Microscopic Approach to The Electric Field Effect in The Kitaev Quantum Spin Liquid

키타예프 양자 스핀 액상에서 전기장 효과에 대한 미시적 접근

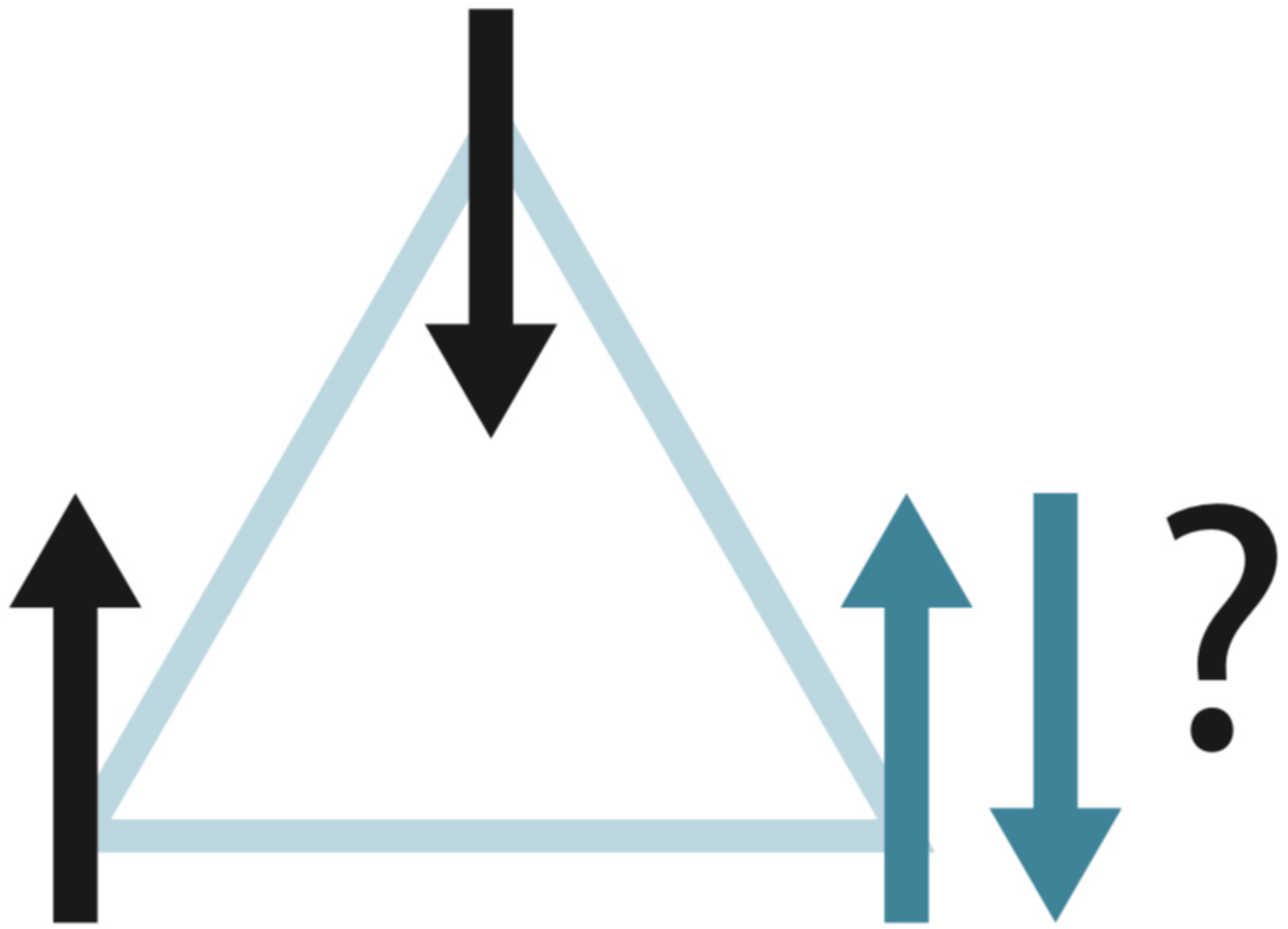
G202245001 물리학과 권성준

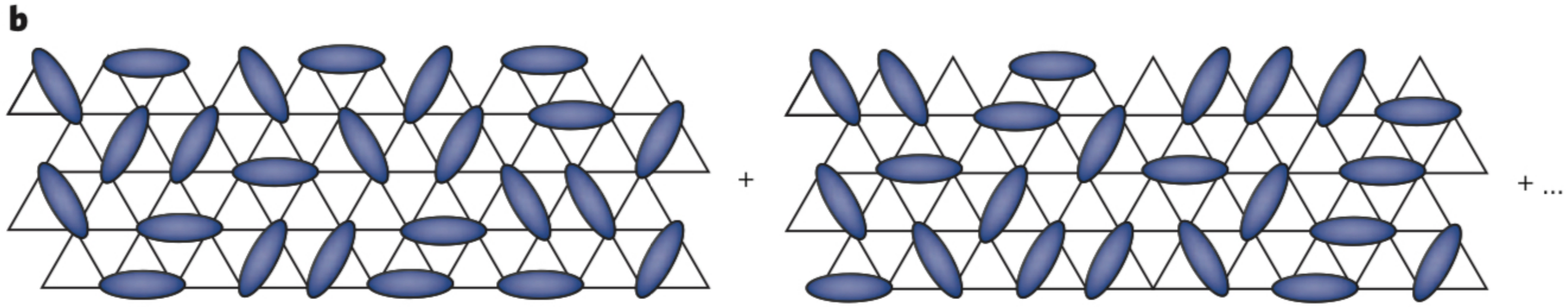
Introduction

Introduction

Quantum Spin Liquid

- magnetic frustration in anti-ferromagnetic material





“Spin liquids in frustrated magnets”, Nature, L. Balents

“They found hidden patterns in the climate and in other complex phenomena”, The Nobel Prize in Physics 2021

- ground state = superposition of various spin bonding

Introduction
Kitaev Quantum Spin Liquid

- Kitaev quantum spin liquid

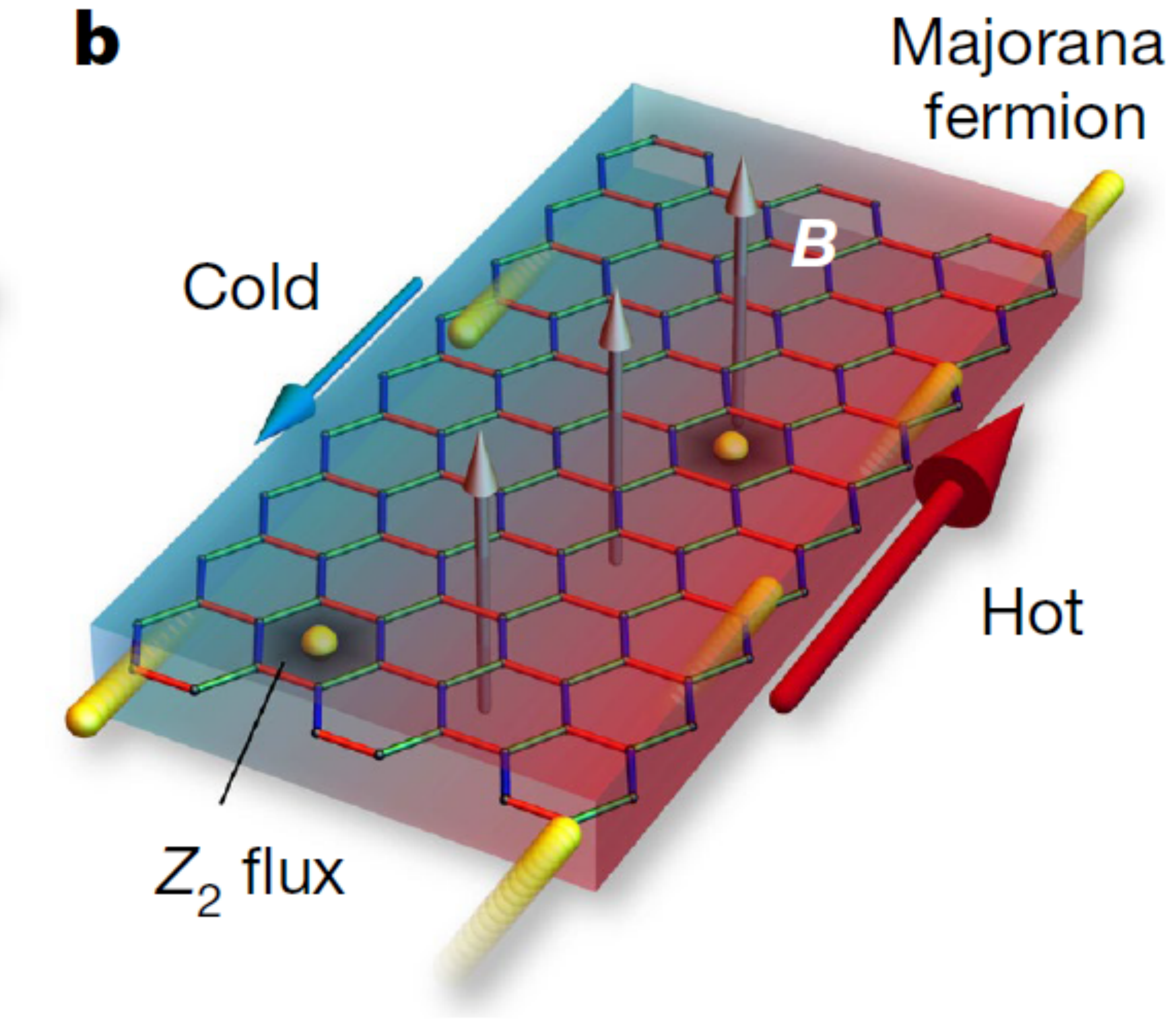
⇒ fractionalized

i.e. exactly solvable in Majorana representation

- similar to the Haldane model

⇒ ∃ Majorana chiral edge mode

- Kitaev material (ex. α-$RuCl_3$, Na_2IrO_3, …)



“Majorana quantization and half-integer thermal quantum Hall effect in a Kitaev spin liquid”, Nature, Y. Kasahara, et al

1. Kitaev Spin Liquid Theory

1. Kitaev Representation

Majorana Operator

- Majorana fermion : Majorana fermion can be its own anti-particle it self
- $\gamma_i^\dagger = \gamma_i \Leftarrow$ particle is its own anti-particle

- algebraic property
- $\{\gamma_{2i-1}, \gamma_{2j-1}\} = 2\delta_{ij}$ and $\gamma_i^2 = 1$ (non-Abelian)
- $\gamma_i \gamma_j = -\gamma_j \gamma_i$

1. Kitaev Representation

Kitaev Spin Operator

- Kitaev representation : describe spin using Majorana operator
- $\Sigma^x = i\gamma^x\gamma^0$ / $\Sigma^y = i\gamma^y\gamma^0$ / $\Sigma^z = i\gamma^z\gamma^0$
- $[\Sigma^a, \Sigma^b] = 2i(\gamma^x\gamma^y\gamma^z\gamma^0)\Sigma^c = 2iD\Sigma^c$ where $D = \gamma^x\gamma^y\gamma^z\gamma^0$

- commutation relation of $\Sigma \neq$ spin commutation relation
- $D_{eig} = \pm 1$ $\Rightarrow$ eigenstate with eigenvalue $D = 1$ satisfies the spin algebra

$\Rightarrow$ project physical state and projection operator : $P = \dfrac{1+D}{2}$

2. Kitaev Model

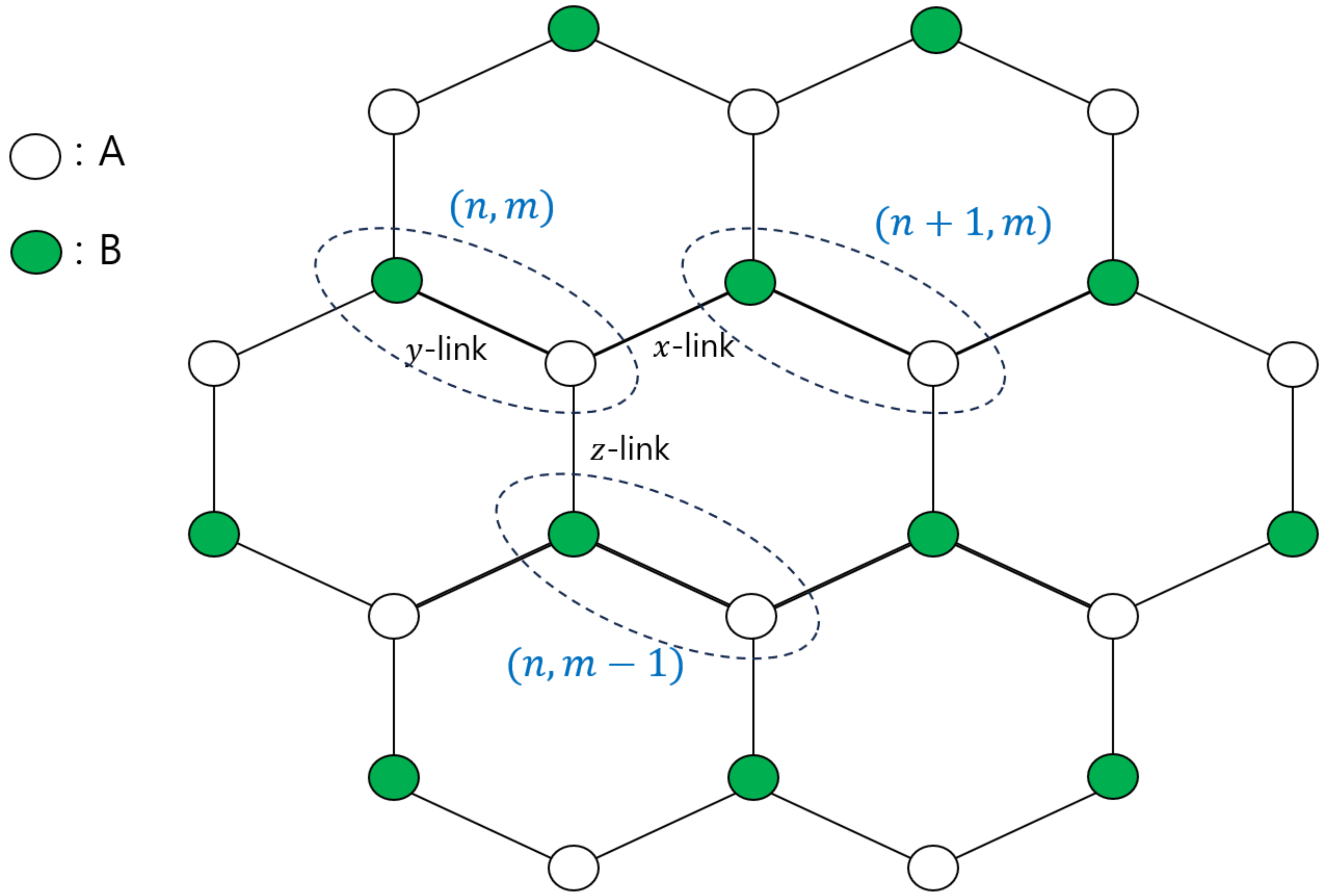
Kitaev Spin Hamiltonian

- $$H = -K_x \sum_{x-link} \sigma_j^x \sigma_k^x - K_y \sum_{y-link} \sigma_j^y \sigma_k^y - K_z \sum_{z-link} \sigma_j^z \sigma_k^z$$

- using Majorana fermion operator,

- $$H = iK_a \sum_{n,m} u^a_{n,m,n',m'} \gamma^0_{A;n,m} \gamma^0_{B;n',m'}$$

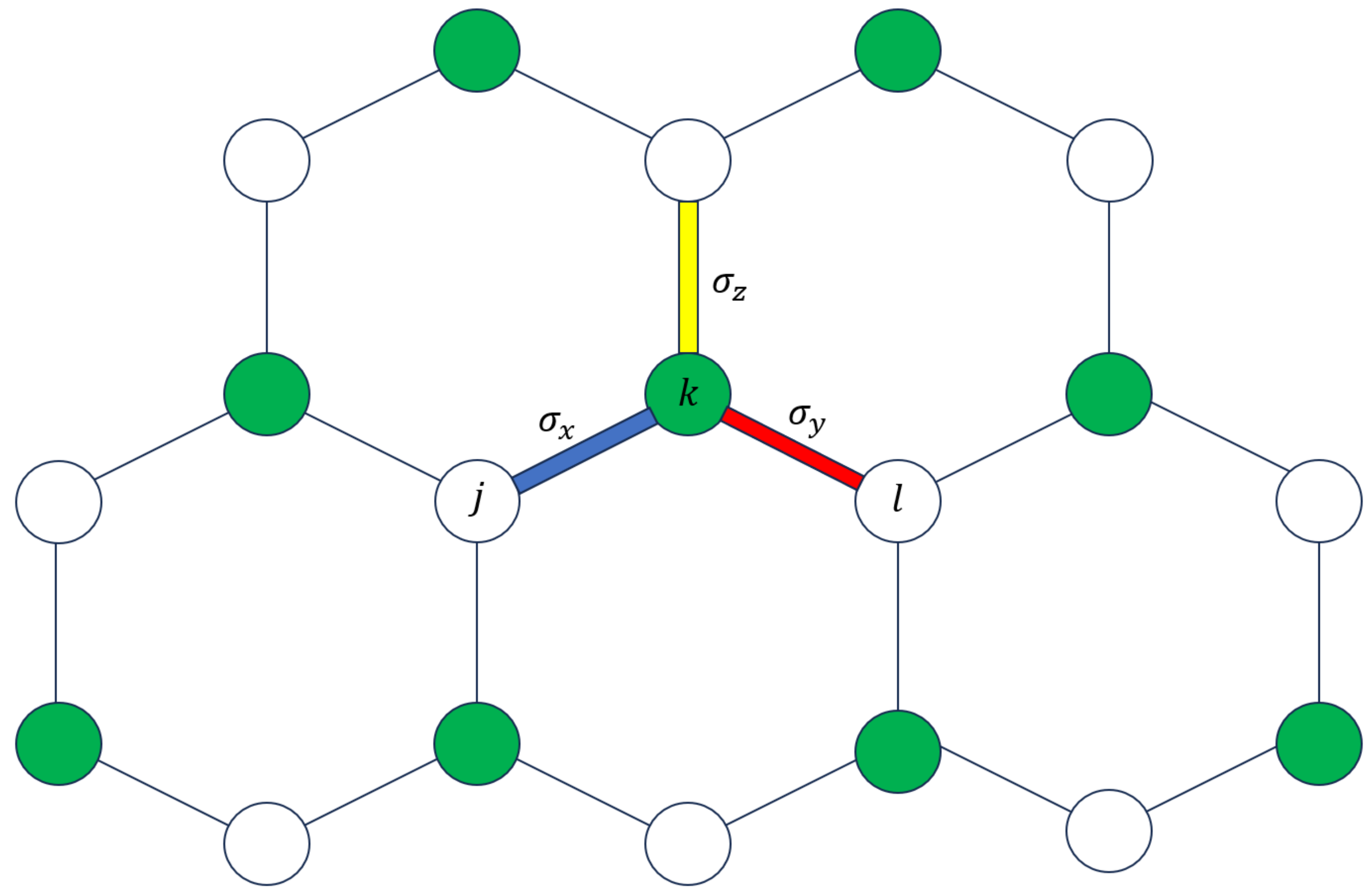
- $\mathbb{Z}_2$ gauge field : $u^a_{n,m,n',m'} = i\gamma^a_{A;n,m}\gamma^a_{B;n',m'}$



2. Kitaev Model

Haldane Like Term

- with perturbative magnetic field,
- $$H' \sim \frac{h_x h_y h_z}{K^2} \sum_{j,k,l} \sigma_j^x \sigma_k^z \sigma_l^y$$

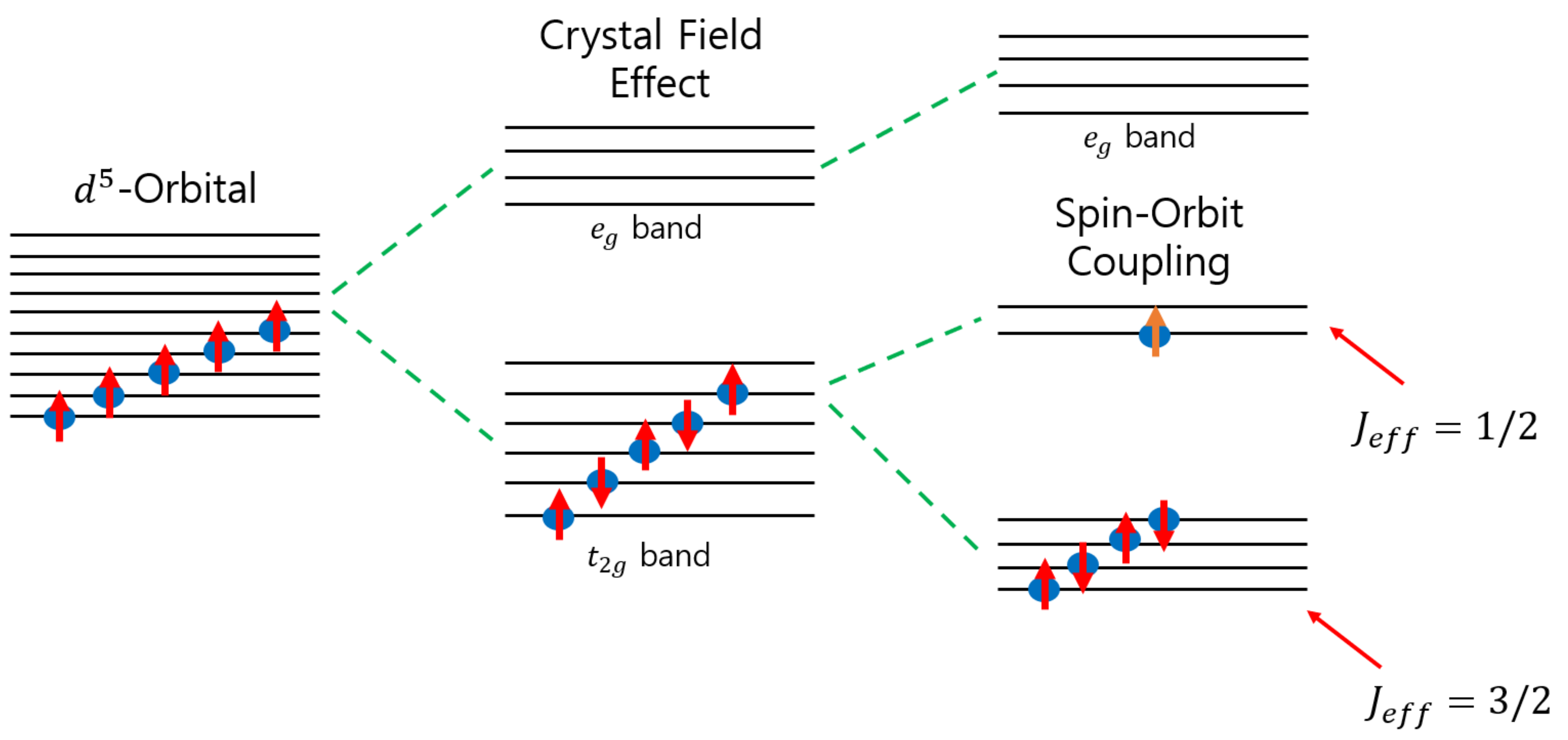


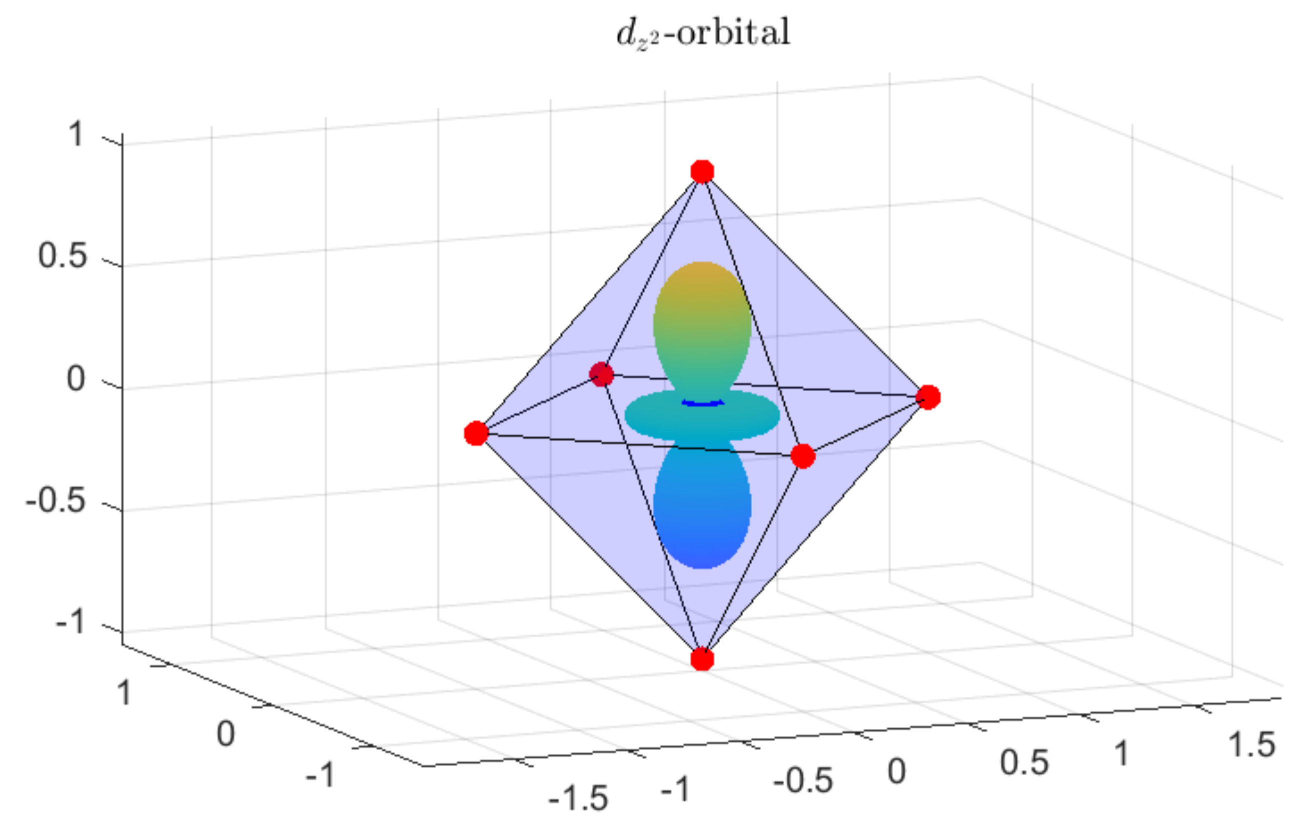
- next nearest hopping term in Majorana basis
- same form with the Haldane's graphene model

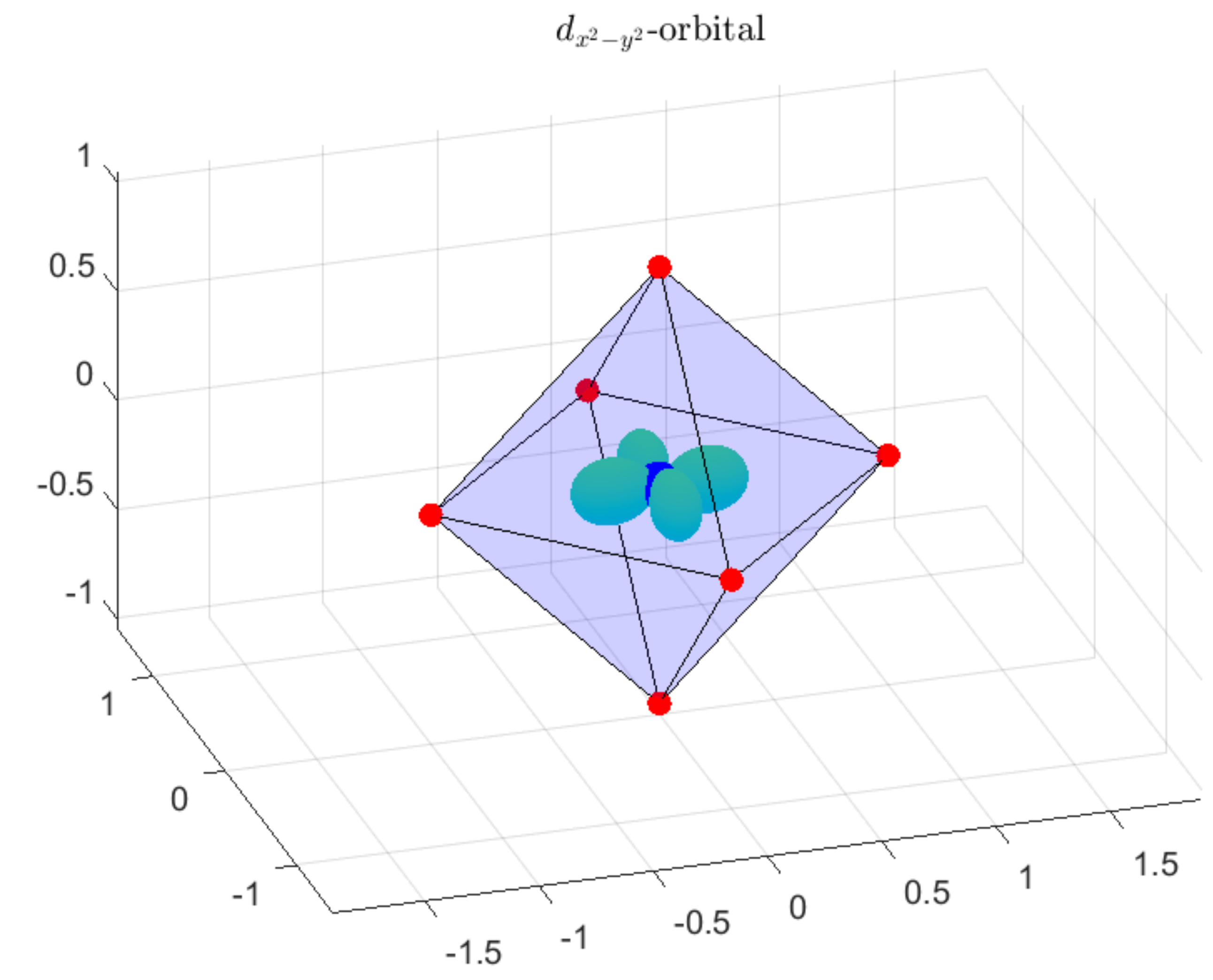
2. Kitaev Material

1. Effective Spin States

$J_{eff} = 1/2$ States



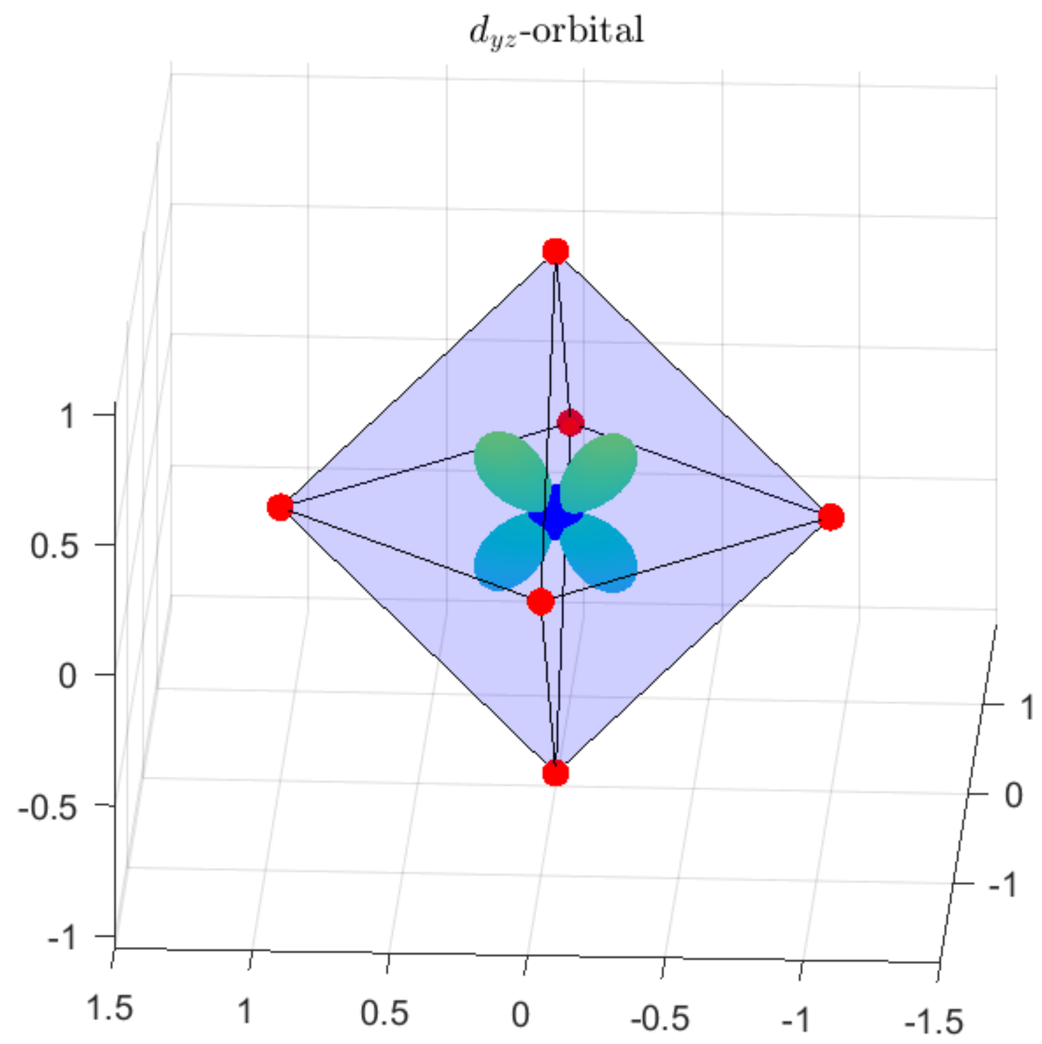




1. Effective Spin States

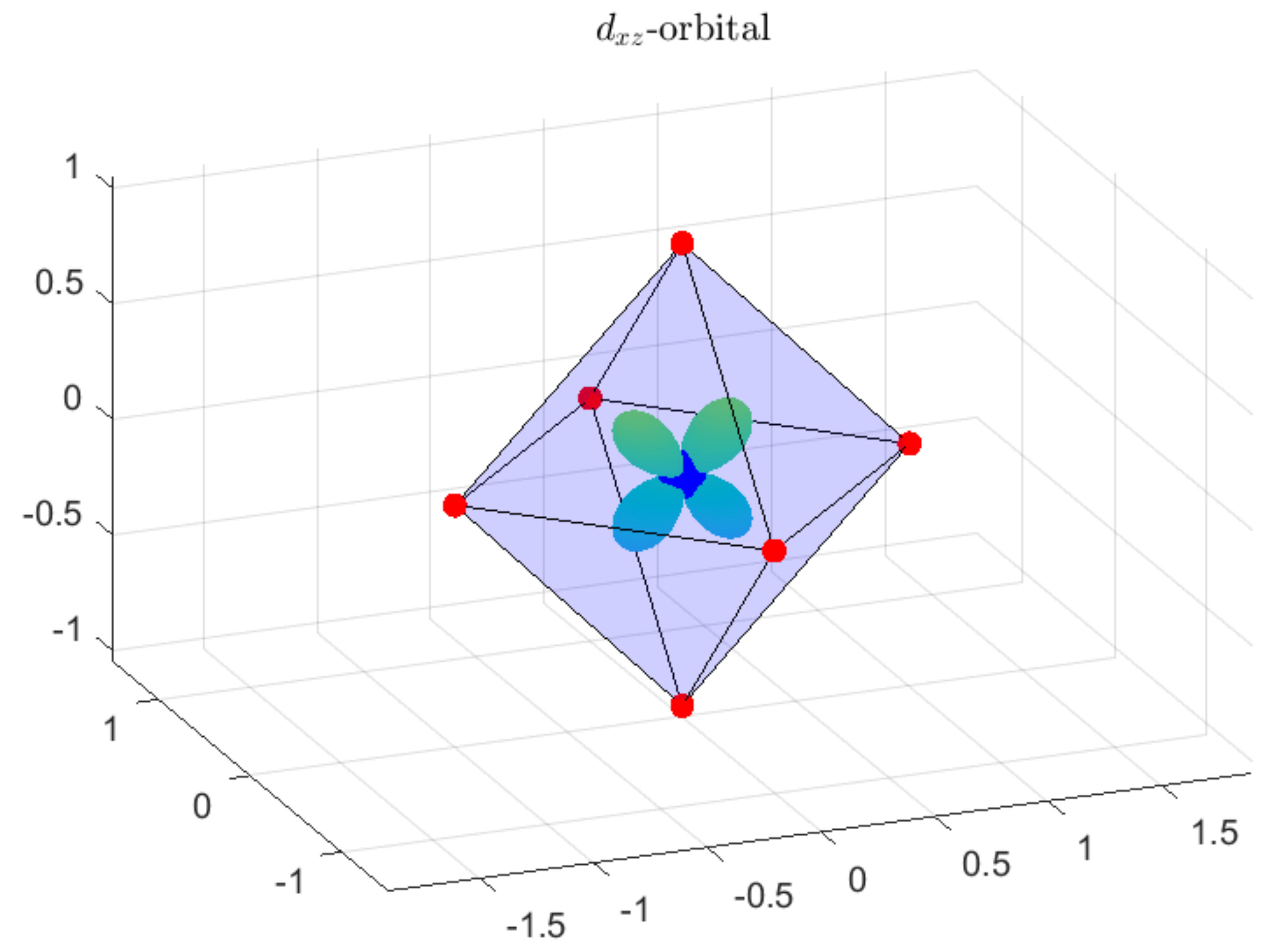
Effective Spin

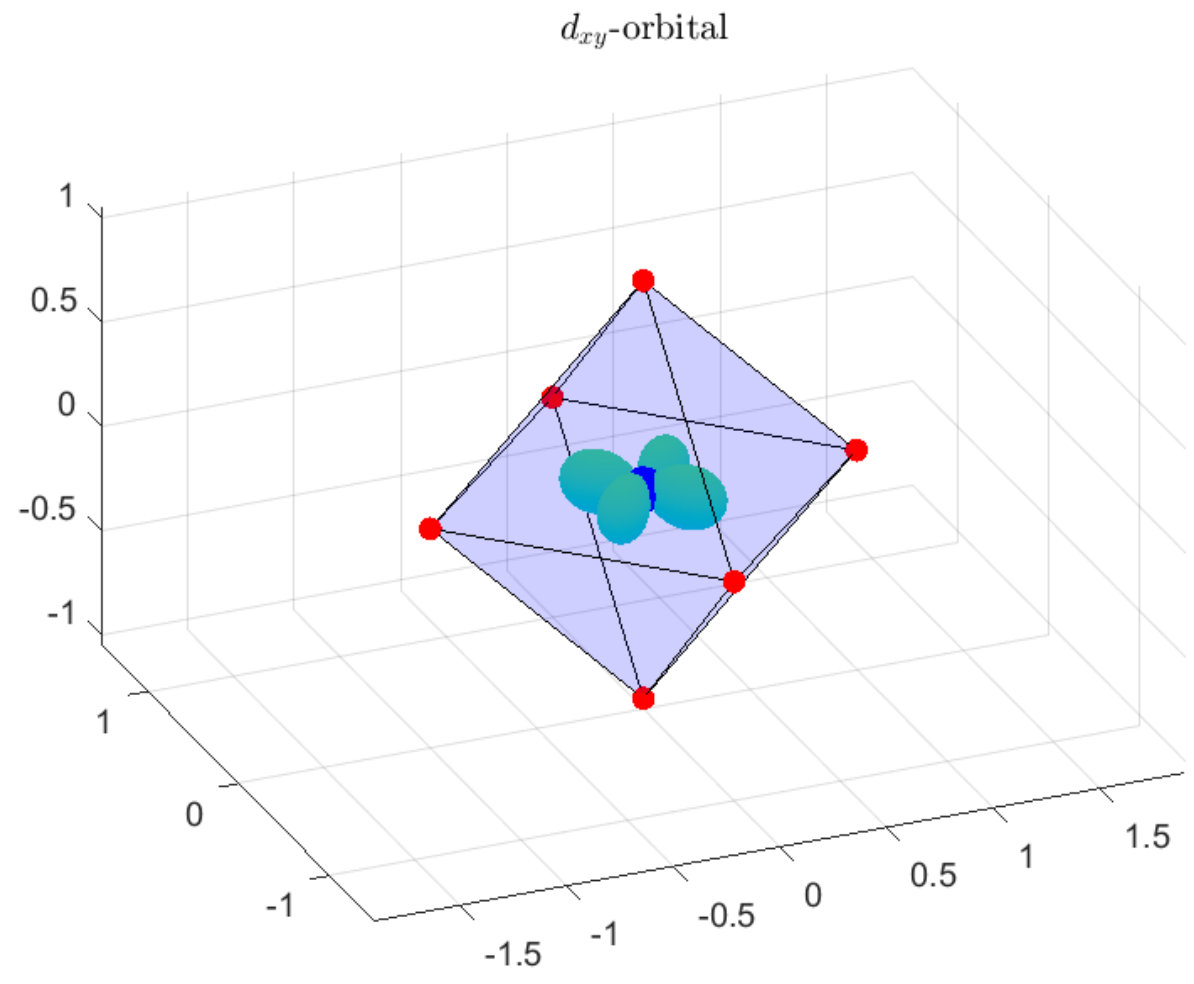
- d-orbital state : $\begin{aligned} \left| yz\text{-orbital} \right\rangle &= \left| x \right\rangle \\ \left| zx\text{-orbital} \right\rangle &= \left| y \right\rangle \\ \left| xy\text{-orbital} \right\rangle &= \left| z \right\rangle \end{aligned}$



- using spherical harmonics

$$\begin{aligned} \left| L_z = 1 \right\rangle &= -\frac{1}{\sqrt{2}}\left(\left| x \right\rangle + i \left| y \right\rangle \right) \\ \left| L_z = 0 \right\rangle &= \left| z \right\rangle \\ \left| L_z = -1 \right\rangle &= \frac{1}{\sqrt{2}}\left(\left| x \right\rangle - i \left| y \right\rangle \right) \end{aligned}$$





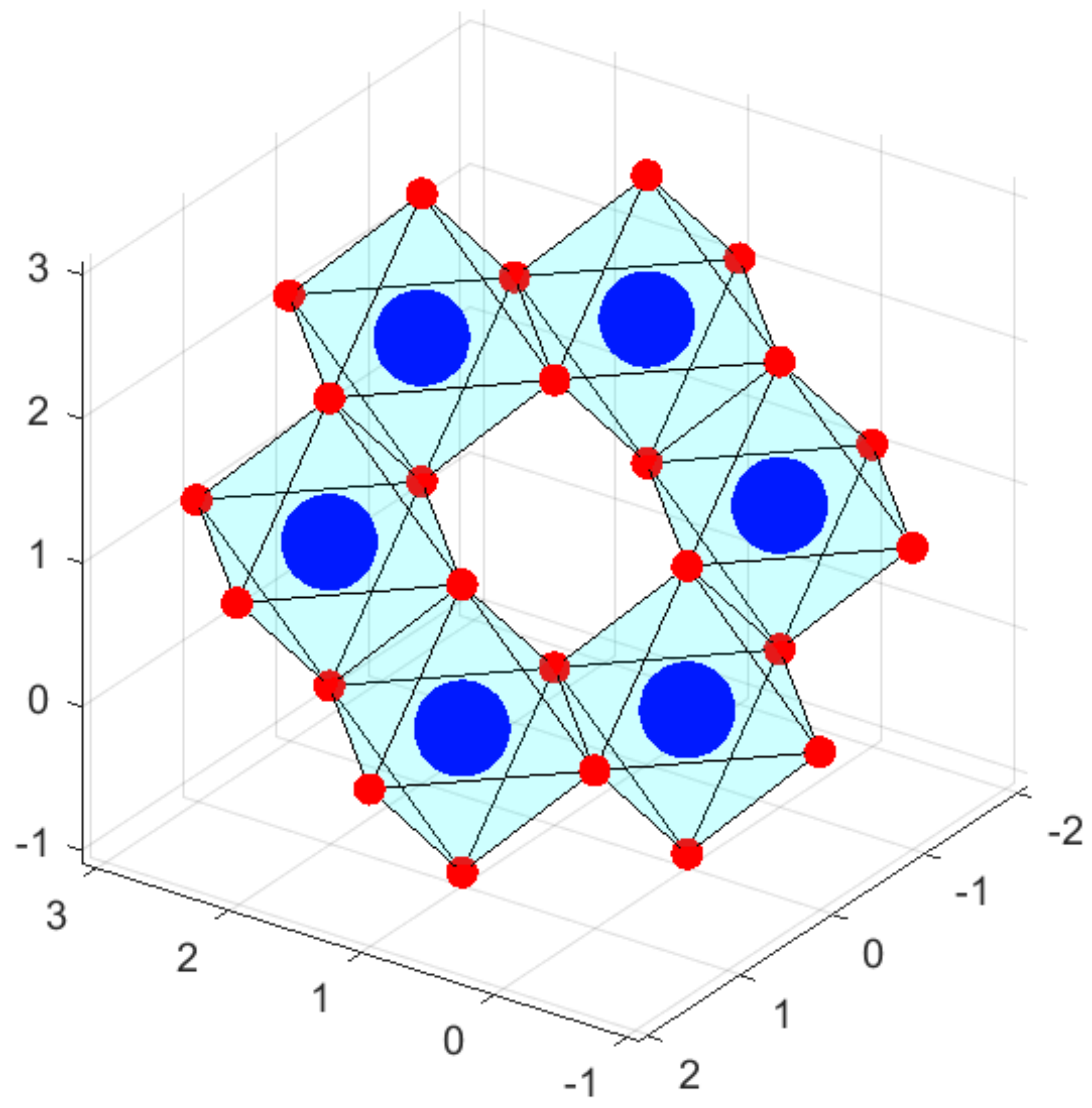
2. Octahedral Structure

Crystal Structure of Kitaev Material

- α-$RuCl_3$ or Na_2IrO_3 have octahedral structure

- core atoms construct honeycomb lattice
- orbital orientation determines spin directions

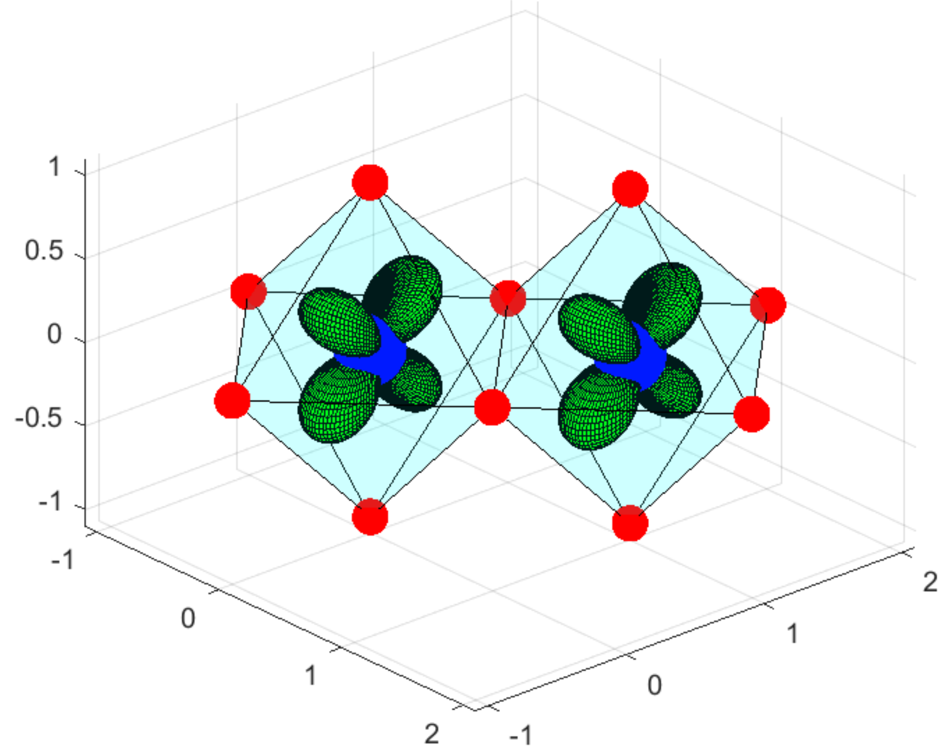
- vertex atoms determine the direction of spin interaction



2. Octahedral Structure

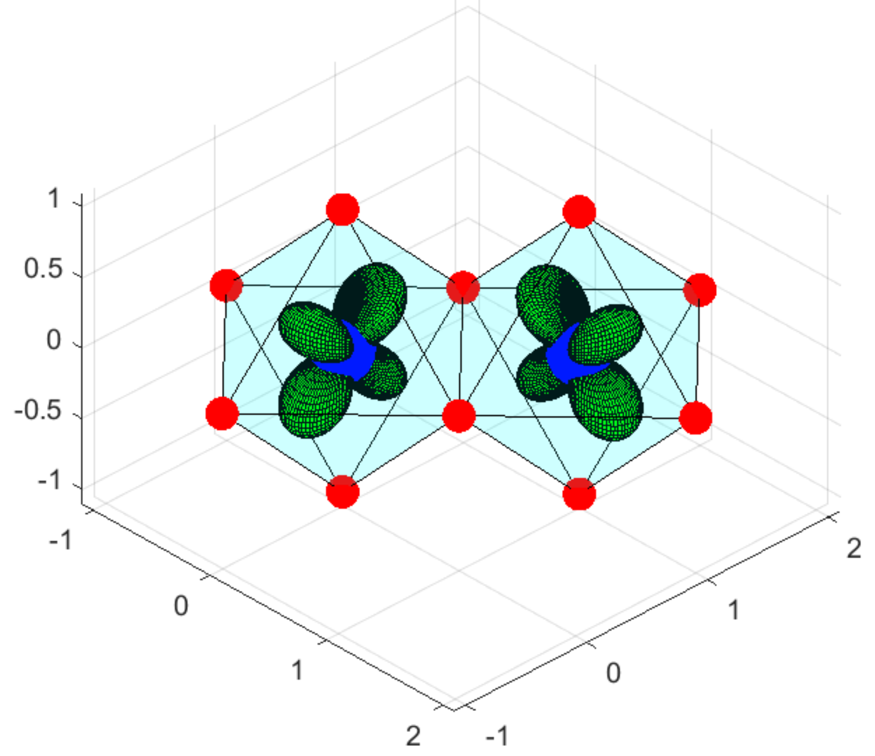
Hopping in Kitaev Material

- $$H_t = \sum_{\sigma} \left[d^{\dagger}_{n,\sigma} F_{n,m} d_{m,\sigma} + d^{\dagger}_{m,\sigma} F_{m,n} d_{n,\sigma} \right]$$
- $$d^{\dagger}_{n,\sigma} = \begin{pmatrix} d^{\dagger}_{n,x,\sigma} & d^{\dagger}_{n,y,\sigma} & d^{\dagger}_{n,z,\sigma} \end{pmatrix}$$
- $$F_{n,m} = \begin{pmatrix} t_1 & t_2 & 0 \\ t_2 & t_1 & 0 \\ 0 & 0 & t_3 \end{pmatrix}$$



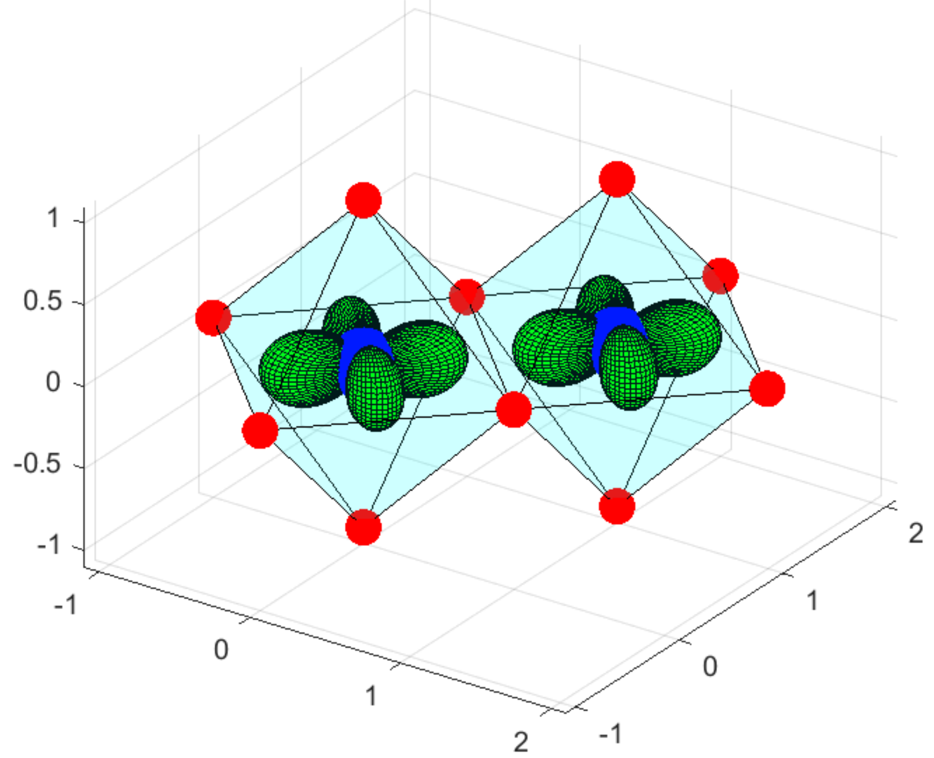
t_1-hopping

($x \to x$ or $y \to y$)



t_2-hopping

($x \to y$ or $y \to x$)



t_3-hopping

($z \to z$)

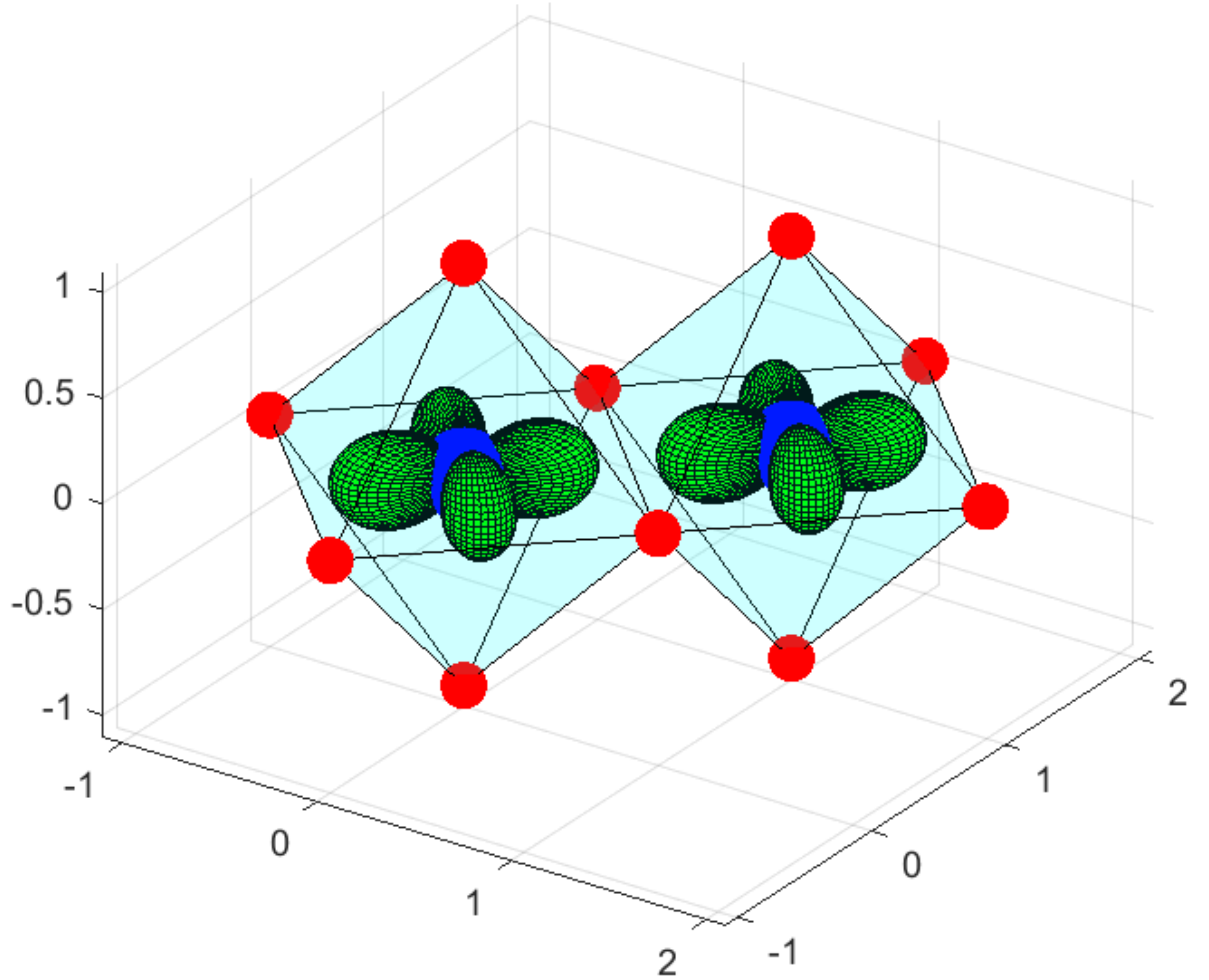
2. Octahedral Structure

Direction Dependent Interaction

- octahedra shares one edge
- orientation of the orbital toward

  shared edge determines bonding direction

- d_z-orbitals orients toward shared edge
- $\Rightarrow$ induce z-direction boding



3. Jackelli-Khaliullin Spin

Jackelli-Khaliullin Representation

- Jackelli-Khaliullin representation

$$\left|J_{eff}=\frac{1}{2}\right\rangle = \sqrt{\frac{1}{3}}\left(\left|x,\downarrow\right\rangle + i\left|y,\downarrow\right\rangle + \left|z,\uparrow\right\rangle\right)$$

$$= \sqrt{\frac{1}{3}}\left(d^{\dagger}_{x,\downarrow} + i d^{\dagger}_{y,\downarrow} + d^{\dagger}_{z,\uparrow}\right)\left|\varnothing\right\rangle$$

- $$\left|J_{eff}=-\frac{1}{2}\right\rangle = \sqrt{\frac{1}{3}}\left(-\left|x,\uparrow\right\rangle + i\left|y,\uparrow\right\rangle + \left|z,\downarrow\right\rangle\right)$$

$$= \sqrt{\frac{1}{3}}\left(-d^{\dagger}_{x,\uparrow} + i d^{\dagger}_{y,\uparrow} + d^{\dagger}_{z,\downarrow}\right)\left|\varnothing\right\rangle$$

3. Effective Spin Interaction

1. Hubbard-Like Model

Hubbard Model

- Hubbard Hamiltonian : $H = -t \sum_{\langle i,j \rangle,\sigma} \left(c^{\dagger}_{i,\sigma} c_{j,\sigma} + c^{\dagger}_{j,\sigma} c_{i,\sigma} \right) + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$

strong interaction term → Mott insulator

perturbative hopping term → anti-ferromagnetism

- $H_t = \sum_{\sigma} \left[d^{\dagger}_{n,\sigma} F_{n,m} d_{m,\sigma} + d^{\dagger}_{m,\sigma} F_{m,n} d_{n,\sigma} \right] \Rightarrow$ perturbative

2. Interaction Coefficient

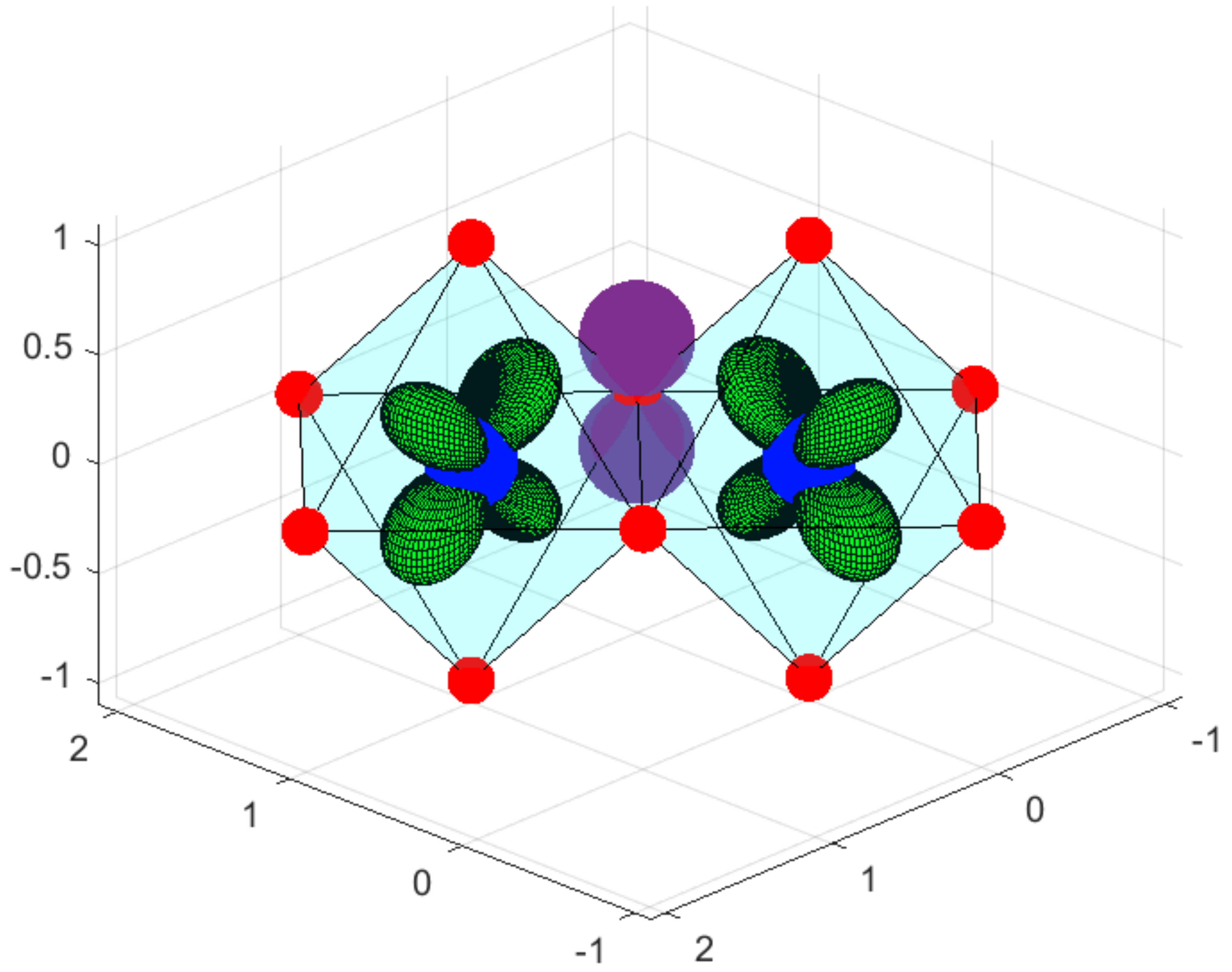
Mediated Hopping

- hopping via p_z-orbital is allowed to t_2-hopping

- mediated hopping is dominant

- preference to specific direction

- $\Rightarrow$ direction dependent hopping



2. Interaction Coefficients

Interaction Coefficients

Heisenberg Interaction : $J = \frac{4}{27}\frac{(2t_1 + t_3)^2}{U + 2J_H} + \frac{8}{27}\frac{(t_1 - t_3)^2}{U - J_H} + \frac{8}{9}\frac{(t_1^2 2t_1 t_3)}{U - 3J_H}$

Kitaev Interaction : $K = \frac{4}{9}\frac{3t_2^2 - (t_1 - t_3)^2}{U - J_H} + \frac{4}{9}\frac{(t_1 - t_3)^2 - 3t_2^2}{U - 3J_H}$

•

Other interaction : $\Gamma = \frac{16J_H}{9}\frac{t_2(t_1 - t_3)}{(U - 3J_H)(U - J_H)}$

- $t_1 = t_3 = 0$ limit $\Rightarrow$ only Kitaev interaction

4. External Field Effect

1. Dzyaloshinskii-Moriya Interaction

Dzyaloshinskii-Moriya Term

- Dzyaloshinskii-Moriya interaction : $H_{DM} = \overrightarrow{D} \cdot (\vec{S}_n \times \vec{S}_m)$

$\Rightarrow$ result of the inversion symmetry breaking

$\Rightarrow$ induced by the external electric filed

- origin of DM interaction = hopping change induced by electric field

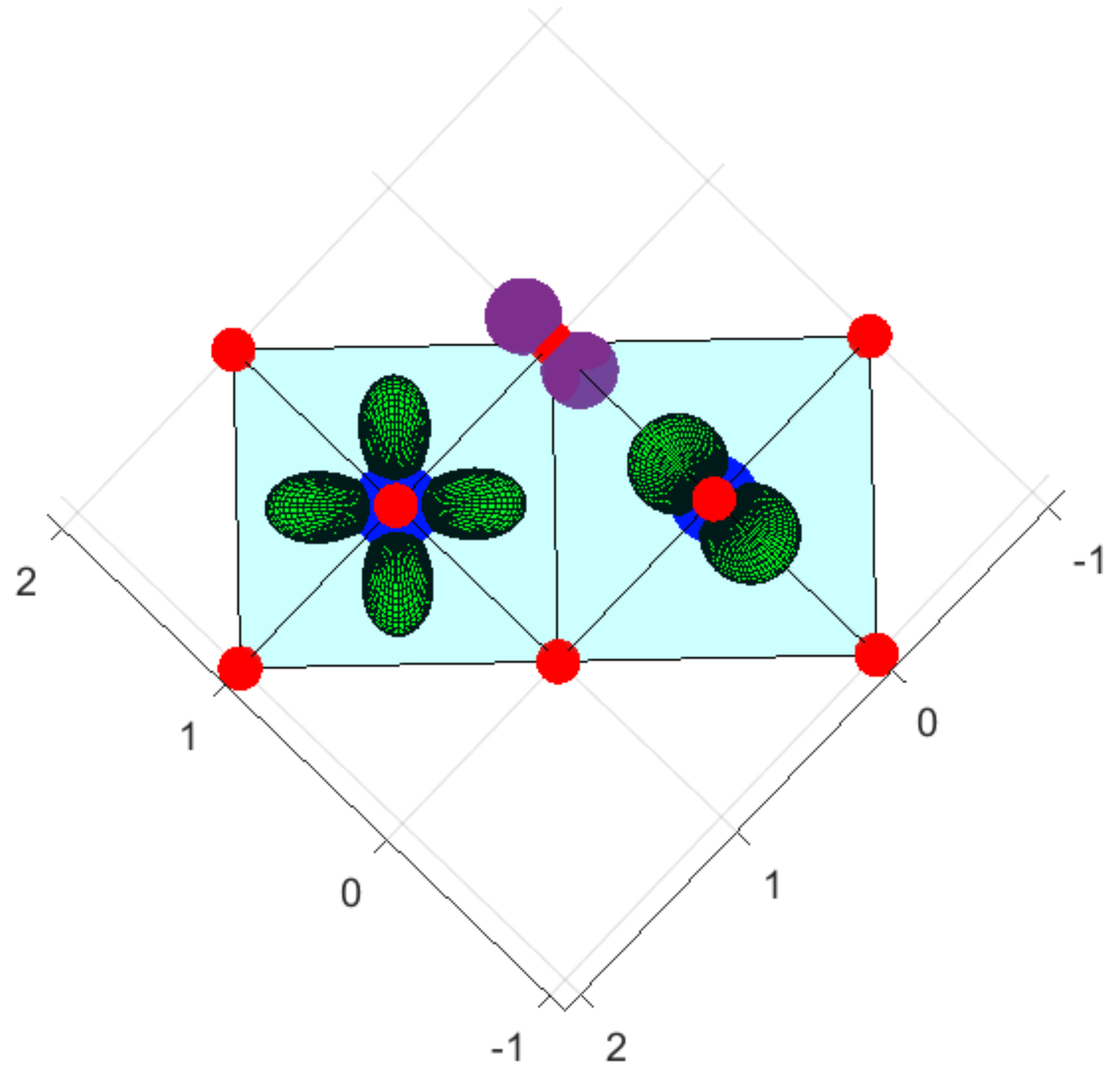
2. Electric Field Effect

Modified Model

- external electric field $\Rightarrow$ distorting orbitals

  $\Rightarrow$ forbidden hopping term

  $\Rightarrow$ t_4-hopping



- hopping matrix : $F_{n,m} = \begin{pmatrix} 0 & t_2 & -t_4 \\ t_2 & 0 & -t_4 \\ t_4 & t_4 & 0 \end{pmatrix}$

- $d_x \rightarrow p_y$ and $d_y \rightarrow p_x$ hopping are allowed by out-of-plane electric fields

2. External Electric Field

Interaction Coefficient

- Dzyaloshinskii-Moriya coefficients
- $D_x = -D_y = -\frac{8}{9}\left[\frac{1}{U-3J_H} - \frac{1}{U-J_H}\right] t_2 t_4$ / $D_z = 0$

- other interaction coefficients
- $$J = \frac{8}{9}\frac{t_4^2}{(U-3J_H)(U-J_H)}$$
  $$K = -\frac{32}{27}\frac{t_4^2}{U+2J_H} + \frac{4}{3}\frac{(t_2^2-t_4^2)}{U-J_H} - \frac{4}{9}\frac{(3t_2^2+5t_4^2)}{U-3J_H}$$
  $$\Gamma = -\frac{32}{27}\frac{t_4^2}{U+2J_H} - \frac{4}{3}\frac{t_4^2}{U-J_H} - \frac{20}{9}\frac{t_4^2}{U-3J_H}$$

3. Conclusion
Conclusion

- external electric field $\Rightarrow$ Dzyloshinskii-Moriya interaction
- $\exists\ t_4$-dependent interaction $\Rightarrow$ result of inversion symmetry breaking
- measuring the strength of the Dzyloshinskii-Moriya intercation

$\Rightarrow$ evidence of the stable Kitaev spin liquid phase