plotted points show the errors in C_1 and S_1 on a logarithmic scale; since for a given value of x the error oscillates with increasing y, the points will not lie on a smooth curve, but

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the general behaviour is represented by a smooth curve drawn as low as possible without being below any of these points).

From exploratory results of this kind, the appropriate quadrature formula to use for different regions of the (x, y) plane was determined. For the calculations to give the final results, two quadratures, using processes (Qn) and $(Qn)^2$, were carried out for each value of x, to provide a check and to verify that truncation errors were not becoming unacceptably large.

An interesting feature of these results is that in a considerable part of the range of x and y the truncation error is only a very small fraction of the value which would be estimated from the formal expression for this error. The truncation error T for the process (Qn) ($2n$-point Gauss formula) is (3)

$$T = \frac{1}{4n+1}\left(\frac{(2n!)^2}{(4n)!}\right)^2 \frac{f^{(4n)}(\alpha)}{(4n)!}(2\beta)^{4n+1}, \tag{19}$$

where α is some number in the range of integration $-\beta \leqslant \theta \leqslant \beta$. Since the value of α is unknown, the only useful estimate that can be based on this formula is the overestimate obtained by giving $|f^{(4n)}(\alpha)|$ its greatest possible value. Now

$$f(\theta) = \exp[ir\cos(\theta+\chi)],$$

and for large r, the range of $r\cos(\theta+\chi)$ is several multiples of 2π, so the greatest value of $|f^{(4n)}(\theta)|$ is of order r^{4n}, and evaluation of the numerical coefficient for $n = 6$ gives approximately for $(Q6)$

$$|T| < (r/36)^{24}. \tag{20}$$

For $r = 32$, for example, this gives $|T| < 0{\cdot}06$; actually for $x = 32, y = 0$, $T = 9 \times 10^{-6}$ approximately, so formula (2) has overestimated $|T|$ by a factor of about 15,000. This shows that the appropriate value of $f^{(4n)}(\alpha)$ to be inserted in formula (19) may be so small a fraction of the greatest value of $|f^{(4n)}(\theta)|$ that this formula gives an overestimate of the error which is so exaggerated that it is of little value.

Further, from formula (19) it might be expected that the truncation error for the processes $(Qn)^2$ would be about $1/2^{4n}$ times that for the process (Qn); for $n = 6$ this ratio is about $1/10^7$. Actually the ratio is more nearly $1/10^3$ to $1/10^5$. If only results for $(Q6)$ and $(Q6)^2$ were available, one might at first sight hope to correct for the truncation errors in the results for $(Q6)^2$ by using the difference between the results for $(Q6)$ and $(Q6)^2$ and assuming the errors were in the ratio $2^{24}/1$. The present results show that this would not be valid, and would give an exaggerated estimate of the accuracy of the $(Q6)^2$ results.

Results for $x = 0\,(8)\,32$ were calculated by quadrature. For $x = 32$, 40, 48 results were also calculated by integration of the y-equation (15) for I_0, followed by use of equation (18) this expression being evaluated only at those values of y at which results were printed. The integration for $x = 32$ was done mainly to check the program for this integration.

The rapid increase in the rounding error with y at fixed x means that although integration of the differential equation for I_0 as a function of y has to be used for the higher values of x, say $x > 32$, in order to cover the range of y required, the initial conditions for such an integration can be evaluated by quadrature for greater values of x.

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Integration of the x-equation on $y = 0$ (equation (17)) was carried out for $x = 12$ to 40 to provide a further check on the values of C_0, S_0, $\partial C_0/\partial x$, $\partial S_0/\partial x$ used in deriving the starting conditions for the solution of the y-equation, and to examine the truncation errors of this integration. For the integration process used (EDSAC library tape $G\,1$) (6), the truncation error is of order $(\delta x)^5$ in one interval, hence of order $(\delta x)^4$ in the aggregate over a given range of x; this suggests that the leading terms in the truncation errors might be eliminated by a process of 'h^4-extrapolation' similar to Richardson's 'h^2-extrapolation' (5). Some results are given in Table 1, and illustrate the improvement obtained by application of this process to the results calculated with $\delta x = \frac{1}{4}$ and $\frac{1}{8}$.

Table 1. *Integration of equation* (17) *from* $x = 12$ *to* $x = 40$; *results at* $x = 40$

	C_0	S_0	$\partial C_0/\partial x$	$\partial S_0/\partial x$
$\delta x = \frac{1}{4}$	0·0667997	0·2886230	−0·2866296	0·0504450
$\frac{1}{8}$	5635	6663	6676	2103
$\frac{1}{16}$	5505	6674	6705	1954
	h^4-extrapolated results			
$\delta x = \frac{1}{4}$ and $\frac{1}{8}$	0·0665497	0·2886692	−0·2866701	0·0501947
$= \frac{1}{8}$ and $\frac{1}{16}$	5495	6675	6707	1944
	By quadrature using $(Q\,8)^2$			
	0·0665495	0·2886676	−0·2866706	0·0501945

5. *Summary.* The calculation of the diffraction pattern for an out-of-focus line source viewed through an axially symmetrical lens involves the evaluation of the integral

$$I_1(x,y) = (1/2\beta)\int_{-\beta}^{\beta} [\exp i(x\cos\theta - y\sin\theta)]\cos\theta\, d\theta$$

for a constant value of β (related to the numerical aperture of the lens) and a range of values of x and y. For small values of x and y this can best be done by quadrature; for larger values of x or y or both it is more practicable to use numerical evaluation of an appropriate ordinary differential equation. It is shown that the variation of

$$I_0(x,y) = (1/2\beta)\int_{-\beta}^{\beta} \exp i(x\cos\theta - y\sin\theta)\, d\theta$$

with x for $y = 0$, and with y for $x =$ const., can both be expressed by second-order ordinary differential equations of a convenient form for numerical integration; the evaluation of $I_1(x,y)$ from solutions of these equations is straightforward. For comparison with experiment, results are required in the form of $I_1(x,y)$ and a derived quantity as functions of y, at relatively widely spaced values of x; numerical work for $\beta = 0{\cdot}72$ has been carried out on the EDSAC and has been organized to produce the results in the required form directly, without interpolation.

Comparison of results obtained by using different Gauss quadrature formulae and different interval lengths show some interesting features of the errors of high-order

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integration formulae, and show that care is necessary in estimating these errors from the differences between quadratures carried out with intervals of different lengths.

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