Group Representations

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November 5, 2012

Group Theory

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

A feeling

Triangle

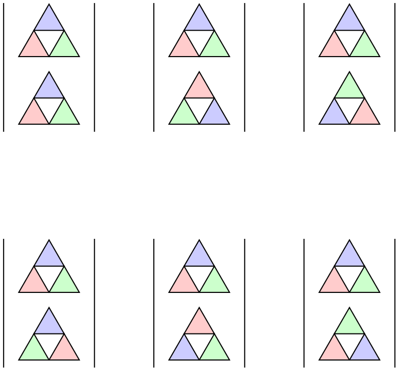
What are you allowed to do to the triangle to keep it unchanged?

Circle

What operations are you allowed to do to the circle that leave it unchanged?

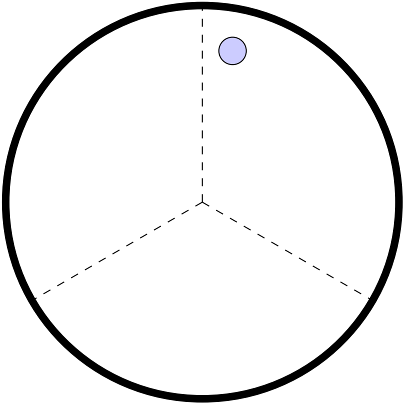
Triangle

What operations can we do that leave the triangle invariant?



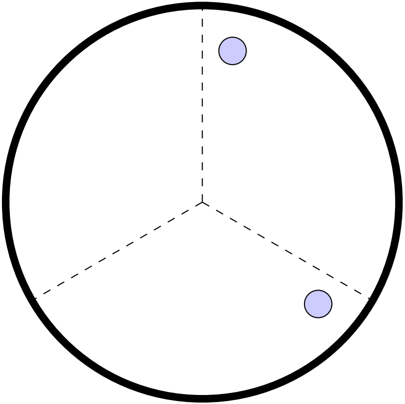
There are six total

C_{3v}



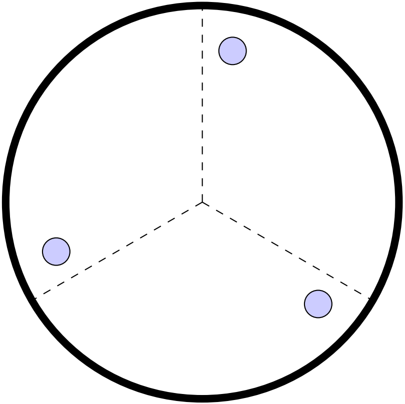
- We can also represents groups with these stereographic pictures.
- It is a way to create an object with the same symmetry.
- Imagine a plate with a single peg.

C_{3v}



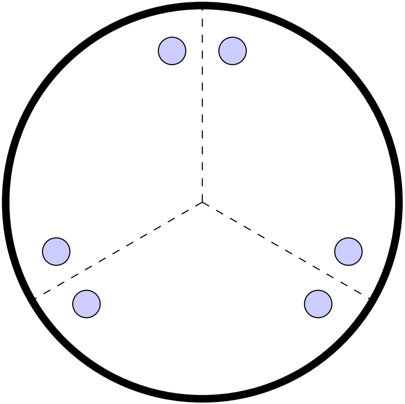
- Now start applying symmetry operations until done.
- First apply a rotation, we have to create a new peg.

C_{3v}



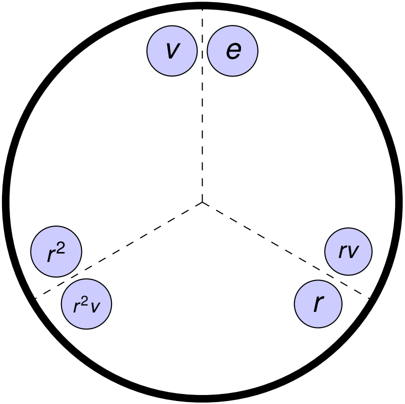
Rotate again and we create another.

C_{3v}



- 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

C_{3v}



- You can also identify individual pegs with individual group elements.
- Useful for reasoning out group operations.

Multiplication Table

	e	r	r^2	v	rv	r^2v
e	e	r	r^2	v	rv	r^2v
r	r	r^2	e	rv	r^2v	v
r^2	r^2	e	r	r^2v	v	rv
v	v	r^2v	rv	e	r^2	r
rv	rv	v	r^2v	r	e	r^2
r^2v	r^2v	rv	v	r^2	r	e

Group - Informal

Informally, it seems we have some common ground

- You can always do nothing

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- You can always do nothing
- You can always undo

Group - Informal

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.

Group - Formal

Definition

A *group* is a set G and a binary operation $\cdot$, $(G, \cdot)$, such that

- identity: $\exists e \in G, \forall g \in G : \quad g \cdot e = e \cdot g = g$
- inverses: $\forall g \in G, \exists g^{-1} \in G : g \cdot g^{-1} = g^{-1} \cdot g = e$
- closure: $\forall g_1, g_2 \in G : \quad g_1 \cdot g_2 \in G$
- 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

Representation

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

$$\boldsymbol{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Vector Representation of C_{3v}

$$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad R = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} & 0 \\ -\sqrt{3} & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

$$R^2 = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} & 0 \\ \sqrt{3} & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad V = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$RV = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{3} & 0 \\ \sqrt{3} & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \qquad R^2 V = \frac{1}{2}\begin{pmatrix} 1 & -\sqrt{3} & 0 \\ -\sqrt{3} & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

Fun fact: These matrices satisfy exactly the same multiplication table!

Representation - Formally

Definition

A *representation* Γ 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.

Functions

You can also generate new representations easily.
Consider

$$f(\boldsymbol{x})$$

Let's say we want to to transform naturally:

$$f'(\boldsymbol{x}') = f(\boldsymbol{x})$$

This defines some linear operators

$$f'(\boldsymbol{x}') = O_R f(\boldsymbol{x}') = O_R f(R\boldsymbol{x}) = f(\boldsymbol{x})$$

$$O_R f(\boldsymbol{x}) = f(R^{-1}\boldsymbol{x})$$

These $\{O_R\}$ will form a representation.

Similarity Transforms

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

$$R' = S^{-1} R S$$

because we will still satisfy the group algebra

$$R_1 R_2 = R_3 \implies (S^{-1} R_1 S)(S^{-1} R_2 S) = (S^{-1} R_3 S)$$

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.

$$\chi^{\Gamma}(R) = \text{Tr } R = \text{Tr } (S^{-1} R S) = \text{Tr } (S^{-1} S R) = \text{Tr } R$$

Characters

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

For the representation we created above:

$$\chi^{V}(E) = 3$$

$$\chi^{V}(R) = 0 \quad \chi^{V}(R^2) = 0$$

$$\chi^{V}(V) = 1 \quad \chi^{V}(RV) = 1 \quad \chi^{V}(R^2V) = 1$$

Classes

Notice that a lot of these guys have the same character.
A *class* is a collection of group elements that are roughly equivalent

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

In our case we have three classes. The identity (always its own class), the rotations, and the mirror symmetries.

Reducible Representation

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.

Character Table

The irreducible representations for the point groups are well documented, in *character tables*. E.g.

	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0
V	3	0	1

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.

Reducible representation - sums

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

	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0
V	3	0	1
$M = V \otimes V$	9	0	1
$E \otimes E$	4	1	0

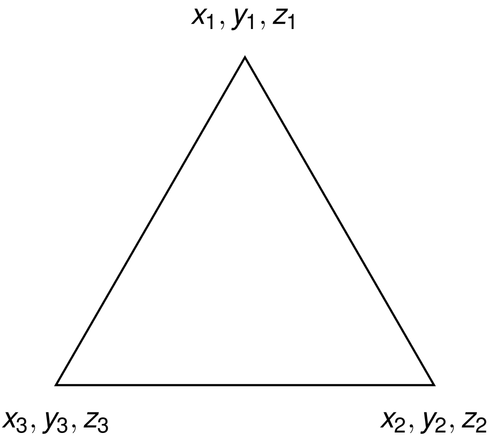
So we see

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

$$E \otimes E = A_1 \oplus A_2 \oplus E$$

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.



Representation

This forms a 9D representation of the group T. What are its characters

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

We already know how to decompose this

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

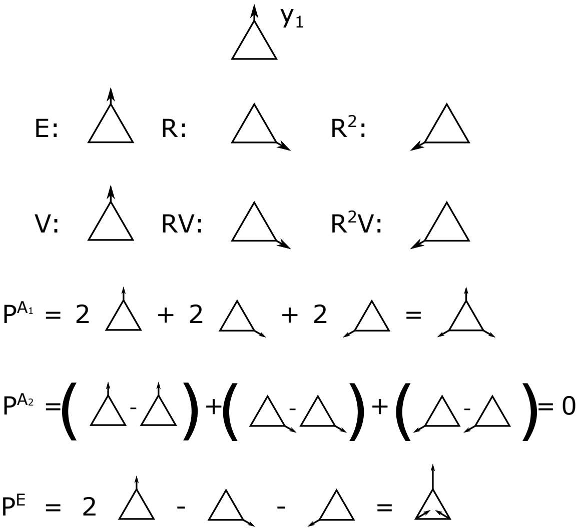
But what do these correspond to?

Projection operator

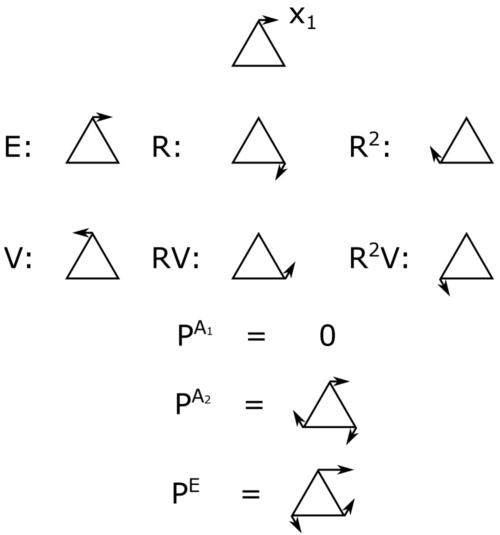
Since the character tables are super orthogonal

$$P^{\Gamma} = \sum_{g} \chi^{\Gamma}(g) D(g)$$

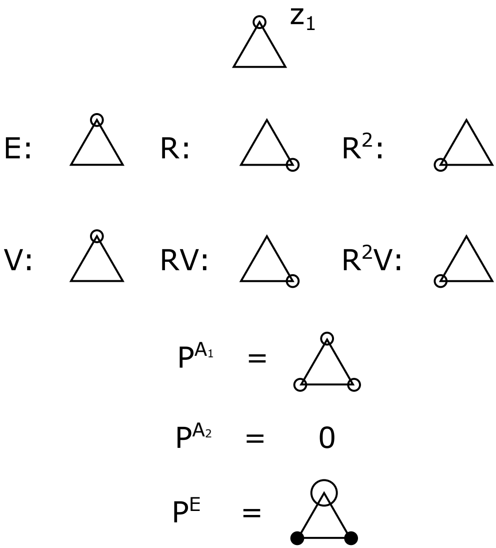
Projecting Down



Projecting Down

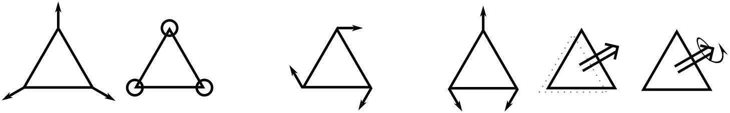


Projecting Down



Normal Modes

$$T = 2\,A_1 + A_2 + 3\,E$$



Continous Groups

There are also all of the continous 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:

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

where ψ is how much rotation you do (the classes)

Vectors

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

$$M_{ii} \qquad (M_{ij} - M_{ji}) \qquad (M_{ij} + M_{ji}) - \frac{1}{3}M_{ii}$$

A matrix has its trace (d=1), antisymmetric part (d=3), and symmetric trace free part (d=5).

2 Parameter Family

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
$l = -(2l + 1), ..., (2l + 1)$.
These parameters are physically important quantum numbers, the angular momentum and the magnetic quantum number.

Fourier Transforms

Consider the group of translations. $x \to x + a$. 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"

Poincare Group

Fun fact: The poincare 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

$$\epsilon_{ij}\epsilon_{kl}$$

$$\{\{V_{SO(3)} \otimes V_{SO(3)}\} \otimes \{V_{SO(3)} \otimes V_{SO(3)}\}\} = 2A_1 \oplus \cdots$$
$$\{\{V_{O_h} \otimes V_{O_h}\} \otimes \{V_{O_h} \otimes V_{O_h}\}\} = 3A_1 \oplus \cdots$$

Graphene

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.

$$Y : \mathbb{R}^2 \to \mathbb{R}^3$$

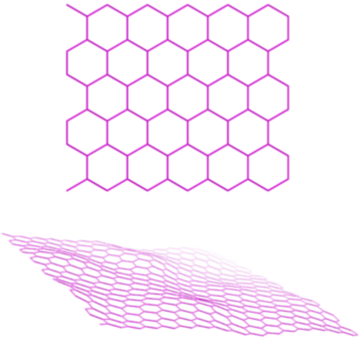
$$X_J = Y_J(x_i)$$

$$dX_J = F_{iJ} dx_i$$

The deformation gradient contains the important information about the deformation.

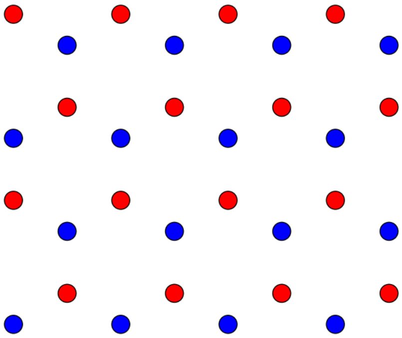
$$F^T F = 1 + 2\epsilon$$

$$F = RU$$



Sublattices

A and B atoms



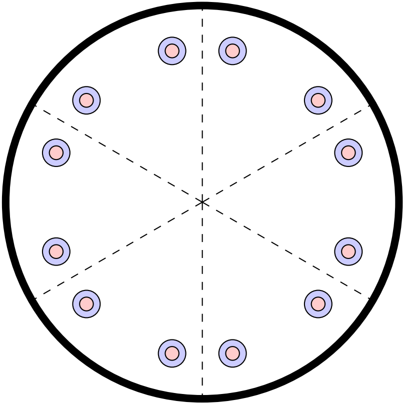
So, actually two functions

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

$$\Delta = Y^A - Y^B$$

$\bar{Y}$ gives rise to F

Point Group Symmetries - D_{6h}



- Graphene has a D_{6h} point group symmetry.
- 24 group elements

D_{6h}

	E	$2C_6$	$2C_3$	C_2	$3C_2'$	$3C_2''$	i	$2S_3$	$2S_6$	σ_h	$3\sigma_d$	$3\sigma_v$
A1g	1	1	1	1	1	1	1	1	1	1	1	1
A2g	1	1	1	1	-1	-1	1	1	1	1	-1	-1
B1g	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1
B2g	1	-1	1	-1	-1	1	1	-1	1	-1	-1	1
E1g	2	1	-1	-2	0	0	2	1	-1	-2	0	0
E2g	2	-1	-1	2	0	0	2	-1	1	2	0	0
A1u	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
A2u	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1
B1u	1	-1	1	-1	1	-1	-1	1	-1	1	-1	-1
B2u	1	-1	1	-1	-1	1	-1	1	-1	1	1	-1
E1u	2	1	-1	-2	0	0	-2	-1	1	2	0	0
E2u	2	-1	-1	2	0	0	-2	1	-1	-2	0	0

Free Energy

Now we can systematically expand the free energy...

- Powers of the strain
- Gradients
- Terms involving Δ

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

$$
\begin{aligned}
F_{iJ} &:(\text{vector on } D_{6h}) \times (\text{vector on } SO(3)) \\
\epsilon_{ij} &:(\text{rank 2 tensor on } D_{6h}) \\
\Delta_J &:(\text{pseudoscalar on } D_{6h}) \times (\text{vector on } SO(3)) \\
\nabla_i &:(\text{vector on } D_{6h})
\end{aligned}
$$

Example Term

Consider an example term

$$A_{IiJjklm}\Delta_I F_{iJ}\epsilon_{jk}\epsilon_{lm}$$

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 $(jk) \leftrightarrow (lm)$

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.

$$T_{ijk} \Delta_l F_{il} \epsilon_{jk} \epsilon_{ll}$$

$$T_{klm} \Delta_l F_{il} \epsilon_{ik} \epsilon_{lm}$$

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...

$$
\begin{aligned}
\mathcal{F} = {} & \alpha_0 \epsilon_{ii} \\
& + \alpha_1 \epsilon_{ii}\epsilon_{jj} + \alpha_2 \epsilon_{ij}\epsilon_{ij} \\
& + \alpha_3 \epsilon_{ii}\epsilon_{jj}\epsilon_{kk} + \alpha_4 \epsilon_{ij}\epsilon_{jk}\epsilon_{ki} + \alpha_5 H_{ijklmn}\epsilon_{ij}\epsilon_{kl}\epsilon_{mn} \\
& + \alpha_6 a_0^2 F_{iI} \nabla_j \nabla_j F_{iI} \\
& + \alpha_7 a_0^4 F_{iI} \nabla_j \nabla_j \nabla_k \nabla_k F_{iI} + \alpha_8 a_0^4 H_{ijklmn} F_{iI} \nabla_j \nabla_k \nabla_l \nabla_m F_{nI} \\
& + \alpha_9 a_0^{-1} T_{ijk} \Delta_I F_{iI} \epsilon_{jk} \\
& + \alpha_{10} a_0^{-1} T_{ijk} \Delta_I F_{iI} \epsilon_{jk} \epsilon_{ll} + \alpha_{11} a_0^{-1} T_{klm} \Delta_I F_{iI} \epsilon_{ik} \epsilon_{lm} \\
& + \alpha_{12} a_0^{-2} \Delta_I \Delta_I \\
& + \alpha_{13} a_0^{-2} \Delta_I F_{Ij} \Delta_J F_{Jj} \\
& + \cdots
\end{aligned}
$$

The End

Thanks.