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Three-dimensional black-and-white Bravais quasilattices with (2+1)-reducible point groups

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Abstract. We have investigated three-dimensional black-and-white Bravais quasilattices (BWBQL) with point groups D_{8h} ($8/mmm$), D_{10h} ($10/mmm$), D_{12h} ($12/mmm$) and D_{5d} ($\bar{5}m$), which are (2+1)-reducible. There exists seven Bravais classes of BWBQLs, $P_{2c}8/mmm$, P_P8/mmm, P_F8/mmm, F_P8/mmm, $P_{2c}10/mmm$, $P_{2c}12/mmm$ and $P_P\bar{5}m$.

1. Introduction

The black-and-white Bravais lattices (BWBLs) are important in the investigation of the order-disorder transformation and magnetic ordering: BWBLs are related to the type IV Shubnikov space groups (Opechowski and Guccione 1965, Bradley and Cracknell 1972, Tolédano 1987). Its generalization to the quasilattice (QL) will be useful in the investigation of similar problems in the case of quasicrystals, which are new ordered states of matter with quasiperiodicity and noncrystallographic point symmetries (Steinhardt and Ostlund 1987, Janssen 1988). We have investigated in a recent paper black-and-white Bravais quasilattices (BWBQLs) with the icosahedral point symmetry (Niizeki 1990). In this paper, we shall investigate BWBQLs associated with octagonal, decagonal, dodecagonal and pentagonal QLs, which are periodic along the c-axis but quasiperiodic only along the plane perpendicular to it.

QLs are basic geometrical objects which provide us with mathematical bases of the structures of the quasicrystals. A QL is obtained with the cut-and-projection method from a periodic lattice in higher dimensions (Janssen 1988); the point group of a QL and that of the relevant lattice in higher dimensions are only isomorphic to each other but are usually identified. Similarly, a BWBQL is obtained with the same method from a BWBL in higher dimensions (Niizeki 1990). Then, enumenrating BWBQLs with a given non-crystallographic point symmetry is reduced to enumerating higher dimensional BWBLs with the same point symmetry.

In section 2, we review general properties of a BWBL as discussed in Niizeki (1990). We investigate in section 3 BWBQLs in two dimensions (2D) and in section 4 those in 3D; the former are basic units of the latter. Section 5 is devoted to discussions.

2. The definition and the properties of a BWBL

A BWBL in d dimensions is composed of the black sublattice L and the white one L', which satisfy the conditions:

(i) L is a Bravais lattice, $L=\{n_1\boldsymbol{e}_1+\ldots+n_d\boldsymbol{e}_d \,|\, n_i\in \boldsymbol{Z}\}$, and L' is its translation, $L'=\boldsymbol{x}_0+L(=\{\boldsymbol{x}_0+\boldsymbol{l}\,|\,\boldsymbol{l}\in L\})$ with $\boldsymbol{x}_0(\notin L)$ being a representative of L'.

(ii) $L_0=L\cup L'$ is also a Bravais lattice and its point group, G, is identical to that of L, where colours of L and L' are neglected in L_0.

We shall call L_0 the host lattice of the BWBL. The space group of L is given by $\mathscr{g}=G*L=\{\{\sigma|\boldsymbol{l}\}\,|\,\sigma\in G, \boldsymbol{l}\in L\}$, i.e. the semidirect product of G and L. It is a subgroup of $\mathscr{g}_0=G*L_0$ with index 2; $\mathscr{g}_0=\mathscr{g}+\{0|\boldsymbol{x}_0\}\mathscr{g}$; L is a superlattice of L_0. $\mathscr{g}_0$ is the ordinary space group, which leaves L_0 invariant. $\mathscr{g}_0$ is isomorphic to the 'coloured space group' $\mathscr{g}_c=\mathscr{g}+I_c\{0|\boldsymbol{x}_0\}\mathscr{g}$, where I_c is the colour inversion operation which inverts black and white. $\mathscr{g}_c$ leaves the BWBL invariant. $\mathscr{g}_c$ is written as $G*L_c$ where $L_c=L\cup I_cL'$ is a maximal Abelian subgroup of $\mathscr{g}_c$. We can identify the BWBL with L_c.

Since L and L_0 are invariant against G, so is L'. Therefore, the point group of $\boldsymbol{x}_0$ with respect to the space group $\mathscr{g}$ is isomorphic to G. $\boldsymbol{x}_0$ is called a non-trivial full-symmetry point (NTFSP) of L; a lattice point of L is a trivial full-symmetry point. L' represents a class of NTFSPs which are translationally equivalent to one another.

Let L^* and L_0^* be the reciprocal lattices to L and L_0, respectively. Then L_0^* is a superlattice of L^*; $L^*=L_0^*\cup L_1^*$ with $L_1^*=\boldsymbol{q}+L_0^*$, where $\boldsymbol{q}$ is a representative reciprocal lattice vector in $L_1^*(=L^*-L_0^*)$. $\boldsymbol{q}$ is a NTFSP of L_0^*. Let us introduce a 'planewave state' by $\phi_{\boldsymbol{q}}(\boldsymbol{l})=\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{l})$ with $\boldsymbol{l}\in L_0(=L\cup L')$. Then $\phi_{\boldsymbol{q}}(\boldsymbol{l})=1$ or -1 according as $\boldsymbol{l}\in L$ or L', respectively. It follows that wavevectors in L_1^* $(=\boldsymbol{q}+L_0^*)$ represent the superlattice lines which appear when the Bravais lattice of the system degrades from L_0 to L.

The above considerations are summarized as follows:

(i) A Bravais lattice L can be a black sublattice of a BWBL if and only if L has a NTFSP $\boldsymbol{x}_0$; the BWBL is given by $L\cup I_cL'$ with $L'=\boldsymbol{x}_0+L$.

(ii) A Bravais lattice L_0 can be the host lattice of a BWBL if and only if its reciprocal lattice L_0^* has a NTFSP $\boldsymbol{q}$; the BWBL is given by $L\cup I_cL'$ with $L=\{\boldsymbol{l}\,|\,\boldsymbol{l}\in L_0, \phi_{\boldsymbol{q}}(\boldsymbol{l})=1\}$ and $L'=\{\boldsymbol{l}\,|\,\boldsymbol{l}\in L_0, \phi_{\boldsymbol{q}}(\boldsymbol{l})=-1\}$.

A NTFSP of a lattice L is a special high-symmetry point of L; a high-symmetry point of L is a point whose point symmetry with respect to the space group of L is higher than those of neighbouring points (Niizeki 1990).

3. Octagonal, decagonal and dodecagonal BWBQLs in 2D

The point groups of the Bravais-type octagonal, decagonal and dodecagonal QLs in 2D are D_8 ($8mm$), D_{10} ($10mm$) and D_{12} ($12mm$). These QLs are obtained from 4D periodic lattices $P8mm$, $P10mm$ and $P12mm$, respectively (Janssen 1988). The reciprocal lattice of each of these 4D lattices belongs to the same Bravais class as that of the real lattice. The high-symmetry points of these lattices have been completely listed (Niizeki 1989); of the three lattices, only the octagonal lattice has NTFSPs, which form a single class. It follows that there exists only one BWBL with the octagonal point symmetry but there are no BWBLs with the decagonal or dodecagonal point symmetry.

These results are similar to the fact that, in 2D, there exists only one BWBL with the tetragonal point symmetry, i.e. the checker lattice (P_P4mm), but there are no BWBLs with the hexagonal point symmetry.

In what follows, the indices of a real lattice vector (or a reciprocal one) are enclosed with brackets (or parentheses).

We can take a 4D simple hypercubic lattice, L_P, as the representative of the 4D octagonal Bravais class ($P8mm$); $L_P=\{\Sigma_i n_i\boldsymbol{e}_i\,|\,n_i\in\boldsymbol{Z}\}$, where $\boldsymbol{e}_i$, $i=1,\ldots,4$, are the basis vectors satisfying $e_i \cdot e_j = a^2 \delta_{i,j}$. The reciprocal lattice L_P^* to L_P is also a simple hypercubic lattice in 4D. The basis vectors e_i^* of L_P^* satisfies $e_i^* \cdot e_j^* = (a^*)^2 \delta_{i,j}$ with $a^* = 2\pi/a$. $\boldsymbol{q} = (1111)/2$ is a representative of NTFSPs of L_P^*. ϕ_q divides L_P into its two face-centred sublattices L_F and L'_F, where $L_F = \{[n_1 n_2 n_3 n_4] \mid n_i \in \boldsymbol{Z}, \Sigma\, n_i = \text{even}\}$ and $L'_F = e_1 + L_F$. Since L_F as well as L_P belongs to the 4D primitive octagonal Bravais class, $P8mm$, (Niizeki 1990), the present BWBL, $L_F \cup I_c L'_F$, is denoted as $P_P 8mm$.

The 2D octagonal BWBQL, $Q_{8,c}$, obtained from $L_c = L_F \cup I_c L'_F$ is shown in figure 1. The two sublattices of $Q_{8,c} = Q_8^{(1)} \cup I_c Q_8^{(2)}$ are the projections of the cuts of those of L_c onto the real space (a 2D subspace).

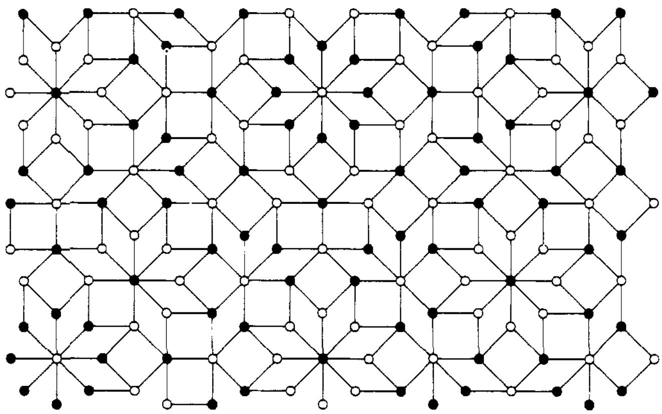

Figure 1. The octagonal BWBQL in 2D.

The relationship between $Q_{8,c}$ and the 3D BWBQLs to be investigated in the next section is similar to that between the checker lattice and the 3D tetragonal BWBLs. Therefore, we shall refer to $Q_{8,c}$ as the checker quasilattice and to the 4D BWBL L_c $(= L_F \cup I_c L'_F)$ as the 4D checker lattice.

4. 3D BWBQLs with (2 + 1)-reducible point groups

We investigate 3D BWBQLs associated with the QLs whose point groups are D_{8h} ($8/mmm$), D_{10h} ($10/mmm$), D_{12h} ($12/mmm$) and D_{5d} ($\bar{5}m$). The 3D Euclidean space E_3 is reduced by these point groups into two invariant subspaces; $E_3 = E_2 \oplus E_1$, where E_1 refers to the c-axis of the QLs and E_2 to the plane perpendicular to the c-axis. Accordingly, these QLs are called $(2+1)$-reducible.

There exist five Bravais classes of 5D lattices associated with the $(2+1)$-reducible QLs with these point groups, namely, three primitive lattices P8/*mmm*, *P*10/*mmm* and *P*12/*mmm*, the centred octagonal lattice, *F*8/*mmm* (=*I*8/*mmm*), and the pentagonal lattice, $P\bar{5}m$ (Janssen 1988, Gähler 1990). The presence of the centred octagonal lattice in 5D is closely related to the fact that the 4D octagonal lattice (*P*8*mm*) has an NTFSP. We emphasize that *F*8/*mmm* and *I*8/*mmm* are equivalent (Niizeki 1990). The fifth axis of each 5D lattice is identified with the c-axis of the relevant QL.

The five 5D lattices are periodic stackings of the 4D octagonal, decagonal or dodecagonal lattices in section 3 along the c-axis. In particular, a primitive lattice is a simple stacking; *PN*/*mmm* with $N = 8$, 10 or 12 is a direct product of *PNmm* and

$L_1 = \{nc \mid n \in \mathbf{Z}\}$, the 1D Bravais lattice. The reciprocal lattice of each 5D lattice belongs to the same Bravais class as that of the real lattice itself (Niizeki 1990a). The basis vectors of a 5D lattice (or its reciprocal lattice) are denoted as $\boldsymbol{\varepsilon}_i$ (or $\boldsymbol{\varepsilon}_i^*$). The high-symmetry points of these 5D lattices have been listed completely (Niizeki 1990a). We will pick up NTFSPs in the following arguments from the tables in Niizeki (1990a).

4.1. *The case of primitive N-gonal lattices*

The reciprocal lattice of a primitive N-gonal lattice PN/mmm with $N = 8$, 10 or 12 has an NTFSP of the form $\boldsymbol{q} = \boldsymbol{\varepsilon}_5^*/2$ $(= (0, 0, 0, 0, c/2))$. As mentioned above, PN/mmm is a stacking of the type $\ldots AAAA \ldots$ with A being the 4D N-gonal lattice ($PNmm$). This lattice is changed with the use of ϕ_q into a 5D BWBL which is an alternating stacking of black layers and white ones like $\ldots A^{\bullet}A^{\circ}A^{\bullet}A^{\circ} \ldots$, where the black layer $A^{\bullet}$ and the white one A° are identical to A except the colours. This BWBL is denoted as $P_{2c}N/mmm$, where the suffix $2c$ stands for the period along the c-axis (we follow the notation by Opechowski and Guccione (1965)).

The reciprocal lattice of PN/mmm with $N = 10$ or 12 has no other classes of NTFSPs and there are no other 5D BWBLs with decagonal or dodecagonal point symmetry.

4.2. *The case of the centred octagonal lattice*

We consider here other 5D octagonal BWBLs than $P_{2c}8/mmm$. The basis vectors of the 5D primitive octagonal lattice, L_P $(= P8/mmm)$, satisfy $\boldsymbol{\varepsilon}_i \cdot \boldsymbol{\varepsilon}_j = a^2\delta_{i,j}$ but $\boldsymbol{\varepsilon}_5 \cdot \boldsymbol{\varepsilon}_5 = c^2$. The reciprocal lattice L_P^* to L_P is a similar lattice to L_P but with the lattice constants $a^* = 2\pi/a$ and $c^* = 2\pi/c$. L_P^* has three classes of NTFSPs; their representatives are given by $\boldsymbol{q} = (00001)/2$ $(= \boldsymbol{\varepsilon}_5^*/2)$, $\boldsymbol{q}' = (11110)/2$ and $\boldsymbol{q}'' = (11111)/2$. $\phi_{q'}$ divides L_P into another two primitive lattices, $L = \{[n_1 n_2 \ldots n_5] \mid n_i \in \mathbf{Z}, n_1 + n_2 + n_3 + n_4 = \text{even}\}$ and $L' = \boldsymbol{\varepsilon}_1 + L$. The resulting BWBL, $L \cup I_c L'$, is denoted as $P_P 8/mmm$, which is a simple stacking of the 4D checker lattice ($P_P 8mm$) along the c-axis.

On the other hand, $\phi_{q''}$ divides L_P into two centred octagonal lattices, $L_F = \{[n_1 n_2 \ldots n_5] \mid n_i \in Z, \Sigma_i n_i = \text{even}\}$ and $L'_F = \boldsymbol{\varepsilon}_1 + L_F$ $(= \boldsymbol{\varepsilon}_5 + L_F)$. The resulting BWBL, $L \cup I_c L'$, is denoted as $P_F 8/mmm$ $(= P_I 8/mmm)$. This BWBL is an alternating stacking of 4D checker lattices, A $(= P_P 8mm)$ and B $(= [1000] + A)$ along the c-axis as $\ldots ABAB \ldots$; the colour pattern of every 4D layer is inverted alternately because $B = I_c A$.

$\boldsymbol{x}_0 = [1 1111]/2$ is a NTFSP of L_P $(= P8/mmm)$ and we obtain the fourth 5D octagonal BWBL, $L_P \cup I_c L'_P$ with $L'_P = \boldsymbol{x}_0 + L_P$. The host lattice is the body-centred lattice, $L_I = L_P \cup L'_P$ $(= I8/mmm)$, so that the BWBL is represented as $I_P 8/mmm$ $(= F_P 8/mmm)$. L_I is an alternating stacking as $\ldots ABAB \ldots$, where A and B are 4D octagonal lattices ($P8mm$) being related to each other by $B = [1111]/2 + A$. Accordingly, $I_P 8/mmm$ is a stacking as $\ldots A^{\bullet}B^{\circ}A^{\bullet}B^{\circ} \ldots$.

The reciprocal lattice of $P8/mmm$ has three classes of NTFSPs but that of $F8/mmm$ $(= I8/mmm)$ has only one. Therefore, there exist three (or one) octagonal BWBLs whose host lattices are $P8/mmm$ (or $F8/mmm$) and the enumeration of 5D octagonal BWBLs has been completed. The presence of many 5D BWBLs with the octagonal symmetry is closely related to the presence of the 4D checker lattice ($P_P 8mm$). Note that the four 5D octagonal BWBLs have their analogues in the 3D tetragonal BWBLs (for the latter BWBLs, see Opechowski and Guccione 1965).

4.3. *The case of the pentagonal lattice*

There remains to investigate a 5D BWBL associated with the 5D pentagonal lattice, $L_5 = P\bar{5}m$. The reciprocal lattice L_5^* to L_5 belongs also to the same Bravais class, $P\bar{5}m$. The 5D simple hypercubic lattice is a special case of L_5 where $\varepsilon_i \cdot \varepsilon_j = a^2\delta_{i,j}$; the c-axis is parallel to [11111]. L_5 is a periodic stacking of 4D decagonal lattices ($P10mm$) along the c-axis; one period is composed of five layers, *ABCDE*, which are related to each other by translations along the 4D subspace (Niizeki 1990a).

L_5^* as well as L_5 has only one class of NTFSPs whose representative is $q = (11111)/2$. ϕ_q divides L_5 into $L_F = \{[n_1 n_2 \ldots n_5] | n_i \in \mathbf{Z}, \Sigma_i n_i = \text{even}\}$ and $L'_F = \varepsilon_1 + L_F$. The stacking in L_F is of the type $\ldots ACEDB \ldots$ which can be changed into $\ldots ABCDE \ldots$ by a rotation arround the c-axis, so that L_F belongs also to $P\bar{5}m$†. The pentagonal BWBL, $L_F \cup I_c L'_F$, is denoted as $P_P\bar{5}m$, which is an alternating stacking as $\ldots A^{\bullet}B^{\circ}C^{\bullet}D^{\circ}E^{\bullet}A^{\circ}B^{\bullet}C^{\circ}D^{\bullet}E^{\circ} \ldots$; one period is composed of ten layers. This BWBL is analogous to the 3D rhombohedral BWBL, $R_R\bar{3}m$, which is an alternating stacking as $\ldots A^{\bullet}B^{\circ}C^{\bullet}A^{\circ}B^{\bullet}C^{\circ} \ldots$.

5. Discussions

If a 5D BWBL investigated in section 4 is projected along the c-axis, we obtain a 4D pattern with point symmetry Nmm, where $N = 8$, 10 or 12. Most of the 4D pattern obtained in this way are 'grey' 4D Bravais lattices ($PNmm$) because black lattice points and the white ones overlap on the projection. The two cases, P_P8/mmm and F_P8/mmm, are exceptional; their projections are the 4D checker lattice (P_P8mm).

A (2+1)-reducible 3D QL is a periodic stacking of 2D QLs. Similarly, a (2+1)-reducible 3D BWBQL is a periodic stacking of coloured 2D QLs, which are obtained from the 4D layers of a 5D BWBL. Therefore, the stacking of the 4D layers in a BWBL investigated in section 4 applies also to the stacking of the 2D layers in the corresponding 3D BWBQLs. For example, a 3D BWBQL of the type P_P8/mmm is a simple stacking of the checker QL in figure 1 as $\ldots AAA \ldots$ but that of the type P_F8/mmm is an alternating stacking like $\ldots ABAB \ldots$ with $B = I_cA$. On the other hand, the projection of the 3D octagonal BWBQL, I_P8/mmm, along the c-axis is similar to the checker QL in figure 1; every black (or white) layer in the 3D BWBQL is projected onto the black (or white) sublattice of figure 1.

The Penrose lattice is a 2D decagonal QL formed by the vertices of the Penrose tiling. It can be changed into a similar black-and-white QL to the checker QL in figure 1. However, this is not in contradiction with the absence of a 2D decagonal BWBQL becuase the Penrose lattice is a non-Bravais-type QL. This is understandable also by the fact that the macroscopic point symmetry of the black-and-white Penrose lattice is pentagonal ($5m$).

A BWBL is considered to be the ordered structure in an order–disorder transformation; the host lattice is, then, a grey lattice which represents the structure of the disordered phase. It can be shown generally that the order–disorder transformation associated with a BWBL (or BWBQL) can be a second-order phase transition (Niizeki

† L_F is a 5D Bravais lattice and its point group is D_{5d}, so that L_F must belong to $P\bar{5}m$, which is an alternative proof. By a similar reason, the body-centred pentagonal lattice, $L_I = L_5 \cup ([11111]/2 + L_5)$, belongs $P\bar{5}m$. That is, $P\bar{5}m = F\bar{5}m = I\bar{5}m$. Note, however, that the orientations of the axes are different among L_5, L_F and L_I.

1990b). Thus, the present investigation provides us with various examples of possible second-order order-disorder transformations of quasicrystals.

The present investigation will be a basis of the enumeration of type IV Schubnikov space-group (Opechowski and Guccione 1965) associated with QLs with (2+1)-reducible point groups.

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