Group Representations

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You’ve been using it this whole time. Things I hope to cover

- And Introduction to Groups
- Representation theory
- Crystallagraphic Groups
- Continuous Groups
- Eigenmodes
- Fourier Analysis
- Graphene
## Triangle

What are you allowed to do to the triangle to keep it unchanged?

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## Circle

What operations are you allowed to do to the circle that leave it unchanged?
What operations can we do that leave the triangle invariant?

There are six total
• We can also represent groups with these stereographic pictures.
• It is a way to create an object with the same symmetry.
• Imagine a plate with a single peg.
Now start applying symmetry operations until done.

First apply a rotation, we have to create a new peg.
Rotate again and we create another.
• Now apply the mirror symmetry.
• We’re done, these pegs all transform into one other, we don’t create any more.
• This plate-peg guy has the same symmetry as our triangle
You can also identify individual pegs with individual group elements.

Useful for reasoning out group operations.
## Multiplication Table

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Informally, it seems we have some common ground

- You can always do nothing
Informally, it seems we have some common ground

- You can always do nothing
- You can always undo
Informally, it seems we have some common ground

- You can always do nothing
- You can always undo
- You can compose operations to get another one.
A group is a set $G$ and a binary operation $\cdot$, $(G, \cdot)$, such that

- **identity**: $\exists e \in G, \forall g \in G : g \cdot e = e \cdot g = g$
- **inverses**: $\forall g \in G, \exists g^{-1} \in G : g \cdot g^{-1} = g^{-1} \cdot g = e$
- **closure**: $\forall g_1, g_2 \in G : g_1 \cdot g_2 \in G$
- **associativity**: $\forall g_1, g_2, g_3 \in G : g_1 \cdot (g_2 \cdot g_3) = (g_1 \cdot g_2) \cdot g_3$
Other Examples

Some examples:

- The symmetry operations of a triangle, square, cube, sphere, ... (really anything)
- The rearrangements of $N$ elements (the symmetric group of order $N$)
- The integers under addition
- The set $(0,..,n-1)$ under addition mod $n$
- The real numbers (less zero) under multiplication

Some non examples:

- The integers under multiplication. (no inverses in general)
- The renormalization group (no inverses)
- Bierbaum
This is all and well, but if we want to do some kind of physics, we need to know how our group transforms things of interest. Take

\[ \mathbf{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \]
Vector Representation of $C_{3v}$

\[ E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad R = \frac{1}{2} \begin{pmatrix} -1 & \sqrt{3} & 0 \\ -\sqrt{3} & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \]

\[ R^2 = \frac{1}{2} \begin{pmatrix} -1 & -\sqrt{3} & 0 \\ \sqrt{3} & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad V = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \]

\[ RV = \frac{1}{2} \begin{pmatrix} 1 & \sqrt{3} & 0 \\ \sqrt{3} & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad R^2 V = \frac{1}{2} \begin{pmatrix} 1 & -\sqrt{3} & 0 \\ -\sqrt{3} & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \]

Fun fact: These matrices satisfy exactly the same multiplication table!
A representation $\Gamma$ is a mapping from the group set $G$ to $M_{n,n}$ such that $\Gamma_{ik}(g_1)\Gamma_{kj}(g_2) = \Gamma_{ij}(g_1 \cdot g_2)$, $\forall g_1, g_2 \in G$.

That is, you represent the group elements by matrices, ensuring that you maintain the multiplication table.
Example Representations of $C_{3v}$

Some examples:

- Represent *every* group element by the number 1. (The trivial representation)
- Represent, $(e, r, r^2)$ by 1 and $(v, rv, r^2v)$ by -1
- Use the matrices we had before (the vector representation?)
- The *regular representation*, in which you make matrices of the multiplication table. (treat each element as an orthogonal vector)

Note: You can form representations of *any* dimension.
You can also generate new representations easily. Consider

\[ f(x) \]

Let’s say we want to transform naturally:

\[ f'(x') = f(x) \]

This defines some linear operators

\[ f'(x') = O_R f(x') = O_R f(Rx) = f(x) \]

\[ O_R f(x) = f(R^{-1} x) \]

These \( \{ O_R \} \) will form a representation.
This representation is far from unique. Any invertible matrix can form a new representation

\[ S = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \]

can generate a new representation

\[ R' = S^{-1} RS \]

because we will still satisfy the group algebra

\[ R_1 R_2 = R_3 \implies (S^{-1} R_1 S)(S^{-1} R_2 S) = (S^{-1} R_3 S) \]
Because of this, we would like some invariant quality of the representation. How about the trace, define the *character* of a group element in a particular representation as the trace of its matrix.

\[ \chi^\Gamma(R) = \text{Tr } R = \text{Tr } (S^{-1}RS) = \text{Tr } (S^{-1}SR) = \text{Tr } R \]
Characters

Because of this, we would like some invariant quality of the representation. How about the trace, define the character of a group element in a particular representation as the trace of its matrix.

\[
\chi^\Gamma(R) = \text{Tr } R = \text{Tr } (S^{-1}RS) = \text{Tr } (S^{-1}SR) = \text{Tr } R
\]

For the representation we created above:

\[
\chi^V(E) = 3 \\
\chi^V(R) = 0 \quad \chi^V(R^2) = 0 \\
\chi^V(V) = 1 \quad \chi^V(RV) = 1 \quad \chi^V(R^2V) = 1
\]
Notice that a lot of these guys have the same character. A *class* is a collection of group elements that are roughly equivalent

\[ g_1 \equiv g_2 \text{ if } \exists s \in G : s^{-1}g_2s = g_1 \]

In our case we have three classes. The identity (always its own class), the rotations, and the mirror symmetries.
Note also that in this case, our representation is *reducible*. We have an invariant subspace, namely the 2D space \((x, y)\), which always transforms into itself, as well as \(z\) which doesn’t transform.

An *irreducible representation* is one that cannot be reduced, i.e. it has no invariant subspaces.

There are a finite number of (equivalent) *irreducible representations* for a finite group.
The irreducible representations for the point groups are well documented, in *character tables*. E.g.

<table>
<thead>
<tr>
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<th>$3\sigma_v$</th>
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Super orthogonality! Across both rows and columns.
Orthogonality

Turns out, there is a sort of orthogonality for the irreducible representations of a group.

\[
\sum_g \left[ D^i_{\alpha\beta}(g) \right]^* D^j_{\gamma\delta}(g) = \frac{h}{n_i} \delta_{ij} \delta_{\alpha\gamma} \delta_{\beta\delta}
\]

Think of this as \( \alpha \times \beta \) different \( h \) dimensional vector spaces, with the matrix elements being the coordinates. We have orthogonality.
Agreeing with our intuition, we see that our 3D representation is reducible into a 2D one and 1D one. We say it is the *direct sum* of the two:

\[ V = A_1 \oplus E \]

In fact all of its matrices were block diagonal (2x2 and 1x1)

\[
\begin{pmatrix}
  a & b & 0 \\
  c & d & 0 \\
  0 & 0 & e
\end{pmatrix}
\]
Direct Product Representations

Another useful way to generate new representations is by forming direct product representations. This happens a lot of in physics, like tensors. We had a representation that acted on vectors,

\[ v'_i = R_{ij} v_j \]

How do you transform tensors? You act on each index.

\[ M'_{ij} = R_{ik} R_{jl} M_{kl} \]

The characters of a the direct product representation are the products of the characters

\[ \chi(R \otimes R) = \text{Tr} \ R_{ik} R_{jl} = R_{ii} R_{ii} = (\text{Tr} \ R)^2 = \chi(R)^2 \]
Matrices

So we see

\[ M = 2A_1 \oplus A_2 \oplus 3E \]

\[ E \otimes E = A_1 \oplus A_2 \oplus E \]
Eigenmodes

Let’s consider a triangle of masses connected by springs. Let’s saw we want to know the eigenmodes of the system. First, let’s form our representation.
This forms a 9D representation of the group $T$. What are its characters

$$\chi(E) = 9 \quad \chi(R) = 0 \quad \chi(V) = 1$$

We already know how to decompose this

$$T = 2A_1 \oplus A_2 \oplus 3E$$

But what do these correspond to?
Projection operator

Since the character tables are super orthogonal

\[ P^\Gamma = \sum_g \chi^\Gamma(g) D(g) \]
Projecting Down

\[ y_1 \]

\[ \begin{align*}
E: & \quad \uparrow \\
R: & \quad \triangleleft \\
R^2: & \quad \triangleleft \\
\end{align*} \]

\[ \begin{align*}
V: & \quad \uparrow \\
RV: & \quad \triangleleft \\
R^2V: & \quad \triangleleft \\
\end{align*} \]

\[ \begin{align*}
P^{A_1} & = 2 \triangle + 2 \triangle + 2 \triangle = \triangle \\
P^{A_2} & = (\triangle - \triangle) + (\triangle - \triangle) + (\triangle - \triangle) = 0 \\
P^E & = 2 \triangle - \triangle - \triangle = \triangle \\
\end{align*} \]
Projecting Down

E: \[ \begin{align*}
\triangle & \\
\text{PA}_1 & = 0
\end{align*} \]

V: \[ \begin{align*}
\triangle & \\
\text{PA}_2 & = \begin{align*}
\triangle
\end{align*}
\]

PE: \[ \begin{align*}
\triangle & \\
\text{PE} & = \begin{align*}
\triangle
\end{align*}
\]
Projecting Down

\[ Z_1 \]

\[ E: \quad V: \quad R: \quad R^2: \]

\[ PA_2 = 0 \]
\[ PA_1 = PE = \]

\[ P^{A_2} = 0 \]
\[ P^{E} = \]
Normal Modes

\[ T = 2 A_1 + A_2 + 3 E \]
Continuous Groups

There are also all of the continuous groups. Consider $SO(3)$, the group of 3D rotations. The irreducible representations are the spherical harmonics.

$$Y_{lm} = e^{im\phi} P_l^m(\cos \theta)$$

With dimensionality

$$d = (2l + 1)$$

The characters are:

$$\chi^l(\psi) = \frac{\sin \left[ (l + \frac{1}{2}) \psi \right]}{\sin \left( \frac{\psi}{2} \right)}$$

where $\psi$ is how much rotation you do (the classes)
Orthogonality becomes integral

\[ \delta_{ij} = \frac{1}{\pi} \int_{0}^{\pi} d\psi \ (1 - \cos \psi) \chi^i(\psi) \chi^j(\psi) \]

Consider the vector representation

\[ \chi^V(\psi) = 1 + 2 \cos \psi \]

So we can decompose this

\[ V = 1 \]
and its direct product (read matrices)

\[ \chi^V \otimes V = (1 + 2 \cos \psi)^2 \]

decomposes as

\[ V \otimes V = 0 \oplus 1 \oplus 2 \]

but you already knew that

\[
\begin{align*}
M_{ii} & \quad (M_{ij} - M_{ji}) & \quad (M_{ij} + M_{ji}) - \frac{1}{3} M_{ii}
\end{align*}
\]

A matrix has its trace (d=1), antisymmetric part (d=3), and symmetric trace free part (d=5).
Looking again at the irreducible representations of the rotation group, we note that it was a 2 parameter family, \((j, l)\) with the group theory telling us that \(j\) was an integer, and
\[ l = -(2l + 1), \ldots, (2l + 1). \]
These parameters are physically important quantum numbers, the angular momentum and the magnetic quantum number.
Consider the group of translations. \( x \rightarrow x + a \). Forms a group. It’s irreducible representations are

\[
f(x) = e^{ikx}
\]

\[
f(x + a) = e^{ik(x+a)} = e^{ikx}e^{ika} = ce^{ikx}
\]

look familiar?
And the orthogonality theorem tells us that these are all orthogonal. Sound familiar?
Irreps form a one parameter family, corresponding to \( k \), or "momentum"
Fun fact: The Poincaré group, the full symmetry group of Minkowski space (translation in space or time, boosts, rotations) has as its unitary irreducible representations a two parameter family \((m, s)\) with these also being physically relevant quantum numbers, namely mass and spin.
Elastic Constants

Why do isotropic solids have 2 (linear) elastic constants, while cubic materials have 3?
Linear elasticity is all of the scalars in

\[ \varepsilon_{ij}\varepsilon_{kl} \]

\[
\left\{ \left\{ V_{SO(3)} \otimes V_{SO(3)} \right\} \otimes \left\{ V_{SO(3)} \otimes V_{SO(3)} \right\} \right\} = 2A_1 \oplus \cdots
\]

\[
\left\{ \left\{ V_{Oh} \otimes V_{Oh} \right\} \otimes \left\{ V_{Oh} \otimes V_{Oh} \right\} \right\} = 3A_1 \oplus \cdots
\]
Now let’s talk a bit about graphene.

**The goal**

To enumerate all possible terms in the free energy
Symmetries of Graphene

Whatever the energy function is, we know it has a lot of invariants:

- Discrete crystallographic translations
- 3D rotations of deformed sheet
- Graphene point group symmetries

The translations I know how to handle – Plane wave basis / Fourier Transforms. What about the others?
The Deformation Gradient

Think of elasticity as an embedding.

\[ Y : \mathbb{R}^2 \rightarrow \mathbb{R}^3 \]

\[ X_J = Y_J(x_i) \]

\[ dX_J = F_{ij}dx_i \]

The deformation gradient contains the important information about the deformation.

\[ F^T F = 1 + 2\varepsilon \]

\[ F = RU \]
A and B atoms

So, actually two functions

\[ \bar{Y} = \frac{1}{2} \left( Y^A + Y^B \right) \]

\[ \Delta = Y^A - Y^B \]

\( \bar{Y} \) gives rise to \( F \)
Graphene has a $D_{6h}$ point group symmetry.

- 24 group elements
### $D_{6h}$

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Free Energy

Now we can systematically expand the free energy...

• Powers of the strain
• Gradients
• Terms involving $\Delta$

The possible terms in our free energy are severely restricted by symmetry

\[ F_{ij} : \text{(vector on } D_{6h}) \times \text{(vector on } SO(3)) \]
\[ \epsilon_{ij} : \text{(rank 2 tensor on } D_{6h}) \]
\[ \Delta_J : \text{(pseudoscalar on } D_{6h}) \times \text{(vector on } SO(3)) \]
\[ \nabla_i : \text{(vector on } D_{6h}) \]
Consider an example term

\[ A_{lijjk\ell} \Delta I F_{ij} \epsilon_{jk} \epsilon_{\ell m} \]

We have a bunch of conditions (basically)

- Every little index must be invariant under \( D_{6h} \)
- Every big index must be invariance under \( SO(3) \)
- We must be able to swap \((jk) \leftrightarrow (\ell m)\)

This term forms a representation of our symmetries, namely

\[
\left[ V_{D_{6h}} \right] \otimes \left[ V_{D_{6h}} \otimes V_{SO(3)} \right] \otimes \left\{ \left[ V_{D_{6h}} \otimes V_{SO(3)} \right] \otimes \left[ V_{D_{6h}} \otimes V_{SO(3)} \right] \right\}
\]
Why I do it

There could have been

\[ 3 \times (2 \times 3) \times (2 \times 2) \times (2 \times 2) = 288 \]

Terms.

But turns out there are only 2 allowed.

\[ T_{ijk} \Delta I F_{iI} \epsilon_{jk} \epsilon_{ll} \]

\[ T_{klm} \Delta I F_{iI} \epsilon_{ik} \epsilon_{lm} \]

where

\[ T_{111} = T_{122} = T_{212} = T_{221} = 0 \]
\[ T_{112} = T_{222} = -1 \]
\[ T_{121} = T_{211} = 1 \]
Expand the Free Energy

Paying attention to symmetry...

\[ \mathcal{F} = \alpha_0 \epsilon_{ii} + \alpha_1 \epsilon_{ii} \epsilon_{jj} + \alpha_2 \epsilon_{ij} \epsilon_{ij} + \alpha_3 \epsilon_{ii} \epsilon_{jj} \epsilon_{kk} + \alpha_4 \epsilon_{ij} \epsilon_{jk} \epsilon_{ki} + \alpha_5 H_{ijklmn} \epsilon_{ij} \epsilon_{kl} \epsilon_{mn} + \alpha_6 a_0^2 F_{ii} \nabla_j \nabla_j F_{ii} + \alpha_7 a_0^4 F_{il} \nabla_j \nabla_j \nabla_k \nabla_k F_{il} + \alpha_8 a_0^4 H_{ijklmn} F_{il} \nabla_j \nabla_k \nabla_l \nabla_m F_{nl} + \alpha_9 a_0^{-1} T_{ijk} \Delta_l F_{il} \epsilon_{jk} + \alpha_{10} a_0^{-1} T_{ijk} \Delta_l F_{il} \epsilon_{jk} \epsilon_{ll} + \alpha_{11} a_0^{-1} T_{klm} \Delta_l F_{il} \epsilon_{ik} \epsilon_{lm} + \alpha_{12} a_0^{-2} \Delta_l \Delta_l + \alpha_{13} a_0^{-2} \Delta_l F_{lj} \Delta_j F_{Jj} + \ldots \]
Thanks.