Cluster Mott insulators and spin liquids in Mo-based cluster magnets

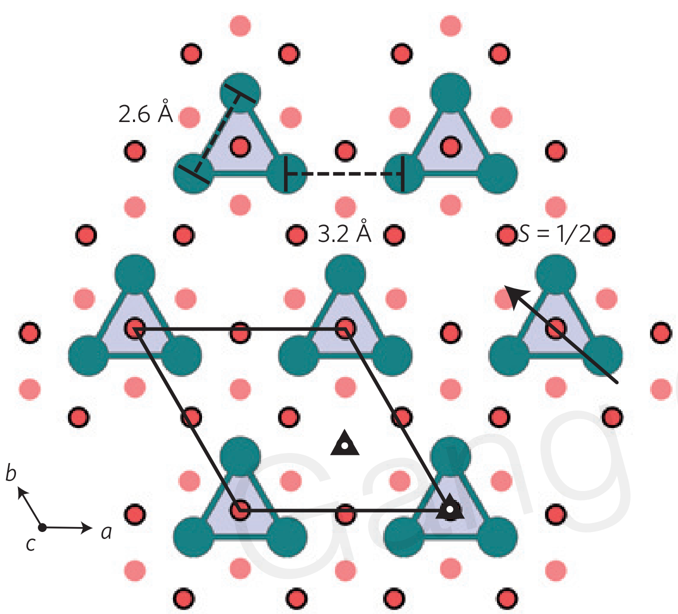
Gang Chen
(Univ of Toronto)

Collaborators: Hae-Young Kee, Yong-Baek Kim

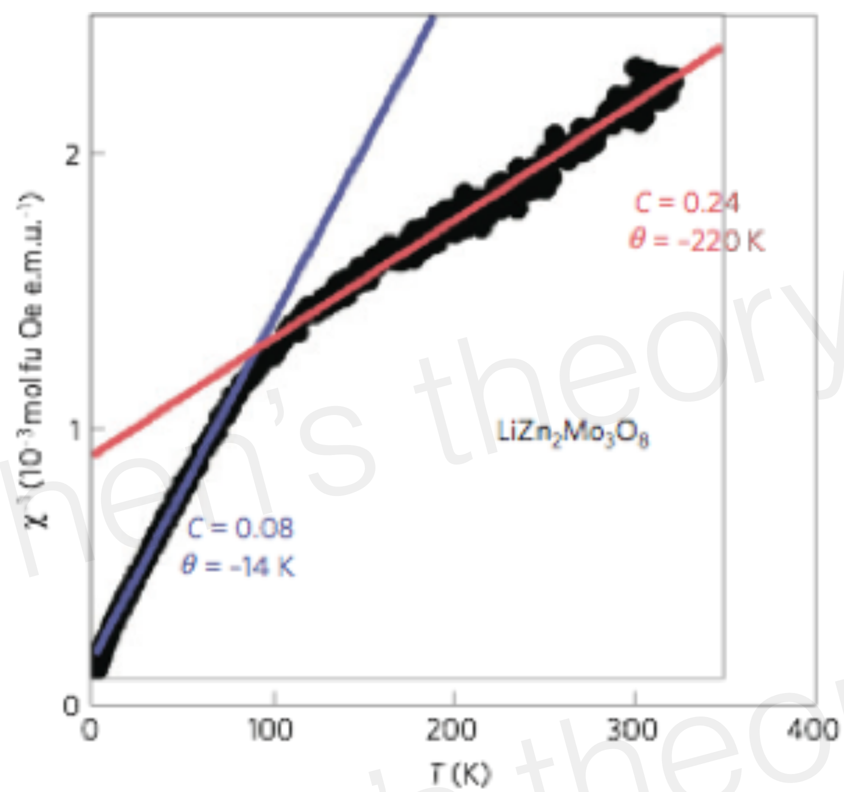
ArXiv 1402.5425 (**Phys. Rev. Lett. 113, 197202 (2014)**)
ArXiv 1408.1963 ????

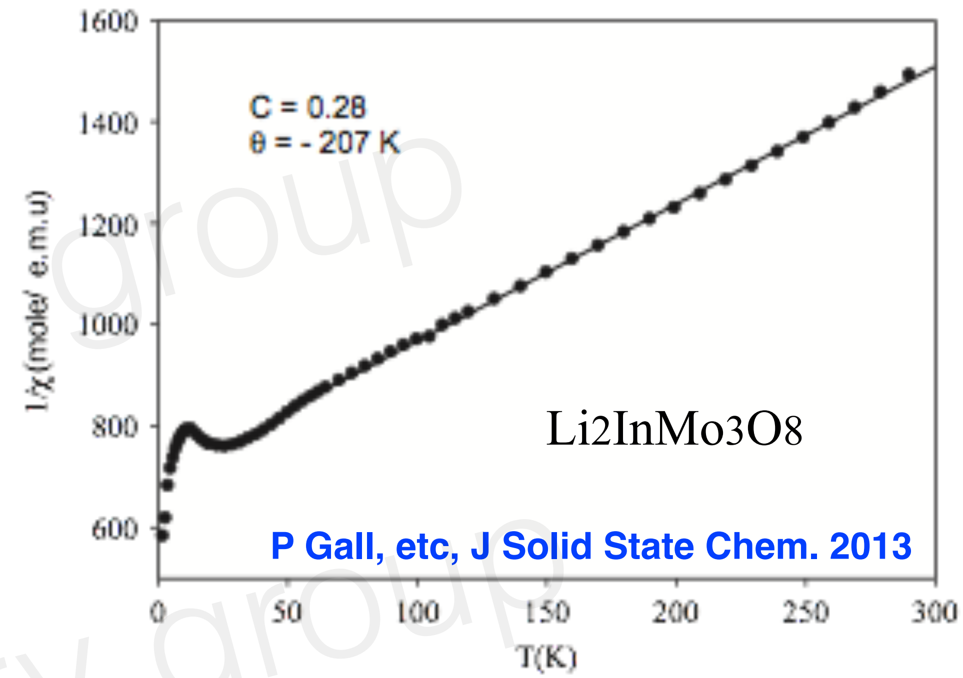
Two Curie-Weiss regimes in $LiZn_2Mo_3O_8$

T. McQueen



Nature Material 2012



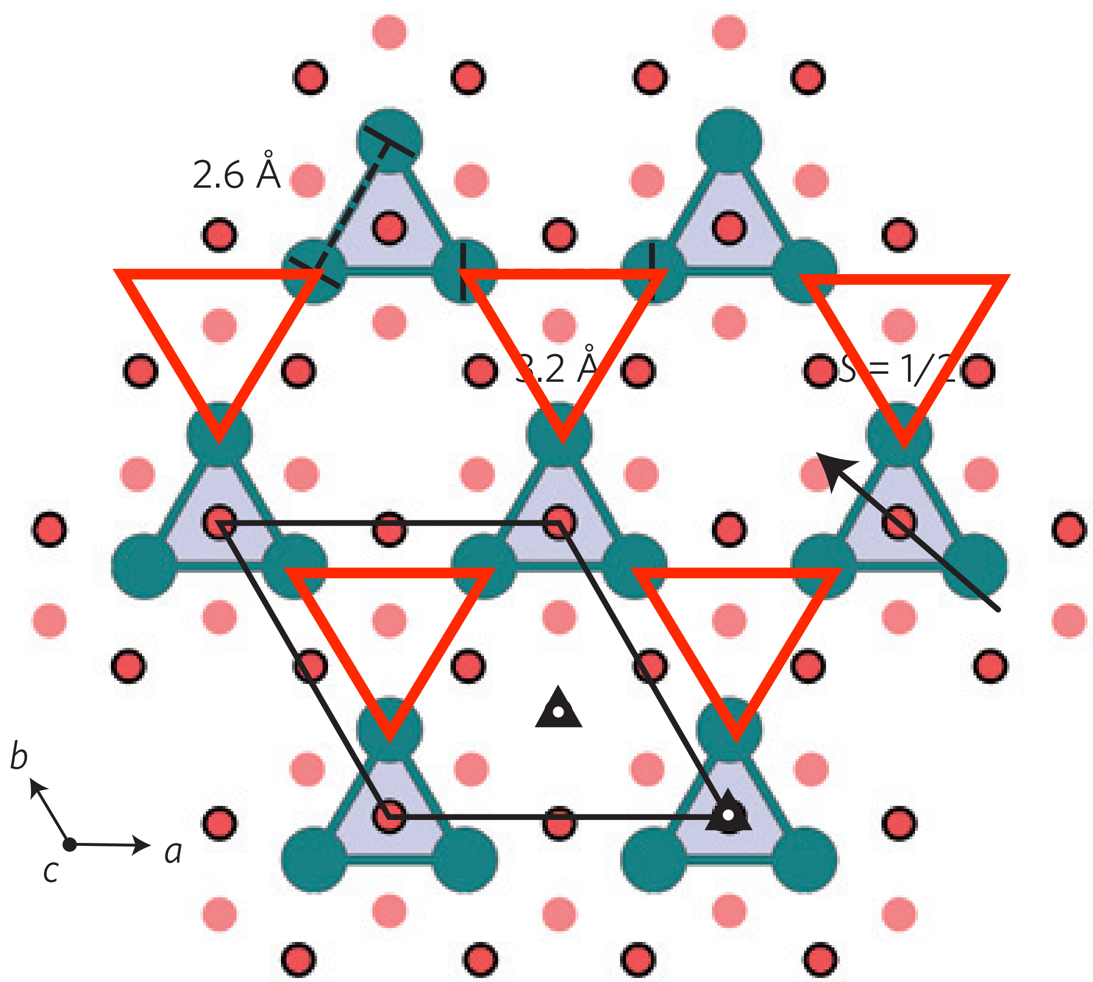


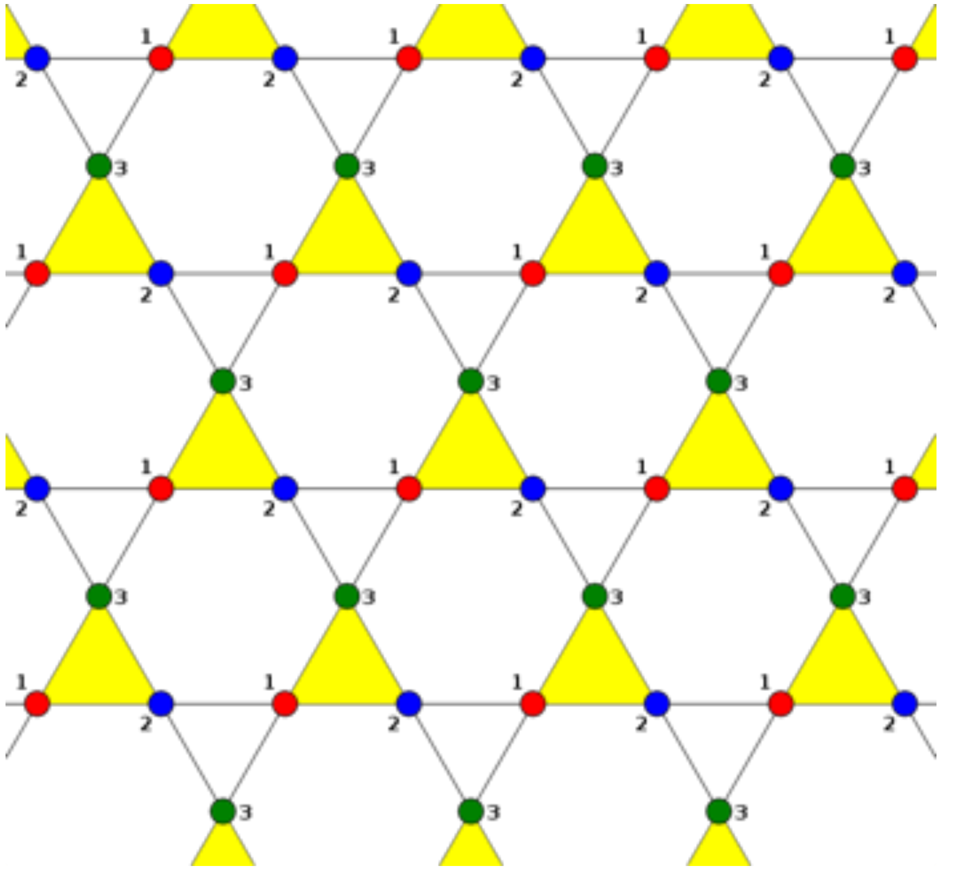
isostructural material

- The result does not fit into our understanding spin-1/2 triangular system.

- Further low-temperature experiments: NMR, muSR, neutron scattering, proposed as a spin liquid candidate.

The Mo structure: anisotropic Kagome



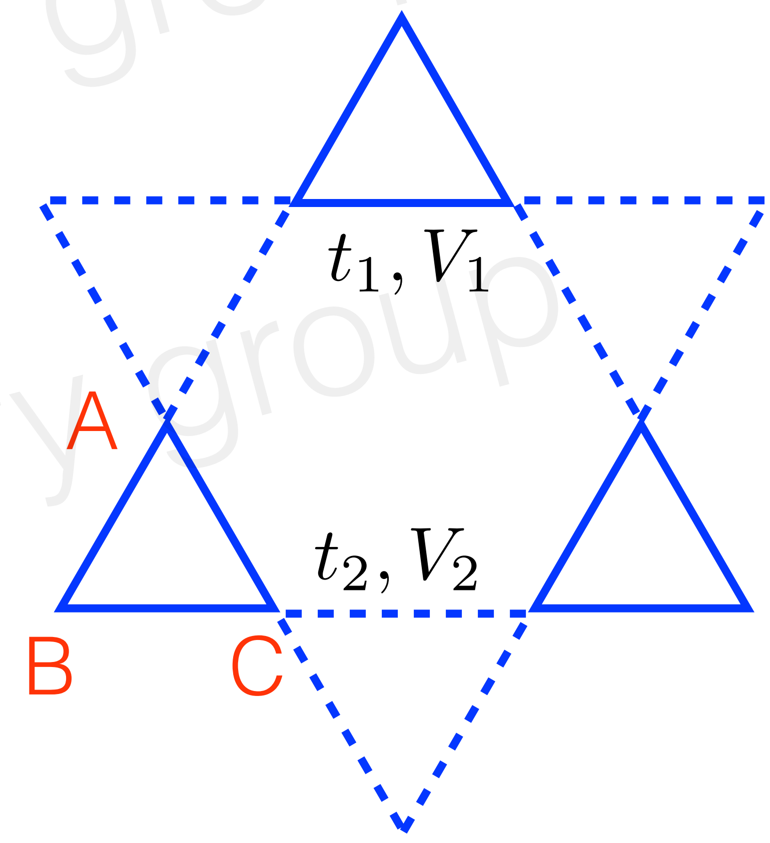


Model

Claim: a single-band extended Hubbard model on an anisotropic Kagome lattice with **1/6 electron filling.**

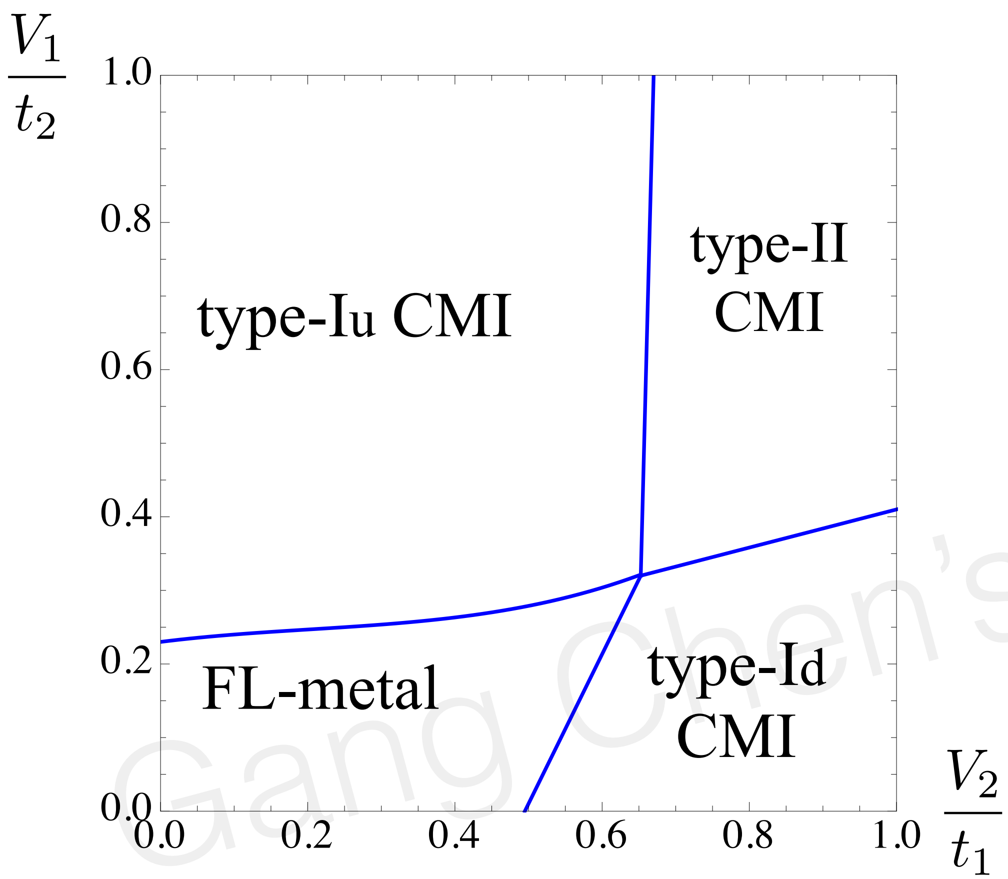
- Minimal model allowed by symmetry [require quantum chemistry understanding]

$$
\begin{aligned}
H = &\sum_{\langle ij \rangle \in \mathrm{u}} [-t_1(c^\dagger_{i\sigma} c_{j\sigma} + h.c.) + V_1 n_i n_j] \\
&+ \sum_{\langle ij \rangle \in \mathrm{d}} [-t_2(c^\dagger_{i\sigma} c_{j\sigma} + h.c.) + V_2 n_i n_j] \\
&+ \sum_i \frac{U}{2}(n_i - \frac{1}{2})^2,
\end{aligned}
$$



* Large U alone **cannot** localize the electron.
* V_1 and V_2 are needed: because it is 4d orbital, and also to localize the electron in the clusters.

Generic phase diagram



spin sector is spin liquid

Here **t1/t2** = 4, no qualitative difference for different **t1/t2**

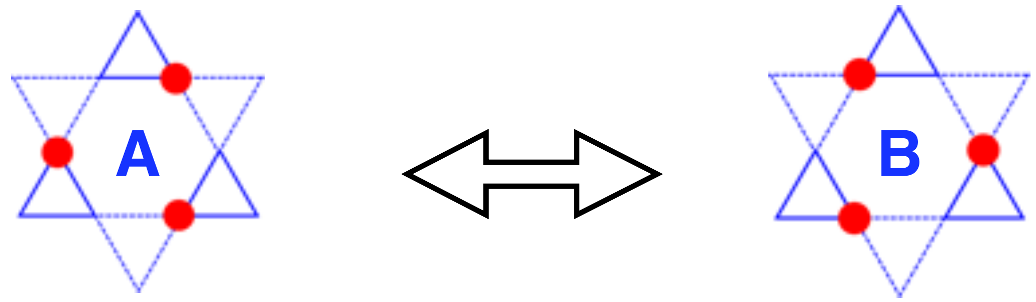
V2 is small, V1 is large

snapshots of electron occupation in type-I CMI

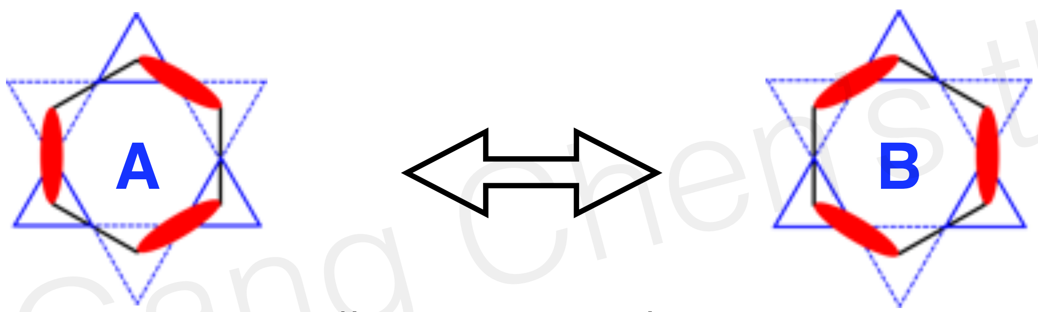
- A "simple" understanding:

* Electrons are localized in **one** type of triangles in type-I CMI;
* Electrons are localized in **both** types of triangles in type-II CMI.

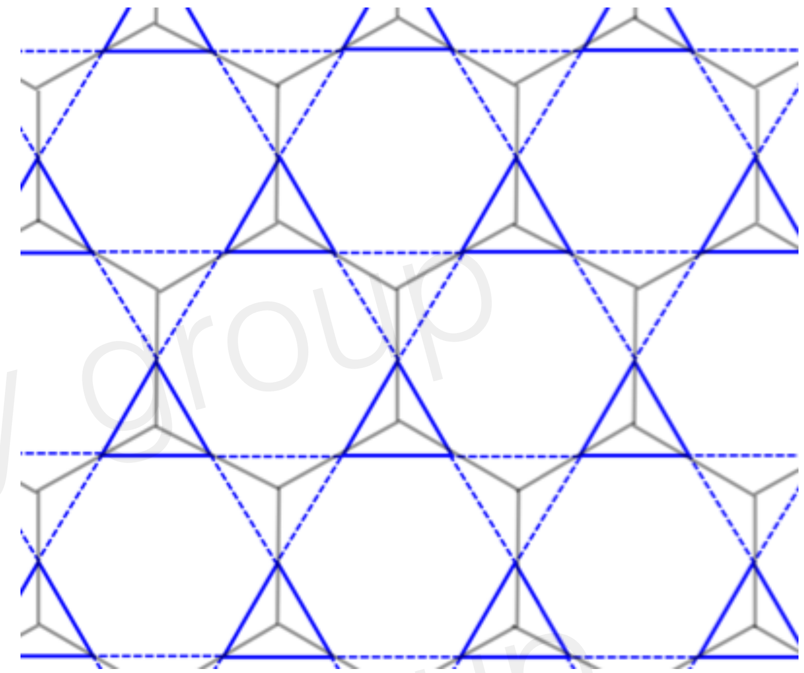
Sub-Mott-gap process: correlated electron motion



3rd order process in type-II CMI

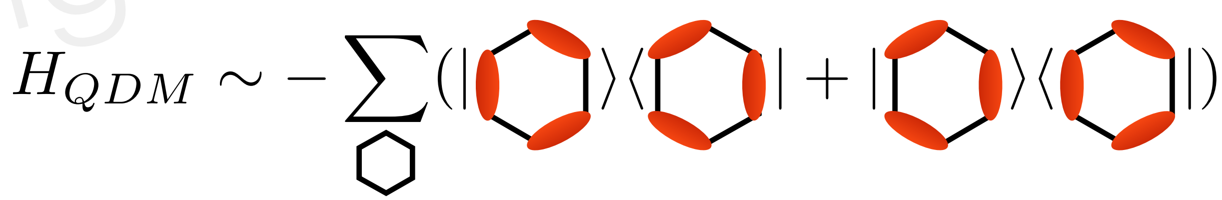


dimer resonating



Dual honeycomb lattice and Kagome lattice

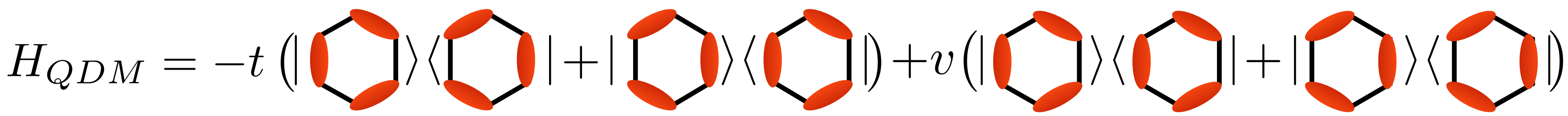
This collective tunnelling process **preserves the center of mass** of 3 electrons !

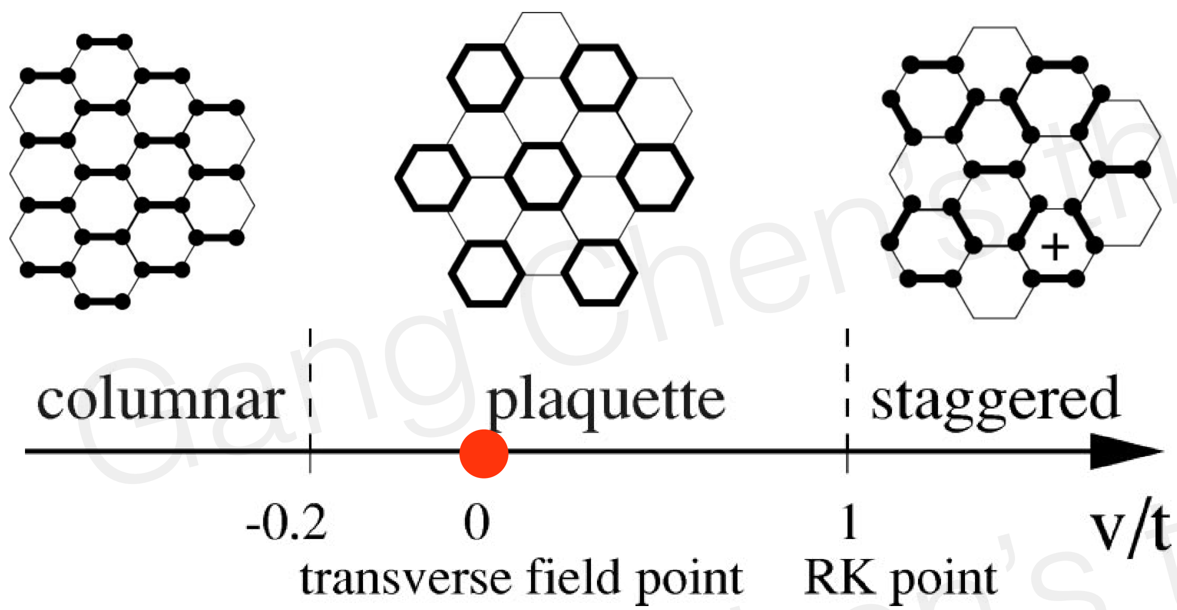


Type-II CMI: plaquette charge order via QDM


R. Moessner S. Sondhi P. Chandra

- A model study in 2001





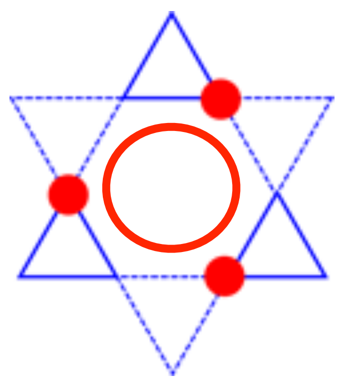
- **plaquette charge order**

- Remarks:

  * The plaquette charge order is a **local charge "RVB"**.
    (This is not Anderson's spin singlet RVB).
  * One may simply view each resonating hexagon as a benzene molecule.
  * It is a collective behaviour of 3 electrons.
  * It is a **quantum** effect.

Charge order reconstructs the spin state

- Spin state reconstruction

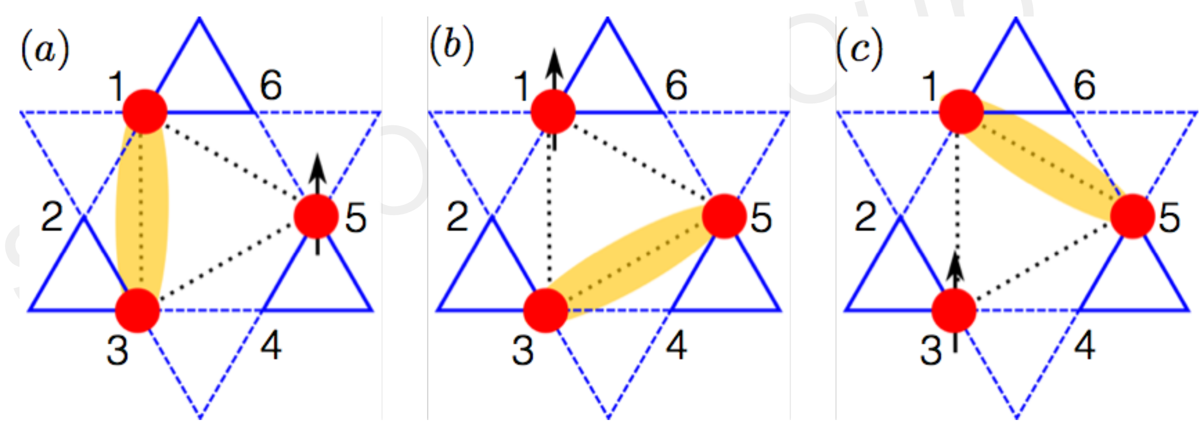


$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = \frac{1}{2} \oplus \frac{1}{2} \oplus \cancel{\frac{3}{2}}$$

K. Kugel

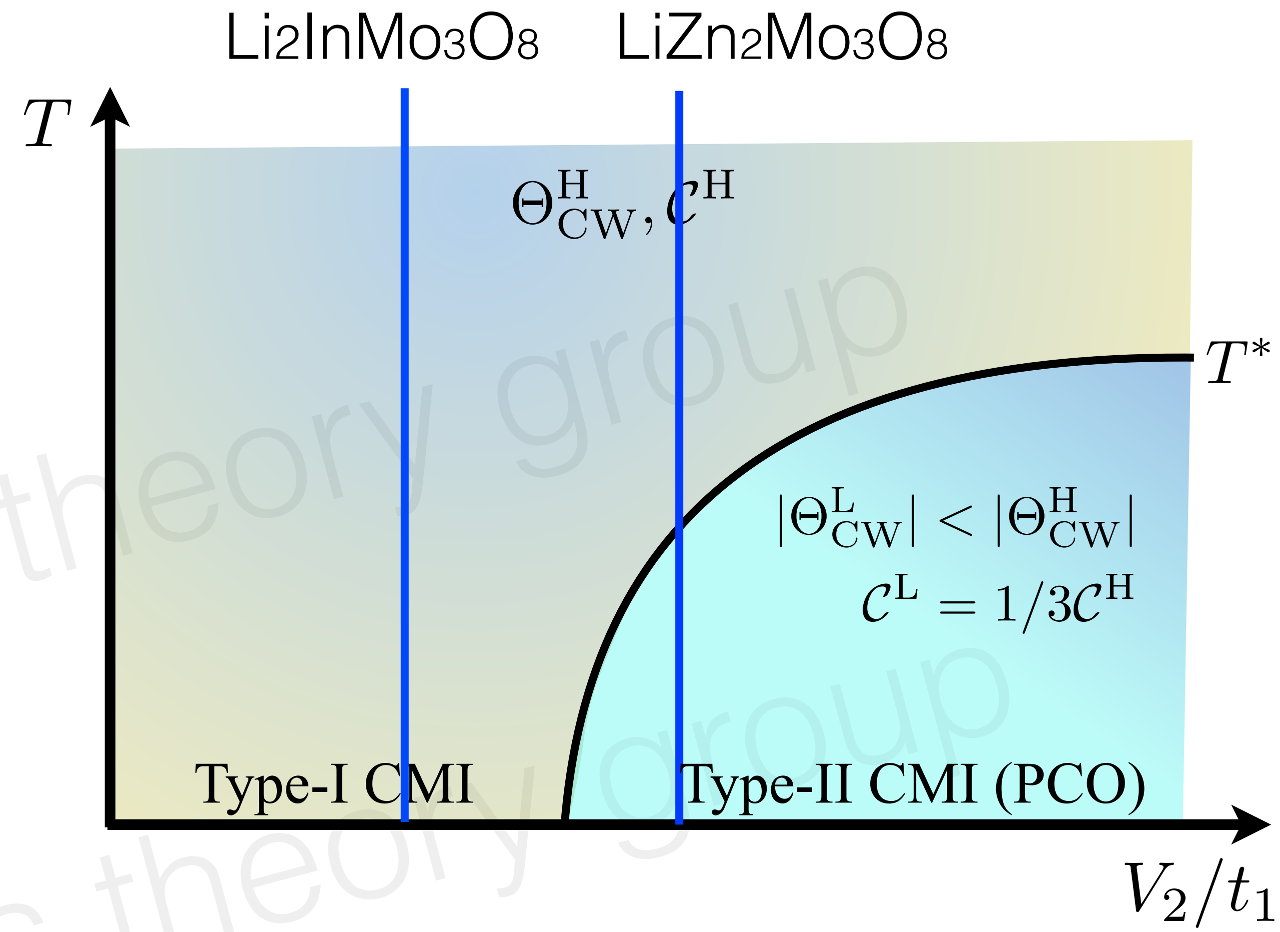
D. Khomskii

The total spin $S_{tot} = 1/2$;
Pseudospin $\mathcal{T} = 1/2$, nonmagnetic



An effective Kugel-Khomskii model on the **emergent triangular lattice**

Explanation for fractional spin susceptibility at finite temperatures



type-II CMI (PCO)

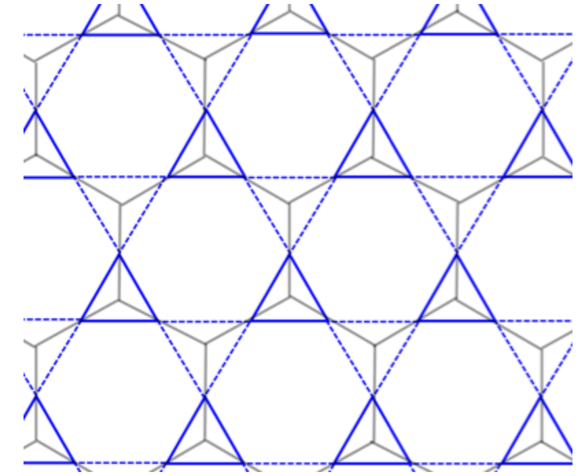
There exists a peak in the heat capacity around 100K, which is consistent with phase transition.

Hastings' theorem implies both CMIs are spin liquids.

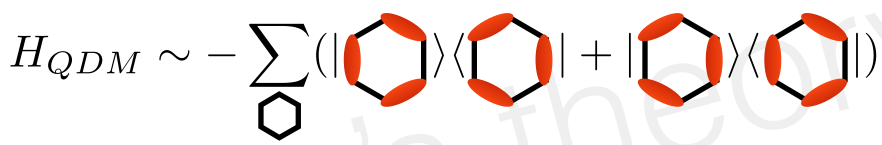

E Fradkin

S Kivelson

S. Sondhi

R. Moessner


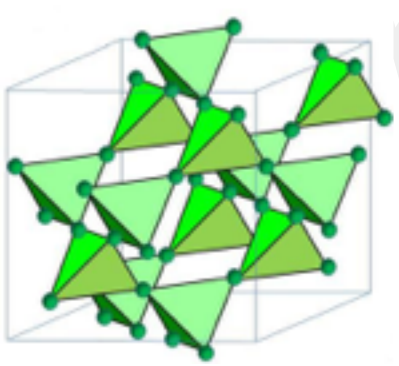
- **Quantum Dimer Model = Lattice Gauge Theory**;
  bipartite: compact U(1) gauge theory,
  non-bipartite: Z_2 gauge theory.

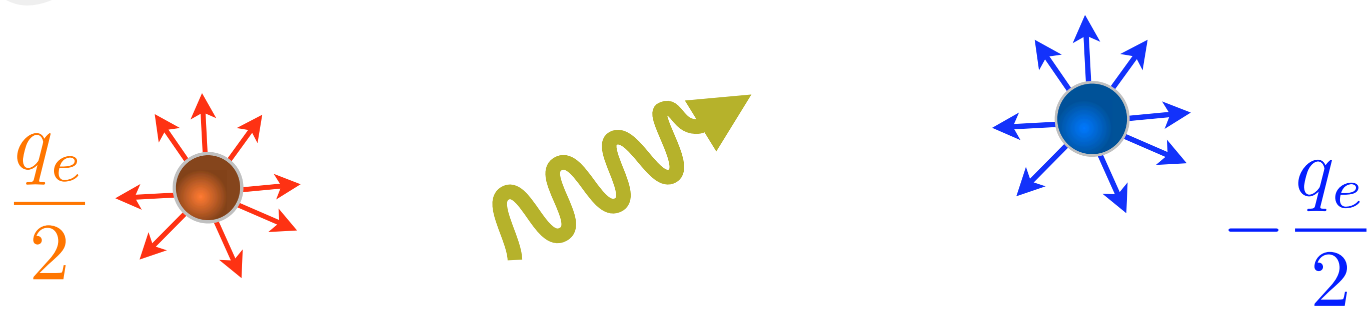



A. Polyakov

- The PCO in type-II CMI can be understood as the confining phase of compact U(1) gauge theory in 2D.

- This implies 3D CMI supports **quantum charge liquid & charge fractionalization** !





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Summary

- I provide specific examples to illustrate some of the physics in cluster Mott insulators.
- There is a very interesting interplay between the charge and spin degrees of freedom in both 2D and 3D cluster Mott insulators, maybe also with **disorders** in the future!
- Cluster Mott insulators are new physical systems that may host various emergent and exotic physics.