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Polychromatic symmetry and physical properties

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Abstract. A group theoretic method of obtaining the maximum number of non-vanishing independent constants required to describe a chosen physical property by the 18 polychromatic classes is presented. These numbers, in conjunction with the magnetic constants already obtained during the earlier study by this author in respect of these colour classes, may help identify the class of crystals that bear the possible geometric configuration envisaged by Indenbom *et al.* The effect of spins in crystals in their magnetic state on the non-magnetic physical properties is theoretically studied and a brief discussion of the results is presented.

1. Introduction

Since the beginning of the 19th century many notable contributions have been made to the study of the physical properties of crystals by several (group) theoretical physicists. Some examples are the character method (Bhagavantam and Suryanarayana 1949) based on the computation of the character, for deriving the number of independent constants for the various physical properties of crystals; and other general methods (Jahn 1949, Bhagavantam and Venkatarayudu 1951, Juretschke 1951) also based on group theory, to find the number of physical constants. The book by Bhagavantam (1966) further enhances the use of the character method in studying the magnetic properties of crystals. In all these studies, interest was concentrated upon the 32 conventional crystallographic point groups and the 58 magnetic (double colour) point groups derived from them. Whereas Bhagavantam (1966) enumerated the number of independent constants required to describe the three magnetic properties by the 58 magnetic point groups, Krishnamurty and Appalanarasimham (1970) obtained the non-vanishing number of physical constants, required for the description of some identified physical property like photo-elasticity, in their magnetic state.

Following the interpretation of antisymmetry as two-colour symmetry, the concept of polychromatic symmetry came to light (Belov and Tarkhova 1956). Consequently Indenbom *et al* (1960), with the help of the 10 crystallographic point groups containing one-dimensional (1D) complex irreducible representations (IR), derived the 18 polychromatic point groups and associated them with the 18 pairs of 1D complex IR of the generator groups. As the 58 magnetic (double colour) groups could not adequately describe the magnetic symmetry of screw (helicoidal) and certain other geometric

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structures, the polychromatic apparatus and thereby the polychromatic groups gained in physical significance to completely account for such a typical situation, as has been indicated by Naish (1963).

In a recent paper, the author (Rama Mohana Rao 1987) has carried out a group theoretic study of the magnetic properties of these 18 important polychromatic classes and enumerated the magnetic constants required by each of them to describe a considered magnetic property like piezomagnetism. In what follows attention is turned to the study of their physical properties such as pyro-electricity (see table 1). Since the 10 conventional crystallographic point groups that generate the 18 polychromatic classes exhibit magnetic properties (Bhagavantam 1966), the question of the existence of the converse of this proposition, i.e. whether the 18 polychromatic classes in their magnetic state exhibit non-magnetic physical properties, is significant and is investigated in this paper.

In § 2 some known physical properties exhibited by crystals, and their computed character, is shown (table 1). The group theoretical method of obtaining the physical constants by the polychromatic classes is outlined and the procedure illustrated in § 3 for the class $6^{(3)}$. Results obtained in respect of the other 17 classes are provided in table 2 and a discussion is given in § 4. The non-vanishing number of independent physical constants enumerated here in respect of the six known physical properties, in conjunction with the non-vanishing number of magnetic constants already obtained in the preceding paper (Rama Mohana Rao 1987)—a total picture providing their physical symmetry more elaborately—may help physicists in identifying the classes of

Table 1. Classification of some known physical properties and their computed character†.

S number	Physical property representing relation between	Computed character $\chi_\rho^{(\Gamma)}(R_\phi)$	Physical property known	Maximum number of constants required
1	Scalar and vector	$2c \pm 1$	Pyro-electricity; production of charges by hydrostatic pressure	3
2	Scalar and symmetric tensor (same as vector and vector with $c_{ik} = c_{ki}$, $k = 1, 2, 3$)	$4c^2 \pm 2c$	Thermal expansion; optical, dielectric and magnetic polarisation; thermal and electrical conductivities; thermo-electricity	6
3	Vector and symmetric tensor	$(2c \pm 1)(4c^2 \pm 2c)$	Piezo-electricity; electro-optical Kerr effect	18
4	Symmetric tensor and symmetric tensor	$(4c^2 \pm 2c)^2$	Photo-elasticity; effect of pressure on electrical conductivity	36
5	Vector and square of symmetric tensor ($c_{ik} = c_{ki}$; i, $k = 1$-6)	$(2c \pm 1)$ $(16c^4 \pm 8c^3 - 4c^2 + 1)$	Piezo-electric coefficients	63
6	Symmetric tensor and square of symmetric tensor ($c_{ik} = c_{ki}$; i, $k = 1$-6)	$(4c^2 \pm 2c)$ $(16c^4 \pm 8c^3 - 4c^2 + 1)$	Photo-elastic coefficients	126

† In this table, c denotes $\cos \phi$. The positive or negative sign in the computed character $\chi_\rho^{(\Gamma)}$ indicates that R_ϕ is a pure rotation or rotation reflection through an angle ϕ, respectively.

Table 2. Number of independent physical constants (n_i) needed for the description of the six chosen physical properties by the 18 polychromatic classes

S number	Polychromatic class	n_i needed to describe the physical property					
		1	2	3	4	5	6
1	$6^{(6)}$	1	1	4	6	12	20
2	$\bar{3}^{(6)}$	1	0	6	0	21	0
3	$3^{(3)}/\mathrm{m}'$	0	1	2	6	9	20
4	$6^{(3)}$	0	1	2	6	9	22
5	$\bar{3}^{(3)}$	0	2	0	12	0	42
6	$3^{(3)}/\mathrm{m}$	1	1	4	6	12	22
7	$6^{(6)}/\mathrm{m}$	1	0	4	0	12	0
8	$6^{(3)}/\mathrm{m}$	0	1	0	6	0	22
9	$6^{(6)}/\mathrm{m}'$	0	1	0	6	0	20
10	$6^{(3)}/\mathrm{m}'$	0	0	2	0	9	0
11	$3^{(3)}$	1	2	6	12	21	42
12	$4^{(4)}$	1	1	5	8	17	29
13	$\bar{4}^{(4)}$	1	1	5	8	17	29
14	$4^{(4)}/\mathrm{m}$	1	0	5	0	17	0
15	$4^{(4)}/\mathrm{m}'$	0	1	0	8	0	29
16	$3^{(3)}/2$	0	1	0	4	4	13
17	$\bar{6}^{(3)}/2$	0	1	0	4	0	13
18	$\bar{6}^{(6)}/2$	0	0	1	0	4	0

crystals that bear the possible geometric configuration envisaged by Indenbom *et al* (1960).

2. Physical properties of crystals

It is well known that physical properties of substances depend on the relation between two quantities—each of which may be a scalar, vector or a symmetric tensor of second rank, etc. In all the cases, each of the relations requires a certain number of independent constants connecting the components of the quantities involved for its complete description. The number of constants required for any property depends on the property chosen and on the crystallographic symmetry of the material, if we are dealing with the solid state. However, the maximum number is given in general by the product of the number of components of the two parameters, the relation between which the physical property represents and remains as such in the triclinic asymmetric class of the crystals. The system of an independent number of non-vanishing constants for the various physical properties in respect of the 32 crystal classes was derived in considerable detail using tensor and group theoretical methods by Bhagavantam and Venkatarayudu (1951), Bhagavantam (1966), Wooster (1973), Nye (1985), etc.

Table 1 gives some known physical properties arranged systematically in order of increasing complexity with the computed character $\chi_p^{(\Gamma)}(R_\phi)$ corresponding to a symmetry element R_ϕ in the representation being provided by the particular physical property under consideration. The list of physical properties in any row, as given by Bhagavantam and Venkatarayudu (1951) and provided here, is only representative and is not complete.

3. Enumeration of physical constants

The maximum number of independent constants required to describe the three magnetic properties by the 18 polychromatic (3-, 4- and 6-coloured) classes was obained by this author in a previous paper through establishing an important theorem (Rama Mohana Rao 1987, theorem 3). It pertains to the equality of the number of constants (n_i) required to describe a magnetic or physical property and occurring before an IR μ of a factor group G/H and that number needed by the corresponding colour group induced by the IR λ of G, for the same property under consideration, where the IR λ of G is engendered by the IR μ of G/H. The physical constants of these 18 classes pertaining to the six identified physical properties listed in table 1 are obtained in this section by adopting much the same procedure that has already been described in § 4 of that paper (Rama Mohana Rao 1987). The actual evaluation of the desired constants is done now by considering the relevant IR of the appropriate factor group G/H with the 10 generating crystallographic point groups containing 1D complex IR and utilising (*a*) the formula for the computed character $\chi_\rho^{(\Gamma)}$ for each property provided in table 1; (*b*) the definition of the character of a coset (Krishnamurty *et al* 1977); (*c*) theorems 3.1–3.3 of Rama Mohana Rao (1987) and (*d*) the known formula (Bhagavantam and Venkatarayudu 1951):

$$n_i = \frac{1}{g}\sum_\rho h_\rho \bar{\chi}_\rho^{(\Gamma_i)} \chi_\rho^{(\Gamma)} \tag{3.1}$$

with the usual notation.

The procedure is illustrated with the help of the point group 6 that induces the polychromatic classes $6^{(3)}$ and $6^{(6)}$, for a physical property, say pyro-electricity, the computed character of which, as provided by table 1, is

$$\chi_\rho^{(\Gamma)}(R_\phi) = 2c \pm 1. \tag{3.2}$$

For the polychromatic variant $6^{(3)}$, consider the normal subgroup 2 of the point group 6 and the factor group $6/2 \simeq 3$. The point group 2 is a subgroup of index 3 to the point group 6 and the group 6 can be written as a union of cosets

$$6 = E2 \cup C_3^+2 \cup C_3^-2.$$

The character of table of $6/2 \simeq 3$ is given in table 3.

It has already been observed (Bhagavantam and Venkatarayudu 1951, Bhagavantam 1966) that the point group 2 requires one pyro-electric constant. So 1 can be taken as the character of the identity element in 6/2. The coset C_3^+2 contains the elements C_3^+ and C_6^-. The character of these elements in respect to pyro-electricity is 0 and 2 respectively. Following the definition of the character of the coset, the character of C_3^+2 for pyro-electricity is seen to be equal to 1. Adopting a similar procedure, it can be shown that the character of C_3^-2 is equal to 1. These characters, when substituted in equation (3.1), show that the variant $6^{(3)}$ requires zero pyro-electric constant. The results obtained for the other physical properties for this variant are shown in table 3. Similarly, considering the factor group 6/1, one can find that 1 pyro-electric constant is required for the variant $6^{(6)}$.

This method when extended, with a suitable choice of the normal subgroups and forming the appropriate factor groups, to the rest of the 9 point groups containing 1D complex IR gives the number of pyro-electric constants required for the rest of the polychromatic classes. A similar procedure, when adopted for the rest of the five

Table 3. Number of independent physical constants (n_i) needed by the polychromatic class $6^{(3)}$ for the 6 chosen physical properties.

6/2	$E2$	C_3^-2	C_3^+2	Polychromatic class induced	n_i needed for the description of the physical property 1	2	3	4	5	6
A′	1	1	1							
$1'_E$	1	ω	ω^2	$6^{(3)}$	0	1	2	6	9	22
$2'_E$	1	ω^2	ω							

$\chi_p^{(\Gamma)}$	$E2$	C_3^-2	C_3^+2
1	1	1	1
2	4	1	1
3	8	2	2
4	20	2	2
5	29	2	2
6	68	2	2

physical properties, yields the corresponding constants needed to describe the chosen physical property. The constants thus enumerated are provided in table 2.

4. Discussion

The IR of a point group are connected with the geometry of the crystal. The 18 polychromatic variants associated with the 18 pairs of 1D complex IR are the 3-, 4- or 6-colour symmetry point groups in which each colour may represent a transformable physical property. These colour symmetry point groups have wide-ranging applications in the derivation and description of similarity symmetry groups and also in the description of stem and layer symmetry groups in higher-dimensional space, as has been appreciated by Roman (1959) and Zamorzaev (1963).

The enumeration of physical constants by the method adopted in this paper gives the constants needed to describe all six physical properties simultaneously for a chosen class—they need not be dealt with separately. It can be noted that the group theoretical method provides exact results whereas the tensor and other methods yield approximate ones through a cumbersome procedure.

Bhagavantam (1966) opines that a symmetry operation (g) of a point group and its complement (R_2g) will have the same effect on any physical property. This leads one to believe that there is no distinction between a point group and its variant in so far as a physical property is concerned. Thus in the case of a physical property, say for instance photo-elasticity, following this hypothesis, the crystal class 2mm and its magnetic variants 2m′m′, 2′mm′ should require the same number of 12 photo-elastic constants. However, it was observed earlier (Krishnamurty and Appalanarasimham 1970) that the magnetic variants 2m′m′ and 2′mm′ each require only eight photo-elastic constants. For another physical property, namely pyro-electricity, when the crystal class 2mm needs only one pyro-electric constant, its magnetic variants 2m′m′ and 2′mm′ can be seen to require zero and one pyro-electric constants respectively. In the case of polychromatic variants (with the generating colour symmetry operation $R_n g$, $n = 3, 4$ or 6) in this work, the point group G and its polychromatic variants $G^{(p)}$ are found to describe a similar phenomenon. For example, the point group 6 can be seen to require one pyro-electric constant and its polychromatic variants $6^{(3)}$ and $6^{(6)}$ are found to require zero and one constants respectively.

In the light of the results obtained in this work, one can note that, in general, the physical properties of the polychromatic point groups are different from those of the magnetic point groups as can be seen by noting their differing number of independent constants (n_i). Similarly, the number of constants (n_i) required to describe a chosen physical property in the magnetic state of a crystal may differ, generally, from the corresponding number in the normal state whilst in other cases these numbers coincide, indicating that the presence of spin does not necessarily affect their physical properties.

The above conclusions of this theoretical study suggest experimental investigation with a view to throwing some light on the influence of spins in crystals in their magnetic state on the non-magnetic physical properties.

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References

Belov N V and Tarkhova T N 1956 *Kristallogr.* **1** 4 (Engl. transl. 1956 *Sov. Phys.-Crystallogr.* **1** 5)
Bhagavantam S 1966 *Crystal Symmetry and Physical Properties* (New York: Academic)
Bhagavantam S and Suryanarayana D 1949 *Acta Crystallogr.* A **2** 21
Bhagavantam S and Venkatarayudu T 1951 *Theory of Groups and its Application to Physical Problems* (Waltair: Andhra University Press)
Indenbom V L, Belov N V and Neronova N N 1960 *Kristallogr.* **5** 497 (Engl. transl. 1961 *Sov. Phys.-Crystallogr.* **5** 477)
Jahn H A 1949 *Acta Crystallogr.* A **2** 30
Juretschke J H 1951 *Lecture Notes* (New York: Polytechnic Institute of Brooklyn)
Krishnamurty T S G and Appalanarasimham V 1970 *Acta Crystallogr.* A **26** 293
Krishnamurty T S G, Appalanarasimham V and Rama Mohana Rao K 1977 *Acta Crystallogr.* A **33** 338
Naish V E 1963 *Izv. Akad. Nauk.* **27** 1496 (Engl. transl. 1963 *Bull. Acad. Sci. USSR, Phys. Ser.* **27** 1468)
Nye J F 1985 *Physical Properties of Crystals* (Oxford: Clarendon)
Rama Mohana Rao K 1987 *J. Phys. A: Math. Gen.* **20** 47
Roman T 1959 *Dokl. Acad. Nauk* **128** 6
Wooster W A 1973 *Tensors and Group Theory for the Physical Properties of Crystals* (Oxford: Clarendon)
Zamorzaev A M 1963 *Kristallogr.* **8** 307 (Engl. transl. 1963 *Sov. Phys.-Crystallogr.* **8** 241)