

The Art of Guessing Hamiltonian in Honeycomb Lattice and Beyond

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This short practice is a reflection of the power of symmetry in contemporary condensed matter physics. We will try to find out all possible forms of allowed Hamiltonian of nearest neighbor level or even next nearest neighbor level with spin orbit coupling (SOC) in the honeycomb lattice (for instance, $\alpha\text{-RuCl}_3$), and classify them with the help of representation theory of *little group*. After that we will impose t/U expansion to verify our results and try to express the electric polarization operator for nearest neighbor or even next nearest neighbor sites with spin degrees of freedom.

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I. INTRODUCTION

A. Pure Hubbard Model

For *pure* Hubbard model without spin-orbit coupling (SOC), Hamiltonian

$$H = -t \sum_{\langle ij \rangle, \alpha} c_{i\alpha}^\dagger c_{j\alpha} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

is invariant under *global* $SU(2)$ spin-rotation symmetry $c_{i\alpha} \mapsto U_{\alpha\beta} c_{i\beta}$ as well as *time-reversal symmetry, parity symmetry*, and some specific *cystalline symmetry*, depending on what kind of lattice we are working with.

Throughout this paper, we only focus on honeycomb lattice, or more specifically, iridates family $A_2\text{IrO}_4$ with $A = \text{Na}^{2+}, \text{Li}^{2+}$, which is believed to be the candidate realizing Kitaev spin chain [1]. In this case the symmetry group is generated by two *oblique-crossing* translation T_1, T_2 , *three-fold* rotation C_3 , horizontal mirror symmetry P and time-reversal symmetry T

$$SG = \{T_1, T_2, C_3, P, T\}$$

with the confinement [2] on group elements

$$\begin{aligned} T^2 &= P^2 = C_6^6 = 1, \\ TUT^{-1}U^{-1} &= 1, \quad U = T_1, T_2, C_3, P, \end{aligned}$$

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$$\begin{aligned}
T_1 T_2 T_1^{-1} T_2^{-1} &= 1, \\
T_1^{-1} P T_1 P &= 1, \\
T_2^{-1} P T_1 T_2^{-1} P &= 1, \\
P C_6 P C_6 &= 1, \\
T_2^{-1} C_6 T_1 C_6 &= 1, \\
T_1^{-1} C_6 T_1 T_2^{-1} C_6 &= 1.
\end{aligned}$$

But how to use these spacial group? In fact, given the coupling between arbitrary nearest neighbor links, one can immediately push it to all the other links of the lattice under the action of the spacial group we listed above. And because Hamiltonian is the summation of *local* operators, we can fully recovered the Hamiltonian from such local details. So the question of classifying *pure* Hubbard Hamiltonian is narrowed to classification of the possible form of coupling on the link, say, the one between site i and site j .

B. Spin Hamiltonian

Physical interesting things occur at *half-filling* under *strong-coupling limit*. But the first thing is to write down the low-energy effective Hamiltonian from (1). Standard t/U expansion will be discussed in the third section. In the first two sections, we try to guess the allowed form purely based on symmetric analysis.

Under strong-coupling limit, each site is occupied by one electron [3]. So by identifying $|n_{i\uparrow} = 1\rangle \equiv |\uparrow\rangle$ and $|n_{i\downarrow} = 1\rangle \equiv |\downarrow\rangle$ (this is certainly a one-to-one mapping), one can always express the fermionic form of Hamiltonian with spin degree of freedom on each site [4].

Focusing on the nearest-neighbor i and j , we have spin operator \mathbf{S}_i and \mathbf{S}_j in hand. The question is how to assembly them? One may naively say that there is no constraint so arbitrary form of coupling is OK. However, no matter which order of perturbation we are working with, after decomposition and projection of many-body Hilbert space [4, 5], we must end up with the combinations of terms holding the same symmetry as original Hamiltonian. And because original Hubbard Hamiltonian is invariant under $SU(2)$ spin-rotation, so should our low-energy effective Hamiltonian be under the strong-coupling limit. All the other forms of assembly are forbidden by symmetry, except for

$$H_{ij} \propto \mathbf{S}_i \cdot \mathbf{S}_j$$

because of the strong dependence of the identity $\boldsymbol{\sigma}_{\alpha\beta} \cdot \boldsymbol{\sigma}_{\mu\nu} = 2\delta_{\alpha\nu}\delta_{\beta\mu} - \delta_{\alpha\beta}\delta_{\mu\nu}$, ensuring

$$\mathbf{S}_i \cdot \mathbf{S}_j = \sum_{\alpha\beta\mu\nu} c_{i\alpha}^\dagger \frac{\boldsymbol{\sigma}_{\alpha\beta}}{2} c_{i\beta} \cdot c_{j\mu}^\dagger \frac{\boldsymbol{\sigma}_{\mu\nu}}{2} c_{j\mu} = \text{simple combinations of four fermionic operators},$$

which is explicitly invariant under spin rotations.

C. Spin-orbit Coupling

It is the *independence* of spin-rotational symmetry and crystalline symmetry for the original Hamiltonian (1) that extremely simplify our work of classification (as is shown above, there is merely one kind allowed).

But when SOC starts to play the role in Hamiltonian, say

$$H_{\text{SOC}} = \lambda \mathbf{L} \cdot \mathbf{S}, \quad (2)$$

all the discussion break down because now spin-rotational symmetry couple with crystalline symmetry in the sense that, if we have known the local Hamiltonian H_{ij} on one link i, j and want to push it by rotation, inversion, and translation as we have done before, then unfortunately the spin form of H_{ij} will also be altered. For example, in Kitaev spin chain [1], if the local Hamiltonian for one link is given, say, $S_i^x S_j^x$, then after $\pi/3$ and $2\pi/3$ rotations, we end up with $S_i^y S_k^y$ and $S_i^z S_\ell^z$ respectively. They are no longer the same.

II. CLASSIFICATION OF HAMILTONIAN

At the nearest-neighbor level, Hamiltonian can be generally expressed as

$$H = \sum_{\square} \sum_{\langle ij \rangle \in \square} \gamma_{\mu\nu}^{\langle ij \rangle} S_i^\mu S_j^\nu. \quad (3)$$

where $\gamma_{\mu\nu}$ are complex coefficient waiting to be determined by symmetry. We will start with classifying Hamiltonian on one link

$$H_{ij} = \gamma_{\mu\nu}^{\langle ij \rangle} S_i^\mu S_j^\nu. \quad (4)$$

A. Hamiltonian on a Link

Although SOC term leads orbital rotation coupling with spin rotation, time-reversal symmetry as well as parity inversion symmetry still survive for H_{ij} . In terms of group action on group representation, we have

$$\rho(g) H_{ij} \rho^\dagger(g) = H \quad (5)$$

for $g = T$ or P , giving

$$\rho(T) H_{ij} \rho^\dagger(T) = \gamma_{\mu\nu}^{\langle ij \rangle *} (-S_i^\mu)(-S_j^\nu) \equiv H_{ij} \implies \gamma_{\mu\nu}^{\langle ij \rangle *} \equiv \gamma_{\mu\nu}^{\langle ij \rangle}, \quad (6)$$

$$\rho(P) H_{ij} \rho^\dagger(P) = \gamma_{\mu\nu}^{\langle ij \rangle} S_j^\mu S_i^\nu \equiv H_{ij} \implies \gamma_{\mu\nu}^{\langle ij \rangle} \equiv \gamma_{\nu\mu}^{\langle ij \rangle}, \quad (7)$$

respectively. Therefore, coefficient matrix γ is *real* and *symmetric*.

But this is far less the end of the story. In fact, when we include the entire space group of our A_2IrO_3 lattice, there is one more group action keeping the link ij unchanged — the (spin) rotation along local \hat{Y} direction, or global $\frac{1}{\sqrt{2}}(-\hat{x} + \hat{y})$ direction. This is clear from the two octahedral structures in FIG 1.

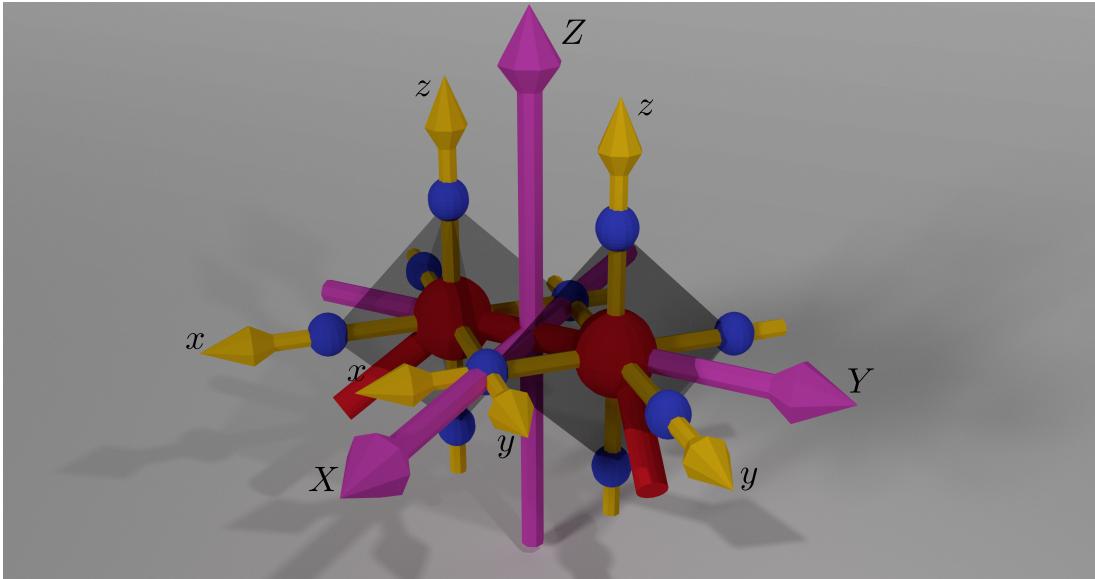


FIG. 1: **Ir-Ir Link:** For each link we assign a local (purple) frame with \hat{Y} in Ir-Ir direction and global spin (yellow) frame pointing three orthogonal Ir-O directions of an octahedra.

Therefore, if we express γ matrix in local spin frame (and denote it as $\tilde{\gamma}_{\mu\nu}$), then because

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tilde{\gamma}_{\mu\nu}^{\langle ij \rangle} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \equiv \tilde{\gamma}_{\mu\nu}^{\langle ij \rangle}$$

we can only write

$$\tilde{\gamma}_{\mu\nu}^{\langle ij \rangle} = \begin{pmatrix} A & 0 & D \\ 0 & B & 0 \\ D & 0 & C \end{pmatrix}. \quad (8)$$

For further discussion of orbital rotation, it's helpful to go back to global spin frame (so that the coupling of spin rotation with orbital rotation is definitely decided)

$$\tilde{\mathbf{S}} = P\mathbf{S}, \text{ or } \begin{pmatrix} \tilde{S}^X \\ \tilde{S}^Y \\ \tilde{S}^Z \end{pmatrix} = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ -1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} S^x \\ S^y \\ S^z \end{pmatrix}.$$

So

$$\gamma_{\mu\nu}^{\langle ij \rangle} = \begin{pmatrix} \frac{a}{2} + \frac{b}{2} & \frac{b}{2} - \frac{a}{2} & \frac{d}{\sqrt{2}} \\ \frac{b}{2} - \frac{a}{2} & \frac{a}{2} + \frac{b}{2} & \frac{d}{\sqrt{2}} \\ \frac{d}{\sqrt{2}} & \frac{d}{\sqrt{2}} & c \end{pmatrix} \quad (9)$$

and

$$H_{ij} = J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j + K_{ij}S_i^z S_j^z + \Gamma_{ij}(S_i^x S_j^y + S_i^y S_j^x) + \Gamma'_{ij}(S_i^x S_j^z + S_i^z S_j^x + S_i^y S_j^z + S_i^z S_j^y), \quad (10)$$

where for physical reason Heisenberg-like term is splitted out and

$$J_{ij} \equiv \frac{a+b}{2}, \quad K_{ij} \equiv c - \frac{a+b}{2}, \quad \gamma_{ij} \equiv \frac{b-a}{2}, \quad \Gamma'_{ij} \equiv \frac{d}{\sqrt{2}}.$$

This result is in consistent with t/U expansion study of [6], chemical calculation of [7], and first-principle study of [8].

B. Hamiltonian on the Entire Lattice

We are interested in the trivial representation of translation transformation, i.e.,

$$\rho(T_1)S_i^\mu\rho^\dagger(T_1) \equiv S_{T_1^{-1}(i)}^\mu, \quad \rho(T_2)S_i^\mu\rho^\dagger(T_2) \equiv S_{T_2^{-1}(i)}^\mu,$$

So the left work of classification of Hamiltonian can be concentrated to the discussion of the honeycomb

$$H_{\bigcirclearrowleft} \equiv \sum_{\langle ij \rangle \in \bigcirclearrowleft} \gamma_{\mu\nu}^{\langle ij \rangle} S_i^\mu S_j^\nu. \quad (11)$$

Fortunately, once global spin orientation is chosen, the coupling of orbital rotation with spin rotation is no longer ambiguous and can be read directly from FIG. 2.

For instance, if we focus on link Ir₁-Ir₂ in FIG. 2, then C_3 rotation will transform it to link Ir₃-Ir₄, in which

$$\rho(C_3)S_i^x\rho^\dagger(C_3) = S_{C_3(i)}^z, \quad \rho(C_3)S_i^y\rho^\dagger(C_3) = S_{C_3(i)}^x, \quad \rho(C_3)S_i^z\rho^\dagger(C_3) = S_{C_3(i)}^y. \quad (12)$$

Unlike above C_3 rotation just connecting two links, C_2 rotation along Ir₂-Ir₅ axis will connect Ir₁-Ir₂ with Ir₃-Ir₂, Ir₆-Ir₁ with Ir₄-Ir₃, and Ir₅-Ir₆ with Ir₅-Ir₄. Still taking Link Ir₁-Ir₂ as example, we have

$$\rho(C_2)S_2^x\rho^\dagger(C_2) = -S_2^x, \quad \rho(C_2)S_1^x\rho^\dagger(C_2) = -S_3^z, \quad (13a)$$

$$\rho(C_2)S_2^y\rho^\dagger(C_2) = -S_2^y, \quad \rho(C_2)S_1^y\rho^\dagger(C_2) = -S_3^y, \quad (13b)$$

$$\rho(C_2)S_2^z\rho^\dagger(C_2) = -S_2^z, \quad \rho(C_2)S_1^z\rho^\dagger(C_2) = -S_3^x. \quad (13c)$$

Therefore, we conclude that coefficients in (10) are the same for all the links. Namely,

$$H_{\bigcirclearrowleft} = \sum_{\langle ij \rangle \in \bigcirclearrowleft} J\mathbf{S}_i \cdot \mathbf{S}_j + KS_i^z S_j^z + \Gamma(S_i^x S_j^y + S_i^y S_j^x) + \Gamma'(S_i^x S_j^z + S_i^z S_j^x + S_i^y S_j^z + S_i^z S_j^y). \quad (14)$$

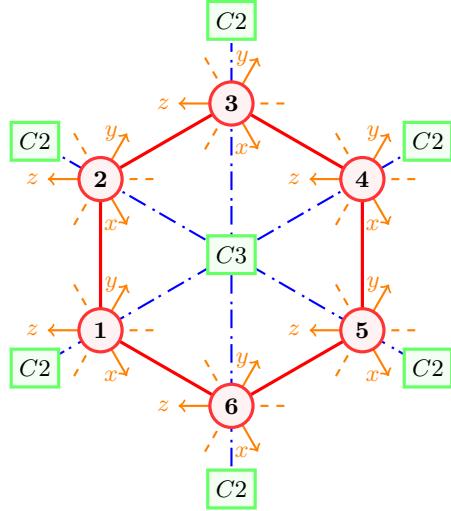


FIG. 2: **Global Spin Orientation on a Hexagon:** SOC term makes C2 rotation and C3 rotation along each Ir

III. ELECTRIC POLARIZATION OPERATOR

Unlike Hamiltonian, polarization operator is *odd* under parity inversion of bond center. Therefore with the same time-reversal symmetry, we can write

$$P_{ij} = \lambda_{\mu\nu}^{(ij)} S_i^\mu S_j^\nu \quad (15)$$

with real but antisymmetric coefficient matrix

$$\lambda_{\mu\nu} = \begin{pmatrix} 0 & A & B \\ -A & 0 & C \\ -B & -C & 0 \end{pmatrix}.$$

To analyze symmetry allowed form of polarization operator, we still start from a link and classify with little group action. For $C2$ rotation along \hat{Z} direction,

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tilde{\lambda}_{\mu\nu}^{(ij)} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \equiv \tilde{\lambda}_{\mu\nu}^{(ij)}$$

gives

$$\tilde{\lambda}_{\mu\nu}^{(ij)} = \begin{pmatrix} 0 & 0 & A \\ 0 & 0 & 0 \\ -A & 0 & 0 \end{pmatrix}. \quad (16)$$

In global spin frame,

$$\lambda_{\mu\nu}^{(ij)} = \begin{pmatrix} 0 & 0 & \frac{A}{\sqrt{2}} \\ 0 & 0 & \frac{A}{\sqrt{2}} \\ -\frac{A}{\sqrt{2}} & -\frac{A'}{\sqrt{2}} & 0 \end{pmatrix} \quad (17)$$

So

$$P_{ij} = \frac{A}{\sqrt{2}} (S_i^x S_j^z - S_i^z S_j^x + S_i^y S_j^z - S_i^z S_j^y),$$

or in a more compact form

$$P_{ij} = A(\mathbf{S}_i \times \mathbf{S}_j) \cdot \hat{e}_{ij}, \quad (18)$$

where $\hat{\mathbf{e}}_{ij}$ is identified with $\hat{\mathbf{e}}_{ij}$ in FIG. 2 so that $\hat{\mathbf{e}}_{ij} \equiv \frac{1}{\sqrt{2}}(-\hat{\mathbf{y}} + \hat{\mathbf{z}})$.

With the same discussion on the remaining C_3 rotation and C_2 rotation (and trivial T_1 and T_2 translation) transformation, we can easily push P_{12} to the entire lattice. Finally, we obtain

$$P_{\bigcirclearrowleft} \equiv \sum_{\langle ij \rangle \in \bigcirclearrowleft} P_{ij} = A \sum_{\langle ij \rangle \in \bigcirclearrowleft} (\mathbf{S}_i \times \mathbf{S}_j) \cdot \hat{\mathbf{e}}_{ij}. \quad (19)$$

This result is in consistent with that in [9].

IV. t/U EXPANSION

But this is exactly true only if $t/U \rightarrow \infty$. In reality where t is small but finite, chances are electrons hopping among sites and forming doubly occupied states.

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