

A walk through of the maths behind Bertaut's method of representational analysis of magnetic structures – ERICE Workshop, June 2019

Andrew S. Wills

Department of Chemistry, University College London

<http://fermat.chem.ucl.ac.uk/spaces/willsgroup>

ver: June 2019

This text presents a walk through of the basic matrix maths of calculating the basis vectors of a magnetic structure using the representational analysis techniques developed by Felix Bertaut. Its goals are to show clearly how to apply the key equations, and to enable the reader to better understand results presented in the literature and created by SARA h -Representational Analysis¹.

¹<http://fermat.chem.ucl.ac.uk/spaces/willsgroup>

1 Symmetry in the Solid State

1.1 Introduction

The aim of this section of the course is to reiterate the concepts of symmetry that you are hopefully already familiar with. A very important extension will also be made to describe the translational properties of extended lattices and the following discussion will be restricted to solids that have long-range translational order, *i.e.* to crystals.

Reading:

- Chemical Applications of Group Theory, F. A. Cotton (John Wiley and Sons, New York 1971) Chapters 4-6.
- Symmetry Principles and Magnetic Symmetry in Solid State Physics, S.J. Joshua (Adam Hilger, Bristol, 1991) Chapters 2 and 3.

1.2 Extending Symmetry Operations From a Molecule to a Solid

I will assume that the reader is familiar with the concepts of molecular symmetry: of point groups, their symmetry operations, the character tables of their irreducible representations, and the basis functions associated with them that can be used to describe the atomic orbitals or molecular vibrations. What we will now do is expand upon these ideas and bring them into the context of the crystalline solid: a system with translational symmetry.

The first things that we must extend when we go from a molecule to a crystalline solid are the symmetry operations themselves. While for a molecule and a point group there are 5 types of symmetry operation (Table 1), in a solid, translations are also possible. These give rise to 2 new types of symmetry operations (Table 2).

The simplest mathematical description of a symmetry operation is a matrix that acts to change the coordinates of a point. If we are dealing with a molecule and a symmetry operations

Symmetry operation	Symmetry element	Symbol
Identity (do nothing)		E
Rotation by $360^\circ/n$ (a 'proper' rotation)	n -fold axis	C_n
Reflection	mirror plane	σ_v, σ_h or σ_d
Inversion	Centre of inversion	i
Rotation by $360^\circ/n$ followed by inversion (an 'improper' rotation)	n -fold axis + a centre of inversion	S_n

Table 1: Symmetry operations in point groups (isolated molecules).

Symmetry operation	Symmetry element	Symbol
Rotation + translation	Screw axis	N_j
Reflection + translation	Glide plane	a, b, c, n, d

Table 2: Additional symmetry operations present in extended solids (crystals).

without translations, they can be represented as 3×3 matrices. For example, the operations E , I , and C_{2z} can be represented by the following matrices:

$$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (1)$$

$$I = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \quad (2)$$

$$C_{2z} = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (3)$$

The operation of a rotational symmetry element, R , on an atomic position vector r to create the new position vector r' is therefore

$$r' = Rr \quad (4)$$

As an example let's apply these symmetry operations to a position with the coordinates

(x, y, z) . The position generated by the application of E to (x, y, z) is:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \quad (5)$$

The position generated by the application of the inversion centre, I , to (x, y, z) is:

$$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \bar{x} \\ \bar{y} \\ \bar{z} \end{pmatrix} \quad (6)$$

The position generated by the application of the reflection C_{2z} to (x, y, z) is:

$$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \bar{x} \\ \bar{y} \\ z \end{pmatrix} \quad (7)$$

In the case of screw axes and glide planes, *i.e.* symmetry operations that involve a translation, we can either write the action of the symmetry operation on the point (x, y, z) in a form with separate rotational and translational parts. As an example, let's look at the screw axis made up of the C_{2z} rotation and the translation $(0.75 \ 0.25 \ 0.5)$. This can be written in separate parts as a rotation followed by a translation:

$$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0.75 \\ 0.25 \\ 0.5 \end{pmatrix} \quad (8)$$

or as a combined (4×4) matrix

$$\begin{pmatrix} \bar{1} & 0 & 0 & 0.75 \\ 0 & \bar{1} & 0 & 0.25 \\ 0 & 0 & 1 & 0.5 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (9)$$

For clarification, the combined form is made up of the rotational part:

$$\begin{pmatrix} \bar{1} & 0 & 0 & - \\ 0 & \bar{1} & 0 & - \\ 0 & 0 & 1 & - \\ - & - & - & - \end{pmatrix} \quad (10)$$

and the translational part:

$$\begin{pmatrix} - & - & - & 0.75 \\ - & - & - & 0.25 \\ - & - & - & 0.5 \\ - & - & - & - \end{pmatrix} \quad (11)$$

, with some zeros and a '1' that are required to finish the matrix

$$\begin{pmatrix} - & - & - & - \\ - & - & - & - \\ - & - & - & - \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (12)$$

Question: Work through the above matrix equation to convince yourself that the application of the 4×4 matrix is indeed equivalent to use of a 3×3 matrix and a separate translation part.

1.3 From 32 Point Groups to 230 Space Groups

Now that we have extended our notions of symmetry operations from a point to a crystalline solid, it is useful to introduce the concept of a space group. Just as the set of rotational symmetry operations that describe a point is called a point group, the set of rotation-translation operations that describe a propagating space is called a space group. The properties of a space group are exactly the same as those of a point group - they both follow the mathematical rules for a group. If G is a group, the symmetry elements A, B, C, \dots follow the rules shown in Table 3:

Given these rules and the different types of translational symmetry (screw axes and glide planes) that are possible in a solid, it can be shown that there are 230 types of space groups for three dimensional systems- solids are therefore far more complex than molecules, where commonly only 32 point groups are used.

1.	they are a set of elements	A, B, C, \dots
2.	the product of 2 elements is also a member of the group	$AB \in G$
3.	the product is associative	$A(BC) = (AB)C$
4.	there exists a unique identity element	E
5.	every element has a unique inverse	$AA^{-1} = A^{-1}A = E$

Table 3: The definition of the Group G in terms of its symmetry elements.

In the rest of this text we will use the notation G_0 to represent the space group of the crystal before the magnetic transition.

1.4 Propagation of a magnetic structure through a crystal– Bloch waves

Crystal structures are constructed from a unit cell that is repeated along the three directions of the crystal axes. Collective phenomena, such as vibrations or electronic bands, also propagate through the crystal structure. The propagation of magnetic structures through a solid can be described using plane waves, *Bloch* waves. These define the atomic moments of any atom by relating it to that of the related atom in the zeroth unit cell using a phase relation. The phase relation is defined by the translational separation, \vec{t} , of the two atoms and a propagation vector, \vec{k} .²

If the moment vector of an atom in the zeroth cell, atom i , is given by $\vec{V}_i = (m_{ai} \ m_{bi} \ m_{ci})$ and $\vec{V}_j = (m_{aj} \ m_{bj} \ m_{cj})$ corresponds to that for another equivalent atom, atom j , that is related to the first by the translation $\vec{t} = \vec{V}_j - \vec{V}_i$. The magnetic moment of atom j with respect to atom i is given by:

$$\vec{V}_j = \vec{V}_i \exp(-2\pi\vec{k} \cdot \vec{t}) \quad (13)$$

which is the equation of a plane wave. Expanding the exponential this can be written:

²I am using the arrow vector notation to emphasise that we are working with vectors as it is very important to follow the phases determined from related scalar products.

$$\tilde{V}_j = \tilde{V}_i [\cos(-2\pi\vec{k} \cdot \vec{t}) + i\sin(-2\pi\vec{k} \cdot \vec{t})] \quad (14)$$

If \vec{k} and \vec{t} are such that the sine component vanishes, we see that the moment vector propagates as a cosine function.

$$\tilde{V}_j = \tilde{V}_i \cos(-2\pi\vec{k} \cdot \vec{t}) \quad (15)$$

From this we see that \vec{k} corresponds to a frequency of the wave measured in terms of unit cells. (As it is a reciprocal space vector, it is also the inverse of the wavelength.)

1.4.1 The Little Group G_k

The symmetry operations of G_0 that are consistent with the translational periodicity defined by \vec{k} are those that leave the \vec{k} vector invariant. Only the rotational parts of the symmetry operations change \vec{k} . Therefore, if the action of the rotational part of a symmetry operation on \vec{k} is written

$$\vec{k}' = \vec{k}R \quad (16)$$

, then the symmetry operations that leave \vec{k} invariant are those that obey the equation

$$\vec{k}' = \vec{k} \pm \vec{\tau} \quad (17)$$

where $\vec{\tau}$ is a primitive lattice vector. The group of symmetry operations that obey this relation are called the ‘group of the propagation vector’, or the little group G_k .

Confusion can often be caused when working with space groups in a centred setting, for example $\vec{k} = (0 \ 0 \ 1)$ in a body-centred lattice corresponds to $\vec{k} = (0.5 \ 0.5 \ 0.5)$ in a primitive setting. For ease, it is recommended to convert propagation vectors and space group symmetry operations to a primitive setting when determining the little groups G_k .

An extension to G_k can be made by bringing together several symmetry-related propagation vectors, $\vec{k}_1, \vec{k}_2, \dots$ to form $G_{\{k\}}$. Such magnetic structures are termed multi-k structures. Particularly important with using Landau theory is the extended group $G_{k,-k}$ as this brings together complex basis vectors with their complex conjugate to make real moments.

1.4.2 From Space Groups, G_0 , to Little Groups, G_k

At the moment we have discussed only crystallographic space groups. It is important to realise that other types of space groups are possible: ones made up of only some of the elements of a crystallographic space group. While these space groups follow all the rules of groups, they do not contain enough symmetry elements to describe a crystal structure - they are subgroups of the crystallographic space groups. To make the subgroups of a group, its symmetry operations are divided in such a way that each subgroup contains the same number of symmetry operations, *i.e.* the subgroups are of the same order. No symmetry operations are shared between the subgroups and they are independent groups.

In this section we introduced the propagation vector, \vec{k} , and divide the space groups into symmetry elements according to how they changed \vec{k} ; we classified the symmetry operations according to the symmetry of how they affect \vec{k} : whether they change it or leave it invariant. As an example, let's look at the primitive orthorhombic space group ($Pmn2_1$, number 31) which has the following symmetry operations:

- $g_1: x, y, z$
- $g_2: \bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$
- $g_3: x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$
- $g_4: \bar{x}, y, z$

Let's first consider the application of these operations on the following propagation vectors $\vec{k}_1 = (0\ 0\ 0)$, $\vec{k}_2 = (0\ 0\ 0.5)$, $\vec{k}_3 = (0.1\ 0\ 0)$. **(Remember that only the rotational part is used.)**

Trivially, we see that for $\vec{k}_1 = (0\ 0\ 0)$ all the symmetry elements leave it invariant

$$\vec{k}_2 = (0\ 0\ 0.5) \text{ gives } g_1 \vec{k}_2 = (0\ 0\ 0.5)$$

similarly

$$\vec{k}_2 g_2 = (0\ 0\ 0.5)$$

$$\vec{k}_2 g_3 = (0\ 0\ 0.5)$$

$$\vec{k}_2 g_4 = (0\ 0\ 0.5)$$

Again, all the symmetry operations leave this propagation vector invariant

Now changing to $\vec{k}_3 = (0.1\ 0\ 0)$, as find that action of these symmetry operations on \vec{k}_3 gives:

$$\vec{k}_3 g_1 = (0.1\ 0\ 0)$$

$$\vec{k}_3 g_2 = (-0.1\ 0\ 0)$$

$$\vec{k}_3 g_3 = (0.1\ 0\ 0)$$

$$\vec{k}_3 g_4 = (-0.1\ 0\ 0)$$

so we see that the action of the symmetry operations on the last propagation vector, \vec{k}_3 , separates them into 2 classes: those that leave \vec{k}_3 invariant (g_1 and g_3), and those that form the symmetry-related propagation vector : \vec{k}_3 , *i.e.* g_2 and g_4 .

1.5 Effects of Symmetry Operations on an Atom and its Magnetic Moment

Once we have defined the periodicity of how the magnetic structure propagates through the crystal and found which symmetry operators are compatible with it, *i.e.* those that leave the propagation \vec{k} invariant, we can begin to look at the symmetry of the magnetic atoms. The start-

ing place is to examine the symmetry of the atom under the symmetry operations compatible with the magnetic structures propagation vector.

The application of a symmetry operation on a vibrating atom in a solid has two distinct effects:

1. To move the atom, *i.e.* to change the atom's position
2. To change the direction of the axial vector that we use to represent the moment of that atom

The operations of all the symmetry elements of the group on all the atomic positions and all of the displacement vectors, can be described using a large matrix called the *magnetic representation*, Γ_{mag} . We will now explore in detail the action of the symmetry operations separately on the atomic positions and their atomic moment vectors.

1.5.1 Effects of Symmetry Operations on an Atom position- The Permutation Representation, Γ_{perm}

The first thing that we will look at is how the atomic positions are changed by the symmetry operations of a space group, G_0 .

Recap: a crystal appears invariant under all of the symmetry operations of its space group. However, equivalent atoms can be **interchanged**, or **permuted**, under the different symmetry operations.

If \vec{r}_i is the atomic position vector, the operation of a symmetry element, g , on an atomic position can be symbolically stated as

$$g(\vec{r}_i) = \vec{r}_j \quad (18)$$

If we label the atoms $a, b, c, \text{etc.}$, the symmetry operation will permute some of the atomic labels.

An example: Take three equivalent positions: $a = (0.25 \ 0.5 \ 0)$, $b = (-0.25 \ -0.5 \ 0)$, $c = (0 \ 0 \ 0)$. Application of the symmetry operation $g = C_{2z}$ to each of these creates the following positions:

$$g(a) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0.25 \\ 0.5 \\ 0 \end{pmatrix} = \begin{pmatrix} -0.25 \\ -0.5 \\ 0 \end{pmatrix} = b \quad (19)$$

$$g(b) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -0.25 \\ -0.5 \\ 0 \end{pmatrix} = \begin{pmatrix} 0.25 \\ 0.5 \\ 0 \end{pmatrix} = a \quad (20)$$

$$g(c) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} = c \quad (21)$$

If we represent the set of atomic labels by a column matrix, P , this operation can be written as

$$g(P) = P' \quad (22)$$

$$g \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} b \\ a \\ c \end{pmatrix} \quad (23)$$

The way that all the symmetry operations of a group permute the labels of all equivalent atoms can be represented by a large matrix, called the *permutation representation*, Γ_{perm} , whose matrix representative is of order N , where N is the number of equivalent atoms that we are looking at. Strictly, the permutation representation corresponds to all the different positions in a crystal, but we can limit ourselves to initial positions in the primitive nuclear cell.

Example: the point group C_2 has 2 symmetry operations: the identity, E , and the 2-fold rotation C_{2z} . The permutation of the three equivalent positions: $a = (0.25 \ 0.5 \ 0)$, $b = (-0.25 \ -0.5 \ 0)$, $c = (0 \ 0 \ 0)$ under the symmetry operation E is

$$E \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad (24)$$

and so the matrix representative, is

$$\Gamma_{perm}^E(P) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad (25)$$

Under C_{2z} the labels permute as

$$C_{2z} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} b \\ a \\ c \end{pmatrix} \quad (26)$$

and so

$$\Gamma_{perm}^{C_{2z}}(P) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad (27)$$

The character of the permutation representation for a symmetry operation, $\chi_{perm}(g)$ is simply the number of position labels that are unchanged under its action, *e.g.* in this case

$$\chi_{perm}(C_{2z}) = 1 \quad (28)$$

$$\chi_{perm}(E) = 3 \quad (29)$$

It is important to note that when a symmetry operation results in an atomic position that is outside the *zeroth* cell, a phase factor must be included that relates the generated position to that in the *zeroth* cell. This phase is simply given by:

$$\theta = -2\pi \vec{k} \cdot \vec{r}_{rtn} \quad (30)$$

where $\vec{\tau}_{rtn}$ is the translation vector, that relates the position vectors of the original (seed) and generated atoms: $\vec{r}_{seed} = \vec{r}_{new} + \vec{\tau}_{rtn}$. This translation is applied to phase the Bloch wave of the generated atom, back to the seed atom in accordance with the k -vector.

1.5.2 Magnetic Moments: (Pseudo) Axial Vectors

An atomic moment is described by an axial vector, for convenience, in the axis system of the point or space group that we are using. We will always refer to moment components defined with respect to the crystallographic axes, not Cartesian projections. (Symmetry theory is always simpler in an axis system matched to the problem, and in this case that is the crystal structure.) Taking the moment vector of an atom to be $\vec{V} = (m_a, m_b, m_c)$, then the action of a rotational symmetry element is simply

$$\vec{V}' = R\vec{V} \times \det(R) \quad (31)$$

Where the determinant $\det(R)$ is required to describe the current loop type symmetry of an axial vector, *i.e.* that is is not reversed by the inversion operation.

If $R = C_{2z}$, with $\det(R) = 1$ we have

$$R = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (32)$$

then

$$\vec{V}' = (-m_a, -m_b, m_c) \quad (33)$$

The axial vector representation, Γ_{axial} , describes how the components of a moment vector are changed by the different symmetry operations. The character for a given symmetry operation describes what component of the a component is left unchanged, the b component that is

unchanged, and the c component that is unchanged. Numerically, it is simply the trace (the sum of the leading diagonal elements) of the rotation matrix of the symmetry operation multiplied by the determinant of the rotation matrix.

Thus, for the point group C_2 ,

$$\chi_{axial}(E) = (1 + 1 + 1) \times 1 = 3 \quad (34)$$

and

$$\chi_{axial}(C_{2z}) = (-1 - 1 + 1) \times 1 = -1 \quad (35)$$

1.5.3 The Magnetic Representation

The magnetic representation, Γ_{vib} , describes both the result of the symmetry operation on the atomic positions and on the axial vectors that describe the atomic moments. As these effects are independent, the magnetic representation is given by their direct product:

$$\Gamma_{mag} = \Gamma_{axial} \times \Gamma_{perm} \quad (36)$$

Or, in terms of the matrices for the representations themselves

$$D_{mag} = D_{axial} \times D_{perm} \quad (37)$$

The characters of these representations are related according to:

$$\chi_{mag} = \chi_{axial} \times \chi_{perm} \quad (38)$$

1.6 Irreducible Representations of the Space Groups

1.6.1 Irreducible Representations Revisited

Recap: Irreducible representations are matrices that map onto the algebra of the space group symmetry operations. Irreducible representations are of particular significance because they are the smallest unique blocks out of which all other representations can be made. In other words, any representation can be written in terms of the different irreducible representations of the group: the representation can be decomposed into irreducible representations. The dimensionality of an irreducible representation is the dimensionality of the matrix representatives of the representation.

1.6.2 Basis Vectors and Basis Vector Space

Symmetry adapted linear combinations, also called *basis vectors*, are obtained by projection from test functions components that are compatible with one row of an irreducible representation matrix. Only functions that have the same symmetry as the irreducible representations under all of the different symmetry operations of the group give non-zero results – these are the *symmetry adapted linear combinations*.

1.7 Decomposition of the Magnetic Representation into Irreducible Representations of G_k

Γ_{mag} describes how the atomic moments change under all the different symmetry operations of a space group. It is reducible and can be written in terms of the irreducible representations of the space group, *i.e.* Γ_{mag} can be decomposed into the irreducible representations of the space group G_k . In this case, the magnetic representation for an atomic site can be decomposed into contributions from the irreducible representations of the little group:

$$\Gamma_{vib} = \sum_{\nu} n_{\nu} \Gamma_{\nu} \quad (39)$$

where n_{ν} is the number of times the irreducible representation Γ_{ν} appears in the vibrations representation Γ_{vib} . n_{ν} is given by:

$$n_{\nu} = \frac{1}{n(G_k)} \sum_{g \in G_k} \chi_{\Gamma_{mag}}(g) \chi_{\Gamma_{\nu}}(g)^* \quad (40)$$

Here, $\chi_{\Gamma_{mag}}(g)$ is the character of the magnetic representation and $\chi_{\Gamma_{\nu}}(g)^*$ is the complex conjugate of the character of the irreducible representation with index ν for element g .

The decomposition of Γ_{mag} into the irreducible representations of the little group G_k gives the number of basis vectors that contribute to Γ_{mag} from each irreducible representation, *e.g.* if the decomposition reads

$$\Gamma_{mag} = 1\Gamma_1^{(1)} \oplus 1\Gamma_2^{(2)} \quad (41)$$

(Here I am using a notation where the superscript represents the order of the irreducible representation and the subscript is its index or label.) We see that Γ_{mag} contains irreducible representation number 1 (which is of order 1) once, and irreducible representation number 2 (which is of order 2) once. This means that Γ_{mag} contains one basis vector associated with Γ_1 and two associated with Γ_2 . The \oplus indicates that the symmetry spaces are joined : this operation is also called the *direct sum*.

1.8 Projection of the Basis Vectors for Atomic Moments– Magnetic Structure Symmetry Types

Calculation of the basis vectors is done using the projection operator technique, which involves taking a test function and projecting from it the part that transforms according to each of the irreducible representations. We will use the notation $\vec{\psi}_n$ as the basis vector that transforms

according to the μ dimensional representation Γ_ν^μ , and D_ν is the matrix representative of the irreducible representation with index ν . The test functions that we will use are

$$\vec{\phi}_1 = (1 \ 0 \ 0) \quad (42)$$

$$\vec{\phi}_2 = (0 \ 1 \ 0) \quad (43)$$

$$\vec{\phi}_3 = (0 \ 0 \ 1) \quad (44)$$

The projection process determines the component of the test function that transforms according to the irreducible representation that is under investigation. If there is, it gives it (this is what the basis vector is). If there isn't, it gives zero. The projection operator formula is:

$$\vec{\psi}_{\alpha\nu}^\lambda = \sum_{g \in G_k} D_\nu^{\lambda*}(g) \sum_i \delta_{i,gi} R_g \vec{\phi}_\alpha \det(R_g) \quad (45)$$

Explaining each symbol from left to right:

- $\vec{\psi}_{\alpha\nu}^\lambda$ is the basis vector projected from the λ th row of the ν th irreducible representation using the test vector $\vec{\phi}_\alpha$
- $g \in G_k$ means that the sum is over the symmetry elements that are in G_k
- $D_\nu^{\lambda*}(g)$ is the complex conjugate of the element of the matrix representative that is being examined: it is the λ th row of the matrix representative of the ν th irreducible representation, for symmetry operation g
- \sum_i means that the following summation is over all of the atomic positions that are related by the symmetry elements of the space group

- $\delta_{i,gi}$ is the Kronecker delta and means that effectively the sum is only over the symmetry elements that move an atom to a position that has the same label
- R_g is the rotational part of the symmetry operation g . (The translational parts are only required when looking at the effects of the symmetry operation on the atomic positions, and not on the polar vector which describes the displacement)
- $\vec{\phi}_\alpha$ is our test function.
- $\det(R_g)$ is the determinant of the rotation operation R_g

During the projection process we:

1. Chose an irreducible representation
2. Chose a row

for **each** element of that row we

1. Chose $\vec{\phi}_1$ (i.e. $\alpha = 1$)
2. Project out any components of $\vec{\phi}_1$ that correspond to that element of the matrix representative and note the atomic position generated
3. If the total basis function component that results, $\vec{\psi}_{\alpha\nu}^\lambda$, is non-zero for an atomic position, we keep it
4. Chose $\vec{\phi}_2$ (i.e. $\alpha = 2$)
5. Project out any components of $\vec{\phi}_2$ that correspond to that element of the matrix representative and note the atomic position generated

6. If the sum of the basis function components that results for an atomic position is non-zero, we keep it
7. Chose $\vec{\phi}_3$ (i.e. $\alpha = 3$)
8. Project out any components of $\vec{\phi}_3$ that correspond to that element of the matrix representative and note the atomic position generated
9. If the sum of the basis function components that results for an atomic position is non-zero, we keep it

This process is repeated for all elements of *one* row and then repeated for the next irreducible representation, *etc.* Of course, the number of non-zero unique projected components for a representation is of course the same as calculated using

$$n_\nu = \frac{1}{n(G_k)} \sum_{g \in G_k} \chi_{\Gamma_{mag}}(g) \chi_{\Gamma_\nu}(g)^* \quad (46)$$

1.9 Example of Projection of Symmetry Adapted Displacement Vectors

1.9.1 Required information

Space group: *Ama2*

k vector : (0 0 0)

Calculate the magnetic basis functions for an atom at position X_1 : (0 0 0)

The symmetry operators in G_0 are :

$$g_1 = (x, y, z) \quad (47)$$

$$g_2 = (-x, -y, z) \quad (48)$$

$$g_3 = \left(x + \frac{1}{2}, -y, z\right) \quad (49)$$

$$g_4 = \left(-x + \frac{1}{2}, y, z\right) \quad (50)$$

1.9.2 How does the propagation vector $\vec{k} = (0, 0, 0)$ change under the symmetry operations of G_0 ?

(Remember that we only need to consider the rotational part for this)

$$\vec{k}R_1 = (0\ 0\ 0) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (51)$$

$$\vec{k}R_2 = (0\ 0\ 0) \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (52)$$

$$\vec{k}R_3 = (0\ 0\ 0) \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (53)$$

$$\vec{k}R_4 = (0\ 0\ 0) \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (54)$$

Under all the symmetry operations \vec{k} is changed into \vec{k} , that is to say that they all leave it unchanged. Therefore all the symmetry operators are in G_k and $G_k = G_0$.

1.9.3 How does the atomic position $X_1 : (0\ 0\ 0)$ change under the symmetry operations of G_k ?

Application (of the rotational/translational operations) to position $X_1 : (0\ 0\ 0)$ gives:

$$g_1 X_1 = (0\ 0\ 0) \quad (55)$$

$$g_2 X_1 = (0\ 0\ 0) \quad (56)$$

$$g_3 X_1 = (0.5\ 0\ 0) \quad (57)$$

$$g_4 X_1 = (0.5\ 0\ 0) \quad (58)$$

There are therefore 2 symmetry related positions generated by the application of G_0 to position X_1 : $X_1 = (0\ 0\ 0)$ and $X_2 = (0.5\ 0\ 0)$.

How do these positions (the *equivalent positions* of a Wyckoff site) permute under the symmetry operations in G_k ?

	$X_1 : (0\ 0\ 0)$	$X_2 : (0.5\ 0\ 0)$
g_1	(0 0 0)	(0.5 0 0)
g_2	(0 0 0)	(-0.5 0 0)
g_3	(0.5 0 0)	(1 0 0)
g_4	(0.5 0 0)	(0 0 0)

Table 4: Table showing how the atom positions and labels permute under the symmetry operations of G_k .

As a crystal structure is made up of unit cells that translate in space, the position (1 0 0) is related to the seed position (0 0 0). The vector that relates positions generated in a neighbouring cell to that in the zeroth cell gives rise to a translational phase. So, this table can be written:

	$X_1 : (0\ 0\ 0)$	$X_2 : (0.5\ 0\ 0)$
g_1	(0 0 0)	$(0.5\ 0\ 0) + \vec{\tau} = (0.5\ 0\ 0); \vec{\tau} = (0\ 0\ 0)$
g_2	(0 0 0)	$(-0.5\ 0\ 0) + \vec{\tau} = (0.5\ 0\ 0); \vec{\tau} = (1\ 0\ 0)$
g_3	(0.5 0 0)	$(1\ 0\ 0) + \vec{\tau} = (0\ 0\ 0); \vec{\tau} = (-1\ 0\ 0)$
g_4	(0.5 0 0)	$(0\ 0\ 0) + \vec{\tau} = (0\ 0\ 0); \vec{\tau} = (0\ 0\ 0)$

Table 5: Table showing how the atom positions and labels permute under the symmetry operations of G_k with some of the translation vectors that return the generated position to the seed position, $\vec{\tau}$.

The permutation of the atom labels and the character of the permutation representation involves a phase related to the k-vector and this returning vector, $\exp(-2\pi i \vec{k} \cdot \vec{\tau})$, and is therefore:

	$X_1 : (0\ 0\ 0)$	$X_2 : (0.5\ 0\ 0)$	$\chi_{perm}(g_n)$
g_1	X_1	X_2	2
g_2	X_1	$X_2 \cdot \exp(0)$	2
g_3	X_2	$X_1 \cdot \exp(0)$	0
g_4	X_2	$X_1 \cdot \exp(0)$	0

Table 6: Table showing how the atom labels permute under the symmetry operations of G_k and the character of the permutation representation.

1.9.4 What is the character of the axial vector representation, Γ_{axial} ?

The character of the axial vector is the trace of the rotational part of the symmetry operators multiplied by the determinant of the rotation matrix. For all the following operations $\det(g) = +1$, so the character $\chi(g)$ is simply the trace of the rotation matrix :

$$R_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (59)$$

$$\text{trace } R_1 = (1 + 1 + 1) \times 1 = 3$$

$$R_2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (60)$$

$$\text{trace } R_2 = (-1 - 1 + 1) \times 1 = -1$$

$$R_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (61)$$

$$\text{trace } R_3 = (1 - 1 + 1) \times -1 = -1$$

$$R_4 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (62)$$

$$\text{trace } R_4 = (-1 + 1 + 1) \times -1 = -1$$

1.9.5 Calculate the decomposition of the magnetic representation into the irreducible representations of G_k

The first step is to calculate the character of the axial representation, χ_{axial}

	g_1	g_2	g_3	g_4
$\chi_{perm}(g_n)$	2	2	0	0
$\chi_{axial}(g_n)$	3	-1	-1	-1
$\chi_{mag}(g_n)$	6	-2	0	0

Table 7: Table showing the characters of the permutation, axial and magnetic representations.

The irreducible representations of G_k are

	g_1	g_2	g_3	g_4
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1	-1	-1	1
Γ_4	1	-1	1	-1

Table 8: Table showing the irreducible representations of the little group G_k .

Given

$$n_\nu = \frac{1}{n(G_k)} \sum_{g \in G_k} \chi_{\Gamma_{mag}}(g) \chi_{\Gamma_\nu}(g)^* \quad (63)$$

for $\nu = 1$ (i.e. Γ_1) we have

$$n_1 = 1/4[1 \times 6 + 1 \times (-2) + 1 \times 0 + 1 \times 0] = 1/4[4] = 1 \quad (64)$$

for $\nu = 2$ (i.e. Γ_2)

$$n_2 = 1/4[1 \times 6 + 1 \times (-2) + (-1) \times 0 + (-1) \times 0] = 1/4[4] = 1 \quad (65)$$

for $\nu = 3$ (i.e. Γ_3)

$$n_3 = 1/4[1 \times 6 + (-1) \times (-2) + (-1) \times 0 + 1 \times 0] = 1/4[8] = 2 \quad (66)$$

for $\nu = 4$ (i.e. Γ_4)

$$n_4 = 1/4[1 \times 6 + (-1) \times (-2) + 1 \times 0 + (-1) \times 0] = 1/4[8] = 2 \quad (67)$$

The decomposition of Γ_{mag} into irreducible representations of G_k is therefore

$$\Gamma_{mag} = 1\Gamma_1 \oplus 1\Gamma_2 \oplus 2\Gamma_3 \oplus 2\Gamma_4 \quad (68)$$

1.9.6 Calculate the basis vectors associated with each irreducible representation

Given the equation for the projection operation:

$$\vec{\psi}_{\alpha\nu}^{\lambda} = \sum_{g \in G_k} D_{\nu}^{\lambda*}(g) \sum_i \delta_{i,gi} R_g \vec{\phi}_{\alpha} \det(R_g) \quad (69)$$

, project out the basis functions associated with the irreducible representations of G_k .

for Γ_1	$R_1:$	$R_2:$	$R_3:$	$R_4:$
R_n	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
operate on X_1	X_1	X_1	X_2	X_2
D_1^{1*}	1	1	1	1
$D_1^{1*} \times R_n \times \det(R)$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
$\vec{\phi}_1$	(1 0 0)	(1 0 0)	(1 0 0)	(1 0 0)
$D_1^{1*} \times R_n \times \det(R) \times \vec{\phi}_1$	(1 0 0)	(-1 0 0)	(-1 0 0)	(1 0 0)
Sum basis vectors of each atom type	(0 0 0)		(0 0 0)	
$\vec{\phi}_2$	(0 1 0)	(0 1 0)	(0 1 0)	(0 1 0)
$D_1^{1*} \times R_n \times \det(R) \times \vec{\phi}_2$	(0 1 0)	(0 -1 0)	(0 1 0)	(0 -1 0)
Sum basis vectors of each atom type	(0 0 0)		(0 0 0)	
$\vec{\phi}_3$	(0 0 1)	(0 0 1)	(0 0 1)	(0 0 1)
$D_1^{1*} \times R_n \times \det(R) \times \vec{\phi}_3$	(0 0 1)	(0 0 1)	(0 0 -1)	(0 0 -1)
Sum basis vectors of each atom type	(0 0 2)		(0 0 -2)	

Table 9: Table showing the projection of basis vectors from Γ_1 for the positions $X_1 = (0\ 0\ 0)$ and $X_2 = (0.5\ 0\ 0)$.

So the non-zero basis vector components on each atom are:

	X_1	X_2
$\vec{\psi}_1$	(0 0 2)	(0 0 -2)

for Γ_2	$R_1:$	$R_2:$	$R_3:$	$R_4:$
R_n	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
operate on X_1	X_1	X_1	X_2	X_2
D_2^{1*}	1	1	-1	-1
$D_2^{1*} \times R_n \times \det(R)$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$\vec{\phi}_1$	(1 0 0)	(1 0 0)	(1 0 0)	(1 0 0)
$D_2^{1*} \times R_n \times \det(R) \times \vec{\phi}_1$	(1 0 0)	(-1 0 0)	(1 0 0)	(-1 0 0)
Sum basis vectors of each atom type	(0 0 0)		(0 0 0)	
$\vec{\phi}_2$	(0 1 0)	(0 1 0)	(0 1 0)	(0 1 0)
$D_2^{1*} \times R_n \times \det(R) \times \vec{\phi}_2$	(0 1 0)	(0 -1 0)	(0 -1 0)	(0 1 0)
Sum basis vectors of each atom type	(0 0 0)		(0 0 0)	
$\vec{\phi}_3$	(0 0 1)	(0 0 1)	(0 0 1)	(0 0 1)
$D_2^{1*} \times R_n \times \det(R) \times \vec{\phi}_3$	(0 0 1)	(0 0 1)	(0 0 1)	(0 0 1)
Sum basis vectors of each atom type	(0 0 2)		(0 0 2)	

Table 10: Table showing the projection of basis vectors from Γ_2 for the positions $X_1 = (0\ 0\ 0)$ and $X_2 = (0.5\ 0\ 0)$.

So the non-zero basis vector components on each atom are:

	X_1	X_2
$\vec{\psi}_2$	(0 0 2)	(0 0 2)

for Γ_3	$R_1:$	$R_2:$	$R_3:$	$R_4:$
R_n	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
operate on X_1	X_1	X_1	X_2	X_2
D_3^{1*}	1	-1	-1	1
$D_3^{1*} \times R_n \times \det(R)$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
$\vec{\phi}_1$	(1 0 0)	(1 0 0)	(1 0 0)	(1 0 0)
$D_3^{1*} \times R_n \times \det(R) \times \vec{\phi}_1$	(1 0 0)	(1 0 0)	(1 0 0)	(1 0 0)
Sum basis vectors of each atom type	(2 0 0)		(2 0 0)	
$\vec{\phi}_2$	(0 1 0)	(0 1 0)	(0 1 0)	(0 1 0)
$D_3^{1*} \times R_n \times \det(R) \times \vec{\phi}_2$	(0 1 0)	(0 1 0)	(0 -1 0)	(0 -1 0)
Sum basis vectors of each atom type	(0 2 0)		(0 -2 0)	
$\vec{\phi}_3$	(0 0 1)	(0 0 1)	(0 0 1)	(0 0 1)
$D_3^{1*} \times R_n \times \det(R) \times \vec{\phi}_3$	(0 0 1)	(0 0 -1)	(0 0 1)	(0 0 -1)
Sum basis vectors of each atom type	(0 0 0)		(0 0 0)	

Table 11: Table showing the projection of basis vectors from Γ_3 for the positions $X_1 = (0\ 0\ 0)$ and $X_2 = (0.5\ 0\ 0)$.

So the non-zero basis vector components on each atom are:

	X_1	X_2
$\vec{\psi}_3$	(2 0 0)	(2 0 0)
$\vec{\psi}_4$	(0 2 0)	(0 -2 0)

for Γ_4	$R_1:$	$R_2:$	$R_3:$	$R_4:$
R_n	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
operate on X_1	X_1	X_1	X_2	X_2
D_4^{1*}	1	-1	1	-1
$D_4^{1*} \times R_n \times \det(R)$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$\vec{\phi}_1$	(1 0 0)	(1 0 0)	(1 0 0)	(1 0 0)
$D_4^{1*} \times R_n \times \det(R) \times \vec{\phi}_1$	(1 0 0)	(1 0 0)	(-1 0 0)	(-1 0 0)
Sum basis vectors of each atom type	(2 0 0)		(-2 0 0)	
$\vec{\phi}_2$	(0 1 0)	(0 1 0)	(0 1 0)	(0 1 0)
$D_4^{1*} \times R_n \times \det(R) \times \vec{\phi}_2$	(0 1 0)	(0 1 0)	(0 1 0)	(0 1 0)
Sum basis vectors of each atom type	(0 2 0)		(0 2 0)	
$\vec{\phi}_3$	(0 0 1)	(0 0 1)	(0 0 1)	(0 0 1)
$D_4^{1*} \times R_n \times \det(R) \times \vec{\phi}_3$	(0 0 1)	(0 0 -1)	(0 0 -1)	(0 0 1)
Sum basis vectors of each atom type	(0 0 0)		(0 0 0)	

Table 12: Table showing the projection of basis vectors from Γ_4 for the positions $X_1 = (0\ 0\ 0)$ and $X_2 = (0.5\ 0\ 0)$.

So the non-zero basis vector components on each atom are:

	X_1	X_2
$\vec{\psi}_5$	(2 0 0)	(-2 0 0)
$\vec{\psi}_6$	(0 2 0)	(0 2 0)

The basis vectors are therefore

		X_1	X_2
Γ_1	$\vec{\psi}_1$	(0 0 2)	(0 0 - 2)
Γ_2	$\vec{\psi}_2$	(0 0 2)	(0 0 2)
Γ_3	$\vec{\psi}_3$	(2 0 0)	(2 0 0)
	$\vec{\psi}_4$	(0 2 0)	(0 - 2 0)
Γ_4	$\vec{\psi}_5$	(2 0 0)	(-2 0 0)
	$\vec{\psi}_6$	(0 2 0)	(0 2 0)

There are 6 basis vectors in agreement with the decomposition equation $\Gamma_{mag} = 1\Gamma_1 \oplus 1\Gamma_2 \oplus 2\Gamma_3 \oplus 2\Gamma_4$, and the number of equivalent positions for this atom (2 positions, each with 3 degrees of freedom = 6 degrees of freedom). Symmetry has now allowed us to classify these degrees of freedom into SALCs. (Important- symmetry does not reduce the number of degrees of freedom, it only classifies it.)³

1.10 The degrees of freedom of a magnetic structure

In general, any linear combination of the basis vectors associated with an irreducible representation will have the symmetry of that irreducible representation. If this linear combination is written

$$\vec{M} = \sum_n C_n \vec{\psi}_n \quad (70)$$

that is to say

$$\vec{M} = C_1 \vec{\psi}_1 \oplus \dots \oplus C_n \vec{\psi}_n \quad (71)$$

³My preference is never to normalise the basis vectors as it their ability to be scaled is an intrinsic aspect of their application.

then at any given instant these propagate through the solid according to the wave equation

$$\vec{M}_j = \vec{M}_i \exp(-2\pi i \vec{k} \cdot \vec{t}) \quad (72)$$

where \vec{M}_i and \vec{M}_j are the moment vectors **from** of atoms i and j . Just as the normal modes of a vibrating molecule are orthogonal, the magnetic structure basis functions of the different IRs are normal modes and are orthogonal.