# Relization of Kitaev Model

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## Outline

Obital degrees of freedom is important for generating the Kitaev type of couplings, which are highly anisotropic and orientation-selective. The strong spin obital coupling gives rise to the formation of Kramer's doublet, which provides the orbital dependent pseudo spin. Electons on different pseudo spin state undergoes vertual hopping though different pathes, thus pseudo spin coupling along different bounds can be different. The effective coupling is given by the super-exchange mechanism. The Hund's rule interaction is the most important for the Kitaev coupling to appear.

**Keywords:** Kramer's doublet, spin-orbital coupling, super-exchange, Kitaev model.

# Origin of The Kitaev Coupling

## Spin-Orbital Coupling in Ir Atom

### $t_{2g}$ Orbital Angularmomentum

In the crystal field, the $d$-orbitals in Ir atom split into the $t_{2g}$ and $e_g$ manifolds. Consider the three $t_{2g}$ orbitals $\alpha = \text{xz, xy, yz}$. They form a $l = 1$ representation for the SO(3) group. They are related to the angular momentum eigen states $m = +1,\ 0,\ -1$ by

$$|0\rangle = |\text{xy}\rangle, \tag{1}$$

$$|\pm 1\rangle = \frac{1}{\sqrt{2}}(|\text{xz}\rangle \pm i\,|\text{yz}\rangle). \tag{2}$$

The orbital representation and the angular momentum representation are related by the unitary transform

$$\langle \alpha \mid m\rangle = \begin{pmatrix} 2^{1/2} & 0 & 2^{1/2} \\ 0 & 1 & 0 \\ i\,2^{1/2} & 0 & -i\,2^{1/2} \end{pmatrix}. \tag{3}$$

### Spin-Orbital Coupling (in l-s Rep)

Assume that the $d$-orbital electron (in fact hole) experiences a strong spin-orbital coupling $\lambda$

$$\epsilon_{(\text{ls})} = \lambda\, \boldsymbol{l}\cdot\boldsymbol{s} + \Delta\, l_z^2 \simeq \lambda\, \boldsymbol{l}\cdot\boldsymbol{s}. \tag{4}$$

The $\Delta$ term is a small lattice distortion term, which may be omitted for now.

In the $l$-$s$ representation: $[\ +1\uparrow\ \ +1\downarrow\ \ 0\uparrow\ \ 0\downarrow\ \ -1\uparrow\ \ -1\downarrow\ ]$.

$$\epsilon_{(\text{ls})} = \begin{pmatrix} \frac{\lambda}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\lambda}{2} & \frac{\lambda}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{\lambda}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\lambda}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & \frac{\lambda}{\sqrt{2}} & -\frac{\lambda}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\lambda}{2} \end{pmatrix} \tag{5}$$

For $l = 1$, $s = 1/2$, $l + s \to\ 1/2,\ 3/2$. The Kramers doublet is the resulting spin $1/2$ subspace, given by the eigen

space of $\boldsymbol{l}\cdot\boldsymbol{s}$ operator with eigenvalue $-1$.

## Spin-Orbital Coupling (in Orbital Rep)

$\epsilon_{(\mathrm{ls})}$ is written in the angular momentum representation, $\epsilon_{(\mathrm{ls})} = \langle m\,|\hat{\epsilon}|\,m'\rangle$. We can use the unitary transformation $\langle\alpha\,|\,m\rangle$ to transform it into orbital representation [ xz↑ xz↓ xy↑ xy↓ yz↑ yz↓ ]. The formula reads

$$\epsilon = \langle\alpha\,|\hat{\epsilon}|\,\alpha'\rangle = \langle\alpha\,|\,m\rangle\,\langle m\,|\hat{\epsilon}|\,m'\rangle\,\langle m'\,|\,\alpha'\rangle, \tag{6}$$

and the result is

$$\epsilon = \begin{pmatrix} 0 & 0 & 0 & \frac{\lambda}{2} & -\frac{i\lambda}{2} & 0 \\ 0 & 0 & \frac{\lambda}{2} & 0 & 0 & \frac{i\lambda}{2} \\ 0 & \frac{\lambda}{2} & 0 & 0 & 0 & -\frac{i\lambda}{2} \\ \frac{\lambda}{2} & 0 & 0 & 0 & \frac{i\lambda}{2} & 0 \\ \frac{i\lambda}{2} & 0 & 0 & -\frac{i\lambda}{2} & 0 & 0 \\ 0 & -\frac{i\lambda}{2} & \frac{i\lambda}{2} & 0 & 0 & 0 \end{pmatrix}. \tag{7}$$

The eigenvalues of $\epsilon$ are made up of 2 fold degenerated $(-\lambda)$ (Kramer's doublet) and 4 fold degenerated $(\lambda/2)$. The ground state energy is $(-\lambda)$. The ground state manifold spans a 2-dim Hilbert space $\tilde{\mathcal{H}}$, the Hilbert space for pseudo-spin.

$$|\tilde{\uparrow}\rangle = \frac{|\mathrm{xz}\downarrow\rangle - |\mathrm{xy}\uparrow\rangle + i\,|\mathrm{yz}\downarrow\rangle}{\sqrt{3}}, \tag{8}$$

$$|\tilde{\downarrow}\rangle = \frac{|\mathrm{xz}\uparrow\rangle - |\mathrm{xy}\downarrow\rangle - i\,|\mathrm{yz}\uparrow\rangle}{\sqrt{3}}. \tag{9}$$

### Hamiltonian and its eigenvalues

### Script: In Case of Finite Δ

## Pseudo-Spin Projection

The Kramer's doublets form a projector to project the obtial-spin Hilbert space $\mathcal{H}$ to the pseudo-spin Hilbert space $\tilde{\mathcal{H}}$,

$$\tilde{\mathcal{P}} = \frac{1}{\sqrt{3}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \\ -1 & 0 \\ 0 & -1 \\ 0 & -i \\ i & 0 \end{pmatrix}. \tag{10}$$

Under this projection, the Hamiltonian is projected into the ground state manifold,

$$\tilde{\mathcal{P}}^{\dagger}\,\epsilon\,\tilde{\mathcal{P}} = -\lambda\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{11}$$

We will use this projection to ectrac the effective pseudo-spin coupling in the Kramer's doublet space.

## On-Site Single Particle Hamiltonian

Introduce the 6-component electron field $c_1$ (on Ir 1) and $c_2$ (on Ir 2). Each contains $c_i = [\,c_{\mathrm{xz}\uparrow}\;\; c_{\mathrm{xz}\downarrow}\;\; c_{\mathrm{xy}\uparrow}\;\; c_{\mathrm{xy}\downarrow}\;\; c_{\mathrm{yz}\uparrow}\;\; c_{\mathrm{yz}\downarrow}\,]$. Then can write down the single particle Hamiltonian on site,

$$H_0 = c_1^{\dagger}\,\epsilon\,c_1 + c_2^{\dagger}\,\epsilon\,c_2. \tag{12}$$

To deduce the effective coupling between pseudo spins on nearest neighboring sites up to the second order perturbation, it is suficient to focus on two sites only.

# Anisotropic Hopping Mediated by O Atom

## 90° Bound Effective Hopping

Consider the 90° bound in the xy plane. The $p_z$ obital of O couples the nearest neighboring Ir $d_{xz}$ and $d_{yz}$ orbital together. The effective hopping in the obtial representation is given by

$$H_t = c_1^\dagger\, t_z\, c_2 + h.c., \tag{13}$$

$$t_z = -t\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \otimes \sigma_0, \tag{14}$$

$$t = \frac{t_{\text{pd}}^2}{\Delta_{\text{pd}}}. \tag{15}$$

It can be deduced from the following model Hamiltonian in the representation $\begin{bmatrix} \text{xz} & \text{xy} & \text{yz} & p_z^{(1)} & p_z^{(2)} \end{bmatrix}$

$$H_{\text{pd}} = \begin{pmatrix} 0 & 0 & 0 & -t_{\text{pd}} & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & t_{\text{pd}} \\ 0 & 0 & -t_{\text{pd}} & \Delta_{\text{pd}} & 0 \\ t_{\text{pd}} & 0 & 0 & 0 & \Delta_{\text{pd}} \end{pmatrix} \otimes \sigma_0 \to \begin{pmatrix} 0 & 0 & -t \\ 0 & 0 & 0 \\ -t & 0 & 0 \end{pmatrix} \otimes \sigma_0 = t_z. \tag{16}$$

$H_{\text{pd}}$ is not Hermitian because it is not a diagonal block.

Let call $t_z$ the $z$-type hopping. For bounds lying in different plane the hopping type is different. For bounds in yz plane, we have the $x$-type hopping

$$t_x = -t\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \otimes \sigma_0, \tag{17}$$

and for bounds in xz plane, we have the $y$-type hopping

$$t_y = -t\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \otimes \sigma_0. \tag{18}$$

# Electron Interaction in Ir Atom

## Interaction Terms

Consider the on-site interaction of electrons in the Ir $d$-orbitals,

$$\begin{aligned} H_I &= \frac{1}{2}\sum_{\sigma,\sigma'}\int d^3x\, d^3x'\, c_\sigma^\dagger(x)\, c_\sigma(x)\, V(x-x')\, c_{\sigma'}^\dagger(x')\, c_{\sigma'}(x') \\ &= \frac{1}{2}\sum_{\sigma,\sigma'}\sum_{\alpha_1,\alpha_2,\alpha_3,\alpha_4} c_{\alpha_1\sigma}^\dagger\, c_{\alpha_2\sigma'}^\dagger\, c_{\alpha_3\sigma'}\, c_{\alpha_4\sigma}\int d^3x\, d^3x'\, \psi_{\alpha_1}(x)\,\psi_{\alpha_2}(x')\, V(x-x')\,\psi_{\alpha_3}(x')\,\psi_{\alpha_4}(x), \end{aligned} \tag{19}$$

where $\sigma$, $\sigma' = \uparrow, \downarrow$ labels the spins, $\alpha_{1,2,3,4} = $ xz, xy, yz labels the orbitals. Due to symmetry, orbitals must come in pairs,

$$\begin{aligned} H_I = &\frac{1}{2}U\sum_{\sigma,\sigma'}\sum_{\alpha} c_{\alpha\sigma}^\dagger\, c_{\alpha\sigma'}^\dagger\, c_{\alpha\sigma'}\, c_{\alpha\sigma} + \frac{1}{2}V\sum_{\sigma,\sigma'}\sum_{\alpha\neq\alpha'} c_{\alpha\sigma}^\dagger\, c_{\alpha'\sigma'}^\dagger\, c_{\alpha'\sigma'}\, c_{\alpha\sigma} + \\ &\frac{1}{2}J\sum_{\sigma,\sigma'}\sum_{\alpha\neq\alpha'} c_{\alpha\sigma}^\dagger\, c_{\alpha'\sigma'}^\dagger\, c_{\alpha\sigma'}\, c_{\alpha'\sigma} + \frac{1}{2}J\sum_{\sigma,\sigma'}\sum_{\alpha\neq\alpha'} c_{\alpha\sigma}^\dagger\, c_{\alpha\sigma'}^\dagger\, c_{\alpha'\sigma'}\, c_{\alpha'\sigma}, \end{aligned} \tag{20}$$

where $U = U_{\alpha\alpha}$ (diagonal), $V = U_{\alpha\beta}$ (off-diagonal),

$$U_{\alpha\alpha'} = \int d^3x\, d^3x'\, \psi_\alpha(x)\,\psi_{\alpha'}(x')\, V(x-x')\,\psi_{\alpha'}(x')\,\psi_\alpha(x), \tag{21}$$

$$J = \int d^3x\, d^3x'\, \psi_\alpha(x)\,\psi_{\alpha'}(x')\, V(x-x')\,\psi_\alpha(x')\,\psi_{\alpha'}(x). \tag{22}$$

There is a relation between $U$, $V$ and $J$ for $d$-orbital[1]: $U = V + 2J$. $U$ term is the (intra-orbital) Hubbard interaction. $V$ term is the inter-orbital direct interaction. The first $J$ term is the Hund's rule exchange interaction, and the

second $J$ term is the pair hopping interaction.

# Representations

## Two-Particle Hilbert Spaces

Let $a = \alpha\sigma$ be the label of both the orbital and the spin. The on-site two-particle Hilbert space $\mathcal{H}_I$ is spaned by 15 states

$$\mathcal{H}_I = \left\{ c^\dagger_{1\,a}\, c^\dagger_{1\,a'} \,|\mathrm{vac}\rangle \;\middle|\; \forall\, a = 1:6,\ \forall\, a' = (a+1):6 \right\}. \tag{23}$$

The inter-site two-particle Hilbert space $\mathcal{H}_0$ is spaned by 36 states

$$\mathcal{H}_0 = \left\{ c^\dagger_{1\,a}\, c^\dagger_{2\,a'} \,|\mathrm{vac}\rangle \;\middle|\; \forall\, a = 1:6,\ \forall\, a' = 1:6 \right\}. \tag{24}$$

## Projection Operator

Hopping terms $H_t$ relates the two Hilbert psaces $\mathcal{H}_0$ and $\mathcal{H}_I$. Naively acting $H_t$ on the 36 inter-site states (in $\mathcal{H}_0$) seems to result in 36 different on-site states (in $\mathcal{H}_I$), however because the on-site fermions are identital, so actually there are only 15 indepenent on-site fermion states. A projection $\mathcal{P}_t$ is needed to project the 36 resulting states to the 15 fermion states.

This can be seen by acting $H_t$ on $\mathcal{H}_0$

$$H_t\,\mathcal{H}_0 = \mathcal{H}_I^* = \left\{ c^\dagger_{1\,a}\, c^\dagger_{1\,a'} \,|\mathrm{vac}\rangle \;\middle|\; \forall\, a = 1:6,\ \forall\, a' = 1:6 \right\}. \tag{25}$$

$\mathcal{H}_I^*$ seems to contain more states than $\mathcal{H}_I$, but they are not linearly independent. So a projection $\mathcal{P}_t$ is needed to bring $\mathcal{H}_I^*$ back to $\mathcal{H}_I$

$$\mathcal{P}_t :\ \mathcal{H}_I^* \to \mathcal{H}_I, \tag{26}$$

so that

$$\mathcal{P}_t : c^\dagger_{1\,a}\, c^\dagger_{1\,a'} \,|\mathrm{vac}\rangle \mapsto :c^\dagger_{1\,a}\, c^\dagger_{1\,a'}: \,|\mathrm{vac}\rangle, \tag{27}$$

where $:c^\dagger\, c^\dagger:$ means to normal order the operators such that their indexes follow a canonical order. $\mathcal{P}_t$ actually takes care of the fermion sign that is generated during the hopping process.

$\mathcal{P}_t$ can be represented by a 15×36 matrix, whose nonzero entries are listed as follows

$$\begin{aligned}
&\mathcal{P}_{t:\,1,2} = 1,\\
&\mathcal{P}_{t:\,1,7} = -1,\\
&\mathcal{P}_{t:\,2,3} = 1,\\
&\mathcal{P}_{t:\,2,13} = -1,\\
&\mathcal{P}_{t:\,3,4} = 1,\\
&\mathcal{P}_{t:\,3,19} = -1,\\
&\mathcal{P}_{t:\,4,5} = 1,\\
&\mathcal{P}_{t:\,4,25} = -1,\\
&\mathcal{P}_{t:\,5,6} = 1,\\
&\mathcal{P}_{t:\,5,31} = -1,\\
&\mathcal{P}_{t:\,6,9} = 1,\\
&\mathcal{P}_{t:\,6,14} = -1,\\
&\mathcal{P}_{t:\,7,10} = 1,\\
&\mathcal{P}_{t:\,7,20} = -1,\\
&\mathcal{P}_{t:\,8,11} = 1,\\
&\mathcal{P}_{t:\,8,26} = -1,\\
&\mathcal{P}_{t:\,9,12} = 1,\\
&\mathcal{P}_{t:\,9,32} = -1,\\
&\mathcal{P}_{t:\,10,16} = 1,\\
&\mathcal{P}_{t:\,10,21} = -1,\\
&\mathcal{P}_{t:\,11,17} = 1,\\
&\mathcal{P}_{t:\,11,27} = -1,
\end{aligned} \tag{28}$$

$$\mathcal{P}_{t:12,18} = 1,$$
$$\mathcal{P}_{t:12,33} = -1,$$
$$\mathcal{P}_{t:13,23} = 1,$$
$$\mathcal{P}_{t:13,28} = -1,$$
$$\mathcal{P}_{t:14,24} = 1,$$
$$\mathcal{P}_{t:14,34} = -1,$$
$$\mathcal{P}_{t:15,30} = 1,$$
$$\mathcal{P}_{t:15,35} = -1.$$

### The Projection Matrix

## Spin-Obital Coupling in $\mathcal{H}_0$

The representation of $H_0$ in the inter-site two-particle Hilbert space $\mathcal{H}_0$ is

$$H_0 = \epsilon \otimes \mathbb{1} + \mathbb{1} \otimes \epsilon, \tag{29}$$

where $\mathbb{1}$ denotes the identity matrix of dimension 6.

## Hopping Between $\mathcal{H}_0$ and $\mathcal{H}_I$

Let us first consider the representation of the hopping from site 2 to site 1. It is not a square matrix for it connects two Hilbert spaces of unequal dimensions.

$$H_t = \mathcal{P}_t(\mathbb{1} \otimes t_z). \tag{30}$$

## Interaction in $\mathcal{H}_I$

The interaction term can be expand into matrix $H_I$ in the on-site two-particle representation, which results in a 15×15 matrix. The none zero entries are listed as follows

$$H_{I:1,1} = U,$$
$$H_{I:1,10} = J,$$
$$H_{I:1,15} = J,$$
$$H_{I:2,2} = -J + V,$$
$$H_{I:3,3} = V,$$
$$H_{I:3,6} = -J,$$
$$H_{I:4,4} = -J + V,$$
$$H_{I:5,5} = V,$$
$$H_{I:5,8} = -J,$$
$$H_{I:6,3} = -J,$$
$$H_{I:6,6} = V,$$
$$H_{I:7,7} = -J + V,$$
$$H_{I:8,5} = -J,$$
$$H_{I:8,8} = V,$$
$$H_{I:9,9} = -J + V,$$
$$H_{I:10,1} = J,$$
$$H_{I:10,10} = U,$$
$$H_{I:10,15} = J,$$
$$H_{I:11,11} = -J + V,$$
$$H_{I:12,12} = V,$$
$$H_{I:12,13} = -J,$$
$$H_{I:13,12} = -J,$$
$$H_{I:13,13} = V,$$
$$H_{I:14,14} = -J + V,$$

(31)

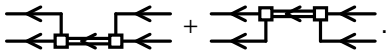
$$H_{I:\,15,1} = J,$$
$$H_{I:\,15,10} = J,$$
$$H_{I:\,15,15} = U.$$

### Matrix Form of $H_I$

## Perturbation Theory

### Small $t$ Perturbation

Consider the small $t$ perturbation to the second order. Let us calculate the self-energy correction to the two-particle propagator according to the following diagram



(32)

The diagram involves two process: super-exchange through site 1 and that through site 2. They should give the same contribution to the self-energy, so we just calculate one of them and double the result. Therefore the self-energy reads,



$$\begin{aligned} &= -2\, H_t^\dagger\, H_I^{-1}\, H_t \\ &= -2\left(\mathbb{1}\otimes t_z^\dagger\right)\mathcal{P}_t^\dagger\, H_I^{-1}\,\mathcal{P}_t(\mathbb{1}\otimes t_z), \end{aligned} \tag{33}$$

where $t_z$ is given by Eq. (14), $\mathcal{P}_t$ by Eq. (28), and $H_I$ by Eq. (31).

### Projection to the Pseudo-Spin Space

To obtain the effective coupling between pseudo-spin on site 1 and site 2, we need to impliment the pseudo-spin projection $\tilde{\mathcal{P}}$ given in Eq. (10). Note that we are now in the two-particle Hilbert space $\mathcal{H}_0 = \mathcal{H}\oplus\mathcal{H}$ which is doubled from the single particle Hilbert space $\mathcal{H}$, so that the correct projection operator is $\tilde{\mathcal{P}}\otimes\tilde{\mathcal{P}}$.

Therefore the effective pseudo-spin coupling can be obtained by projecting the self-energy $\Sigma$ to the pseudo-spin subspace

$$\begin{aligned} \tilde{\Sigma} &= \left(\tilde{\mathcal{P}}\otimes\tilde{\mathcal{P}}\right)^\dagger \Sigma\left(\tilde{\mathcal{P}}\otimes\tilde{\mathcal{P}}\right) \\ &= -2\left(\tilde{\mathcal{P}}\otimes\tilde{\mathcal{P}}\right)^\dagger \left(\mathbb{1}\otimes t_z^\dagger\right)\mathcal{P}_t^\dagger\, H_I^{-1}\,\mathcal{P}_t(\mathbb{1}\otimes t_z)\left(\tilde{\mathcal{P}}\otimes\tilde{\mathcal{P}}\right). \end{aligned} \tag{34}$$

With all the matrices we defined above, one can evaluate Eq. (34) explicitly, we find

$$\tilde{\Sigma} = J_0 + J_{ij}\,\sigma_i\otimes\sigma_j, \tag{35}$$

where $\sigma_i$ $(i = x,\ y,\ z)$ are the Pauli matrices, and the coupling coefficients are

$$J_0 = \frac{4\,t^2}{9}\left(\frac{2}{J-U} + \frac{7}{J-V} - \frac{3}{J+V}\right), \tag{36}$$

$$J_{xx} = J_{yy} = \frac{8\,t^2}{9}\left(\frac{1}{J-U} + \frac{1}{J+V}\right), \tag{37}$$

$$J_{zz} = \frac{4\,t^2}{9}\left(\frac{2}{-J+U} + \frac{3}{J-V} + \frac{1}{J+V}\right), \tag{38}$$

$$J_{xy} = J_{yz} = J_{zx} = J_{yx} = J_{zy} = J_{xz} = 0. \tag{39}$$

Using the constrain $U = V + 2\,J$, we can eliminate $V$, then

$$J_0 = \frac{8\,t^2(11\,J - 6\,U)}{9\left(3\,J^2 - 4\,J\,U + U^2\right)}, \tag{40}$$

$$J_{xx} = J_{yy} = 0, \tag{41}$$

$$J_{zz} = -\frac{8\,t^2\,J}{3\left(3\,J^2 - 4\,J\,U + U^2\right)}. \tag{42}$$

We foud that the $J_{xx}$ and $J_{yy}$ terms vanish exactly, remaining the $J_{zz}$ coupling. $J_{zz}$ is ferromagnetic for $J < U/3$, and becomes antiferromagnetic for $J > U/3$. $J = U/3$ will be a resonance point for this model.

We have also checked that by changing $t_z \to t_x \to t_y$, the coupling rotates $J_{zz} \to J_{xx} \to J_{yy}$ accordingly. So we have shown that Kitaev coupling between Ir atoms can be generated as a super-exchange coupling bridged by O atom.

### Further Discussions

$J_{zz}$ is propotional to the Hund's rule interaction $J$ only, why? Why does the contribution of $U$ cancel out finally? Why it turns out to be a ferromagnetic coupling (comparing to the AFM coupling for ordinary super-exchange)? What are the super-exchange pathes that contributes to $J_{zz}$ and $J_0$? Any possible generalization of the formulism to other geometry? What about $e_g$ obitals?

### Program (Old Version)

### Checking the Interactions

### Exchange Path

## The Reversed Energy Level

## Symmetry Protection

## Effective Hopping

### Reference

[1] C. Castellani, C. R. Natoli, and J. Ranninger, Phys. Rev. B **18**, 4945 (1978).