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An Approximate Functional Form of the Joint Distribution $p(E_1, \ldots, E_m)$ in $P\bar{1}$

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(*Received 17 May 1988; accepted 6 February 1989*)

Abstract

A compact approximate formula is presented for the joint distribution $p(E_1, \ldots, E_m)$ of m structure factors for an equal-atom structure in the space group $P\bar{1}$. The formula is based on the peculiar behaviour at infinity of suitable approximations of the characteristic function of $p(E_1, \ldots, E_m)$. The case $(E_1, E_2) = (E_{2\mathbf{h}}, E_{\mathbf{h}})$ is considered for values $|U_{2\mathbf{h}}|$, $|U_{\mathbf{h}}| \leq 0{\cdot}45$. The conditional probability $P_+(E_{2\mathbf{h}}|E_{\mathbf{h}})$ that is obtained with the above method is compared with the tangent formula of Cochran & Woolfson [*Acta Cryst.* (1955), **8**, 1-12].

1. Introduction

Let us consider m normalized structure factors

$$E_{\mathbf{h}_k} = 2N^{-1/2} \sum_{j=1}^{N/2} \cos(2\pi \mathbf{h}_k \cdot \mathbf{x}_j) \quad (k = 1, 2, \ldots, m)$$

for the space group $P\bar{1}$ and a unit cell containing N equal atoms. We shall suppose that $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ ($n = N/2$) are n independent random vectors ranging uniformly over the unit cell and we denote by $p(E_1, E_2, \ldots, E_m)$ the joint probability density of the m random variables $\hat{E}_k$ ($\equiv \hat{E}_{\mathbf{h}_k}$); we use the notation $\hat{E}_{\mathbf{h}}$ to denote $E_{\mathbf{h}}$ but considered as a random variable. For phase determination we are primarily interested in a good approximation of $\exp(\frac{1}{2}\sum_k E_k^2) p(E_1, E_2, \ldots, E_m)$ rather than $p(E_1, E_2, \ldots, E_m)$. It has been indicated by Brosius (1987) that a Gram–Charlier series expansion of $p(E_1, E_2, \ldots, E_m)$ is a poor approximation to $\exp(\frac{1}{2}\sum_k E_k^2) p(E_1, \ldots, E_m)$ for moderately high $|E|$ values. A way to cope with this problem was to develop $\log p(E_1, \ldots, E_m)$ according to an asymptotic series expansion (*e.g.* Karle & Hauptman, 1953). This is believed to work fine for moderately high E values and not too high m. A serious annoyance of the latter method is that it will be practically impossible to calculate the error of truncating $\log p(E_1, \ldots, E_m)$ at some order, whereas it should in principle be possible to do it for the Gram–Charlier expansion of $p(E_1, \ldots, E_m)$ [the case $m = 1$ is treated by Brosius (1988)]. Furthermore, the formal expansion of $\log p(E_1, \ldots, E_m)$ will hide some basic forms in it; to be more precise, it has been shown by Heinerman, Krabbendam & Kroon (1977) that $\log p(E_1, \ldots, E_m)$ contains a Karle–Hauptman determinant at least if one considers $\log p(E_1, \ldots, E_m)$ to order N^{-1}. But if one inspects the terms of order $(NN^{1/2})^{-1}$ it is also clear that something else is in play, the influence of which might become greater for larger m. Another example is given by the well known Cochran & Woolfson (1955) formula that gives the conditional probability of $E_{2\mathbf{h}}$ given the value $|E_{\mathbf{h}}|$. In their formula the expression $\frac{1}{2}E_{2\mathbf{h}}(E_{\mathbf{h}}^2 - 1)N^{-1/2}$ appears. Clearly, the part $(1/2N^{1/2})E_{2\mathbf{h}}E_{\mathbf{h}}^2$ has something to do with the Harker–Kasper inequality $U_{\mathbf{h}}^2 \leq \frac{1}{2}(1 + U_{2\mathbf{h}})$ (Harker & Kasper, 1948). But where the term $-(1/2N^{1/2})E_{2\mathbf{h}}$ comes from remains a mystery.

Recently, the search for the functional form and for a better approximation of $p(E_1, E_2, \ldots, E_m)$ has regained interest (*e.g.* Wilson, 1981, 1983, 1986, 1987; Shmueli & Weiss, 1985; Shmueli & Wilson, 1981). Our approach differs from approaches like that of Shmueli, Weiss, Kiefer & Wilson (1984) in that we present a modification of the usual asymptotic development.

2. The formula

$$\begin{aligned} p(E_1, E_2, \ldots, E_m) &= (2\pi)^{-m/2} \{\det[\sigma_{ij}(\mathscr{E}_1, \mathscr{E}_2, \ldots, \mathscr{E}_m)]\}^{-1/2} \\ &\quad \times \prod_{k=1}^{m} \exp(-E_k \mathscr{E}_k) I_0(2\mathscr{E}_k / N^{1/2})^{N/2} \\ &\quad \times \rho(\mathscr{E}_1, \mathscr{E}_2, \ldots, \mathscr{E}_m)^{N/2} \delta_N(\mathscr{E}_1, \ldots, \mathscr{E}_m) \quad (1) \end{aligned}$$

0108-7673/89/070453-04$03.00

where $x\to I_n(x)$ denotes the modified Bessel function of order n; $\alpha_n(x)=I_n(x)/I_0(x)$ for every real x;

$$(u_1,\ldots,u_m)\to\varphi(u_1,\ldots,u_m)^{N/2}$$

is the characteristic function of the random vector $(\hat{E}_1,\hat{E}_2,\ldots,\hat{E}_m)$;

$$\psi(u_1,u_2,\ldots,u_m)=\varphi(-iu_1,-iu_2,\ldots,-iu_m);$$

$$\rho(\mathscr{E}_1,\mathscr{E}_2,\ldots,\mathscr{E}_m)=\psi(\mathscr{E}_1,\ldots,\mathscr{E}_m)\Big/\prod_{k=1}^{m}I_0(2\mathscr{E}_k/N^{1/2});$$

$(\mathscr{E}_1,\mathscr{E}_2,\ldots,\mathscr{E}_m)$ is the solution of the m equations

$$E_k\psi(\mathscr{E}_1,\ldots,\mathscr{E}_m)=\frac{N}{2}\frac{\partial}{\partial u_k}\psi(u_1,\ldots,u_m)|_{(u_1,\ldots,u_m)=(\mathscr{E}_1,\ldots,\mathscr{E}_m)}\qquad(2)$$

$$(k=1,2,\ldots,m);$$

$$\sigma_{ij}(\mathscr{E}_1,\ldots,\mathscr{E}_m)=-\frac{2}{N}E_iE_j+\frac{N}{2}\frac{1}{\psi(\mathscr{E}_1,\ldots,\mathscr{E}_m)}\times\frac{\partial^2}{\partial u_i\,\partial u_j}\psi(u_1,\ldots,u_m)|_{(u_1,\ldots,u_m)=(\mathscr{E}_1,\ldots,\mathscr{E}_m)}$$

$$(1\le i,j\le m);$$

$$\delta_N(\mathscr{E}_1,\ldots,\mathscr{E}_m)=1+O(1/N).$$

We usually take $\delta_N(\mathscr{E}_1,\ldots,\mathscr{E}_N)=1$ for N sufficiently large. For the definition of δ_N we refer to the derivation of this formula in § 3.

Some comments should be made here. We expect that δ_N may be approximated by 1 for sufficiently large N. Also (1) is only valid whenever $\det(\sigma_{ij})\neq 0$. We think that the set (2) of m equations always admits a solution whenever $E_1,\ldots,E_m$ are 'acceptable values', *i.e.* whenever there exist n vectors $\mathbf{r}_1,\ldots,\mathbf{r}_n$ $(n=N/2)$ such that

$$E_{\mathbf{h}_k}=2N^{-1/2}\sum_j\cos(2\pi\mathbf{h}_k\,.\,\mathbf{r}_j)\quad\text{for }k=1,\ldots,m;$$

but this is still an open question. However it is not difficult to show that a solution must be unique whenever $\det(\sigma_{ij})\neq 0$. Finally, for the case $m=1$ it has been shown (Brosius, 1987) that

$$\lim_{\det(\sigma_{ij})\to 0}\det(\sigma_{ij})^{-1/2}\left[\prod_{k=1}^{m}\exp(-E_k\mathscr{E}_k)\times I_0(2\mathscr{E}_k)/N^{1/2})^{N/2}\right]\rho(\mathscr{E}_1,\ldots,\mathscr{E}_m)^{N/2}=0$$

whenever $N\ge 5$. It is not known if anything similar is valid for general m. Finally, let us notice that in practice we shall usually look for values of $\mathscr{E}_1,\mathscr{E}_2,\ldots,\mathscr{E}_m$ that solve the m equations (2) to a good approximation.

3. The derivation of formula (1)

Let $\Phi(u_1,\ldots,u_m)=\langle\exp(iu_1\hat{E}_1+\ldots+iu_m\hat{E}_m)\rangle$ be the characteristic function of $(\hat{E}_1,\ldots,\hat{E}_m)$,

$$\Phi(u_1,\ldots,u_m)=\lim_{r\to\infty}\Phi_r(u_1,\ldots,u_m)$$

where $\Phi_r(u_1,\ldots,u_m)$ is a suitable approximation of $\Phi(u_1,\ldots,u_m)$ defined as

$$\Phi_r(u_1,\ldots,u_m)=\left\{\left\langle\prod_{s=1}^{m}[J_0(2u_s/N^{1/2})+2\sum_{k=1}^{r}i^kJ_k(2u_s/N^{1/2})\cos(2\pi k\mathbf{h}_s\,.\,\mathbf{x})]\right\rangle\right\}^{N/2}.$$

Since

$$J_n(z)\simeq(2/\pi z)^{1/2}\{\cos(z-\tfrac{1}{2}n\pi-\tfrac{1}{4}\pi)+\exp(|\mathrm{Im}\,z|)O(|z|^{-1})\}\quad\text{for }|z|\to\infty\quad(|\arg z|<\pi),$$

it follows from a slight generalization of the method given by Brosius (1987) that the Fourier transform $p_r(E_1,\ldots,E_m)$ of $\Phi_r(u_1,\ldots,u_m)$ is also given by

$$p_r(E_1,\ldots,E_m)=(1/2\pi)^m\int_{-\infty}^{+\infty}\mathrm{d}u_1\ldots\int_{-\infty}^{+\infty}\mathrm{d}u_m\times\exp\left[-i\sum_k(-i\mathscr{E}_k+u_k)E_k\right]\times\Phi_r(-i\mathscr{E}_1+u_1,\ldots,-i\mathscr{E}_m+u_m)\qquad(3a)$$

for all real values of $\mathscr{E}_1,\ldots,\mathscr{E}_m$. If we assume that the joint density distribution $p(E_1,\ldots,E_m)$ of $(\hat{E}_1,\ldots,\hat{E}_m)$ exists, we clearly have

$$p(E_1,\ldots,E_m)=\lim_{r\to\infty}p_r(E_1,\ldots,E_m).$$

So (3a) becomes

$$p(E_1,\ldots,E_m)=(1/2\pi)^m\int_{-\infty}^{+\infty}\mathrm{d}u_1\ldots\int_{-\infty}^{+\infty}\mathrm{d}u_m\times\exp[-i\sum(-i\mathscr{E}_k+u_k)E_k]\times\Phi(-i\mathscr{E}_1+u_1,\ldots,-i\mathscr{E}_m+u_m)\qquad(3b)$$

for all real values of $\mathscr{E}_1,\mathscr{E}_2,\ldots,\mathscr{E}_m$. One then gets

$$p(E_1,\ldots,E_m)=\exp\left(-\sum_k E_k\mathscr{E}_k\right)\Phi(-i\mathscr{E}_1,\ldots,-i\mathscr{E}_m)\times(1/2\pi)^m\int_{-\infty}^{+\infty}\mathrm{d}u_1\ldots\int_{-\infty}^{+\infty}\mathrm{d}u_m\exp\left(-i\sum_k u_kE_k\right)\times\Phi_{\mathscr{E}}(u_1,\ldots,u_m)\qquad(4)$$

where

$$\Phi_{\mathscr{E}}(u_1,\ldots,u_m)=\frac{\Phi(-i\mathscr{E}_1+u_1,\ldots,-i\mathscr{E}_m+u_m)}{\Phi(-i\mathscr{E}_1,\ldots,-i\mathscr{E}_m)} \quad (5)$$

is a *characteristic function.* More precisely one has

$$\Phi_{\mathscr{E}}(u_1,\ldots,u_m)=\varphi_{\mathscr{E}}(u_1,\ldots,u_m)^n \quad (n=N/2) \quad (6)$$

where $\varphi_{\mathscr{E}}(u_1,\ldots,u_m)$ is a *characteristic function.* Hence, for large n, $\varphi_{\mathscr{E}}(u_1,\ldots,u_m)^n$ can be developed asymptotically as

$$\varphi_{\mathscr{E}}(u_1,\ldots,u_m)^n = \exp\Big[i\sum_k \mu_k(\mathscr{E}_1,\ldots,\mathscr{E}_m)u_k - \tfrac{1}{2}\sum_i\sum_j \sigma_{ij}(\mathscr{E}_1,\ldots,\mathscr{E}_m)u_iu_j + O(1/N^{1/2})\Big] \quad (7)$$

where

$$\mu_k(\mathscr{E}_1,\ldots,\mathscr{E}_m) = \frac{1}{i}\frac{\partial}{\partial u_k}\ln\Phi(-i\mathscr{E}_1+u_1,\ldots,-i\mathscr{E}_m+u_m)\big|_{u_1=u_2=\ldots=u_m=0}$$

$$\sigma_{ij}(\mathscr{E}_1,\ldots,\mathscr{E}_m) = -\frac{\partial^2}{\partial u_i\,\partial u_j}\ln\Phi(-i\mathscr{E}_1+u_1,\ldots,-i\mathscr{E}_m+u_m)\big|_{u_1=\ldots=u_m=0}. \quad (8)$$

One then obtains

$$(1/2\pi)^m\int_{-\infty}^{+\infty}\mathrm{d}u_1\ldots\int_{-\infty}^{+\infty}\mathrm{d}u_m \times\exp\Big(-i\sum_k u_kE_k\Big)\Phi_{\mathscr{E}}(u_1,\ldots,u_m)$$
$$=(1/2\pi)^m\int_{-\infty}^{+\infty}\mathrm{d}u_1\ldots\int_{-\infty}^{+\infty}\mathrm{d}u_m \times\exp\Big[-i\sum_k(E_k-\mu_k)u_k-\tfrac{1}{2}\sum_i\sum_j\sigma_{ij}u_iu_j\Big]\varepsilon_N \quad (9)$$

with

$$\varepsilon_N=1+O(1/N^{1/2}).$$

Now choose $\mathscr{E}_1,\ldots,\mathscr{E}_m$ such that $|E_k-\mu_k|$ is as small as possible. So, if we suppose that there exist values $\mathscr{E}_1,\ldots,\mathscr{E}_m$ such that $E_k=\mu_k$ for every k then the part on the right of (9) becomes

$$(1/2\pi)^{m/2}\delta_N[\det(\sigma_{ij})]^{-1/2} \quad [\text{if } \det(\sigma_{ij})\neq 0] \quad (10)$$

where $\delta_N=1+O(1/N)$. In general we hope that δ_N can be approximated by 1 when N is large enough even when $\det(\sigma_{ij})$ is small (but positive). The term δ_N has been partially analysed (Brosius, 1987). It is now straightforward to obtain the final form of (1).

4. An application: the case $(E_1, E_2)=(E_{2\mathbf{h}}, E_{\mathbf{h}})$

For convenience, let us put

$$\beta=2N^{-1/2}. \quad (11)$$

One then obtains, using (*A*4) of the Appendix,

$$\varphi(u_1,u_2)=J_0(\beta u_1)J_0(\beta u_2)-2iJ_1(\beta u_1)J_2(\beta u_2)+O(1/N^3)$$

and thus

$$\psi(\mathscr{E}_1,\mathscr{E}_2)=I_0(\beta\mathscr{E}_1)I_0(\beta\mathscr{E}_2)+2I_1(\beta\mathscr{E}_1)I_2(\beta\mathscr{E}_2)+O(1/N^3) \quad (12)$$

$$\rho(\mathscr{E}_1,\mathscr{E}_2)=1+2\alpha_1(\beta\mathscr{E}_1)\alpha_2(\beta\mathscr{E}_2)+O(1/N^3). \quad (13)$$

For $U_k=E_kN^{-1/2}$ and using (*A*1), equations (2) become

$$U_1\rho(\mathscr{E}_1,\mathscr{E}_2)=\alpha_1(\beta\mathscr{E}_1)+\alpha_2(\beta\mathscr{E}_2)+\alpha_2(\beta\mathscr{E}_1)\alpha_2(\beta\mathscr{E}_2)+\text{higher-order terms}$$
$$U_2\rho(\mathscr{E}_1,\mathscr{E}_2)=\alpha_1(\beta\mathscr{E}_2)+\alpha_1(\beta\mathscr{E}_1)\alpha_1(\beta\mathscr{E}_2)+\alpha_1(\beta\mathscr{E}_1)\alpha_3(\beta\mathscr{E}_2)+\text{higher-order terms.} \quad (14)$$

Inspection of the tables of $I_n(x)$ shows that a good approximation to the solution of (14) within the range $|U_1|$, $|U_2|\le 0{\cdot}45$ is given by

$$U_1\simeq\alpha_1(\beta\mathscr{E}_1) \quad\text{and}\quad U_2\simeq\alpha_1(\beta\mathscr{E}_2).$$

We may then approximate $\alpha_2(\beta\mathscr{E}_1)$, $\alpha_3(\beta\mathscr{E}_1)$, *etc.* by $\frac{1}{2}U_1^2$, $\frac{1}{6}U_1^3$, *etc.* and analogous approximations may be given for $\alpha_n(\beta\mathscr{E}_2)$. It then follows that

$$\rho(\mathscr{E}_1,\mathscr{E}_2)\simeq 1+U_1U_2^2+O(1/N^3), \quad (15)$$

and after using (*A*2)

$$\sigma_{11}(\mathscr{E}_1,\mathscr{E}_1)\simeq 1-\tfrac{3}{2}U_1^2$$
$$\sigma_{22}(\mathscr{E}_1,\mathscr{E}_2)\simeq U_2$$
$$\sigma_{22}(\mathscr{E}_1,\mathscr{E}_2)\simeq 1+U_1-\tfrac{3}{2}U_2^2. \quad (16)$$

Hence

$$\det[\sigma_{ij}(\mathscr{E}_1,\mathscr{E}_2)]\simeq 1+U_1-\tfrac{3}{2}U_1^2-\tfrac{5}{2}U_2^2. \quad (17)$$

Since for this approximation sign $(\mathscr{E}_k)$ = sign (E_k) $(k=1,2)$ we only need to consider the part $\rho(\mathscr{E}_1,\mathscr{E}_2)^{N/2}|\det[\sigma_{ij}(\mathscr{E}_1,\mathscr{E}_2)]|^{-1/2}$,

$$\rho(\mathscr{E}_1,\mathscr{E}_2)^{N/2}\{\det[\sigma_{ij}(\mathscr{E}_1,\mathscr{E}_2)]\}^{-1/2}\simeq\frac{(1+U_1U_2)^{N/2}}{[1+U_1-\frac{3}{2}U_1^2-\frac{5}{2}U_2^2]^{1/2}} \quad (18)$$

of $p(E_1,E_2)$ [see (1)] in order to derive the conditional probability $P_+(E_{2\mathbf{h}}||E_{\mathbf{h}}|)$ that the sign of $E_{2\mathbf{h}}$ is positive given the magnitude of $E_{\mathbf{h}}$. Define

$$a_+(E_1,E_2)=1+|U_1|-\tfrac{3}{2}U_1^2-\tfrac{5}{2}U_2^2$$
$$a_-(E_1,E_2)=1-|U_1|-\tfrac{3}{2}U_1^2-\tfrac{5}{2}U_2^2. \quad (19)$$

Then one obtains

$$P_+(E_{2\mathbf{h}}||E_{\mathbf{h}}|) = \left\{1+\left[\frac{a_+(E_1,E_2)}{a_-(E_1,E_2)}\right]^{1/2}\exp(-|U_1|E_2^2)\right\}^{-1}. \quad (20)$$

Let us compare this with the classical tangent formula (Cochran & Woolfson, 1955) for $E_2^2=1$. It then follows from (20) that (if N is high enough)

$$P_+(E_{2\mathbf{h}}||E_{\mathbf{h}}|=1) = \left[1+\left(\frac{1+|U_1|-\frac{3}{2}U_1^2}{1-|U_1|-\frac{3}{2}U_1^2}\right)^{1/2}\right]^{-1}. \quad (21)$$

This gives $P_+=0{\cdot}41$ for $|U_1|=0{\cdot}3$ whereas the classical formula would have given $P_+=0{\cdot}5$.

5. Concluding remarks

Besides the problem of proving that the m equations (2) always give a solution for acceptable values of $E_1,\ldots,E_m$ it also remains to investigate the term δ_N. We believe that δ_N can be approximated very well by 1 (and some heuristic arguments point to that direction), but a lot of research has still to be done.

APPENDIX
Some useful relations

$$\frac{d}{dx}I_n(x)=\tfrac{1}{2}I_{n-1}(x)+\tfrac{1}{2}I_{n+1}(x). \quad (A1)$$

$$\frac{d^2}{dx^2}I_n(x)=\tfrac{1}{4}I_{n-2}(x)+\tfrac{1}{2}I_n(x)+\tfrac{1}{4}I_{n+2}(x). \quad (A2)$$

$$J_n(ix)=i^nI_n(x);\quad J_{-n}(x)=(-1)^nJ_n(x);$$
$$I_{-n}(x)=(-1)^nI_n(x). \quad (A3)$$

$$\exp(iz\cos\varphi)=J_0(z)+2\sum_{k=1}^{\infty}i^kJ_k(z)\cos(k\varphi). \quad (A4)$$

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Acta Cryst. (1989). A**45**, 456-463

The Direct Method Based on a Fitting of Distributions of Semi-Invariants

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(*Received* 5 *May* 1988; *accepted* 6 *February* 1989)

Abstract

A new direct method (called *TRYMIN*) for phase-problem solution is described. At first a methodical procedure is presented for the construction of a direct method. The aim of the calculation is formulated as a consistency between theoretical and calculated distributions of invariants. A minimized function is obtained and an algorithm for its minimization is proposed. The algorithm is based on the partial decomposition of phases into three subsets and on the cyclical improvement of the estimate of local minima. The efficiency of the method has been tested on 23 structures and a short evaluation of the results of computer experiments with test structures is presented.

Definition of the problem

The direct method for the solution of the phase problem is based on a theory that gives for a great number of functions Y_i of phases φ a forecast of their values for the correct phases φ^*. For arbitrary values l_i, u_i the theory affords the probability that the theoretically correct value $Y_i^*=Y_i(\varphi^*)$ satisfies

$$l_i < Y_i^* < u_i.$$

Implementing this theory we can formulate the following task: to construct an algorithm for the generation of a limited number of sets $\bar{\varphi}$ for which the values $\bar{Y}_i=Y_i(\bar{\varphi})$ will satisfy inequalities $l_i<\bar{Y}_i<u_i$ (for *a priori* given l_i, u_i) with frequency in correspondence with the theory.

0108-7673/89/070456-08$03.00