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# From a Partial to the Complete Crystal Structure


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## Abstract

The joint probability distribution method is applied in order to estimate phases when part of the crystal structure is correctly positioned. The mathematical approach is briefly described and the conclusive formulas are compared with those given by previous authors.


## Symbols and abbreviations

Throughout the paper a number of symbols will find frequent application. For the sake of simplicity they are here listed together.

$\mathbf{h} \equiv (h,k,l)$: vectorial index of a reflection. We will also use $\mathbf{k}$ and $\mathbf{h}+\mathbf{k}$.
$f(\mathbf{h})$: atomic scattering factor. The thermal factor is included: anomalous dispersion is not considered.
$F_{\mathbf{h}}$: structure factor with vectorial index $\mathbf{h}$.
$N$: number of atoms in the unit cell.
$p$: number of atoms (symmetry equivalents included) whose positions are *a priori* known.
$q$: number of atoms (symmetry equivalents included) whose positions are unknown: $q = N - p$.
$F_{\mathbf{h}}$, $E_{\mathbf{h}}$: structure factor and normalized structure factor with vectorial index $\mathbf{h}$.
$\varphi_{\mathbf{h}}$, $\varphi_{\mathbf{k}}$, $\varphi_{\mathbf{h}+\mathbf{k}}$: phase values of $E_{\mathbf{h}}$, $E_{\mathbf{k}}$, $E_{\mathbf{h}+\mathbf{k}}$.
$R_{\mathbf{h}}$, $R_{\mathbf{k}}$, $R_{\mathbf{h}+\mathbf{k}}$: moduli of $E_{\mathbf{h}}$, $E_{\mathbf{k}}$, $E_{\mathbf{h}+\mathbf{k}}$.
$\Phi = \varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} - \varphi_{\mathbf{h}+\mathbf{k}}$.
$E_{p,\mathbf{h}}$, $E_{p,\mathbf{k}}$, $E_{p,\mathbf{h}+\mathbf{k}}$ = pseudo-normalized structure factors of the partial structure with $p$ atoms in the unit cell.
$R_{p,\mathbf{h}}$, $R_{p,\mathbf{k}}$, $R_{p,\mathbf{h}+\mathbf{k}}$: moduli of $E_{p,\mathbf{h}}$, $E_{p,\mathbf{k}}$, $E_{p,\mathbf{h}+\mathbf{k}}$.
$\varphi_{p,\mathbf{h}}$, $\varphi_{p,\mathbf{k}}$, $\varphi_{p,\mathbf{h}+\mathbf{k}}$ = phase values of $E_{p,\mathbf{h}}$, $E_{p,\mathbf{k}}$, $E_{p,\mathbf{h}+\mathbf{k}}$.
$\Phi_p = \varphi_{p,\mathbf{h}} + \varphi_{p,\mathbf{k}} - \varphi_{p,\mathbf{h}+\mathbf{k}}$.
$E_{q,\mathbf{h}}$, $E_{q,\mathbf{k}}$, $E_{q,\mathbf{h}+\mathbf{k}}$ = pseudo-normalized structure factors of the unknown part of the structure.
$R_{q,\mathbf{h}}$, $R_{q,\mathbf{k}}$, $R_{q,\mathbf{h}+\mathbf{k}}$ = moduli of $E_{q,\mathbf{h}}$, $E_{q,\mathbf{k}}$, $E_{q,\mathbf{h}+\mathbf{k}}$.

$$\Sigma_q(\mathbf{h}) = \sum_{j=p+1}^{N} f_j^2(\mathbf{h}).$$

$t_j(\mathbf{h})$: $f_j(\mathbf{h})/[|F_{p,\mathbf{h}}|^2 + \Sigma_q(\mathbf{h})]^{1/2}$ for the $j$th atom.

$$b(\mathbf{h}) = \sum_{j=p+1}^{N} t_j^2(\mathbf{h}) = \Sigma_q(\mathbf{h})/[|F_{p,\mathbf{h}}|^2 + \Sigma_q(\mathbf{h})].$$

$$c = \sum_{j=p+1}^{N} t_j(\mathbf{h})\, t_j(\mathbf{k})\, t_j(\mathbf{h}+\mathbf{k}).$$

Other locally used symbols are defined in the text.

## 1. Introduction

Main (1976) generalized Cochran's (1955) formula for the phase probability of a triple product in order to exploit some *a priori* knowledge about the structure. He considered four kinds of information: (*a*) randomly positioned atoms; (*b*) randomly positioned and randomly oriented atomic groups; (*c*) randomly positioned but correctly oriented atomic groups; (*d*) correctly positioned atoms.

A mathematical derivation of Main's formula was given by Heinerman (1977) (see also Heinerman, Krabbendam & Kroon, 1977). In its formulation the normalized structure factor $E_{\mathbf{h}}$ is defined by

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$$E_{\mathbf{h}} = \frac{F_{\mathbf{h}}}{\langle |F_{\mathbf{h}}|^2 \rangle_{\text{p.r.v.}}^{1/2}}, \tag{1}$$

where $\langle |F_{\mathbf{h}}|^2 \rangle_{\text{p.r.v.}}$ denotes the average of $|F_{\mathbf{h}}|^2$, the variable being the primitive random variables.

If a group of $p$ atoms is assumed to be correctly positioned and the other $N-p$ atomic positions are the primitive random variables, (1) may be written in $P1$ or $P\bar{1}$ as

$$E_{\mathbf{h}} = \frac{F_{\mathbf{h}}}{\left\langle \sum_{i,j=1}^{N} f_i f_j \exp 2\pi i \mathbf{h}(\mathbf{r}_i - \mathbf{r}_j) \right\rangle_{\text{p.r.v.}}^{1/2}} = \frac{F_{\mathbf{h}}}{[|F_{p,\mathbf{h}}|^2 + \Sigma_q]^{1/2}}. \tag{2}$$

We define here $E_{p,\mathbf{h}}$ and $E_{q,\mathbf{h}}$:

$$E_{p,\mathbf{h}} = \frac{F_{p,\mathbf{h}}}{[|F_{p,\mathbf{h}}|^2 + \Sigma_q]^{1/2}}, \quad E_{q,\mathbf{h}} = \frac{F_{q,\mathbf{h}}}{[|F_{p,\mathbf{h}}|^2 + \Sigma_q]^{1/2}}.$$

We explicitly note that $E_{p,\mathbf{h}}$ is not a variable in our approach and always $|E_{p,\mathbf{h}}| \leq 1$. On the other hand, $E_{q,\mathbf{h}}$ is a variable, but it is not a normalized structure factor *stricto sensu*. Indeed, $\langle |E_{q,\mathbf{h}}|^2 \rangle = b(\mathbf{h}) \leq 1$. For the sake of simplicity in the text we will denote $E_{p,\mathbf{h}}$ and $E_{q,\mathbf{h}}$ as pseudo-normalized structure factors.

When $p$ atoms have *a priori* known positions, Main's formula reduces to

$$P(\Phi | R_{\mathbf{h}}, R_{\mathbf{k}}, R_{\mathbf{h}+\mathbf{k}}) \simeq \frac{1}{2\pi I_0(Q)} \exp\{Q \cos(\Phi - q)\}, \tag{3}$$

where

$$Q \exp(iq) = 2R_{\mathbf{h}} R_{\mathbf{k}} R_{\mathbf{h}+\mathbf{k}} (R_{p,\mathbf{h}} R_{p,\mathbf{k}} R_{p,\mathbf{h}+\mathbf{k}} \exp i\varphi_p + c)$$

and $I_0$ is the modified Bessel function of order zero. In $P\bar{1}$ Main's formula leads to

$$P_+(E_{\mathbf{h}} E_{\mathbf{k}} E_{\mathbf{h}+\mathbf{k}}) \simeq 0{\cdot}5 + 0{\cdot}5 \tanh(R_{\mathbf{h}} R_{\mathbf{k}} R_{\mathbf{h}+\mathbf{k}} E_{p,\mathbf{h}} E_{p,\mathbf{k}} E_{p,\mathbf{h}+\mathbf{k}} + c), \tag{4}$$

where $P_+(E_{\mathbf{h}} E_{\mathbf{k}} E_{\mathbf{h}+\mathbf{k}})$ is the probability that the product $E_{\mathbf{h}} E_{\mathbf{k}} E_{\mathbf{h}+\mathbf{k}}$ is positive. Heinerman observed that (3) and (4) were not quite satisfactory and concluded that only high-order terms of the distributions could improve the accuracy of the formulas.

In this paper (§§ 2, 3, 4, 7) we introduce a mathematical approach which does not coincide with Heinerman's procedure and leads to conclusive formulas very promising for practical applications. For the sake of brevity we do not give a full account of our procedure: the reader is referred to a recent book (Giacovazzo, 1980) for the basic ideas. We only say here that: (*a*) the atomic positions are assumed to be the random variables; (*b*) any normalized structure factor $E_{\mathbf{h}}$ is considered as the sum of a fixed term $E_{p,\mathbf{h}}$ arising from the atoms with known positions and a random term $E_{q,\mathbf{h}}$ arising from the atoms with unknown positions: $E_{\mathbf{h}} = E_{p,\mathbf{h}} + E_{q,\mathbf{h}}$.

In the text we give explicitly the characteristic functions of the various distributions because they do not coincide with those given by Heinerman. In addition to Main's formula other procedures are widely used for recovering the full structure from a partial. In §5 we briefly discuss them in the light of the results here presented. In § 8 the use of our theory in the determinantal approach is described. Practical considerations are given in §§ 6 and 9.

## 2. The conditional probability density $P(E_{\mathbf{h}}|E_{p,\mathbf{h}})$ and related distributions

In this section our approach is applied to obtain some results concerning $P(E_{\mathbf{h}}|E_{p,\mathbf{h}})$ and related distributions. The results are not new, however they are stressed because: (*a*) they are given in terms of the normalized and pseudo-normalized structure factors defined by (2); (*b*) they play a central role in some widely used procedures which try to obtain the whole structure from a partial one.

For the sake of brevity $E$ and $E_p$ will denote $E_{\mathbf{h}}$ and $E_{p,\mathbf{h}}$. We will deal here only with $P\bar{1}$ and $P1$: the corresponding distributions can be applied to all centrosymmetric and non-centrosymmetric space groups, respectively.

### $P\bar{1}$

The characteristic function of the distribution $P(E|E_p)$ is

$$C(u) \simeq \exp(iuE_p) \exp\left(-\frac{u^2}{2} b\right),$$

where $u$ is a carrying variable associated with $E$. Then

$$P(E|E_p) \simeq \frac{1}{2\pi} \int_{-\infty}^{+\infty} C(u) \exp(-iuE)\, du = \frac{1}{(2\pi b)^{1/2}} \exp\left\{-\frac{(E-E_p)^2}{2b}\right\}. \tag{5}$$

Equation (5) is a normal distribution of type $N[E_p; b^{1/2}]$: $E_p$ is the expected value of $E$ and $b^{1/2}$ the standard deviation. $b$ always lies in the interval (0,1). Furthermore, $b = 1$ if $p = 0$: then $E_p = 0$ and (5) coincides with Wilson's distribution; $b = 0$ if $p = N$: then (5) reduces to a delta function centred on $E = E_p$.

From (5) the distribution $P(|E||E_p)$ is readily obtained:

$$P(|E||E_p) \simeq \left(\frac{2}{\pi b}\right)^{1/2} \exp\left\{-\frac{(E^2 + E_p^2)}{2b}\right\} \cosh\left(\frac{|EE_p|}{b}\right). \tag{6}$$

The distribution (6) is equivalent to a previous result obtained by Srinivasan & Chandrasekharan in 1966 (for reference see Srinivasan & Parthasarathy, 1976, p. 86) in terms of structure factors.

The probability that $E$ and $E_p$ have the same sign is given by

$$P(s = s_p) \simeq 0{\cdot}5 + 0{\cdot}5 \tanh \frac{|EE_p|}{b}, \qquad (7)$$

which is equivalent to a previous result obtained by Woolfson (1956, equation 4) in terms of unitary structure factors.

*P*1

The characteristic function of the distribution $P(A,B|A_p,B_p)$ is

$$C(u,v) \simeq \exp i(uA_p + vB_p) \exp\left[-\left(\frac{u^2}{4} + \frac{v^2}{4}\right) b\right],$$

where $A$, $A_p$ and $B$, $B_p$ are the real and imaginary parts of $E$ and $E_p$ respectively, $u$ and $v$ are carrying variables associated with $A$ and $B$. Then

$$P(A,B|A_p,B_p) \simeq \frac{1}{\pi b} \exp\left\{-\frac{1}{b}[(A - A_p)^2 + (B - B_p)^2]\right\}, \qquad (8)$$

which is a two-dimensional normal distribution of two uncorrelated random variables with identical standard deviation $(b/2)^{1/2}$. In polar form (8) is written as

$$P(R,\varphi|R_p,\varphi_p) \simeq \frac{R}{\pi b} \exp\left\{-\frac{1}{b}[R^2 + R_p^2 - 2RR_p \cos(\varphi - \varphi_p)]\right\}, \qquad (9)$$

which was first obtained by Sim (1959) in terms of structure factors. From (9), (10) and (11) are readily obtained:

$$P(R|R_p,\varphi) \simeq \frac{2R}{b} \exp\left\{-\frac{(R^2 + R_p^2)}{b}\right\} I_0(G), \qquad (10)$$

$$P(\varphi|R,R_p,\varphi_p) \simeq \frac{1}{2\pi I_0(G)} \exp[G \cos(\varphi - \varphi_p)], \qquad (11)$$

where $G = 2RR_p/b$. Equation (11) is a von Mises distribution: $\varphi_p$ is the expected value of $\varphi$ and the reliability of the distribution $\varphi \simeq \varphi_p$ increases with $G$.

### 3. The conditional joint probability distribution $P(E_\mathbf{h}, E_\mathbf{k}, E_{\mathbf{h}+\mathbf{k}}|E_{p,\mathbf{h}}, E_{p,\mathbf{k}}, E_{p,\mathbf{h}+\mathbf{k}})$ and related distributions in $P\bar{1}$

Let us denote

$$E_1 = E_\mathbf{h}, \quad E_2 = E_\mathbf{k}, \quad E_3 = E_{\mathbf{h}+\mathbf{k}},$$
$$E_{p1} = E_{p,\mathbf{h}}, \quad E_{p2} = E_{p,\mathbf{k}}, \quad E_{p3} = E_{p,\mathbf{h}+\mathbf{k}}.$$

The joint probability distribution

$$P(E_1,E_2,E_3|E_{p1},E_{p2},E_{p3})$$

retaining only terms up to $1/(q)^0$ order is

$$[P(E_1,E_2,E_3|\ldots)]_{1/(q)^0} \simeq (2\pi)^{-3/2}(b_1 b_2 b_3)^{-1/2} \exp\left\{-\frac{(E_1 - E_{p1})^2}{2b_1} - \frac{(E_2 - E_{p2})^2}{2b_2} - \frac{(E_3 - E_{p3})^2}{2b_3}\right\}, \qquad (12)$$

which is a three-dimensional normal distribution. $E_{p1}$, $E_{p2}$, $E_{p3}$ are the expected values of $E_1$, $E_2$, $E_3$, respectively and $b_1^{1/2}$, $b_2^{1/2}$, $b_3^{1/2}$ the standard deviations. No correlation coefficient exists among the variables so that they may be considered as independent of one another. From (12) no information additional to that provided by (5) may be obtained for a single $E_i$. We note that $b_i = 1$, $i = 1, 2, 3$, when $p = 0$: then (12) reduces to the product of three Wilson's distributions. On the other hand, $b_i = 0$, $i = 1, 2, 3$, if $p = N$: then (12) reduces to the product of three delta functions centred on $E_{p1}$, $E_{p2}$, $E_{p3}$.

Additional information may be obtained if terms of order $1/q^{1/2}$ are taken into account in the characteristic function of the trivariate distribution. Such terms will perturbate the distribution (12) by introducing a correlation coefficient among the variables. The characteristic function is then

$$C(u_1,u_2,u_3) \simeq \exp\{i(u_1 E_{p1} + u_2 E_{p2} + u_3 E_{p3})\} \times \exp\left(-b_1\frac{u_1^2}{2} - b_2\frac{u_2^2}{2} - b_3\frac{u_3^2}{2} - icu_1u_2u_3\right),$$

where $u_1$, $u_2$, $u_3$ are carrying variables associated with $E_1$, $E_2$, $E_3$, respectively, and $b_1$, $b_2$, $b_3$ stand for $b(\mathbf{h})$, $b(\mathbf{k})$, $b(\mathbf{h}+\mathbf{k})$.

After some calculation we obtained

$$P(E_1,E_2,E_3|E_{p1},E_{p2},E_{p3}) \simeq (2\pi)^{-3/2}(b_1 b_2 b_3)^{-1/2} \exp\left\{-\frac{(E_1 - E_{p1})^2}{2b_1} - \frac{(E_2 - E_{p2})^2}{2b_2} - \frac{(E_3 - E_{p3})^2}{2b_3} + \frac{c}{b_1 b_2 b_3}(E_1 - E_{p1})(E_2 - E_{p2})(E_3 - E_{p3})\right\}. \qquad (13)$$

Equation (13) coincides with the trivariate distribution obtained by Karle & Hauptman (1956) when $p = 0$ (see § 6). In Appendix *A* we give some distributions related to (13) which are used in this paper. We only state here:

(*a*) the conditional expected value of $E_1$:

$$(\langle E_1\rangle|E_2,E_3,E_{p1},E_{p2},E_{p3}) \simeq E_{p1} + \frac{c}{b_2 b_3}(E_2 - E_{p2})(E_3 - E_{p3}). \quad (14)$$

In contrast with (5), the expected value of $E_1$ is no longer $E_{p1}$ but $E_{p1}$ plus an additional contribution often larger than $E_{p1}$;

(*b*) the conditional expected value of $E_2E_3$:

$$(\langle E_2E_3\rangle|E_1,E_{p1},E_{p2},E_{p3}) \simeq E_{p2}E_{p3} + \frac{c}{b_1}(E_1 - E_{p1}). \quad (15)$$

Equations (14) and (15) will be useful in the determinantal approach, as described in § 8.

In practical direct procedures the estimation of the signs of structure factors or of their products are usually required. Let us now calculate the probability that

$$(E_1 - E_{p1})(E_2 - E_{p2})(E_3 - E_{p3}) > 0.$$

From the distribution (13) we obtain

$$P_+(E_{q1}E_{q2}E_{q3} > 0) \simeq 0{\cdot}5 + 0{\cdot}5\tanh\left\{\frac{c}{b_1 b_2 b_3}|E_{q1}E_{q2}E_{q3}|\right\}, \quad (16)$$

which gives a first indication of the differences between Main's and our theory. According to (4), $E_1E_2E_3E_{p1}E_{p2}E_{p3}$ is expected to be positive if: (i) $E_{p1}E_{p2}E_{p3}$ is positive; (ii) $E_{p1}E_{p2}E_{p3}$ is negative and $c > R_1R_2R_3R_{p1}R_{p2}R_{p3}$. According to (16),

$$(E_1 - E_{p1})(E_2 - E_{p2})(E_3 - E_{p3})$$

is always expected to be positive. An important point to be emphasized is the following: when from the trivariate distribution (13) we pass to (16) we lose the information about the correlations between the pairs $E_i$ and $E_{pi}$. In practice, the application of (16) reduces the problem of finding the sign of a triplet in an $N$-atom structure with $p$ atoms in known positions to the problem of estimating the sign of a triplet in a structure with $q$ atoms [see the analysis of the factor $c/(b_1b_2b_3)$ in § 6]. Thus (16) is nothing but the classical Woolfson relationship which is not very useful in this context unless the information about the correlations of the pairs $E_i$ and $E_{pi}$ are introduced in the procedure by additional information.

The probability that the sign of $E_1E_2E_3$ is positive may be calculated *via* (13). Let $P(s_1,s_2,s_3)$ be the value of (13) when the signs $s_1$, $s_2$, $s_3$ are associated with $E_1$, $E_2$, $E_3$, respectively. Then

$$P(s_1s_2s_3 = +) = P(+,+,+) + P(+,-,-) + P(-,+,-) + P(-,-,+),$$

$$P(s_1s_2s_3 = -) = P(-,-,-) + P(-,+,+) + P(+,-,+) + P(+,+,-),$$

from which the normalized sign probability formula may be derived:

$$P(s_1s_2s_3 = +)/[P(s_1s_2s_3 = +) + P(s_1s_2s_3 = -)]. \quad (17)$$

Such an approach does not lose information as (16). In a similar way the probabilities that $E_2E_3$, $E_1E_2$, $E_1E_3$ have positive sign or the probability that $E_1E_2E_3$ and $E_{p1}E_{p2}E_{p3}$ have the same sign may be calculated.

The sign probability (17) is rather prolix and, for the sake of simplicity, we do not give here its explicit expression. However, it is not very useful in the practice where a more immediate application has the estimation of the sign probability of $E_1$ when $E_2$, $E_3$, $E_{p1}$, $E_{p2}$, $E_{p3}$ are known. We obtain

$$P_+(E_1) \simeq 0{\cdot}5 + 0{\cdot}5\tanh\left\{|E_1|\left[\frac{E_{p1}}{b_1} + \frac{c}{b_1b_2b_3}\times(E_2 - E_{p2})(E_3 - E_{p3})\right]\right\}. \quad (18)$$

Equation (18) is basic for practical applications and will be discussed in § 6.

## 4. The conditional joint probability $P(R_h, R_k, R_{\overline{h+k}}, \varphi_h, \varphi_k, \varphi_{\overline{h+k}}, R_{p,h}, R_{p,k}, R_{p,\overline{h+k}}, \varphi_{p,h}, \varphi_{p,k}, \varphi_{p,\overline{h+k}})$ in $P1$

Let $\rho_i$, $\psi_i$, $i = 1, 2, 3$, be carrying variables associated with $R_i$, $\varphi_i$, $i = 1, 2, 3$, respectively. The characteristic function of the distribution $P(R_i, \varphi_i, i = 1, 2, 3|R_{pi}, \varphi_{pi}, i = 1, 2, 3)$ is

$$C(\rho_i, \psi_i, i = 1, 2, 3) \simeq \exp\left\{-\frac{1}{4}(b_1\rho_1^2 + b_2\rho_2^2 + b_3\rho_3^2)\right\} \times \exp i\left\{\rho_1R_{p1}\cos(\varphi_1 - \psi_1) + \rho_2R_{p2}\cos(\varphi_2 - \psi_2) + \rho_3R_{p3}\cos(\varphi_3 - \psi_3) - \frac{c}{4}\rho_1\rho_2\rho_3\cos(\psi_1 + \psi_2 + \psi_3)\right\}.$$

Its Fourier transform gives the required distribution

$$P(R_1,R_2,R_3,\varphi_1,\varphi_2,\varphi_3|R_{p1},R_{p2},R_{p3},\varphi_{p1},\varphi_{p2},\varphi_{p3})$$
$$\simeq (\pi)^{-3}(b_1b_2b_3)^{-1}R_1R_2R_3\exp\left\{-\sum_{i=1}^{3}\frac{1}{b_i}[R_i^2+R_{pi}^2 - 2R_iR_{pi}\cos(\varphi_i-\varphi_{pi})]\right.$$
$$+\frac{2c}{b_1b_2b_3}[R_1R_2R_3\cos(\varphi_1+\varphi_2+\varphi_3)$$
$$-R_{p1}R_{p2}R_{p3}\cos(\varphi_{p1}+\varphi_{p2}+\varphi_{p3})$$
$$-R_{p1}R_2R_3\cos(\varphi_{p1}+\varphi_2+\varphi_3)$$
$$-R_1R_{p2}R_3\cos(\varphi_1+\varphi_{p2}+\varphi_3)$$
$$-R_1R_2R_{p3}\cos(\varphi_1+\varphi_2+\varphi_{p3})$$
$$+R_{p1}R_{p2}R_3\cos(\varphi_{p1}+\varphi_{p2}+\varphi_3)$$
$$+R_{p1}R_2R_{p3}\cos(\varphi_{p1}+\varphi_2+\varphi_{p3})$$
$$\left.+R_1R_{p2}R_{p3}\cos(\varphi_1+\varphi_{p2}-\varphi_{p3})]\right\}. \quad (19)$$

Equation (19) is basic for the following applications. It coincides with the classical trivariate distribution of Karle & Hauptman when $p = 0$. In Appendix $B$ we give some distributions related to (19) of which use is made in this paper. We only state here:

($a$) the conditional expected value of $E_2E_3$:

$$\langle(E_2E_3|\ldots)\rangle = \langle R_2R_3\exp i(\varphi_2+\varphi_3)\rangle$$
$$= E_{p2}E_{p3}+\frac{c}{b_1}(E_1-E_{p1}); \quad (20)$$

($b$) the conditional expected value of $\varphi_1$:

$$P(\varphi_1|\varphi_2,\varphi_3,R_i,R_{pi},\varphi_{pi},i=1,2,3)$$
$$\simeq [2\pi I_0(G)]^{-1}\exp[G\cos(\varphi_1-\xi)], \quad (21)$$

where $G^2 = a_1^2 + a_2^2$,

$$a_1 = 2R_1\left\{\frac{R_{p1}}{b_1}\cos\varphi_{p1}+\frac{c}{b_1b_2b_3}[R_2R_3\cos(\varphi_2+\varphi_3) - R_{p2}R_3\cos(\varphi_{p2}+\varphi_3)-R_2R_{p3}\cos(\varphi_2+\varphi_{p3}) + R_{p2}R_{p3}\cos(\varphi_{p2}+\varphi_{p3})]\right\},$$

$$a_2 = 2R_1\left\{\frac{R_{p1}}{b_1}\sin\varphi_{p1}+\frac{c}{b_1b_2b_3}[-R_2R_3\sin(\varphi_2+\varphi_3) + R_{p2}R_3\sin(\varphi_{p2}+\varphi_3)+R_2R_{p3}\sin(\varphi_2+\varphi_{p3}) - R_{p2}R_{p3}\sin(\varphi_{p2}+\varphi_{p3})]\right\},$$

$$\cos\xi = a_1/G, \quad \sin\xi = a_2/G.$$

Considerations about the use of (21) are made in § 6.

## 5. A comparison with preceding approaches

In the light of the theory so far described we briefly analyse in this section some theories or practical procedures aiming at recovering, *via* the reciprocal space, the entire structure from a partial one.

### ($a$) *Weighted Fourier syntheses*

Woolfson (1956) and Sim (1960) (see also Main, 1979) suggested that the use of Fourier syntheses with weighted terms $W|F|(\exp i\varphi_p)$ would reveal the unknown atomic positions better than the usual syntheses with $|F|\exp(i\varphi_p)$. These and related Fourier methods use essentially the information contained in the distributions (7) and (11).

### ($b$) *Tangent recycling methods* (*Karle*, 1970; *see also Hull & Irwin*, 1978)

A phase $\varphi_p$ is accepted if $|F_p| > \eta|F|$, where $\eta$ is the fraction of the total scattering power contained in the fragment and where $|F|$ is associated with an $|E| \geq 1{\cdot}5$. This approach empirically exploits distributions (7) and (11) because it aims to select high products $|E_pE|$. Tangent recycling uses a large starting set of $\varphi_p$'s in order to compensate for wrong estimations. In each tangent cycle the *a priori* structural information is only used for defining a good starting set.

### ($c$) *Tangent recycling methods applied to difference structure factors*

In the procedure proposed by Beurskens, Prick, Doesburg & Gould (1979) difference structure factors $\Delta F = (|F| - |F_p|)\exp i\varphi_p$ are calculated and, in favourable cases, accepted for a first estimation of $F_q$. Weighted tangent formula is applied to the $\Delta F$ values in order to convert them to more probable $F_q$ values.

A related approach was suggested by Hull & Irwin (1978). From (11) the expected cosine value

$$\langle\cos(\varphi-\varphi_p)\rangle = D_1\left(\frac{2RR_p}{b}\right)$$

follows. Since $R_q^2 = R^2 + R_p^2 + 2RR_p\cos(\varphi-\varphi_p)$, the expected value of $R_q^2$ is $R_q^2 = R^2 + R_p^2 + 2RR_pD_1(2RR_p/b)$. The normalized structure factors are input for a weighted tangent formula refinement. For both these procedures it may be observed: (1) they involve difference structure factors in tangent refinement instead of structure factors, and introduce the information about the correlation between $E$ and $E_p$ by suitable statistical criteria based on (7) and (11). According to our theory they appear more theoretically sound than procedure ($b$); (2) unfortunately they are unable to use the true $F_q$'s and strict theoretical distribution involving contemporaneously $E_i$, $E_{pi}$, $\varphi_i$, $\varphi_{pi}$.

### 6. Practical considerations about conclusive formulas

Let us suppose that $\varphi_2$, $\varphi_3$, $R_i$, $R_{pi}$, $\varphi_{pi}$, $i = 1, 2, 3$, are known. Centrosymmetrical or non-centrosymmetrical phases $\varphi_1$ can be estimated *via* (18) or (21), respectively. The parameters $c$ and $b_i$ play a central role in the formulas. The $b_i$'s are the expected values of $|E_{pi}|^2$. In the statistical sense small values of $b_i$ favour a reliable estimation of $\varphi_1$.

If $p = 0$ then the $b_i$'s assume the maximum value (= 1) and

$$c = \sum_{j=1}^{N} f_j(\mathbf{h}) f_j(\mathbf{k}) f_j(\mathbf{h}+\mathbf{k}) \left[\sum_{j=1}^{N} f_j^2(\mathbf{h})\right]^{-1/2} \times \left[\sum_{j=1}^{N} f_j^2(\mathbf{k})\right]^{-1/2} \left[\sum_{j=1}^{N} f_j^2(\mathbf{h}+\mathbf{k})\right]^{-1/2}.$$

Furthermore, assuming that all the atoms have the same unitary scattering factor, $c$ reduces to $[\sigma_3/\sigma_2^{3/2}]_N$, where

$$[\sigma_r]_N = \sum_{j=1}^{N} Z_j^r$$

and $Z_j$ is the atomic number of $j$. Consequently, (18) and (21) reduce to the widely used Woolfson and Cochran formulas.

In general, the reliability of a phase indication *via* (18) and (21) depends on the cooperative effect of two terms: the first, of order $1/(q)^0$, and the second, of order $1/(q)^{1/2}$, having the coefficient

$$\begin{aligned}\frac{c}{b_1 b_2 b_3} = \sum_{j=p+1}^{N} & f_j(\mathbf{h}) f_j(\mathbf{k}) f_j(\mathbf{h}+\mathbf{k}) [\Sigma_q(\mathbf{h})]^{-1/2} \\ & \times [\Sigma_q(\mathbf{k})]^{-1/2} [\Sigma_q(\mathbf{h}+\mathbf{k})]^{-1/2} \\ & \times \{[|F_{p1}|^2 + \Sigma_q(\mathbf{h})] [|F_{p2}|^2 + \Sigma_q(\mathbf{k})] \\ & \times [|F_{p3}|^2 + \Sigma_q(\mathbf{h}+\mathbf{k})] \\ & \times [\Sigma_q(\mathbf{h}) \Sigma_q(\mathbf{k}) \Sigma_q(\mathbf{h}+\mathbf{k})]^{-1}\}^{1/2} \\ = A \times B. \qquad & (22)\end{aligned}$$

For a simple analysis of (22) we suppose again that all the atoms have the same unitary scattering factor. Then $A$ is equal to $[\sigma_3/\sigma_2^{3/2}]_q \leq [\sigma_3/\sigma_2^{3/2}]_N$ (for equal atoms $A = 1/q^{1/2}$). The value of $B$ is larger than unity and depends on the ratios $|F_{pi}|/|\Sigma_{qi}|$.

In the practical applications $B$ may often assume values larger than 2 or 3. We conclude that the contribution of the term of order $1/(q)^{1/2}$ is in general not negligible with respect to that of order $1/(q)^0$. Such a property is strengthened if more than one triplet is available for estimating $\varphi_1$ (see § 7). Important special cases in which the contribution of order $1/(q)^{1/2}$ plays a central role occur when the known part of the structure does not evenly contribute to all parity groups. Then $E_1$ may be large but $E_{p1}$ may be near zero (*i.e.* a sublattice extinct reflection). In such cases (18) and (21) may provide a reliable phase indication for $\varphi_1$ provided the real part of

$$\frac{2c}{b_1 b_2 b_3} (E_2 - E_{p2})(E_3 - E_{p3})$$

is large enough.

### 7. The estimation of $\varphi_1$ *via* more triplets

Suppose that more triplets $\mathbf{h}$, $\mathbf{k}_i$, $\overline{\mathbf{h}+\mathbf{k}_i}$ may be exploited in order to estimate $\varphi_{\mathbf{h}}$. Then, from the distribution $P(E_{\mathbf{h}}, E_{\mathbf{k}_1}, E_{\mathbf{h}+\mathbf{k}_1}, E_{\mathbf{k}_2}, E_{\mathbf{h}+\mathbf{k}_2}, \ldots, E_{p,\mathbf{h}}, E_{p,\mathbf{k}_1}, E_{p,\mathbf{h}+\mathbf{k}_1} E_{p,\mathbf{k}_2}, E_{p,\mathbf{h}+\mathbf{k}_2}, \ldots)$, we obtain:

(*a*) for the centrosymmetric case:

$$P_+(E_1) \simeq 0{\cdot}5 + 0{\cdot}5 \tanh\left\{|E_1|\left[\frac{E_{p1}}{b_1} + \sum_{\text{triplets}} \frac{c}{b_1 b_2 b_3} \times (E_2 - E_{p2})(E_3 - E_{p3})\right]\right\}. \qquad (23)$$

We note that proper values of $c/b_1 b_2 b_3$ must be calculated for each triplet;

(*b*) for the non-centrosymmetric case:

$$P(\varphi_1|\ldots) \simeq [2\pi I_0(\alpha)]^{-1} \exp[\alpha \cos(\varphi_1 - \xi)], \qquad (24)$$

where $\alpha^2 = a_1^2 + a_2^2$,

$$\begin{aligned} a_1 = 2R_1 \Bigg\{ & \frac{R_{p1}}{b_1} \cos\varphi_{p1} + \sum_{\text{triplets}} \frac{c}{b_1 b_2 b_3} \\ & \times [R_2 R_3 \cos(\varphi_2 + \varphi_3) - R_{p2} R_3 \cos(\varphi_{p2} + \varphi_3) \\ & - R_2 R_{p3} \cos(\varphi_2 + \varphi_{p3}) \\ & + R_{p2} R_{p3} \cos(\varphi_{p2} + \varphi_{p3})] \Bigg\}, \end{aligned}$$

$$\begin{aligned} a_2 = 2R_1 \Bigg\{ & \frac{R_{p1}}{b_1} \sin\varphi_{p1} + \sum_{\text{triplets}} \frac{c}{b_1 b_2 b_3} \\ & \times [-R_2 R_3 \sin(\varphi_2 + \varphi_3) + R_{p2} R_3 \sin(\varphi_{p2} + \varphi_3) \\ & + R_2 R_{p3} \sin(\varphi_2 + \varphi_{p3}) \\ & - R_{p2} R_{p3} \sin(\varphi_{p2} + \varphi_{p3})] \Bigg\}, \end{aligned}$$

$$\cos\xi = a_1/\alpha, \quad \sin\xi = a_2/\alpha.$$

From (24) the tangent formula (25) arises:

$$\tan\varphi_1 \simeq a_1/a_2. \qquad (25)$$

## 8. Use of the partial structure in the determinantal approach

Let us conform our notation to that usually employed in the determinantal approach. Let $\mathbf{h}_{0i_1}$ be a 'generating' reciprocal vector and $\mathbf{h}_{i_1 i_2} = \mathbf{h}_{0i_2} - \mathbf{h}_{0i_1}$. In accordance with (15) and (20) the conditional expected values $\langle (E_{0i_1} E^*_{0i_2} | E_{p,0i_1}, E_{p,0i_2}, E_{i_1 i_2}, E_{p,i_1 i_2}) \rangle$ are:

(i) for centrosymmetric space groups:

$$\langle E_{0i_1} E_{0i_2} | \ldots \rangle = E_{p,0i_1} E_{p,0i_2} + \frac{c}{b(\mathbf{h}_{i_1 i_2})} (E_{i_1 i_2} - E_{p,i_1 i_2}),$$

where

$$c = \sum_{j=p+1}^{N} t_j(\mathbf{h}_{0i_1})\, t_j(\mathbf{h}_{0i_2})\, t_j(\mathbf{h}_{i_1 i_2});$$

(ii) for non-centrosymmetric space groups:

$$\langle E_{0i_1} E^*_{0i_2} | \ldots \rangle = E_{p,0i_1} E^*_{p,0i_2} + \frac{c}{b(\mathbf{h}_{i_1 i_2})} (E^*_{i_1 i_2} - E^*_{p,i_1 i_2}).$$

To obtain higher-order relationships dependent only upon the covariance we invoke the central-limit theorem which leads to the following conditional distributions (Tsoucaris, 1970):

(i) for non-centrosymmetric space groups:

$$P(E_{01}, \ldots, E_{0m} | \ldots) \simeq \pi^{-m} D_m^{-1} \exp(-Q_m), \qquad (26)$$

where

$$Q_m = \sum_{i_1, i_2 = 1}^{m} (E^*_{0i_1} - E^*_{p,0i_1})\, D_{i_1 i_2} (E_{0i_2} - E_{p,0i_2}) \qquad (27)$$

(ii) for centrosymmetric space groups:

$$P(E_{01}, \ldots, E_{0m} | \ldots) \simeq \frac{1}{(2\pi)^{m/2}} \frac{1}{D_m^{1/2}} \exp(-\tfrac{1}{2} Q_m). \qquad (28)$$

$D_m$ is the determinant of the correlation matrix and $D_{i_1 i_2}$ is an element of the inverse correlation matrix. Now the phases of the generating reflections may be calculated by standard methods. For example, the expected value of the phase of any generating reflection, say $E_{0r}$, may be calculated by the statistical regression of $E_{0r}$ upon all others (de Rango, Tsoucaris & Zelwer, 1974). The specific case $m = 2$ is discussed in Appendix *C*.

## 9. Conclusions

A probabilistic theory is described which gives new insight into the methods aiming at recovering the full structure from a partial one. The new approach exploits the *a priori* information in a way which appears to be more promising than in previous methods and may find application for the structure solution of small as well as large crystal structures, and for the improvement of electron-microscope images (Ishizuka, Miyazaki & Uyeda, 1982).

The additional following practical considerations are a consequence of the present theory: (*a*) the crystal structures often have different parity groups of reflections with different average values of the intensities. Renormalization in order to obtain always $\langle |E|^2 \rangle = 1$ for each parity group is not advised, in order to avoid violation of Sayre's equation; (*b*) very often the application of triplets to such structures provides a partial structure. Then reflections should be renormalized in accordance with (2) and the formulas described in §§ 3, 4, 7, 8 should be applied. Those formulas are derived in $P\bar{1}$ and $P1$ but can be applied in all centrosymmetric and non-centrosymmetric space groups, respectively; (*c*) space-group algebra is not taken into account in this paper. Thus the theory does not hold for special cases such as those described by Giacovazzo (1980, pp. 286–287) and by Pontenagel & Krabbendam (1983).

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## APPENDIX *A*

From the joint probability distribution (13) the following conditional probability distributions are obtained:

(*a*) $P(E_1 | E_2, E_3, E_{p1}, E_{p2}, E_{p3})$

$$\simeq (2\pi b_1)^{-1/2} \exp\left\{ -\frac{1}{2b_1} (E_1 - E_{p1})^2 + \frac{c}{b_1 b_2 b_3} (E_1 - E_{p1})(E_2 - E_{p2})(E_3 - E_{p3}) \right\}, \quad (A1)$$

from which (14) arises;

(*b*) $P(E_2, E_3 | E_1, E_{p1}, E_{p2}, E_{p3})$

$$\simeq (2\pi)^{-1} (b_2 b_3)^{-1/2} \exp\left\{ -\frac{(E_2 - E_{p2})^2}{2b_2} - \frac{(E_3 - E_{p3})^2}{2b_3} + \frac{c}{b_1 b_2 b_3} (E_1 - E_{p1})(E_2 - E_{p2})(E_3 - E_{p3}) \right\}, \quad (A2)$$

from which (15) arises.

## APPENDIX *B*

From the joint probability distribution (19) the following conditional probability distributions are obtained:

(*a*) $P(\varphi_1, \varphi_2, \varphi_3 | R_i, R_{pi}, \varphi_{pi}, i = 1, 2, 3)$

$$\simeq \frac{1}{L} \exp\left\{ \sum_{i=1}^{3} \frac{2}{b_i} R_i R_{pi} \cos(\varphi_i - \varphi_{pi}) + \frac{2c}{b_1 b_2 b_3} \right.$$
$$\times [R_1 R_2 R_3 \cos(\varphi_1 + \varphi_2 + \varphi_3)$$
$$- R_{p1} R_2 R_3 \cos(\varphi_{p1} + \varphi_2 + \varphi_3)$$
$$- R_1 R_{p2} R_3 \cos(\varphi_1 + \varphi_{p2} + \varphi_3)$$
$$- R_1 R_2 R_{p3} \cos(\varphi_1 + \varphi_2 + \varphi_{p3})$$
$$+ R_{p1} R_{p2} R_3 \cos(\varphi_{p1} + \varphi_{p2} + \varphi_3)$$
$$+ R_{p1} R_2 R_{p3} \cos(\varphi_{p1} + \varphi_2 + \varphi_{p3})$$
$$\left. + R_1 R_{p2} R_{p3} \cos(\varphi_1 + \varphi_{p2} + \varphi_{p3})] \right\}; \qquad (B1)$$

(*b*) $P(R_2, R_3, \varphi_2, \varphi_3 | R_1, \varphi_1, R_{pi}, \varphi_{pi}, i = 1, 2, 3)$

$$\simeq \pi^{-2} (b_2 b_3)^{-1} R_2 R_3 \exp\left\{ \sum_{i=2}^{3} \frac{1}{b_i} |E_i - E_{pi}|^2 + \frac{2c}{b_1 b_2 b_3} \right.$$
$$\left. \times \mathrm{Re}[(E_1 - E_{p1})(E_2 - E_{p2})(E_3 - E_{p3})] \right\}, \qquad (B2)$$

where Re stands for 'real part of' and

$$|E - E_p|^2 = R^2 + R_p^2 - 2RR_p \cos(\varphi - \varphi_p).$$

From (*B*2) the expected value (20) arises;

(*c*) $P(R_1, \varphi_1 | R_2, R_3, \varphi_2, \varphi_3, R_{pi}, \varphi_{pi}, i = 1, 2, 3)$

$$\simeq (\pi b_1)^{-1} R_1 \exp\left\{ -\frac{1}{b_1} |E_1 - E_{p1}|^2 + \frac{2c}{b_1 b_2 b_3} \right.$$
$$\left. \times \mathrm{Re}[(E_1 - E_{p1})(E_2 - E_{p2})(E_3 - E_{p3})] \right\}, \qquad (B3)$$

from which (21) arises.

## APPENDIX *C*

Let us apply (28) when $m = 2$ and when $\mathbf{k}$, $\mathbf{h} + \mathbf{k}$ are the generating reciprocal vectors. It is supposed that $E_{\mathbf{h}}$, $E_{p,\mathbf{h}}$, $E_{p,\mathbf{k}}$, $E_{p,\mathbf{h}+\mathbf{k}}$ is the *a priori* available information. We obtain:

$$\langle (E_{\mathbf{k}} | E_{\mathbf{h}}, E_{p,\mathbf{h}}, E_{p,\mathbf{k}}, E_{p,\mathbf{h}+\mathbf{k}}) \rangle = E_{p,\mathbf{k}}$$
$$\langle (E_{\mathbf{h}+\mathbf{k}} | \ldots) \rangle = E_{p,\mathbf{h}+\mathbf{k}}$$
$$\langle |E_k|^2 | \ldots \rangle = \langle |E_{\mathbf{h}+\mathbf{k}}|^2 | \ldots \rangle = 1$$

according to which

$$\langle (E_k - \langle E_k \rangle)^2 \rangle = 1 - |E_{p,\mathbf{k}}|^2;$$
$$\langle (E_{\mathbf{h}+\mathbf{k}} - \langle E_{\mathbf{h}+\mathbf{k}} \rangle)^2 \rangle = 1 - |E_{p,\mathbf{h}+\mathbf{k}}|^2;$$
$$\langle (E_{\mathbf{k}} - \langle E_{\mathbf{k}} \rangle)(E_{\mathbf{h}+\mathbf{k}} - \langle E_{\mathbf{h}+\mathbf{k}} \rangle) \rangle = \frac{c}{b(\mathbf{h})} (E_{\mathbf{h}} - E_{p,\mathbf{h}}).$$

Correctly, the variances of $E_{\mathbf{k}}$ and $E_{\mathbf{h}+\mathbf{k}}$ vanish if $|E_{p,\mathbf{k}}|$ and $|E_{p,\mathbf{h}+\mathbf{k}}|$ equal unity. Indeed, that occurs only if $p = N$. The same observation holds for the covariance term.

The value of $D_2$ is then

$$D_2 = (1 - |E_{p,\mathbf{k}}|^2)(1 - |E_{p,\mathbf{h}+\mathbf{k}}|^2) - \left| \frac{c}{b(\mathbf{h})} (E_{\mathbf{h}} - E_{p,\mathbf{h}}) \right|^2$$

so that

$$P(E_{\mathbf{k}}, E_{\mathbf{h}+\mathbf{k}} | E_{\mathbf{h}}, E_{p,\mathbf{h}}, E_{p,\mathbf{k}}, E_{p,\mathbf{h}+\mathbf{k}})$$
$$\simeq (2\pi)^{-1} D_2^{-1/2} \exp\left\{ -\frac{1}{2} \frac{(1 - E_{p,\mathbf{h}+\mathbf{k}}^2)}{D_2} \left[ (E_{\mathbf{k}} - E_{p,\mathbf{k}})^2 \right.\right.$$
$$+ \frac{(1 - E_{p,\mathbf{k}}^2)}{D_2} (E_{\mathbf{h}+\mathbf{k}} - E_{p,\mathbf{h}+\mathbf{k}})^2$$
$$- \frac{2c}{D_2 b(\mathbf{h})} (E_{\mathbf{h}} - E_{p,\mathbf{h}})(E_{\mathbf{k}} - E_{p,\mathbf{k}})$$
$$\left.\left. \times (E_{\mathbf{h}+\mathbf{k}} - E_{p,\mathbf{h}+\mathbf{k}}) \right] \right\}.$$

The sign probability for $E_{\mathbf{h}+\mathbf{k}}$ may be calculated by a statistical regression of $E_{\mathbf{h}+\mathbf{k}}$ on $E_{\mathbf{k}}$. We obtain

$$P^+(E_{\mathbf{h}+\mathbf{k}}) \simeq \tfrac{1}{2} + \tfrac{1}{2} \tanh\left\{ \frac{|E_{h+k}|}{D_2} \left[ E_{p,\mathbf{h}+\mathbf{k}} \right.\right.$$
$$\left.\left. + \frac{c}{b(\mathbf{h})} (E_{\mathbf{h}} - E_{p,\mathbf{h}})(E_{\mathbf{k}} - E_{p,\mathbf{k}}) \right] \right\}.$$

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