

On Homometric Sets. II. Sets Obtained by Singular Transformations

BY R. K. BULLOUGH

Department of Mathematics, The Manchester College of Science and Technology, Manchester 1, England

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The theorem that sets which have the same weighted vector set continue to do so when subjected to the same non-singular affine transformation is extended to singular transformations, but it does not follow that homometric sets (h.s.) necessarily remain homometric under singular transformations although they may do so. It is also shown that sets which are not homometric may become homometric under singular transformations. The singular transformation of periodic sets offers special difficulties. It is shown that 'almost all' singular transformations of periodic sets do not exist.

The (enumerable) infinity of transformations which do exist can be a source of new h.s., but the recognition of distinct homometric pairs (h.p.) is usually not simple. It is shown that every h.s. is a degenerate example of a larger h.s. and this occasions a re-examination of the definition of distinct h.s. An investigation is made of sets which become the 4-point pair Π_4 of part I under the same particular singular transformation. An argument which seems to be fairly general is used to prove that two 5-point pairs with this property are distinct but they are only two of many sets which transform to Π_4 . It is shown that an (enumerable) infinity of distinct h.s. can be reduced to Π_4 .

It is suggested that h.s. obtained by singular transformations cannot be considered to be examples of their generating sets as are h.s. obtained by non-singular transformations.

A group property of h.s. obtained by singular transformations is touched upon.

1. Introduction

In an earlier paper (Bullough, 1961), hereafter referred to as I, it was shown (I, Lemma 1) that if two periodic or non-periodic point sets were homometric to each other they remained homometric when each was subjected to the same affine transformation

$$\mathbf{T}x = \mathbf{A}x + \mathbf{c} \quad (1)$$

in which \mathbf{A} is a real non-singular m -dimensional square matrix. Accordingly it was argued that all homometric pairs (h.p.) related one to another by non-singular transformations should be counted as the same h.p.: h.p. are then invariant under the full affine group.

The notation of (1) for $\mathbf{T}x$ means that x , which is to be interpreted as an m -dimensional column vector, is subjected to transformation by the matrix \mathbf{A} followed by translation by the vector \mathbf{c} : $\mathbf{A}x$ is matrix multiplication. In I the notation $\mathbf{A} \cdot x$ was used to distinguish matrix multiplication from the operation signified by $\mathbf{T}x$. It is convenient no longer to make this distinction: the more usual notation $\mathbf{A}x$ for matrix multiplication is adopted and the transpose of \mathbf{A} (or x) is denoted by \mathbf{A}' (or x'); 'transformation under \mathbf{A}' means transformation by \mathbf{T} with matrix \mathbf{A} . The remaining notation of I is adopted without further explanation.

Now it is known (Hosemann & Bagchi, 1954, Figs. 2 and 3) that sets homometric in $m(>1)$ dimensions can remain homometric when subjected to the same singular transformation. Thus if \mathbf{V} is a singular affine transformation with matrix

$$\mathbf{B} = \begin{bmatrix} \beta & \gamma \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

in which β is a non-singular r -dimensional square matrix ($r < m$) then, in the notation of I, if S_1 —(S_2 in m dimensions, it may be that $\mathbf{V}S_1$ —($\mathbf{V}S_2$ in r dimensions. More generally if \mathbf{B} is of rank r it may be that $\mathbf{V}S_1$ —($\mathbf{V}S_2$ in r dimensions. But any r -dimensional vector $x'_r = (x_1, \dots, x_r)$ can be treated as an m -dimensional vector x'_m by adjoining $m-r$ constant components, e.g. $x'_m = (x_1, \dots, x_r, 0, \dots, 0)$ with $m-r$ noughts is an m -dimensional vector. Hence if \mathbf{B} is of rank r , $\mathbf{V}S_1$ —($\mathbf{V}S_2$ in m dimensions. One question which now arises is whether S_1 and $\mathbf{V}S_1$ are the same h.s. even though V is singular.

In I it was briefly noted that a generalization of the 1-dimensional h.p. Π_4 of I (8) and I, example (i) to two dimensions was

$$\left. \begin{aligned} S_1 &= ((0, 0), (a, b), (\frac{1}{4} + a, \frac{1}{4} + b), (\frac{1}{2}, \frac{1}{2}); 1, 1, 1, 1) \\ S_2 &= ((0, 0), (a, b), (\frac{3}{4} + a, \frac{3}{4} + b), (\frac{1}{2}, \frac{1}{2}); 1, 1, 1, 1) \end{aligned} \right\} \quad (2)$$

and that under the singular matrix

$$\mathbf{B} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \quad (3)$$

it became

$$\left. \begin{aligned} \mathbf{V}S_1 &= ((0, 0), (u, u), (\frac{1}{4} + u, \frac{1}{4} + u), (\frac{1}{2}, \frac{1}{2}); 1, 1, 1, 1) \\ \mathbf{V}S_2 &= ((0, 0), (u, u), (\frac{3}{4} + u, \frac{3}{4} + u), (\frac{1}{2}, \frac{1}{2}); 1, 1, 1, 1) \end{aligned} \right\} \quad (4)$$

which is a particular example of (2) with $a=b(=u)$.* Hence it was argued in I that in the absence of other information S_1 and $\mathbf{V}S_1$ should be counted as identical. In this paper (II) singular transformations are examined more completely: it is shown that whilst S_1 and $\mathbf{V}S_1$ may be the same set they are in general distinct. This is perhaps more consistent with the fact that \mathbf{V}^{-1} does not exist: for then, as we show,

$$\mathbf{V}S_1) \text{---} (\mathbf{V}S_2 \leftrightarrow S_1) \text{---} (S_2, S_1) \text{---} (S_2 \leftrightarrow \mathbf{V}S_1) \text{---} (\mathbf{V}S_2.$$

But distinction between h.s. can be difficult and is sometimes necessarily arbitrary. For example, the equivalence of h.s. under the affine group is very much less simple than envisaged in I: three examples which show an unexpected affine equivalence are noted in (29) (the pairs P_2 and P_3), (30), and (42) below yet these pairs are in some sense obviously distinct. At the same time it is shown (Theorem 16) that all h.s. are degenerate examples of larger h.s. and in § 5 the definition of distinct h.s. is re-examined in the light of this theorem.

It is also shown in the present paper (II) that if two non-periodic sets S_1 and S_2 have the same weighted vector set in m -dimensions, *i.e.* $\widehat{S_1\bar{S}_1} = \widehat{S_2\bar{S}_2}$, then they continue to do so in r ($\leq m$) dimensions under any affine transformation whatsoever, singular or non-singular, *i.e.* if $S_1^* = \mathbf{T}S_1$, $S_2^* = \mathbf{T}S_2$, $\widehat{S_1^*\bar{S}_1^*} = \widehat{S_2^*\bar{S}_2^*}$ for any \mathbf{T} and any matrix \mathbf{A} . The result for non-singular transformations was proved in I (6), and it was also applicable to periodic sets; but the extension to singular transformations offers difficulty on two counts. The first difficulty, the presence in the result of $\det \mathbf{A}^{-1}$, which does not exist when \mathbf{A} is singular, is more apparent than real; the second difficulty, that of the interpretation of all but a relatively small class of h.s. transformed by singular transformations when those h.s. are periodic, seems to be fundamental. It appears that transformed periodic sets are not necessarily meaningful when they are derived by singular transformations and although the result above remains true as a formal limit if necessary, it can be interpreted only for an enumerable set of singular transformations. On the other hand, an investigation of h.p. under singular transformations cannot be confined to the simpler case of non-periodic h.p. for (*cf.* I, and § 4 below) the class of periodic h.p. includes all non-periodic h.p. together with pairs which are homometric only when infinite and periodic.

A further indication of the motivation for the content of the present paper is the evident truth of the following theorem:

* The considerations of § 4 show that this result is to some extent fortuitous (*cf.* the example (20) below where under \mathbf{B} single projected lattice unit cells do not have the same vector set).

THEOREM 17: If $\widehat{S_1\bar{S}_1} = \widehat{S_2\bar{S}_2}$ and an affine transformation \mathbf{T} non-singular or singular exists (in the sense of Theorem 14 below in the second case) such that $\mathbf{T}S_1) \text{---} (\mathbf{T}S_2$, then $S_1) \text{---} (S_2$.

For if \mathbf{T} is non-singular, then if $S_1^* = \mathbf{T}S_1$, $S_2^* = \mathbf{T}S_2$

$$S_1^*) \text{---} (S_2^* \rightarrow \mathbf{T}^{-1}S_1^*) \text{---} (\mathbf{T}^{-1}S_2^* \text{ (by I, Lemma 1)})$$

or

$$S_1) \text{---} (S_2 .$$

If \mathbf{T} is singular

$$\widehat{S_1\bar{S}_1} = \widehat{S_2\bar{S}_2} \rightarrow S_1 \equiv S_2, S_1 \sim S_2 \text{ or } S_1) \text{---} (S_2 .$$

But

$$S_1 \equiv S_2 \rightarrow S_1^* \equiv S_2^*, S_1 \sim S_2 \rightarrow S_1^* \sim S_2^* .$$

The theorem asserts that if two sets have the same weighted vector set in $m > 1$ dimensions and can be shown to project to a h.p. in a smaller number of dimensions they are necessarily homometric in m dimensions. This theorem is invaluable in the building up of m -dimensional h.p. from 1-dimensional h.p. as will be shown in part III of this series; for although it is often easy to generate m -dimensional pairs with the same vector sets it is not always easy to show that such pairs constitute a h.p. This difficulty was already evident in the arguments of the earlier paper (I).

One only of the conditions of Theorem 17 is not sufficient and its converse is not true: $S_1^*) \text{---} (S_2^* \leftrightarrow \widehat{S_1\bar{S}_1} = \widehat{S_2\bar{S}_2}$ (and *a fortiori* $\leftrightarrow S_1) \text{---} (S_2$ as noted above) as is shown in Example (ii) of § 5; and $S_1) \text{---} (S_2$ ($\rightarrow \widehat{S_1\bar{S}_1} = \widehat{S_2\bar{S}_2} \rightarrow S_1^*\bar{S}_1^* = S_2^*\bar{S}_2^*$ by Theorems 13 and 15 below) $\leftrightarrow S_1^*) \text{---} (S_2^*$.

2. Vector sets under linear transformations

If S is a point set as in I, $\widehat{S\bar{S}}$ is its vector set. In order to prove Lemma 1 of I it was shown (I(6)) that if \mathbf{A} is non-singular and S is a point set of N m -dimensional δ -functions of weights z_0, \dots, z_{N-1} , then if $\mathbf{T}S = S^*$,

$$\mathbf{T}(\widehat{S\bar{S}}) = |\det \mathbf{A}|^{-1} S^* \bar{S}^* . \quad (\text{I(6)})$$

This result is sufficient to prove I, Lemma 1 when $\det \mathbf{A} \neq 0$ but becomes meaningless when \mathbf{T} is singular and $\det \mathbf{A} = 0$. But the extension of I(6) to this latter case is possible because the presence of $\det \mathbf{A}$ in I(6) is in fact illusory. Equation I(6) as proved is actually applicable to any function $S(\mathbf{x})$ whatsoever (provided S is integrable and $\widehat{S\bar{S}}$ exists). We shall first show that $\det \mathbf{A} (\neq 0)$ does not appear

in I(6) if $\mathbf{T}(\widehat{S\bar{S}})$ and S^* are properly normalized and S is any non-periodic function, we then prove I(6) when $\det \mathbf{A} = 0$ for any properly normalized non-

periodic set, S , of δ -functions; in § 3 and § 4 we then extend the proof to periodic sets but this requires an investigation of the meaning of $S^* = \mathbf{T}S$ when S is periodic and \mathbf{T} singular.

In the proof of I(6) S and $\mathbf{T}S$ were assumed to be such that to every point \mathbf{x} in S corresponds $\mathbf{T}\mathbf{x}$ in $\mathbf{T}S$. Hence

$$\mathbf{T}S(\mathbf{x}) = S(\mathbf{T}^{-1}\mathbf{x}). \tag{5}$$

If S has a certain total weight Z ,

$$Z = \int S(\mathbf{x}) d\tau$$

where, since S is assumed non-periodic, the integration is over all space. The weight of $\mathbf{T}S$ is therefore

$$\int S(\mathbf{T}^{-1}\mathbf{x}) d\tau = |\det \mathbf{A}| \int S(\mathbf{x}) d\tau = |\det \mathbf{A}|Z.$$

If this total weight is to be unchanged in the transformation induced by \mathbf{T} we must use not (5) but

$$\mathbf{T}S = |\det \mathbf{A}|^{-1} S(\mathbf{T}^{-1}\mathbf{x}). \tag{6}$$

We can now complete the proof of I(6): we give it in full since I(6) contains a small error. We have

$$\begin{aligned} \mathbf{T}(\widehat{S\bar{S}}) &= |\det \mathbf{A}|^{-1} \int S(\mathbf{y}) S(\mathbf{y} - \mathbf{T}^{-1}\mathbf{x}) d\tau \\ &= |\det \mathbf{A}|^{-2} \int S(\mathbf{T}^{-1}\mathbf{y}) S(\mathbf{T}^{-1}\mathbf{y} - \mathbf{T}^{-1}\mathbf{x}) d\tau, \end{aligned}$$

but it was not noted in I(6) that

$$\begin{aligned} \mathbf{T}^{-1}\mathbf{y} - \mathbf{T}^{-1}\mathbf{x} &= \mathbf{A}^{-1}(\mathbf{y} - \mathbf{c}) - \mathbf{A}^{-1}(\mathbf{x} - \mathbf{c}) \\ &= \mathbf{A}^{-1}(\mathbf{y} - \mathbf{x}) = \mathbf{T}^{-1}(\mathbf{y} - \mathbf{x} + \mathbf{c}). \end{aligned}$$

Hence, if

$$S^* = \mathbf{T}S = |\det \mathbf{A}|^{-1} S(\mathbf{T}^{-1}\mathbf{x}),$$

then in the notation of I, Definition 1

$$\mathbf{T}(\widehat{S\bar{S}}) = \widehat{S^*\bar{S}^*} + \mathbf{c} \tag{7a}$$

and

$$\mathbf{T}(\widehat{S\bar{S}}) \equiv \widehat{S^*\bar{S}^*} \tag{7b}$$

changing the equality in I(6) to identity.

The argument fails when \mathbf{T}^{-1} does not exist. Suppose for the moment that $\det \mathbf{A} \neq 0$. The matrix \mathbf{A} is not symmetric in general, but (*cf.* Appendix) we can always write

$$\mathbf{A} = \mathbf{C}\mathbf{O}$$

where \mathbf{C} is a symmetric m -dimensional square matrix and \mathbf{O} is m -dimensional orthogonal ($\det \mathbf{O} = \pm 1$). The dimensionality of $\mathbf{C}\mathbf{O}$ is then $\frac{1}{2}m(m+1) + \frac{1}{2}m(m-1) = m^2$ equal to that of \mathbf{A} . The matrix \mathbf{O} is non-singular and simply introduces a combination of rotations and reflexions which can be ignored because (I, Lemma 1) if, and only if, S_1)—(S_2 then

$\mathbf{O}S_1$)—($\mathbf{O}S_2$.* Because \mathbf{C} is real symmetric it has real eigen values and may be diagonalized by appropriate choice of the coordinate axes. If we now consider a singular transformation as the limit of a non-singular one, the only singular matrices are diagonal ones. This is considered more completely in (i) of the Appendix.

As in I, suppose that S is a set of N m -dimensional δ -functions:

$$S(\mathbf{x}) = \sum_{i=0}^{N-1} z_i \delta(\mathbf{x} - \mathbf{x}_i). \tag{8}$$

When \mathbf{C} is non-singular diagonal

$$\mathbf{C} = \text{diag}(c_1, \dots, c_m); \quad c_r \neq 0, \quad 1 \leq r \leq m;$$

also

$$\delta(\mathbf{x} - \mathbf{x}_i) = \prod_{r=1}^m \delta(x_r - x_r^{(i)})$$

where

$$\mathbf{x}' = (x_1, \dots, x_m), \quad \mathbf{x}'_i = (x_1^{(i)}, \dots, x_m^{(i)}),$$

and so

$$\begin{aligned} \mathbf{C}\delta(\mathbf{x} - \mathbf{x}_i) &= |\det \mathbf{C}|^{-1} \prod_{r=1}^m \delta(c_r^{-1}x_r - x_r^{(i)}) \\ &= \prod_{r=1}^m c_r^{-1} \delta\{c_r^{-1}(x_r - c_r x_r^{(i)})\}. \end{aligned}$$

But from the definition of the δ -function it follows that

$$\delta\{c_r^{-1}(x_r - c_r x_r^{(i)})\} = c_r \delta(x_r - c_r x_r^{(i)})$$

and

$$\mathbf{C}\delta(\mathbf{x} - \mathbf{x}_i) = \prod_{r=1}^m \delta(x_r - c_r x_r^{(i)}).$$

This shows that, when S is of the form (8) and $\mathbf{T}S$ is defined as in (6), S and $\mathbf{T}S$ are such that a point of weight z_i at \mathbf{x}_i in S becomes a point of the same weight at $\mathbf{T}\mathbf{x}_i$ in $\mathbf{T}S$ as was originally required in I. This will always be the meaning of $\mathbf{T}S$ in the future whether \mathbf{T} is non-singular or not. When \mathbf{T}^{-1} exists this interpretation is precisely equivalent to (6). When any c_r , say c_s , tends to zero, $\mathbf{C}\delta(\mathbf{x} - \mathbf{x}_i)$ is an m -dimensional δ -function located on the point $(c_1 x_1^{(i)}, \dots, 0, \dots, c_m x_m^{(i)})$ with 0 in the s th place. It follows that

$$\mathbf{T}(\widehat{S\bar{S}}) = \widehat{S^*\bar{S}^*} + \mathbf{c} \equiv \widehat{S^*\bar{S}^*} \tag{9}$$

whether \mathbf{C} is non-singular or not. Since \mathbf{A} is arbitrary the argument is in no way restricted to the *orthogonal*† ‘projections’ resulting when $c_s = 0$. The number, N , of points in the set S can be as large as one pleases, but S is for the moment assumed non-periodic.

The result (9) is almost trivial since if \mathbf{T} is to have the property of changing \mathbf{x}_i in S to $\mathbf{T}\mathbf{x}_i$ leaving

* $\mathbf{O}S$, in which \mathbf{O} is a matrix is used to mean the set $\mathbf{T}S$ in which \mathbf{T} is such that $\mathbf{T}\mathbf{x} = \mathbf{O}\mathbf{x}$, *i.e.* is a homogeneous affine transformation.

† An orthogonal basis is assumed here but this is of course not necessary (see the discussion in (ii) and (iii) of the Appendix).

z_i unchanged, \mathbf{x}_i and \mathbf{x}_j become $\mathbf{T}\mathbf{x}_i$ and $\mathbf{T}\mathbf{x}_j$ leaving z_i and z_j unchanged, whilst $(\mathbf{x}_i - \mathbf{x}_j)$ becomes $\mathbf{T}(\mathbf{x}_i - \mathbf{x}_j)$ leaving $z_i z_j$ unchanged, and this is true even when \mathbf{T} is of rank $r < m$ (restricting $\mathbf{T}\mathbf{x}_i$, $\mathbf{T}\mathbf{x}_j$ and $\mathbf{T}(\mathbf{x}_i - \mathbf{x}_j)$ to an r -dimensional sub-space of the m -dimensional space). Its essential simplicity should not obscure its importance: we have, in fact

THEOREM 13. If S_1 and S_2 are not periodic and $\widehat{S_1 S_1} = \widehat{S_2 S_2}$, and if $S_1^* = \mathbf{T}S_1$, $S_2^* = \mathbf{T}S_2$ where \mathbf{T} is any real affine transformation whatsoever, then

$$\widehat{S_1^* S_1^*} = \widehat{S_2^* S_2^*}.$$

The equality follows from (9) because

$$\widehat{S_1^* S_1^*} + \mathbf{c} = \widehat{S_2^* S_2^*} + \mathbf{c}.$$

The theorem is equally true when \mathbf{A} has complex elements but this does rather less than extend the theorem to $2m$ dimensions. An incomplete proof of (9) is also given in (iii) of the Appendix for sets much more general than (8). The theorem is much less obvious here since it appears to require the particular interpretation (43) of $\mathbf{A}S$.

Theorem 13 is applicable to periodic sets when \mathbf{T} is non-singular. When \mathbf{T}^{-1} exists I(7) and I, Lemma 1 follow. Whether \mathbf{T}^{-1} exists or not we always have $S_1 \equiv S_2 \rightarrow S_1^* \equiv S_2^*$, $S_1 \sim S_2 \rightarrow S_1^* \sim S_2^*$, but when \mathbf{T}^{-1} does exist, it cannot be inferred from Theorem 13 that $S_1) - (S_2 \rightarrow S_1^*) - (S_2^*$. Moreover the converse of Theorem 13 does not necessarily hold: when \mathbf{T}^{-1} does not exist

$$\widehat{S_1^* S_1^*} = \widehat{S_2^* S_2^*} \leftrightarrow \widehat{S_1 S_1} = \widehat{S_2 S_2}.$$

Hence it is possible to obtain h.p. by singular transformations of pairs which are not homometric. Indeed, when \mathbf{T}^{-1} does not exist S_1^* , S_2^* imply little about S_1, S_2 : so much so indeed that we can have $S_3 \neq S_1, S_4 \neq S_2, S_3^* = S_1^*, S_4^* = S_2^*, S_1^*) - (S_2^*$ whether or not either or both of $S_3) - (S_4, S_1) - (S_2$ obtain, and the correspondence of $S_1) - (S_2$ to $S_1^*) - (S_2^*$ can at least be many-one. It follows that when \mathbf{T} is singular S_1 and $S_1^* = \mathbf{T}S_1$ cannot be the same h.s. in general. Examples of these various relations appear in § 3 and § 4.

3. Transformations of periodic sets.

The difficulty associated with the transformation of periodic sets arises because such sets necessarily contain an infinite number of points. An obvious example is that occurring when \mathbf{A} is the singular matrix

$$\mathbf{A} = \begin{bmatrix} \alpha & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

where α is non-singular and $(m-1)$ -dimensional, pro-

jecting S down the m axis. If S is periodic, an infinity of points exist with coordinates (x_1, \dots, x_{m-1}, a) each with different a , and $\mathbf{T}S$ contains a set of points with infinite weights lying in the plane $x_m = 0$. But it is clearly sufficient to project only those points lying between $x_m = 0$ and $x_m = 1$ onto $x_m = 0$, since the remaining part of the lattice only superposes copies of the projected set. The obvious way to submit a periodic lattice to a singular transformation is therefore to submit only a fundamental portion of it to the transformation. The particular fundamental portion is determined by the particular transformation.

We consider only orthogonal projections: these do not necessarily include all possible projections since although the lattice may be sheared in such a way as to make the subsequent projection orthogonal the resulting lattice is no longer a primitive cubic lattice. However, there seems to be no difference in principle between orthogonal and non-orthogonal projections.

We can project orthogonally in an arbitrary fashion from m to $m-1$ dimensions but the result may not be meaningful. For we can project orthogonally in an arbitrary direction \mathbf{n} (with transpose $\mathbf{n}' = (n_1, \dots, n_m)$) in m dimensions onto an $(m-1)$ dimensional hyperplane normal to \mathbf{n} . A hyperplane passing through a lattice point at the origin is $\mathbf{n}'\mathbf{r} = 0$. A vector $\lambda\mathbf{n}$ passing through the origin must either intersect no more lattice points or it must intersect an infinity of them. For if it intersects one for $\lambda = \lambda_1$ (say), then $\lambda_1\mathbf{n}$ is a lattice translation and there are lattice points at $\nu\lambda_1\mathbf{n}$ for any positive or negative integer ν . If $\lambda_1\mathbf{n}$ is a lattice vector and there is no value of λ lying in $0 < \lambda < |\lambda_1|$ such that $\lambda\mathbf{n}$ is a lattice vector then, extending a usage of (H.W., 29),* the point with position vector $\lambda_1\mathbf{n}$ will be called a 'visible point': any direction \mathbf{n} which defines a 'visible point' $\lambda\mathbf{n}$ for some λ will be called a 'visible direction'.

If $\lambda_1\mathbf{n}$ is a visible point then it is sufficient to project down \mathbf{n} onto $\mathbf{n}'\mathbf{r} = 0$ all points which lie between the planes $\mathbf{n}'\mathbf{r} = 0, \mathbf{n}'\mathbf{r} = \lambda_1$, satisfying (for $\lambda_1 > 0$) $0 \leq \mathbf{n}'\mathbf{r} < \lambda_1$. Combined with this condition the matrix for the projection must be such that \mathbf{r} becomes \mathbf{s} where $\mathbf{n}'\mathbf{s} = 0$ and

$$\mathbf{r} + \mu\mathbf{n} = \mathbf{s}.$$

Hence $\mu = -\mathbf{n}'\mathbf{r}$ and

$$\mathbf{s} = \mathbf{r} - \mathbf{n}(\mathbf{n}'\mathbf{r}) = (\mathbf{I}_m - \mathbf{M}_m)\mathbf{r}$$

where \mathbf{I}_m is the m -dimensional unit matrix and \mathbf{M}_m is an m -dimensional square matrix with components

$$(\mathbf{M})_{ij} = n_i n_j. \quad (10)$$

The required matrix is therefore

$$\mathbf{A}_m = \mathbf{I}_m - \mathbf{M}_m$$

* As in I, (H.W., k) refers to page k of Hardy & Wright (1954).

and provided visible directions can always be found* $\mathbf{A}_m, \mathbf{A}_{m-1}, \dots, \mathbf{A}_{m-r}$ will perform any projection from m to r dimensions. The projected set is clearly periodic in $(m-1)$ dimensions since any lattice vector \mathbf{u} in S becomes

$$(\mathbf{I}_m - \mathbf{M}_m)\mathbf{u} = \mathbf{v} \text{ (say)}$$

in $\mathbf{T}S$ and $\nu\mathbf{u}$ becomes $\nu\mathbf{v}$ and the sets are therefore periodic in r dimensions.

If \mathbf{n} is not a visible direction, *i.e.* $\lambda\mathbf{n}$ intersects no lattice points other than the origin, there are at most N points on the line $\lambda\mathbf{n}$; for if $\lambda\mathbf{n}$ is not a lattice vector it cannot intersect more than one equivalent of any of the N points in the unit cell. Hence no difficulty arises from the superposition of an infinite number of points in the projection and it is sufficient to project all points lying on the line

$$\mathbf{r} = \mathbf{s} + \lambda\mathbf{n}$$

onto the point \mathbf{s} by the matrix $(\mathbf{I}_m - \mathbf{M}_m)$. The projected set necessarily remains periodic but the difficulty is now that the unit of repeat has a zero hyperarea in the plane $\mathbf{n}'\mathbf{r} = 0$. This is so because no two cells of the lattice superpose on this plane yet the total number of cells of the lattice must be preserved: the projected cells necessarily overlap and, since the number of points of the lattice is enumerable in each of m linearly independent directions whilst that of the projected set is enumerable in only $m-1$ linearly independent directions, there are other lattice points of the projected set arbitrarily close to any one lattice point of the projected set. Projected sets of this type obviously require a special interpretation and may be meaningful only as a formal limit. *A fortiori* successive projections of sets of this type may not be meaningful and, when \mathbf{n} is not a visible direction, it is not obvious that projections from m to $r < m-1$ dimensions are still possible. However, it may be possible to project directly as in the following.

We consider the important case of orthogonal projection from m to 1 dimensions by a matrix of rank 1. If \mathbf{T} has such a matrix it transforms every point lying in the hyperplane

$$\mathbf{n}'\mathbf{r} = p$$

into the point $p\mathbf{n}$. The required matrix is therefore the matrix \mathbf{M}_m : for convenience we henceforth drop the subscript. If the origin is a lattice point then either $\mathbf{n}'\mathbf{r} = 0$ contains no other lattice points or it contains an infinity of them. In the first case it is sufficient to project *every* point in $\mathbf{n}'\mathbf{r} = p$ onto $p\mathbf{n}$.

* It is shown below that if \mathbf{n} is visible $\mathbf{n}'\mathbf{r} = 0$ contains lattice points repeating in $(m-1)$ linearly independent directions: this is also true only if \mathbf{n} is visible. Therefore successive projections from m to r dimensions are always possible if every \mathbf{n} is visible but may not be possible if \mathbf{n} at any stage is not visible.

In the second case $\mathbf{n}'\mathbf{r} = 0$ will contain in general a periodic set of lattice points repeating along up to $m-1$ linearly independent directions. For if $\lambda\mathbf{u}_1$ is a lattice point in this plane so is $\nu\lambda\mathbf{u}_1$, and if $\mu\mathbf{u}_2$ is a lattice point ($\mathbf{u}_2 \neq \kappa\mathbf{u}_1$) so is $\nu_1\lambda\mathbf{u}_1 + \nu_2\mu\mathbf{u}_2$, and so on. If $\mathbf{n}'\mathbf{r} = 0$ contains a periodic set repeating in up to $(m-1)$ linearly independent directions, then it is sufficient to project exactly one of each inequivalent point (with maximum number N) lying in $\mathbf{n}'\mathbf{r} = p$ onto $p\mathbf{n}$ by the matrix \mathbf{M} .

The line $\lambda\mathbf{n}$ through the origin will intersect either none or an infinity of other lattice points. Suppose \mathbf{n} is visible with a visible point $\lambda_1\mathbf{n}$. Under \mathbf{T} with matrix $\mathbf{M}S$ becomes $\mathbf{T}S$ periodic with one period $|\lambda_1|\mathbf{n}$. But in fact the period is $\leq |\lambda_1|\mathbf{n}$.* For if the hyperplane $\mathbf{n}'\mathbf{r} = 0$ contains a lattice repeating along $m-1$ linearly independent directions it contains a cell of finite hyperarea A such that $|\lambda_1|A$ contains an integral number of lattice unit cells. Hence the period of the projected set lying along \mathbf{n} is $1/A$. For it is clear that, since every lattice point is equivalent to every other, any lattice point projected onto the line $\lambda\mathbf{n}$ must be equivalent to any other and if $\lambda_1\mathbf{n}$ contains $|\lambda_1|A$ projected lattice points the set on $\lambda\mathbf{n}$ repeats every $1/A$.

The area A of the unit cell in the hyperplane can be found as follows. Since $\lambda_1\mathbf{n}$ is visible, it is a lattice point and is such that for $0 < \lambda < |\lambda_1|$, $\lambda\mathbf{n}$ is not a lattice point. If

$$\lambda_1\mathbf{n}' = (p, q, \dots, w)$$

then, by the first property, the m components p, q, \dots, w are integers which, by the second property, have no common factor. The positive integers $|p|, |q|, \dots, |w|$ are therefore relatively prime but not necessarily relatively prime in pairs (H.W., 48). If the hyperplane $\mathbf{n}'\mathbf{r} = 0$ contains lattice points repeating in $(m-1)$ linearly independent directions with unit cell of area A , this cell is the base of a 'unit cell' of a volume $|\lambda_1|A$ which contains an integral number of lattice points and must therefore be an integer. Since

$$|\lambda_1| = (p^2 + q^2 + \dots + w^2)^{\frac{1}{2}}$$

and $|\lambda_1|A$ is an integer for every choice of the integers p, q, \dots, w we must have

$$A = (p^2 + q^2 + \dots + w^2)^{\frac{1}{2}} f(p, q, \dots, w) \quad (11)$$

where $f(p, q, \dots, w)$ is a homogeneous polynomial in p, q, \dots, w with integral coefficients.

To determine the function f we use an argument specifically for four dimensions ($m=4$) which can obviously be generalized to $m > 4$. We require three linearly independent lattice vectors with components x, y, z, v necessarily integral satisfying

$$px + qy + rz + sv = 0 \quad (12)$$

* *i.e.* the length of the period in the direction \mathbf{n} is $\leq |\lambda_1|$.

in which the components of $(p, q, r, s) = \lambda_1 \mathbf{n}'$ are also integers. A set is

$$\mathbf{u}'_1 = (s, 0, 0, -p), \quad \mathbf{u}'_2 = (r, 0, -p, 0), \quad \mathbf{u}'_3 = (q, -p, 0, 0) \quad (13)$$

and this is true for all integral p, q, r, s . Incidentally, this and its generalization demonstrate that if $\lambda_1 \mathbf{n}$ is a visible point and \mathbf{n} a visible direction the points of the hyperplane perpendicular to \mathbf{n} necessarily repeat in $m-1$ linearly independent directions (see footnote on p. 299). The cell defined by the vectors (13) is a unit of repeat in the hyperplane (12) but it is not necessarily the smallest such unit: in particular, if *e.g.* p and s have a common factor d , \mathbf{u}'_1 should be replaced by

$$\mathbf{u}'_1 = (s/d, 0, 0, -p/d).$$

The hyperarea of the cell defined by (13) is therefore an integral multiple of (11).

The area of the base of the cell defined by the vectors $\mathbf{u}_1, \mathbf{u}_2$ is

$$[\mathbf{u}_1^2 \mathbf{u}_2^2 - (\mathbf{u}'_1 \mathbf{u}_2)^2]^{\frac{1}{2}} = p(p^2 + s^2 + r^2)^{\frac{1}{2}}. \quad (14)$$

A perpendicular to \mathbf{u}_1 and \mathbf{u}_2 lying in the plane (12) is the vector

$$(p, \alpha, r, s); \quad \alpha = -(p^2 + r^2 + s^2)/q.$$

This is of length

$$l = (p^2 + r^2 + s^2 + \alpha^2)^{\frac{1}{2}} = (p^2 + r^2 + s^2)^{\frac{1}{2}} \times (p^2 + q^2 + r^2 + s^2)^{\frac{1}{2}}/q.$$

The projection of \mathbf{u}_3 in this direction is

$$(pq - \alpha p)/l = p(p^2 + q^2 + r^2 + s^2)^{\frac{1}{2}}(p^2 + r^2 + s^2)^{-\frac{1}{2}}$$

and the hyperarea of the cell is

$$p^2(p^2 + q^2 + r^2 + s^2)^{\frac{1}{2}}. \quad (15)$$

It is clear that for $m=5$ one can consider vectors

$$\mathbf{u}'_1 = (t, 0, 0, 0, -p), \quad \mathbf{u}'_2 = (s, 0, 0, -p, 0), \\ \mathbf{u}'_3 = (r, 0, -p, 0, 0), \quad \mathbf{u}'_4 = (q, -p, 0, 0, 0),$$

instead of (13), and (15)* replaces (14). The argument then continues as from (14) and the hyperarea is

$$p^3(p^2 + q^2 + r^2 + s^2 + t^2)^{\frac{1}{2}},$$

and in general the hyperarea is

$$p^{m-2}(p^2 + q^2 + \dots + w^2)^{\frac{1}{2}}. \quad (16)$$

Since (16) is an integral multiple of (11) and $f(p, q, \dots, w)$ is homogeneous in p, q, \dots, w it follows that the hyperarea A of the unit cell in the plane $\mathbf{n}'\mathbf{r}=0$ is

$$A = (p^2 + q^2 + \dots + w^2)^{\frac{1}{2}}.$$

In particular when $m=2$,

$$A = (p^2 + q^2)^{\frac{1}{2}}$$

which is known from simpler considerations.

When \mathbf{n} is a visible direction $|p|, |q|, \dots, |w|$ are relatively prime. When \mathbf{n} is not visible we consider this as the limit of $|p|, |q|, \dots, |w|$ tending to ∞ in such a way that they remain relatively prime, *i.e.* so that at least one ratio *e.g.* $|p|/|q|$ is irrational. In this case A tends to ∞ and lattice points in $\mathbf{n}'\mathbf{r}=0$ repeat in at most $m-2$ linearly independent directions. At the same time the length $1/A$ of the unit of repeat of the set projected on the direction \mathbf{n} tends to zero.

The magnitude of the unit of repeat of the projected set remains equal to unity if instead of the matrix \mathbf{M} of (10) we use

$$(p^2 + q^2 + \dots + w^2)^{\frac{1}{2}} \mathbf{M}. \quad (17)$$

This matrix exists for every set of integers (p, q, \dots, w) . Hence we can project periodic sets orthogonally onto all visible directions. The matrix does not exist when $|p|, |q|, \dots, |w|$ tend to ∞ and the projection is not possible when \mathbf{n} is not a visible direction. On the other hand, when \mathbf{n} is not a visible direction, we can project onto directions \mathbf{m} which approach \mathbf{n} as closely as we please. Nevertheless, since the number of lattice points is enumerable the number of visible points is enumerable and the matrix (17) does not exist for 'almost all' directions \mathbf{n} . The matrix \mathbf{M} of (10) exists for all \mathbf{n} but the unit cell of the projected set has 'almost always' nothing but formal significance — as far as the theory is developed here. We shall therefore say that a projection onto the direction \mathbf{n} exists only when (17) exists. Analogous matrices which may exist or not will also occur in the singular transformations of m -dimensional sets to $r (< m)$ dimensions.

We have proved the theorem:

THEOREM 14. Orthogonal projections of rank 1 of periodic sets S onto directions \mathbf{n} exist if, and only if, \mathbf{n} is visible.

We have also proved the

COROLLARY: 'Almost all' such projections do not exist.

Provided the projection \mathbf{T} onto a direction \mathbf{n} exists we can extend Theorem 13 to the case of periodic sets. Theorem 13 is valid for sets S_1 and S_2 containing arbitrary numbers of points N_1 and N_2 but even when the projection is interpreted in the sense of the discussion above this does not mean the extension is immediate. Certainly if S_1 and S_2 are periodic the implication that N_1 and N_2 are enumerably infinite now causes no difficulty *per se*: the real difficulty in the direct appeal to Theorem 13 is that when two infinite periodic sets are convoluted the resultant periodic set is meaningful only when 'factored' once by the periodic set of lattice points. Suppose C_1 is the content of the unit cell of S_1 and L is its lattice.

* With r, s, t replacing p, r, s respectively.

Then as in §4 below (but there with a different interpretation of C_1) $S_1 = \widehat{C_1 L}$, but $\widehat{S_1 \bar{S}_1}$ is $\widehat{C_1 \bar{C}_1 L}$ and not $\widehat{C_1 \bar{C}_1 L \bar{L}}$. Since $L = \bar{L}$, $\widehat{S_1 \bar{S}_1}$ is 'factored' once by L .

This is necessary because $\widehat{L \bar{L}}$ is a periodic lattice of δ -functions in which each δ -function has infinite weight: L is, therefore, a 'renormalized' $\widehat{L \bar{L}}$ and Theorem 13 could be applicable only if the renormalization could be carried through.

When the projection \mathbf{T} exists (so that \mathbf{n} is visible) both the superposition of points and the renormalization are avoided by projecting only finite parts of S_1 and S_2 (which we call their 'cells for projection' in §4): this means that the two finite sets to be projected are not necessarily homometric — for it was noted in I and §1 here, that certain sets are homometric only when their unit cells lie in (m -dimensional) infinite lattices. Paradoxically this second difficulty is avoided when \mathbf{n} is not visible provided only finite superpositions of points occur in the projection of the whole lattice; and this is certainly so in the extreme case when the plane normal to \mathbf{n} contains no more than one equivalent of each point, *i.e.* when every ratio $p/q, p/r, q/r$, *etc.* is irrational.

But now although $\mathbf{T}S_1, \mathbf{T}S_2$ and $\mathbf{T}(\widehat{S_1 \bar{S}_1}) = \mathbf{T}(\widehat{S_2 \bar{S}_2})$ can be said to exist as everywhere 'dense' (H.W. 121) projections of all the points of each set, still the convolution of $\mathbf{T}S_1$ and $\mathbf{T}S_2$ could be taken only by factoring out one convolution of the projected set of lattice points. Moreover since $\mathbf{T}S_1$ and $\mathbf{T}S_2$ contain δ -functions located on lattice and other points arbitrarily close to other δ -functions on lattice and other points, both the process of convolution and the process of integration itself is now undefined. The sense in which Theorem 13 remains true for periodic lattices when the projecting matrix 'does not exist' (in particular in the sense that (17) does not exist except for visible \mathbf{n} when the rank is 1) is thus of considerable mathematical interest but requires an extension of interpretation that we shall not attempt in the present paper. When (17) exists, however, the same result which we prove as Theorem 15 below is of interest because the unit cells of S overlap in the projection, forming new unit cells, and the projected set S^* can be very different from the set S . Hence the possibility exists of obtaining essentially new h.s. in r dimensions by the projection of h.s. in $m(>r)$ dimensions.

4. Transformations of periodic vector sets

We assume that the situation for transformations \mathbf{T} of a rank r ($< m$) is strictly analogous to the situation considered in detail above for transformations of rank 1. If the transformation exists, hyperareas of magnitude A of which one has lattice points at its

corners are projected onto each point of a second hyperarea of magnitude A' also with lattice points at its corners, and the two areas with lattice points at their corners define a cell (for orthogonal projection of volume AA') in the m -dimensional periodic set S which we can call a cell for projection (c.p.). If

$\widehat{S_1 \bar{S}_1} = \widehat{S_2 \bar{S}_2}$, S_1 and S_2 must have a common lattice which as usual we choose to be primitive cubic with unit lattice constant. The c.p. of S_1 is then identical with that of S_2 and it is also the c.p. of $\widehat{S_1 \bar{S}_1}$ and $\widehat{S_2 \bar{S}_2}$.

If S_1 and S_2 have the same weighted vector set it does not necessarily follow that the content C_1 and C_2 of the c.p.s. of S_1 and S_2 have the same vector set. Suppose first they have.

The simplest case of this occurs when the contents of the *unit cells* of S_1 and S_2 have the same weighted vector set. In this case the contents of the unit cells can be abstracted from their lattices and have the same weighted vector set when projected in any direction whatsoever according to Theorem 13. They may then be inserted in a new periodic lattice in the projected space and will still have the same weighted vector set.

An example is that of Hosemann & Bagchi (1954). Their Fig. 1 contains the non-periodic h.p.

$$S_1 = ((-1, 0), (-1, -1), (0, -2), (1, -1), (1, 1), (2, 1); 1, 1, 1, 1, 1, 1)$$

$$S_2 = ((-1, 0), (0, -1), (0, 1), (1, -1), (2, 1), (2, 2); 1, 1, 1, 1, 1, 1)$$

in an orthogonal system of axes. Under the singular matrix

$$\begin{bmatrix} 4 & -1 \\ 0 & 0 \end{bmatrix}$$

this h.p. becomes their Fig. 3 namely

$$S_1^* = (-4, -3, 2, 5, 3, 7; 1, 1, 1, 1, 1, 1)$$

$$S_2^* = (-4, 1, -1, 5, 7, 6; 1, 1, 1, 1, 1, 1).$$

S_1^* and S_2^* have the same 1-dimensional non-periodic vector set according to Theorem 13, and in fact they constitute a h.p.

It is interesting to observe that, from one point of view, S_1 and S_2 are unchanged in H.B.'s Fig. 2: only the *basis* of the vectorspace is changed. With the new basis S_1^* and S_2^* are still obtained from S_1 and S_2 of the Fig. 2 by the *same* singular matrix. The h.p.s. of H.B.'s Figs. 1 and 2 are, therefore, the same h.p. and differ only in the choice of basis: from this point of view, but more generally, affine equivalents under I, Lemma 1 differ only in the choice of basis. But if \mathbf{T} is singular, and S_1^* — (S_2^* , and S_1) — (S_2 , the two pairs differ in the choice of vector space — a real difference as is suggested in this paper.

If C_1 and C_2 do have the same vector set, then

— because when the numbers of points N_1 and N_2 in the unit cells of S_1 and S_2 are finite, Theorem 13 is certainly applicable to the finite sets C_1 and C_2 — the projected sets C_1^* and C_2^* have

$$\widehat{C_1^* C_1^*} = \widehat{C_2^* C_2^*}.$$

Since S_1 and S_2 have the same lattice, they have the same lattice L (say) of c.p.s. and the same lattice L^* of projected c.p.s.†. Now it is clear that if convolution — is taken over all space

$$S_1^* = C_1^* L^*, \quad S_2^* = C_2^* L^*, \quad S_1^* \widehat{S_1^*} = \widehat{C_1^* C_1^*} L^*.$$

Hence

$$\widehat{S_1^* \widehat{S_1^*}} = \widehat{C_1^* \widehat{C_1^*}} L^* = \widehat{C_2^* \widehat{C_2^*}} L^* = \widehat{S_2^* \widehat{S_2^*}}.$$

Because

$$\widehat{S_1 \widehat{S_1}} = \widehat{C_1 \widehat{C_1}} L, \quad (18)$$

we can still have

$$\widehat{S_1 \widehat{S_1}} = \widehat{S_2 \widehat{S_2}}, \quad \widehat{C_1 \widehat{C_1}} \neq \widehat{C_2 \widehat{C_2}}. \quad (19)$$

Suppose the c.p. is defined by vectors $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_m$. Then if (19) holds $\widehat{C_1 \widehat{C_1}}$ and $\widehat{C_2 \widehat{C_2}}$ differ from the content of the c.p. of $\widehat{S_1 \widehat{S_1}}$ (or $\widehat{S_2 \widehat{S_2}}$) in that at least one vector \mathbf{x} in $\widehat{S_1 \widehat{S_1}}$ is \mathbf{y}_1 in $\widehat{C_1 \widehat{C_1}}$ and \mathbf{y}_2 in $\widehat{C_2 \widehat{C_2}}$ where

$$\begin{aligned} \mathbf{x} &= \mathbf{y}_1 + \kappa_1 \mathbf{u}_1 + \dots + \kappa_m \mathbf{u}_m \\ &= \mathbf{y}_2 + \mu_1 \mathbf{u}_1 + \dots + \mu_m \mathbf{u}_m \end{aligned}$$

in which the κ_i, μ_i are integers, positive, negative or zero. This is so because convolution with L as in (18) (taken over all space) simply adds vectors $\kappa_1 \mathbf{u}_1 + \dots + \kappa_m \mathbf{u}_m$ for every set of integers κ_i to each vector \mathbf{y}_1 of $\widehat{C_1 \widehat{C_1}}$. Hence, since from (9)

$$\begin{aligned} \widehat{C_1^* \widehat{C_1^*}} &= \mathbf{T}(\widehat{C_1 \widehat{C_1}}) - \mathbf{c} \\ \widehat{C_2^* \widehat{C_2^*}} &= \mathbf{T}(\widehat{C_2 \widehat{C_2}}) - \mathbf{c} \end{aligned}$$

these two sets differ by at least one pair of vectors $\mathbf{A}\mathbf{y}_1$ and $\mathbf{A}\mathbf{y}_2$ (where as usual \mathbf{A} is the matrix of \mathbf{T}): and the difference between these is

$$\mathbf{A}(\mathbf{y}_1 - \mathbf{y}_2) = \mathbf{A}(\nu_1 \mathbf{u}_1 + \dots + \nu_m \mathbf{u}_m)$$

for some set of integers ν_i . This is true for any \mathbf{x}, \mathbf{y}_1 , and \mathbf{y}_2 : hence,

$$\widehat{C_1^* \widehat{C_1^*}} L^* = \widehat{C_2^* \widehat{C_2^*}} L^*.$$

We therefore have the theorem:

THEOREM 15. If \mathbf{T} exists for the periodic sets S_1 and S_2 , then

† If \mathbf{T} is of rank 1 projecting onto a visible direction \mathbf{n} with a visible point $\lambda_1 \mathbf{n}$, L^* is a set of δ -functions of weight 1 at points $\nu \lambda_1 \mathbf{n}$ for all integers ν .

$$\widehat{S_1 \widehat{S_1}} = \widehat{S_2 \widehat{S_2}} \rightarrow S_1^* \widehat{S_1^*} = S_2^* \widehat{S_2^*}.$$

As an example of the considerations of this section consider the 2-dimensional 5 point periodic h.p.

$$\begin{aligned} &((0, 0), (\frac{1}{4}, \frac{3}{4} + b), (\frac{1}{2}, b), (\frac{1}{2}, \frac{1}{2}), (\frac{3}{4}, \frac{3}{4} + b); \\ &\quad z_0, z_3, z_2, z_0, z_1) \\ &((0, 0), (\frac{1}{4}, \frac{1}{4} + b), (\frac{1}{2}, b), (\frac{1}{2}, \frac{1}{2}), (\frac{3}{4}, \frac{1}{4} + b); \\ &\quad z_0, z_1, z_2, z_0, z_3) \end{aligned} \quad (20)$$

projected onto the line $y = x$. Here $p = q = 1$ and the required matrix is

$$\mathbf{C} = \sqrt{(2)} \mathbf{B}$$

where \mathbf{B} is defined in (3). The c.p. has volume 2 and contains two unit cells. Under \mathbf{B} the projected pair is not

$$\begin{aligned} S_1^* &\equiv ((0, 0), (\frac{1}{2} + b, \frac{1}{2} + b), (\frac{1}{4} + b, \frac{1}{4} + b), (\frac{1}{2}, \frac{1}{2}), \\ &\quad (\frac{3}{4} + b, \frac{3}{4} + b); z_0, z_3, z_2, z_0, z_1) \\ S_2^* &\equiv ((0, 0), (\frac{1}{4} + b, \frac{1}{4} + b), (\frac{1}{2}, \frac{1}{2}), (\frac{1}{2} + b, \frac{1}{2} + b); \\ &\quad z_0, z_1 + z_2, z_0, z_3) \end{aligned}$$

repeating every (1, 1) for in this case $\widehat{S_1^* \widehat{S_1^*}} \neq \widehat{S_2^* \widehat{S_2^*}}$: instead it is the superposition of two such pairs with origins separated by $(\frac{1}{2}, \frac{1}{2})$

$$\begin{aligned} S_1^* &\equiv S_2^* \equiv ((0, 0), (b, b), (\frac{1}{4} + b, \frac{1}{4} + b), (\frac{1}{2}, \frac{1}{2}), \\ &\quad (\frac{1}{2} + b, \frac{1}{2} + b), (\frac{3}{4} + b, \frac{3}{4} + b); \\ &\quad 2z_0, z_3, z_1 + z_2, 2z_0, z_3, z_1 + z_2) \end{aligned}$$

for which $\widehat{S_1^* \widehat{S_1^*}} = \widehat{S_2^* \widehat{S_2^*}}$ of necessity. These 1-dimensional sets revert to 2-dimensional ones when put into a square lattice with constants $(0, \frac{1}{2}), (\frac{1}{2}, 0)$.

As a second example consider the 20-point quadruplet

$$\begin{aligned} S_1 &= ((0, 0), (a, 0), (0, b), (a, b), (\frac{1}{6} + a, 0), (\frac{1}{6} + a, b), \\ &\quad (0, \frac{1}{4} + b), (a, \frac{1}{4} + b), (\frac{1}{6} + a, \frac{1}{4} + b), (\frac{1}{3}, 0), (\frac{1}{3}, b), \\ &\quad (0, \frac{1}{2}), (a, \frac{1}{2}), (\frac{1}{6} + a, \frac{1}{2}), (\frac{1}{3}, \frac{1}{4} + b), (\frac{2}{3}, \frac{1}{4} + b), \\ &\quad (\frac{2}{3}, 0), (\frac{2}{3}, b), (\frac{1}{3}, \frac{1}{2}), (\frac{2}{3}, \frac{1}{2}); 1, 1, \dots, 1) \\ S_2 &= ((0, 0), (a, 0), (0, b), (a, b), (\frac{1}{6} + a, 0), (\frac{1}{6} + a, b), \\ &\quad (0, \frac{3}{4} + b), (a, \frac{3}{4} + b), (\frac{1}{6} + a, \frac{3}{4} + b), (\frac{1}{3}, 0), (\frac{1}{3}, b), \\ &\quad (0, \frac{1}{2}), (a, \frac{1}{2}), (\frac{1}{6} + a, \frac{1}{2}), (\frac{1}{3}, \frac{3}{4} + b), (\frac{2}{3}, \frac{3}{4} + b), \\ &\quad (\frac{2}{3}, 0), (\frac{2}{3}, b), (\frac{1}{3}, \frac{1}{2}), (\frac{2}{3}, \frac{1}{2}); 1, 1, \dots, 1) \\ S_3 &= ((0, 0), (a, 0), (0, b), (a, b), (\frac{5}{6} + a, 0), (\frac{5}{6} + a, b), \\ &\quad (0, \frac{1}{4} + b), (a, \frac{1}{4} + b), (\frac{5}{6} + a, \frac{1}{4} + b), (\frac{1}{3}, 0), (\frac{1}{3}, b), \\ &\quad (0, \frac{1}{2}), (a, \frac{1}{2}), (\frac{5}{6} + a, \frac{1}{2}), (\frac{1}{3}, \frac{1}{4} + b), (\frac{2}{3}, \frac{1}{4} + b), \\ &\quad (\frac{2}{3}, 0), (\frac{2}{3}, b), (\frac{1}{3}, \frac{1}{2}), (\frac{2}{3}, \frac{1}{2}); 1, 1, \dots, 1) \\ S_4 &= ((0, 0), (a, 0), (0, b), (a, b), (\frac{5}{6} + a, 0), (\frac{5}{6} + a, b), \\ &\quad (0, \frac{3}{4} + b), (a, \frac{3}{4} + b), (\frac{5}{6} + a, \frac{3}{4} + b), (\frac{1}{3}, 0), (\frac{1}{3}, b), \\ &\quad (0, \frac{1}{2}), (a, \frac{1}{2}), (\frac{5}{6} + a, \frac{1}{2}), (\frac{1}{3}, \frac{3}{4} + b), (\frac{2}{3}, \frac{3}{4} + b), \\ &\quad (\frac{2}{3}, 0), (\frac{2}{3}, b), (\frac{1}{3}, \frac{1}{2}), (\frac{2}{3}, \frac{1}{2}); 1, 1, \dots, 1); \end{aligned} \quad (21)$$

S_1) — (S_2) — (S_3) — (S_4) — (transitive). When c.p.s of volume 2 containing these points are projected

onto $y=x$ by **B** of (3) they form essentially new h.s. In 1-dimensional form repeating at intervals of one half these are

$$\begin{aligned}
 S_1^* &= (0, a, b, a+b, \frac{1}{12}+a, \frac{1}{12}+a+b, \frac{1}{8}+b, \frac{1}{8}+a+b, \\
 &\quad \frac{5}{24}+a+b, \frac{1}{6}, \frac{1}{6}+b, \frac{1}{4}, \frac{1}{4}+a, \frac{1}{3}+a, \frac{7}{24}+b, \frac{11}{24}+b, \\
 &\quad \frac{1}{3}, \frac{5}{12}, \frac{1}{3}+b, \frac{1}{12}; 1, 1, \dots, 1) \\
 S_2^* &= (0, a, b, a+b, \frac{1}{12}+a, \frac{1}{12}+a+b, \frac{3}{8}+b, \frac{3}{8}+a+b, \\
 &\quad \frac{11}{24}+a+b, \frac{1}{6}, \frac{1}{6}+b, \frac{1}{4}, \frac{1}{4}+a, \frac{1}{3}+a, \frac{1}{24}+b, \frac{5}{24}+b, \\
 &\quad \frac{1}{3}, \frac{5}{12}, \frac{1}{3}+b, \frac{1}{12}; 1, 1, \dots, 1) \\
 S_3^* &= (0, a, b, a+b, \frac{5}{12}+a, \frac{5}{12}+a+b, \frac{1}{8}+b, \frac{1}{8}+a+b, \\
 &\quad \frac{1}{24}+a+b, \frac{1}{6}, \frac{1}{6}+b, \frac{1}{4}, \frac{1}{4}+a, \frac{1}{6}+a, \frac{7}{24}+b, \frac{11}{24}+b, \\
 &\quad \frac{1}{3}, \frac{5}{12}, \frac{1}{3}+b, \frac{1}{12}; 1, 1, \dots, 1) \\
 S_4^* &= (0, a, b, a+b, \frac{5}{12}+a, \frac{5}{12}+a+b, \frac{3}{8}+b, \frac{3}{8}+a+b, \\
 &\quad \frac{7}{24}+a+b, \frac{1}{6}, \frac{1}{6}+b, \frac{1}{4}, \frac{1}{4}+a, \frac{1}{6}+a, \frac{1}{24}+b, \frac{5}{24}+b, \\
 &\quad \frac{1}{3}, \frac{5}{12}, \frac{1}{3}+b, \frac{1}{12}; 1, 1, \dots, 1); \tag{22}
 \end{aligned}$$

S_1^* —(S_2^*)—(S_3^*)—(S_4^*)—(transitive) and (21) continues as a quadruplet in projection. But it does not always follow that if S_1, \dots, S_r constitute a multiplet of order r , *i.e.* form an r -tuple, that S_1^*, \dots, S_r^* constitute a multiplet of the same order. The construction of sets of the type of (21) will be considered in part III of this series. Certain of them have the property considered in I of being homometric with other sets which can be obtained from them by non-singular affine transformations. In particular S_1)—(S_1' where $S_1' = \mathbf{T}S_1$ and \mathbf{T} has matrix

$$\mathbf{A} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

when

$$\begin{aligned}
 S_1 &\equiv ((0, 0), (a, 0), (0, a), (\frac{1}{4}+a, 0), (0, \frac{3}{4}+a), (\frac{1}{2}, 0), \\
 &\quad (0, \frac{1}{2}), (a, a), (a, \frac{3}{4}+a), (\frac{1}{4}+a, a), (\frac{1}{4}+a, \frac{3}{4}+a), \\
 &\quad (\frac{1}{2}, a), (a, \frac{1}{2}), (\frac{1}{4}+a, \frac{1}{2}), (\frac{1}{2}, \frac{3}{4}+a), (\frac{1}{2}, \frac{1}{2}); 1, 1, \dots, 1) \\
 S_1' &\equiv ((0, 0), (a, 0), (0, a), (0, \frac{1}{4}+a), (\frac{3}{4}+a, 0), (\frac{1}{2}, 0), \\
 &\quad (0, \frac{1}{2}), (a, a), (\frac{3}{4}+a, a), (a, \frac{1}{4}+a), (\frac{3}{4}+a, \frac{1}{4}+a), \\
 &\quad (\frac{1}{2}, a), (a, \frac{1}{2}), (\frac{1}{2}, \frac{1}{4}+a), (\frac{3}{4}+a, \frac{1}{2}), (\frac{1}{2}, \frac{1}{2}); 1, 1, \dots, 1).
 \end{aligned}$$

Since

$$\mathbf{BA} = \mathbf{B},$$

$S_1^* = S_1'^*$. It is possible to construct more elaborate examples in which multiplets of order r greater than two are similarly reduced to multiplets of order two and greater but still less than r . It is also possible to offer many other examples of h.s. S with essentially new projections S^* .

5. Some generating sets of Π_4

The many-one correspondence between S_1)—(S_2 and S_1^*)—(S_2^* can be illustrated by the many sets which under singular transformation reduce to Π_4 of I(8) and I(i). It is first necessary to make explicitly a point implicit in I, Definition 4 where distinct h.s. are defined.

It is known from an extension of the results of I that the 1-dimensional pairs

$$\left\{ \begin{aligned} &(0, a, c, \frac{1}{4}+a, \frac{1}{2}, \frac{1}{2}+c; z_0, z_1, z_2, z_1, z_0, z_2) \\ &(0, a, c, \frac{3}{4}+a, \frac{1}{2}, \frac{1}{2}+c; z_0, z_1, z_2, z_1, z_0, z_2) \end{aligned} \right. \tag{24}$$

$$\left\{ \begin{aligned} &(0, a, c, a+c, \frac{1}{4}+a, \frac{1}{4}+a+c, \frac{1}{2}, \frac{1}{2}+c; \\ &\quad z_0, z_1, z_0z_2, z_1z_2, z_3, z_2z_3, z_0, z_0z_2) \\ &(0, a, c, a+c, \frac{3}{4}+a, \frac{3}{4}+a+c, \frac{1}{2}, \frac{1}{2}+c; \\ &\quad z_0, z_1, z_0z_2, z_1z_2, z_3, z_2z_3, z_0, z_0z_2) \end{aligned} \right. \tag{25}$$

are h.p.: it can be verified that

$$\left\{ \begin{aligned} &(0, a, a+c, \frac{1}{2}, \frac{1}{2}+a-c; z_0, z_1, z_2, z_0, z_1) \\ &(0, a-c, a, \frac{1}{2}, \frac{1}{2}+a+c; z_0, z_2, z_1, z_0, z_1) \end{aligned} \right. \tag{26}$$

is a h.p. Yet for particular choices of coordinate and weight parameters each of the pairs (24), (25) and (26) reduces to Π_4 . The h.p. Π_4 with $N=4$ is therefore a particular example of at least three pairs with $N > 4$. Indeed it is known from I that as many sets $S_r = (c_r, \frac{1}{2}+c_r; z_r, z_r)$ with arbitrary c_r and z_r can be added to each of the h.s. in the h.p. (24) as is wished; the new sets are h.s. and the new h.p. reduce to Π_4 when all c_r (and the parameter $c=c_0$ in (24)) are zero. The h.p. Π_4 with $N=4$ is therefore a particular example of an infinite number of h.p. with $N > 4$ which reduce to it when, by suitable choice of the parameters in these h.p., points are made to coalesce.

That this is a general result follows from an obvious theorem of the type proved in I:

THEOREM 16. If S_1)—(S_2 and S is any set whatsoever then $\widehat{S_1S}$ and $\widehat{S_2S}$ have the same weighted vector set.

For

$$(\widehat{S_1S})(\widehat{S_1S}) = (\widehat{S_1S_1})(\widehat{SS}) = (\widehat{S_2S_2})(\widehat{SS}).$$

Moreover, since S is arbitrary, $\widehat{S_1S}$)—($\widehat{S_2S}$ in general. Indeed if S_1)—(S_2 in one dimension and

$$S = (0, c_1, c_2, \dots, c_{N-1}; z_0, z_1, \dots, z_{N-1})$$

then

$$\widehat{S_1S})—(\widehat{S_2S}$$

for at least some set of values of the c_i not all zero, whilst if every $c_i=0$, S is a δ -function of weight $\sum_{i=0}^{N-1} z_i$ at the point 0 and

$$\widehat{S_1S} = S_1; \widehat{S_2S} = S_2; \widehat{S_1S} = S_1)—(S_2 = \widehat{S_2S}.$$

Thus every h.s. can be embedded in at least one larger h.s. of which it is a degenerate example. If the smaller h.s. is treated as an example of the larger it then follows that the only distinct h.s. contain an (enumerable) infinity of points and distinct periodic h.s. contain an infinite number of points in their

unit cell ($N = \infty$). But for crystallographic purposes† one requires, in principle at least, the separate exhibition of all particular h.s.; and although the existence of affine equivalents and parametric families of h.s. makes this impossible in practice it is implicit in I, Definition 4 that, even if the h.s. S of N points can be obtained from the h.s. S' of N' points by a suitable choice of its parameters, S is an example of S' if, and only if, $N = N'$. On the other hand given N' , S' embraces all those h.s. S with $N = N'$ which can be obtained from S' by choice of its parameters. It is not necessary that $N_1 = N_2$ in the h.p. S_1 —(S_2 : the pair S'_1)—(S'_2 embraces all h.p. S_1)—(S_2 with $N_1 = N'_1$, $N_2 = N'_2$ which can be obtained from S'_1 and S'_2 by choice of their parameters.

If \mathbf{T} is singular, points in S may coalesce in $\mathbf{T}S$. It is then trivial that S and $\mathbf{T}S$ are distinct h.s. even though when \mathbf{T} is of rank $r < m$ $\mathbf{T}S$ can still be made m -dimensional. For example, the 4-point generalization of Π_4 of I(8), namely:

$$\Pi_4 = \left\{ \begin{array}{l} (0, a, \frac{1}{4}a + \frac{1}{2}, \frac{1}{2}; z_0, z_2, z, z_0) \\ (0, a, \frac{3}{4}a + \frac{1}{2}, \frac{1}{2}; z_0, z_2, z, z_0) \end{array} \right. \quad (27)$$

which will be the h.p. signified by Π_4 in the future is trivially distinct from all 5-point h.p. from which it can be generated by projection on the y axis by the singular matrix

$$\mathbf{C} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}. \quad (28)$$

Amongst these 5-point sets are certainly

$$P_1 = \left\{ \begin{array}{l} ((0, 0), (a + c, \frac{1}{4}a + b), (a, b), (\frac{1}{2}, \frac{1}{2}), (\frac{1}{2} + a - c, \frac{1}{4}a + b); \\ z_0, z_1, z_2, z_0, z_1) \\ ((0, 0), (\frac{1}{2} + a + c, \frac{3}{4}a + b), (a, b), (\frac{1}{2}, \frac{1}{2}), (a - c, \frac{3}{4}a + b); \\ z_0, z_1, z_2, z_0, z_1) \end{array} \right.$$

$$P_2 \ddagger = \left\{ \begin{array}{l} ((0, 0), (\frac{1}{4}a + \frac{3}{4}a + b), (a, b), (\frac{1}{2}, \frac{1}{2}), (\frac{3}{4}a + \frac{3}{4}a + b); \\ z_0, z_1, z_2, z_0, z_3) \\ ((0, 0), (\frac{1}{4}a + \frac{1}{4}a + b), (a, b), (\frac{1}{2}, \frac{1}{2}), (\frac{3}{4}a + \frac{1}{4}a + b); \\ z_0, z_3, z_2, z_0, z_1) \end{array} \right.$$

$$P_3 = \left\{ \begin{array}{l} ((0, 0), (\frac{1}{2} + a, \frac{3}{4}a + b), (a, b), (0, \frac{1}{2}), (a, \frac{3}{4}a + b); \\ z_0, z_3, z_2, z_0, z_1) \\ ((0, 0), (\frac{1}{2} + a, \frac{1}{4}a + b), (a, b), (0, \frac{1}{2}), (a, \frac{1}{4}a + b); \\ z_0, z_3, z_2, z_0, z_1) \end{array} \right. \quad (29)$$

with $z = 2z_1$, or $(z_1 + z_3)$ in (27). The pair Π_4 is therefore obtainable by the same singular transformation from at least three distinct 2-dimensional h.p. and from their generalizations, in the manner of Patterson (1944), to $m > 2$ dimensions.

It must be recognized, however, that the demonstration that two h.p. are distinct can be difficult and that such distinction can be rather arbitrary. In a

† It is also mathematically inconvenient to have $N = \infty$.

‡ This pair was given by Garrido (1951) for $a = \frac{1}{2}$.

later paper it will be shown that in a rather special sense P_2 and P_3 are in fact affine equivalents. It will also be shown for example that a very surprising triplet of affine equivalents of the same type is the triplet of periodic h.p.

$$\left\{ \begin{array}{l} ((0, 0), (a, b), (\frac{1}{14}a + \frac{1}{14}a + b), (\frac{1}{7}, \frac{1}{7}), (\frac{2}{7}, \frac{2}{7}), (\frac{3}{7}, \frac{3}{7}), (\frac{4}{7}, \frac{4}{7}), \\ (\frac{5}{7}, \frac{5}{7}), (\frac{6}{7}, \frac{6}{7}); z_0, z_1, z_2, z_0, z_0, z_0, z_0, z_0) \\ ((0, 0), (a, b), (\frac{13}{14}a + \frac{13}{14}a + b), (\frac{1}{7}, \frac{1}{7}), (\frac{2}{7}, \frac{2}{7}), (\frac{3}{7}, \frac{3}{7}), (\frac{4}{7}, \frac{4}{7}), \\ (\frac{5}{7}, \frac{5}{7}), (\frac{6}{7}, \frac{6}{7}); z_0, z_1, z_2, z_0, z_0, z_0, z_0, z_0) \end{array} \right. \quad (30a)$$

and

$$\left\{ \begin{array}{l} ((0, 0), (a, b), (\frac{3}{14}a + \frac{3}{14}a + b), (\frac{1}{7}, \frac{1}{7}), (\frac{2}{7}, \frac{2}{7}), (\frac{3}{7}, \frac{3}{7}), (\frac{4}{7}, \frac{4}{7}), \\ (\frac{5}{7}, \frac{5}{7}), (\frac{6}{7}, \frac{6}{7}); z_0, z_1, z_2, z_0, z_0, z_0, z_0, z_0) \\ ((0, 0), (a, b), (\frac{11}{14}a + \frac{11}{14}a + b), (\frac{1}{7}, \frac{1}{7}), (\frac{2}{7}, \frac{2}{7}), (\frac{3}{7}, \frac{3}{7}), (\frac{4}{7}, \frac{4}{7}), \\ (\frac{5}{7}, \frac{5}{7}), (\frac{6}{7}, \frac{6}{7}); z_0, z_1, z_2, z_0, z_0, z_0, z_0, z_0) \end{array} \right. \quad (30b)$$

and

$$\left\{ \begin{array}{l} ((0, 0), (a, b), (\frac{5}{14}a + \frac{5}{14}a + b), (\frac{1}{7}, \frac{1}{7}), (\frac{2}{7}, \frac{2}{7}), (\frac{3}{7}, \frac{3}{7}), (\frac{4}{7}, \frac{4}{7}), \\ (\frac{5}{7}, \frac{5}{7}), (\frac{6}{7}, \frac{6}{7}); z_0, z_1, z_2, z_0, z_0, z_0, z_0, z_0) \\ ((0, 0), (a, b), (\frac{9}{14}a + \frac{9}{14}a + b), (\frac{1}{7}, \frac{1}{7}), (\frac{2}{7}, \frac{2}{7}), (\frac{3}{7}, \frac{3}{7}), (\frac{4}{7}, \frac{4}{7}), \\ (\frac{5}{7}, \frac{5}{7}), (\frac{6}{7}, \frac{6}{7}); z_0, z_1, z_2, z_0, z_0, z_0, z_0, z_0) \end{array} \right. \quad (30c)$$

These pairs are Patterson generalizations (P -generalizations) of the 1-dimensional h.p. $\Pi_9^{(1)}$, $\Pi_9^{(2)}$, and $\Pi_9^{(3)}$ of I which are certainly distinct, but it will be shown later that all the P -generalizations of the $\Pi_n^{(i)}$ (for different i) are affine equivalents if $n = p + 2$, p prime. Another example of this unexpected affine equivalence is the pair of h.p. (42) below for which $p = 5$.

As a second example of a plausible but none the less arbitrary distinction between h.p. the periodic pair

$$P_4 = \left\{ \begin{array}{l} ((0, 0), (c, \frac{3}{4}a + b), (0, b), (0, \frac{1}{2}), (1 - c, \frac{3}{4}a + b); \\ z_0, z_1, z_2, z_0, z_1) \\ ((0, 0), (c, \frac{1}{4}a + b), (0, b), (0, \frac{1}{2}), (1 - c, \frac{1}{4}a + b); \\ z_0, z_1, z_2, z_0, z_1) \end{array} \right. \quad (31)$$

becomes Π_4 under the matrix (28), but it is in fact a degenerate example of the P -generalization of the 1-dimensional periodic pair

$$\left\{ \begin{array}{l} (0, a, \frac{1}{4}a + a - c, \frac{3}{4}a + a + c; z_0, z_2, z_0, z_1, z_1) \\ (0, a, \frac{1}{4}a + a - c, \frac{1}{4}a + a + c, \frac{1}{2}; z_0, z_2, z_1, z_1, z_0) \end{array} \right. \quad (32)$$

taken along $x = 0$ (and which is an affine equivalent of the more obvious generalization along $y = x$) with the x parameter a and the y parameter c both zero. The h.p. (32) is the h.p. (26) with c replaced by $\frac{1}{4}a + c$, and the h.p. P_1 is the P -generalization of (26) along $y = x$ with the y parameter $c = \frac{1}{4}a$. P_1 and P_4 are therefore examples of the same pair.

Within the terms of the problem as set, namely that pairs P and P' are to be in some way distinct and satisfy $\mathbf{T}P = \mathbf{T}P' = \Pi_4$ (with an obvious notation),

P_4 and P_1 may still be considered distinct. The same may be said *a fortiori* of P_1 and P_2 for P_1 contains 3 weight- and 3 coordinate-parameters, whereas P_2 contains 4 weight- and 2 coordinate-parameters. In particular, there exists no more general pair P which embraces by choice of parameters both P_1 and P_2 and satisfies $\mathbf{TP} = \mathbf{II}_4$ if \mathbf{T} has matrix (28). This we now prove.

We remark that P_1 is a 5-point h.p. which under

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

is the 5-point h.p. (26). The latter is a h.p. even when $z_0 = z_1 = z_2 = 1$ and if it is in its most general form its coordinate parameters are still most general in this case. But it can be shown by direct calculation that if the coordinates are as in (26) then the most general set of weights is again as in (26). Since (26) is a 5-point projection of the 5-point pair P_1 , P_1 can itself contain at most 3 weight parameters and must be distinct (at least when $\mathbf{TP} = \mathbf{II}_4$ is to be satisfied) from P_2 which contains 4.

We show now that the h.p.

$$\left\{ \begin{array}{l} (0, a, a+c, \frac{1}{2}, \frac{1}{2}+a-c; 1, 1, 1, 1, 1) \\ (0, a-c, a, \frac{1}{2}, \frac{1}{2}+a+c; 1, 1, 1, 1, 1) \end{array} \right. \quad (33)$$

has its most general set of coordinate parameters. If $a > c > 0$, $a+c < \frac{1}{2}$, the coordinates in (33) are in order of increasing magnitude. The two sets of separations between adjacent points are

$$\begin{aligned} (a, c, \frac{1}{2}-a-c, a-c, \frac{1}{2}-a+c) &= (u_1, u_2, u_3, u_4, u_5) \\ (a-c, c, \frac{1}{2}-a, a+c, \frac{1}{2}-a-c) &= (u'_1, u'_2, u'_3, u'_4, u'_5) \end{aligned} \quad (34)$$

with $u_1 = a, u_2 = c$, etc. The 10 separations u_i, u'_i satisfy

$$\left. \begin{aligned} \sum_{i=1}^5 u_i &= \sum_{i=1}^5 u'_i = 1 & (\alpha) \\ u_1 &= u'_1 + u'_2; u'_3 = u_2 + u_3 & (\beta) \\ u_5 &= u'_2 + u'_3; u'_4 = u_1 + u_2 & (\gamma) \\ u_1 + u_5 &= u'_3 + u'_4 & (\gamma) \\ u_2 \text{ or } u_3 \text{ or } u_4 &= u' \text{ or } u'_2 \text{ or } u'_5 & (\delta) \end{aligned} \right\} \quad (35)$$

Equations (35) contain 10 relations between the 10 unknowns u_i and u'_i of which 2 are redundant. For $(\delta) \rightarrow u_2 = u'_1$ or u'_2 or u'_5 and $u_3 = (u'_2$ or $u'_5)$ or $(u'_5$ or $u'_1)$ or $(u'_1$ or $u'_2)$ which determines u_4 as the remaining u'_i . Then (γ) and (δ) imply one relation of (α) . Also from (β) and (α)

$$u_1 + u_2 = u'_4 \rightarrow u_3 + u_4 + u_5 = u'_1 + u'_2 + u'_3 + u'_5,$$

whilst from (γ) and (α)

$$u_2 + u_3 + u_4 = u'_1 + u'_2 + u'_5$$

or

$$u_5 - u_2 = u'_3,$$

and from $u_5 = u'_2 + u'_3$ in (β)

$$u_2 = u'_2,$$

which is one possible relation of (δ) . Hence (if (α) is two relations) (δ) is the one relation with two alternatives

$$u_3 = u'_1 \text{ or } u'_5.$$

The most general pair of sets satisfying the eight independent relations (35) therefore contains two arbitrary coordinate parameters.

Indeed (34) is a solution of (35): putting $u_1 = a, u_2 = u'_2 = c$, we find that if $u_3 = u'_1$ the u_i and u'_i are

$$\begin{aligned} u_i &: a, c, a-c, 1-3a-c, a+c \\ u'_i &: a-c, c, a, a+c, 1-3a-c \end{aligned}$$

which is an enantiomorphic pair; if $u_3 = u'_5$ we obtain (34), which is the set of separations between adjacent points of the h.p. (33). But they are also in a form which is quite general to all 5-point, equal weight, 1-dimensional h.p. It is hoped to show in a later paper that, in such pairs, at least two u_i are identical with two u'_i . Also there must be (α) , one relation like (γ) and at least four relations like (β) : in this case there is also one relation like (δ) . Alternatively there can be six relations like (β) , one like (γ) and none like (δ) . Thus 5-point, equal weight, 1-dimensional pairs contain at most two coordinate parameters. It follows that the coordinates (33) are in their most general form and that P_1 contains at most three weight-parameters.

The major conclusion — that the correspondence of S to S^* is many-one — is fairly obvious however. For at least the following become \mathbf{II}_4 under \mathbf{C} of (28): the 5-point pairs P_1, P_2, P_3, P_4 ; the 4-point P -generalization of \mathbf{II}_4

$$P_5 = \left\{ \begin{array}{l} ((0, 0), (a, b), (a, \frac{1}{4}+b), (0, \frac{1}{2}); z_0, z_1, z, z_0) \\ ((0, 0), (a, b), (a, \frac{3}{4}+b), (0, \frac{1}{2}); z_0, z_1, z, z_0) \end{array} \right. \quad (36)$$

and some of its affine equivalents; a related 4-point pair

$$P_6 = \left\{ \begin{array}{l} ((0, 0), (a, b), (\frac{1}{2}+a, \frac{1}{4}+b), (0, \frac{1}{2}); z_0, z_1, z, z_0) \\ ((0, 0), (a, b), (\frac{1}{2}+a, \frac{3}{4}+b), (0, \frac{1}{2}); z_0, z_1, z, z_0) \end{array} \right. \quad (37)$$

the P -generalization to two dimensions of (25)

$$P_7 = \left\{ \begin{array}{l} ((0, 0), (a, b), (c, d), (a+c, b+d), (\frac{1}{4}+a, \frac{1}{4}+b), \\ (\frac{1}{4}+a+c, \frac{1}{4}+b+d), (\frac{1}{2}, \frac{1}{2}), (\frac{1}{2}+c, \frac{1}{2}+d); \\ z_0, z_1, z_0z_2, z_1z_2, z_3, z_2z_3, z_0, z_0z_2) \\ ((0, 0), (a, b), (c, d), (a+c, b+d), (\frac{3}{4}+a, \frac{3}{4}+b), \\ (\frac{3}{4}+a+c, \frac{3}{4}+b+d), (\frac{1}{2}, \frac{1}{2}), (\frac{1}{2}+c, \frac{1}{2}+d); \\ z_0, z_1, z_0z_2, z_1z_2, z_3, z_2z_3, z_0, z_0z_2) \end{array} \right. \quad (38)$$

with $d=0$; the 2-dimensional P -generalizations of the infinity of distinct pairs which can be obtained from (24) by the addition of sets S_r when $d_r=0$ (where d_r is the y parameter corresponding to c_r or c in (24)), e.g.

$$P_8 = \begin{cases} (0, 0), (a, b), (c, d), (\frac{1}{4}+a, \frac{1}{4}+b), (\frac{1}{2}, \frac{1}{2}), \\ (\frac{1}{2}+c, \frac{1}{2}+d); z_0, z, z_1, z, z_0, z_1 \\ (0, 0), (a, b), (c, d), (\frac{3}{4}+a, \frac{3}{4}+b), (\frac{1}{2}, \frac{1}{2}), \\ (\frac{1}{2}+c, \frac{1}{2}+d); z_0, z, z_1, z, z_0, z_1 \end{cases} \quad (39)$$

with $d=0$; the examples (i) and (ii) below

Example (i): A 2-dimensional h.p. related to $\Pi_{22}^{(1)}$ defined in I, namely

$$P_9 = \begin{cases} ((0, 0), (a, b), \frac{1}{40}+a, \frac{1}{4}+b), (\frac{1}{20}, \frac{1}{2}), (\frac{2}{20}, 0), \\ (\frac{3}{20}, \frac{1}{2}), \dots, (\frac{19}{20}, \frac{1}{2}); z_0, z_1, z_2, z_0, \dots, z_0 \\ (0, 0), (a, b), (\frac{39}{40}+a, \frac{3}{4}+b), (\frac{1}{20}, \frac{1}{2}), (\frac{2}{20}, 0), \\ (\frac{3}{20}, \frac{1}{2}), \dots, (\frac{19}{20}, \frac{1}{2}); z_0, z_1, z_2, z_0, \dots, z_0 \end{cases} \quad (40)$$

There appears to be an example of this type for every analogous 2-dimensional relative of $\Pi_{n+2}^{(1)}$ provided n has a factor 4. This is another example of an enumerable infinity of distinct 2-dimensional h.p. which project to Π_4

Example (ii): Two sets of the form

$$\left\{ \begin{array}{l} S_1 \equiv ((a_1^{(0)}, 0), (a_2^{(0)}, 0), \dots, (a_r^{(0)}, 0), \\ (a_1^{(1)}, a), (a_2^{(1)}, a), \dots, (a_s^{(1)}, a), \\ (a_1^{(2)}, \frac{1}{4}+a), (a_2^{(2)}, \frac{1}{4}+a), \dots, (a_t^{(2)}, \frac{1}{4}+a), \\ (a_1^{(3)}, \frac{1}{2}), (a_2^{(3)}, \frac{1}{2}), \dots, (a_u^{(3)}, \frac{1}{2}); z_i^{(0)}; z_i^{(1)}; z_i^{(2)}; z_i^{(3)} \\ S_2 \equiv ((b_1^{(0)}, 0), (b_2^{(0)}, 0), \dots, (b_r^{(0)}, 0), \\ (b_1^{(1)}, a), (b_2^{(1)}, a), \dots, (b_s^{(1)}, a), \\ (b_1^{(2)}, \frac{3}{4}+a), (b_2^{(2)}, \frac{3}{4}+a), \dots, (b_t^{(2)}, \frac{3}{4}+a), \\ (b_1^{(3)}, \frac{1}{2}), (b_2^{(3)}, \frac{1}{2}), \dots, (b_u^{(3)}, \frac{1}{2}); z_i^{(0)}; z_i^{(1)}; z_i^{(2)}; z_i^{(3)} \end{array} \right. \quad (41)$$

become Π_4 when projected onto the y axis for any values of the $a_i^{(j)}$ and $b_i^{(j)}$ whatsoever, provided only that

$$\sum_{i=1}^r z_i^{(0)} = \sum_{i=1}^{r'} z_i^{(0')} = \sum_{i=1}^u z_i^{(3)} = \sum_{i=1}^{u'} z_i^{(3)'},$$

$$\sum_{i=1}^s z_i^{(1)} = \sum_{i=1}^{s'} z_i^{(1)'}; \quad \sum_{i=1}^t z_i^{(2)} = \sum_{i=1}^{t'} z_i^{(2)'}$$

In this example $S_1 \not\subset S_2$, S_1 and S_2 are not h.s. (in general), yet $S_1^* \equiv S_2^*$: an infinity of distinct non-homometric, 2-dimensional sets projects into Π_4 . Clearly a family of non-homometric sets of this type exists for every 1-dimensional h.p. and indeed for every r -dimensional h.p.

The examples of this section and the arguments of this paper suggest the

DEFINITION 5. If \mathbf{T} is singular (and $S^* = \mathbf{T}S$ exists), S and S^* are distinct unless S^* can be obtained from (an affine equivalent of) S by a particular choice of coordinate parameters. S and S^* are always distinct if they contain a different number of points.

6. A group property of h.s. obtained by singular transformations

Under a singular transformation with matrix

$$\mathbf{C} = (\sqrt{29})^2 \begin{bmatrix} \frac{25}{29} & \frac{10}{29} \\ \frac{10}{29} & \frac{4}{29} \end{bmatrix} = \begin{bmatrix} 25 & 10 \\ 10 & 4 \end{bmatrix}$$

a c.p. containing 29 lattice unit cells of the P -generalization of $\Pi_7^{(1)}$

$$S_1 \equiv ((0, 0), (a, b), (\frac{1}{10}+a, \frac{1}{10}+b), (\frac{1}{5}, \frac{1}{5}), (\frac{2}{5}, \frac{2}{5}), (\frac{3}{5}, \frac{3}{5}), (\frac{4}{5}, \frac{4}{5}); z_0, z_1, z_2, z_0, z_0, z_0, z_0)$$

$$S_2 \equiv ((0, 0), (a, b), (\frac{9}{10}+a, \frac{9}{10}+b), (\frac{1}{5}, \frac{1}{5}), (\frac{2}{5}, \frac{2}{5}), (\frac{3}{5}, \frac{3}{5}), (\frac{4}{5}, \frac{4}{5}); z_0, z_1, z_2, z_0, z_0, z_0, z_0) \quad (42a)$$

is projected onto the line $5y=2x$ as the h.p.

$$\left\{ \begin{array}{l} ((0, 0), (5c, 2c), (\frac{7}{5}+5c, \frac{7}{5}+2c), (2, \frac{4}{5}), (4, \frac{8}{5}), (1, \frac{2}{5}), \\ (3, \frac{6}{5}); z_0, z_1, z_2, z_0, z_0, z_0, z_0 \\ ((0, 0), (5c, 2c), (\frac{3}{5}+5c, \frac{3}{5}+2c), (2, \frac{4}{5}), (4, \frac{8}{5}), (1, \frac{2}{5}), \\ (3, \frac{6}{5}); z_0, z_1, z_2, z_0, z_0, z_0, z_0 \end{array} \right.$$

repeating periodically every $(5, 2)$. In a rectangular lattice with constants 5, 2 this is an affine equivalent of the P -generalization of $\Pi_7^{(2)}$

$$S_3 \equiv ((0, 0), (a, b), (\frac{7}{10}+a, \frac{7}{10}+b), (\frac{1}{5}, \frac{1}{5}), (\frac{2}{5}, \frac{2}{5}), (\frac{3}{5}, \frac{3}{5}), (\frac{4}{5}, \frac{4}{5}); z_0, z_1, z_2, z_0, z_0, z_0, z_0)$$

$$S_4 \equiv ((0, 0), (a, b), (\frac{3}{10}+a, \frac{3}{10}+b), (\frac{1}{5}, \frac{1}{5}), (\frac{2}{5}, \frac{2}{5}), (\frac{3}{5}, \frac{3}{5}), (\frac{4}{5}, \frac{4}{5}); z_0, z_1, z_2, z_0, z_0, z_0, z_0) \quad (42b)$$

with $a=b$ from which it can be obtained under the matrix

$$\begin{bmatrix} 5 & 0 \\ 0 & 2 \end{bmatrix}.$$

Now $\mathbf{C}S_3$ is an example of S_2 , $\mathbf{C}S_2$ is an example of S_4 . Hence if \mathbf{O} is the operation: singular transformation by \mathbf{C} followed by P -generalization to a 2-dimensional rectangular lattice and if \mathbf{O}^2 is \mathbf{O} applied twice, then

$$S_1) - (\mathbf{O}^2 S_1; \mathbf{O} S_1) - (\mathbf{O}^3 S_1; \mathbf{O}^4 S_1 \equiv S_1$$

In this way from the single h.s. S_1 are obtained all four h.s. S_1, S_2, S_3 and S_4 by singular transformation. It will become apparent from later work that, if $\Pi_n^{(1)}$ is P -generalized to $r > 1$ dimensions and $n = p + 2$, p prime, it is possible to obtain all $\Pi_n^{(i)}$ (for different i) by singular transformation followed by P -generalization. The $\Pi_n^{(i)}$ are certainly distinct in one dimension so that this is an example of new h.p. obtained by singular transformations: but from another point of view of course it raises the question of distinction between h.p. It is plain that a cyclic group of order 4 represented by the operations $\mathbf{O}, \mathbf{O}^2, \mathbf{O}^3, \mathbf{O}^4$ is associated with the $2\Pi_7^{(1)}$. It appears that a group of order $n-3 = p-1$, if p is an odd prime, is associated with the $\frac{1}{2}(p-1)\Pi_n^{(1)}$. A better representation of this group is afforded by transformations with non-

singular matrices \mathbf{A} , however, and it is hoped to take this up in a later paper.

APPENDIX

(i) In § 2 we appeal to an extension of the theorem (cf. e.g. Birkhoff & MacLane, 1953) that if \mathbf{A} is real and non-singular with transpose \mathbf{A}' , then

$$\mathbf{A} = \mathbf{C}\mathbf{O},$$

where $\mathbf{C} = (\mathbf{A}\mathbf{A}')^{\frac{1}{2}}$ is real symmetric and $\mathbf{O} = \mathbf{C}^{-1}\mathbf{A}$ is real orthogonal: we extend the theorem to singular \mathbf{A} (and hence singular \mathbf{C}).

We define for singular \mathbf{A}

$$\mathbf{B} = \mathbf{A} + \varepsilon\mathbf{U}, \quad 0 < \varepsilon < \varepsilon_1$$

with for convenience $\det \mathbf{U} \neq 0$, and ε_1 the smallest positive root of

$$\det(\mathbf{A} + \varepsilon\mathbf{U}) = 0.$$

Then

$$\lim_{\varepsilon \rightarrow 0} \mathbf{B} = \mathbf{A}.$$

Since \mathbf{B} is non-singular

$$\mathbf{B} = \mathbf{C}\mathbf{O}; \quad \mathbf{C}^2 = \mathbf{B}\mathbf{B}'; \quad \mathbf{O}\mathbf{O}' = \mathbf{I}.$$

We can then prove

$$\mathbf{Q} = \lim_{\varepsilon \rightarrow 0} \mathbf{O}; \quad \mathbf{D} = \lim_{\varepsilon \rightarrow 0} (\mathbf{B}\mathbf{B}')^{\frac{1}{2}} = (\mathbf{A}\mathbf{A}')^{\frac{1}{2}}$$

exist and that

$$\mathbf{A} = \mathbf{D}\mathbf{Q}; \quad \mathbf{Q}\mathbf{Q}' = \mathbf{I}; \quad \mathbf{D} = \mathbf{D}'.$$

Then we have

$$\mathbf{A} = (\mathbf{A}\mathbf{A}')^{\frac{1}{2}}\mathbf{O}$$

with $\mathbf{C} = (\mathbf{A}\mathbf{A}')^{\frac{1}{2}}$ symmetric and \mathbf{O} (non-singular) orthogonal whether \mathbf{A} is singular or not.

If $\mathbf{O}\mathbf{O}' = \mathbf{I}$, $\det \mathbf{O} \neq 0$ and

$$S_1) - (S_2 \rightarrow \mathbf{O}S_1) - (\mathbf{O}S_2 \text{ (by I, Lemma 1)}).$$

Since \mathbf{C} is symmetric there exists (Birkhoff & MacLane, 1953) a real orthogonal matrix \mathbf{P} such that

$$\mathbf{P}\mathbf{C}\mathbf{P}^{-1} = \text{diag}(c_1, \dots, c_m).$$

Since $\det \mathbf{P} \neq 0$, by I, Lemma 1

$$S_1) - (S_2 \leftrightarrow \mathbf{P}S_1) - (\mathbf{P}S_2; \mathbf{P}^{-1}S_1) - (\mathbf{P}^{-1}S_2 \leftrightarrow S_1) - (S_2).$$

Hence we need only consider singular transformations of h.p. under diagonal matrices as stated in the text.

Perhaps a simpler argument is to appeal to the theorem (Aitken, 1956) that every real m -dimensional matrix of rank r is 'equivalent' to

$$\mathbf{I}_r^{(m)} = \begin{bmatrix} \mathbf{I}_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

where \mathbf{I}_r is the r -dimensional unit matrix: then the

only matrices we need consider are diagonal with diagonal elements 0 or 1. (We can also use this theorem instead of choosing the basis of \mathbf{x} in (ii) following when S is an arbitrary set.)

(ii) Implicit in the argument of (i) (and indeed in the whole context of parts I and II) is the following lemma:

LEMMA. If $S(\mathbf{x})$ is a point set in the sense of (8) above, and $\mathbf{T}, \mathbf{T}_1, \mathbf{T}_2$ are affine transformations such that for any vector \mathbf{x}

$$\mathbf{T}_1\mathbf{x} = \mathbf{A}_1\mathbf{x} + \mathbf{c}_1; \quad \mathbf{T}_2\mathbf{x} = \mathbf{A}_2\mathbf{x} + \mathbf{c}_2$$

$$\mathbf{T}\mathbf{x} = \mathbf{A}\mathbf{x} + \mathbf{c} = \mathbf{A}_2\mathbf{A}_1\mathbf{x} + \mathbf{A}_2\mathbf{c}_1 + \mathbf{c}_2 = \mathbf{T}_2\mathbf{T}_1\mathbf{x},$$

then

$$\mathbf{T}S(\mathbf{x}) = \mathbf{T}_2(\mathbf{T}_1S(\mathbf{x})).$$

If \mathbf{A}_1 and \mathbf{A}_2 are non-singular, and $\mathbf{T}S$ is interpreted in the sense of (6) above

$$\begin{aligned} \mathbf{T}_2(\mathbf{T}_1S(\mathbf{x})) &= \mathbf{T}_2(|\det \mathbf{A}_1|^{-1}S(\mathbf{T}_1^{-1}\mathbf{x})) \\ &= |\det \mathbf{A}_1\mathbf{A}_2|^{-1}S(\mathbf{T}_1^{-1}\mathbf{T}_2^{-1}\mathbf{x}) = \mathbf{T}S(\mathbf{x}). \end{aligned}$$

The lemma is indeed true for any function $S(\mathbf{x})$ in this case.

If one at least of \mathbf{A}_1 and \mathbf{A}_2 (say \mathbf{A}_1) is singular then as in § 2 (between (8) and (9))

$$\begin{aligned} \mathbf{T}_1\delta(\mathbf{x} - \mathbf{x}_i) &= \delta(\mathbf{x} - \mathbf{A}_1\mathbf{x}_i - \mathbf{c}_i) = \delta(\mathbf{x} - \mathbf{T}_1\mathbf{x}_i) \\ \mathbf{T}_2\mathbf{T}_1\delta(\mathbf{x} - \mathbf{x}_i) &= \delta(\mathbf{x} - \mathbf{T}_2\mathbf{T}_1\mathbf{x}_i) = \mathbf{T}\delta(\mathbf{x} - \mathbf{x}_i); \end{aligned}$$

and when $S(\mathbf{x})$ has the form (8)

$$\mathbf{T}S(\mathbf{x}) = \mathbf{T}_2(\mathbf{T}_1S(\mathbf{x})).$$

The lemma can be extended to all integrable sets $S(\mathbf{x})$ for which the relevant integrals exist. The extension is already proved when \mathbf{T}_1 and \mathbf{T}_2 are non-singular. If \mathbf{T}_1 (and \mathbf{A}_1) is singular of rank r , choose a basis of \mathbf{x} so that \mathbf{A}_1 is completely reduced (cf. Weyl, 1931) to the 'sum' of two square matrices in r - and $(m-r)$ -dimensional complementary subspaces, $\mathbf{A}_1^{(r)}$ and $\mathbf{A}_1^{(m-r)}$: by proper choice of basis $\mathbf{A}_1^{(m-r)} = \mathbf{0}^{(m-r)}$, the $(m-r)$ -dimensional zero matrix, and $\det \mathbf{A}_1^{(r)} \neq 0$. Define

$$S^{(r)}(\mathbf{x}) = \mathbf{A}_1S(\mathbf{x}) = \left\{ \mathbf{A}_1^{(r)} \int S(\mathbf{x}) d\mathbf{x}^{(m-r)} \right\} \delta(\mathbf{x}^{(m-r)}), \quad (43)$$

where $\mathbf{x}^{(r)}$ and $\mathbf{x}^{(m-r)}$ lie in the complementary subspaces:

$$\mathbf{x} = \mathbf{x}^{(r)} + \mathbf{x}^{(m-r)}.$$

If \mathbf{A}_2 is of rank $> r$ and $\det \mathbf{A}_2^{(r)} \neq 0$, $\mathbf{A}_2\mathbf{A}_1$ is not in general simultaneously completely reduced with \mathbf{A}_1 but one can find a new basis of \mathbf{x} completely reducing $\mathbf{A}_2\mathbf{A}_1$ to an r -dimensional sub-space: $(\mathbf{A}_2\mathbf{A}_1)S(\mathbf{x})$ is then defined analogously to (43). A proof in two dimensions (omitted here) shows that in terms of the basis of (43) the set $(\mathbf{A}_2\mathbf{A}_1)S(\mathbf{x})$ is exactly the set $\mathbf{A}_2S^{(r)}(\mathbf{x})$. There seems to be no difficulty in principle in extending this proof to $m > 2$ dimensions: its truth hinges on the fact that

the definition (43) leaves $S^{(r)}(\mathbf{x})$ m -dimensional, but it is clear that the subsequent transformation of $S^{(r)}(\mathbf{x})$ under \mathbf{A}_2 requires the transformation of an $(m-r)$ -dimensional δ -function as in § 2. The equivalence of $(\mathbf{A}_1\mathbf{A}_2)S$ and $\mathbf{A}_1(\mathbf{A}_2S)$ with \mathbf{A}_1 singular should follow for the same reason.

(iii) In so far as the point sets of (8) are idealizations of a real situation in which electron density $S(\mathbf{x}) > 0$ at almost all points of space, it is natural to enquire how far the operations of convolution and affine transformation commute for general sets $S(\mathbf{x})$. If \mathbf{T} is non-singular and $S^* = \mathbf{T}S$ is defined as in (6), it is clear from the argument leading to (7) that more generally

$$\mathbf{T}(\widehat{S_1 S_2}) \equiv \widehat{S_1^* S_2^*} \quad (44)$$

for all integrable sets S_1, S_2 for which the convolution $\widehat{S_1 S_2}$ exists. The following is a proof of (44) when \mathbf{T} is singular and S_1 and S_2 are not periodic and have convergent integrals, that is have finite total weights.

By a proper choice of basis in the m -dimensional space, \mathbf{A} of rank $r < m$ is completely reduced to $\mathbf{A}^{(r)} + \mathbf{A}^{(m-r)}$, where $\mathbf{A}^{(m-r)} = \mathbf{0}^{(m-r)}$. Let now

$$g(\mathbf{x}^{(r)}) = \int S(\mathbf{x}) d\mathbf{x}^{(m-r)}.$$

Then using (43) and the interpretation (6)

$$S_1^* = |\det \mathbf{A}^{(r)}|^{-1} g_1((\mathbf{A}^{(r)})^{-1} \mathbf{x}^{(r)}) \delta(\mathbf{x}^{(m-r)}),$$

since from (8) to (9)

$$\mathbf{0}^{(m-r)} \delta(\mathbf{x}^{(m-r)}) = \delta(\mathbf{x}^{(m-r)}).$$

Then

$$\widehat{S_1^* S_2^*} = \{\mathbf{A}^{(r)} \widehat{g_1 g_2}\} \delta(\mathbf{x}^{(m-r)}).$$

Also

$$\begin{aligned} \mathbf{A} \widehat{S_1 S_2} &= \left\{ \mathbf{A}^{(r)} \int \int S_1(\mathbf{y}) S_2(\mathbf{x} - \mathbf{y}) d\mathbf{y} d\mathbf{x}^{(m-r)} \right\} \delta(\mathbf{x}^{(m-r)}) \\ &= \left\{ \mathbf{A}^{(r)} \int S_1(\mathbf{y}) \int S_2(\mathbf{x} - \mathbf{y}) d(\mathbf{x} - \mathbf{y})^{(m-r)} d\mathbf{y} \right\} \delta(\mathbf{x}^{(m-r)}) \\ &= \{\mathbf{A}^{(r)} \widehat{g_1 g_2}\} \delta(\mathbf{x}^{(m-r)}) \end{aligned}$$

which proves the theorem.

The reversal of the integrations puts certain further conditions on S_1 and S_2 ; e.g. sufficient conditions would be continuity of these functions and uniform convergence of their integrals if the range of integration is all space or all of some infinite sub-space. These conditions obtain for any real distribution of electron density.

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General spot-size correction for inclined incident beam: Weissenberg method. By KATHLEEN LONSDALE, *University College, London W.C. 1, England*

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D. C. Phillips (1954, 1956) has derived formulae giving the reflexion spot area variations observed on upper-level Weissenberg photographs. These apply only to the normal-beam and equi-inclination methods. Since the formulae involve the axial coordinate ζ which is dependent upon the wave-length, it follows that the Phillips correction cannot be applied to $K\beta$ spots if the incident beam is set in the equi-inclination position for the $K\alpha$ radiation. It is sometimes, however, very desirable to make use of the intensities of the $K\beta$ spots, for example if the $K\alpha$ are too strong, if they are just outside the

limiting sphere or if they are enhanced by the Renninger effect. It seems necessary, therefore, to give the Phillips equations for the general case.

The nomenclature used is that of section 4.3 of the *International Tables for X-ray Crystallography* (hereinafter *I.T.*) Volume II (1959), which differs from that of Phillips mainly in using φ for the angular coordinate instead of ω . The method consists in determining the reflexion-spot length \mathfrak{L} (parallel to the rotation axis) without any camera translation; and then of determining the additional $\pm \Delta \mathfrak{L}$ introduced by the movement of the