where $k_{0,R}$ and $k_{0,I}$ are the real and imaginary parts of the roots of the equation $d(k)=0$. Then we translate the integral, letting $k'=k-k_{0,R}$. This gives us

$$\Delta_4(x-x';\, z-z') = -\frac{\theta(z-z')A_3C_\Delta}{\pi(B_1-B_2)} \times \exp\{i[(A_1+A_2)(z-z')/2+\alpha k_{0,R}]\} \times \int_{-\infty}^{\infty} \frac{\sin[\beta(k^2+k_{0,I}^2)^{1/2}]}{(k^2+k_{0,I}^2)^{1/2}} \exp(i\alpha k)\mathrm{d}k \qquad \text{(A10)}$$

where $\alpha=(x-x')-(B_1-B_2)(z-z')/2$ and $\beta=[(B_2-B_1)(z-z')/2]>0$. Next, we make two more obvious transformations; first let $k=k_{0,I}\sinh t$ and write out the sine in terms of exponentials. Then, let $\alpha\sinh t+\beta\cosh t=\pm(\beta^2-\alpha^2)^{1/2}\cosh\theta$ where $\beta>0$ and $\beta>\alpha$ and the $+(-)$ goes with the first (second) exponential. These transformations result in the integral in equation (A10) becoming

$$\frac{1}{\pi}\int_{-\infty}^{\infty} \sin[|k_{0,I}|(\beta^2-\alpha^2)^{1/2}\cosh\theta]\mathrm{d}\theta = J_0[|k_{0,I}|(\beta^2-\alpha^2)^{1/2}]\,.$$

We note that $k_{0,R}=(A_1-A_2)/\Omega$ and $k_{0,I}=\pm 2A_3/\Omega$ where $\beta^2-\alpha^2=-(\beta+\alpha)(\alpha-\beta)=-\mu_1\mu_2$; therefore we can write equation (A10) as

$$\Delta_4(x-x';\, z-z') = -\frac{\theta(z-z')C_\Delta A_3}{\Omega}\exp(i\varphi)J_0(\xi)\,. \qquad \text{(A11)}$$

To compute the diagonal elements of Δ, we need the relations:

$$\left(\frac{\partial}{\partial z}+B_1\frac{\partial}{\partial x}\right)\mu_1 = \left(\frac{\partial}{\partial z}+B_2\frac{\partial}{\partial x}\right)\mu_2 = 0$$

and

$$\left(\frac{\partial}{\partial z}+B_1\frac{\partial}{\partial x}\right)\mu_2 = -\left(\frac{\partial}{\partial z}+B_2\frac{\partial}{\partial x}\right)\mu_1 = \Omega\,.$$

Then using these relationships we obtain

$$\Delta_1(x-x';\, z-z') = \theta(z-z')\left\{\delta[\mu_1]\exp[iA_1(z-z')] - \frac{C_\Delta\exp(i\varphi)}{\Omega}\left[(A_1-A_2)J_0(\xi) - iA_3\left(-\frac{\mu_1}{\mu_2}\right)^{1/2}J_1(\xi)\right]\right\} \qquad \text{(A13)}$$

and

$$\Delta_2(x-x';\, z-z') = \theta(z-z')\left\{\delta[\mu_2]\exp[iA(z-z')] - \frac{C_\Delta\exp(i\varphi)}{\Omega}\left[(A_2-A_1)J_0(\xi) - iA_3\left(-\frac{\mu_2}{\mu_1}\right)^{1/2}J_1(\xi)\right]\right\} \qquad \text{(A14)}$$

where the Dirac delta functions are a result of having to differentiate the characteristic functions, while J_1 is a result of having to differentiate J_0.

References

LEWIS, A. L., HAMMOND, R. B. & VILLAGRANA, R. E. (1975). *Acta Cryst.* A**31**, 221–227.

KATO, N. (1968). *J. Appl. Phys.* **39**, 2225–2230, 2231–2237.

KURIYAMA, M. & EARLY, J. G. (1974). *Acta Cryst.* A**30**, 525–535.

TAKAGI, S. (1962). *Acta Cryst.* **15**, 1311–1312.

TAKAGI, S. (1969). *J. Phys. Soc. Japan*, **26**, 1239–1253.

Acta Cryst. (1975). A**31**, 727

The Joint Probability Distribution of Structure Factors: The First-Order Term

BY J. J. L. HEINERMAN

Laboratorium voor Structuurchemie, Rijksuniversiteit, Padualaan 8, *Utrecht, The Netherlands*

(*Received* 25 *March* 1975; *accepted* 1 *April* 1975)

The first-order term of the joint probability distribution of $E_{\mathbf{h}_1+\mathbf{k}},\ldots,E_{\mathbf{h}_m+\mathbf{k}}$, for $\mathbf{h}_1,\ldots,\mathbf{h}_m$ fixed and $\mathbf{k}$ variable, is derived for both space groups $P\bar{1}$ and $P1$. It appears that the first-order term affects the most probable values for the moduli of the structure factors, but that it has no influence on the most probable values for the phases.

Introduction

The main term of the joint probability distribution of an arbitrary number of structure factors has been obtained from the central-limit theorem (Tsoucaris, 1970). From this distribution, formulae for the most probable values of structure factors have been derived (Tsoucaris, 1970; de Rango, Tsoucaris & Zelwer, 1974). The present paper deals with the first-order term of this distribution. To calculate this term use is made of Hauptman's (1971) method for the derivation of the joint probability distributions of two and three

structure factors. The influence of the first-order term on the most probable values for the structure factors is discussed.

Joint probabilities

We shall derive the main term and first-order term of the joint probability distribution $P(X_1,\ldots,X_m)$ of $E_{\mathbf{h}_1+\mathbf{k}},\ldots,E_{\mathbf{h}_m+\mathbf{k}}$, where $\mathbf{h}_1,\ldots,\mathbf{h}_m$ are fixed reciprocal-lattice vectors and $\mathbf{k}$ is a variable one.

For space group $P\bar{1}$ the expressions for the normalized structure factor $E_{\mathbf{h}}$ and the unitary structure factor $U_{\mathbf{h}}$ are

$$E_{\mathbf{h}}=\sum_{j=1}^{N/2}\frac{2Z_j}{\sigma_2^{1/2}}\cos 2\pi\mathbf{h}\,.\,\mathbf{r}_j \qquad (1)$$

and

$$U_{\mathbf{h}}=\sum_{j=1}^{N/2}\frac{2Z_j}{\sigma_1}\cos 2\pi\mathbf{h}\,.\,\mathbf{r}_j\,, \qquad (2)$$

where N is the number of atoms in the unit cell, Z_j is the number of electrons of atom j and

$$\sigma_n=\sum_{j=1}^{N}Z_j^n\,. \qquad (3)$$

By $p_j(\xi_1,\ldots,\xi_m)$ we denote the joint probability distribution of

$$\frac{2Z_j}{\sigma_2^{1/2}}\cos 2\pi(\mathbf{h}_1+\mathbf{k})\,.\,\mathbf{r}_j,\ldots,\frac{2Z_j}{\sigma_2^{1/2}}\cos 2\pi(\mathbf{h}_m+\mathbf{k})\,.\,\mathbf{r}_j\,.$$

The characteristic function $q_j(x_1,\ldots,x_m)$ of $p_j(\xi_1,\ldots,\xi_m)$ is defined by

$$q_j(x_1,\ldots,x_m)=\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\Big[i\sum_{i=1}^{m}x_i\xi_i\Big]\times p_j(\xi_1,\ldots,\xi_m)\,\mathrm{d}\xi_1\ldots\mathrm{d}\xi_m\,. \qquad (4)$$

If $p_1,\ldots,p_{N/2}$ are assumed to be independent, the characteristic function $Q(x_1,\ldots,x_m)$ of $P(X_1,\ldots,X_m)$ equals the product of the q_j's (see *e.g.* Cramér, 1971),

$$Q(x_1,\ldots,x_m)=\prod_{j=1}^{N/2}q_j(x_1,\ldots,x_m)\,. \qquad (5)$$

First we derive an expression for $Q(x_1,\ldots,x_m)$. The next step is the calculation of $P(X_1,\ldots,X_m)$,

$$P(X_1,\ldots,X_m)=\frac{1}{(2\pi)^m}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp\Big[-i\sum_{i=1}^{m}X_ix_i\Big]\times Q(x_1,\ldots,x_m)\,\mathrm{d}x_1\ldots\mathrm{d}x_m\,. \qquad (6)$$

Formula (4) can be written as

$$q_j(x_1,\ldots,x_m)=\left\langle\exp\Big[i\,\frac{2Z_j}{\sigma_2^{1/2}}\sum_{i=1}^{m}x_i\cos 2\pi(\mathbf{h}_i+\mathbf{k})\,.\,\mathbf{r}_j\Big]\right\rangle_{\mathbf{k}}\,. \qquad (7)$$

The sum of the cosines in (7) is replaced by one cosine, analogous to Hauptman's calculations for the cases $m=2$ and $m=3$,

$$\sum_{i=1}^{m}x_i\cos 2\pi(\mathbf{h}_i+\mathbf{k})\,.\,\mathbf{r}_j=A_j\cos(2\pi\mathbf{k}\,.\,\mathbf{r}_j+\varepsilon_j)\,, \qquad (8)$$

where

$$A_j=\Big(\sum_{i_1=1}^{m}\sum_{i_2=1}^{m}x_{i_1}x_{i_2}\cos 2\pi(\mathbf{h}_{i_1}-\mathbf{h}_{i_2})\,.\,\mathbf{r}_j\Big)^{1/2}\,, \qquad (9)$$

$$\cos\varepsilon_j=A_j^{-1}\sum_{i=1}^{m}x_i\cos 2\pi\mathbf{h}_i\,.\,\mathbf{r}_j \qquad (10)$$

and

$$\sin\varepsilon_j=A_j^{-1}\sum_{i=1}^{m}x_i\sin 2\pi\mathbf{h}_i\,.\,\mathbf{r}_j\,. \qquad (11)$$

Next, the exponential form is expanded into Bessel functions, using (Watson, 1966, p. 22)

$$\exp(iz\cos\theta)=J_0(z)+2\sum_{n=1}^{\infty}i^nJ_n(z)\cos n\theta\,. \qquad (12)$$

After averaging, the resulting expression for $q_j(x_1,\ldots,x_m)$ becomes

$$q_j(x_1,\ldots,x_m)=J_0\left(\frac{2Z_j}{\sigma_2^{1/2}}A_j\right)\,, \qquad (13)$$

where it is assumed that there are no atoms which have three rational coordinates. Next, for $Q(x_1,\ldots,x_m)$ we obtain

$$Q(x_1,\ldots,x_m)=\prod_{j=1}^{N/2}J_0\left(\frac{2Z_j}{\sigma_2^{1/2}}A_j\right)\approx\left\{\exp-\frac{1}{\sigma_2}\sum_{j=1}^{N/2}Z_j^2A_j^2\right\}\left\{1-\frac{1}{4\sigma_2^2}\sum_{j=1}^{N/2}Z_j^4A_j^4\right\} \qquad (14)$$

(Hauptman, 1971).

For the exponential we calculate

$$\exp-\frac{1}{\sigma_2}\sum_{j=1}^{N/2}Z_j^2A_j^2=\exp-\left[\sum_{i_1=1}^{m}\sum_{i_2=1}^{m}x_{i_1}x_{i_2}\times\sum_{j=1}^{N/2}\frac{Z_j^2}{\sigma_2}\cos 2\pi(\mathbf{h}_{i_1}-\mathbf{h}_{i_2})\,.\,\mathbf{r}_j\right]=\exp-\tfrac{1}{2}\mathbf{x}'\mathbf{U}\mathbf{x}\,, \qquad (15)$$

in which $\mathbf{x}$ is a column vector with components $x_1,\ldots,x_m$, $\mathbf{x}'$ is the corresponding row vector and $\mathbf{U}$ is a Karle–Hauptman matrix (Karle & Hauptman, 1950). Its components are

$$U_{i_1i_2}=U^s_{\mathbf{h}_{i1}-\mathbf{h}_{i2}}\,, \qquad (16)$$

where $U^s_{\mathbf{h}}$ is a unitary structure factor of the squared structure,

$$U^s_{\mathbf{h}}=\sum_{j=1}^{N/2}\frac{2Z_j^2}{\sigma_2}\cos 2\pi\mathbf{h}\,.\,\mathbf{r}_j\,. \qquad (17)$$

For structures consisting of equal atoms $U^s_{\mathbf{h}}=U_{\mathbf{h}}$. The expression between the second pair of braces in (14) can be written as

$$1-\frac{1}{4\sigma_2^2}\sum_{j=1}^{N/2}Z_j^4A_j^4=1-\tfrac{1}{8}\sum_{i_1=1}^{m}\cdots\sum_{i_4=1}^{m}N_{i_1i_2i_3i_4}x_{i_1}x_{i_2}x_{i_3}x_{i_4}\,, \tag{18}$$

where

$$N_{i_1i_2i_3i_4}=\frac{\sigma_4}{2\sigma_2^2}\,(U^f_{\mathbf{h}_{i1}-\mathbf{h}_{i2}+\mathbf{h}_{i3}-\mathbf{h}_{i4}}+U^f_{\mathbf{h}_{i1}-\mathbf{h}_{i2}-\mathbf{h}_{i3}+\mathbf{h}_{i4}})\,. \tag{19}$$

$U^f_{\mathbf{h}}$ is a unitary structure factor of the structure to the fourth power,

$$U^f_{\mathbf{h}}=\sum_{j=1}^{N/2}\frac{2Z_j^4}{\sigma_4}\cos 2\pi\mathbf{h}\,.\,\mathbf{r}_j\,. \tag{20}$$

For structures consisting of equal atoms $U^f_{\mathbf{h}}=U_{\mathbf{h}}$ and $\sigma_4/\sigma_2^2=1/N$. The most important $N_{i_1i_2i_3i_4}$ are

$$N_{i_1i_1i_2i_2}=\sigma_4/\sigma_2^2 \tag{21}$$

and

$$N_{i_1i_2i_1i_2}=N_{i_1i_2i_2i_1}=\frac{\sigma_4}{2\sigma_2^2}\,(1+U^f_{2\mathbf{h}_{i1}-2\mathbf{h}_{i2}})$$

$$\approx\frac{\sigma_4}{2\sigma_2^2}\,,\quad i_1\neq i_2\,. \tag{22}$$

Neglecting the other $N_{i_1i_2i_3i_4}$, the characteristic function of $P(X_1,\ldots,X_m)$ can be written as

$$Q(x_1,\ldots,x_m)\approx\{\exp\,-\tfrac{1}{2}\mathbf{x}'\mathbf{U}\mathbf{x}\}$$
$$\times\left\{1-\frac{\sigma_4}{8\sigma_2^2}\,(2\sum_{i_1=1}^{m}\sum_{i_2=1}^{m}x_{i_1}^2x_{i_2}^2-\sum_{i=1}^{m}x_i^4)\right\}. \tag{23}$$

Next we use (6). The calculation of the integral involves a transformation of variables $\mathbf{x}=\mathbf{C}\mathbf{y}$ (see Cramér, 1971, p. 119) such that $\mathbf{C}'\mathbf{U}\mathbf{C}$ is the diagonal matrix formed by the eigenvalues of $\mathbf{U}$. For $\sum_{i=1}^{m}x_i^4$, between the second pair of braces in (23), we use the approximation $x_i=y_i$. In fact this means that for the calculation of the first-order term in $P(X_1,\ldots,X_m)$ (order: σ_4/σ_2^2) we assume small off-diagonal elements in the Karle–Hauptman matrix. This assumption is also taken into account after the evaluation of the integral. The following result is obtained,

$$P(X_1,\ldots,X_m)\approx\frac{1}{(2\pi)^{m/2}U^{1/2}}\{\exp\,-\tfrac{1}{2}\mathbf{X}'\mathbf{U}^{-1}\mathbf{X}\}$$
$$\times\left\{1-\frac{\sigma_4}{8\sigma_2^2}\left[2(\sum_{i=1}^{m}X_i^2)^2-\sum_{i=1}^{m}X_i^4\right.\right.$$
$$\left.\left.-(4m+2)\sum_{i=1}^{m}X_i^2+2m^2+m\right]\right\}, \tag{24}$$

in which U and $\mathbf{U}^{-1}$ are the determinant and the inverse of $\mathbf{U}$ respectively, $\mathbf{X}$ is a column vector with components $X_1,\ldots,X_m$ and $\mathbf{X}'$ is the corresponding row vector.

For space group $P1$, where

$$E_{\mathbf{h}}=\sum_{j=1}^{N}\frac{Z_j}{\sigma_2^{1/2}}\exp 2\pi i\mathbf{h}\,.\,\mathbf{r}_j \tag{25}$$

and

$$U_{\mathbf{h}}=\sum_{j=1}^{N}\frac{Z_j}{\sigma_1}\exp 2\pi i\mathbf{h}\,.\,\mathbf{r}_j\,, \tag{26}$$

analogous calculations lead to

$$P(X_1,\ldots,X_m)\approx\frac{1}{\pi^m U}\{\exp\,-\mathbf{X}^\dagger\mathbf{U}^{-1}\mathbf{X}\}$$
$$\times\left\{1-\frac{\sigma_4}{4\sigma_2^2}\,[2(\sum_{i=1}^{m}|X_i|^2)^2-\sum_{i=1}^{m}|X_i|^4\right.$$
$$\left.-4m\sum_{i=1}^{m}|X_i|^2+2m^2]\right\}. \tag{27}$$

In this formula $\mathbf{X}^\dagger$ denotes the complex conjugate of $\mathbf{X}'$. The components of $\mathbf{U}$ are given by (16), now with

$$U^s_{\mathbf{h}}=\sum_{j=1}^{N}\frac{Z_j^2}{\sigma_2}\exp 2\pi i\mathbf{h}\,.\,\mathbf{r}_j\,. \tag{28}$$

Again, for equal-atom structures $U^s_{\mathbf{h}}=U_{\mathbf{h}}$.

The main terms in (24) and (27) have been found by Tsoucaris (1970). $P(X_1,X_2)$ and $P(X_1,X_2,X_3)$, both for structures consisting of equal atoms, have been derived by Hauptman & Karle (1958) for space group $P\bar{1}$ and by Hauptman (1971) for $P1$. For unequal atoms and space group $P\bar{1}$, the joint probability distribution $P(X_1,X_2)$ has been obtained by Heinerman, Krabbendam & Kroon (1975). (24) and (27) are in agreement with those results.

The most probable set of values for the $E_{\mathbf{h}_l+\mathbf{k}}$'s is the one for which $P(X_1,\ldots,X_m)$ is as large as possible. The first-order term does not depend on the phases (signs) of the X_i's. This implies that the first-order term does not affect the most probable values for the phases (signs) of the $E_{\mathbf{h}_l+\mathbf{k}}$'s. It only affects the most probable values for the $|E_{\mathbf{h}_l+\mathbf{k}}|$'s, especially if m is of the order σ_2^2/σ_4 ($=N$ for equal-atom structures). It follows that the maximum-determinant rule for phase determination (Tsoucaris, 1970), which is based on the main terms of (24) and (27), remains valid when the first-order term is included. However, it must be emphasized that the fact that the first-order term has no influence on the most probable values for the phases does not imply that the same holds for the second and higher-order terms.

Conditional probabilities

After bringing the first-order terms in (24) and (27) into the exponent (Karle, 1972) we obtain for space group $P\bar{1}$

$$P(X_1,\ldots,X_m)\approx \frac{1}{(2\pi)^{m/2}U^{1/2}}\exp\left\{-\tfrac{1}{2}\mathbf{X}'\mathbf{U}^{-1}\mathbf{X}\right.$$
$$-\frac{\sigma_4}{8\sigma_2^2}\left[2\Big(\sum_{i=1}^{m}X_i^2\Big)^2-\sum_{i=1}^{m}X_i^4\right.$$
$$\left.\left.-(4m+2)\sum_{i=1}^{m}X_i^2+2m^2+m\right]\right\}, \qquad (29)$$

and for $P1$

$$P(X_1,\ldots,X_m)\approx \frac{1}{\pi^m U}\exp\left\{-\mathbf{X}^\dagger\mathbf{U}^{-1}\mathbf{X}\right.$$
$$-\frac{\sigma_4}{4\sigma_2^2}\left[2\Big(\sum_{i=1}^{m}|X_i|^2\Big)^2-\sum_{i=1}^{m}|X_i|^4\right.$$
$$\left.\left.-4m\sum_{i=1}^{m}|X_i|^2+2m^2\right]\right\}. \qquad (30)$$

Denote $E_{\mathbf{h}_p+\mathbf{k}}$ by E_p. For given values of $E_1,\ldots,E_{q-1}$, $E_{q+1},\ldots,E_m$ the most probable value for E_q (denoted by $\bar{E}_q$) is that value of X_q for which $P(E_1,\ldots,E_{q-1}, X_q, E_{q+1},\ldots,E_m)$ is as large as possible. Following the same procedure as Tsoucaris (1970) and de Rango, Tsoucaris & Zelwer (1974) the following formulae are obtained.

Space group $P\bar{1}$

$$\bar{E}_q\approx -\frac{\sum_{\substack{i=1\\ i\neq q}}^{m}U_{qi}^{-1}E_i}{U_{qq}^{-1}+\frac{\sigma_4}{\sigma_2^2}\left[\sum_{\substack{i=1\\ i\neq q}}^{m}(E_i^2-1)+\tfrac{1}{2}(\bar{E}_q^2-3)\right]}. \qquad (31)$$

Neglecting $\frac{1}{2}(\bar{E}_q^2-3)$ in the denominator we get

$$\bar{E}_q\approx -\frac{\sum_{\substack{i=1\\ i\neq q}}^{m}U_{qi}^{-1}E_i}{U_{qq}^{-1}+\frac{\sigma_4}{\sigma_2^2}\sum_{\substack{i=1\\ i\neq q}}^{m}(E_i^2-1)}. \qquad (32)$$

Except for the first-order term, formula (32) is the same as the result obtained by Tsoucaris and de Rango *et al.* The probability distribution of E_q, given the other E's, is

$$P(X_q|E_1,\ldots,E_{q-1},E_{q+1},\ldots,E_m)$$
$$\approx\frac{1}{(2\pi)^{1/2}\sigma_q}\exp-\frac{(X_q-\bar{E}_q)^2}{2\sigma_q^2}, \qquad (33)$$

where $\bar{E}_q$ is given by (32) and

$$\sigma_q^2=[U_{qq}^{-1}+\frac{\sigma_4}{\sigma_2^2}\sum_{\substack{i=1\\ i\neq q}}^{m}(E_i^2-1)]^{-1}. \qquad (34)$$

Note that in contrast with the result of Tsoucaris and de Rango *et al.*, who found $\sigma_q^2=(U_{qq}^{-1})^{-1}$, our expression for the variance depends on the $|E_i|$'s. As the $|E_i|$'s become larger the variance becomes smaller. This is in agreement with the fact that large $|E_i|$'s give more information than small ones. From (33) we find for the probability that $E_q\bar{E}_q$ is positive

$$P(E_q\bar{E}_q>0|E_1,\ldots,E_{q-1},|E_q|,E_{q+1},\ldots,E_m)$$
$$\approx\tfrac{1}{2}+\tfrac{1}{2}\tanh\frac{A_q}{2}, \qquad (35)$$

in which

$$A_q=\frac{2}{\sigma_q^2}|E_q\bar{E}_q|. \qquad (36)$$

From (32) and (34) it follows that A_q does not depend on the first-order term.

Space group $P1$

$$\bar{E}_q\approx -\frac{\sum_{\substack{i=1\\ i\neq q}}^{m}U_{qi}^{-1}E_i}{U_{qq}^{-1}+\frac{\sigma_4}{\sigma_2^2}\left[\sum_{\substack{i=1\\ i\neq q}}^{m}(|E_i|^2-1)+\tfrac{1}{2}(|\bar{E}_q|^2-2)\right]}. \qquad (37)$$

Neglecting $\frac{1}{2}(|\bar{E}_q|^2-2)$ in the denominator of (37) we obtain (32) with the E_i^2 replaced by $|E_i|^2$. The probability distribution of E_q, given the other E's, is

$$P(X_q|E_1,\ldots,E_{q-1},E_{q+1},\ldots,E_m)$$
$$\approx\frac{1}{\pi\sigma_q^2}\exp-\frac{|X_q-\bar{E}_q|^2}{\sigma_q^2}. \qquad (38)$$

$\bar{E}_q$ and σ_q^2 are given by (32) and (34) respectively, where in both formulae the E_i^2 are replaced by $|E_i|^2$. From (38) we obtain the probability distribution of the phase φ_q of E_q,

$$P(\Phi_q|E_1,\ldots,E_{q-1},|E_q|,E_{q+1},\ldots,E_m)$$
$$\approx\frac{\exp\left[A_q\cos(\Phi_q-\bar{\varphi}_q)\right]}{2\pi I_0(A_q)}, \qquad (39)$$

where A_q is given by (36) and $\bar{\varphi}_q$ is the phase of $\bar{E}_q$.

The first-order term has influence on $|\bar{E}_q|$ and $P(X_q|E_1,\ldots,E_{q-1},E_{q+1},\ldots,E_m)$, especially if the $|E_i|$'s are large, but it has no influence on the phase (sign) and the phase (sign) probability.

The author thanks Drs H. Krabbendam and J. Kroon and Professor A. F. Peerdeman for stimulating discussions and critical reading of the manuscript.

References

CRAMÉR, H. (1971). *Mathematical Methods of Statistics*. Princeton Univ. Press.

HAUPTMAN, H. (1971). *Z. Kristallogr.* **134**, 28–43.

HAUPTMAN, H. & KARLE, J. (1958). *Acta Cryst.* **11**, 149–157.

HEINERMAN, J. J. L., KRABBENDAM, H. & KROON, J. (1975). *Acta Cryst.* A**31**, 731–737.

KARLE, J. (1972). *Acta Cryst.* B**28**, 3362–3369.

KARLE, J. & HAUPTMAN, H. (1950). *Acta Cryst.* **3**, 181–187.

RANGO, C. DE, TSOUCARIS, G. & ZELWER, CH. (1974). *Acta Cryst.* A**30**, 342–353.

TSOUCARIS, G. (1970). *Acta Cryst.* A**26**, 492–499.

WATSON, G. N. (1966). *A Treatise on the Theory of Bessel Functions*. Cambridge Univ. Press.