References

ANANTHARAMAN, T. R., RAMA RAO, P. & LELE, S. (1972). *Recent Developments in Metallurgical Science and Technology*, pp. 407–484. New Delhi: Indian Institute of Metals.
COHEN, J. B. & WAGNER, C. N. J. (1962). *J. Appl. Phys.* **33**, 2073–2077.
GEVERS, R. (1954). *Acta Cryst.* **7**, 337–343.
LELE, S. (1974*a*). *Acta Cryst.* A**30**, 509–513.
LELE, S. (1974*b*). *Acta Cryst.* A**30**, 689–693.
NABARRO, F. R. N. (1967). *Theory of Crystal Dislocations*. Oxford Univ. Press.
PRASAD, B. & LELE, S. (1971). *Acta Cryst.* A**27**, 54–64.
WARREN, B. E. (1959). *Progr. Metal Phys.* **8**, 147–202.

Acta Cryst. (1974). A**30**, 698

Ambiguities in the X-ray Analysis of Crystal Structures*

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A mathematical construction is given for arbitrarily many distinct crystal structures all of which would give the same diffraction pattern. A. L. Patterson's concept of *homometric sets* is analyzed, and examples are given in one, two and three dimensions.

Let $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ be linearly independent vectors in three-dimensional space. Let A be the three-by-three matrix whose columns are the $\mathbf{a}_j$. The vectors $\mathbf{a}_j$ determine a *lattice* of points

$$\mathsf{A}\mathbf{n} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \tag{1}$$

where the n_j are integers. The *basic cell* of the lattice is the set of points

$$\mathbf{x} = \xi_1\mathbf{a}_1 + \xi_2\mathbf{a}_2 + \xi_3\mathbf{a}_3 \text{ with } 0 \le \xi_j < 1 . \tag{2}$$

The *reciprocal lattice* has the matrix

$$\mathsf{B} = (\mathsf{A}^T)^{-1} = (\mathsf{A}^{-1})^T . \tag{3}$$

Its columns $\mathbf{b}_j$ satisfy

$$\begin{aligned} \mathbf{a}_k \,.\, \mathbf{b}_j = \delta_{kj} &= 0 \text{ if } k \neq j \\ &= 1 \text{ if } k = j . \end{aligned} \tag{4}$$

The reciprocal lattice consists of the points $\mathbf{Bh}$, where the h_j are integers (called Miller indices).

Let the atoms in a crystal be located at $\mathbf{r}_1, \ldots, \mathbf{r}_N$ in the basic cell (2) and at all *congruent* points $\mathbf{r}_j + \mathbf{An}$. By X-ray analysis, one tries to find the positions $\mathbf{r}_j$.

The F factor is defined to be

$$F(\mathbf{h}) = \sum_{s=1}^{N} f_s \exp 2\pi i\, \mathbf{h} \,.\, \mathbf{r}_s . \tag{5}$$

For $\mathbf{h}$ in the reciprocal lattice, observations are made of

$$|F(\mathbf{h})|^2 = \sum_{s=1}^{N} \sum_{t=1}^{N} f_s f_t \exp 2\pi i \mathbf{h} \,.\, (\mathbf{r}_t - \mathbf{r}_s) . \tag{6}$$

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The f_s are positive numbers.

If the F factors were observed, the $\mathbf{r}_s$ would be determined uniquely. Ambiguity results from observing $|F^2|$ instead of F.

In the following definitions, let X, Y, ... represent finite non-empty point sets in the real Euclidian space of n dimensions. A set X is allowed to have repeated elements, but no ordering or indexing is prescribed. For instance, if $\mathsf{X} = \{1, 1, 2\}$ in one dimension, then

$$\mathsf{X} = \{1, 2, 1\} \quad \text{but} \quad \mathsf{X} \neq \{1, 2\} .$$

Given X and Y, we define the sets

$$\begin{aligned} \mathsf{X}+\mathsf{Y} &= \{\mathbf{x}+\mathbf{y}\} \ (\mathbf{x} \text{ in X}, \mathbf{y} \text{ in Y}) \\ \lambda\mathsf{X} &= \{\lambda\mathbf{x}\} \ (\mathbf{x} \text{ in X}) \\ -\mathsf{X} &= \{-\mathbf{x}\} \ (\mathbf{x} \text{ in X}) \\ \mathsf{X}+\mathbf{c} &= \{\mathbf{x}+\mathbf{c}\} \ (\mathbf{x} \text{ in X}) \\ \mathsf{X}-\mathsf{Y} &= \mathsf{X}+(-\mathsf{Y}) = \{\mathbf{x}-\mathbf{y}\} \\ \mathsf{D}(\mathsf{X}) &= \mathsf{X}-\mathsf{X} . \end{aligned} \tag{7}$$

Thus, if X has m members, D(X) has m^2 members, including at least m points $\mathbf{0}$.

Suppose

$$\mathsf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\} \text{ and } \mathsf{Y} = \{\mathbf{y}_1, \ldots, \mathbf{y}_m\} . \tag{8}$$

We say

$$\mathsf{X} = \mathsf{Y} \text{ if } \mathbf{x}_1 = \mathbf{y}_{j1}, \ldots, \mathbf{x}_m = \mathbf{y}_{jm}$$

where $j_1, \ldots, j_m$ is some permutation of $1, \ldots, m$.

Let $\mathbf{x}$ and $\mathbf{y}$ be points in real n-dimensional space.

Let A be an $n \times n$ matrix. We write

$$\mathbf{x} \equiv \mathbf{y} \bmod \mathsf{A} \tag{9}$$

to mean

$$\mathbf{x} = \mathbf{y} + \mathsf{A}\mathbf{k}$$

where $\mathbf{k}$ is some vector with integer components, or equivalently

$$\mathbf{x} = \mathbf{y} + k_1\mathbf{a}_1 + \ldots + k_n\mathbf{a}_n$$

where the k_j are integers and the $\mathbf{a}_j$ are the columns of A.

If X and Y are the sets (8) in n dimensions, we say

$$\mathsf{X} \equiv \mathsf{Y} \bmod \mathsf{A} \tag{10}$$

if

$$\mathbf{x}_k \equiv \mathbf{y}_{jk} \bmod \mathsf{A} \ (k = 1, \ldots, m)$$

where $j_1, \ldots, j_m$ is some permutation of $1, \ldots, m$.

If X is a (finite, non-empty, real) set in n dimensions, we define the complex-valued Fourier-sum transform

$$\varphi(\mathbf{h},\mathsf{X}) = \sum_{\mathbf{x}\in\mathsf{X}} \exp 2\pi i \mathbf{h} \cdot \mathbf{x} \tag{11}$$

for all real $\mathbf{h}$ in n dimensions. Note that

$$|\varphi(\mathbf{h},\mathsf{X})|^2 = \varphi[\mathbf{h},\mathsf{D}(\mathsf{X})] \tag{12}$$

$$\varphi(\mathbf{h}, -\mathsf{X}) = \varphi^*(\mathbf{h},\mathsf{X}) \tag{13}$$

$$\varphi(\mathbf{h},\mathsf{X}+\mathsf{Y}) = \varphi(\mathbf{h},\mathsf{X})\varphi(\mathbf{h},\mathsf{Y}) . \tag{14}$$

[By φ^* in (13) we mean the complex conjugate of φ. Thus, φ is real if $\mathsf{X} = -\mathsf{X}$.) The function φ is just an F factor if all the f factors are replaced by 1.

In the basic cell of a crystal, let

$$\mathsf{R} = \{\mathbf{r}_1, \ldots, \mathbf{r}_N\}$$

be the set of positions of the atoms. By observing $|F(\mathbf{h})|^2$ for $\mathbf{h}$ in the reciprocal lattice, one finds D(R) mod A. Note that one does not find D(R), but only D(R) *mod* A. The question is: *to what extent does* D(R) mod A *determine* R?

There are trivial modifications of R that leave the difference set unchanged. If

$$\mathsf{S} \equiv \pm\mathsf{R} + \mathbf{c} \bmod \mathsf{A} \tag{15}$$

where $\mathbf{c}$ is any single vector, then

$$\mathsf{D}(\mathsf{S}) \equiv \mathsf{D}(\mathsf{R}) \bmod \mathsf{A}. \tag{16}$$

If sets R and S satisfy

$$\mathsf{S} \not\equiv \pm\mathsf{R} + \mathbf{c} \bmod A, \text{ but } \mathsf{D}(\mathsf{S}) \equiv \mathsf{D}(\mathsf{R}) \bmod \mathsf{A} \tag{17}$$

we will say that the sets S and R are homometric *mod* A. Patterson (1944) called such sets *homometric* – without explicit reference to the lattice matrix A; but we will reserve the term *homometric* for sets R and S that satisfy

$$\mathsf{S} \neq \pm\mathsf{R} + \mathbf{c}, \text{ but } \mathsf{D}(\mathsf{S}) = \mathsf{D}(\mathsf{R}) . \tag{18}$$

Here equality replaces congruence. Patterson's attention was called to this problem by a practical example discovered by Pauling & Shappell (1930). The mathematical definitions (17) and (18) can be made for sets in n-dimensional space. Patterson gave many examples of homometric sets mod A in one dimension, and he suggested a general perturbation method for constructing homometric sets mod A in higher dimensions.

The purpose of this paper is to give some theory and examples of strictly homometric sets, satisfying (18).

Here is an example of homometric sets mod A in one dimension. It is due to Patterson (1944, p. 197, Fig. 2):

$$\mathsf{R} = \{0,1,4,7\}, \quad \mathsf{S} = \{0,4,5,7\}, \quad \mathsf{A} = 8 . \tag{19}$$

It is easy to verify that $\mathsf{S} \not\equiv \pm\mathsf{R} + \mathbf{c} \bmod 8$ for any $\mathbf{c}$. Next, we look at the difference-sets:

$$\begin{aligned}\mathsf{D}(\mathsf{R}) = \{&0,0,0,0,1,-1,4,-4,7,-7,3,-3,6,-6,\\ &3,-3\}\end{aligned} \tag{20}$$

$$\begin{aligned}\mathsf{D}(\mathsf{S}) = \{&0,0,0,0,4,-4,5,-5,7,-7,1,-1,3,-3,2,\\ &-2\} .\end{aligned}$$

The difference sets are *not* equal; but they are congruent mod 8:

$$\mathsf{D}(\mathsf{R}) \equiv \mathsf{D}(\mathsf{S}) \equiv \{0,0,0,0,1,1,2,3,3,4,4,5,5,6,7,7\} . \tag{21}$$

So these sets are homometric mod A – but not homometric.

Garrido (1951) has also discussed sets that are not homometric, but are homometric *mod* A.

Suppose we know that sets S and R are homometric. Given a non-singular lattice matrix A, we would like to say that S and R are homometric *mod* A. Indeed, the equation $\mathsf{D}(\mathsf{S}) = \mathsf{D}(\mathsf{R})$ implies the congruence $\mathsf{D}(\mathsf{S}) \equiv \mathsf{D}(\mathsf{R}) \bmod \mathsf{A}$. But, unfortunately, the inequality $\mathsf{S} \neq \pm\mathsf{R} + \mathbf{c}$ does *not* imply the incongruence $\mathsf{S} \not\equiv \pm\mathsf{R} + \mathbf{c} \bmod \mathsf{A}$. For example,

$$\{0,1\} \neq \pm\{0,2\} + \mathbf{c} \quad \text{for any } \mathbf{c}$$

but

$$\{0,1\} \equiv \{0,2\} + 1 \bmod 3 .$$

The following theorem implies that, if S and R are homometric, then S and R are also homometric mod $(\lambda\mathsf{A})$ for all scalars λ *near* one. So if we cannot use the matrix A, we can use any nearby matrix $\lambda\mathsf{A}$.

Theorem 1. In real n-dimensional space, let R and S be finite point sets such that

$$\mathsf{S} \neq \pm\mathsf{R} + \mathbf{c} \quad \text{for any } \mathbf{c} . \tag{22}$$

Let A be an $n \times n$ non-singular matrix. Then for some $\varepsilon > 0$

$$\mathsf{S} \equiv \pm\mathsf{R} + \mathbf{c} \bmod (\lambda A) \quad \text{for any } \mathbf{c} \tag{23}$$

provided $0 < |\lambda - 1| < \varepsilon$.

Proof. Let $\sigma = \pm 1$. Suppose

$$\mathsf{S} \equiv \sigma\mathsf{R} + \mathbf{c} \bmod \lambda\mathsf{A}. \tag{24}$$

That means, if R and S each contain m points correspondingly indexed,

$$\mathbf{s}_j = \sigma\mathbf{r}_j + \mathbf{c} + \lambda\mathsf{A}\mathbf{k}_j \quad (j = 1, \ldots, m)$$

where the vectors $\mathbf{k}_j$ have *integer* coordinates. Summation yields

$$m\mathbf{c}=m\mathbf{b}-\lambda\mathsf{A}\mathbf{k} \tag{25}$$

where

$$m\mathbf{b}=\sum_{j=1}^{m}(\mathbf{s}_j-\sigma\mathbf{r}_j) \tag{26}$$

and

$$\mathbf{k}=\sum_{j=1}^{m}\mathbf{k}_j\,. \tag{27}$$

Therefore, for $j=1,\ldots,m$,

$$\mathbf{s}_j=\sigma\mathbf{r}_j+\left(\mathbf{b}-\frac{\lambda}{m}\mathsf{A}\mathbf{k}\right)+\lambda\mathsf{A}\mathbf{k}_j$$

and, for $j=1,\ldots,m$

$$m\mathsf{A}^{-1}(\mathbf{s}_j-\sigma\mathbf{r}_j-\mathbf{b})=\lambda\mathbf{h}_j \tag{28}$$

where $\mathbf{h}_j$ is the vector $m\mathbf{k}_j-\mathbf{k}$, which has *integer* components.

But $\mathsf{S}\neq\sigma\mathsf{R}+\mathbf{b}$. Therefore, some of the vectors $\lambda\mathbf{h}_j$ are non-zero. The non-zero scalar components of these vectors constitute a *finite* set of real numbers, Ω. Now (28) implies that λ is a number in Ω divided by an integer:

$$\lambda=\omega/N(\omega\in\Omega,\ N=\pm1,\pm2,\pm3,\ldots)\,.$$

But these numbers have 0 as their *only* limit point. Therefore, some set $0<|\lambda-1|<\varepsilon$ contains *none* of the numbers $\lambda=\omega/N$. But this is the assertion (23).

Theorem 2. For finite point-sets, the equation

$$\mathsf{X}+\mathsf{Y}=\mathsf{X}+\mathsf{Z}\text{ implies }\mathsf{Y}=\mathsf{Z}\,. \tag{29}$$

Proof. If $\mathsf{X}+\mathsf{Y}=\mathsf{X}+\mathsf{Z}$, then the Fourier sums (11) satisfy

$$\varphi(\mathbf{h},\mathsf{X})\ \varphi(\mathbf{h},\mathsf{Y})=\varphi(\mathbf{h},\mathsf{X})\ \varphi(\mathbf{h},\mathsf{Z})\text{ for all }\mathbf{h}\,. \tag{30}$$

The function $\varphi(\mathbf{h},\mathsf{X})$ is not identically zero, since for $\mathbf{h}=\mathbf{0}$ it equals the number of elements in the non-empty set X. But $\varphi(\mathbf{h},\mathsf{X})$ is an analytic function of the n coordinates $h_1,h_2,\ldots$ of the vector $\mathbf{h}$. Therefore, by the principle of analytic continuation, $\varphi(\mathbf{h},\mathsf{X})$ cannot vanish for all $\mathbf{h}$ in *any* sphere $|\mathbf{h}-\mathbf{c}|<\varepsilon$.

If $\varphi(\mathbf{h},\mathsf{X})\neq0$, (30) implies

$$\varphi(\mathbf{h},\mathsf{Y})=\varphi(\mathbf{h},\mathsf{Z})\,. \tag{31}$$

But we know that if $\varphi(\mathbf{c},\mathsf{X})=0$, then the point $\mathbf{c}$ is the limit of points $\mathbf{h}$ at which $\varphi(\mathbf{h},\mathsf{X})\neq0$. Since both sides of equation (31) are continuous functions of $\mathbf{h}$, this equation must hold for *all* $\mathbf{h}$.

But the identity of the transforms (31) implies the identity of the sets Y and Z. That is because, for any finite set W, the average over all $\mathbf{h}$,

$$\text{average}\,[\varphi(\mathbf{h},\mathsf{W})\,.\,\exp(-2\pi i\mathbf{h}\,.\,\mathbf{p})] \tag{32}$$

equals 0 if $\mathbf{p}$ is not in W or equals the multiplicity with which $\mathbf{p}$ occurs in W if $\mathbf{p}\in\mathsf{W}$. If we multiply the identity (31) by $\exp(-2\pi i\mathbf{h}\,.\,\mathbf{p})$ and average over $\mathbf{h}$, we conclude $\mathsf{Y}=\mathsf{Z}$.

In this proof, we used an average (32) over all $\mathbf{h}$ in real, n-dimensional space. That means this: we integrate over the set

$$-\tfrac{1}{2}L\leq h_j\leq\tfrac{1}{2}L\quad(j=1,\ldots,n)$$

divide by the volume, L^n, and take the limit as $L\to\infty$.]

The analog of Theorem 2 for congruence is false. For example, if $\mathsf{A}=6$ and if

$$\mathsf{X}=\{0,2,4\},\ \mathsf{Y}=\{0,1\},\text{ and }\mathsf{Z}=\{0,3\}$$

then

$$\mathsf{X}+\mathsf{Y}\equiv\mathsf{X}+\mathsf{Z}\equiv\{0,1,2,3,4,5\}\bmod\mathsf{A}$$

but $\mathsf{Y}\not\equiv\mathsf{Z}$ mod A. (In fact, $\mathsf{Y}\not\equiv\pm\mathsf{Z}+\mathbf{c}$ for any $\mathbf{c}$.)

Now we are almost ready to construct some homometric sets. First we need the idea of a centric (or centrosymmetric) set S. This is a set satisfying

$$\mathsf{S}-\mathbf{c}=-(\mathsf{S}-\mathbf{c}) \tag{33}$$

for some $\mathbf{c}$. For *finite* sets, the center of symmetry is unique: it is the center of mass of S if every point is given unit weight;

$$\mathbf{c}=\frac{1}{m}(\mathbf{s}_1+\ldots+\mathbf{s}_m) \tag{34}$$

if $\mathsf{S}=\{\mathbf{s}_1,\ldots,\mathbf{s}_m\}$. If a set R is not centric, we will call it *acentric*. Every acentric set has at least three points.

Theorem 3. If the sets X and Y are both acentric, then the sets $\mathsf{X}+\mathsf{Y}$ and $\mathsf{X}-\mathsf{Y}$ are homometric.

Example 1. In one dimension, let

$$\mathsf{X}=\{0,4,9\}\text{ and }\mathsf{Y}=\{0,1,3\}\,.$$

These sets are acentric. The theorem implies

$$\mathsf{X}+\mathsf{Y}+\mathbf{a}\text{ and }\mathsf{X}-\mathsf{Y}+\mathbf{b}\text{ are homometric} \tag{35}$$

for any $\mathbf{a}$ and $\mathbf{b}$. In this example, we will choose $\mathbf{a}=0$ and $\mathbf{b}=3$. Then (35) yields the two homometric sets

$$\begin{aligned}\mathsf{X}+\mathsf{Y}&=\{0,1,3,4,5,7,9,10,12\}\\ \mathsf{X}-\mathsf{Y}+3&=\{0,2,3,4,6,7,9,11,12\}\,.\end{aligned} \tag{36}$$

Example 2. The theorem permits X to equal Y. Let $\mathsf{X}=\mathsf{Y}=\{0,1,3\}$. Then we get the homometric sets

$$\begin{aligned}\mathsf{X}+\mathsf{Y}&=\{0,1,1,2,3,3,4,4,6\}\\ \mathsf{X}-\mathsf{Y}&=\{-3,-2,-1,0,0,0,1,2,3\}\,.\end{aligned} \tag{37}$$

Here $\mathsf{X}+\mathsf{Y}$ is an acentric set, while $\mathsf{X}-\mathsf{Y}$ is centric; that is true in general if $\mathsf{X}=\mathsf{Y}$ and X is acentric. Both sets have non-distinct points.

Example 3. In two dimensions, let X and Y be the acentric sets

$$\begin{array}{l}x\\ \\ \qquad y\\ x\quad x\end{array}\text{ and }\begin{array}{l}\\ \\ \\ y\ y\end{array}\,.$$

Let $\mathsf{R}=\mathsf{X}+\mathsf{Y}$ and $\mathsf{S}=\mathsf{X}-\mathsf{Y}$:

$$\begin{array}{l}r\qquad\quad s\,s\\ r\,r\qquad\quad\ s\\ r\quad r\qquad s\,s\,s\,s\\ r\,r\,r\,r\end{array}\text{ and }\begin{array}{l}\\ \\ \\ s\quad s\end{array}\,.$$

Example 4. For a non-degenerate three-dimensional analog of the last example, let $\mathsf{X}=\{\mathbf{x}_0,\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3\}$, where

$$\mathbf{x}_0=\begin{pmatrix}0\\0\\0\end{pmatrix},\quad \mathbf{x}_1=\begin{pmatrix}2\\0\\0\end{pmatrix},\quad \mathbf{x}_2=\begin{pmatrix}0\\2\\0\end{pmatrix},\quad \mathbf{x}_3=\begin{pmatrix}0\\0\\2\end{pmatrix}.$$

Let $\mathsf{Y}=\frac{1}{2}\mathsf{X}$. (The multiple $\frac{1}{2}$ is taken in order to achieve homometric sets with *distinct* points). Then $\mathsf{X}+\mathsf{Y}$ and $\mathsf{X}-\mathsf{Y}$ are homometric.

Example 5. Let X and Y be

$$\begin{array}{cc} & x \\ & \\ & y\ y \\ x & x \end{array} \quad \text{and} \quad \begin{array}{cc} & y \\ & \\ & y \\ y & y \end{array}.$$

Let $\mathsf{R}=\mathsf{X}+\mathsf{Y}$ and $\mathsf{S}=\mathsf{X}-\mathsf{Y}$:

$$\begin{array}{cc} r\ r & \\ r & \\ r\ r\ r & \\ r & r \end{array} \quad \text{and} \quad \begin{array}{cc} & s \\ & s\ s \\ & s \\ s & s \end{array}.$$

Although these sets are homometric, they are also equivalent under rigid motions: S can be transformed into R by a rotation through 90° followed by a reflection through a vertical axis. This example and Example 3 show that homometric sets *may* or *may not* be equivalent under rigid motions.

Proof of Theorem 3. First we verify

$$\mathsf{D}(\mathsf{X}-\mathsf{Y})=\mathsf{D}(\mathsf{X})+\mathsf{D}(-\mathsf{Y})=\mathsf{D}(\mathsf{X})+\mathsf{D}(\mathsf{Y})=\mathsf{D}(\mathsf{X}+\mathsf{Y}).$$

Now we must show $\mathsf{X}+\mathsf{Y}\neq\pm(\mathsf{X}-\mathsf{Y})+\mathbf{c}$ for any $\mathbf{c}$.

Suppose

$$\mathsf{X}+\mathsf{Y}=\mathsf{X}-\mathsf{Y}+\mathbf{c}.$$

Then Theorem 2 implies $\mathsf{Y}=-\mathsf{Y}+\mathbf{c}$. Then

$$\mathsf{Y}-\tfrac{1}{2}\mathbf{c}=-(\mathsf{Y}-\tfrac{1}{2}\mathbf{c});$$

so Y would have to be symmetric – a contradiction.

Suppose instead

$$\mathsf{X}+\mathsf{Y}=-(\mathsf{X}-\mathsf{Y})+\mathbf{c}$$

Then

$$\mathsf{X}+\mathsf{Y}=\mathsf{Y}-\mathsf{X}+\mathbf{c}$$

Then Theorem 2 implies $\mathsf{X}=-\mathsf{X}+\mathbf{c}$, so X would have to be symmetric – again a contradiction.

Calderon & Pepinsky (1952) observed that, if $d_1(\mathbf{x})$ and $d_2(\mathbf{x})$ are density functions, then the convolutions

$$d(\mathbf{x})=d_1(\mathbf{x})*d_2(\mathbf{x}) \text{ and } d^1(\mathbf{x})=d_1(\mathbf{x})*d_2(-\mathbf{x})$$

are density functions whose Fourier transforms have the same moduli. [The finite point sets $\mathsf{X}_1+\mathsf{X}_2$ and $\mathsf{X}_1-\mathsf{X}_2$ arise if the densities $d_1(\mathbf{x})$ and $d_2(\mathbf{x})$ are finite sums of delta functions.] Calderon & Pepinsky asserted that, if d_1 and d_2 are non-centrosymmetric, then 'unless d_1 and d_2 satisfy special conditions, d will be essentially different from d^1 – that is, not related to d^1 by a trivial transformation such as a translation, rotation, or other symmetry operation'; but they did not say what the special conditions were.

Following Calderon & Pepinsky we can show that, if X and Y are both *centric*, then the equation $\mathsf{D}(\mathsf{X})=\mathsf{D}(\mathsf{Y})$ implies $\mathsf{X}=\mathsf{Y}+\mathbf{c}$. (Therefore, centric sets X and Y cannot be homometric.) Like Theorem 3, this can be proved by analytic continuation: Let $\mathbf{a}$ and $\mathbf{b}$ be the centroids of X and Y, and let $\mathsf{X}_0=\mathsf{X}-\mathbf{a}$ and $\mathsf{Y}_0=\mathsf{Y}-\mathbf{b}$. Then

$$\mathsf{X}_0=-\mathsf{X}_0,\ \mathsf{Y}_0=-\mathsf{Y}_0, \text{ and } \mathsf{D}(\mathsf{X}_0)=\mathsf{D}(\mathsf{Y}_0).$$

Therefore, for all real vectors $\mathbf{h}$, the functions $\varphi(\mathbf{h},\mathsf{X}_0)$ and $\varphi(\mathbf{h},\mathsf{Y}_0)$ are *real*-valued, and

$$\varphi^2(\mathbf{h},\mathsf{X}_0)=\varphi^2(\mathbf{h},\mathsf{Y}_0).$$

Therefore, for all $\mathbf{h}$,

$$[\varphi(\mathbf{h},\mathsf{X}_0)+\varphi(\mathbf{h},\mathsf{Y}_0)]\,[\varphi(\mathbf{h},\mathsf{X}_0)-\varphi(\mathbf{h},\mathsf{Y}_0)]=0.$$

Since the first factor $[\varphi+\varphi]$ is positive for $\mathbf{h}$ near $\mathbf{0}$, the second factor $[\varphi-\varphi]$ must vanish for $\mathbf{h}$ near $\mathbf{0}$. But $\varphi(\mathbf{h},\mathsf{X}_0)-\varphi(\mathbf{h},\mathsf{Y}_0)$ is an entire analytic function of every component of $\mathbf{h}$; therefore it vanishes for all $\mathbf{h}$. So $\mathsf{X}_0=\mathsf{Y}_0$; and $\mathsf{X}=\mathsf{Y}+\mathbf{c}$, where $\mathbf{c}=\mathbf{a}-\mathbf{b}$.

Piccard (1939, p. 31) presents a theorem concerning finite point sets R and S in one dimension. The theorem states that R and S cannot be homometric if the non-zero members of $\mathsf{D}(\mathsf{R})$ are distinct. This theorem does not contradict Theorem 3, since some non-zero members of $\mathsf{D}(\mathsf{X}\pm\mathsf{Y})$ occur more than once if X and Y both have more than one member.

Theorem 3 can be generalized: we will now show how to construct 2^k sets every two of which are homometric.

Theorem 4. Let $\mathsf{P}_0,\mathsf{P}_1,\ldots,\mathsf{P}_k$ be centric sets. Let each set P_j have centroid $\mathbf{0}$. Let each P_j consist of distinct points. Let each point $\mathbf{p}$ in P_j have Cartesian coordinates that are all rational numbers. Let $\tau_0,\tau_1,\ldots,\tau_k$ be real numbers that are linearly independent over the rationals (for instance, $\tau_k=\pi^k$). For $\sigma_1=\pm1$, $\sigma_2=\pm1,\ldots,\sigma_k=\pm1$ define

$$\mathsf{R}(\sigma_1\ldots,\sigma_k)=\tau_0\mathsf{P}_0+\sum_{j=1}^{k}\sigma_j\tau_j\mathsf{P}_j. \tag{38}$$

Then every two of these sets are homometric.

Proof. All of the sets (38) have the same difference set: $\mathsf{D}[\mathsf{R}(\sigma_1,\ldots,\sigma_k)]=\tau_0\mathsf{D}(\mathsf{P}_0)+\tau_1\mathsf{D}(\mathsf{P}_1)+\ldots+\tau_k\mathsf{D}(\mathsf{P}_k)$. Therefore, we only have to prove that the identity

$$\mathsf{R}(\alpha_1,\ldots,\alpha_k)=\pm\mathsf{R}(\beta_1,\ldots,\beta_k)+\mathbf{c}(\text{for some } \mathbf{c}) \tag{39}$$

(where all the α's and β's are ±1) implies

$$\alpha_1=\beta_1,\ \alpha_2=\beta_2,\ldots,\alpha_k=\beta_k. \tag{40}$$

The equation (39) implies $\mathbf{c}=\mathbf{0}$, since every set P_j is assumed to have centroid $\mathbf{0}$, which implies that every set $\pm\mathsf{R}(\sigma_1,\ldots)$ has centroid $\mathbf{0}$. So we will now suppose (39) holds with $\mathbf{c}=\mathbf{0}$, and try to deduce (40).

Suppose first:

$$\mathsf{R}(\alpha_1,\ldots,\alpha_k)=-\mathsf{R}(\beta_1,\ldots,\beta_k). \tag{41}$$

Let $\mathbf{p}_0$ be some point in P_0 such that $^-\mathbf{p}_0$ is not in P_0. Then (41) implies

$$\tau_0\mathbf{p}_0+\sum_{j=1}^{h}\alpha_j\tau_j\mathbf{p}_j=-(\tau_0\mathbf{q}_0+\sum_{j=1}^{k}\beta_j\tau_j\mathbf{q}_j)$$

for some $\mathbf{q}_0$ in P_0 and some $\mathbf{p}_j$ and $\mathbf{q}_j$ in P_j $(j=1,\ldots,n)$. Then

$$\tau_0(\mathbf{p}_0+\mathbf{q}_0)+\sum_{j=1}^{k}\tau_j(\alpha_j\mathbf{p}_j+\beta_j\mathbf{q}_j)=0\,. \tag{42}$$

But $\mathbf{q}_0\neq-\mathbf{p}_0$, and all the points

$$\mathbf{p}_0+\mathbf{q}_0,\ \alpha_j\mathbf{p}_j+\beta_j\mathbf{q}_j\ (j=1,\ldots,k)$$

have *rational* coordinates. The linear independence of $\tau_0,\ldots,\tau_k$ over the rationals now implies that (42) is impossible. Therefore (41) is impossible.

Suppose instead:

$$\mathsf{R}(\alpha_1,\ldots,\alpha_k)=\mathsf{R}(\beta_1,\ldots,\beta_k)\,. \tag{43}$$

Define the set of indices

$$\mathsf{J}=\{j \text{ such that } \alpha_j\neq\beta_j\}\,. \tag{44}$$

Assume J is not empty. Then (43) and Theorem 3 imply

$$\sum_{j\in\mathsf{J}}\alpha_j\tau_j\mathsf{P}_j=\sum_{j\in\mathsf{J}}\beta_j\tau_j\mathsf{P}_j\,. \tag{45}$$

Now we proceed as before: let h be a particular member of J, and let $\mathbf{p}_h$, but not $-\mathbf{p}_h$, lie in P . Now (44) implies

$$\sum_{\mathsf{J}}\alpha_j\tau_j\mathbf{p}_j=\sum_{\mathsf{J}}\beta_j\tau_j\mathbf{q}_j \tag{46}$$

where $\mathbf{p}_j$ and $\mathbf{q}_j$ are in J. Since $\alpha_j=-\beta_j$ for $j\in$J, we find

$$\sum_{\mathsf{J}}\alpha_j\tau_j(\mathbf{p}_j+\mathbf{q}_j)=\mathbf{0} \tag{47}$$

where $\mathbf{p}_j+\mathbf{q}_j\neq\mathbf{0}$ for $j=h$. But then (47) is impossible because the τ_j are independent over the rationals. Therefore, J must be empty; in other words, (43) implies $\alpha_j=\beta_j(j=1,\ldots,n)$.

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References

CALDERON, A. & PEPINSKY, R. (1952). *Computing Methods and the Phase Problem in X-ray Crystal Analysis*, edited by R. PEPINSKY, Appendix 8, pp. 356–360. X-ray Crystal Analysis Laboratory, Pennsylvania State Univ.

GARRIDO, J. (1951). *Bull. Soc. Fr. Minér. Crist.* **74**, 397.

PATTERSON, A. L. (1944). *Phys. Rev.* **64**, 195–201.

PAULING, L. & SHAPPELL, M. D. (1930). *Z. Kristallogr.* **75**, 128.

PICCARD, S. (1939). *Sur les Ensembles de Distances des Ensembles de Points d'un Espace Euclidien*, Mém. Univ. Neuchâtel, **13**.

Acta Cryst. (1974). A**30**, 702

Probability Distribution of Bijvoet Differences. II*

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The earlier theoretical treatment of the probability distribution of Bijvoet differences [Parthasarathy & Srinivasan (1964). *Acta Cryst.* **17**, 1400–1407], has been extended to four new situations, namely, when the non-anomalous scatterers (Q) take up centrosymmetric configuration with the anomalous scatterers (P) corresponding to $P=$ one, $P=$ two, $P=$ many atoms with centrosymmetric (MC) and $P=$ many atoms with non-centrosymmetric (MNC) configuration. The theoretical distributions have been verified with hypothetical models.

Introduction

The probability distribution of the Bijvoet differences in the presence of anomalous scatterers in a non-centrosymmetric crystal was considered by Parthasarathy & Srinivasan (1964, hereafter referred to as part I). This had led to useful information on the optimum condition for measuring Bijvoet differences. The Bijvoet ratio has been considered by Parthasarathy & Parthasarathi (1973). In all these studies four situations have generally been considered for which probability distributions were derived in part I. These correspond to the Q atoms (light atoms) being non-centrosymmetric with the P atoms (anomalous scatterers) being one of the four types, namely (i) $P=$ one, (ii) $P=$ two, (iii) $P=$ many atoms with centrosymmetric

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