Quantum spin ices and topological phases from dipolar-octupolar doublets on the pyrochlore lattice

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Systems we are interested in

▶ Compound with **pyrochlore** networks, *i.e.* pyrochlores, $A_2B_2O_7$ or spinels AB_2O_4.

- $A_2B_2O_7$ and AB_2O_4., B is d^1 or d^3, A is non-magnetic.(FIG.1)
- $A_2B_2O_7$, A is a trivalent rare earth with partially filled 4f shell, B is non-magnetic[1].

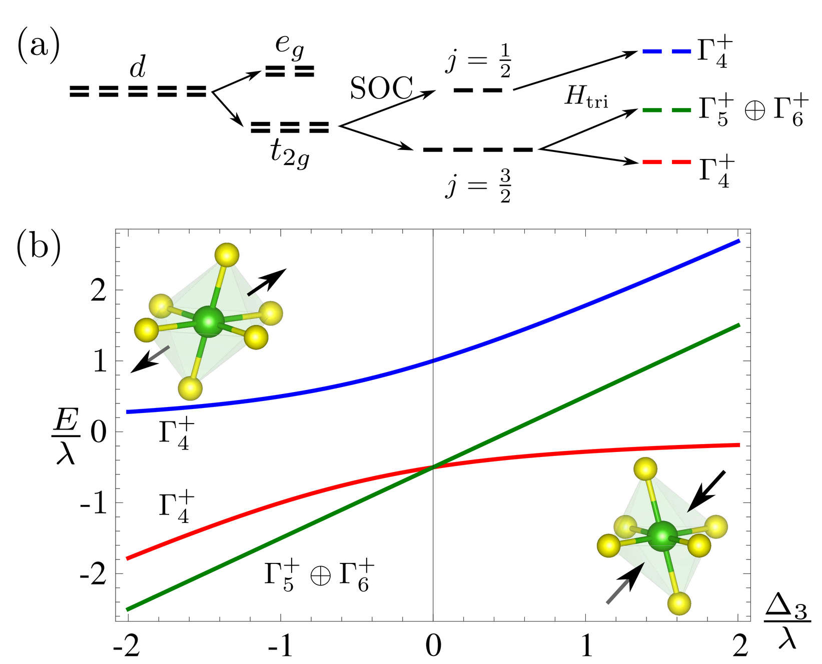

Figure 1: Trigonally distorted crystal field for 5d system.

Motivation/questions

▶ Iridates reveal lots of interesting questions already. However, they are just part of the material with large spin-orbit coupling. How about other 5d transition metal compounds?

▶ System with valence electron configuration $5d^3$ on pyrochlore lattice could also be interesting. The local doublets for $5d^3$ configuration (dipolar-octupolar doublets, DO doublets) transform differently with $5d^5$ configuration. Will different transformation properties of local doublets change the physics? If yes, how?

Pyrochlore network

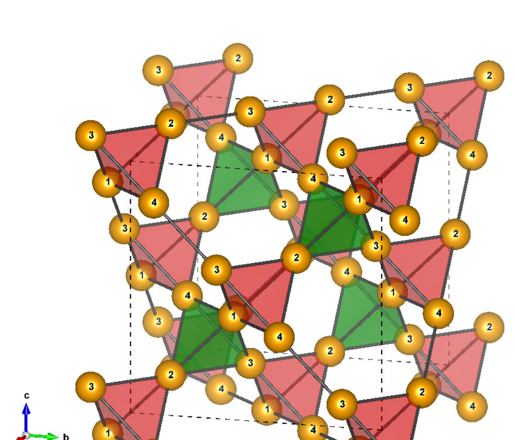

Figure 2: Pyrochlore network

Tight-binding model

$$H_{TB} = \sum_{(\boldsymbol{r},\boldsymbol{r}')} \left[\boldsymbol{c}_{\boldsymbol{r}}^{\dagger} T_{\boldsymbol{r}\boldsymbol{r}'} \boldsymbol{c}_{\boldsymbol{r}} + h.c.\right] \quad (1)$$

▶ For nerest-neighbor case, $T^{nn}_{\boldsymbol{r}\boldsymbol{r}'} = i[t^1_{nn}\sigma^1 + t^3_{nn}\sigma^3]$.→ highly-nested fermi surface: more realistic to consider further hopping.

▶ We construct the symmetry allowed tight-binding model to 4-th nearest-neighbor hopping which is the lowest order that can split the accidental degeneracy at W point.

▶ The D_{3d} site symmetry is generated by a 3-fold rotation C_3, a mirror plane M, and inversion $\mathcal{I}$, with: $C_3 : \tau^\mu \to \tau^\mu$, $M : \tau^{x,z} \to -\tau^{x,z}$, $M : \tau^y \to \tau^y$, and $\mathcal{I} : \tau^\mu \to \tau^\mu$.

Exchange model

Symmetry allowed nearest-neighbor exchange model is $H_{ex} = \sum_{\langle \boldsymbol{r}\boldsymbol{r}'\rangle} J_x \tau^x_{\boldsymbol{r}}\tau^x_{\boldsymbol{r}'} + J_y \tau^y_{\boldsymbol{r}}\tau^y_{\boldsymbol{r}'} + J_z \tau^z_{\boldsymbol{r}}\tau^z_{\boldsymbol{r}'} + J_{xz}(\tau^x_{\boldsymbol{r}}\tau^z_{\boldsymbol{r}'} + \tau^z_{\boldsymbol{r}}\tau^x_{\boldsymbol{r}'})$

▶ Reduce to XYZ model after a global rotation about y-axis in pseudo-spin space

▶ *Dzyaloshinskii-Moriya interaction is forbidden!!*

$$H_{\text{XYZ}} = \sum_{\langle \boldsymbol{r}\boldsymbol{r}'\rangle} \tilde{J}_x \tilde{\tau}^x_{\boldsymbol{r}}\tilde{\tau}^x_{\boldsymbol{r}'} + \tilde{J}_y \tilde{\tau}^y_{\boldsymbol{r}}\tilde{\tau}^y_{\boldsymbol{r}'} + \tilde{J}_z \tilde{\tau}^z_{\boldsymbol{r}}\tilde{\tau}^z_{\boldsymbol{r}'} \quad (2)$$

▶ Comparing with the results of dipolar doublets[2].

▶ Closely related to XXZ model. QSI is robust to arbitrary symmetry breaking perturbations, and thus survives away from the XXZ line.

▶ $E_{\boldsymbol{r}\boldsymbol{r}'} = \tilde{\tau}^z_{\boldsymbol{r}}; e^{iA_{\boldsymbol{r}\boldsymbol{r}'}} = \tilde{\tau}^x_{\boldsymbol{r}} + i\tilde{\tau}^y_{\boldsymbol{r}}$

Important Result

▶ The expected existence of DO doublets on the pyrochlore lattice, and the resulting (surprisingly strong) symmetry constraints on (and simple form of) the tight-binding and spin models that describe many-body physics.

▶ The existence of both dipolar QSI and octupolar QSI phases in the XYZ model obeyed by DO doublets.

Results(I): at itinerant limit

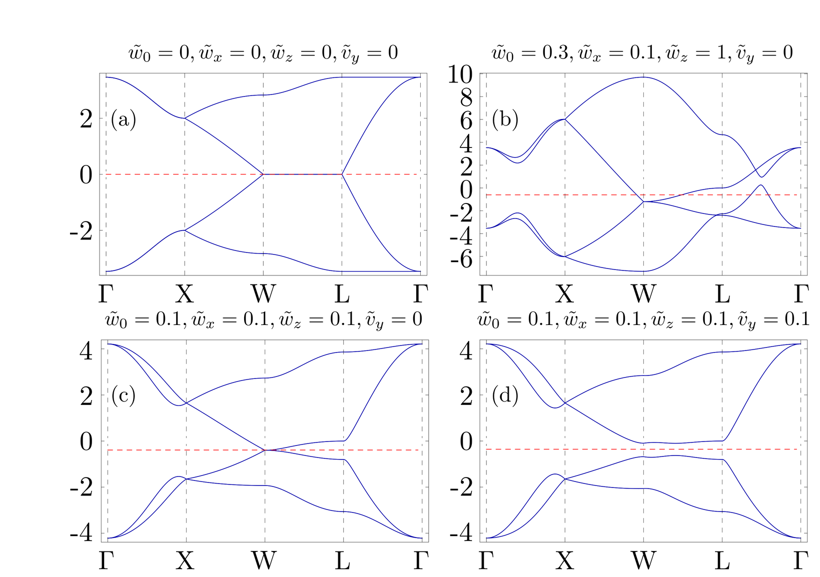

Figure 3: Band structure at different parameters.

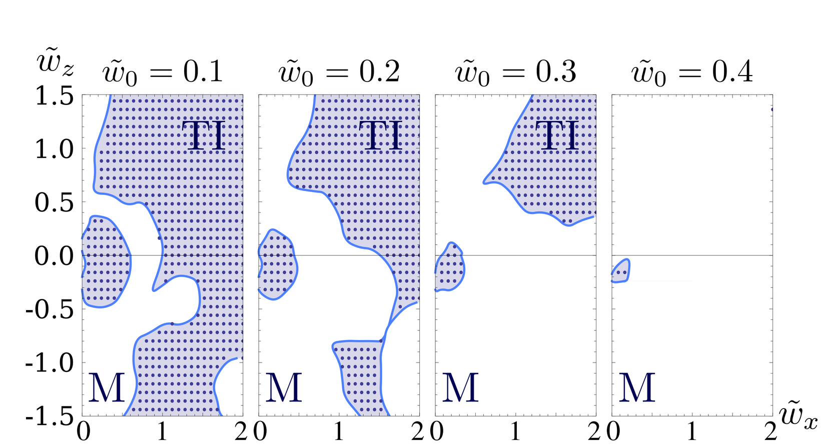

Figure 4: Phase diagram for the tight-binding model.

Results(II):at localized limit

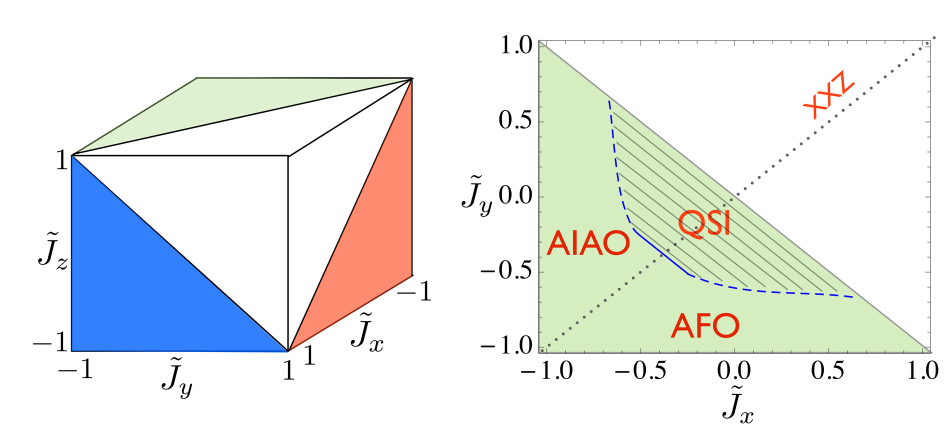

Figure 5: Phase diagram for exchange model

▶ Two distinct SET protected by space group symmetry, dQSI and oQSI.

▶ dQSI(oQSI) phase, so named because the electric field operator $E_{\boldsymbol{r}\boldsymbol{r}'} = \tilde{\tau}^z_{\boldsymbol{r}}(\tilde{\tau}^y_{\boldsymbol{r}}) \to$ dipolar(octupolar).

- Odd under time reversal
- Γ_4^+ (pseudovector) of the O_h point group for dQSI
- Γ_5^+ (neither vector nor pseudovector) of the O_h point group for oQSI

Conclusion

▶ We construct the symmetry allowed models under itinerant limit and localized limit. **DO doublets is highly constrained by space group symmetry, and both models are different with previously studied systems. At itinerant limit, we found topological insulator phase. At localized limit, the model is a *XYZ* model which could support two distinct quantum spin-ice phase protected by space group symmetry.**

Further questions

- Hund's coupling?[3]
- Possible candidates? $Nd_2B_2O_7$, $Nd_2Ir_2O_7$, $CdEr_2Se_4$.
- How to measure it? Both dQSI and oQSI T^3 specific heat from gapless photons; in f-electron realizations, this is expected to be about 1000 times the phonon contribution.
- Equal-time dipolar correlations fall off as r^{-4} in dQSI, but as r^{-8} in oQSI.

References

[1] Jason S. Gardner, Michel J. P. Gingras, and John E. Greedan. *Rev. Mod. Phys.*, 82:53–107, Jan 2010.

[2] Lucile Savary and Leon Balents. *Phys. Rev. Lett.*, 108(3):037202, January 2012.

[3] Yi-Ping Huang, Gang Chen, and Michael Hermele. *Phys. Rev. Lett.*, 112:167203, Apr 2014.

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