

SHORT COMMUNICATIONS

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Character table of the hypercubic point group in six dimensions. By S. DEONARINE, *Physics Department, Bronx Community College of CUNY, University Avenue & West 181st, Bronx, NY 10453, USA* and JOSEPH L. BIRMAN, *Physics Department, City College of CUNY, Convent Avenue at 138th, New York, NY 10031, USA*

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Abstract

By application of a modified Burnside method, based on the explicit determination of class multiplication coefficients h_{ijk} , the character table of the hypercubic point group in six dimensions B_6 – a group of order 46 080 – is obtained. This point group is used in the study of quasicrystals through a projection from six to three dimensions.

Introduction

Recourse is often made to higher-dimensional crystallography in order to explain irregularities or unusual patterns in lower dimensions. The discovery of icosahedral point symmetry in crystals of Al-Mn alloys has spurred interest in $n > 3$ -dimensional space groups, beyond that of mere mathematical curiosity.

Using inductive methods from 3-space Kramer (1987) has shown how a rotation of the hypercubic lattice in 6-space relates periodic cubic order with non-periodic icosahedral order. Further comparisons and projections from six to three dimensions require a knowledge of the character table for B_6 .

B_6 is a Coxeter group and hence can be generated by reflections. It is also the wreath product $Z_2 \uparrow n$ of the two-element group Z_2 . This group is generated by $n \times n$ permutation matrices with elements $\varepsilon_i = \pm 1$ and $n \times n$ permutation matrices. Applying a modification of Burnside's method for obtaining tables for groups of high order (Chen & Birman, 1971) we obtain, by directly computing the class multiplication coefficients h_{ijk} on the VAX-11/780, this table for B_6 . A mechanism for the change from 6-space to 3-space may be based on the Landau theory for phase transitions (Lyubarskii, 1960). We have accordingly identified the polar vector representation of B_6 and determined the Landau and Lifschitz activities of each of the 65 irreducible representations in the table.

Determination of character table for B_6

The point group $G = B_6$ of order $g = 2^6 \times 6! = 46\,080$ may be generated by 720 rotations and 64 reflections in six dimensions (Coxeter & Moser, 1965). An element f of B_6 may be represented as a 2-row symbol (Kramer, 1987)

$$f = \begin{vmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ \varepsilon_1 f(1) & & \dots & & & \varepsilon_6 f(6) \end{vmatrix}$$

where

$$\varepsilon_i f(i) = \pm f(i), \quad i = 1, 2, \dots, 6$$

and $f(1), f(2), \dots, f(6)$ is a permutation of S_6 , the symmetric group of 6! permutations.

Using standard group theory (Burnside, 1955), we obtained 65 classes. These are listed in Table 1, showing respectively the number of elements in each class, a representative element of a class and the order of that element. Only the lower row of the 2-row symbol above is shown.

Let G be a finite group of order g . Let the class C_i of G be of order r_i and the total number of classes be r . The class multiplication coefficients $h_{i,j,k}$ are defined by

$$C_i C_j = \sum_{k=1}^r h_{i,j,k} C_k.$$

For B_6 18 692 independent $h_{i,j,k}$ values were calculated.

Let χ_i^μ be the character of class C_i in the μ th irreducible representation (irrep) R_μ of G , $\mu = 1, \dots, r$. There are four basic equations that the χ_i^μ must satisfy with $d_\mu = \chi_1^\mu$ being the dimension of the μ th irrep:

$$\sum_{\mu=1}^r d_\mu^2 = g \quad (1)$$

$$\sum_{\mu=1}^r r_i \chi_i^\mu \chi_j^{\mu*} = g \delta_{ij} \quad (2)$$

$$\sum_{i=1}^r r_i \chi_i^\mu \chi_i^{\nu*} = g \delta_{\mu\nu} \quad (3)$$

$$r_i r_j \chi_i^\mu \chi_j^\mu = d_\mu \sum_{k=1}^r h_{i,j,k} r_k \chi_k^\mu \quad i, j = 1, \dots, r. \quad (4)$$

The importance of (4) cannot be overstated in verifying a character table. There are some characters that satisfy (1) and orthogonality relations (2) and (3) but fail (4). These pseudo-characters differ from the true ones in sign. Table 2 shows the character table for B_6 .

Activity of the irreps

The Landau theory of phase transitions uses the concepts of order parameters and free energy. The latter is a polynomial expansion of the order parameters that is invariant under all symmetry elements $g \in G$. The order parameters may be chosen from the basis functions of the irreps (Lyubarskii, 1960).

Certain selection rules are used to predict whether a transition from G to a phase of lower symmetry is allowed. The Lifschitz and Landau criteria are respectively

$$(I) \quad \Gamma_1 \notin \Gamma_{\nu} \chi \{ \Gamma_G \}^2$$

$$(II) \quad \Gamma_1 \notin [\Gamma_G]^3$$

Table 1. Class structure of B_6

Class	Number	Element	Order	Class	Number	Element	Order
1	1	1 2 3 4 5 6	1	34	480	1 2 -3 5 6 -4	6
2	6	1 2 3 4 5 -6	2	35	480	1 -2 -3 5 6 4	6
3	15	1 2 3 4 -5 -6	2	36	480	1 -2 -3 5 6 -4	6
4	20	1 2 3 -4 -5 -6	2	37	160	-1 -2 -3 5 6 4	6
5	15	1 2 -3 -4 -5 -6	2	38	160	-1 -2 -3 5 6 -4	6
6	6	1 -2 -3 -4 -5 -6	2	39	640	2 3 1 5 6 4	3
7	1	-1 -2 -3 -4 -5 -6	2	40	1280	2 3 1 5 6 -4	6
8	30	1 2 3 4 6 5	2	41	640	2 3 -1 5 6 -4	6
9	30	1 2 3 4 6 -5	4	42	720	1 2 4 5 6 3	4
10	120	1 2 3 -4 6 5	2	43	720	1 2 4 5 6 -3	8
11	120	1 2 3 -4 6 -5	4	44	1440	1 -2 4 5 6 3	4
12	180	1 2 -3 -4 6 5	2	45	1440	1 -2 4 5 6 -3	8
13	180	1 2 -3 -4 6 -5	4	46	720	-1 -2 4 5 6 3	4
14	120	1 -2 -3 -4 6 5	2	47	720	-1 -2 4 5 6 -3	8
15	120	1 -2 -3 -4 6 -5	4	48	1440	2 1 4 5 6 3	4
16	30	-1 -2 -3 -4 6 5	2	49	1440	2 1 4 5 6 -3	8
17	30	-1 -2 -3 -4 6 -5	4	50	1440	2 -1 4 5 6 3	4
18	180	1 2 4 3 6 5	2	51	1440	2 -1 4 5 6 -3	8
19	360	1 2 4 3 6 -5	4	52	2304	1 3 4 5 6 2	5
20	180	1 2 4 -3 6 -5	4	53	2304	1 3 4 5 6 -2	10
21	360	1 -2 4 3 6 5	2	54	2304	-1 3 4 5 6 2	10
22	720	1 -2 4 3 6 -5	4	55	2304	-1 3 4 5 6 -2	10
23	360	1 -2 4 -3 6 -5	4	56	960	1 3 2 5 6 4	6
24	180	-1 -2 4 3 6 5	2	57	960	1 3 2 5 6 -4	6
25	360	-1 -2 4 3 6 -5	4	58	960	1 3 -2 5 6 4	12
26	180	-1 -2 4 -3 6 -5	4	59	960	1 3 -2 5 6 -4	12
27	120	2 1 4 3 6 5	2	60	960	-1 3 2 5 6 4	6
28	360	2 1 4 3 6 -5	4	61	960	-1 3 2 5 6 -4	6
29	360	2 1 4 -3 6 -5	4	62	960	-1 3 -2 5 6 4	12
30	120	2 -1 4 -3 6 -5	4	63	960	-1 3 -2 5 6 -4	12
31	160	1 2 3 5 6 4	3	64	3840	2 3 4 5 6 1	6
32	160	1 2 3 5 6 -4	6	65	3840	2 3 4 5 6 -1	12
33	480	1 2 -3 5 6 4	6				

where Γ_1 is the identity representation Γ_v is the polar vector representation and Γ_G is an irrep of group G . $\{\Gamma\}^2$ and $\{\Gamma\}^3$, respectively the antisymmetrized square and symmetrized cube of Γ_G , are defined by (Lyubarskii, 1960)

$$(Ia) \quad \{\chi\}^2(g) = \frac{1}{2}\chi^2(g) - \frac{1}{2}\chi(g^2)$$

$$(IIa) \quad [\chi]^3(g) = \frac{1}{3}\chi(g^3) + \frac{1}{2}\chi(g^2)\chi(g) + \frac{1}{6}\chi^3(g).$$

We have found that Γ_v is R_{15} in our table. All the irreps were Lifschitz active. The irreps that did not satisfy the Landau condition were $R_1, R_6, R_{12}, R_{17}, R_{26}, R_{30}, R_{32}, R_{33}, R_{44}, R_{45}, R_{57}, R_{58}, R_{59}, R_{62}$ and R_{63} .

Projection into 3-space

Kramer (1987) uses $i_2, h_2, g_2, g_3, g_4, g_5$ as the generators of cubic and icosahedral groups (I, I_h). They belong to classes 7, 21, 24, 39, 50, 52 respectively in Table 1. Class 52 (2304 elements) is unique among all 65 classes in possessing elements of 5-fold order. We will use its representative element [1 3 4 5 6 2] as g_5 .

	E	$[15e_2]$	$[20e_3]$	$[12e_5]$	$[12e'_5]$
R'_1	1	1	1	1	1
R'_2	3	-1	0	τ	$1-\tau$
R'_3	3	-1	0	$1-\tau$	τ
R'_4	4	0	1	-1	-1
R'_5	5	1	-1	0	0

Character table of icosahedral group I [$\tau = (1 + \sqrt{5})/2$].

If we restrict the elements in B_6 to the corresponding elements of I , we obtain for the 6-dimensional irreps $R_{13},$

$R_{14}, R_{15},$ and R_{16} (Table 2) the characters of a reducible representation Γ_6 in 3-space.

	E	$[15e_2]$	$[20e_3]$	$[12e_5]$	$[12e'_5]$
Γ_6	6	-2	0	1	1
				$\Gamma_6 = R'_2 + R'_3.$	

Hence a unitary (orthogonal) matrix M exists which completely reduces the 6-dimensional representation D_{Γ_6} to block-diagonal form:

$$M D_{\Gamma_6} M^{-1} = \begin{bmatrix} D'_2 & 0 \\ 0 & D'_3 \end{bmatrix},$$

where D'_2 and D'_3 are the 3×3 matrices corresponding to R'_2 and R'_3 respectively. If we focus on g_5 , we can obtain this reduction. The 12 vertices of an icosahedron (edge 2) are given as (Coxeter, 1973)

$$(0, \pm\tau, \pm 1), (\pm 1, 0, \pm\tau), (\pm\tau, \pm 1, 0).$$

Let an axis of 5-fold symmetry in 6-space pass through the vertices $(0, 1, \tau), (0, -1, -\tau)$ in 3-space. The vertices $(\tau, 0, 1), (0, -1, \tau), (-\tau, 0, 1), (-1, \tau, 0)$ and $(1, \tau, 0)$ all lie in a plane in 3-space. By rotating these vertices with g_5 we obtain as one of its representations in 3-space

$$D'_2(g_5) = \begin{bmatrix} \tau^{-1}/2 & \tau/2 & -1/2 \\ -\tau/2 & 1/2 & \tau^{-1}/2 \\ 1/2 & \tau^{-1}/2 & \tau/2 \end{bmatrix}.$$

The 20 vertices of the reciprocal dodecahedron (edge $2\tau^{-1}$) are

$$(0, \pm\tau^{-1}, \pm\tau), (\pm\tau, 0, \pm\tau^{-1}), (\pm\tau^{-1}, \pm\tau, 0), (\pm 1, \pm 1, \pm 1).$$

