

Symmetries in physics

Magnetic groups

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1 Introduction

When speaking of crystals it is impossible to overlook the fact that they are more or less symmetric structures. Consequently, they are like a playground for the theory of discrete groups. Each crystal can be described by a space group, whose elements have the property that they transform crystal lattice back into itself. These transformations are of different kinds: translation, point group transformations (which leave at least one point unchanged) and their combination. However, they are all unitary. Such classical theory of symmetry is essentially a three-dimensional study, i.e. each lattice point can be specified by a vector $\mathbf{r} = (x, y, z)$ and one considers the effect of symmetry operations on it.

However, the study of the theory the symmetry did not advance much between the derivation of 230 space groups just before 1900 and the introduction of the use of the idea of antisymmetry by Schubnikov in 1951. The concept of antisymmetry had been suggested by Heesch [1] long before Schubnikov's work, but its importance was not realized at the time. Schubnikov's basic idea was to give the x, y, z coordinates of a point a fourth coordinate s which can take only two possible values [2]. If we distribute the values of s to atoms in a lattice in some regular fashion, it is possible for part of the symmetry to survive. If we include a new operation, *operation of antisymmetry* r , which changes between values of s , and consider this in a conjunction with all the ordinary point groups and space groups operations, it is possible to obtain a collection of new point groups and space groups which are called *black and white groups*, or *magnetic groups*, or *Heesch-Schubnikov groups*. The real usage of such groups becomes apparent if we think of s as being the two allowed values

of a magnet's direction, then r is the operation which reverses a magnetic moment and is often regarded as being the operation of *time-reversal*. The introduction of neutron diffraction techniques has made it possible to determine the orientation of the magnetic moments of the various atoms or ions in magnetically ordered crystals. Then the magnetic groups proved to be very relevant for the crystallographic description of the symmetry of very large number of magnetic crystals, first example of such usage being given by Donnay et al. (1958).

2 Classification of magnetic or Schubnikov groups

Let us restrict the internal degrees of freedom s to just two values, which can be looked upon as two 'colours' (black-white). A change of state of this internal property can be described by an operator r , which changes colour (black into white and vice versa), so that $r^2 = E$. By enlarging the point groups with r we obtain new groups besides the ordinary geometrical ones.

- **Color or Schubnikov groups of type I** These groups describe object that are monochromatic, i.e. having a definite color, say white. The operator r is then excluded from such group. They are in fact identical to the geometric point groups

$$\mathcal{M}^I = \mathcal{G} \tag{1}$$

In all there are 32 monochromatic point groups.

- **Color or Schubnikov groups of type II (the gray groups)** System with this symmetry type possess identical and overlapping distribution of two colors, say black and white (hence name gray). Such groups may describe the symmetry of paramagnetic or diamagnetic systems where there are equal numbers of up and down spin states, and the application of the operator r will leave the system invariant. The corresponding symmetry group can be expressed as

$$\mathcal{M}^{II} = \mathcal{G} \oplus r\mathcal{G} = \mathcal{G} \otimes \{E, r\} \tag{2}$$

where \mathcal{G} is the geometric point group associated with the atomic arrangement of the system. Here \mathcal{G} is invariant subgroup of \mathcal{M}^{II} with index 2¹. We should notice that equality (2) can be written because r commutes with all the elements of \mathcal{G} .

- **Dichromatic or Schubnikov groups of type III** Groups that belong to this class do not contain r as a separate element, but include elements comprising of products involving r . To elucidate the role of such groups in describing the symmetry of physical systems, we consider the simple dichromatic equilateral triangle shown in Fig. 1.

Obviously r is not a symmetry operation of the colored triangle. Moreover, among the elements of $\mathcal{G} = C_{3v}$ we find that those of the subgroup C_3 (rotations for 120°) leave the colored triangle invariant, while all the reflection operations do not. However, if we multiply these reflections by r , the compound operation leaves the triangle invariant. Thus the elements, $E, C_3, C_3^{-1}, r\sigma_1, r\sigma_2, r\sigma_3$ form a group $\mathcal{M} = C_{3v}^{III}$ which we call a color group. We may notice that in contrast to gray group C_{3v}^{II} , C_{3v}^{III} does not have r as an element by itself. The structure of C_{3v}^{III} is typical of all color point groups, and we may write

$$\mathcal{M}^{III} = \mathcal{N} \oplus r(\mathcal{G} - \mathcal{N}) = \mathcal{N} \oplus rS\mathcal{N}, \quad S \in (\mathcal{G} - \mathcal{N}) \tag{3}$$

¹Index of a subgroup is number of groups elements divided by the number of subgroup elements.

where \mathcal{N} as a normal ². subgroup of \mathcal{G} of index 2. In principle we can take any ordinary point group \mathcal{G} of even order, determine all its subgroups of index 2, and construct from each a new color group. Last equality in (3) is written using the Lagrange's theorem³, since for $S \in (\mathcal{G} - \mathcal{N})$ left coset $S\mathcal{N}$ contains no elements in common with \mathcal{N} .

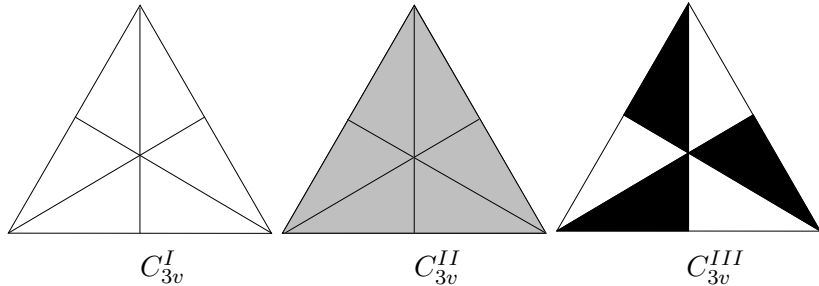


Figure 1: Color point groups of types I, II and III associated with C_{3v}

The number of subgroups of index 2 of a point group \mathcal{G} is given by

$$2^n - 1; \quad \text{where } n \text{ is number of independent generators of } \mathcal{G}. \quad (4)$$

This constitutes the maximum number of color groups that may be constructed from \mathcal{G} . In all there are 58 dichromatic point groups.

3 Dichromatic space groups

Dichromatic Bravais lattices The concept of the color may equally be applied to the translational symmetries as it is applied to point group symmetries. We can construct dichromatic Bravais lattices by introducing a colored translation $r\tau_0$, where τ_0 cannot be identity. A dichromatic translation group \mathcal{T}_c is then defined as

$$\mathcal{T}_c = \mathcal{T}_2 \oplus r\tau_0\mathcal{T}_2 \quad (5)$$

where \mathcal{T}_2 is a subgroup with index 2 of one of the monochromatic 14 Bravais lattices.

In two dimensions, 5 extra dichromatic Bravais nets can be constructed, and are shown in Fig. 2. In three-dimensions there are some restrictions on τ_0 [3] giving together 22 dichromatic classes.

Since a **space group** comprises a combination of some Bravais lattice with a point subgroup it is possible to construct dichromatic space groups by combining either

²A subgroup \mathcal{N} , of a group \mathcal{G} , is called normal subgroup if it is invariant under conjugation; that is, for each element n in \mathcal{N} and each g in \mathcal{G} , the element gng^{-1} is still in \mathcal{N} .

$$\mathcal{N} \triangleleft \mathcal{G} \quad \Leftrightarrow \quad \forall n \in \mathcal{N}, \forall g \in \mathcal{G}, gng^{-1} \in \mathcal{N}$$

³Lagrange's theorem: Let \mathcal{S} be a subgroup (of order n) of \mathcal{G} (of order g). For any $g_i \in \mathcal{G}$ the elements of $\mathcal{S}g_i$ form a right coset. If $g_i \in \mathcal{S}$ the coset is equal to \mathcal{S} . If not the coset contains no elements in common with \mathcal{S} . Given \mathcal{S} a set of g/n elements g_i of \mathcal{G} may be found such that any element of \mathcal{G} may be written in a form $s_p g_i$, $s_p \in \mathcal{S}$. Equally for the left coset.

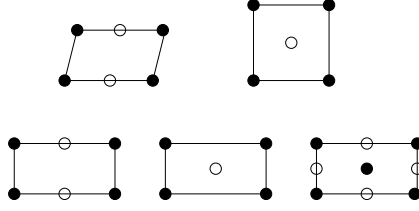


Figure 2: Two-dimensional dichromatic Bravais nets.

- (a) a dichromatic point group with a monochromatic Bravais lattice
- (b) a dichromatic Bravais lattice with a monochromatic point group.

4 The time-reversed representation

One most obvious application of color groups is description of magnetic crystals. The r operator which changes color is in this case the time reversal operator \mathcal{T} . \mathcal{T} is a symmetry operator for the Hamiltonians of many physical systems. For a crystalline system with time-reversal symmetry the full point group will then be the product of the ordinary point group with the identity and the time-reversal, since the latter commutes with the point group operations. In language introduced above this would be the gray group.

However, this can only be true for non-magnetic crystals, since \mathcal{T} reverses the direction of currents and spins and consequently the direction of magnetization in magnetically ordered crystals. Reversion of color is manifested in reversion of spin. Still magnetic crystals may be invariant under an operation, which is a product of \mathcal{T} with a rotation, even though it is not invariant under \mathcal{T} itself. Recalling the definition of color group of type III we see that the symmetry group of such crystals is just the latter.

As an example, we consider a ferromagnetic crystal which, disregarding the time-reversal, has symmetry group D_3 . Above critical temperature T_N , in the magnetically disordered state the inclusion of time-reversal lead to larger gray group $D_3 \otimes \{E, \mathcal{T}\}$, since there is no magnetic moment. Below T_N , the crystal becomes ferromagnetic with magnetization along the three-fold axis. Since the two-fold rotations C_2 about axes in the xy-plane reverse the direction of magnetization they are no longer symmetry operations and nether is \mathcal{T} . However, the product $\mathcal{T}C_2$ remains as symmetry operations and the new symmetry group contains $\{E, C_3, C_3^{-1}, \mathcal{T}C_2^1, \mathcal{T}C_2^2, \mathcal{T}C_2^3\}$. We should notice that three-fold rotations C_3 consist a subgroup of original D_3 , which is normal subgroup of index 2. For visual presentation one can still use the dichromatic Fig. 1.

4.1 Theory of corepresentations

In order to construct the representations of magnetic groups we first need to study the effect of \mathcal{T} on a representation (Rep) basis set. We consider, in particular the case when \mathcal{T} , and to this effect any antilinear operator, is applied to a Rep basis function following the action of some linear (or antilinear) operator \mathcal{O} .

$$\mathcal{T}\mathcal{O}\psi_\mu = \mathcal{T} \sum \psi_\nu \Gamma_{\nu\mu}(\mathcal{O}) = \sum (\mathcal{T}\psi_\nu) \Gamma_{\nu\mu}^*(\mathcal{O}) = \sum_{\nu\lambda} \psi_\lambda \Sigma_{\lambda\nu}(\mathcal{T}) \Gamma_{\nu\mu}^*(\mathcal{O}) \quad (6)$$

since \mathcal{T} complex-conjugates (c-conjugates) all quantities to its right. This shows that the product of the two operators does not lead to just a product of the corresponding matrix representation, but leads, in addition, to a c-conjugation of the matrix representative of \mathcal{O} . Therefore, when \mathcal{T} is included in a symmetry group, we must seek not ordinary matrix representations, but representations consistent with (6) (so called *corepresentations* (CoRep)).

4.1.1 Construction of corepresentations

We consider magnetic group \mathcal{M} , which we write as

$$\mathcal{M} = \mathcal{N} \oplus \mathcal{AN} \quad (7)$$

where \mathcal{N} is a unitary subgroup of index 2 of \mathcal{M} , and $\mathcal{A} \notin \mathcal{N}$ is an antiunitary element of \mathcal{M} (either $\mathcal{A} = \mathcal{T}$ (for gray \mathcal{M}) or $\mathcal{A} = \mathcal{TS}$, $S \in \mathcal{G} - \mathcal{N}$ (for dichromatic \mathcal{M})). We denote the elements of \mathcal{N} by R, T and those of \mathcal{AN} by \mathcal{A}, \mathcal{B} , but we should remember that $\mathcal{A}^2, \mathcal{AB} \in \mathcal{N}$ (since \mathcal{N} is normal).

We start with applying R to a basis set $\{\psi_\mu\} \equiv \Psi$ which engenders an Irrep Δ of \mathcal{N} , namely,

$$\begin{aligned} R\psi_\mu &= \sum_\nu \psi_\nu \Delta_{\nu\mu}(R), \quad R \in \mathcal{N} \\ R\Psi &= \Psi\Delta(R). \end{aligned} \quad (8)$$

Next, we define the time-reversed set $\Phi \equiv \{\phi_\mu\} = \{\mathcal{T}\psi_\mu\}$ such that

$$R\Phi = \Phi\check{\Delta}(R), \quad (9)$$

but since $\mathcal{TR} = RT$, we have

$$\begin{aligned} RT\Psi &= \mathcal{T}(R\Psi) = \mathcal{T}(\Psi\Delta(T)) \\ &= (\mathcal{T}\Psi)\Delta^*(R) = \Phi\Delta^*(R) \end{aligned} \quad (10)$$

$$\boxed{\check{\Delta}(R) = \Delta^*(R)} \quad (11)$$

The time-reversed representation $\check{\Delta}$ is **identical** to the complex conjugate representation Δ^* .

If we set $\mathcal{A} = S\mathcal{T}$, where $S \in (\mathcal{M} - \mathcal{N})$, then the basis vectors $\mathcal{A}\Psi$ generate a *generalized time-reversed representation*, namely,

$$R(\mathcal{A}\Psi) = (\mathcal{A}\Psi) \mathcal{A}\Delta(R) \quad (12)$$

$$\begin{aligned} &= RST\Psi = S(S^{-1}RS)\mathcal{T}\Psi \\ &= (ST\Psi)\Delta^*(S^{-1}RS) = (\mathcal{A}\Psi)\Delta^*(S^{-1}RS) \end{aligned} \quad (13)$$

$$\boxed{\mathcal{A}\Delta(R) = \Delta^*(S^{-1}RS)} \quad (14)$$

where $\Delta(S^{-1}RS)$ is an Irrep conjugate to $\Delta(R)$, since \mathcal{N} is a normal subgroup.

We now construct the Rep Γ engendered by the combined basis $F = [\Psi, \mathcal{A}\Psi]$,

$$\begin{aligned} RF &= F\Gamma(R) \\ &= [\Psi, \mathcal{A}\Psi] \begin{pmatrix} \Delta(R) & 0 \\ 0 & \Delta^*(S^{-1}RS) \end{pmatrix}, \quad \forall R \in \mathcal{N} \end{aligned} \quad (15)$$

Next we apply an operation $\mathcal{B} = \mathcal{A}T, T \in \mathcal{N}$ and obtain

$$\begin{aligned}\mathcal{B}\Psi &= \mathcal{A}T\Psi = \mathcal{A}\Psi\Delta(T) = (\mathcal{A}\Psi)\Delta^*(T) = (\mathcal{A}\Psi)\Delta^*(\mathcal{A}^{-1}\mathcal{B}) \\ \mathcal{B}(\mathcal{A}\Psi) &= \mathcal{B}\mathcal{A}\Psi = \Psi\Delta(\mathcal{B}\mathcal{A}), \quad \mathcal{B}\mathcal{A} \in \mathcal{N}\end{aligned}\tag{16}$$

Therefore

$$\begin{aligned}\mathcal{B}F &= F\Gamma(\mathcal{B}) \\ &= [\Psi, \mathcal{A}\Psi] \begin{pmatrix} 0 & \Delta(\mathcal{B}\mathcal{A}) \\ \Delta^*(\mathcal{A}^{-1}\mathcal{B}) & 0 \end{pmatrix}, \quad \forall \mathcal{B} \in \mathcal{AN}\end{aligned}\tag{17}$$

It is easy to see that the matrix representatives Γ do not obey the ordinary multiplication relations associated with unitary groups, but rather

$$\begin{aligned}\Gamma(R)\Gamma(S) &= \Gamma(RS) & \Gamma(R)\Gamma(\mathcal{B}) &= \Gamma(R\mathcal{B}) \\ \Gamma(\mathcal{B})\Gamma^*(R) &= \Gamma(\mathcal{B}R) & \Gamma(\mathcal{B})\Gamma^*(\mathcal{C}) &= \Gamma(\mathcal{B}\mathcal{C})\end{aligned}\tag{18}$$

where $R, S \in \mathcal{N}$ and $\mathcal{B}, \mathcal{C} \in \mathcal{AN}$.

The set of unitary matrices defined by (15) and (17) form a *corepresentation* of \mathcal{M} , derived from unitary Irrep Δ of its normal subgroup \mathcal{N} and satisfying the multiplication rules (18)

4.1.2 Reality of Irreps

All the CoReps comprise of Irreps Δ , their c-conjugates Δ^* and conjugate Irreps derived from Δ and Δ^* . Therefore it is useful to know, whether Δ and Δ^* are equivalent, which is connected with the concept of *reality*.

We consider an Irrep Δ^{\Re} to be real if

$$\Delta^{\Re}(R) = (\Delta^{\Re}(R))^*, \quad \forall R \in \mathcal{N}.\tag{19}$$

An Irrep Δ is *potentially real* if it is equivalent to a Δ^{\Re} , even when Δ is complex. Moreover, a potentially real Δ is equivalent to its complex conjugate Δ^* , since

$$\begin{aligned}\Delta^{\Re} &= U^{-1}\Delta(R)U = (U^*)^{-1}\Delta^*(R)U^* \\ \Delta^*(R) &= (U(U^*)^{-1})^{-1}\Delta(R)(U(U^*)^{-1}) \sim \Delta(R)\end{aligned}\tag{20}$$

However, Δ may be equivalent to Δ^* but may not be equivalent to any real Irrep.

To find the nature of Irrep Frobenius/Schur character sum rules prove to be very useful. They state that [3]

$$\sum_{R \in \mathcal{N}} {}^{(\mu)}\chi(R^2) = \begin{cases} n & {}^{(\mu)}\Delta \text{ is a real Irrep,} \\ 0 & {}^{(\mu)}\Delta \text{ is a complex Irrep,} \\ -n & {}^{(\mu)}\Delta \text{ is a pseudo-real Irrep.} \end{cases}$$

4.1.3 Equivalence of CoIrreps

Before studying the reducibility of representations, we explore the equivalence relationship among CoIrreps of the group \mathcal{M} . We already know that if we apply unitary transformation U of the basis F , representation of unitary R in the transformed set $\Gamma'(R)$ is connected to the original $\Gamma(R)$ through

$$\Gamma'(R) = U^{-1}\Gamma(R)U \quad (21)$$

In order to obtain the transformation of $\Gamma(\mathcal{B})$ under U , we consider the action of \mathcal{B} on $F' = FU$

$$\begin{aligned} \mathcal{B}F' &= F'\Gamma'(\mathcal{B}) = FU\Gamma'(\mathcal{B}) \\ \mathcal{B}F' &= \mathcal{B}FU = F\Gamma(\mathcal{B})U^* = (FU)U^{-1}\Gamma(\mathcal{B})U^*. \end{aligned} \quad (22)$$

which yields

$$\Gamma'(\mathcal{B}) = U^{-1}\Gamma(\mathcal{B})U^*. \quad (23)$$

Equations (21) and (23) define the equivalence between Γ' and Γ .

4.1.4 Reducibility of Γ

The question of reducibility of Γ entails whether there exists a unitary transformation that will render an equivalent block-diagonal Rep Γ^{block} or not. We need to find a transformation that block-diagonalizes $\Gamma(R)$ and $\Gamma(\mathcal{B})$ instantaneously. Because of the structure of Γ , we should examine the relationship between the Irreps $\Delta(R)$ and ${}^{\mathcal{A}}\Delta = \Delta^*(S^{-1}RS)$.

We separate different cases:

- (i) $\Delta(R) \not\sim {}^{\mathcal{A}}\Delta = \Delta^*(S^{-1}RS)$. We examine the reducibility of Γ by exploring the possibility of constructing a unitary matrix U that reduces Γ

$$\begin{aligned} \Gamma(R) \quad U &= U \quad \Gamma'(R) \\ \begin{bmatrix} \Delta(R) & 0 \\ 0 & {}^{\mathcal{A}}\Delta(R) \end{bmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} &= \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{bmatrix} \Delta'(R) & 0 \\ 0 & \Delta''(R) \end{bmatrix} \\ \begin{bmatrix} \Delta(R)a & \Delta(R)b \\ {}^{\mathcal{A}}\Delta(R)c & {}^{\mathcal{A}}\Delta(R)d \end{bmatrix} &= \begin{bmatrix} a\Delta'(R) & b\Delta''(R) \\ c\Delta'(R) & d\Delta''(R) \end{bmatrix} \end{aligned} \quad (24)$$

Since $\Delta \not\sim \Delta''$ and ${}^{\mathcal{A}}\Delta \not\sim \Delta'$, b and c must be zero. Then U is block-diagonal matrix and therefore cannot block-diagonalize $\Gamma(\mathcal{B})$. Hence the corresponding Γ is irreducible.

- (ii) If $\Delta(R) \sim {}^{\mathcal{A}}\Delta = \Delta^*(S^{-1}RS)$ procedure is longer and can be found in [3]. The result is that Γ can be reduced in this case.

All together we have tree possible types of CoIrreps:

- (a) $\mathcal{A}\Psi = \Phi$ reproduces the set Ψ . The CoRep ${}^{(\mu)}\Gamma$ of \mathcal{M} corresponds to a single Irrep ${}^{(\mu)}\Delta$ of \mathcal{N} , and has the same dimension.

In this case no new degeneracy is introduced by the coset \mathcal{AN} .

(b) $\mathcal{A}\Psi$ produces the set Φ which is independent of the set Ψ , but which also forms a basis for $^{(\mu)}\Delta$ of \mathcal{N} . The CoRep $^{(\mu)}\Gamma$ of \mathcal{M} corresponds again to a single Irrep $^{(\mu)}\Delta$ of \mathcal{N} , but with twice the dimension. In this case the dimension of $^{(\mu)}\Delta$ is doubled.

Possible extra degeneracy may appear.

(c) The set $\Phi = \mathcal{A}\Psi$ is independent of Ψ , and forms a basis for the Irrep $^{(\nu)}\Delta$ of \mathcal{N} which is inequivalent to $^{(\mu)}\Delta$. In this case the CoRep $^{(\mu)}\Gamma$ corresponds to two inequivalent Irrep of \mathcal{N} . Whole Γ is irreducible as we discussed in case (i).

The antiunitary operators cause $^{(\mu)}\Delta$ and $^{(\nu)}\Delta$ to become degenerate.

This classification is summarized in the following table:

Type	$\chi^{\mathcal{A}}(R)$	Equivalence	Symmetry	$^{\mathcal{A}}\Delta = \Delta(R)$
(a)	$= \chi(R)$	$^{\mathcal{A}}\Delta(R) = V^{-1}\Delta(R)V$	$V^*V = +\Delta(S^2)$	if $\Delta(S^2) = \Delta(E)$
(b)	$= \chi(R)$	$^{\mathcal{A}}\Delta(R) = V^{-1}\Delta(R)V$	$V^*V = -\Delta(S^2)$	if $\Delta(S^2) = -\Delta(E)$
(c)	$\neq \chi(R)$	$^{\mathcal{A}}\Delta(R) \not\sim \Delta(R)$	-	No

In the above classification an extra degeneracy was meant in respect to the case where the classical group \mathcal{N} is the appropriate symmetry group. This can be illustrated with eigenfunctions and eigenvalues of a Hamiltonian H , Fig. 3. Here ψ_i is an eigenfunction of H belonging to Irrep $^{(i)}\Delta$ and E_i is its corresponding eigenvalue; $\phi_i = \mathcal{A}\psi_i$ is the function from the transformed set. In case (b) the degeneracy will arise between two different eigenfunctions which belong to the same Irrep of \mathcal{N} , but in case (c) this degeneracy will arise between a pair of eigenfunctions which belong to inequivalent Irreps of \mathcal{N} . One can imagine what consequences this leaves to the spectrum. The discussion holds also for the gray groups. It is then easy to see what will happen to the energy spectrum is case we add to the 'classical' symmetries of the Hamiltonian also the time-reversal symmetry.

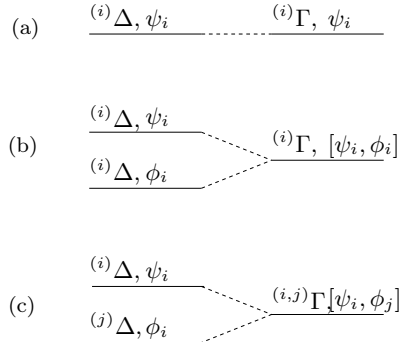


Figure 3: Changes in the degeneracies of the eigenfunctions and eigenvalues for different types of CoIrreps.

4.1.5 Dimmock and Wheeler's character sum rule

To identify the type of CoIrrep associated with a given Irrep Δ of \mathcal{N} , Dimmock and Wheeler [4] devised a test in terms of a character sum rule similar to that of Frobenius and Schur for identifying

the reality type of an Irrep.

$$\sum_{\mathcal{B} \in \mathcal{AN}} {}^{(\mu)}\chi(\mathcal{B}^2) = \begin{cases} n & \text{type (a),} \\ -n & \text{type (b),} \\ 0 & \text{type (c).} \end{cases}$$

4.2 Example: CoIrreps of dichromatic groups derived from \mathcal{D}_4 (422)

The unitary group \mathcal{D}_4 has three subgroups of index 2: $\mathcal{C}_4, \mathcal{D}_2, \mathcal{D}'_2$. These subgroups consist of element: $\mathcal{C}_4 = \{E, C_4, C_4^{-1}, C_2\}$, $\mathcal{D}_2 = \{E, C_2, U^1, U^2\}$ and $\mathcal{D}'_2 = \{E, C_2, U_d^1, U_d^2\}$. Fig. 4 shows the axis of rotation for these group elements.

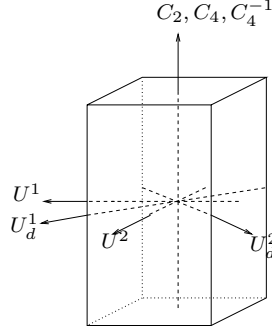


Figure 4: Axes of rotation for group \mathcal{D}_4

The character tables for Irreps of $\mathcal{D}_4, \mathcal{C}_4$ and \mathcal{D}_2 are: We examine different possible subgroups:

	Irreps of \mathcal{D}_4					Irreps of \mathcal{C}_4				Irreps of \mathcal{D}_2					
	E	$2C_4$	C_2	$2U$	$2U_d$	E	C_4	C_4^{-1}	C_2	E	C_2	U^1	U^2	U_d^1	U_d^2
$(1)\Gamma$	1	1	1	1	1	$(1)\Delta$	1	1	1	1	$(1)\Delta$	1	1	1	1
$(2)\Gamma$	1	1	1	-1	-1	$(2)\Delta$	1	-1	-1	1	$(2)\Delta$	1	1	-1	-1
$(3)\Gamma$	1	-1	1	1	-1	$(3)\Delta$	1	i	$-i$	-1	$(3)\Delta$	1	-1	1	-1
$(4)\Gamma$	1	-1	1	-1	1	$(4)\Delta$	1	$-i$	i	-1	$(4)\Delta$	1	-1	-1	1
$(5)\Gamma$	2	0	-2	0	0										

Figure 5: Irreps of $\mathcal{D}_4, \mathcal{C}_4$ and \mathcal{D}_2

- (i) $\mathcal{N} = \mathcal{D}_2$ and $\mathcal{A} = \mathcal{TC}_4$.

This induces the dichromatic point group $\underline{422}$.

The DW sum-rule test yields

$$\begin{aligned} \sum_{\mathcal{B} \in \mathcal{AN}} {}^{(\mu)}\chi(\mathcal{B}^2) &= {}^{(\mu)}\chi((\mathcal{TC}_4)^2) + {}^{(\mu)}\chi((\mathcal{TC}_4^{-1})^2) + {}^{(\mu)}\chi((\mathcal{TU}_d^1)^2) + {}^{(\mu)}\chi((\mathcal{TU}_d^2)^2) \\ &= 2{}^{(\mu)}\chi(C_2) + 2{}^{(\mu)}\chi(E) \end{aligned}$$

and applying this test to the Irreps of \mathcal{D}_2 , we obtain

$$\sum_{\mathcal{B} \in \mathcal{AN}} {}^{(\mu)}\chi(\mathcal{B}^2) = \begin{cases} 4 & \text{for } {}^{(1)}\Delta, {}^{(2)}\Delta, \\ 0 & \text{for } {}^{(3)}\Delta, {}^{(4)}\Delta \end{cases}$$

From this we can conclude that Irreps ${}^{(1)}\Delta$ and ${}^{(2)}\Delta$ are of type (a), so that $\Delta(\mathcal{B}) = \Delta(R)$ where $\mathcal{B} = R\mathcal{A}$. The CoIrreps of the nonunitary $\underline{422}$ obtained from ${}^{(1)}\Delta$ and ${}^{(2)}\Delta$ of \mathcal{D}_2 are given in Fig. 6.

For the ${}^{(3)}\Delta$ and ${}^{(4)}\Delta$, the DW test specifies they are type (c). If we start with ${}^{(4)}\Delta$ we can check that ${}^{(4)}\Delta(S^{-1}RS) = {}^{(3)}\Delta$.

R	$\mathcal{A}^{-1}RA$	${}^{(4)}\Delta(R)$
E	E	${}^{(4)}\Delta(E) = 1$
C_2	C_2	${}^{(4)}\Delta(C_2) = -1$
U^1	U^2	${}^{(4)}\Delta(U^2) = 1$
U^2	U^1	${}^{(4)}\Delta(U^1) = -1$

According to (15) and (17) we can construct the two-dimensional CoRep of $\underline{422}$ from ${}^{(3)}\Delta$ and ${}^{(4)}\Delta$, $\Gamma({}^{(3,4)}\Delta)$. It is given in Fig. 6.

$\underline{422}$	E	C_2	U^1	U^2	ΘC_4	ΘC_4^{-1}	ΘU_d^1	ΘU_d^2
$\underline{422}$	E	C_2	U_d^1	U_d^2	ΘC_4	ΘC_4^{-1}	ΘU^1	ΘU^2
$\Gamma({}^{(1)}\Delta)$	1	1	1	1	1	1	1	1
$\Gamma({}^{(2)}\Delta)$	1	1	-1	-1	1	1	-1	-1
$\Gamma({}^{(3,4)}\Delta)$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$	$\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$

Figure 6: CoIrreps of $\underline{422}$ and $\underline{422}$. Θ stands for time-reversal operation \mathcal{T} .

(ii) $\mathcal{N} = \mathcal{C}_4$ and $\mathcal{A} = \mathcal{T}U^1$.

This induces the dichromatic point group $\underline{422}$.

Since $(\mathcal{T}U^1)^2 = (\mathcal{T}U^2)^2 = (\mathcal{T}U_d^1)^2 = (\mathcal{T}U_d^2)^2 = E$, the DW sum-rule yields +4 for all the Irreps of \mathcal{C}_4 . Hence, all the CoIrreps of $\underline{422}$ are of type (a). Table of CoIrreps of $\underline{422}$ is given in Fig. 7

	E	C_4	C_4^{-1}	C_2	ΘU^1	ΘU^2	ΘU_d^1	ΘU_d^2
$\Gamma^{(1)\Delta}$	1	1	1	1	1	1	1	1
$\Gamma^{(2)\Delta}$	1	-1	-1	1	1	1	-1	-1
$\Gamma^{(3)\Delta}$	1	i	$-i$	-1	1	-1	i	$-i$
$\Gamma^{(4)\Delta}$	1	$-i$	i	-1	1	-1	$-i$	i

Figure 7: Character table for the CoIrreps of $4\bar{2}2$. Θ stands for time-reversal operation \mathcal{T} .

5 Symmetry properties and degeneracies in the electronic band structure of a magnetic crystalline material

Now that we are familiar with the mathematical point of view, we would like to make use of it in a physical context. Beside the fundamental description of magnetically ordered crystals there are many more applications of symmetry arguments.

Because of translational symmetry the wave functions in a crystal can be characterized with wave vector \mathbf{k} and are of the form $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r})$ (Bloch theorem). Because it should possess the translational symmetry, $u_{\mathbf{k}}(\mathbf{r})$ must be invariant under the translations for a vector of Bravais lattice. Since Hamiltonian is invariant under the whole space group of the crystal, for a particular symmetry operation R , in case $\psi(\mathbf{r})$ is an eigenfunction of Hamiltonian then $P_R\psi(\mathbf{r})$ should also be an eigenfunction with the same energy. Let R be an element from point group \mathcal{P} . Since

$$P_R\psi_{\mathbf{k}}(\mathbf{r}) = e^{iR\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(R^{-1}\mathbf{r}) = e^{iR\mathbf{k}\cdot\mathbf{r}}\tilde{u}_{R\mathbf{k}}(\mathbf{r}) = \psi_{R\mathbf{k}}(\mathbf{r})$$

where we used the fact that $\tilde{u}_{R\mathbf{k}}(\mathbf{r})$ is again some periodic function. We can see that all Bloch functions with $\mathbf{k}' = R\mathbf{k}$ will have the same energy

$$E_{\mathbf{k}} = E_{R\mathbf{k}}.$$

If the system possesses also time-reversal symmetry,

$$E_{\mathbf{k}} = E_{-\mathbf{k}},$$

since

$$\mathcal{T}\psi_{\mathbf{k}}(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}^*(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}}\tilde{u}_{-\mathbf{k}}(\mathbf{r}).$$

In this case all the wave vectors transformed under the point group $P' = \mathcal{P} \oplus I\mathcal{P}$, where I is inversion, will have the same energy.

Suppose that the symmetry of a magnetic crystal is described by the non-unitary group $\mathcal{M} = \mathcal{N} \oplus \mathcal{A}\mathcal{N}$, $\mathcal{A} = \mathcal{T}\mathcal{S}$, then it can be shown that the anti-unitary elements cause the energy eigenvalues at \mathbf{k} and $S\mathbf{k}$ to be identical [5]. Then energies corresponding to eigenvectors transformed under the elements of point group $\mathcal{P}' = \mathcal{P} \oplus I\mathcal{S}\mathcal{P}$ will be equal. It should be noted that P' is a classical, type I Schubnikov group.

Set of vectors $R\mathbf{k}$ is called a 'star'. For some special wave vectors \mathbf{k} there might exist operations R under which they are invariant. Group of all such operations R is called the *little group of \mathbf{k}* . The functions $u_{\mathbf{k}}(R^{-1}\mathbf{r})$ form basis vectors for its irreducible representations.

Previously mentioned invariance of wave vectors is meant in a broader sense. When considering only unitary point group operations $R \mathbf{k}$ is equivalent to $\mathbf{k} + \mathbf{K}$ for any reciprocal lattice vector \mathbf{K} . For magnetic space groups the definition of *magnetic little group of $\mathcal{M}^{\mathbf{k}}$* is slightly different. It consists of:

(i) those unitary elements ($\in \mathbf{G}^{\mathbf{k}}$) of the magnetic space group that 'send' \mathbf{k} into $\mathbf{k} + \mathbf{K}$

(ii) those anti-unitary elements ($\in \mathcal{T}\mathbf{G}_{\Gamma}^{\mathbf{k}}$) of the magnetic space group that 'send'⁴ \mathbf{k} into $-\mathbf{k} + \mathbf{K}$

where \mathbf{K} is again a vector of reciprocal lattice. Therefore we may write

$$\mathcal{M}^{\mathbf{k}} = \mathbf{G}^{\mathbf{k}} \oplus \mathcal{T}\mathbf{G}_{\Gamma}^{\mathbf{k}}.$$

The little groups are important for determination of irreducible corepresentations of dichromatic *space* groups, since the procedure discussed in 4 gives us decomposition into CoIrreps only for the dichromatic *point* group. Since Hamiltonian is invariant under the whole dichromatic space group it is the decomposition of space group into its CoIrreps from which we can read the degeneracies in energy spectrum and study the symmetry of eigenstates.

6 Spin waves

When describing the structure of magnetically ordered crystals we have assumed that each individual magnetic moment, or spin, is pointing statically. However at any temperature rather than zero this is not true and we have some fluctuation of the spins. Furthermore, with external influence we can produce spin excitations in the ordered crystal. Using symmetry arguments we can predict possible degeneracies in the spectra of spin excitations, their interaction with lattice vibrations, allowed transitions due to external neutrons and photons, etc.

It is convenient to analyse the variation in the orientation of the spin in terms of normal modes (characterized with wave vector \mathbf{k}) where the quanta is called 'magnon'. The number of allowed magnon frequencies for a given wave vector \mathbf{k} in a magnetic crystal is determined by the number of magnetic atoms in the unit cell of the crystal. One thing we can address using the theory of corepresentations is the symmetry properties of spin-wave relations. Namely, we can label the magnon dispersion relations with the labels of the corepresentation of the appropriate magnetic space group and predict the degeneracies at various points in the Brillouine zone. More precisely, the wave function of a magnon with wave vector \mathbf{k} must belong to one of the irreducible corepresentations of magnetic little group $\mathcal{M}^{\mathbf{k}}$.

6.1 Magnon interaction with phonons

Traditionally it is common to assume that to a very good approximation the lattice vibrations of a crystal are unaffected by the behaviour of any magnetic moments associated with atoms in crystal. Therefore we usually assume that magnetic moments are frozen in their equilibrium positions and not involved in any translational motions. However, so called magnetoelastic waves, which involve

⁴Group element $\mathcal{T}S$ 'sends' \mathbf{k} into $-\mathbf{k} + \mathbf{K}$ in a sense that

$$\hat{p}\mathcal{T}S\psi_{\mathbf{k}} = \mathcal{T}\mathcal{T}^{-1}\hat{p}\mathcal{T}S\psi_{\mathbf{k}} = \mathcal{T}(-\hbar S\mathbf{k})\psi_{S\mathbf{k}} = \hbar(-\mathbf{k} + \mathbf{K})\mathcal{T}S\psi_{\mathbf{k}}$$

where we used that $\mathcal{T}^{-1}\hat{p}\mathcal{T} = -\hat{p}$ and $S\psi_{\mathbf{k}} = \psi_{S\mathbf{k}}$.

both displacement in the position of the atoms and the orientation of the spin vectors were expected theoretically, but also proved experimentally[6]. What is interesting is that it was measured that a given magnon may interact appreciably with certain phonons but not with others [7]. Explanation to that lies in the symmetry.

If \mathcal{H} is the Hamiltonian used to describe the coupled magnetoelastic vibrations of a magnetically ordered crystal, any given magnetoelastic wave must belong to one or other of the irreducible representations of the group of \mathcal{H} , which will be determined by the symmetry of the crystal itself.

In connection with experiments it is tempting to establish selection rules for magnon-phonon interaction, and it should be done for special lines of symmetry in the Brillouin zone. By this we mean the possibility of lifting of an accidental degeneracy between a phonon and a magnon with the same value of \mathbf{k} , caused by magnon-phonon interaction. Rule goes as follows: *If \mathbf{k} is on line of symmetry, the degeneracy can only be lifted if the magnon and the phonon have the same symmetry, i.e. they belong to the same irreducible representations, or corepresentation, of the space group of the crystal*[8]. Since for phonon symmetries it is common to use the classical space group, say \mathcal{G} , in testing the compatibilities it is necessary to use the grey group derived from \mathcal{G} .

Let us assume that group theory has been used to determine which irreducible representations or corepresentations describe the phonons and magnons in crystal, and that it may be possible to distribute these uniquely among the observed branches of the dispersion relations. Then it is possible to see whether any given magnon branch which intersects a certain phonon branch in the non-interaction approximation will be expected to couple with the phonon branch when magnon-phonon interaction is included. Fig. 8 shows experimental result [6] indicating the magnon-phonon interaction measured in uranium dioxide. For temperature $T = 90K$ well above the (transition) Neel temperature they first measured pure phononic dispersion relation $\omega(\mathbf{k})$. Whereas for temperature $T = 9K$ which is below the Neel temperature, so that crystal is magnetically ordered, dispersion is altered due to interaction with magnons, whose dispersion would in the non-interacting limit intersect with the phononic one. This is sketched in the left part of 8.

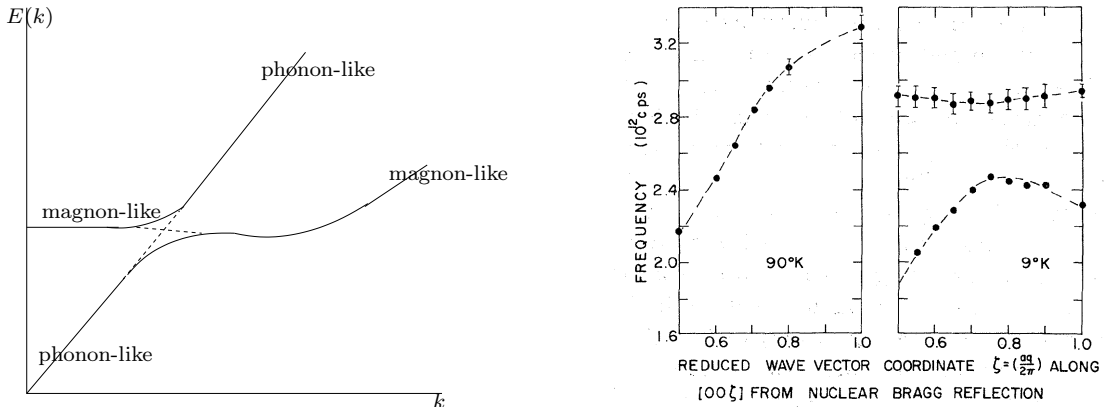


Figure 8: Left: Sketch of degeneracy lifting between the phonon and magnon dispersion as opposed to the non-interacting limit, right: the dispersion curves for the excitations of uranium dioxide in the $[00\xi]$ direction at 9 and $90^\circ K$. At $90^\circ K$ the curve corresponds to the acoustic phonon branch which is modified at $9^\circ K$ by the magnon-phonon interaction[6].

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A Supplement: The time-reversal operator

Let us assume that Hamiltonian is time invariant. From the structure of Schrödinger equation and its conjugation, we can conclude that we need to apply the time inversion to the latter to retain the form of former

$$\begin{aligned}\mathcal{H}\Psi(x, t) &= i\hbar\frac{\partial}{\partial t}\Psi(x, t), \\ \mathcal{H}\Psi^*(x, t) &= -i\hbar\frac{\partial}{\partial t}\Psi^*(x, t) \quad \Rightarrow \quad \mathcal{H}\Psi^*(x, -t) = i\hbar\frac{\partial}{\partial t}\Psi^*(x, t)\end{aligned}\quad (25)$$

which demonstrates that if $\Psi(x, t)$ is a wavefunction that satisfies the Schrödinger equation, then $\Psi^*(x, -t)$ must be a degenerate solution.

Thus time-reversal must involve both complex conjugation and time-inversion operation

$$\mathcal{T} = U\mathcal{K}_0 \quad (26)$$

where U is a unitary operator and \mathcal{K}_0 the conjugation operator, which satisfies $\mathcal{K}_0^2 = \mathbb{I}, \mathcal{K}_0^{-1} = \mathcal{K}_0$. \mathcal{T} has the properties:

- It is *antilinear*

$$\mathcal{T}(a\Psi + b\Phi) = a^*\mathcal{T}\Psi + b^*\mathcal{T}\Phi \quad (27)$$

- It is *antiunitary*

$$(\mathcal{T}\Psi, \mathcal{T}\Phi) = (\Phi, \Psi) \quad (28)$$

- The elements of a point or space group, associated with a physical system, *commute with the time-reversal operator*

$$\mathcal{T}R = R\mathcal{T} \quad (29)$$

and therefore have real representations.

- Transformations of the wavefunction $\psi(x) = \langle x|\psi\rangle$ in the absence of spin under \mathcal{T} :

$$\mathcal{T}|\psi\rangle = \int d^3x \psi^*(x) |x\rangle, \quad \text{where we set the phase } \mathcal{T}|x\rangle = |x\rangle \quad (30)$$

- Transformations of the operators under \mathcal{T} :

$$\mathcal{T}B\mathcal{T}^{-1} = \epsilon_B B, \quad \epsilon_B = \pm 1 \text{ for a general unitary } B \quad (31)$$

$$\mathcal{T}x\mathcal{T}^{-1} = x \quad (32)$$

$$\mathcal{T}p\mathcal{T}^{-1} = -p \quad (33)$$

$$\mathcal{T}L\mathcal{T}^{-1} = -L \quad (34)$$

For the nonrelativistic spin- $\frac{1}{2}$ particles we demand

$$\mathcal{T}S\mathcal{T}^{-1} = -S \quad \rightarrow \quad \mathcal{T}J\mathcal{T}^{-1} = -J \quad (35)$$

which is satisfied with $\mathcal{T} = e^{-i\pi S_y/\hbar} K_0$, $\mathcal{D}(\mathcal{T}^2) = -\mathbb{I}$