an observation in a sample of size j drawn from a normal population with zero mean and unit variance is given exactly by

$$\xi_{1/2}(i|j) = \frac{2j!}{(j-i)!\,(i-1)!} \times \int_0^\infty \frac{x \exp(-x^2/2)}{\sqrt{2\pi}} (2P-1)^{j-i}(2-2P)^{i-1}\mathrm{d}x \quad (2)$$

where

$$P = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{X} \exp(-\alpha^2/2)\mathrm{d}\alpha.$$

A comparison of exact [equation (2)] and approximate expected magnitudes of the ranked half-normal order statistics, for three values of j, is given in Table 2. The exact moduli, for values of $j = 2[1]\ 41$, for all values of i (to our knowledge, not previously published) are presented in Table 3. The normal approximation is satisfactory for intermediate values of i (*cf.* Table 2), but remains in error by about 2% for values of j as high as 400. The extreme smallest value has a limiting exact value which is double that for the normal approximation, although the *absolute* difference between exact and approximate values is of no practical importance for large values of j.

Complete values of the full- and half-normal order statistics will appear in Volume 4 of *International Tables for X-ray Crystallography*.

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Multiple diffraction effects in neutron single-crystal diffractometry.

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(*Received* 1 *February* 1971)

The n-beam dynamical theory of diffraction is applied to multiple neutron diffraction. A computer program has been adapted to the neutron case from one originally developed for high energy electron diffraction in reflection. The integrated intensities are computed for the two and multibeam cases of the 002 reflection and compared with experiment. It is shown that only a negligible fraction of the incident beam satisfies the conditions for multiple diffraction.

The importance of multiple neutron diffraction in the Bragg case was recognized early by Moon & Shull (1961) and subsequently by Borgonovi & Caglioti (1962). The latter authors found remarkable effects in the 002 reflection from mosaic crystals such as nickel, aluminum, and pyrite, whereas they were not able to observe any appreciable effect in relatively perfect crystals such as LiF and NaCl. Since multiple diffraction is essentially related to a dynamical interaction among diffracted beams, the reason for this negative result is not clear, and a theoretical evaluation of these effects seems worthwhile.

The appropriate tool for this interpretation is the n-beam dynamical theory of diffraction and, for this purpose, a computer program originally developed for high energy electron diffraction in reflection (Colella, 1971; Colella & Menadue, 1971) has been adapted to the neutron case with a few minor modifications.

In Borgonovi & Caglioti's experiment, the crystal was oriented for the 002 Bragg reflection and then rotated around the [002] normal. The intensity was measured as a function of φ, the azimuthal angle. The divergence of the incident beam in the diffraction plane, of the order of several minutes of arc (Caglioti & Ricci, 1962), was much higher than the Darwin width of the crystal. In this situation, the intensity measured by the counter corresponds to the integrated intensity of the diffraction profile for an ω scan. For the sake of comparison with Borgonovi & Caglioti's experiment, the 002 integrated intensity for an ω scan (Bragg case) was computed when one or two strong reflections other than 002 were simultaneously excited. In relation to the nickel 002 azimuthal plot obtained by Borgonovi & Caglioti, numerous multibeam rocking curves for LiF and NaCl single crystals were computed in the vicinity of $\varphi = 36$–$37°$, where the 002 intensity suffers the most drastic changes.† The results are reported in Table 1. The 002 integrated intensity

† The azimuthal angle $\varphi = 0$ corresponds to a [010] axis lying in the diffraction plane.

Table 1. *The effects of simultaneous reflections on the* 002 *integrated intensity*

The simultaneous reflections are listed in the second column from the left. When two simultaneous reflections are involved (four-beam case), their *hkl* indices are indicated by parentheses. The maximum and minimum percentage changes of the 002 integrated intensity are indicated, along with the angular width on the azimuthal scale. I_2 is the 002 two-beam integrated intensity.

Crystal	*hkl*	$\Delta I/I_2$ (×100)	$\Delta\varphi$ (sec)
LiF	$\bar{1}31$	−15 +466	14
	$\binom{042}{040}$	+33 −30	8·3
NaCl	$\bar{1}31$	−2·5 +31·4	3·1

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can be either increased or decreased by simultaneous diffraction, and the extreme values are given in Table 1. For every multibeam case, a particular azimuth φ_0 is computed corresponding to a situation in which one or two reciprocal lattice nodes lie on the Ewald sphere. When the actual azimuth φ differs from φ_0 by more than $\Delta\varphi/2$ as given in Table 1, the 002 integrated intensity is practically restored to the two-beam value.

Table 1 shows that these effects are by no means negligible, especially in the case of the $\bar{1}31$. However, the azimuthal width for the $\bar{1}31$ (14 sec) must be compared with the vertical divergence, *i.e.* perpendicular to the diffraction plane, of the incident beam in Borgonovi & Caglioti's experiment. This vertical divergence amounts to 76 minutes, as calculated from a description of the experimental set up given by Caglioti & Ricci (1962). It is clear, therefore, that only a negligible fraction of the incident beam satisfies the conditions for multiple diffraction. The remaining portion undergoes two-beam 002 diffraction and is totally collected by the counter. The net effect turns out to be of the order of 1·7% which is within the limits of the experimental error.

Thanks are due to Professor B. W. Batterman and to the U.S. Advanced Research Projects Agency for partial support of this work.

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Analytical solution for the X-ray absorption factor for cylinders in two special cases.

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(*Received* 18 *August* 1971)

The equation for the absorption factor at Bragg angles of 0 and 90° is integrable, resulting in simple equations that are functions of well-known higher transcendental functions. Numerical results are easily obtained, and a comparison with those obtained using numerical integration is made.

For small-angle scattering studies of cylindrical samples, it is useful to calculate the absorption factor at zero Bragg angle directly, in a manner that does not require a large amount of computer storage. Also, direct calculations at Bragg angles of 0 and 90° allow checks to be made on absorption factors calculated by numerical integration.

The general equation for the transmission factor A that is the reciprocal of the absorption factor A^* is

$$A = \frac{1}{V}\int_V \exp(-\mu L)\mathrm{d}V, \qquad (1)$$

where V is the sample volume, μ is the linear absorption coefficient, and L is the total path length of the X-ray beam in the sample.

After introducing boundary conditions for the sample shape, transformation of coordinates, and integration by parts, definite integrals, for which solutions are well known, were obtained from equation (1) for Bragg angles of 0 and 90°. The equations for the transmission factors for these two special cases are:

$$A = 2[I_2\{z\} - \mathbf{L}_2\{z\} + (I_1\{z\} - \mathbf{L}_1\{z\})/z - (2z)/(3\pi)] \quad (\theta = 0°) \quad (2)$$
$$= 2[(I_0\{z\} - \mathbf{L}_0\{z\}) - (I_1\{z\} - \mathbf{L}_1\{z\})/z],$$

$$A = [I_1\{2z\} - \mathbf{L}_1\{2z\}]/z, \qquad (\theta = 90°) \quad (3)$$

where $z = 2\mu R$, R is the radius of the cylinder, and I_ν and $\mathbf{L}_\nu$ are the modified Bessel function and the modified Struve function respectively of order ν (Erdélyi, Magnus, Oberhettinger & Tricomi, 1953).†

The numerical values of I_ν and $\mathbf{L}_\nu$ can be obtained using series solutions only slightly more complicated than those for the simple transcendental functions, such as the sine. Because series solutions are simple to evaluate on a computer, it is quite simple to solve for the absorption correction directly for the two special cases.

For large values of the arguments of the modified Bessel and Struve functions, these functions become very large,

† Proofs of equations (2) and (3) are available from the author.

Table 1. *Values of A**

	$\theta = 0°$		$\theta = 90°$	
μR	A^*	% Error‡	A^*	% Error
0·5	2·300	0·43	2·050	0.01
1·0	5·091	0·61	3·389	0·04
1·5	10·75	0·45	4·863	0·15
2·0	21·44	0·63	6·389	0·17
2·5	40·10	0·74	7·936	0·30
3·0	70·12	0·88	9·492	0·40
4·0	177·0	1·11	12·62	0·66
5·0	363·0	1·11	15·75	0·97

‡ Percent error in A^* values in *International Tables for X-ray Crystallography* (1959) when compared with A^* values given in this table.