Irreducible Representation Analysis

Lecture 1

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PCG Intensive Summer School in Physical Crystallography

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Overview

- What is a representation?
- Irreducible representations of point groups
- Reducing a representation
- A physical interpretation of irreps
- The link between irreps and Eigen vectors
- Irrep degeneracy and dimensionality
- Irreps extended to space groups

Representation Theory

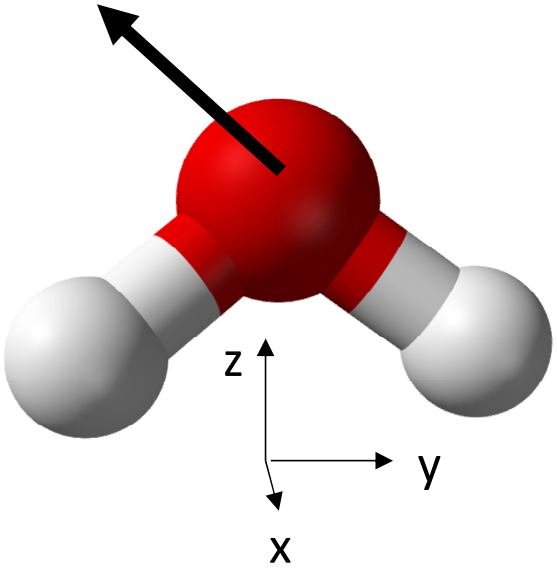
- Representation theory is a well established branch of mathematics and group theory.
- *"The goal of group representation theory is to study groups via their actions on vector spaces."* (Representation Theory of Finite Groups, Benjamin Steinberg).
- As solid state scientists, our motivation is slightly different. We wish to understand phase transitions (group-subgroup relationships) by studying representations of groups.
- In this context, the representation is the **transformational properties** of the collection of atomic displacements, site or magnetic orderings, which drive some phase transitions from a high symmetry structure to a lower symmetry structure.

Representations – some terminology

- The collection of atomic displacements, site or magnetic orderings that happen when some high symmetry structure undergoes a phase transition is often referred to as the "**vector space**" .
- A representation of a group G is a **structure-preserving (1 to 1) mapping** of the elements in G for some finite-dimensional vector space.
- For a three dimensional (polar) vector (x,y,z) and a single symmetry operator (g_1) of a group G:
  - g_1(x,y,z) = (x,y,z) D(g_1)
  - In this case D(g_1) is a 3x3 matrix and the complete set of D(g_1),D(g_2)…D(g_n) for all n g_1,g_2,..g_n symmetry elements is a representation of the group.

Constructing representations

- Consider the point group C_{2v} (*mm2*). What is the representation of a polar vector (x,y,z)?
  - E(x,y,z) $= (x,y,z)\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
  - m_x(x,y,z) $= (x,y,z)\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
  - m_y(x,y,z) $= (x,y,z)\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
  - 2_z(x,y,z) $= (x,y,z)\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$



- For a polar vector with its tail at the origin, these are just the symmetry operators in matrix form!

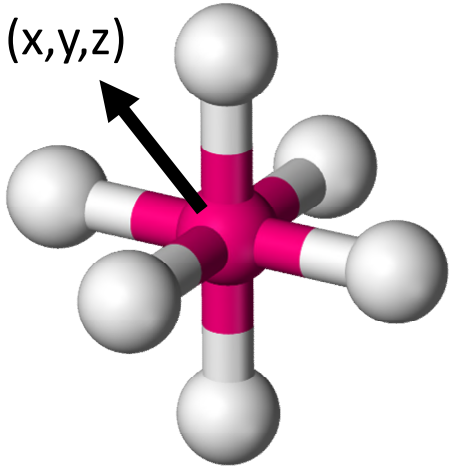
Irreducible representations

- For certain choices of vector spaces (e.g. a specific pattern of atomic displacements), the representations have the special property that they are irreducible.
  - $D'(g) = S^{-1}D(g)S$
- Irreducible in this context means that they **cannot be** expressed as a linear combination of any of the other irreducible representations of the group.
- Since this definition is somewhat cyclical, I will illustrate what irreducible means with several examples.

Irreducible representations of point groups

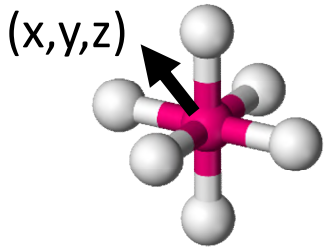
- Ultimately we are interested in studying solid state phase transitions, and hence irreps of space groups.
- However, we will start with something a bit more familiar, by playing around with character tables of point groups.

- Consider a 6-coordinate atom at the centre of a octahedron. For sake of argument this could be a TiO_6 octahedron in the perovskite structure $BaTiO_3$.



O_h (*m*-3*m*)

m-3m Character tables



O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2=(C_4)^2$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$	linear functions, rotations	quadratic functions
m-3m	1	8 3[111]	6 2[110]	6 4[100]	3 2[100]	-1	6 4[100]	8 3[111]	3 m[100]	6 m[110]		
A_{1g}	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	-	$x^2+y^2+z^2$
A_{2g}	+1	+1	-1	-1	+1	+1	-1	+1	+1	-1	-	-
E_g	+2	-1	0	0	+2	+2	0	-1	+2	0	-	$(2z^2-x^2-y^2, x^2-y^2)$
T_{1g}	+3	0	-1	+1	-1	+3	+1	0	-1	-1	(R_x, R_y, R_z)	-
T_{2g}	+3	0	+1	-1	-1	+3	-1	0	-1	+1	-	(xz, yz, xy)
A_{1u}	+1	+1	+1	+1	+1	-1	-1	-1	-1	-1	-	-
A_{2u}	+1	+1	-1	-1	+1	-1	+1	-1	-1	+1	-	-
E_u	+2	-1	0	0	+2	-2	0	+1	-2	0	-	-
T_{1u}	+3	0	-1	+1	-1	-3	-1	0	+1	+1	(x, y, z)	-
T_{2u}	+3	0	+1	-1	-1	-3	+1	0	+1	-1	-	-

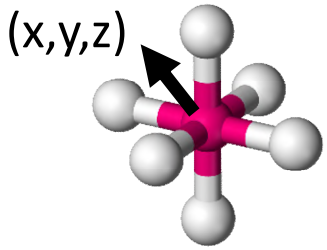
Characters of irreps

- In this case, the representation of the vector (x,y,z) in point group *m-3m* is already irreducible: T_{1u}.
- The T indicates that it is triply degenerate - a displacement along x would be equivalent to one along y or z in *m-3m*.
- The u indicates that it is antisymmetric w.r.t. inversion – the vector is polar after all!
- The character table gives the characters(!) of the irreps, which are the sum of the diagonal component of the irrep matrixes.
- E(x,y,z) = (x,y,z) $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ sum of diagonal is 3, hence triply degenerate.

Characters of irreps

- Considering a mirror plane perpendicular to *x*, m[100].
  - (x,y,z) $\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ = (-x,y,z)
  - The Character is 1+1 -1 = 1
- Consider a 3 fold about [111], 3[111]:
  - (x,y,z) $\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$ = (z,x,y)
  - The Character is 0 + 0 + 0 = 0

m-3m Character tables

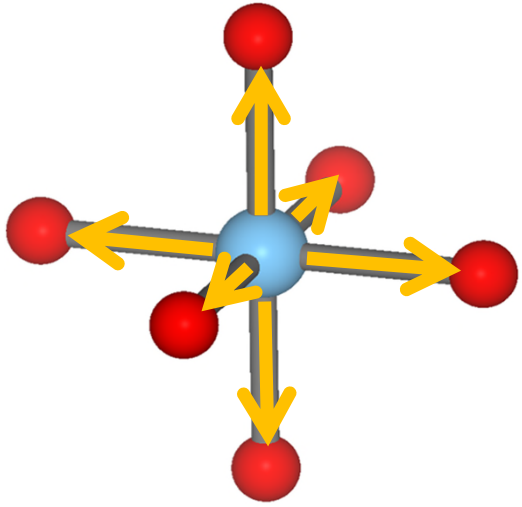


O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2=(C_4)^2$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$	linear functions, rotations	quadratic functions
m-3m	1	8 3[111]	6 2[110]	6 4[100]	3 2[100]	-1	6 - 4[100]	8 - 3[111]	3 m[100]	6 m[110]		
A_{1g}	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	-	$x^2+y^2+z^2$
A_{2g}	+1	+1	-1	-1	+1	+1	-1	+1	+1	-1	-	-
E_g	+2	-1	0	0	+2	+2	0	-1	+2	0	-	$(2z^2-x^2-y^2, x^2-y^2)$
T_{1g}	+3	0	-1	+1	-1	+3	+1	0	-1	-1	(R_x, R_y, R_z)	-
T_{2g}	+3	0	+1	-1	-1	+3	-1	0	-1	+1	-	(xz, yz, xy)
A_{1u}	+1	+1	+1	+1	+1	-1	-1	-1	-1	-1	-	-
A_{2u}	+1	+1	-1	-1	+1	-1	+1	-1	-1	+1	-	-
E_u	+2	-1	0	0	+2	-2	0	+1	-2	0	-	-
T_{1u}	+3	0	-1	+1	-1	-3	-1	0	+1	+1	(x, y, z)	-
T_{2u}	+3	0	+1	-1	-1	-3	+1	0	+1	-1	-	-

Other irreps of point group m-3m

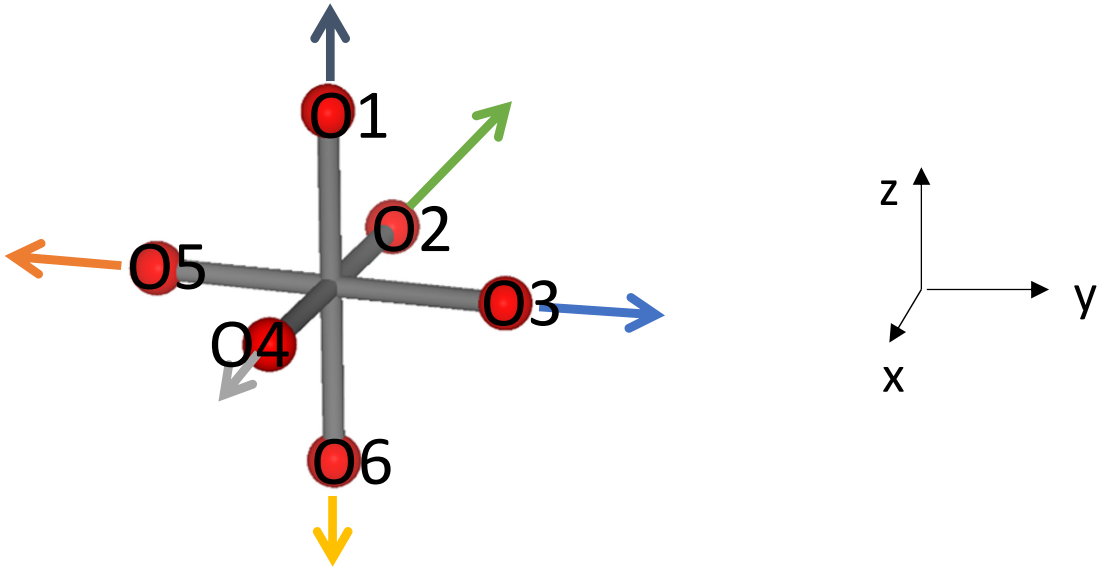
- Let us chose a different vector space that has the following transformational property:
  - $(x_2,0,0) \equiv (0,y_2,0) \equiv (0,0,z_2) \equiv (-x_2,0,0) \equiv (0,-y_2,0) \equiv (0,0,-z_2)$.
  - e.g. what I am describing is a breathing mode of the octahedron.
  - This is now a scalar and not a vector and requires just a single value to describe its magnitude.

- As this vector space is invariant under all symmetry elements of m-3m, the associated representation is now the totally symmetry irrep A_{1g}.
- Any 1 dimensional rep will always be an irrep.



Reducing representations

- In the two previous examples I chose vector spaces deliberately, such that the associated representations were irreducible.
- However, I could have chosen the lowest symmetry pattern of bond stretches that I could imagine.



Reps of the vector space

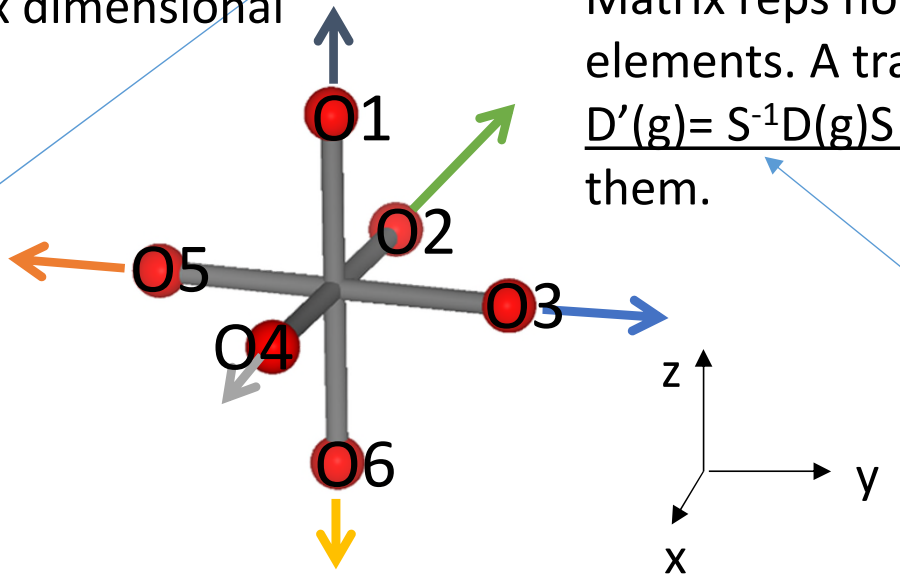
- $m_x(z_1,x_2,y_3,x_4,y_5,z_6) = \begin{pmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{pmatrix} (z_1,\mathbf{-x_4},y_3,\mathbf{-x_2},y_5,z_6)$
- $m_z(z_1,x_2,y_3,x_4,y_5,z_6) = \begin{pmatrix} 0 & \cdots & -1 \\ \vdots & \ddots & \vdots \\ -1 & \cdots & 0 \end{pmatrix} (\mathbf{-z_6},x_2,y_3,x_4,y_5,\mathbf{-z_1})$

The vector space is now six dimensional

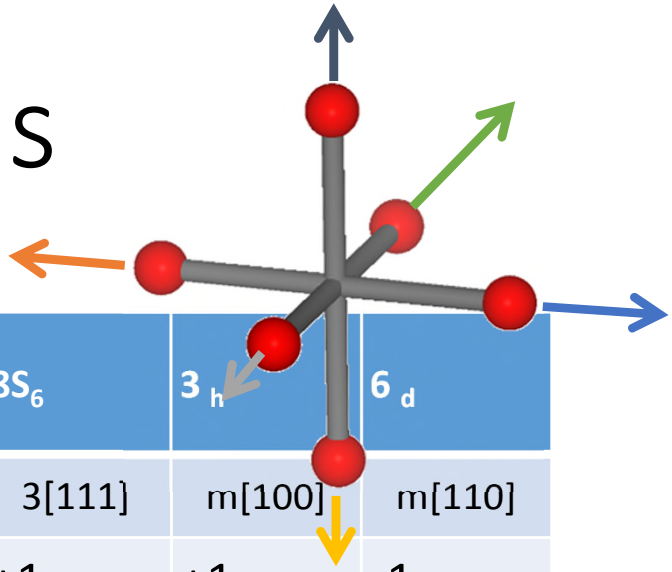
Now the rep is a 6x6 matrix

Matrix reps now have off-diagonal elements. A transformation of kind $D'(g)= S^{-1}D(g)S$ is required to reduce them.

This looks like a basis transformation

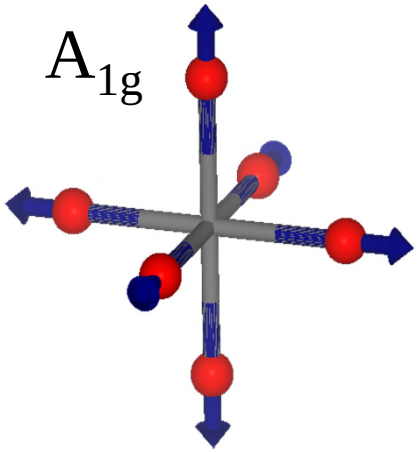


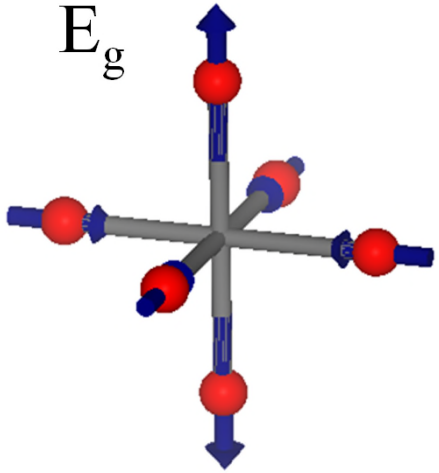
Reducing representations

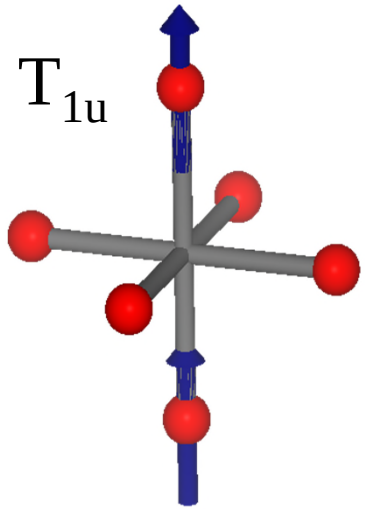


O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2 = (C_4)^2$	i	$6S_4$	$8S_6$	$3\,\sigma_h$	$6\,\sigma_d$
m-3m	1	3[111]	2[110]	4[100]	2[100]	-1	4[100]	3[111]	m[100]	m[110]
A_{2g}	+1	+1	-1	-1	+1	+1	-1	+1	+1	-1
E_g	+2	-1	0	0	+2	+2	0	-1	+2	0
T_{1g}	+3	0	-1	+1	-1	+3	+1	0	-1	-1
T_{2g}	+3	0	+1	-1	-1	+3	-1	0	-1	+1
A_{1u}	+1	+1	+1	+1	+1	-1	-1	-1	-1	-1
A_{2u}	+1	+1	-1	-1	+1	-1	+1	-1	-1	+1
E_u	+2	-1	0	0	+2	-2	0	+1	-2	0
T_{1u}	+3	0	-1	+1	-1	-3	-1	0	+1	+1
T_{2u}	+3	0	+1	-1	-1	-3	+1	0	+1	-1
Γ_{Bonds}	6	0	0	2	2	0	0	0	4	2

Reducing representations







(Basis vectors of the vector space)

The representation was 6 dimensional, the sum of the irrep dimensionality (degeneracy) is 6.

Irreducibility

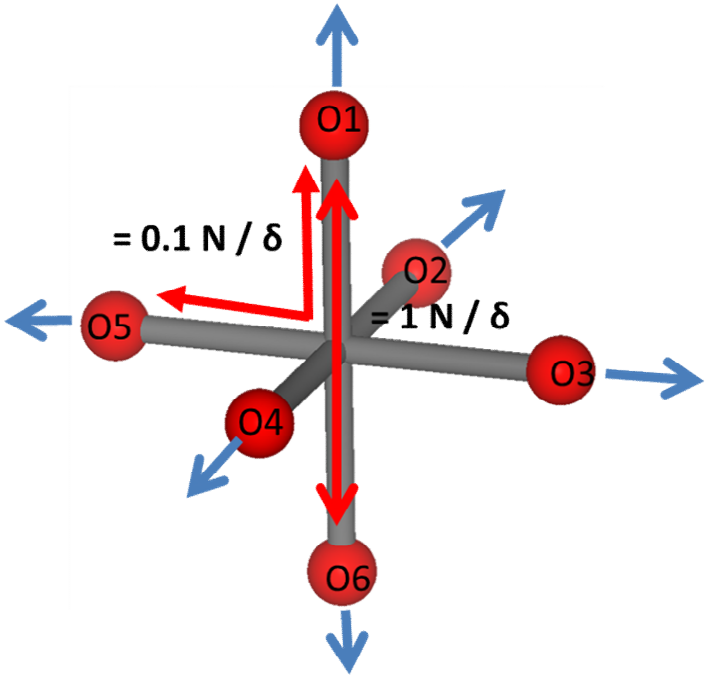
- Deriving the irreducible representations of *m-3m* (or indeed any point group with a significant number of operators) is non trivial.
- However it is easy to show that irreps are irreducible by showing that the dot product of the characters of the irreps with each other is "0".

O_h	E	$\underline{8}C_3$	$\underline{6}C_2$	$\underline{6}C_4$	$\underline{3}C_2=(C_4)^2$	i	$\underline{6}S_4$	$\underline{8}S_6$	$\underline{3}\,\sigma_h$	$\underline{6}\,\sigma_d$	linear functions, rotations	quadratic functions
m-3m	1	8 3[111]	6 2[110]	6 4[100]	3 2[100]	-1	6 4[100]	8 3[111]	3 m[100]	6 m[110]		
A_{1g}	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	-	$x^2+y^2+z^2$
E_g	+2	-1	0	0	+2	+2	0	-1	+2	0	-	$(2z^2-x^2-y^2, x^2-y^2)$
T_{1u}	+3	0	-1	+1	-1	-3	-1	0	+1	+1	T_{1u}	+3

Careful, in doing this you need to consider the <u>number of each symmetry operator</u> when multiplying the individual elements together.

Analogy with molecular vibrations

- Consider how one might calculate the stretching frequencies of a ABO_6 molecule - Construct a FCM.



	O1	O2	O3	O4	O5	O6
O1	1.4	0.1	0.1	0.1	0.1	1
O2	0.1	1.4	0.1	1	0.1	0.1
O3	0.1	0.1	1.4	0.1	1	0.1
O4	0.1	1	0.1	1.4	0.1	0.1
O5	0.1	0.1	1	0.1	1.4	0.1
O6	1	0.1	0.1	0.1	0.1	1.4

- Local coordinate system +ve for motion towards B and -ve for motion away from B.

Diagonalizing the FCM

Eigen Vectors:	E1	E2	E3	E4	E5	E6
O1	-0.408	-0.707	-0.056	-0.577	0.391	0.21
O2	-0.408	0	-0.492	0.289	0.173	0.259
O3	-0.408	0	0.504	0.289	-0.563	0.624
O4	-0.408	0	0.492	0.289	0.173	-0.259
O5	-0.408	0	-0.504	0.289	-0.563	-0.624
O6	-0.408	0.707	0.056	-0.577	0.391	-0.21

	Eigen Values
E1	2.8
E2	0.4
E3	0.4
E4	2.2
E5	2.2
E6	0.4

Eigen vectors: Related to the transformational matrix (**M**) required to bring the FCM into diagonal form, via similarity transformation $\mathbf{M^{-1}\ FCM\ M}$

Eigen values: The diagonal elements of the diagonal matrix.

You can have a play around with this using an online matrix calculator (http://www.bluebit.gr/matrix-calculator/) to take some of the pain out of inverting 3x3 matrices.

Visualising Eigen Vectors

	E1	E2	E3	E4	E5	E6
O1	-0.408	-0.707	-0.056	-0.577	0.391	0.21
O2	-0.408	0	-0.492	0.289	0.173	0.259
O3	-0.408	0	0.504	0.289	-0.563	0.624
O4	-0.408	0	0.492	0.289	0.173	-0.259
O5	-0.408	0	-0.504	0.289	-0.563	-0.624
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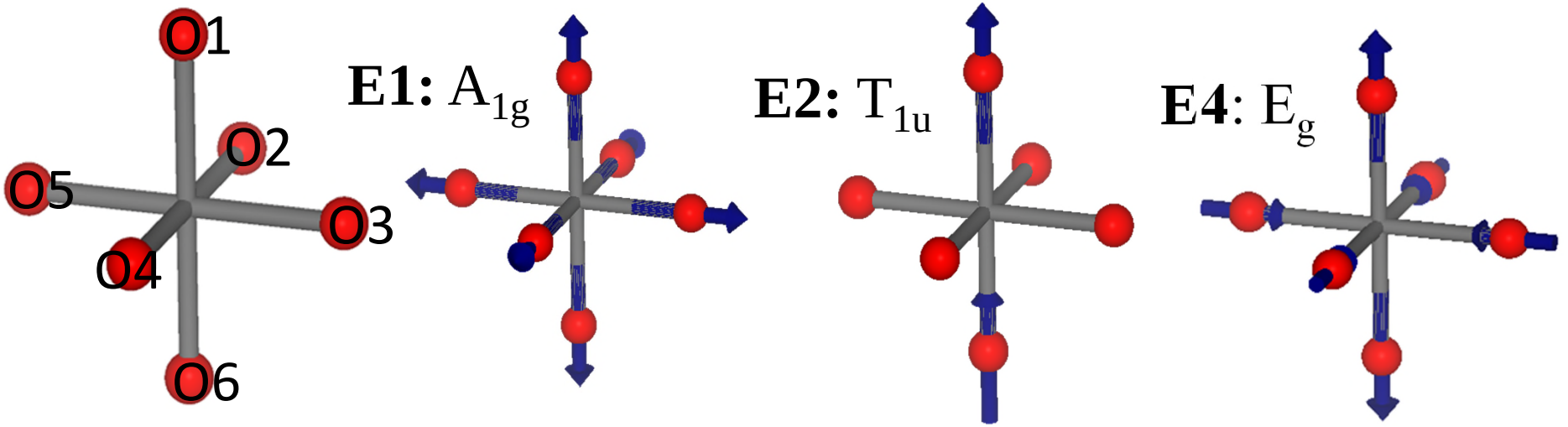


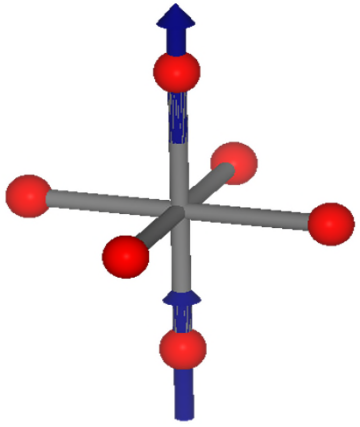
Why does this work?

- When assigning the forces to our BO_6 molecule we respected the symmetry of m-3m.
- We hence encoded the symmetry of the system in the FCM.
- It is worth reflecting that, in effect, symmetry predetermines the Eigen vectors of this system (the allowed vibration modes).
- The basis change involved in going from FCM to Eigen vectors is analogous in many ways to the “basis change” involved in going from representations to irreps.
- Reducing reps using the characters of irreps is considerably less work than diagonalising a FCM – especially for more complex systems!

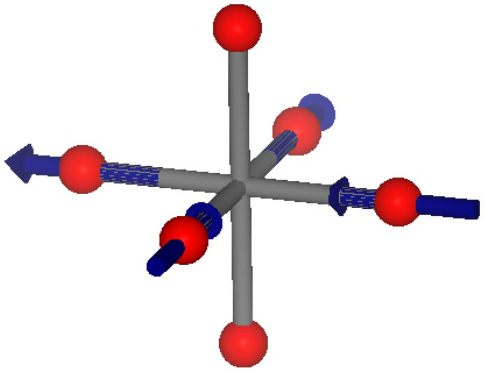
Irrep degeneracy

- You may notice that I glossed over the fact earlier that not all of the Eigen vectors degenerating in energy correspond nicely to the triply degenerate anti-symmetric and doubly degenerate symmetric stretches that we are used to visualising:

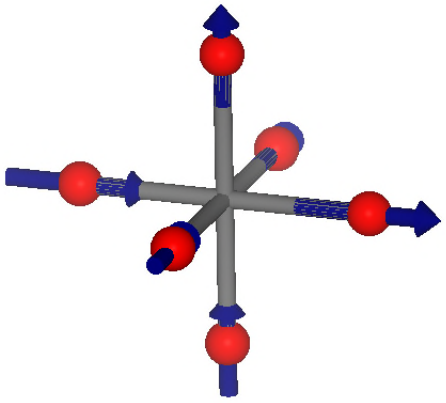
	E2	E3	E6
O1	-0.707	-0.056	0.21
O2	0	-0.492	0.259
O3	0	0.504	0.624
O4	0	0.492	-0.259
O5	0	-0.504	-0.624
O6	0.707	0.056	-0.21



E2: T_{1u}

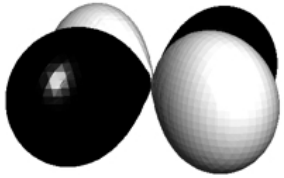


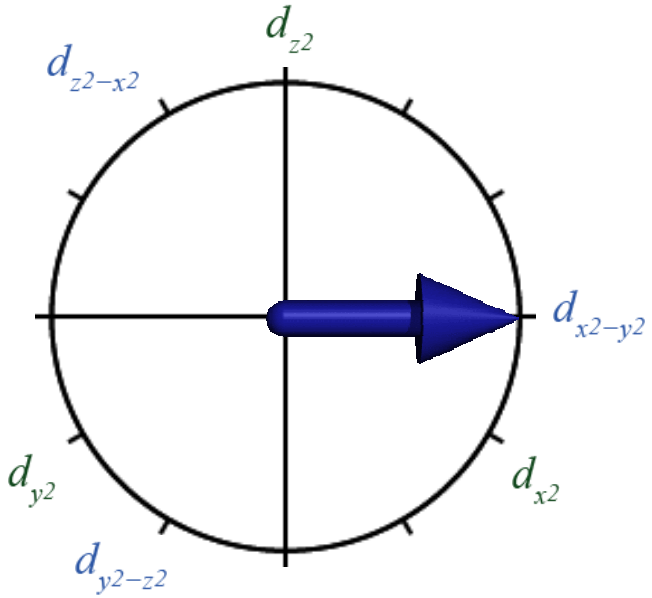
E3: T_{1u}

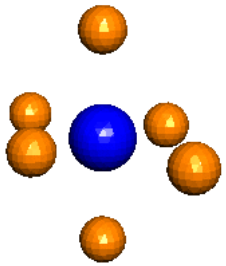


E6: T_{1u}

Irrep degeneracy – E_g







Credit: Goodwin Group

Irrep degeneracy

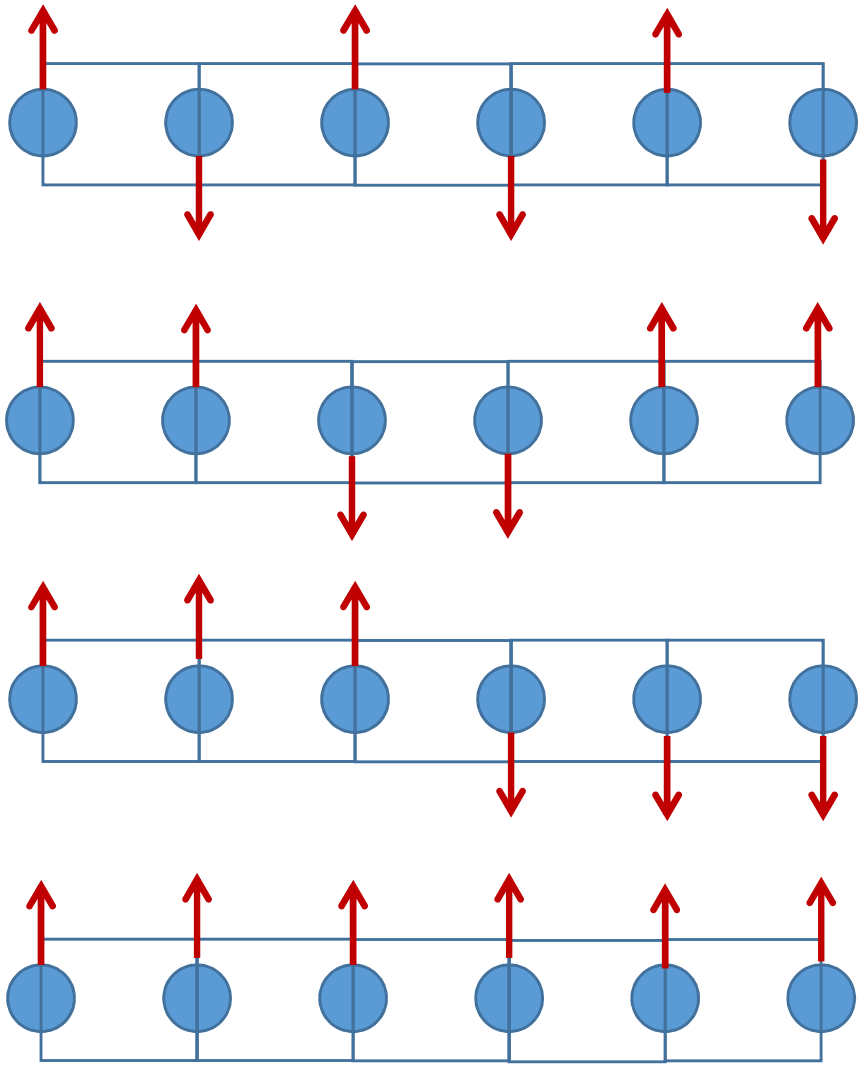
- Occurs because the associated degeneracy leaves an additional ambiguity with respect to the basis vectors that are used.
- Irrep analysis uniquely defines the basis vectors of your vector space up to the degeneracy/dimensionality of the irreps.
- Additional choices have been made in tabulating irreps such that the resulting basis vectors are compatible with Cartesian axes and/or are physically intuitive.
- The FCM approach does not know anything about our preferences.
- In the harmonic approximation, a vibration of character corresponding to any of these triply degenerate eigen vectors / irreps or any linear combination thereof is strictly equivalent in energy.

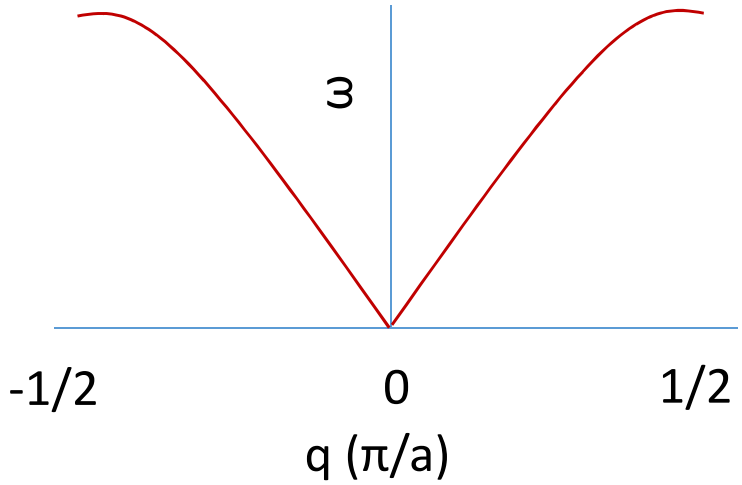
Irreps of space groups

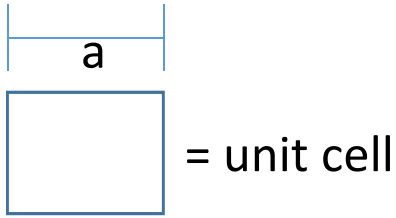
- We will now consider how these ideas extend to space groups and additional complications that arise.
- For space groups we have to consider not only the additional symmetry elements such as glide and screw axes, but also lattice translational symmetry.
- Since a lattice is in principle infinite, we might expect an infinite number of irreps!
- Thankfully, symmetry in reciprocal space helps us reduce and classify these into a manageable form.

Propagation vectors

- Propagation vector or crystal momentum k:



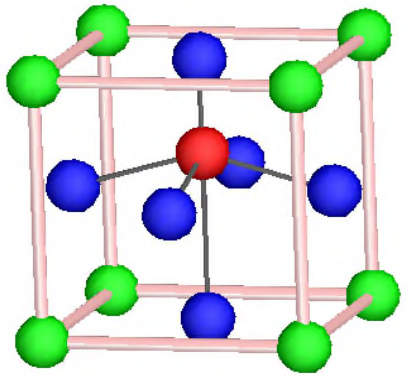




Space group irrep tabulations

- As for phonon Eigen vector calculations, the irreps concerned with vector spaces with different propagation vectors can be calculated independent of each other.
- There are thankfully tabulations that have been made by various authors.
- These have been made predominantly for the high symmetry point of the BZ, but more recent tabulations of low symmetry lines and points are also available online.
- We will use exclusively the “2011 version” of the irrep matrices calculated by Stokes, Campbell and Cordes (Acta Cryst. (2013). A69, 388–395), as implemented in the current version of ISODISPLACE.

Irreps of Pm-3m at Γ



- We will start by extending our point group example of a BO_6 molecule to a ABO_3 perovskite with setting A(0,0,0), B(½,½,½), O(½, ½, 0).
- Consider again a vector space corresponding to an off-centre displacement of B.
- This corresponds to irrep Γ_4^- in Miller and Love notation.
- The letter always denotes k. k = (0 0 0) always for Γ
- "-" denotes antisymmetric nature w.r.t the **inversion centre at (0,0,0)**.

Irrep dimensionality

- Miller-Love notation contains extra information on the propagation vector, but does not describe the dimensionality / degeneracy of irreps, as is done with Mulliken symbols.
- To counter this, often a string of letters of a length equal to the dimensionality is given after the irrep label.
- As Γ_4^- is three dimensional, three letters are needed.
- Γ_4^-(a,b,c) corresponds to the most general (lowest symmetry) displacement of the B site along x, y and z.
- Higher symmetry Γ_4^-(a,a,a), Γ_4^-(a,0,0) and so on are possible.
- Note: since symmetry imposes no constraint on the basis vectors of Γ_4^-, the irrep matrices need not necessarily be chosen such that they have a nice correspondence with a high symmetry lattice direction. However, programs like ISODISRORT normally endeavor to do so.

Irreps of Pm-3m at Γ

Character

Irrep matrices

IR GM4- Symmetry operator

Star of k: (0,0,0),

(1)	(2)	(3)
1:(x,y,z)	3	(1, 0, 0 /0, 1, 0 /0, 0, 1)
2[100]:(x,-y,-z)	-1	(1, 0, 0 /0, -1, 0 /0, 0, -1)
2[010]:(-x,y,-z)	-1	(-1, 0, 0 /0, 1, 0 /0, 0, -1)
2[001]:(-x,-y,z)	-1	(-1, 0, 0 /0, -1, 0 /0, 0, 1)
3[111]:(z,x,y)	0	(0, 0, 1 /1, 0, 0 /0, 1, 0)
3[-1-1-1]:(y,z,x)	0	(0, 1, 0 /0, 0, 1 /1, 0, 0)
3[-111]:(-y,z,-x)	0	(0, -1, 0 /0, 0, 1 /-1, 0, 0)
3[1-1-1]:(-z,-x,y)	0	(0, 0, -1 /-1, 0, 0 /0, 1, 0)
3[1-11]:(-y,-z,x)	0	(0, -1, 0 /0, 0, -1 /1, 0, 0)
3[-11-1]:(z,-x,-y)	0	(0, 0, 1 /-1, 0, 0 /0, -1, 0)
3[11-1]:(y,-z,-x)	0	(0, 1, 0 /0, 0, -1 /-1, 0, 0)
3[-1-11]:(-z,x,-y)	0	(0, 0, -1 /1, 0, 0 /0, -1, 0)
4[100]:(x,-z,y)	1	(1, 0, 0 /0, 0, -1 /0, 1, 0)
4[-100]:(x,z,-y)	1	(1, 0, 0 /0, 0, 1 /0, -1, 0)
4[010]:(z,y,-x)	1	(0, 0, 1 /0, 1, 0 /-1, 0, 0)
4[0-10]:(-z,y,x)	1	(0, 0, -1 /0, 1, 0 /1, 0, 0)
4[001]:(-y,x,z)	1	(0, -1, 0 /1, 0, 0 /0, 0, 1)
4[00-1]:(y,-x,z)	1	(0, 1, 0 /-1, 0, 0 /0, 0, 1)
2[110]:(y,x,-z)	-1	(0, 1, 0 /1, 0, 0 /0, 0, -1)
2[-110]:(-y,-x,-z)	-1	(0, -1, 0 /-1, 0, 0 /0, 0, -1)
2[101]:(z,-y,x)	-1	(0, 0, 1 /0, -1, 0 /1, 0, 0)
2[-101]:(-z,-y,-x)	-1	(0, 0, -1 /0, -1, 0 /-1, 0, 0)
2[011]:(-x,z,y)	-1	(-1, 0, 0 /0, 0, 1 /0, 1, 0)
2[0-11]:(-x,-z,-y)	-1	(-1, 0, 0 /0, 0, -1 /0, -1, 0)
-1:(-x,-y,-z)	-3	(-1, 0, 0 /0, -1, 0 /0, 0, -1)
-2[100]:(-x,y,z)	1	(-1, 0, 0 /0, 1, 0 /0, 0, 1)
-2[010]:(x,-y,z)	1	(1, 0, 0 /0, -1, 0 /0, 0, 1)
-2[001]:(x,y,-z)	1	(1, 0, 0 /0, 1, 0 /0, 0, -1)
-3[111]:(-z,-x,-y)	0	(0, 0, -1 /-1, 0, 0 /0, -1, 0)
-3[-1-1-1]:(-y,-z,-x)	0	(0, -1, 0 /0, 0, -1 /-1, 0, 0)
-3[-111]:(y,-z,x)	0	(0, 1, 0 /0, 0, -1 /1, 0, 0)
-3[1-1-1]:(z,x,-y)	0	(0, 0, 1 /1, 0, 0 /0, -1, 0)
-3[1-11]:(y,z,-x)	0	(0, 1, 0 /0, 0, 1 /-1, 0, 0)
-3[-11-1]:(-z,x,y)	0	(0, 0, -1 /1, 0, 0 /0, 1, 0)
-3[11-1]:(-y,z,x)	0	(0, -1, 0 /0, 0, 1 /1, 0, 0)
-3[-1-11]:(z,-x,y)	0	(0, 0, 1 /-1, 0, 0 /0, 1, 0)
-4[100]:(-x,z,-y)	-1	(-1, 0, 0 /0, 0, 1 /0, -1, 0)
-4[-100]:(-x,-z,y)	-1	(-1, 0, 0 /0, 0, -1 /0, 1, 0)
-4[010]:(-z,-y,x)	-1	(0, 0, -1 /0, -1, 0 /1, 0, 0)
-4[0-10]:(z,-y,-x)	-1	(0, 0, 1 /0, -1, 0 /-1, 0, 0)
-4[001]:(y,-x,-z)	-1	(0, 1, 0 /-1, 0, 0 /0, 0, -1)
-4[00-1]:(-y,x,-z)	-1	(0, -1, 0 /1, 0, 0 /0, 0, -1)
-2[110]:(-y,-x,z)	1	(0, -1, 0 /-1, 0, 0 /0, 0, 1)
-2[-110]:(y,x,z)	1	(0, 1, 0 /1, 0, 0 /0, 0, 1)
-2[101]:(-z,y,-x)	1	(0, 0, -1 /0, 1, 0 /-1, 0, 0)
-2[-101]:(z,y,x)	1	(0, 0, 1 /0, 1, 0 /1, 0, 0)
-2[011]:(x,-z,-y)	1	(1, 0, 0 /0, 0, -1 /0, -1, 0)
-2[0-11]:(x,z,y)	1	(1, 0, 0 /0, 0, 1 /0, 1, 0)
1:(x+1,y,z)	3	(1, 0, 0 /0, 1, 0 /0, 0, 1)
1:(x,y+1,z)	3	(1, 0, 0 /0, 1, 0 /0, 0, 1)
1:(x,y,z+1)	3	(1, 0, 0 /0, 1, 0 /0, 0, 1)

48 + 3

ISODISTORT: http://stokes.byu.edu/iso/isodistort.php

Γ-point irreps of Pm-3m

- The output of ISODISTORT gives the full list of symmetry operators rather than grouping these together according to operator type.
- The output of ISODISTORT includes the full irreducible representation matrices rather than just the characters.
- There are three additional entries such as 1:(x,y,z+1) 3 (1, 0, 0 /0, 1, 0 /0, 0, 1) that deal with the lattice translational symmetry.
- Note that in space groups with translational symmetry elements the extension from point groups, even for irreps at the Γ-point, is somewhat more complicated.

End of Lecture 1