

SYMMETRIES IN TRANSITIONAL METAL COMPOUNDS

GROUP THEORY TOOLS FOR THEORETICAL PHYSICS IN SOLIDS

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Short notes like this are not my original discovery, but I still uploaded them for pedagogical purposes of my own. The application part is related to my current project concerning $RuCl_3$, whose mechanisms responsible for non-trivial properties¹ are still open questions. **The symmetry groups mentioned in this file include: space group, cubic symmetry for octahedrons, Lie group, double group and spin-space group.** I will keep updating this file.

¹ Specify the term "non-trivial"

1 Symmorphic and Nonsymmorphic Space Groups

The notation for a general space group operation is $\{\mathbf{R}_\alpha|\tau\}$, where \mathbf{R}_α is a point group group operation of rotations, improper rotations, reflections and inversions, while τ is a translational operation. The α denotes one group element of the full rotational group. For instance,

$$\begin{aligned} \{\varepsilon|0\}, & \text{ identity,} \\ \{\alpha|0\}, & \text{ pure rotation,} \\ \{\varepsilon|\tau\}, & \text{ pure translation.} \end{aligned} \tag{1}$$

The effect if the operation $\{\alpha|\tau\}$ ² on a vector \mathbf{r} is

$$\{\alpha|\tau\}\mathbf{r} = \mathbf{r}' \Leftrightarrow \alpha\mathbf{r} + \tau. \tag{2}$$

² Its inverse is $\{\alpha^{-1}| - \alpha\tau\}$.

In crystals of infinite size, periodicity makes points that differ by a multiple of primitive translations equivalent. A general space group operation can rephrased as

$$\{\mathbf{R}_\alpha|\tau\} = \{\mathbf{R}_\alpha|\mathbf{R}_n + \tau_{<}\} = \{\varepsilon|\mathbf{R}_n\}\{\mathbf{R}_\alpha|\tau_{<}\}, \tag{3}$$

where $\tau = \mathbf{R}_n + \tau_{<}$, \mathbf{R}_n is a linear combination of Bravais vectors, and $\tau_{<}$ is a translation within a unit cell. The definitions of a symmorphic and nonsymmorphic space group are as follows:

Definition 1

A **symmorphic** or simple space group is a group with all elements satisfying

$$\{\mathbf{R}_\alpha|\tau\} = \{\varepsilon|\mathbf{R}_n\}\{\mathbf{R}_\alpha|\tau_{<}\} = \{\varepsilon|\mathbf{R}_n\}\{\mathbf{R}_\alpha|0\}, \tag{4}$$

while a **nonsymmorphic** space group is a group with at least one element which has nonzero $\tau_{<}$.

2 Translation Subgroup

To clarify the difference between symmorphic and nonsymmorphic space groups, we first review the relation between the translation subgroup T and the space group G . First, the translations $\{\varepsilon|\tau\}$ form a **self-conjugate subgroup**³ T of the space group G . An arbitrary conjugate of a group element $\{\varepsilon|\tau\}$ is

$$\begin{aligned} \{\mathbf{R}_\alpha|\tau\}\{\varepsilon|\tau'\}\{\mathbf{R}_\alpha|\tau\}^{-1} &= \{\mathbf{R}_\alpha|\tau\}\{\varepsilon|\tau'\}\{\mathbf{R}_\alpha^{-1}| - \mathbf{R}_\alpha^{-1}\tau\} \\ &= \{\mathbf{R}_\alpha|\tau\}\{\mathbf{R}_\alpha^{-1}| - \mathbf{R}_\alpha^{-1}\tau + \tau'\} \\ &= \{\varepsilon|\mathbf{R}_\alpha\tau'\}, \end{aligned} \tag{5}$$

where $\{\varepsilon|\mathbf{R}_\alpha\tau'\}$ is *by definition*⁴ another translation in the subgroup T .

Remark

The translation subgroup T defines the Bravais lattice. In 2D and 3D spaces, there are 5 and 14 Bravais lattices, respectively.

³ self-conjugate = normal = invariant

For 3D crystals, the total 230 space groups are the *combinations* of 32 **crystallographic point groups** and 14 Bravais lattices. For a nonsymmorphic space group, the point

⁴ I haven't showed to myself that $\mathbf{R}_\alpha\tau'$ is just another translation, but by def., it is!

group g acquired by setting the translational part to zero is a subgroup of a **holohedral group**⁵, but it is not a subgroup of G . To obtain the rotational part of a nonsymmorphic group, one of the procedures is to find its factor group G/T .

Theorem 1 The cosets of the self-conjugate subgroup T form the factor group of the space group G . G/T is isomorphic to the rotational parts of the operators of the space group G .

Besides, the Bloch functions $\psi_{\mathbf{k}} = e^{i\mathbf{k}\cdot\mathbf{r}} \mathbf{u}_{\mathbf{k}}(\mathbf{r})$ are the basis functions of the translation group T . The wave vector \mathbf{k} are the quantum numbers of of translation and the label for irreducible representations of translation group. A translation group is abelian so fits in the properties above.

Definition 2 A **class** is a set of group elements which are the conjugates of a given element; if all elements commute, the group is called an **abelian** group.

Theorem 2 The number of irreducible representations is equal to the number of classes.

Theorem 3 From the orthogonality theorem, the order of a group h and the dimensionality l_i of the irreducible representations Γ_j have the relation

$$\sum l_j^2 = h. \quad (6)$$

Remark Since the elements of an abelian group commute,

$$XAX^{-1} = B, \text{ or } XA = BX = AX, \quad (7)$$

every elements of an abelian group is **self-conjugate** and forms a class. Because the number of irreducible representation is equal to the number of classes, each irreducible representation is one-dimensional.

3 Representations and Little Groups of \mathbf{k}

To understand the star of the the wave vector \mathbf{k} , we review some basis properties of Bloch functions. Consider a symmorphic group.

Definition 3 Since G/T is isomorphic to the point group g , the small representations for the little group of wave vector \mathbf{k} are given by

$$D_{\mathbf{k}}^{\Gamma_i}(\{\mathbf{R}_\alpha | \mathbf{R}_n\}) = e^{i\mathbf{k}\cdot\mathbf{R}_n} D^{\Gamma_i}(\mathbf{R}_\alpha), \quad (8)$$

where Γ_i is the i^{th} irreducible representation of the point group. The character has similar relation,

$$\chi_{\mathbf{k}}^{\Gamma_i}(\{\mathbf{R}_\alpha | \mathbf{R}_n\}) = e^{i\mathbf{k}\cdot\mathbf{R}_n} \chi^{\Gamma_i}(\mathbf{R}_\alpha). \quad (9)$$

Remark For $\mathbf{k} = \mathbf{0}$, the representations and characters are identical as that of the case of the point group and factor group.

3.1 Representation Theory

Definition 4 A **(linear) representation** of a group G is a homomorphism $D : G \rightarrow End(\mathcal{V})$, where \mathcal{V} is a vector space of dimension $\dim(\mathcal{V})$, and $End(\mathcal{V})$ is the space of the endomorphism of \mathcal{V} , or the space of operators $D(G)$. The representation is **faithful**

⁵ The 32 crystallographic point groups are categorized into 7 crystal families. In each family, the group of highest order is called the holohedral group.

if $D(G)$ is an isomorphism.

The representations, or the operators, should be independent of choices of basis. The most formal way to write down the difference is as follows

$$D(G)|e_i\rangle = |e_i\rangle D_{ik}^{(n)}, \quad (10)$$

where $D_{ik}^{(n)} \in GL(n, \mathbb{C})$ is a $n \times n$ matrix. If a representation is **irreducible**, it means that for the vector space this representation operates on, there is no nontrivial⁶ invariant subspace $\mathcal{V}_1 \subset \mathcal{V}$. In contrast, the reduction of a **reducible** representation $D^\psi(G)$ is

$$\begin{aligned} D^\psi(G) &= D^{\Gamma_1}(G) \oplus D^{\Gamma_1}(G) \oplus \cdots \oplus D^{\Gamma_2}(G) \oplus D^{\Gamma_2}(G) \oplus \cdots \\ &= n_{\Gamma_1} D^{\Gamma_1}(G) \oplus n_{\Gamma_2} D^{\Gamma_2}(G) \oplus \cdots \\ &= \bigoplus_{\Gamma} n_{\Gamma} D^{\Gamma}(G). \end{aligned} \quad (11)$$

⁶ The trivial subspaces are the \mathcal{V} itself and the null space.

3.2 Basis Functions for Irreducible Representations

Theorem 4

The great orthogonality theorem Consider all the inequivalent irreducible, unitary representations of a group, Then

$$\sum_{\mathbf{R}} \Gamma^{(i)}(\mathbf{R})_{\mu\nu}^* \Gamma^{(j)}(\mathbf{R})_{\alpha\beta} = \frac{h}{l_i} \delta_{ij} \delta_{\mu\alpha} \delta_{\nu\beta}, \quad (12)$$

where the summation \mathbf{R} runs over all group elements E, A_2, \dots, A_h , and l_i is the dimensionality of $\Gamma^{(i)}$.

Representations of dimensionality greater than 1 come from the noncommuting elements. For the j^{th} IR of dimension N , a set of basis functions $\{\phi_{\lambda_1}^{(j)}, \dots, \phi_{\lambda_N}^{(j)}\}$ are called **partners** to each other. An operation on one basis function $\phi_k^{(j)}$ is written as

$$P_R \phi_k^{(j)} = \sum_{\lambda=1}^{l_j} \phi_{\lambda}^{(j)} \Gamma_{\lambda k}^{(j)}. \quad (13)$$

This can be understood in the following way. Take $l_j = 3$, $k = 1$ as an example⁷,

$$\begin{aligned} \phi^{(j)} &= \{\hat{\phi}_1^{(j)}, \hat{\phi}_2^{(j)}, \hat{\phi}_3^{(j)}\}, \\ \Gamma^{(j)} &= \begin{bmatrix} \Gamma_{11}^{(j)} \Gamma_{12}^{(j)} \Gamma_{13}^{(j)} \\ \Gamma_{21}^{(j)} \Gamma_{22}^{(j)} \Gamma_{23}^{(j)} \\ \Gamma_{31}^{(j)} \Gamma_{32}^{(j)} \Gamma_{33}^{(j)} \end{bmatrix}, \end{aligned} \quad (14)$$

$$P_R \hat{\phi}_1^{(j)} = \sum_{\lambda=1}^{l_j} \phi_{\lambda}^{(j)} \Gamma_{\lambda 1}^{(j)} = \Gamma_{11}^{(j)} \hat{\phi}_1^{(j)} + \Gamma_{21}^{(j)} \hat{\phi}_2^{(j)} + \Gamma_{31}^{(j)} \hat{\phi}_3^{(j)},$$

⁷ This is not correct. To be revised

which is exactly the transformation of unit vectors in undergraduate linear algebra. Eq. (13) shows how a unit vector transforms under operation $\Gamma^{(j)}$. To see this in another way, we write down the transformation of an arbitrary vector $\sum_k^{l_j} v_k \phi_k^{(j)}$,

$$P_R \sum_k^{l_j} v_k \phi_k^{(j)} = \sum_k^{l_j} (P_R \phi_k^{(j)}) v_k = \sum_{\lambda=1}^{l_j} \phi_{\lambda}^{(j)} \sum_k^{l_j} \Gamma_{\lambda k}^{(j)} v_k = \sum_{\lambda=1}^{l_j} v'_{\lambda} \phi_{\lambda}^{(j)}. \quad (15)$$

The point is, the terms $\sum_{\lambda=1}^{l_j} \phi_{\lambda}^{(j)} \Gamma_{\lambda k}^{(j)}$ and $\sum_k^{l_j} \Gamma_{\lambda k}^{(j)} v_k$ only differ in convention, but we need to be careful about what $\phi_{\lambda}^{(j)}$ and v_k are. For instance, $\sum_k^{l_j} v_{\lambda} \Gamma_{\lambda k}^{(j)}$ is a wrong transform. Multiply Eq. (13) by $\Gamma_{\lambda' k'}^{(i)}(\mathbf{R})^*$,

$$\sum_{\mathbf{R}} \Gamma_{\lambda' k'}^{(i)}(\mathbf{R})^* P_R \phi_k^{(j)} = \sum_{\lambda=1}^{l_j} \phi_{\lambda}^{(j)} \sum_{\mathbf{R}} \Gamma_{\lambda' k'}^{(i)}(\mathbf{R})^* \Gamma_{\lambda k}^{(j)}(\mathbf{R}) = \sum_{\lambda=1}^{l_j} \phi_{\lambda}^{(j)} \frac{h}{l_i} \delta_{ij} \delta_{\lambda \lambda'} \delta_{kk'}. \quad (16)$$

Consider the cases with nonzero result on the RHS, we define an operator

$$\mathcal{P} \equiv \frac{l_i}{h} \sum_{\mathbf{R}} \Gamma_{\lambda k}^{(j)}(\mathbf{R})^* P_R \quad (17)$$

$$\mathcal{P} \phi_k^{(j)} = \sum_{\lambda=1}^{l_j} \phi_{\lambda}^{(j)}. \quad (18)$$

An alternative method to find the basis functions for 2D irreps is to construct a basis

$$|\Gamma_n \alpha\rangle = a_1 + \omega a_2 + \cdots + \omega^{n-1} a_n \quad (19)$$

which is a eigenstate of principal axis rotation C_n . $|\Gamma_n \beta\rangle$, the complex conjugate of $|\Gamma_n j\rangle$, is the other eigenstate of C_n rotation.

4 Lie Groups

A very simple but perplexing problem is whether a 2×2 matrix is diagonalizable or not. To answer this question concretely and understand the symmetries of orbitals in real materials, we must go through the basics of representations of continuous groups.

Definition 5

A **matrix Lie group** is a subgroup G of $GL(n, \mathbb{C})$, complex invertible $n \times n$ matrices, such that if A_n is a sequence of matrices in G and converges to A , then $A \in G$ or it is noninvertible. Then G is a closed subgroup of $GL(n, \mathbb{C})$.

The Dresselhaus's textbook states that the 2D irreps found through Eq. 18 could have some problem. For instance, the matrices are not unitary.

5 Cubic Crystal Field

The so-called **cubic crystal field** is an electron distribution of a cubic cell. For many transition metal compounds, the ligands form an octahedral cage with charges centered at the vertices of the cage. A regular octahedron has $O_h = O \otimes i$ symmetry, where the subscript h means inversion symmetry⁸. The decomposition of $\Gamma_{l=2}$ is shown in Table(2).

rep	irreps	E	$8C_3$	$3C_2 = 3C_4^2$	$6C'_2$	$6C_4$
$\Gamma_{l=2}$	$E + T_2$	5	-1	1	1	-1

Table 1. Angular momenta of l are irreducible representations of $SO(3)$. This table shows that, for instance, $\Gamma_{l=2}$ become reducible under a lower symmetry O . These characters can be obtained by from the expression of the characters for rotation α along the z axis $\chi^{(l)}(\alpha) = \frac{\sin[(l+\frac{1}{2})\alpha]}{\sin[\alpha/2]}$, where α is the rotation degree.

⁸ The subscript d means a reflection.

Under inversion, the spherical harmonics transform by a factor $(-1)^l$

$$\hat{P}_I Y_m^l(\theta, \phi) \rightarrow Y_m^l(\pi - \theta, \pi + \theta) = (-1)^l Y_m^l(\theta, \phi), \quad (20)$$

which shows that

$$\chi^{(l)}(i) = \sum_{m=-l}^{m=l} (-1)^l = (-1)^l(2l+1), \quad (21)$$

and for odd l , the spherical harmonics, or say the orbital angular momenta, are not invariant under inversion. $Y_m^l(\theta, \phi)$ are irreducible representations of $SO(3)$, but for a lower group like O , $Y_m^l(\theta, \phi)$ are reducible representations of O for $l > 2$. What do angular momenta look like in the real symmetry O_h of an octahedron? Now here is the argument: Since O_h is the direct product⁹ of O and i , their characters follow the rule

$$\chi^{(a \otimes b)}(A_k B_l) = \chi^{(a)}(A_k) \chi^{(b)}(B_l), \quad (22)$$

where a, b is the dimension of each irreducible representation and A_k and B_l are the elements of group A and B . Let's take angular momenta $l = 2$ as an example. The representation $\Gamma_{l=2}$ is decomposed into irreducible representations

$$\begin{aligned} \Gamma_{l=2} &= E + T_2, \text{ for group } O, \\ \Gamma_{l=2} &= 5A, \text{ for group } C_i. \end{aligned} \quad (23)$$

We can first observe from Eq.(20) that $Y_m^{l=2}(\theta, \phi)$ is even under inversion, so we need not to worry about Γ_B irreducible representation of C_i . According to Eq.(22),

$$\begin{aligned} \chi^{(E \otimes A)}(O_k C_{i,l}) &= \chi^{(E)}(O_k) \chi^{(A)}(C_{i,l}) \equiv \chi^{(E_g)}(O_{h,k,l}), \\ \chi^{(T_2 \otimes A)}(O_k C_{i,l}) &= \chi^{(T_2)}(O_k) \chi^{(A)}(C_{i,l}) \equiv \chi^{(T_{2g})}(O_{h,k,l}), \end{aligned} \quad (24)$$

whose values are listed in Table (2). One can review this chapter if he/she needs to decompose a representation into irreducible ones of a direct product group.

reps	E	$8C_3$	$3C_2 = 3C_4^2$	$6C'_2$	$6C_4$	i	$8iC_3$	$3iC_2 = 3iC_4^2$	$6iC'_2$	$6iC_4$
E_g	2	-1	2	0	0	2	-1	2	0	0
T_{2g}	3	0	-1	1	-1	3	0	-1	1	-1
$\Gamma_{l=2}$	5	-1	1	1	-1	5	-1	1	1	-1

Table 2. The indices k and l denote the classes of each group, so the number of classes in O_h group is $k \times l = 5 \times 2 = 10$. In O_h group, since angular momenta $l = 2$ are even under inversion, the irreducible representations of concern are those with index g , which means even under inversion, and then $\Gamma_{l=2} = E_g + T_{2g}$.

6 Double Group and Spin-Space Group

proper and improper rotation and the effects on vector/pseudovector

6.1 Double Group

Double cover of a point group refer to a mathematical extension of it that includes spinor properties and spinor representation. For instance, $SU(2)$ is the double cover of $SO(3)$.

From quaternions to double cover of $SO(3)$

Quaternion is a number system \mathbf{V} that generalized complex numbers, whose element q and relative rules are written as \mathbf{V} is isomorphic to R^4

$$q = q_0 + q_1\mathbf{i} + q_2\mathbf{j} + q_3\mathbf{k}, q_\mu \in \mathbf{R}, \quad (25)$$

$$\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = -1, \quad (26)$$

⁹ An improper rotation is a compound operation which can be written as the direct product of a proper rotation and an inversion(mirror plane). To see more derivation, check Chap.6 of Dresselhaus's book.

$$\mathbf{i}\mathbf{j} = \mathbf{k}, \mathbf{j}\mathbf{k} = \mathbf{i}, \mathbf{k}\mathbf{i} = \mathbf{j}, \quad (27)$$

$$\bar{q} = q_0 - q_1\mathbf{i} - q_2\mathbf{j} - q_3\mathbf{k}, q_\mu \in \mathbf{R}, \quad (28)$$

$$|q|^2 = q\bar{q} = q_0^2 + q_1^2 + q_2^2 + q_3^2, \quad (29)$$

$$\bar{u}\bar{v} = \bar{v}\bar{u}. \quad (30)$$

$$|uv|^2 = uv\bar{u}\bar{v} = uv\bar{v}\bar{u} = |u|^2|v|^2. \quad (31)$$

The quaternions q of length-1 form a group called $sp(1)$. The inverse element is defined as

$$q^{-1} = \frac{\bar{q}}{|q|^2} = \bar{q}. \quad (32)$$

The unit sphere $S^3 \subset \mathbf{R}^4$ is

$$q_0^2 + q_1^2 + q_2^2 + q_3^2 = 1. \quad (33)$$

Let (u, v) be the element in the product group $sp(1) \times sp(1)$. The cover mapping from $sp(1) \times sp(1)$ to $SO(4)$ is

$$\Phi_{cover} : (u, v) \in sp(1) \times sp(1) \rightarrow \{q \rightarrow uqv^{-1}\} \in SO(4). \quad (34)$$

This mapping shows that $sp(1) \times sp(1)$ "double covers" $SO(4)$. The double cover of $SO(3)$ is $sp(1)$. To show that we start with the subgroup of $sp(1) \times sp(1)$ (or $spin(4)$), $spin(3)$, which acts on 3 dimensions of quaternions

$$q \equiv p = p_1\mathbf{i} + p_2\mathbf{j} + p_3\mathbf{k}, \quad (35)$$

which lies in a subspace \mathcal{Q} of quaternions. In the following we will show that $sp(1)$ (or $spin(3)$) is the double cover of $SO(3)$ by showing that $upu^{-1} \in \mathcal{Q}$. This can be done by simple math,

$$\begin{aligned} u &= u_0 + u_1\mathbf{i} + u_2\mathbf{j} + u_3\mathbf{k}, \\ p &= p_0 + p_1\mathbf{i} + p_2\mathbf{j} + p_3\mathbf{k}, p_0 = 0. \end{aligned} \quad (36)$$

$$\begin{aligned} up &= u_0p_0 - u_1p_1 - u_2p_2 - u_3p_3 + \mathbf{i}(u_0p_1 + p_0u_1 + u_2p_3 - u_3p_2) \\ &\quad + \mathbf{j}(u_0p_2 + p_0u_2 + u_3p_1 - u_1p_3) + \mathbf{k}(u_0p_3 + p_0u_3 + u_1p_2 - u_2p_1) \end{aligned} \quad (37)$$

Picking out the real number of upu^{-1} ,

$$\begin{aligned} &u_0p_0u_0 - u_1p_1u_0 - u_2p_2u_0 - u_3p_3u_0 \\ &\quad + u_0p_1u_1 + p_0u_1u_1 + u_2p_3u_1 - u_3p_2u_1 \\ &\quad + u_0p_2u_2 + p_0u_2u_2 + u_3p_1u_2 - u_1p_3u_2 \\ &\quad + u_0p_3u_3 + p_0u_3u_3 + u_1p_2u_3 - u_2p_1u_3 = 0. \end{aligned} \quad (38)$$

The element after transformation is still a 3-dimensional quaternion whose real component is zero. Thus,

$$\begin{aligned} &upu^{-1} \in \mathcal{Q}, \\ &\Phi : (u, u) \in spin(3) \rightarrow \{p \rightarrow upu^{-1}\} \in SO(3). \end{aligned} \quad (39)$$

We also have Lie group $sp(n)$, but it is not significant in quantum mechanics.

acts non-trivially? Why?

Result 6.1. The element of $sp(1)$ group is a quaternion of unit length; by tensor product $sp(1) \times sp(1)$, one can get $spin(4)$ group, which is the double cover of $SO(4)$. $spin(3)$, a subgroup of $spin(4)$, is the double cover of $SO(3)$.

If the isomorphism between quaternions and 2 by 2 complex matrices is developed, then we could go on to argue that $SU(2)$ is the double cover of $SO(3)$. This approach is not so intuitive, though. I found a better material that could help us build the idea of a double cover.

Projection Representations

A projection representation keeps the multiplication rule up to a phase

$$D(g)D(h) = \omega(g, h)D(gh), \quad (40)$$

where $\omega(g, h) \in \mathbb{C}$ for all g, h is called **cocycle**, and the associativity is kept as well. The irreducible representations of an abelian group are all one dimensional, whereas the irreducible projective representation of an abelian group can be two-dimensional. The simplest example of projective representation is probably that of $Z_2 \times Z_2$ abelian group $\{E, \sigma, \tau, \sigma\tau\}$. the projective representations of $G = Z_2 \times Z_2$ are

$$D(\sigma) = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, D(\tau) = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, D(\sigma\tau = \tau\sigma) = iY \equiv \Lambda = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (41)$$

You can check that the algebraic structure of $\mathbb{Z}_2 \times \mathbb{Z}_2$ in this representation is preserved up to a phase. For instance, $D(\tau)D(\sigma) = -D(\tau\sigma)$. A non-abelian group¹⁰ $\tilde{G} = \{\pm E, \pm X, \pm Z, \pm \Lambda\}$ is a "double cover"¹¹ of $G = Z_2 \times Z_2$. The **quaternion group**, on the other hand, is $\pm E, \pm iX, \pm iZ, \pm \Lambda$. The extension of group G can be obtained by a procedure called an **exact sequence of homomorphism**. Let us skip it for now¹². One of the famous example is $SU(2)$ as the double cover of $SO(3)$, i.e., $SU(2)/\mathbb{Z}_2 \sim SO(3)$. Every $R \in SO(3)$ can be mapped to two elements $\pm U \in SU(2)$

$$\begin{aligned} U\sigma^\alpha U^\dagger &= R_{\alpha\beta}\sigma^\beta, \\ R_{\alpha\beta}(\xi) &= n^\alpha n^\beta + (\delta^{\alpha\beta} - n^\alpha n^\beta) \cos \xi - \epsilon_{\alpha\beta\gamma} n^\gamma \sin \xi \end{aligned} \quad (42)$$

$R_{\alpha\beta}(\xi)$ is the $SO(3)$ rotation along arbitrary direction.

$$\begin{aligned} U(\xi, \mathbf{n}) &= \exp\left(-\frac{i}{2}\xi \hat{\mathbf{n}} \cdot \boldsymbol{\sigma}\right) = \cos \frac{\xi}{2} I - i \sin \frac{\xi}{2} (\mathbf{n} \cdot \boldsymbol{\sigma}), \\ -U(\xi, \mathbf{n}) &= -\cos \frac{\xi}{2} I + i \sin \frac{\xi}{2} (\mathbf{n} \cdot \boldsymbol{\sigma}) = \cos \frac{\xi + 2\pi}{2} I - i \sin \frac{\xi + 2\pi}{2} (\mathbf{n} \cdot \boldsymbol{\sigma}) = U(\xi + 2\pi, \mathbf{n}). \end{aligned} \quad (43)$$

From Eq.(43), rotation U by ξ and $\xi + 2\pi$ has the same effect on σ^α .

7 Applications

7.1 Spin-Spin Couplings for 2D Kitaev Material

This subsection is part of the content of my master's thesis and contains immature notations. In the above derivations, we only consider the hopping due to orbital overlaps and the only Coulomb interaction term that affects the electron configurations of the lowest energies is the Hubbard potential. If we consider Hund's coupling and derive the

¹⁰ There are only two non-abelian groups of order eight: the D_4 group and quaternion group.

¹¹ Usually the the collocation cover group refers to the central extension of a Lie group.

¹² If being interested, one could check the mathematics of $H^2(G, U(1))$. You can learn the similarity between "double covers" like D_4 and $SU(2)$.

second-order effective Hamiltonian, we can get other nearest neighbor hopping terms

$$\begin{aligned} S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha, \\ S_i^\alpha S_j^\gamma + S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta + S_i^\gamma S_j^\alpha. \end{aligned} \quad (44)$$

These terms are important since they are believed to stabilize the antiferromagnetic zigzag state, which is the ground state of monolayer $\alpha - RuCl_3$. The perturbation approach to obtain terms in Eq.(44) is cumbersome and theoretically, it only includes the hopping mechanism caused by orbital overlaps. Therefore it is worth a shot that we try identifying the symmetry-allowed terms. Consider the nearest neighboring bonds, the couplings should be invariant under the symmetry transformation of the tetrahedron. The symmetries of n.n. bonds form a C_{2h} group: E, I, C_2, σ_h . Since $\sigma_h = IC_2$, a coupling invariant under both symmetry transformations C_2 and I is automatically invariant under σ_h transformation. To find the invariant couplings, we have to do three things:

1. transform each basis vectors
2. find the transformed results of the constructed operators, e.g. Pauli matrices
3. "guess/list" the invariant couplings.

Recall that

$$\begin{aligned} |\psi_{E_1}^{(1)}\rangle &= \frac{-i}{\sqrt{3}}|\tilde{0}, \uparrow\rangle + \frac{\sqrt{2}}{\sqrt{3}}|\tilde{1}, \downarrow\rangle \equiv |\tilde{\downarrow}\rangle, \\ |\psi_{E_1}^{(2)}\rangle &= \frac{1}{\sqrt{3}}|\tilde{0}, \downarrow\rangle + \frac{-i\sqrt{2}}{\sqrt{3}}|\tilde{1}, \uparrow\rangle \equiv |\tilde{\uparrow}\rangle. \end{aligned} \quad (45)$$

and the basis vectors contain real space components and spin components. Notice that we want to check the transformation effects of symmetry \hat{O} on operators, we check the effects of \hat{O}^\dagger instead.

7.1.1 Inversion symmetry

The effect of inversion on the real space components are:

$$\begin{aligned} \langle \theta, \phi | \hat{I}^\dagger | \tilde{0} \rangle_1 &= \langle \hat{I}\theta, \hat{I}\phi | \tilde{0} \rangle_1 = \langle \theta', \phi' | \tilde{0} \rangle_2 = \langle \theta, \phi | \tilde{0} \rangle_2, \\ \langle \theta, \phi | \hat{I}^\dagger | \tilde{1} \rangle_1 &= \langle \hat{I}\theta, \hat{I}\phi | \tilde{1} \rangle_1 = \langle \theta', \phi' | \tilde{1} \rangle_2 = \langle \theta, \phi | \tilde{1} \rangle_2, \\ \langle \theta, \phi | \hat{I}^\dagger | \tilde{1} \rangle_1 &= \langle \hat{I}\theta, \hat{I}\phi | \tilde{1} \rangle_1 = \langle \theta', \phi' | \tilde{1} \rangle_2 = \langle \theta, \phi | \tilde{1} \rangle_2. \end{aligned} \quad (46)$$

The spin components are also invariant under inversion symmetry. Only the positions exchange. Therefore,

$$\begin{aligned} I^\dagger |\tilde{\uparrow}\rangle_1 &= |\tilde{\uparrow}\rangle_2, \\ I^\dagger |\tilde{\downarrow}\rangle_1 &= |\tilde{\downarrow}\rangle_2, \end{aligned} \quad (47)$$

and

$$S_1^\gamma \longrightarrow S_2^\gamma. \quad (48)$$

7.1.2 C_2 rotation symmetry

Consider its effect on coordinates:

$$C_2(x, y, z) = (y, x, -z), \quad (49)$$

The real space components change like:

$$\begin{aligned} |\tilde{0}\rangle &\rightarrow |\tilde{0}\rangle \\ |\tilde{1}\rangle &\rightarrow i|\tilde{-1}\rangle \\ |\tilde{-1}\rangle &\rightarrow -i|\tilde{1}\rangle \end{aligned} \quad (50)$$

For the spin components, the rotation changes the spin state with the operator

$$e^{-i\frac{\vec{S}\cdot\hat{n}}{\hbar}\phi} = 1 \cdot \cos(\phi/2) - i\vec{\sigma}\cdot\hat{n} \sin(\phi/2), \quad (51)$$

$$e^{-i\frac{\vec{S}\cdot\hat{n}}{\hbar}\phi}|\pm n\rangle = e^{\mp i\frac{\phi}{2}}|\pm n\rangle \quad (52)$$

Since we want to rotate the states with respect to the axis $\hat{n} = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$, we change the basis

$$\begin{aligned} |+\rangle &= |n\rangle\langle n|+ + |-n\rangle\langle -n|+, \\ |-\rangle &= |n\rangle\langle n|- + |-n\rangle\langle -n|-, \end{aligned} \quad (53)$$

where $|\pm n\rangle$ are

$$\begin{aligned} |+n\rangle &= \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix}_{\theta=\frac{\pi}{2}, \phi=\frac{\pi}{4}} \rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \frac{1+i}{\sqrt{2}} \end{pmatrix} \\ |-n\rangle &= \begin{pmatrix} -\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2}e^{i\phi} \end{pmatrix}_{\theta=\frac{\pi}{2}, \phi=\frac{\pi}{4}} \rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ \frac{1+i}{\sqrt{2}} \end{pmatrix} \end{aligned} \quad (54)$$

Simplify the states $|\pm\rangle$,

$$\begin{aligned} |+\rangle &= \frac{1}{\sqrt{2}}(|n\rangle - |-n\rangle), \\ |-\rangle &= \frac{1}{\sqrt{2}}e^{-i\frac{\pi}{4}}(|n\rangle + |-n\rangle). \end{aligned} \quad (55)$$

Rotate 180 degrees with C_2^\dagger the states $|\pm n\rangle$ get phases $\pm i$,

$$(e^{i\frac{\vec{S}\cdot\hat{n}}{\hbar}\phi})_{\phi=\pi}|\pm n\rangle = (e^{\pm i\frac{\phi}{2}})_{\phi=\pi}|\pm n\rangle = e^{\pm i\frac{\pi}{2}}|\pm n\rangle = \pm i|\pm n\rangle. \quad (56)$$

Our states $|\pm\rangle$ become

$$\begin{aligned} C_2^\dagger|+\rangle &= \frac{1}{\sqrt{2}}(i|n\rangle + i|-n\rangle) = e^{i\frac{3\pi}{4}}|-\rangle, \\ C_2^\dagger|-\rangle &= \frac{1}{\sqrt{2}}e^{-i\frac{\pi}{4}}(i|n\rangle - i|-n\rangle) = e^{i\frac{\pi}{4}}|-\rangle. \end{aligned} \quad (57)$$

The effect of C_2^\dagger on isospin up and down states are

$$\begin{aligned} C_2^\dagger|\tilde{\uparrow}\rangle &= C_2^\dagger\left(\frac{1}{\sqrt{3}}|\tilde{0},+\rangle - \frac{\sqrt{2}}{\sqrt{3}}|\tilde{1},-\rangle\right) \\ &= e^{i\frac{3\pi}{4}}\left(\frac{1}{\sqrt{3}}|\tilde{0},-\rangle - \frac{\sqrt{2}}{\sqrt{3}}|\tilde{-1},+\rangle\right) = e^{i\frac{3\pi}{4}}|\tilde{\downarrow}\rangle, \\ C_2^\dagger|\tilde{\downarrow}\rangle &= C_2^\dagger\left(\frac{1}{\sqrt{3}}|\tilde{0},-\rangle - \frac{\sqrt{2}}{\sqrt{3}}|\tilde{-1},+\rangle\right) \\ &= e^{i\frac{\pi}{4}}\left(\frac{1}{\sqrt{3}}|\tilde{0},+\rangle - \frac{\sqrt{2}}{\sqrt{3}}|\tilde{1},-\rangle\right) = e^{i\frac{\pi}{4}}|\tilde{\downarrow}\rangle. \end{aligned} \quad (58)$$

Therefore

$$\begin{aligned} S_1^x &\rightarrow -S_1^y, \\ S_1^y &\rightarrow -S_1^x, \\ S_1^z &\rightarrow -S_1^z. \end{aligned} \quad (59)$$

Now we can find the symmetry-allowed n.n. couplings. For the γ bonds between site i and site j , the invariant couplings are

$$\begin{aligned} &S_i^\gamma S_j^\gamma, \\ &S_i^\alpha S_j^\alpha + S_i^\beta S_j^\beta, \\ &S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha, \\ &S_i^\alpha S_j^\gamma + S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta + S_i^\gamma S_j^\alpha. \end{aligned} \quad (60)$$

Result 7.1. The most general spin model for $\alpha - RuCl_3$ with the nearest neighboring couplings($const(N)$) is eliminated by changing the zero-point energy) is

$$H_{spin} = \frac{1}{2} \sum_{\langle i,j \rangle} J \vec{S}_i \cdot \vec{S}_j + 2K S_i^\gamma S_j^\gamma + \Gamma(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) + \Gamma'(S_i^\alpha S_j^\gamma + S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta + S_i^\gamma S_j^\alpha). \quad (61)$$

The bonds denoted by the index $\langle i,j \rangle$ are anisotropic. A bond with Kitaev coupling $2K S_i^\gamma S_j^\gamma$ in γ direction is called a γ bond and α, β represents the other two real space directions. To be more specific, for x bonds, y bonds and z bonds, the indices $\{\alpha, \beta, \gamma\}$ are $\{y, z, x\}$, $\{z, x, y\}$ and $\{x, y, z\}$, respectively.

Result 7.2. Write it more specifically,

$$\begin{aligned} H_{spin} &= \sum_{\substack{x, x = \langle i,j \rangle \\ \in \{x \text{ bond}\}}} H_{spin,x} + \sum_{\substack{y, y = \langle i,j \rangle \\ \in \{y \text{ bond}\}}} H_{spin,y} + \sum_{\substack{z, z = \langle i,j \rangle \\ \in \{z \text{ bond}\}}} H_{spin,z} \\ &= \frac{1}{2} \sum_{\substack{\langle i,j \rangle \in \\ \{x \text{ bond}\}}} J \vec{S}_i \cdot \vec{S}_j + 2K S_i^x S_j^x + \Gamma(S_i^y S_j^z + S_i^z S_j^y) + \Gamma'(S_i^y S_j^x + S_i^z S_j^x + S_i^x S_j^z + S_i^x S_j^y) \\ &\quad + \frac{1}{2} \sum_{\substack{\langle i,j \rangle \in \\ \{y \text{ bond}\}}} J \vec{S}_i \cdot \vec{S}_j + 2K S_i^y S_j^y + \Gamma(S_i^z S_j^x + S_i^x S_j^z) + \Gamma'(S_i^z S_j^y + S_i^x S_j^y + S_i^y S_j^x + S_i^y S_j^z) \\ &\quad + \frac{1}{2} \sum_{\substack{\langle i,j \rangle \in \\ \{z \text{ bond}\}}} J \vec{S}_i \cdot \vec{S}_j + 2K S_i^z S_j^z + \Gamma(S_i^x S_j^y + S_i^y S_j^x) + \Gamma'(S_i^x S_j^z + S_i^y S_j^z + S_i^z S_j^y + S_i^z S_j^x). \end{aligned} \quad (62)$$

The subsets $\{x \text{ bond}\}$, $\{y \text{ bond}\}$ and $\{z \text{ bond}\}$ distinguish the anisotropic spin couplings in $\{\langle i,j \rangle\}$.

Write $H_{spin,x/y/z}$ in matrix form,

$$\begin{aligned}
H_{spin,x} &= (S_i^x \ S_i^y \ S_i^z) \begin{bmatrix} J+2K & \Gamma' & \Gamma' \\ \Gamma' & J & \Gamma \\ \Gamma' & \Gamma & J \end{bmatrix} \begin{pmatrix} S_j^x \\ S_j^y \\ S_j^z \end{pmatrix}, \\
H_{spin,y} &= (S_i^x \ S_i^y \ S_i^z) \begin{bmatrix} J & \Gamma' & \Gamma \\ \Gamma' & J+2K & \Gamma' \\ \Gamma & \Gamma' & J \end{bmatrix} \begin{pmatrix} S_j^x \\ S_j^y \\ S_j^z \end{pmatrix}, \\
H_{spin,z} &= (S_i^x \ S_i^y \ S_i^z) \begin{bmatrix} J & \Gamma & \Gamma' \\ \Gamma & J & \Gamma' \\ \Gamma' & \Gamma' & J+2K \end{bmatrix} \begin{pmatrix} S_j^x \\ S_j^y \\ S_j^z \end{pmatrix}.
\end{aligned} \tag{63}$$

In general, we can add external magnetic field to the general spin model in Eq.(61),

$$\begin{aligned}
H_{spin} = & \frac{1}{2} \sum_{\langle i,j \rangle} J \vec{S}_i \cdot \vec{S}_j + 2K S_i^\gamma S_j^\gamma + \Gamma (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) \\
& + \Gamma' (S_i^\alpha S_j^\gamma + S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta + S_i^\gamma S_j^\alpha) - \sum_i \vec{h}_i \cdot \vec{S}_i.
\end{aligned} \tag{64}$$

where $\vec{h}_i = \mu_B \vec{B}_i$, $\mu_B = \frac{e\hbar}{2m_e} \sim 5.8 \times 10^{-5} eV/T$ is the Bohr magneton. In an experimental setting, we often choose a uniform magnetic field $\vec{B}_i = \vec{B}$. We want to emphasize that the spin operator here is dimensionless and the coupling strength $\{J, K, \Gamma, \Gamma', h\}$ is of energy dimension.

In the next chapter, we will use the Holstein-Primakoff transformation to derive the magnon Hamiltonian and calculate its properties. During the transformation a spin operator S_i^α is of angular momentum dimension to keep track of the physical meaning of magnon, and we make the symbol S_i^α dimensionless again after the transformation finishes.

7.2 Magnetoelastic Couplings Constrained by C_{6v} Point Group

The point group of phonons on honeycomb lattice is C_{6v} group, or D_6 dihedral group, where D_n is the symmetry group of a planar n -gon. Phonon (lattice vibration) itself cannot see spin couplings, i.e., it simply deform the crystal lattice, or displace the atoms. With this awareness, lattice deformation(phonon) also have C_{6v} point group symmetry. This statement suggests that phonons(on 2D honeycomb lattice), as the representation of C_{6v} point group, can be identified as the linear combination of certain irreducible representations(irreps). The strain tensor from general elasticity (See Appendix ??)

$$\epsilon_{\alpha\beta} = \frac{1}{2} \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right) \tag{65}$$

can be identified as quadratic functions, and therefore transforms as the quadratic functions under C_{6v} point group. By checking the character table(Table. ??), we identify that for 2D system, the strain tensor transforms as A_1 and E_2 irreps with basis functions $\epsilon_{xx} + \epsilon_{yy}$ and $(\epsilon_{xx} - \epsilon_{yy}, \epsilon_{xy})$, respectively. The magnetoelastic coupling is

$$H_c(\mathbf{r}) \sim \mathbf{M}_\eta \cdot (\mathbf{M}_\eta \cdot \nabla) \mathbf{u}(\mathbf{r}) S_{\mathbf{r}}^\eta S_{\mathbf{r}+M_\eta}^\eta. \tag{66}$$

To see the microscopic derivation of it, see the notes about **bands of magnon and phonons**¹³.

¹³ ADD link here

Goal 7.1

| Reproduce the magnetoelastic couplings

$$\begin{aligned} & (\epsilon_{xx} + \epsilon_{yy}) f_{A_1}(S_{\mathbf{r}}^\eta S_{\mathbf{r}+M_\eta}^\eta), \\ & (\epsilon_{xx} - \epsilon_{yy}, \epsilon_{xy}) \otimes \left(f_{E_2}^{(1)}(S_{\mathbf{r}}^\eta S_{\mathbf{r}+M_\eta}^\eta), f_{E_2}^{(2)}(S_{\mathbf{r}}^\eta S_{\mathbf{r}+M_\eta}^\eta) \right), \end{aligned} \quad (67)$$

where f_{A_1} and $(f_{E_2}^{(1)}, f_{E_2}^{(2)})$ are functions of quadratic spin couplings $S_r^\eta S_{r+M_\eta}^\eta$. These functions along with $(\epsilon_{xx} + \epsilon_{yy})$ and $(\epsilon_{xx} - \epsilon_{yy}, \epsilon_{xy})$ are also bases for A_1 and E_2 irreps, respectively. To make sure the meaning of Eq. (67) is clear from the bottom up, we want to go through the following topics:

- generalized elasticity and its symmetry (**ongoing**)
- symmetry operation on hexagonal spin lattice (**done study**)
- A_1 irreps of magnetoelastic couplings (**?unknown**)

7.2.1 Basis Functions for an Irreducible Representation

Before discussing the transformation of spin-spin couplings, let's examine the transformation of the vectors $\mathbf{v} = v_1\hat{\mathbf{x}} + v_2\hat{\mathbf{y}}$ on 2D planar plane. Take the E_2 irreps of C_6 rotation

$$\mathcal{R}_{E_2}(C_6(z)) = \begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix} \quad (68)$$

as an example. Any vector \mathbf{v} in the ordered basis $\{\hat{\mathbf{x}}, \hat{\mathbf{y}}\}$ would transform as Eq. (68)

$$\mathcal{R}_{E_2}(C_6(z)) \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} \frac{1}{2}v_1 - \frac{\sqrt{3}}{2}v_2 \\ \frac{\sqrt{3}}{2}v_1 + \frac{1}{2}v_2 \end{pmatrix} \quad (69)$$

If we change the ordered basis $\alpha = \{\hat{\mathbf{x}}, \hat{\mathbf{y}}\}$ to $\beta = \{\hat{\mathbf{x}}', \hat{\mathbf{y}}'\}$ via a similarity transformation $\mathcal{S}_{\beta\alpha}$

$$\mathcal{S}_{\beta\alpha} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}_\alpha = \begin{pmatrix} v'_1 \\ v'_2 \end{pmatrix}_\beta \quad (70)$$

in the new basis β the transformation becomes

$$\begin{aligned} \mathcal{R}_{E_2}(C_6(z))_{\beta\beta} \begin{pmatrix} v'_1 \\ v'_2 \end{pmatrix}_\beta &= \mathcal{S}_{\beta\alpha} \mathcal{R}_{E_2}(C_6(z))_{\alpha\alpha} \mathcal{S}_{\alpha\beta}^{-1} \mathcal{S}_{\beta\alpha} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}_\alpha \\ &= \mathcal{S}_{\beta\alpha} \mathcal{R}_{E_2}(C_6(z))_{\alpha\alpha} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}_\alpha \\ &= \mathcal{S}_{\beta\alpha} \begin{pmatrix} \frac{1}{2}v_1 - \frac{\sqrt{3}}{2}v_2 \\ \frac{\sqrt{3}}{2}v_1 + \frac{1}{2}v_2 \end{pmatrix}_\alpha \\ &= \mathcal{S}_{\beta\alpha} \begin{pmatrix} \frac{1}{2}v_1 - \frac{\sqrt{3}}{2}v_2 \\ \frac{\sqrt{3}}{2}v_1 + \frac{1}{2}v_2 \end{pmatrix}_\alpha \end{aligned} \quad (71)$$

Eq. (71) is a basic idea in linear algebra: **the operation on a vector** is independent of the chosen basis. However, **the matrix representation of the operation**, e.g., $\mathcal{R}_{E_2}(C_6(z))$, depends on the basis we choose since in general,

$$\mathcal{R}_{E_2}(C_6(z))_{\beta\beta} = \mathcal{S}_{\beta\alpha} \mathcal{R}_{E_2}(C_6(z))_{\alpha\alpha} \mathcal{S}_{\alpha\beta}^{-1} \neq \mathcal{R}_{E_2}(C_6(z))_{\alpha\alpha}. \quad (72)$$

However, two similar matrices have the same character since trace is independent of the chosen basis

$$\text{tr}(\mathcal{R}_{E_2}(C_6(z))_{\beta\beta}) = \text{tr}(\mathcal{R}_{E_2}(C_6(z))_{\alpha\alpha}) \quad (73)$$

and therefore both are legitimate E_2 irreps of C_6 operation.

Result 7.3. To derive Eq.(71), we went through the following steps: (1) write down an E_1 irrep for C_6 operation (2) identify the vector space as a 2D plane (3) choose an arbitrary vector which transforms like the irreps (4) change the ordered basis to rewrite the vector and operation. The premise for steps (2)-(4) is that we know the **actual transformation of vecotrs in the real world**; we need to know how our targeted system transforms under symmetries before jump into any character table. Usually (3) is more doable than (2).

To find A_1 irreps in spin-phonon tensor product space, i.e., A_1^{sp-ph} , it's important to be careful about the basis functions chosen for the irreps E_2^{sp} , E_2^{ph} . Eq.(72) and (73) suggest that the irreps in Table ?? is not universal.

Table 3. The character table for C_{6v} point group

h=12	E	$2C_6(z)$	$2C_3(z)$	$C_2(z)$	$3\sigma_v$	$3\sigma_d$		
A_1	1	1	1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	1	1	-1	-1	R_z	
B_1	1	-1	1	-1	1	-1		
B_2	1	-1	1	-1	-1	1		
E_1	2	1	-1	-2	0	0	$(x, y), (R_x, R_y)$	(xz, yz)
E_2	2	-1	-1	2	0	0		$(x^2 - y^2, xy)$

Table 4. The A_1 and E_2 irreps of C_{6v} point group, whose source is a wikipedia for group properties[?].

h=12	E	$2C_6(z)$	$2C_3(z)$	$C_2(z)$	$3\sigma_v$	$3\sigma_d$
A_1	1	1	1	1	1	1
E_2	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$	$\begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

7.2.2 Spin-Spin Couplings under Point Group Operations

A formal method to find basis functions through projection operator is written in Appendix 3.2. In this section, The spin-spin couplings transform under σ_v (Fig.3a) and C_6 (Fig.3b) operations as the following:

$$\begin{aligned} \mathcal{R}(\sigma_v) S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x &\rightarrow S_{\mathbf{r}'}^x S_{\mathbf{r}'-M_y}^x \\ \mathcal{R}(\sigma_v) S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y &\rightarrow S_{\mathbf{r}'}^y S_{\mathbf{r}'-M_x}^y \\ \mathcal{R}(\sigma_v) S_{\mathbf{r}}^z S_{\mathbf{r}+M_z}^z &\rightarrow S_{\mathbf{r}'}^z S_{\mathbf{r}'-M_z}^z \end{aligned} \quad (74)$$

$$\begin{aligned} \mathcal{R}(C_6) S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x &\rightarrow S_{\mathbf{r}'}^x S_{\mathbf{r}'-M_z}^x \\ \mathcal{R}(C_6) S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y &\rightarrow S_{\mathbf{r}'}^y S_{\mathbf{r}'-M_x}^y \\ \mathcal{R}(C_6) S_{\mathbf{r}}^z S_{\mathbf{r}+M_z}^z &\rightarrow S_{\mathbf{r}'}^z S_{\mathbf{r}'-M_y}^z \end{aligned} \quad (75)$$

By observing the total spin-spin couplings

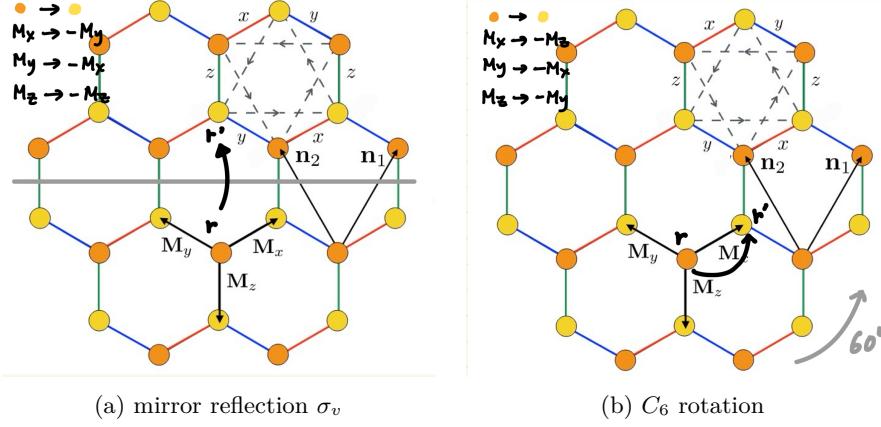


Figure 1. Operations in Eqs.(74) and (75). The exchange between orange and yellow sites means the exchange of sublattice indices.

$$H_c = \frac{1}{2} \sum_{\mathbf{r}, \eta} S_{\mathbf{r}}^{\eta} S_{\mathbf{r}+M_{\eta}}^{\eta} = \frac{1}{2} \sum_{\mathbf{r}_A, \eta} S_{\mathbf{r}_A}^{\eta} S_{\mathbf{r}_A+M_{\eta}}^{\eta} + \frac{1}{2} \sum_{\mathbf{r}_B, \eta} S_{\mathbf{r}_B}^{\eta} S_{\mathbf{r}_B-M_{\eta}}^{\eta}, \quad (76)$$

we could find that transformations in Eq.(74) and Eq.(75), surprisingly, can be viewed as the exchange of sublattices $\mathbf{r}_A \leftrightarrow \mathbf{r}_B$, $M_{\eta} \leftrightarrow -M_{\eta}$, and the permutation of the vectors $\{M_x, M_y, M_z\}$. The former causes no difference if we know the expression in Eq.(76), but the latter makes some changes.

The E_2 irreps of σ_v suggests that the second component of the basis $(f_{E_2}^{(1)}, f_{E_2}^{(2)})$ is antisymmetric under operation $\mathcal{R}_{E_2}(\sigma_v)$. The first guess for $f_{E_2}^{(2)}$ is

$$f_{E_2}^{(2)} = \sum_r \left(S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y \right) \quad (77)$$

since x and y components of spin operators exchange in Eq.(74).

$$\begin{aligned} \mathcal{R}(\sigma_v) \left(\sum_r \left(S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y \right) \right) &\rightarrow \sum_{r'} S_{\mathbf{r}'}^x S_{\mathbf{r}'-M_y}^x - S_{\mathbf{r}'}^y S_{\mathbf{r}'-M_x}^y, \\ \sum_{r'} S_{\mathbf{r}'}^x S_{\mathbf{r}'-M_y}^x - S_{\mathbf{r}'}^y S_{\mathbf{r}'-M_x}^y &= \sum_r S_{\mathbf{r}}^x S_{\mathbf{r}+M_y}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_x}^y = - \sum_r \left(S_{\mathbf{r}}^y S_{\mathbf{r}+M_x}^y - S_{\mathbf{r}}^x S_{\mathbf{r}+M_y}^x \right). \end{aligned} \quad (78)$$

Remember the conclusion we obtained in Eq. 71: the transformation of a vector makes the vector itself unchanged; it's the coordinates that changed. So the "coordinates" for the function $f_{E_2}^{(2)}$ in Eq.(77) is

$$\begin{aligned} f_{E_2}^{(2)} &= \sum_r \left(S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y \right) \rightarrow (M_x - M_y) \\ \mathcal{R}f_{E_2}^{(2)} &\rightarrow (M_y - M_x) = -(M_x - M_y) \end{aligned} \quad (79)$$

With the same logic, the effects of C_6 rotations could be identified as

$$M(S^x S^x, S^y S^y, S^z S^z) = (M_x, M_y, M_z) \rightarrow (M_z, M_x, M_y) \quad (80)$$

Could we say this is anti-symmetric?

Now our goal is to find a function $f_{E_2}^{(1)}$ which transform as

$$\begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix} \begin{pmatrix} f_{E_2}^{(1)}(M_x, M_y, M_z) \\ M_x - M_y \end{pmatrix} = \begin{pmatrix} -\frac{1}{2}f_{E_2}^{(1)} - \frac{\sqrt{3}}{2}(M_x - M_y) \\ \frac{\sqrt{3}}{2}f_{E_2}^{(1)} - \frac{1}{2}(M_x - M_y) \end{pmatrix} \\ = \begin{pmatrix} f_{E_2}^{(1)}(M_z, M_x, M_y) \\ M_z - M_x \end{pmatrix}. \quad (81)$$

From the Eq.(81) we have

$$f_{E_2}^{(1)} = -\frac{1}{\sqrt{3}}(M_x + M_y - 2M_z). \quad (82)$$

This result can be used to general models for Kitaev material candidate since only the change of M_η matters. Notice that we assume that the local axes for spins **do not change** under symmetry operations. To show the rotation of local axes more explicitly, we may add a label \hat{n} for local axes into Eqs. (79) and (82),

$$f_{E_2}^{(2)} = \sum_r \left(S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y \right) \rightarrow \hat{n} \otimes (M_x - M_y) \quad (83)$$

$$\mathcal{R}f_{E_2}^{(2)} \rightarrow \hat{n}' \otimes (M_y - M_x) = -\hat{n}' \otimes (M_x - M_y)$$

$$f_{E_2}^{(1)} = -\frac{1}{\sqrt{3}}\hat{n} \otimes (M_x + M_y - 2M_z). \quad (84)$$

What does this mean? What is the possible scenario for this to happen?

Result 7.4. The basis functions for an E_2 irreps in terms of spin-spin coupling is

$$(f_{E_2}^{(1)}, f_{E_2}^{(2)}) = (M_x + M_y - 2M_z, -\sqrt{3}(M_x - M_y)), \quad (85)$$

or

$$(f_{E_2}^{(1)}, f_{E_2}^{(2)}) = \left(\sum_{\mathbf{r}} \left(S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x + S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y - 2S_{\mathbf{r}}^z S_{\mathbf{r}+M_z}^z \right), \sqrt{3} \sum_{\mathbf{r}} \left(S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y \right) \right) \quad (86)$$

This result can be extended to any general x , y , and z bonds. For instance, the general bonds for general Kitaev model in my thesis. However, **whether the change of local axes could be ignored for anisotropic couplings is still unknown.**

7.2.3 Reproduce the 2D Basis Functions for E_2 Irreducible Representations via Permutations

Strain tensor in the system of C_{6v} symmetry is the direct sum of A_1 and E_2 irreps. By proof of exhaustion, there are only two possibilities to acquire A_1^{sp-ph} irreps by tensor product: $A_1^{sp} \otimes A_1^{ph}$ or $E_2^{sp} \otimes E_2^{ph}$, where

$$E_2^{sp} \otimes E_2^{ph} = A_1^{sp-ph} \oplus A_2^{sp-ph} \oplus E_2^{sp-ph}. \quad (87)$$

Our goal is to find the basis for A_1^{sp} and E_2^{sp} . An easier way to derive the basis for A_1^{sp} and E_2^{sp} irreps (In this section we use the simpler term A_1 and E_2) is to follow Eq. (19). In the following derive it step by step. Since every (point) group is isomorphic to a permutation group(Cayley's theorem), it's useful to identify Kitaev model as a 3-tuple (x, y, z) , where the first element is the coupling lying on M_x direction; the second and

third element are the couplings lying on M_y and M_z direction respectively (See Fig. ??). The effects of group operations on Kitaev model can thus be identified as the permutation of the elements x , y and z .

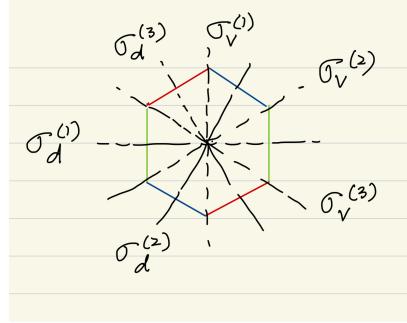


Figure 2. Mirror operations.

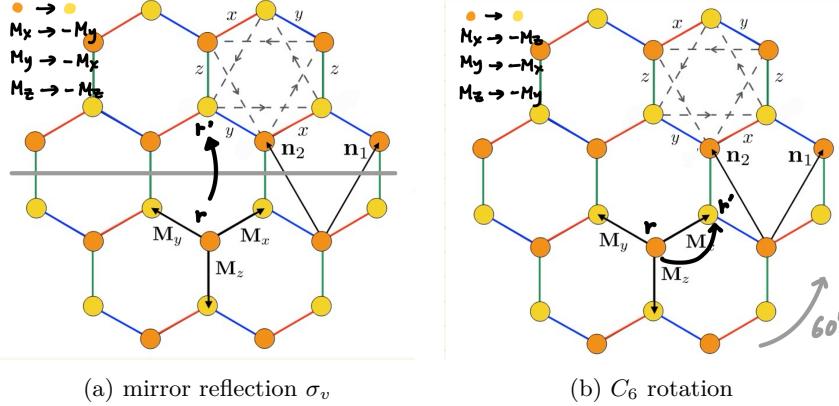


Figure 3. The exchange between orange and yellow sites means the exchange of sublattice indices. To make it clear we treat the bonds as vectors, so that we could see the difference between two sublattices.

We could absolutely write down the resulted 3-tuples for the operations of C_{6v} group. After the operation acting on (x, y, z) , we get

$$\begin{aligned} \hat{P}_E(x, y, z) &\rightarrow (x, y, z), \hat{P}_{\sigma_v^{(1)}}(x, y, z) \rightarrow (y, x, z), \\ \hat{P}_{C_6}(x, y, z) &\rightarrow (y, z, x), \hat{P}_{\sigma_v^{(2)}}(x, y, z) \rightarrow (x, z, y), \\ \hat{P}_{C_6^{-1}}(x, y, z) &\rightarrow (z, x, y), \hat{P}_{\sigma_v^{(3)}}(x, y, z) \rightarrow (z, y, x), \\ \hat{P}_{\sigma_v^{(1)}}(x, y, z) &\rightarrow (y, x, z), \hat{P}_{C_3}(x, y, z) \rightarrow (z, x, y), \\ \hat{P}_{C_3^{-1}}(x, y, z) &\rightarrow (y, z, x), \hat{P}_{\sigma_v^{(2)}}(x, y, z) \rightarrow (z, y, x), \\ \hat{P}_{C_2}(x, y, z) &\rightarrow (x, y, z), \hat{P}_{\sigma_v^{(3)}}(x, y, z) \rightarrow (x, z, y). \end{aligned} \quad (88)$$

Through reduction formula, we found this representation Γ_n is the direct sum of A_1 and E_2 irreps

$$\Gamma_n = \Gamma_{A_1} \oplus \Gamma_{E_2} \quad (89)$$

The basis of Γ_{A_1} is $(x + y + z)$, which can be found through the projection operator. Although the basis of Γ_{E_2} could also be found in the same way, it's more convenient to follow the recipe

$$|\Gamma_n\alpha\rangle = (x + \omega y + \omega^2 z), |\Gamma_n\beta\rangle = (x + \omega^2 y + \omega z), \quad (90)$$

where $\omega = e^{2\pi i/3}$, Then

$$\begin{aligned} \hat{P}_{C_6}(x + \omega y + \omega^2 z) &= (y + \omega z + \omega^2 x) = \omega^2(x + \omega y + \omega^2 z) \\ \hat{P}_{C_6}(x + \omega^2 y + \omega z) &= (y + \omega^2 z + \omega x) = \omega(x + \omega^2 y + \omega z) \end{aligned} \quad (91)$$

$$Tr \begin{bmatrix} \omega^2 & 0 \\ 0 & \omega \end{bmatrix} = -1 \quad (92)$$

We try to find the dim-2 basis through the rotation along the principle axis and reach to our conclusion: $|\Gamma_n\alpha\rangle$ and $|\Gamma_n\beta\rangle$ form the basis for Γ_{E_2} irreps! Through linear combinations, we find another ordered basis $\{|\Gamma_{E_2}1\rangle, |\Gamma_{E_2}2\rangle\}$

$$\begin{aligned} |\Gamma_{E_2}1\rangle &\equiv e^{2\pi i/3}|\Gamma_n\alpha\rangle + e^{-2\pi i/3}|\Gamma_n\beta\rangle = -(x + y - 2z), \\ |\Gamma_{E_2}2\rangle &\equiv e^{2\pi i/3}|\Gamma_n\alpha\rangle - e^{-2\pi i/3}|\Gamma_n\beta\rangle = i\sqrt{3}(x - y), \end{aligned} \quad (93)$$

which are exactly the basis functions written in the reference paper except for the phase differences. This result perfectly matches the paper, but we didn't consider the effect of these operations on the spin states and crystal structures. In the next section we'll go through this part.

References:

- Dresselhaus, Section 4.6
 - Eq. (6) in the paper "Phonon dynamics in the Kitaev spin liquid"
-



7.2.4 Crystal Structure and Spin Operators under Group Operations

In the last section we see the effect of C_{6v} group operation on the Kitaev model. Is it the same case for Kitaev mateiral candidates? To see this we need to review an important question: do we really have anisotropic couplings in the Kitaev material candidates? If the answer is positive, how do we justify the reasoning?

First, the machinery for producing nearest neighboring spin-spin couplings is two octahedrons with shared edges. From the second-order effective perturbative method, we get an effective Hamiltonian H_{eff} of quartic terms

$$H_{eff} = -\frac{1}{U} \left(\sum_{\langle i,j \rangle \mu' \mu} [H_{1,ij}]_{\mu\mu} [H_{1,ji}]_{\mu'\mu'} d_{i,\mu}^\dagger d_{j,\mu} d_{j,\mu'}^\dagger d_{i,\mu'} \right), \quad (94)$$

which arises from the symmetry-allowed hoppings that could happen in the given system. For systems with large enough spin-orbit couplings, we could focus on those interactions happening on the manifold spanned by the isospins

$$\begin{aligned} |\tilde{\uparrow}\rangle &= \sin \theta |0, \uparrow\rangle - \cos \theta |1, \downarrow\rangle, \\ |\tilde{\downarrow}\rangle &= \sin \theta |0, \downarrow\rangle - \cos \theta |-1, \uparrow\rangle. \end{aligned} \quad (95)$$

Notice that the corresponding H_{eff} in terms of $d_{i\uparrow}, d_{i,\uparrow}^\dagger$ can be written down after identifying the possible hopping routes. The form $d_{i\uparrow}, d_{i,\uparrow}^\dagger$ in H_{eff} and the isospins $|\tilde{\uparrow}\rangle$

and $|\tilde{\downarrow}\rangle$ implies the choice of basis has been made. Here's comes the point: for one machinery, we could always change its basis, which is completely arbitrary. However, for the same site i , the other two nearest neighboring bondings come from exactly the same type of machineries but tilted in different angles, which rotates their own bases $\{|\tilde{\uparrow}\rangle, |\tilde{\downarrow}\rangle\}$. By actually rotating the bases, we found the operators S_i^x, S_i^y, S_i^z in the tilted bases permute and make S_i^z become S_i^x (or S_i^y). For more details you could see Appendix ???. We can thus conclude that the origin of anisotropic couplings in Kitaev material candidate is the crystal structure, or say the relative angles between the machineries of bond formation.

An octahedron has 8 faces, 12 edges and 6 vertices. Since the couplings come from shared edges(ligands), for instance, there are four ways of sharing edges which can form z bonds. It's the same cases for x and y bonds. We want to make sure the crystal structure is unchanged under all C_{6v} group symmetry operations, i.e., the transformation of quantization axes and that of shared edges should be consistent. What does an inconsistent case look like? Let's label the bonds using the quantization axes and shared edges(using the midpoints):

$$\begin{aligned} x &: \left(\hat{x}, \frac{\hat{z} - \hat{y}}{2} \right) \\ y &: \left(\hat{y}, \frac{\hat{x} - \hat{z}}{2} \right) \\ z &: \left(\hat{z}, \frac{\hat{y} - \hat{x}}{2} \right) \end{aligned} \quad (96)$$

For instance, If a transformed result is $\left(\hat{x}, \frac{\hat{y} - \hat{z}}{2} \right)$, it means that the shared edge has changed! Rotate the system 120 degree about the axes $\hat{n} = (\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$,

$$\begin{aligned} \hat{x} &\rightarrow \hat{y}, \\ \hat{y} &\rightarrow \hat{z}, \\ \hat{z} &\rightarrow \hat{x}, \\ x \text{ bonds} &\rightarrow y \text{ bonds}, \\ y \text{ bonds} &\rightarrow z \text{ bonds}, \\ z \text{ bonds} &\rightarrow x \text{ bonds}. \end{aligned} \quad (97)$$

Mirror(Take one mirror plane as an example):

$$\begin{aligned} \hat{x} &\rightarrow \hat{y}, \\ \hat{y} &\rightarrow \hat{x}, \\ \hat{z} &\rightarrow \hat{z}, \\ x \text{ bonds of r site} &\rightarrow y \text{ bonds of r' site}, \\ y \text{ bonds of r site} &\rightarrow x \text{ bonds of r' site}, \\ z \text{ bonds of r site} &\rightarrow z \text{ bonds of r' site}. \end{aligned} \quad (98)$$

From the above simple examination, we know the two major operations—rotation and mirror reflection—won't make any inconsistency in crystal structure.

References:

- master thesis, around Section 2.3.1

- Jackeli, et al. "Mott Insulators in the Strong Spin-Orbit Coupling Limit: From Heisenberg to a Quantum Compass and Kitaev Models"

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7.2.5 Spin Lattice under Group Operations

Combining the transformation of crystal structure and spin operators, we write own our version of spin lattice transformation under C_{6v} group operations,

$$\begin{aligned}
 \hat{P}_E(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (x, y, z, (\sigma_x, \sigma_y, \sigma_z)) \\
 \hat{P}_{C_6}(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (y, z, x, (\frac{2}{3}\sigma_x + \frac{2}{3}\sigma_y - \frac{1}{3}\sigma_z, -\frac{1}{3}\sigma_x + \frac{2}{3}\sigma_y + \frac{2}{3}\sigma_z, \frac{2}{3}\sigma_x - \frac{1}{3}\sigma_y + \frac{2}{3}\sigma_z)) \\
 \hat{P}_{C_6^{-1}}(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (z, x, y, (\frac{2}{3}\sigma_x - \frac{1}{3}\sigma_y - \frac{2}{3}\sigma_z, +\frac{2}{3}\sigma_x + \frac{2}{3}\sigma_y - \frac{1}{3}\sigma_z, -\frac{1}{3}\sigma_x + \frac{2}{3}\sigma_y + \frac{2}{3}\sigma_z)) \\
 \hat{P}_{C_3}(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (z, x, y, (\sigma_y, \sigma_z, \sigma_x)) \\
 \hat{P}_{C_3^{-1}}(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (y, z, x, (\sigma_z, \sigma_x, \sigma_y)) \\
 \hat{P}_{C_2}(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (x, y, z, (-\frac{1}{3}\sigma_x + \frac{2}{3}\sigma_y + \frac{2}{3}\sigma_z, \frac{2}{3}\sigma_x - \frac{1}{3}\sigma_y + \frac{2}{3}\sigma_z, \frac{2}{3}\sigma_x + \frac{2}{3}\sigma_y - \frac{1}{3}\sigma_z)) \\
 \hat{P}_{\sigma_v^{(1)}}(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (y, x, z, (-\sigma_y, -\sigma_x, -\sigma_z)) \\
 \hat{P}_{\sigma_v^{(2)}}(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (x, z, y, (-\sigma_x, -\sigma_z, -\sigma_y)) \\
 \hat{P}_{\sigma_v^{(3)}}(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (z, y, x, (-\sigma_z, -\sigma_y, -\sigma_x)) \\
 \hat{P}_{\sigma_v^{(1)}}(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (y, x, z, (-\sigma_y, -\sigma_x, -\sigma_z)) \\
 \hat{P}_{\sigma_v^{(2)}}(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (z, y, x, (-\sigma_z, -\sigma_y, -\sigma_x)) \\
 \hat{P}_{\sigma_v^{(3)}}(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (x, z, y, (-\sigma_x, -\sigma_z, -\sigma_y))
 \end{aligned} \tag{99}$$

References:

- written notes

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8 Magnetoelastic Couplings Constrained by $C_{2/m}$ Space Group

The transformation of spin space should be considered carefully.

8.1 Spin lattice under group operations

Experimentally, it is not realistic to grow a monolayer sample with its ideal 2D symmetry due to the substrate underneath. We analyze the magnetoelastic couplings allowed by the bulk symmetry $C_{2/m}$, which is a symmorphic group with corresponding point group C_{2h} . The character table is listed below (Table 5).

$$\begin{aligned}
 \hat{P}_E(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (x, y, z, (\sigma_x, \sigma_y, \sigma_z)), \\
 \hat{P}_{C_2}(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (y, x, z, (-\sigma_y, -\sigma_x, -\sigma_z)), \\
 \hat{P}_i(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (x, y, z, (-\sigma_x, -\sigma_y, -\sigma_z)) + \text{sublattice exchange}, \\
 \hat{P}_{\sigma_h}(x, y, z, (\sigma_x, \sigma_y, \sigma_z)) &\rightarrow (y, x, z, (\sigma_y, \sigma_x, \sigma_z)) + \text{sublattice exchange}.
 \end{aligned} \tag{100}$$

Consider only the spin-spin ocouplings $S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x, S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y$ and $S_{\mathbf{r}}^z S_{\mathbf{r}+M_z}^z$. Under C_{2h} point group operations, a linear combination $S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y$ transforms as

Due to stacking faults, There are three possible space group symmetries: $C_{2/m}$, $R\bar{3}$ and $P_{31}12$ (Fig. 4).

Table 5. The character table for C_{2h} point group

$h=4$	E	$C_2(y)$	i	σ_h		
A_g	1	1	1	1	R_y	x^2, y^2, z^2, xz
B_g	1	-1	1	-1	R_x, R_z	yz, xy
A_u	1	1	-1	-1	y	
B_u	1	-1	-1	1	x, z	

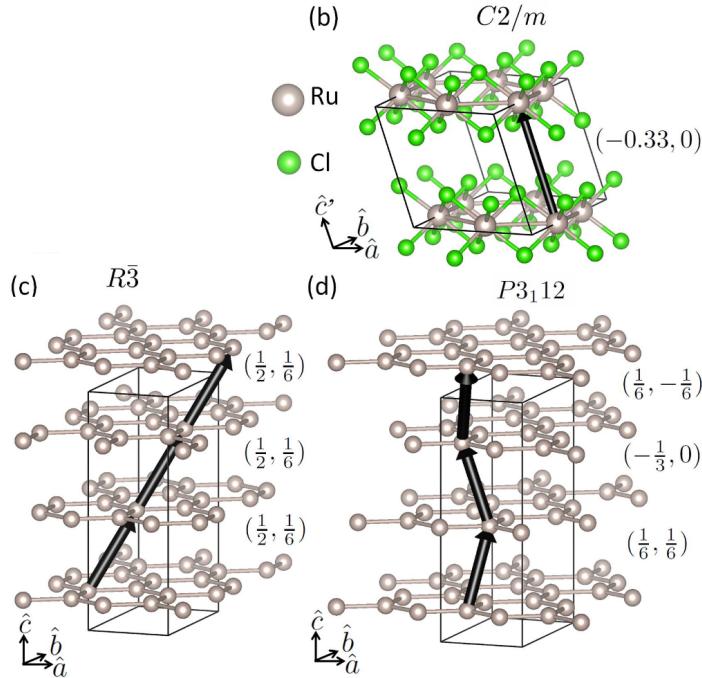


FIG. 1: Antiferromagnetic zig-zag unit cells of α -RuCl₃. (a) In-plane magnetic structure with red and blue arrows denoting anti-parallel spins. Out-of-plane stacking structure for space groups (b) $C2/m$ (No. 12), (c) $R\bar{3}$ (No. 148) and (d) $P3_112$ (No. 151), with black arrows indicating stacking shifts expressed in in-plane lattice vectors. Cl atoms are shown in (b) only.

Figure 4. A screenshot of different space groups. The symmetry center for C_{2h} point group is between the monolayers.

$$\begin{aligned}
 S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y &\xrightarrow{\hat{P}_E} S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y, \\
 S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y &\xrightarrow{\hat{P}_{C_2}} - \left(S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y \right), \\
 S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y &\xrightarrow{\hat{P}_i} S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y, \\
 S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y &\xrightarrow{\hat{P}_{\sigma_h}} - \left(S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y \right),
 \end{aligned} \tag{101}$$

which suggests that $S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^x$ is exactly one basis of Γ_{B_g} irreps.

B_g irreps of phonons

For long wavelength limit, lattice vibration are properly expressed in strain tensor ϵ_{kl} , whose indices k and l represent the propagation direction and polarization, respectively. According to Table. 5, B_g irreps of strain tensor ϵ_{yx} , ϵ_{yz} , ϵ_{zy} and ϵ_{xy} along with B_g irreps of spin-spin couplings $S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^x$ form an A_g irreps of C_{2h} point group, i.e.,

$$\Gamma_{A_g} = \Gamma_{B_g} \otimes \Gamma_{B_g}, \quad (102)$$

and the tensor products

$$\begin{aligned} & \left(S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^x \right) \otimes \epsilon_{yx}, \\ & \left(S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y \right) \otimes \epsilon_{yz}, \\ & \left(S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^y \right) \otimes \epsilon_{zy}, \\ & \left(S_{\mathbf{r}}^x S_{\mathbf{r}+M_x}^x - S_{\mathbf{r}}^y S_{\mathbf{r}+M_y}^x \right) \otimes \epsilon_{xy}, \end{aligned} \quad (103)$$

are the A_g irreps of C_{2h} point group. In the next subsection, we will discuss the physical meaning of these magnetoelastic modes.

References:

- Bilbao Crystallographic Server
- notes (not written down)
- screenshot from "The Role of the Third Dimension in Searching Majorana Fermions in α - $RuCl_3$ via Phonons"



8.2 Intuitions on B_{2g} irreps of strain tensor

Fig. 5 illustrates the effects of strain tensors allowed in our construction Eq. 103. Since we only consider the long wavelength modes, the adjacent sites in Fig. 5 have no relative displacements. Thus, the pink lines representing the polarizations are exaggerated.

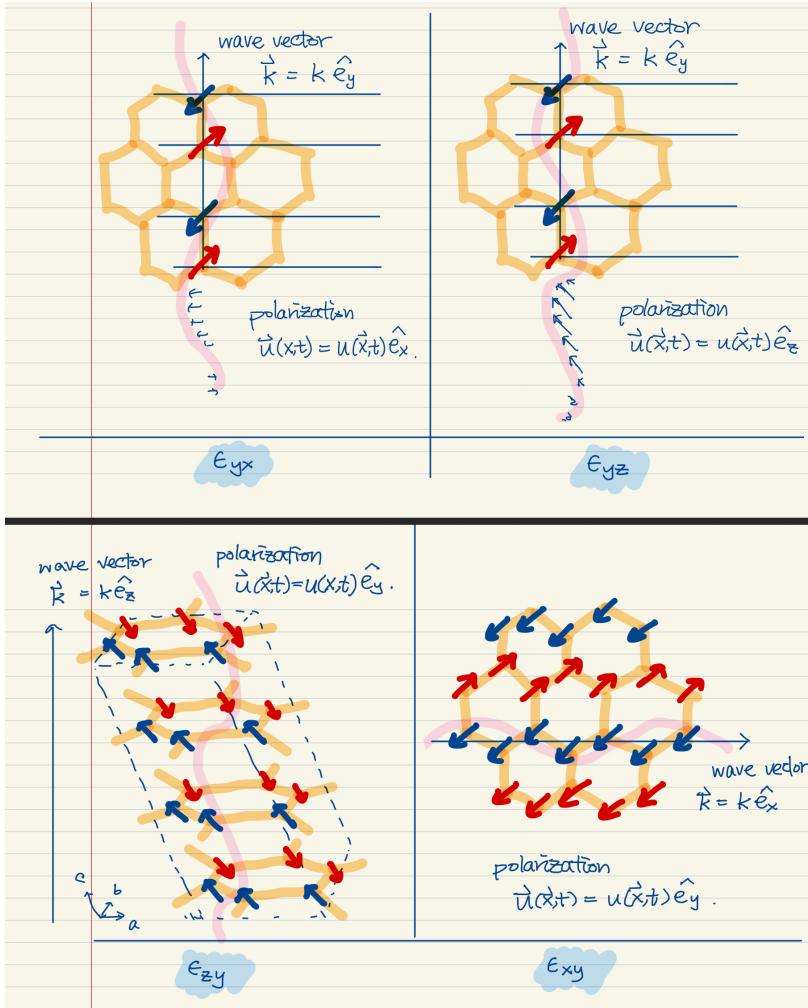


Figure 5. Upper panel: vibrations propagate along y axis with polarization in x and z directions. Lower panel: vibrations with polarization in y direction propagating along x and z axes. Only the component ϵ_{zy} produces the relative motion between layers. These vibration modes have quantum numbers $\mathbf{k} \approx 0$.