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LETTER TO THE EDITOR

Icosahedral black-and-white Bravais quasilattices and order–disorder transformations of icosahedral quasicrystals

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Abstract. It is shown that there exist only two black-and-white Bravais quasilattices ($P_F\bar{5}\bar{3}m$ and $I_P\bar{5}\bar{3}m$) with icosahedral point symmetry; the former is related to a division of the primitive icosahedral quasilattice ($P\bar{5}\bar{3}m$) into two face-centred ones ($F\bar{5}\bar{3}m$) and the latter to a division of the body-centred quasilattice ($I\bar{5}\bar{3}m$) into two primitive ones. It is shown also that an order-disorder transformation of an icosahedral quasicrystal can be a second-order transition, if the ordering is associated with either of the two sublattice divisions.

The checker lattice (CL) is composed of the black sublattice L and the white one L', both of which are square lattices with the same lattice constant. The point group of L (and L') is D_4 ($4mm$). If we disregard the 'colours' of the lattice points, the CL coincides with the third square lattice L_0 ($=L\cup L'$), whose lattice constant is $1/\sqrt{2}$ times that of L. L, L' and L_0 are sets of points in the two-dimensional (2D) Euclidean space E_2, into which they are embedded. Alternatively, we can consider these lattices as the sets of 2D vectors. If the Cartesian coordinate system of E_2 is so chosen that its origin coincides with a lattice point of L, then L and L_0 are considered to be additive groups (2D Z-modules) with two generators.

The following are three important properties of the CL.

(i) L is a Bravais lattice and L' is its translation; $L'=x_0+L$ ($=\{x_0+l\,|\,l\in L\}$) with x_0 ($\in L$) being a representative of L'.

(ii) $2x_0\in L$, so that $L_0=L\cup L'$ is also a Bravais lattice. That is, L is a subgroup of L_0 with index 2; $L+L=L$, $L+L'=L'+L=L'$ and $L'+L'=L$.

(iii) L and L_0 have a common point group G, and L', as well as L and L_0, is invariant against G.

The space group $\mathscr{g}$ of the CL is the same as that of L. That is, $\mathscr{g}=\mathrm{G}*L=\{\{\sigma|l\}\,|\,\sigma\in\mathrm{G}, l\in L\}$ with $\mathrm{G}=D_4$, where the symbol $*$ stands for a semidirect product. In fact, the CL has a larger symmetry than $\mathscr{g}$. Let I_c be the colour inversion operation, which inverts black and white. Then, $I_c\{\sigma|l\}$ with $\sigma\in\mathrm{G}$ and $l\in L'$ is also a symmetry element of the CL. It follows that the CL is invariant against the coloured space group $\mathscr{g}_c=\mathscr{g}\cup I_c\{\{\sigma|l\}\,|\,\sigma\in\mathrm{G}, l\in L\}$; $\mathscr{g}$ is a subgroup of $\mathscr{g}_c$ with index 2. The maximal Abelian subgroup of $\mathscr{g}_c$ is $L_c=L\cup I_cL'$, which can be identified with the CL. $\mathscr{g}_c$ is a semidirect product of L_c and G; $\mathscr{g}_c=G*L_c$. By these properties, the CL is called a black-and-white Bravais lattice (BWBL) (see, for example, Opechowski and Guccione 1965, Bradley and Cracknell 1972).

If two lattices L and L' in any dimensions are given, the set of the conditions (i)-(iii) above are necessary and sufficient conditions for them to give a BWBL, L_c ($=L\cup I_cL$). G is called the point group of L_c. L is a superlattice of L_0. L and L' are

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interpenetrated into each other. The roles of L and L' can be exchanged if the origin of the Cartesian coordinate system is shifted to the other sublattice. A BWBL is useful in the investigation of an order–disorder transformation or a magnetic transition (Opechowski and Guccione 1965, Tolédano and Tolédano 1987). BWBLs in 2D and 3D have been completely classified.

It has been established recently that quasicrystals are new ordered states of matter with non-crystallographic point symmetries (Steinhardt and Ostlund 1987, Janssen 1988); their structures are not periodic but quasiperiodic. The quasilattices are basic geometrical objects which provide us with mathematical bases of the structures of the quasicrystals; a quasilattice is obtained with the cut-and-projection method from a periodic lattice in higher dimensions. Therefore, it is an urgent problem to generalize various concepts in the ordinary crystallography to the case of quasilattices.

In this letter we shall generalize the black-and-white Bravais lattices. A black-and-white Bravais quasilattice (BWBQL) is defined naturally as 'coloured' quasiperiodic pattern obtained with the cut-and-projection method from a BWBL in higher dimensions. Then, enumerating BWBQLs with a given non-crystallographic point symmetry is reduced to enumerating higher-dimensional BWBLs with the same point symmetry†.

We begin with investigating a general method of constructing a d-dimensional BWBL, $L_c = L \cup I_c L'$, with a given point group G. Let x_0 be a representative of the white sublattice L'. Then $\rho x_0 \equiv x_0 \bmod L\ \forall \rho \in \mathrm{G}$ because $L' = x_0 + L$ and both L and L' are invariant against G. It follows that the point symmetry $\mathrm{G}(x_0)$ of x_0 with respect to the space group $\mathcal{G} = \mathrm{G} * L$ is isomorphic to G; this is obvious in the case of the checker lattice. A point in E_d with a similar property to that of x_0 shall be called a full symmetry point of L. A lattice point of L is obviously a full symmetry point of L; it is, however, trivial. A point x_0 satisfying both $G(x_0) \simeq G$ and $x_0 \notin L$ is called a non-trivial full symmetry point (NTFSP) of L. The present consideration proves the first half of the following theorem:

Theorem. A necessary and sufficient condition for a Bravais lattice L to be a black sublattice of a BWBL is that L has a NTFSP.

We will prove that the condition of the theorem is sufficient. We first recall that G includes the inversion operation I $(Ix = -x\ \forall x \in E_d)$ since L is a Bravais lattice. Let x_0 be a NTFSP of L. Then, $Ix_0 \equiv x_0 \bmod L$ and, accordingly, $2x_0 \equiv 0 \bmod L$. Moreover, $L' \equiv x_0 + L$ is invariant against G; L' represents a class of NTFSPs which are translationally equivalent to x_0. It follows that L and L' satisfy the conditions (i)–(iii) for $L_c = L \cup I_c L'$ to be a BWBL.

A 2D square lattice (P$4mm$) has only one class of NTFSPs and the corresponding BWBL is the checker lattice. This BWBL is represented as $\mathrm{P_P}\,4mm$ (we follow the notation of Opechowski and Guccione 1965). On the other hand, a 2D triangular lattice (P$6mm$) has no NTFSPs and there exist no BWBLs with the hexagonal point symmetry, $\mathrm{G} = \mathrm{D}_6$. More generally, if a d-dimensional Bravais lattice L is given, a BWBL having L as its black sublattice is obtained only when L has an NTFSP. If L has two or more classes of NTFSPs, we can obtain two or more BWBLs.

In this letter, we investigate the case of 6D icosahedral BWBLs which yield 3D icosahedral BWBQLs. The relevant point group is Y_h ($\bar{5}\bar{3}m$). There exist three Bravais

† Strictly speaking, the point group of a BWBL is not identical to that of the relevant BWBQL but is only isomorphic because the dimensions of the spaces onto which they act are different. However, the two point groups are usually identified.

classes of 6D icosahedral lattices (Janssen 1988), $P\bar{5}\bar{3}m$, $F\bar{5}\bar{3}m$ and $I\bar{5}\bar{3}m$, whose representatives are chosen to be the 6D simple hypercubic lattice, L_P, the face-centred one, L_F, and the body-centred one, L_I. The basis vectors ε_i of L_P satisfy $\varepsilon_i \cdot \varepsilon_j = a^2 \delta_{i,j}$. $l = \Sigma_i n_i \varepsilon_i \in L_P$ is indexed as $l = [n_1 n_2 \ldots n_6]$. The three Bravais lattices are written with this index scheme as $L_P = \{[n_1 n_2 \ldots n_6] | n_i \in Z\}$, $L_F = \{[n_1 n_2 \ldots n_6] | n_i \in Z, \Sigma\, n_i = \text{even}\}$ and $L_I = \{[n_1 n_2 \ldots n_6]/2 | n_i \in Z,\ n_i$ are all even or all odd$\}$. The high symmetry points of these lattices have been listed completely (Janssen 1988, Niizeki 1989); of the three Bravais lattices, L_P and L_F have NTFSPs but L_I does not.

L_F is a sublattice of L_P, $L_P = L_F \cup L'_F$ with $L'_F = \varepsilon_1 + L_F$. ε_1 ($=[10000] \equiv x_0$) is a NTFSP of L_F. Therefore, $L_F \cup I_c L'_F$ is a 6D icosahedral BWBL, which is represented as $P_F\bar{5}\bar{3}m$. L_F has two other classes of NTFSPs whose representatives are $x_1 = [111111]/2$ and $x_2 = [\bar{1}11111]/2$ and we can obtain another two 6D icosahedral BWBLs. Unfortunately, these two BWBLs belong to the same black-and-white Bravais class as $P_F\bar{5}\bar{3}m$. This is because x_1 and x_2 are transformed to x_0 by affine transformations which are automorphisms of L_F and preserve the icosahedral point symmetry (Niizeki 1989)†. Thus, L_F gives only one BWBL.

L_I is divided into two sublattices, $L_I = L_P \cup L'_P$ with $L'_P = x_1 + L_P$, where $x_1 = [111111]/2$ is a NTFSP of L_P. Accordingly, we obtain a new 6D icosahedral BWBL, $I_P\bar{5}\bar{3}m = L_P \cup I_c L'_P$. L_P has no other classes of NTFSPs.

Let L_P^* and L_I^* be the reciprocal lattices of L_P and L_I, respectively. Then, L_P^* (or L_I^*) is a simple (or face-centred) hypercubic lattice in 6D. The basis vectors ε_i^* of L_P^* satisfy $\varepsilon_i^* \cdot \varepsilon_j^* = (a^*)^2 \delta_{i,j}$ with $a^* = 2\pi/a$. $g = \Sigma_i n_i \varepsilon_i^* \in L_P^*$ is indexed as $g = (n_1 n_2 \ldots n_6)$. L_I^* is written with this index scheme as $L_I^* = \{(n_1 n_2 \ldots n_6) | n_i \in Z, \Sigma n_i = \text{even}\}$.

$k = (111111)/2$ is an NTFSP of L_P^*. Let $l \in L_P$ ($= L_F \cup L'_F$). Then, $\exp(ik \cdot l)$ takes 1 or -1 depending on whether $l \in L_F$ or L'_F, respectively. Thus, the 6D plane-wave state $\phi_k = \exp(ik \cdot r)$ ($r \in E_6$) forms a 1D irreducible representation (IR) of the space group $P\bar{5}\bar{3}m$ ($= Y_h * L_P$). Here, it is essential that k is an NTFSP of L_P^*; $\rho k \equiv k \bmod L_P^*\ \forall \rho \in Y_h$. This IR is closely related to the presence of the BWBL $P_F\bar{5}\bar{3}m$. Similarly, the plane-wave state ϕ_q with $q = (100000)$ being an NTFSP of L_I^* forms a 1D IR of $I\bar{5}\bar{3}m$ ($= Y_h * L_I$) and is related to the presence of the BWBL $I_P\bar{5}\bar{3}m$.

The identity representation Γ_0 is a 1D IR of the space group $\mathcal{G}_0$ ($= G * L_0$) of a Bravais lattice L_0. It is, however, a trivial 1D IR because it represents the identity representation of both G and L_0. On the other hand, if k is an NTFSP of the reciprocal lattice of L_0, it can easily be shown that the 1D IR Γ given by the plane-wave state ϕ_k divides L_0 into two sublattices L and L' which form a BWBL $L \cup I_c L'$. In this case, the product representation $\Gamma \times \Gamma \times \Gamma$ is identical to Γ. Moreover, the antisymmetrized representation $\{\Gamma^2\}$ does not exist because Γ is one-dimensional. Then, the Landau theory of the phase transformation (Landau and Lifshitz 1968, Tolédano and Tolédano 1987)) tells us that the phase transition which freezes a mode with symmetry Γ will be a second-order transition. The Bravais lattice of the system changes from L_0 to L on the transition and, accordingly, the unit cell is doubled without changing the point symmetry. Furthermore, the superlattice lines appear at wavevectors in $L^*(k) = k + L^*$.

It follows that a primitive (or a body-centred) icosahedral quasicrystal can transform to a face-centred one (or a primitive one) through a second-order transition. Therefore, the reported order-disorder transformation from the primitive icosahedral

† These transformations are related to the self-similarity of the face-centred icosahedral quasilattice obtained from L_F.

quasicrystal to the face-centred one is probably a second-order transition (Devaud-Rzepski *et al* 1989, Hiraga *et al* 1989).

In conclusion, there exist only two black-and-white Bravais quasilattices ($P_F\bar{5}\bar{3}m$ and $I_P\bar{5}\bar{3}m$) with icosahedral point symmetry; the former is related to a division of the primitive icosahedral quasilattice ($P\bar{5}\bar{3}m$) into two face-centred ones ($F\bar{5}\bar{3}m$) and the latter to a division of the body-centred quasilattice ($I\bar{5}\bar{3}m$) into two primitive ones. Moreover, an order–disorder transformation of an icosahedral quasicrystal can be a second-order transformation, if the ordering is associated with either of the two sublattice divisions.

The 2D and 3D BWBQLs with octagonal, decagonal and dodecagonal point symmetries are discussed in Niizeki (1990).

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