Color Groups

Maciek Borysiuk

June 13, 2007

1 Introduction

Color group also known as Shubnikov group or magnetic group is an extension of a concept of a crystallographic point group first developed by a russian physicst A.V.Shubnikov. This text focuses specifically on two colour point groups or black and white groups and their application to magnetically ordered systems.

2 Point Groups

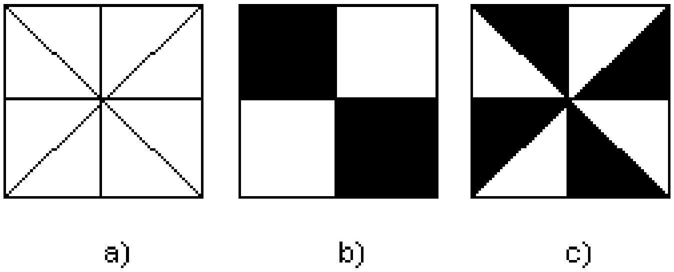
Point group is a finite group which can be used to describe symmetry properties of an object such as a molecule or a crystal. Color point group is an extension of that concept which allows one to describe an additional degree of freedom for example magnetic ordering or ferroelectricity.

2.1 Theory

Color groups are constructed out of 32 ordinary crystallographic point groups G. Which are as it is well known finite unitary groups. In order to create color group M point group G is extended with an antiunitary operation R such that $R^2 = E$. (Antiunitarity of an operator means that $\langle XA \,||\, AY\rangle = \langle XY\rangle^\star = \langle YX\rangle$ as oposed to unitarity U which gives $\langle XU \,||\, UY\rangle = \langle XY\rangle$.) Operator R doesn't operate on regular coordinate space only on the color space so it commutes with regular group operations which only transform spatial coordinates. Graphically the R operation can be illustrated as color changing (black to white) physically can correspond to reversing spin or equivalently time reversal. That is because one can see spin ($\uparrow$)as a current loop which is $\frac{dq}{dt}$ so inverting the time $\frac{dq}{d(-t)}$ is equivalent to inverting the current $-\frac{dq}{dt}$ which is the same as inverting the spin ($\downarrow$). This properties of R make color groups useful in describing magnetically ordered systems. As with ordinary point groups each operation which brings the object back to itself belongs to the given group.

For example from ordinary group C_{4v} one can build two black and white groups (see figure 1). By coloring some parts of the square black and others white we break the symmetry so that the effect of some of the original operations of C_{4v} brings us outside of the group but by adding aformentioned antiunitary

Figure 1: In this example we see two color groups b), c) made out of one ordinary point group in a). Four lines crisscrossing a) are mirror lines $m_v$and m_d rotation axis goes trough the middle of the square: a)C_{4v} $\{E, 2C_4, C_2, 2m_d, 2m_v\}$ b) $C_{4v}(C_{2v})$ $\{E, C_2, 2m_d, 2R{*}C_4, 2R{*}m_v\}$ c) $C_{4v}(C_4)$ $\{E, 2C_4, C_2, 2R{*}m_d, 2R{*}m_v\}$



a) b) c)

operator to those elements $A = RU$ we bring them back to the group. So that our new group consists of Unitary elements U and antiunitary elements A. We will represent the unitary subgroup of G as H. Similar considerations can be done for all 32 point groups. Introducing R increases number of point groups from 32 to the total of 122. Newly created groups can be divided into one of 3 following ways.

- *First* we have 32 colorless groups which are simply equal to the ordinary crystallographic point groups $M = G$.
- *Second* 32 grey groups made by taking R with each element of the group $M = G \times \{E, R\} = G + RG$. Those groups could be used to represent a paramgnetic system.
- *Third* are 58 black and white groups $M = H + R(G/H)$ which can be constructed same way as the two color groups of C_{4v} here H is agian unitary subgroup R(G/H) are the remaining antiunitary elements

All 58 black and white groups and the 32 colorless groups can be easily constructed from one dimensional representations of ordinary point groups. In table 1 we can see one dimensional characters of the C_{4v} group. Instead of inspecting all the operations we use a following method. Take the fully symmetric one dimensional representation to be type one color group in all the remaining one dimensional representations $+1$ value of character means that the particular operation/class of operations belongs to H if character is -1 it then belongs to G/H. Ignore all the degnerate and complex representations. We see that we get back same result as in figure 1.

Table 1: One dimensional characters of the C_{4v} group

representation	E	$2 * C_4$	C_2	$2 * \sigma_v$	$2 * \sigma_d$	Group H
Γ_1	1	1	1	1	1	C_{4v}
Γ_2	1	1	1	-1	-1	C_4
Γ_3	1	-1	1	-1	1	C_{2v}
Γ_4	1	-1	1	1	-1	C_{2v}

2.2 Representations

Irreducible representations of color groups are constructed out of the ordinary point group representations. Since the magnetic group is non-unitary we can not use regular representation theory to achive that goal. Solution to this problem was derived by wigner [1]. Given that D^i is an irreducible representation for a colored group and d^i is same for a colorless one also that U refers to unitary element and A to antiunitary one then one can observe three distinct cases. First two occur if $\chi\{d^i(U)\} = \chi\{\overline{d^i}(U)\}$ where we have that $\overline{d^i}(U) = d^i(A_0^{-1}UA_0)^*$ then we can write $\overline{d^i}(U) = \beta^{-1}d^i(U)\beta$ meaning that those two elements only differ by a similarity transformation.

1. If
   $$\beta\beta^* = d^i(A_0^2)$$
   then
   $$D^i(U) = d^i(U)$$
   and
   $$D^i(A) = d^i(AA_0^{-1})\beta$$
   so that one unitary representation corresponds to one nonunitary with the same dimension.

2. If
   $$\beta\beta^* = -d^i(A_0^2)$$
   then
   $$D^i(U) = (\begin{matrix} d^i(U) & 0 \\ 0 & d^i(U) \end{matrix})$$
   and
   $$D^i(A) = (\begin{matrix} 0 & d^i(AA_0^{-1})\beta \\ -d^i(AA_0^{-1})\beta & 0 \end{matrix})$$
   and we have that one unitary representation corresponds to one nonunitary but D^i has double the dimension.

---

[1] Wigner 1959 “Group theory and its application to the qunatum mechanics of Atomic Spectra”

3. If $\chi\{d^i(U)\} \neq \chi\{\overline{d^i}(U)\}$ where once agian $\overline{d^i}(U) = d^i(A_0^{-1}UA_0)$ we have

   $$D^i(U) = (\begin{array}{cc} d^i(U) & 0 \\ 0 & \overline{d^i}(U) \end{array})$$

   and

   $$D^i(A) = (\begin{array}{cc} 0 & d^i(AA_0) \\ d^i(A_0^{-1}A)^* & 0 \end{array})$$

   so that one nonunitary representation consists of two unitary ones.

Question now is how to easily find which one of the 3 cases we are dealing with. After some derivation one can arive at a simple result.

1. $\sum_k \chi\{A_k^2\} = +n$
2. $\sum_k \chi\{A_k^2\} = -n$
3. $\sum_k \chi\{A_k^2\} = 0$

here $A_k = U_k A_0$ and $A_0 = U_0 R$ also n equals the number of elements in H. Now we have everything we need to construct the irreducible representaions of magnetic point groups.

3 Space Groups

To fully describe a symmetry of magnetic material it is not enough to know its point group same as for a nonmagnetic one we must define its space group. Color space groups are built up in the same way as regular space groups namely out of lattice and a point group. Color point group and or color lattice means a magnetically ordered system.

3.1 Color lattice

We extend regular 14 crystal lattices by maknig it possible for each lattice site to have a color associated with it. We do that by definig vector τ which point from black to white lattice points This way we get additional 22 crystal lattices.

3.2 Space Group

If we consider color groups and color lattices total numer of space groups grows to 1651 groups. They can be categorized in a following way.

1. *230 colorless groups.* They are simply the 230 ordinary space groups. Ordinary point group + colorless lattice.

2. *230 grey groups.* Grey point groups with colorless lattices (one of the original 14).

3. *674 black and white groups with colorless lattices.* Third type of point group plus one of the colorless lattices.
4. *517 black and white groups with colored lattices.* Third type point group plus one of the new 22 colored lattices.

4 References

Most of the information in this work comes from the book “Symmetry Principles and Magnetic Symmetry in solid state physics” S.J Joshua (Adam Hilger 1991).