**Title:** Microscopic Roadmap to a Yao-Lee Spin-Orbital Liquid **Speakers:** Hae-Young Kee **Collection/Series:** Quantum Matter **Subject:** Condensed Matter **Date:** November 12, 2024 - 3:30 PM **URL:** https://pirsa.org/24110069

## **Abstract:**

The exactly solvable spin-1/2 Kitaev model on a honeycomb lattice has drawn significant interest, as it offers a pathway to realizing the long-sought after quantum spin liquid. Building upon the Kitaev model, Yao and Lee introduced another exactly solvable model on an unusual star lattice featuring non-abelian spinons. The additional pseudospin degrees of freedom in this model could provide greater stability against perturbations, making this model appealing. However, a mechanism to realize such an interaction in a standard honeycomb lattice remains unknown. I will present a microscopic theory to obtain the Yao-Lee model on a honeycomb lattice by utilizing strong spin-orbit coupling of anions edge-shared between two eg ions in the exchange processes. This mechanism leads to the desired bond-dependent interaction among spins rather than orbitals, unique to our model, implying that the orbitals fractionalize into gapless Majorana fermions and fermionic octupolar excitations emerge. Since the conventional Kugel-Khomskii interaction also appears, the phase diagram including these interactions using classical Monte Carlo simulations and exact diagonalization techniques will be presented. Several open questions will be also discussed.

# Microscopic Roadmap to Yao-Lee Spin-Orbital Liquid & Open Questions

Hae-Young Kee University of Toronto









**NSERC** 

**CRSNG** 

Perimeter Institute, Waterloo, Nov. 12, 2024

# **Quantum Spin Liquids**



## Exchange Interaction frustration

### example of bond-dependent interactions





 $|\xi\rangle \in \mathcal{M}$  if and only if  $D|\xi\rangle = |\xi\rangle$ , where  $D = b^x b^y b^z c$ . : physical subspace



Kitaev quantum spin liquid: emergent particles - Majorana fermion and vortices

# **Generic Spin Model in 2D honeycomb**



nearest neighbour: ideal honeycomb

$$
H = \sum_{\gamma \in x, y, z} H^{\gamma},
$$

bond-dep. interactions

$$
H^z = \sum_{\langle ij \rangle \in z-bond} [K_z S_i^z S_j^z + \Gamma_z (S_i^x S_j^y + S_i^y S_j^x)] + J \mathbf{S}_i \cdot \mathbf{S}_j
$$

 $H^x = H^z(x \to y \to z \to x)$ 

G. Jackeli & G. Khaliulin, PRL (2009); J. Rau, E. Lee, HYK, PRL (2014)



Kitaev spin liquid is fragile under other interactions

## Candidates: layered quasi-2D honeycomb with SOC





Iridium oxides:  $A_2$ Ir $O_3$ 

Y. Singh, et al, PRB 82, 064412 (2010); PRL 108, 127203 (2012);....

alpha-RuCl<sub>3</sub>

K. Plumb,... HYK, Y-J. Kim, PRB 90 041112(R) (2014); ...

All candidates: Magnetic ordering at low T

non-Kitaev interactions are present

I. Rousochatzakis, N. Perkins, Q. Luo, HYK, Reports on Progress in Physics (2024)

# Candidates: layered quasi-2D honeycomb with SOC



Iridium oxides:  $A_2$ IrO<sub>3</sub>

Y. Singh, et al, PRB 82, 064412 (2010); PRL 108, 127203 (2012);....



K. Plumb,... HYK, Y-J. Kim, PRB 90 041112(R) (2014); ...

All candidates: Magnetic ordering at low T

Kitaev materials: Kitaev interaction is dominant! but small other interactions move it away from the Kitaev spin liquid

I. Rousochatzakis, N. Perkins, Q. Luo, HYK, Reports on Progress in Physics (2024)

# more stable Quantum Spin Liquids?

# **Another exactly solvable model: Flavored Kitaev; Yao-Lee model**



Fermionic Magnons, Non-Abelian Spinons, and the Spin Quantum Hall Effect from an Exactly Solvable Spin-1/2 Kitaev Model with SU(2) Symmetry

Hong Yao and Dung-Hai Lee



Star lattice (decorated honeycomb lattice)

$$
H = J \sum_{i} S_{i}^{2} + \sum_{\lambda-\text{link}\langle ij \rangle} J_{\lambda} [\tau_{i}^{\lambda} \tau_{j}^{\lambda}][S_{i} \cdot S_{j}],
$$
  

$$
J \gg J_{\lambda}
$$
  

$$
H = \frac{1}{4} \sum_{\lambda-\text{link}\langle ij \rangle} J_{\lambda} [\tau_{i}^{\lambda} \tau_{j}^{\lambda}][\vec{\sigma}_{i} \cdot \vec{\sigma}_{j}],
$$
  
Pseudospin & spin

$$
H = J \sum_{i} \mathbf{S}_{i}^{2} + \sum_{\lambda-\text{link}\langle ij\rangle} J_{\lambda} [\tau_{i}^{\lambda} \tau_{j}^{\lambda}] [\mathbf{S}_{i} \cdot \mathbf{S}_{j}],
$$
  
\nIntractriangle  
\n
$$
\tau_{i}^{x} = 2(\mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2} + 1/4)
$$
  
\n
$$
\tau_{i}^{y} = 2(\mathbf{S}_{i,1} \cdot \mathbf{S}_{i,3} - \mathbf{S}_{i,2} \cdot \mathbf{S}_{i,3})/\sqrt{3}
$$
  
\n
$$
\tau_{i}^{z} = 4\mathbf{S}_{i,1} \cdot (\mathbf{S}_{i,2} \times \mathbf{S}_{i,3})/\sqrt{3}
$$
  
\n
$$
[\mathbf{S}_{i}^{2}, \mathbf{S}_{j}] = 0
$$
  
\n
$$
[\tau_{i}^{\alpha}, \tau_{i}^{\beta}] = 2i\epsilon^{\alpha\beta\gamma}\tau_{i}^{\gamma}
$$
  
\n
$$
[\mathbf{S}_{i}^{2}, \tau_{j}^{\lambda}] = 0
$$

$$
\mathbf{S}_{i} = \mathbf{S}_{i,1} + \mathbf{S}_{i,2} + \mathbf{S}_{i,3}
$$

$$
[\mathbf{S}_{i}^{2}, \mathbf{S}_{j}] = 0
$$

$$
[\mathbf{S}_{i}^{2}, \tau_{j}^{\lambda}] = 0
$$



**Star lattice** 

$$
J \gg J_{\lambda} \qquad \qquad H = \frac{1}{4} \sum_{\lambda-\text{link}\langle ij \rangle} J_{\lambda} \left[ \tau_{i}^{\lambda} \tau_{j}^{\lambda} \right] \left[ \vec{\sigma}_{i} \cdot \vec{\sigma}_{j} \right],
$$
 Pseudospin & spin

 $\tau^x_i$ 

 $\tau_i^y$ 

 $\tau^z_i$ 

 $H = \frac{1}{4} \sum_{\lambda \text{-link}(i)} J_{\lambda} [\tau_i^{\lambda} \tau_j^{\lambda}] [\vec{\sigma}_i \cdot \vec{\sigma}_j],$  $\sigma_i^{\alpha} \tau_i^{\beta} = i c_i^{\alpha} d_i^{\beta}, \qquad \sigma_i^{\alpha} = -\frac{\epsilon^{\alpha \beta \gamma}}{2} i c_i^{\beta} c_i^{\gamma},$  $\tau_i^{\alpha} = -\frac{\epsilon^{\alpha\beta\gamma}}{2}i d_i^{\beta} d_i^{\gamma},$  $D_i|\Psi\rangle_{\text{phys}} = |\Psi\rangle_{\text{phys}}, \quad \forall i,$  $D_i = -ic_i^x c_i^y c_i^z d_i^x d_i^y d_i^z$ .

$$
\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} u_{ij} [ic_i^x c_j^x + i c_i^y c_j^y + i c_i^z c_j^z], \quad J_{ij} = J_{\lambda}/4
$$

$$
u_{ij} = -i d_i^{\lambda} d_j^{\lambda}
$$

$$
[u_{ij}, \mathcal{H}] = 0 \qquad [u_{ij}, u_{i'j'}] = 0
$$

Z2 gauge transformation:

 $c_i^{\alpha} \rightarrow \Lambda_i c_i^{\alpha}$  and  $u_{ij} \rightarrow \Lambda_i u_{ij} \Lambda_j$ ,  $\Lambda_i = \pm 1$ .

GS has 0 flux

3 types of Majorana fermions couple with Z2 gauge field

When TRS is broken: two localized  $S_z = 1/2$  spinons occur by creating two vortex excitations



### More stable to some perturbations than original Kitaev model

PHYSICAL REVIEW LETTERS 125, 257202 (2020)

#### Fractionalized Fermionic Ouantum Criticality in Spin-Orbital Mott Insulators

Urban F. P. Seifert, <sup>1</sup> Xiao-Yu Dong, <sup>2</sup> Sreejith Chulliparambil<sup>o</sup>,<sup>1,3</sup> Matthias Vojta, <sup>1</sup> Hong-Hao Tu<sup>o</sup>,<sup>1</sup> and Lukas Janssen<sup>o</sup><sup>1</sup>



Exact deconfined gauge structures in the higher-spin Yao-Lee model: a quantum spin-orbital liquid with spin fractionalization and non-Abelian anyons

> Zhengzhi Wu,\* Jing-Yun Zhang,\* and Hong Yao<sup>†</sup> Institute for Advanced Study, Tsinghua University, Beijing 100084, China (Dated: April 12, 2024)

### Topological transitions in the Yao-Lee spin-orbital model and effects of site disorder

Vladislav Poliakov, <sup>1,\*</sup> Wen-Han Kao, <sup>2,\*</sup> and Natalia B. Perkins<sup>2,†</sup>

<sup>1</sup>Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA  $2$ School of Physics and Astronomy, University of Minnesota, Minneapolis, MN 55455, USA

#### **ARTICLE OPEN**

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# Kitaev spin-orbital bilayers and their moiré superlattices

Emilian Marius Nica  $\mathbb{D}^{1,2}$ <sup>52</sup>, Muhammad Akram<sup>1,3</sup>, Aayush Vijayvargia<sup>1</sup>, Roderich Moessner<sup>4</sup> and Onur Erten<sup>1</sup>

#### PHYSICAL REVIEW B 102, 201111(R) (2020)

**Rapid Communications** 

#### Microscopic models for Kitaev's sixteenfold way of anyon theories

Sreejith Chulliparambil  $\bullet$ ,<sup>1,2</sup> Urban F. P. Seifert,<sup>1</sup> Matthias Vojta,<sup>1</sup> Lukas Janssen  $\bullet$ ,<sup>1</sup> and Hong-Hao Tu $\bullet$ <sup>1,\*</sup> <sup>1</sup>Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany <sup>2</sup>Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany

### Maybe Yao-Lee model from spin &orbital degree of freedom?

### Typically, we have the Kugel-Khomskii Model



There is no angular momentum change nor spin change during the exchange processes: no bond-dependence

## Kugel-Khomskii SU(4) model on honeycomb lattice

$$
\mathcal{H} = \sum_{\langle i,j \rangle} \Biggl( 2\mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{2} \Biggr) \Biggl( 2\mathbf{T}_i \cdot \mathbf{T}_j + \frac{1}{2} \Biggr)
$$
  

$$
|\bullet\rangle = |\uparrow a\rangle, |\bullet\rangle = |\downarrow a\rangle, |\bullet\rangle = |\uparrow b\rangle, |\bullet\rangle = |\downarrow b\rangle
$$





P. Corboz, et al, PRX 2, 041013 (2012)



 $S_{\alpha}^{\beta} = |\alpha\rangle\langle\beta|$  are the generators of SU(4)

Algebraic spin-orbital (SO) liquids



Figure credit: J. Rau, E. Lee, HYK, ARCMP (2016)

## **Edge sharing lattice structure**





**z-bond:**  $H_K = KS_i^z S_j^z$  $K \propto -\frac{t_0^2(J_H)}{U^2} \propto t_0^2(\frac{1}{U-J_H}-\frac{1}{U-3J_H})$  With only p-orbital mediate (interorbital) hopping



bond-dependent Ising interaction is due to orbital that bridges pseudospin interaction via SOC!

Kitaev Exchange  $\sum S_i^{\gamma} S_j^{\gamma}$  $K_{\parallel}$  $\langle \overline{\overline{ij}} \rangle \in \gamma$ 

G. Jackeli, G. Khaliullin, Phys. Rev. Lett. 102, 017205 (2009)



**z-bond:**  $H_K = KS_i^z S_j^z$ 

$$
j=\frac{1}{2}
$$

$$
K\propto -\frac{t_0^2(J_H)}{U^2}\propto t_0^2(\frac{1}{U-J_H}-\frac{1}{U-3J_H})
$$

multi-orbital systems with SOC and Hund's coupling

Once we have SOC to generate bond-dependent Kitaev interaction, H reduces to pseudospin interaction like the original Kitaev (or compass model of J operators) model.

Conversely, if we leave the orbital d.o.f., we are back to Kugel-Khomskii model (or compass model), as there is no SOC that bridges the spin interaction?

> How do we generate Yao-Lee interaction, and what are other interactions generated during the exchange the processes?

How do we generate such Yao-Lee-like interaction in honeycomb lattice?

Let us consider two orbitals which are degenerate such as d<sup>7</sup> or d<sup>9</sup>  $\bullet$ 





where  $T_i$  and  $S_i$  are orbital and spin degrees of freedom



## Consider direct exchange between nearest neighbour M sites



$$
t_a \approx t_b \implies H_{\text{eff}} = \frac{t^2}{U} \sum_{\langle ij \rangle} \left( S_i \cdot S_j + \frac{1}{4} \right) \left( T_i \cdot T_j + \frac{1}{4} \right)
$$

Kugel-Khomskii model: no bond-dependence - due to missing spin-orbit coupling!

Consider interorbital hopping that changes the angular momentum



Consider an intermediate ligand (A site, p<sup>6</sup> configuration) with strong SOC



Hopping between M sites through ligands becomes spin-dependent!

$$
t_{\text{eff}} = \frac{t_{pd\sigma}^2}{4\sqrt{3}} \left( \frac{1}{\Delta_{pd} - \frac{\lambda}{2}} - \frac{1}{\Delta_{pd} + \lambda} \right)
$$



$$
H_{\text{eff}} = -J \sum_{\langle ij \rangle_{\gamma}} \left[ \left( \mathbf{S}_{i} \cdot \mathbf{S}_{j} - 2S_{i}^{\gamma} S_{j}^{\gamma} - \frac{1}{4} \right) \otimes \left( \mathbf{T}_{i} \cdot \mathbf{T}_{j} - 2T_{i}^{y} T_{j}^{y} - \frac{1}{4} \right) \right], \ J \propto \frac{t_{\text{eff}}^{2}}{U}
$$

$$
T_{i}^{x} \to \tilde{T}_{i}^{x}, \quad T_{i}^{y} \to (-1)^{i} \tilde{T}_{i}^{y}, \quad T_{i}^{z} \to \tilde{T}_{i}^{z}
$$

$$
H_{\text{eff}} = -J \sum_{\langle ij \rangle_{\gamma}} \left[ \left( \mathbf{S}_{i} \cdot \mathbf{S}_{j} - 2S_{i}^{\gamma} S_{j}^{\gamma} - \frac{1}{4} \right) \otimes \left( \tilde{\mathbf{T}}_{i} \cdot \tilde{\mathbf{T}}_{j} - \frac{1}{4} \right) \right]
$$
**Yao-Lee interaction**



$$
H_{\mathsf{KK}} = \frac{t^2}{U} \sum_{\langle ij \rangle} \left( S_i \cdot S_j + \frac{1}{4} \right) \left( T_i \cdot T_j + \frac{1}{4} \right)
$$

$$
H_{\text{eff}} = -J \sum_{\langle ij \rangle_{\gamma}} \left[ \left( \mathbf{S}_{i} \cdot \mathbf{S}_{j} - 2S_{i}^{\gamma} S_{j}^{\gamma} - \frac{1}{4} \right) \otimes \left( \tilde{\mathbf{T}}_{i} \cdot \tilde{\mathbf{T}}_{j} - \frac{1}{4} \right) \right]
$$

Introduce  $\alpha$  and  $\ \beta$  and investigate the phase diagram

$$
H_{\text{model}} = -\sum_{\langle ij \rangle_{\gamma}} \left[ \left( \alpha \mathbf{S}_{i} \cdot \mathbf{S}_{j} - 2S_{i}^{\gamma} S_{j}^{\gamma} - \beta \right) \otimes \left( \tilde{\mathbf{T}}_{i} \cdot \tilde{\mathbf{T}}_{j} - \beta \right) \right].
$$



Yao-Lee limit

$$
H_{\text{model}} = -\sum_{\langle ij \rangle_{\gamma}} \left[ \left( \alpha \mathbf{S}_{i} \cdot \mathbf{S}_{j} - 2S_{i}^{\gamma} S_{j}^{\gamma} - \beta \right) \otimes \left( \tilde{\mathbf{T}}_{i} \cdot \tilde{\mathbf{T}}_{j} - \beta \right) \right].
$$

 $S(Q) = \frac{1}{N^2} \sum_{ij} \langle (S_i \cdot S_j) \rangle e^{-iQ \cdot (r_i - r_j)}$ 

 $T(Q) = \frac{1}{N^2} \sum_{ij} \langle (T_i \cdot T_j) \rangle e^{-iQ \cdot (r_i - r_j)}$ 

 $ST(Q) = \frac{1}{N^2} \sum_{ij} \left\langle (S_i \cdot S_j) (T_i \cdot T_j) \right\rangle e^{-iQ \cdot (r_i - r_j)}$ 



Disordered in ST(Q)

$$
H_{\text{model}} = -\sum_{\langle ij \rangle_{\gamma}} \left[ \left( \alpha \mathbf{S}_{i} \cdot \mathbf{S}_{j} - 2S_{i}^{\gamma} S_{j}^{\gamma} - \beta \right) \otimes \left( \tilde{\mathbf{T}}_{i} \cdot \tilde{\mathbf{T}}_{j} - \beta \right) \right].
$$



Nematic Paramagnet 1

$$
H_{\text{model}} = -\sum_{\langle ij \rangle_{\gamma}} \biggl[ \biggl( \alpha \mathbf{S}_{i} \cdot \mathbf{S}_{j} - 2 S_{i}^{\gamma} S_{j}^{\gamma} - \beta \biggr) \otimes \biggl( \tilde{\mathbf{T}}_{i} \cdot \tilde{\mathbf{T}}_{j} - \beta \biggr) \biggr].
$$



$$
H_{\text{model}} = -\sum_{\langle ij \rangle_{\gamma}} \left[ \left( \alpha \mathbf{S}_{i} \cdot \mathbf{S}_{j} - 2S_{i}^{\gamma} S_{j}^{\gamma} - \beta \right) \otimes \left( \tilde{\mathbf{T}}_{i} \cdot \tilde{\mathbf{T}}_{j} - \beta \right) \right]
$$



## Exactly solvable point

Define Majorana operators  $S_i^{\alpha} = -\frac{i}{4} \epsilon^{\alpha\beta\gamma} c_i^{\beta} c_i^{\gamma}$  and  $T_i^{\alpha} = -\frac{i}{4} \epsilon^{\alpha\beta\gamma} d_i^{\beta} d_i^{\gamma}$ 

Then when  $\alpha = 0, \ \beta = 0$  defining the fermionic operator  $f_i^y = \frac{1}{\sqrt{2}}(d_i^z - id_i^x)$ 

$$
H = \frac{1}{8} \sum_{\langle ij \rangle} \hat{u}_{ij} \left( 2 \left( i f_{i,y}^\dagger f_{j,y} - i f_{j,y}^\dagger f_{i,z} \right) - i d_i^y d_j^y \right)
$$

The ground state lies in the zero-flux sector by Lieb's theorem

Fermions created by  $f_{i,y}^{\dagger}$ : fermonic octupolar excitation

Since 
$$
T^y = P^T \left( \frac{1}{3\sqrt{5}} O_{xyz} \right) P
$$
, where  $O_{xyz} = \frac{\sqrt{15}}{6} \overline{L_x L_y L_z}$   
of:  $T_x = \frac{1}{2\sqrt{3}} Q_{x^2 - y^2}$   $T_z = \frac{1}{2\sqrt{3}} Q_{3z^2 - y^2}$ 

# Summary

- Provide a microscopic mechanism to obtain a flavoured (Yao-Lee-like) Kitaev interaction on a honeycomb lattice  $\bullet$
- Show certain d<sup>7</sup> (d<sup>9</sup>) compounds lie near swaths of nematic phases engulfing a Quantum Spin-Orbital Liquid (QSOL)  $\bullet$ point
- Revealed interesting features of the QSOL: fractionalized orbitals, octupolar fermionic excitation  $\bullet$



# Open questions

- Nature of transition between two SO liquids  $\bullet$
- Candidate materials  $(Cu^{2+}, Co^{2+}, Ni^{3+}$  surrounded by heavy ions making a honeycomb)  $\bullet$
- Finite size effects; different numerical techniques are needed  $\bullet$
- Effects of other interactions; compass terms are generated in orbital part:  $\bullet$ 
	- if small, they are not going to affect the final result

 $\cdots$ 

# Summary

- Provide a microscopic mechanism to obtain a flavoured (Yao-Lee-like) Kitaev interaction on a honeycomb lattice  $\bullet$
- Show certain d<sup>7</sup> (d<sup>9</sup>) compounds lie near swaths of nematic phases engulfing a Quantum Spin-Orbital Liquid (QSOL)  $\bullet$ point
- Revealed interesting features of the QSOL: fractionalized orbitals, octupolar fermionic excitation  $\bullet$

