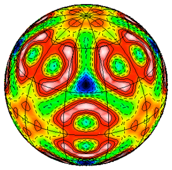
Iridates

The New Frontier

Mike Norman

Materials Science Division
Argonne National Laboratory



KITP, Feb. 12, 2010

Spin Liquids are insulators that have large Curie-Weiss temperatures, but do not order or show spin glass behavior. Particularly relevant are those with S=1/2.

PHYSICS

An End to the Drought of Quantum Spin Liquids

Patrick A. Lee

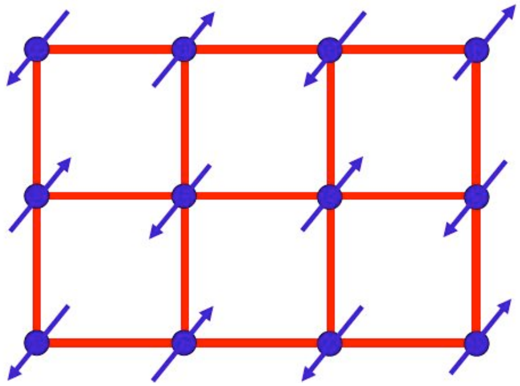
After decades of searching, several promising examples of a new quantum state of matter have now emerged.

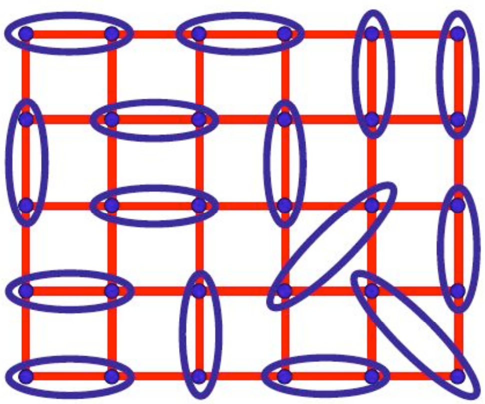
Science 321, 1306 (2008)

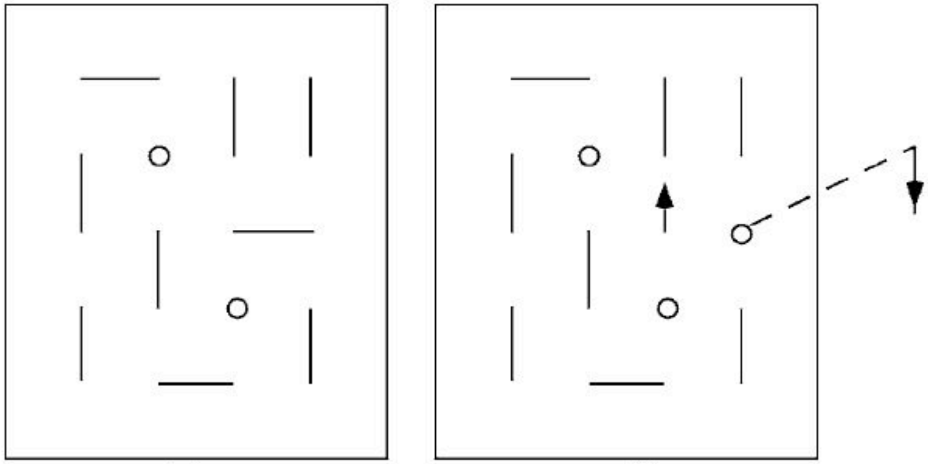
- κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ (triangular)
- ZnCu$_3$(OH)$_6$Cl$_2$ (kagome)
- Na$_4$Ir$_3$O$_8$ (hyper-kagome)

(See also article in Physics Today by Barbara Goss Levi, page 16, February 2007)

RVB - a liquid of spin singlets



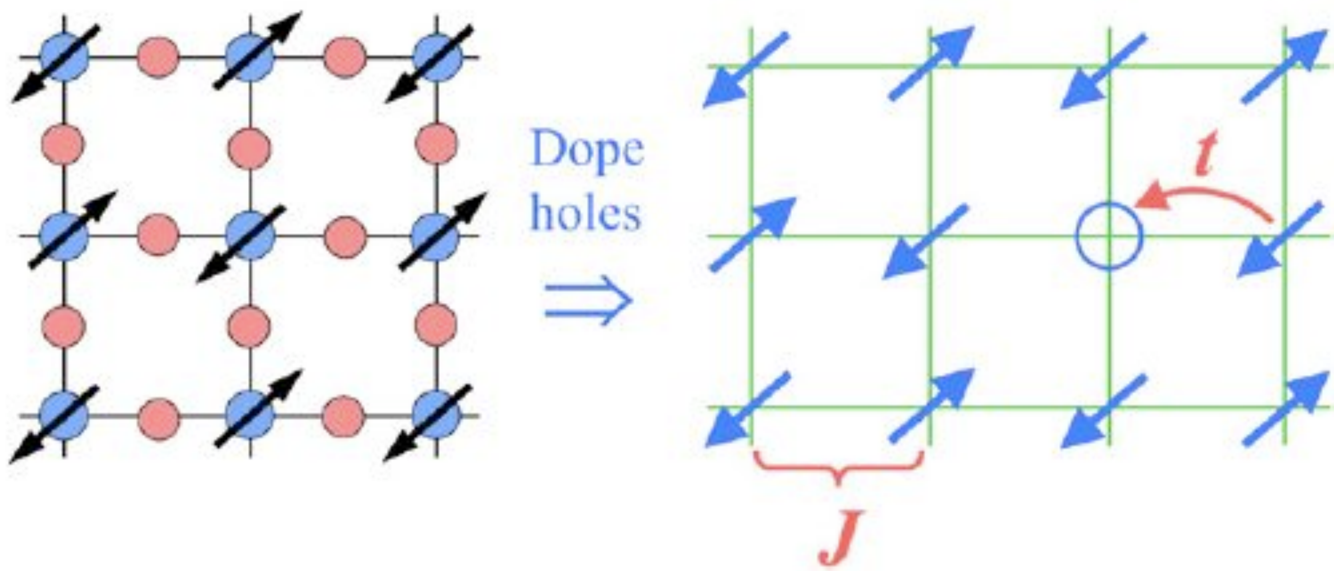




(a) (b)

In the uniform RVB state, the S=1/2 excitations (spinons) possess a zero energy Fermi surface (Anderson, 1987)

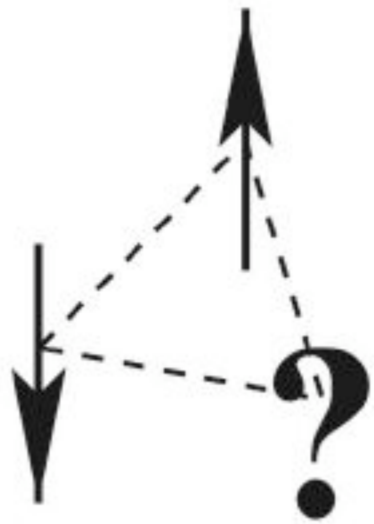
Square Lattice (Anderson, 1987)

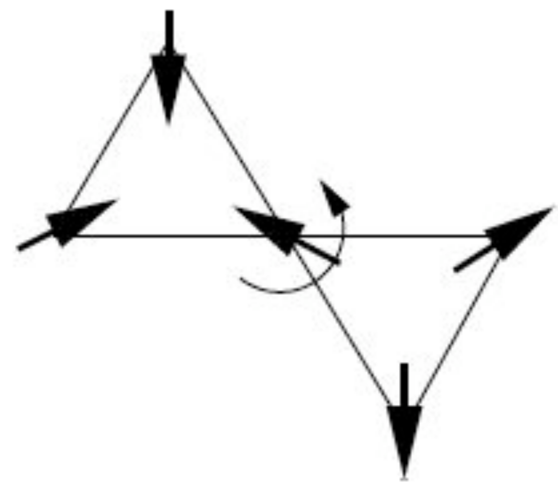


J S·S where J = 2 t^2/U
for S=1/2
Neel - J/4 per bond - S_zS_z
Singlet - 3J/4 per bond - S(S+1)

Lee, Rep. Prog. Phys. 71, 012501 (2008)

Frustration on the Triangular Lattice (Anderson, 1973)





$$\chi^{-1} = T - \Theta_{CW}$$

κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$

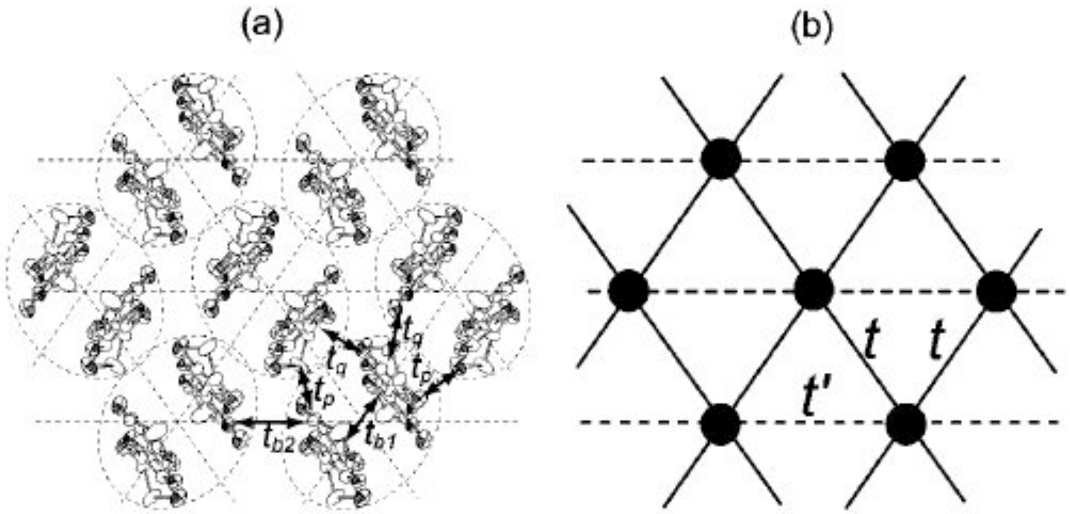
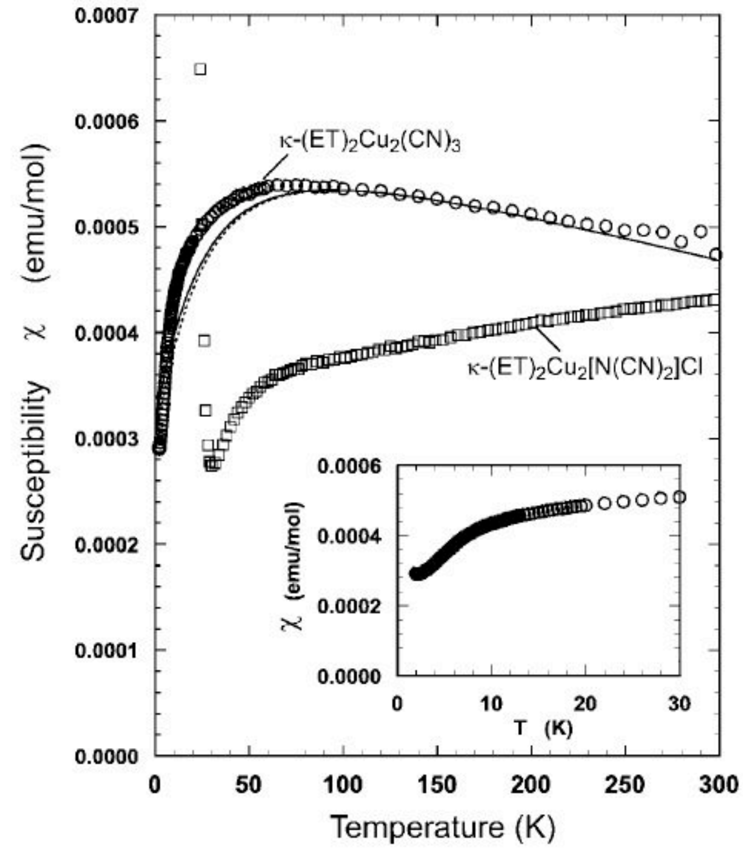
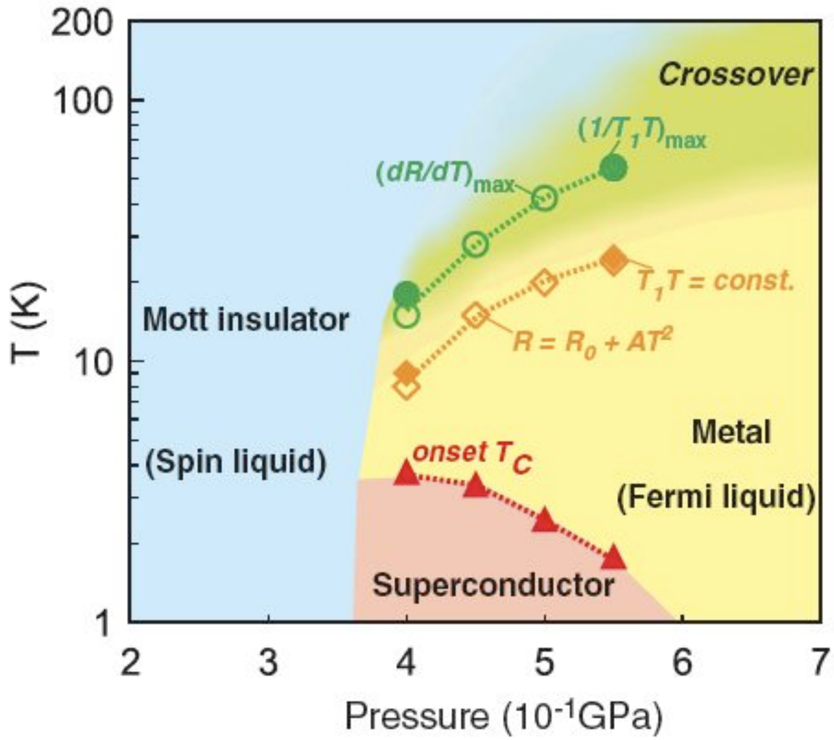


FIG. 1. (a) Crystal structure of an ET layer of κ-(ET)$_2$Cu$_2$(CN)$_3$ viewed along the long axes of ET molecules

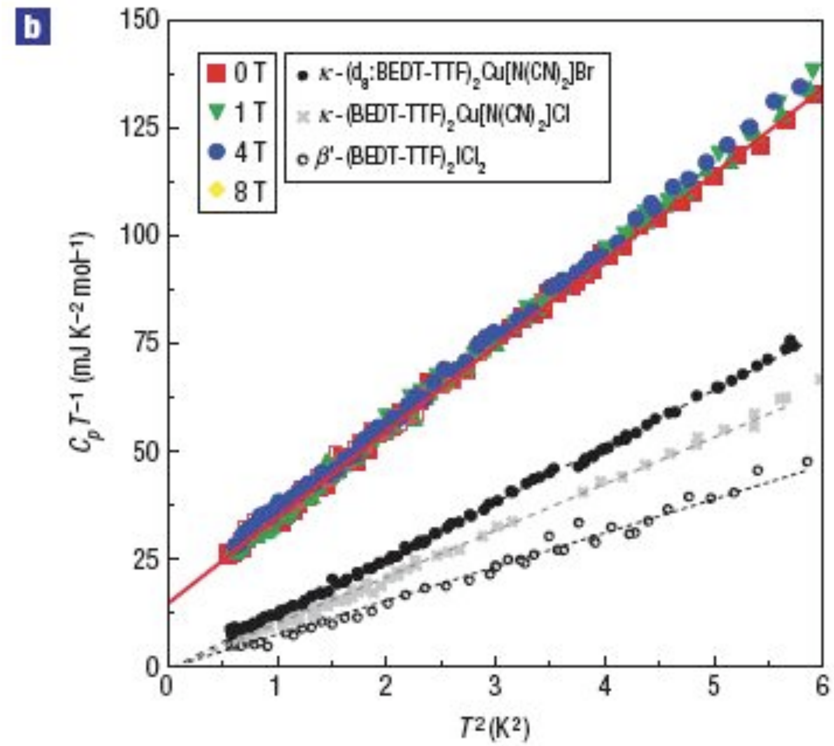
Geiser *et al*., Inorg. Chem. 30, 2586 (1991)



Shimizu *et al*., PRL 91, 107001 (2003)

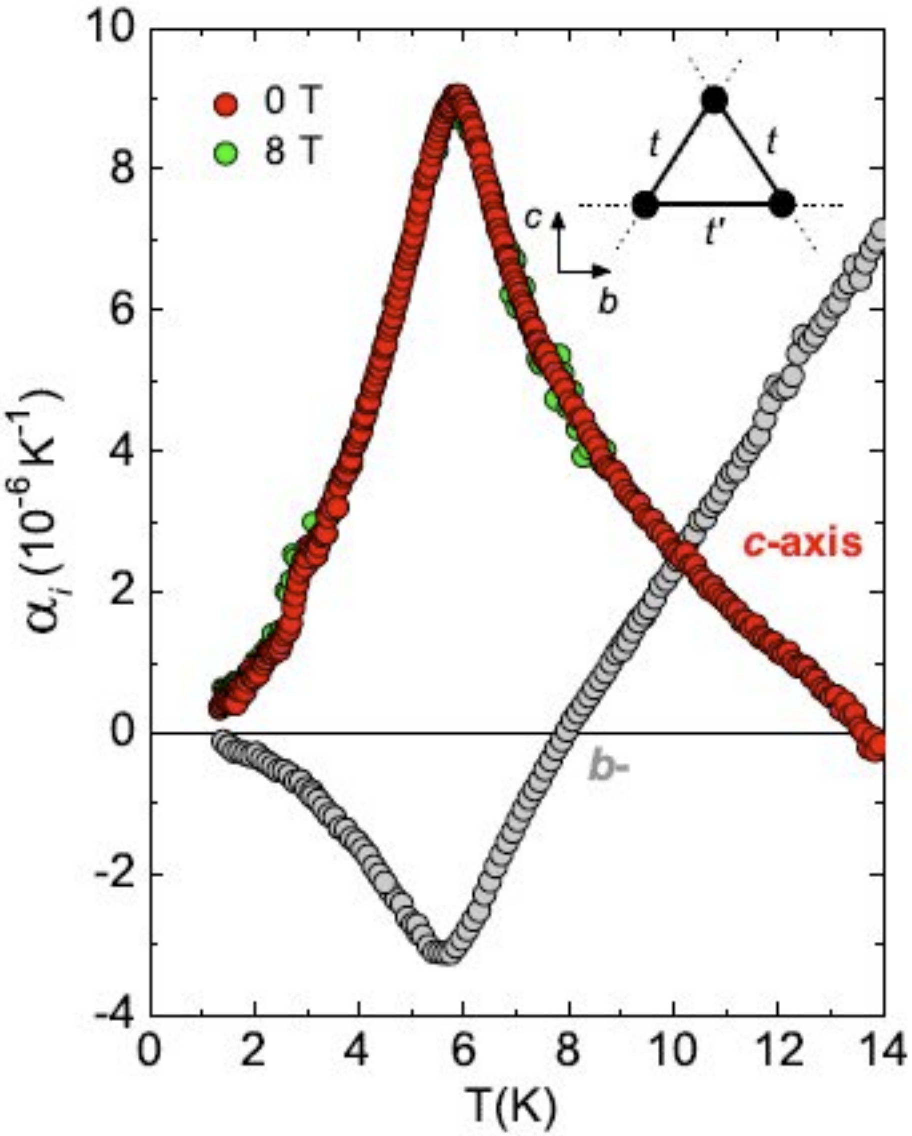


Kurosaki *et al*., PRL 95, 177001 (2005)



Yamashita *et al*., Nat. Phys. 4, 459 (2008)

Ordering at 6 K?



Manna *et al*., PRL 104, 016403 (2010)

The Universe is a String-Net Liquid

Herbertsmithite

Zeeya Merali, New Scientist (15 March 2007)

Herbertsmithite $ZnCu_3(OH)_6Cl_2$

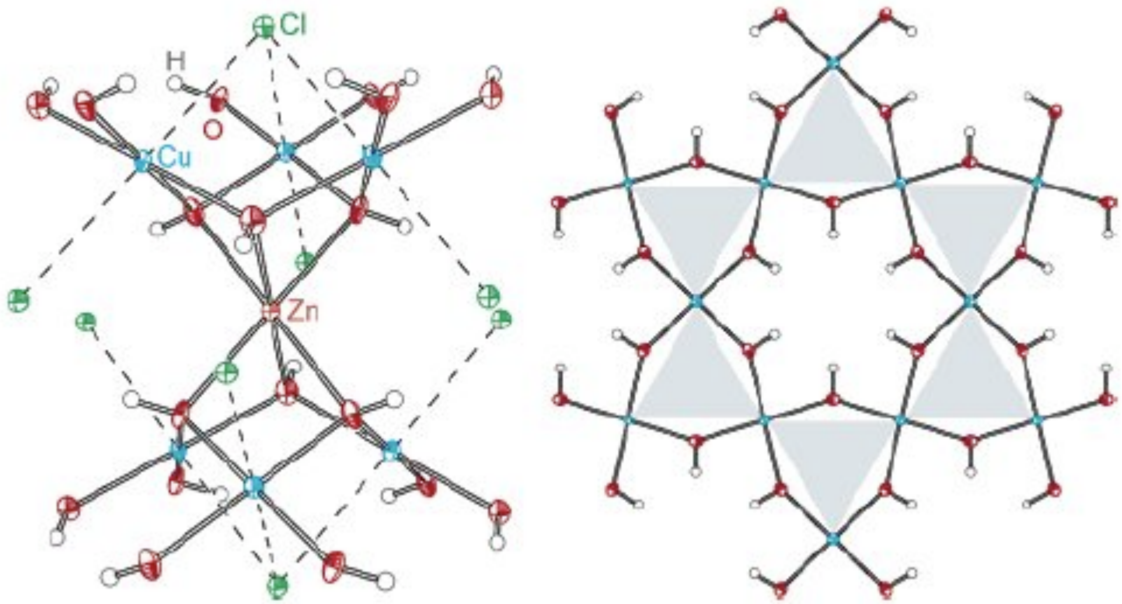
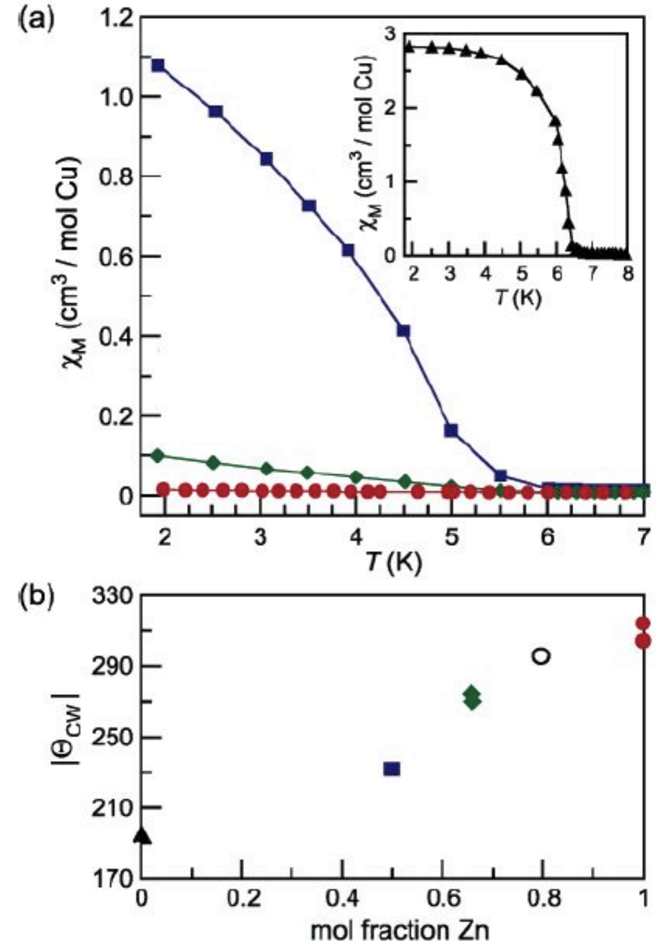
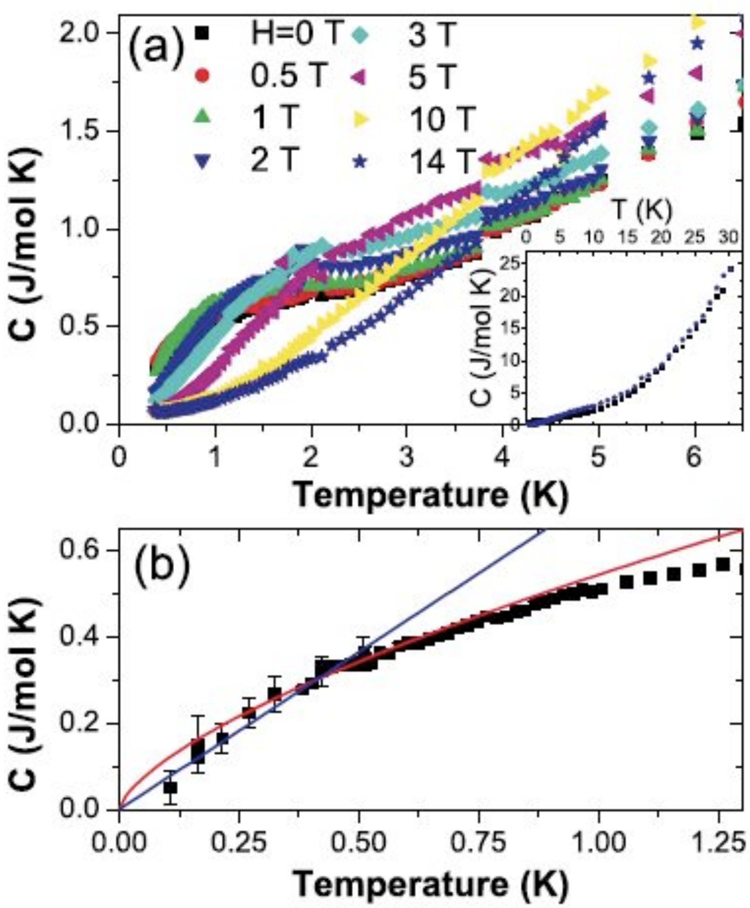


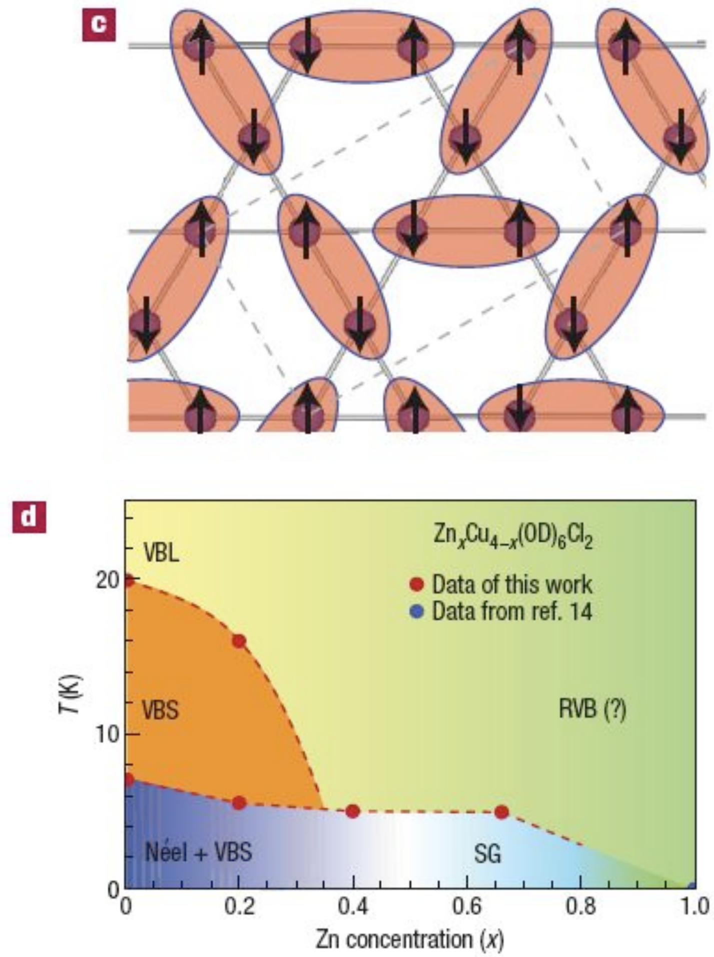
Figure 1. Crystal structure of Zn−paratacamite (**1**), $Zn_{0.33}Cu_{3.67}(OH)_6Cl_2$.



Shores *et al.*, JACS 127, 13462 (2005)

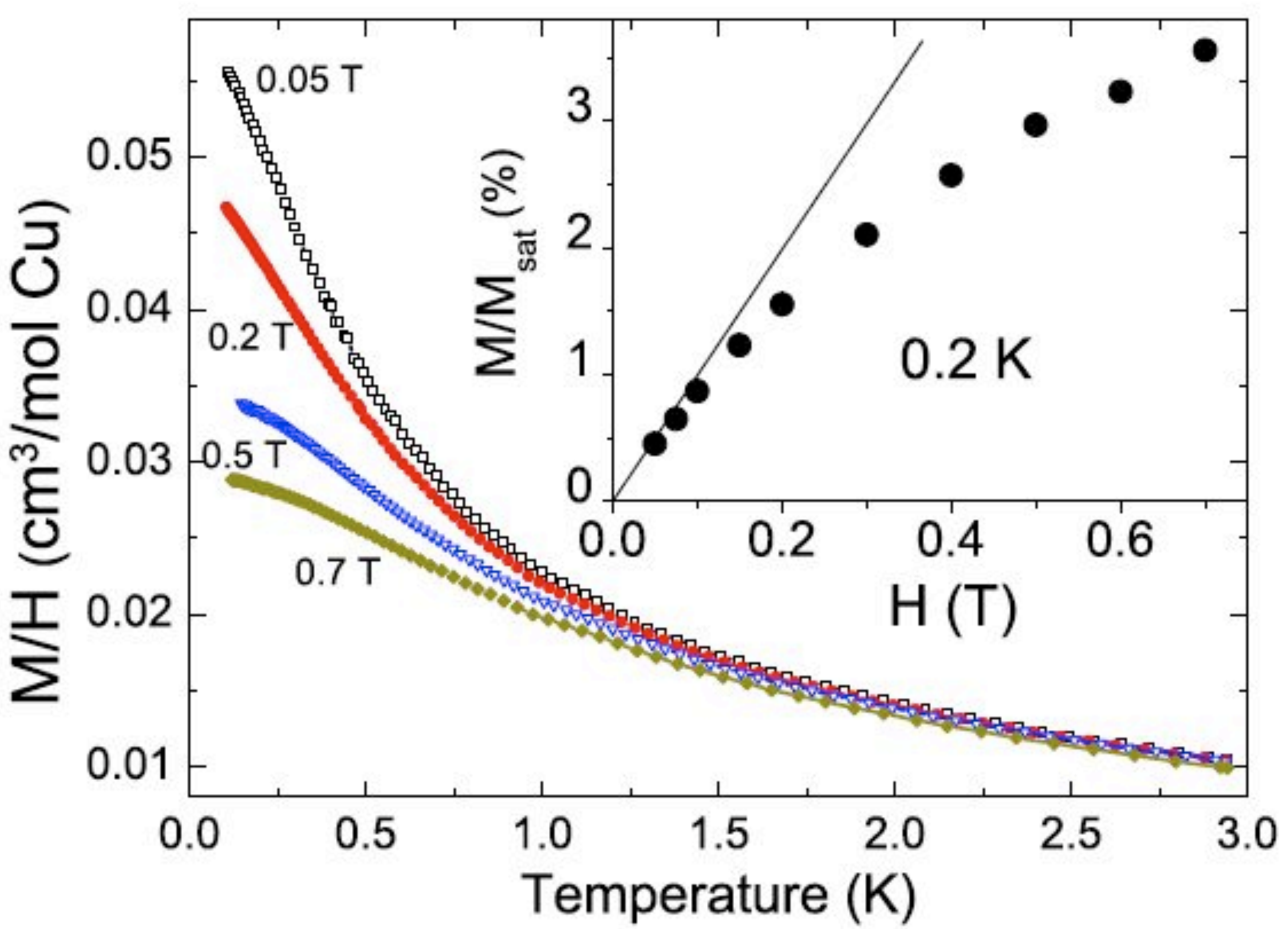


Helton *et al*., PRL 98, 107204 (2007)



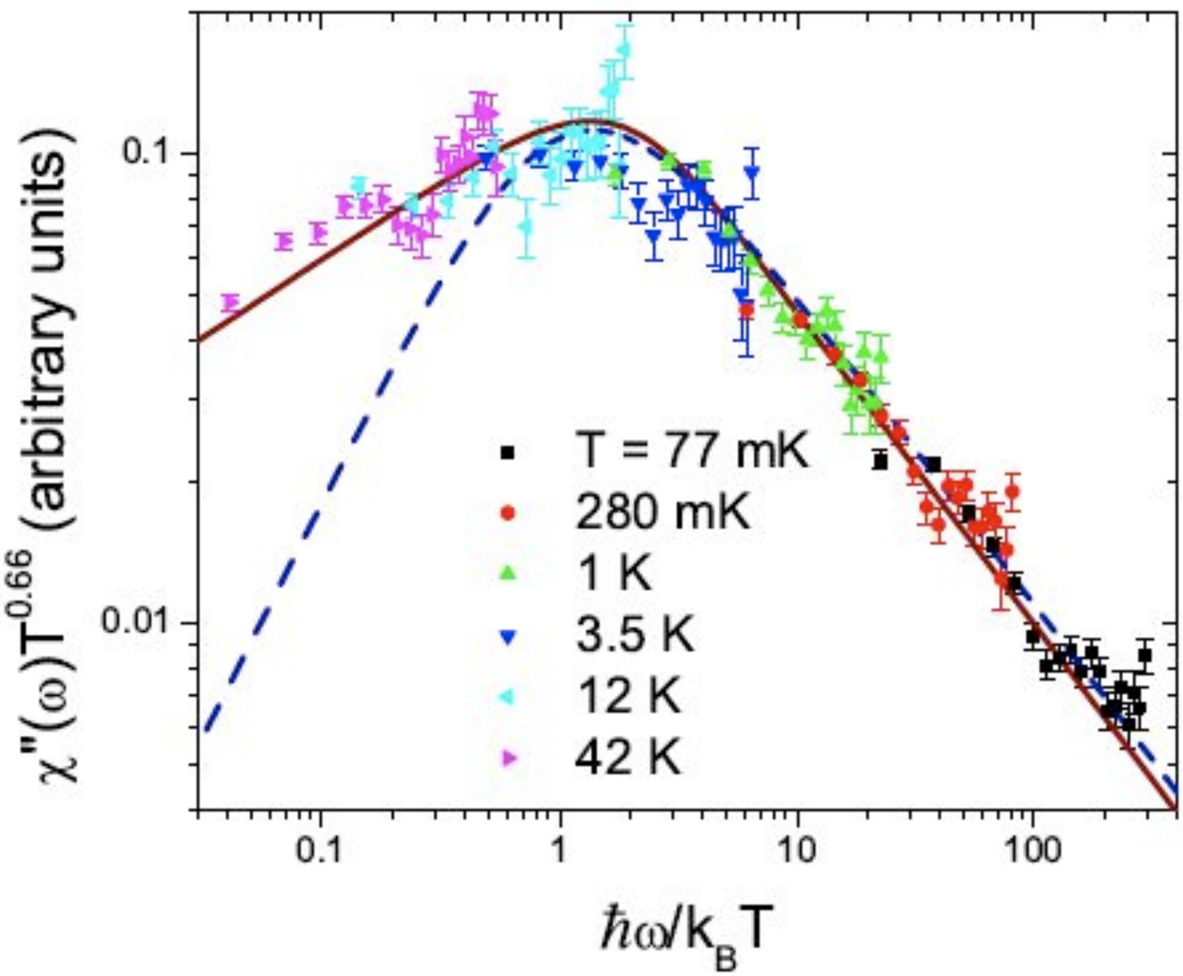
Lee *et al*., Nat. Matls. 6, 853 (2007)

But, there is a large defect concentration (Cu - Zn)



Bert *et al*., PRB 76, 132411 (2007)

ω/T scaling



Helton *et al*., arXiv:1002.1091

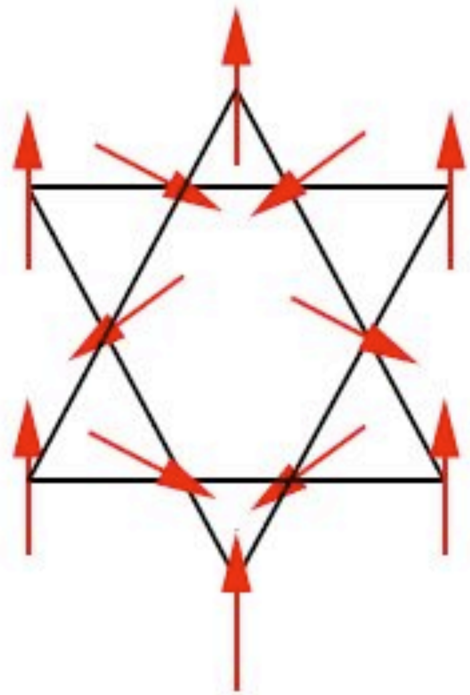
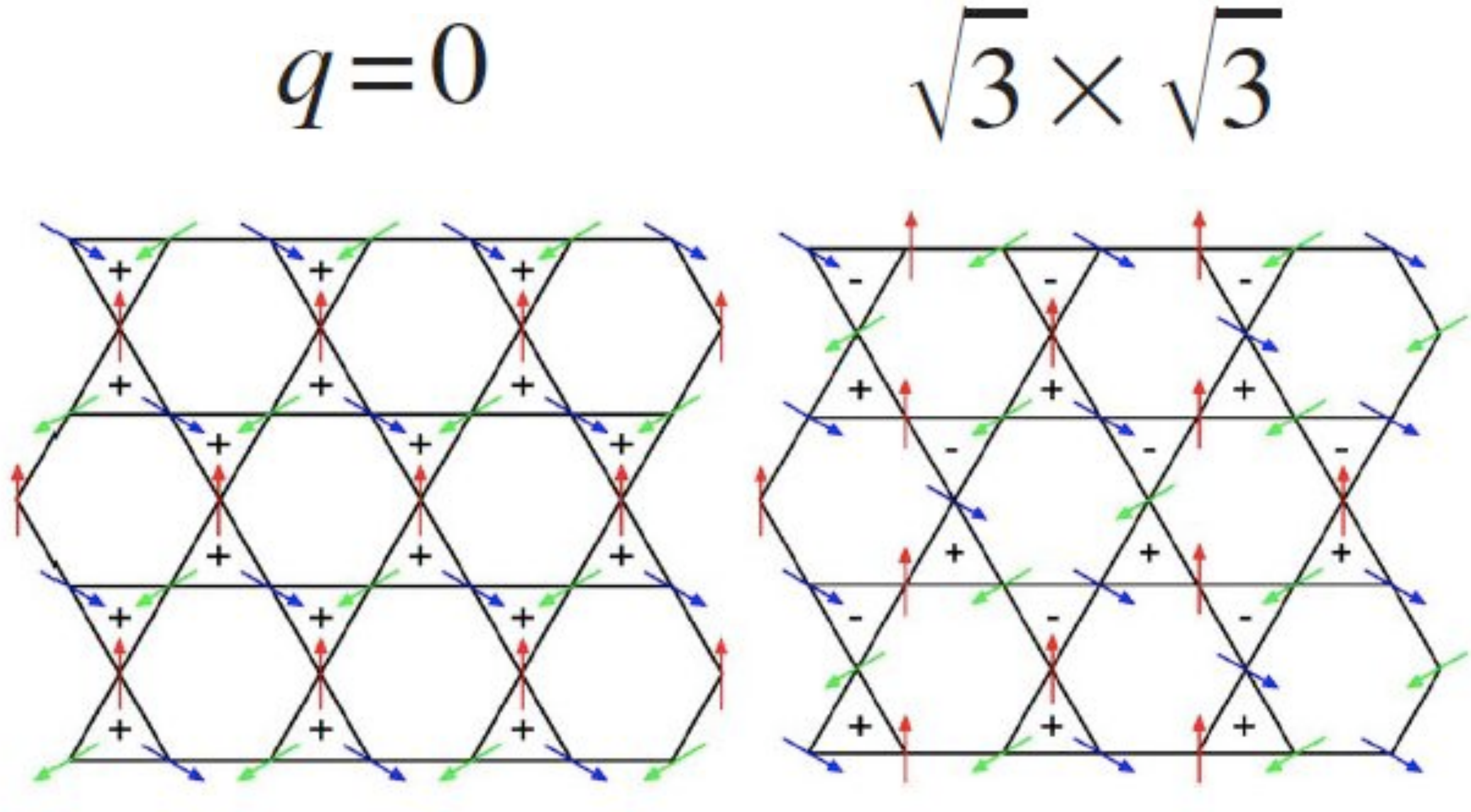


Fig. 1.5. Illustration of how ground state degrees of freedom arise for the Heisenberg model on the kagome lattice: spins on the central hexagon may be rotated together through any angle about the axis defined by the outer spins, without leaving the ground state.

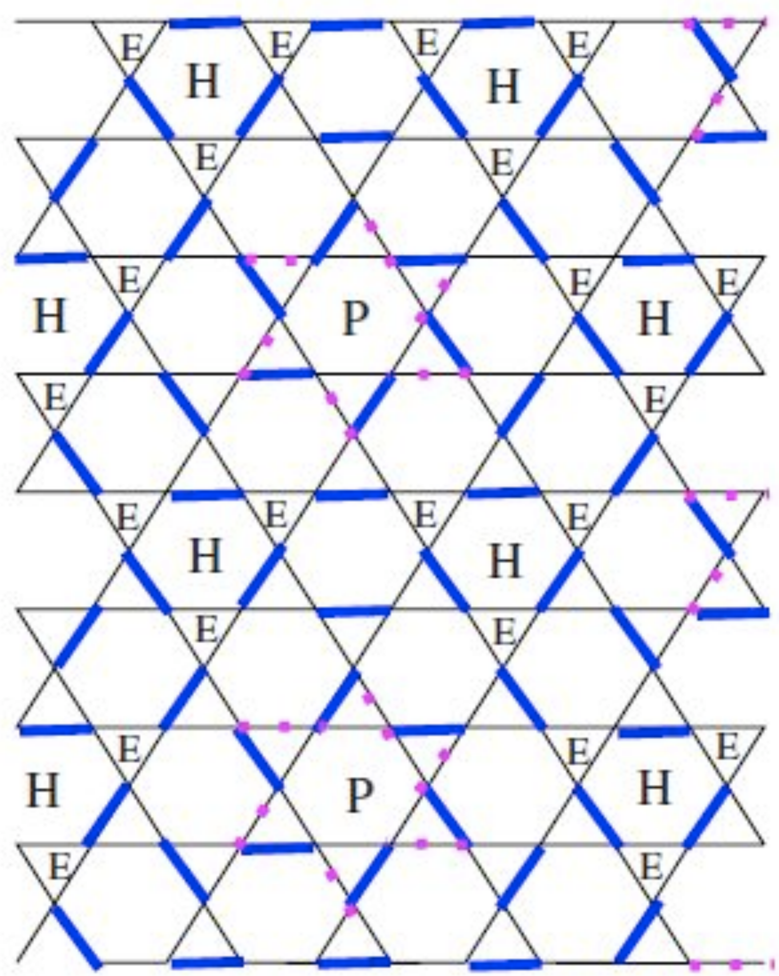
Chalker, arXiv:0901.3492

Classical Kagome Ground States



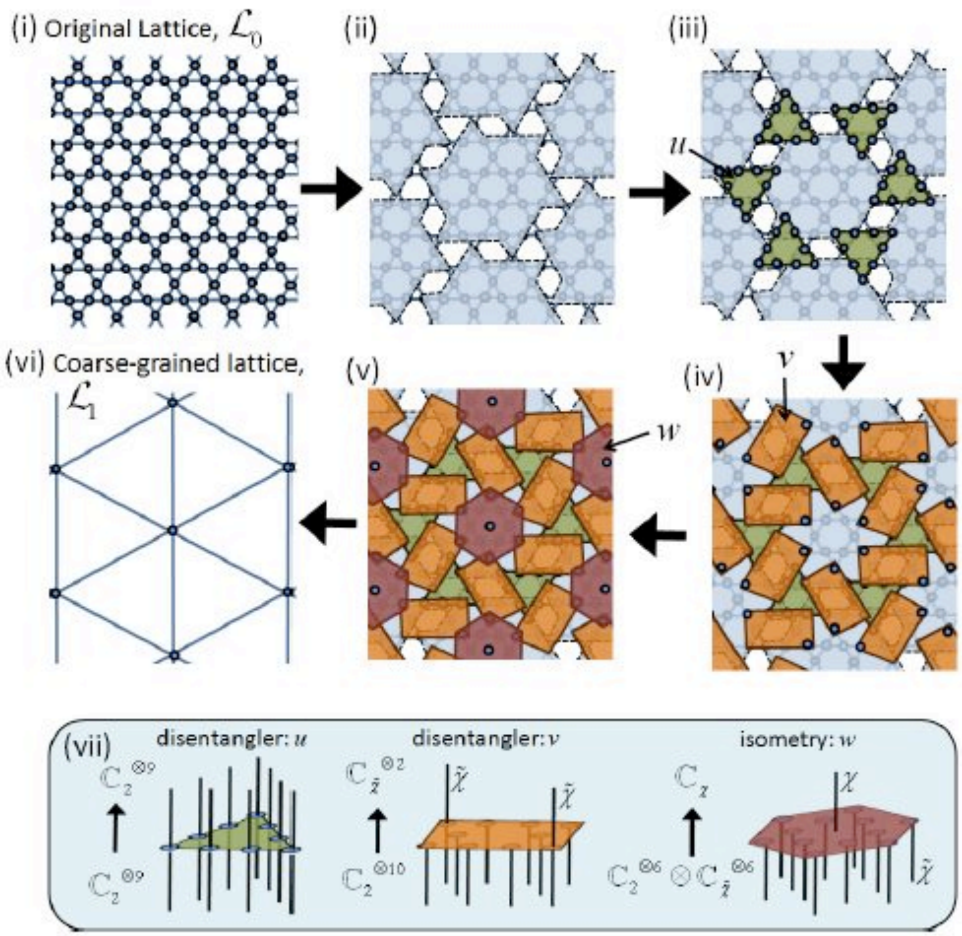
Ryu *et al.*, PRB 75, 184406 (2007)

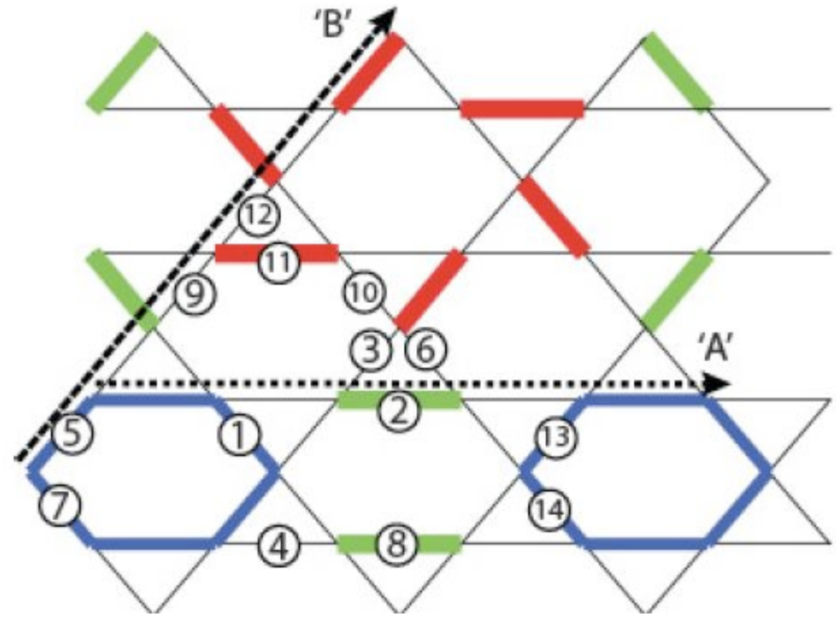
Valence Bond Ground State for Kagome?



Singh & Huse, PRB 76, 180407 (2007)

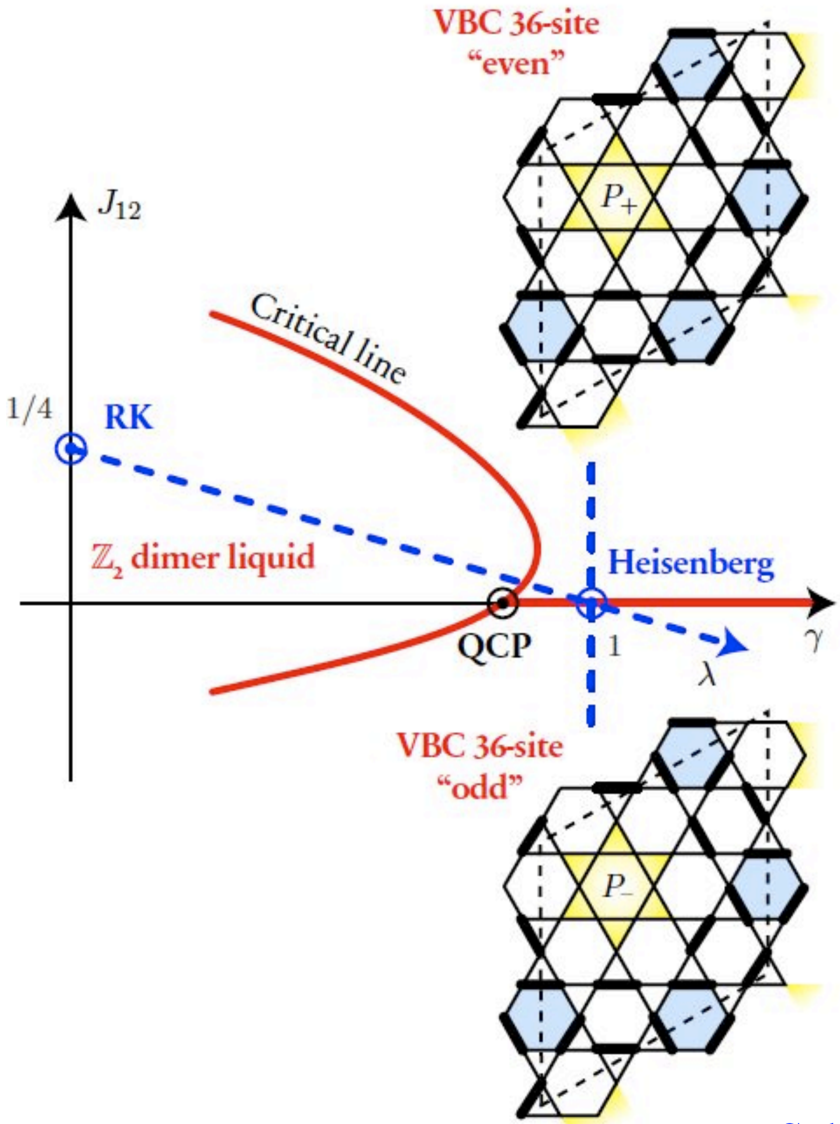
Multi-scale entanglement renormalization ansatz (MERA)





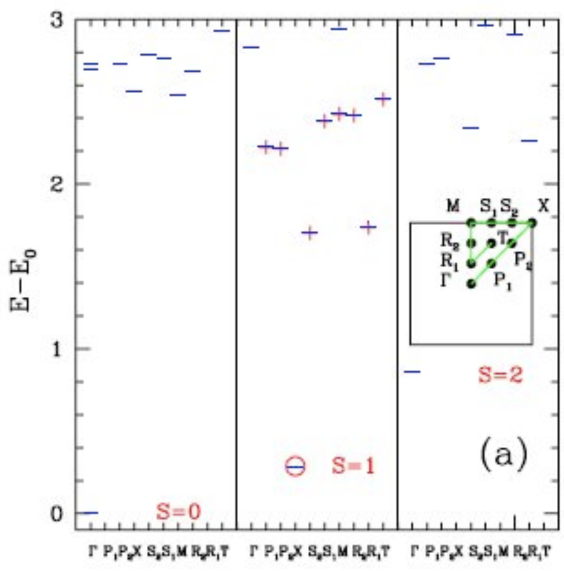
Evenbly & Vidal, arXiv:0904.3383

Close to a Quantum Critical Point?

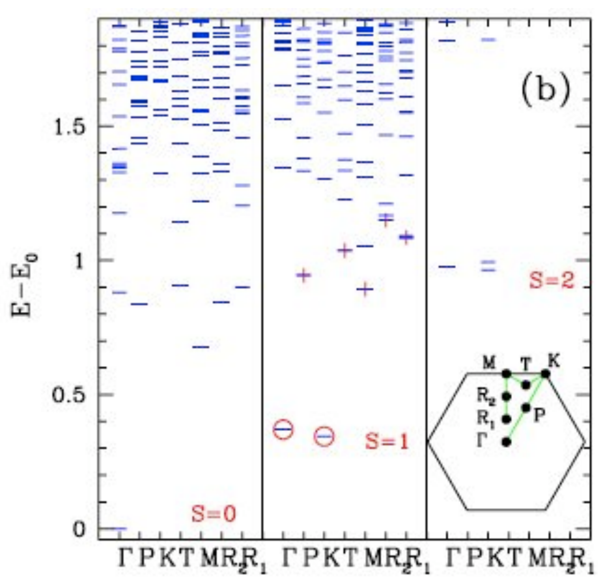


Schwandt *et al.*, arXiv:1002.0774

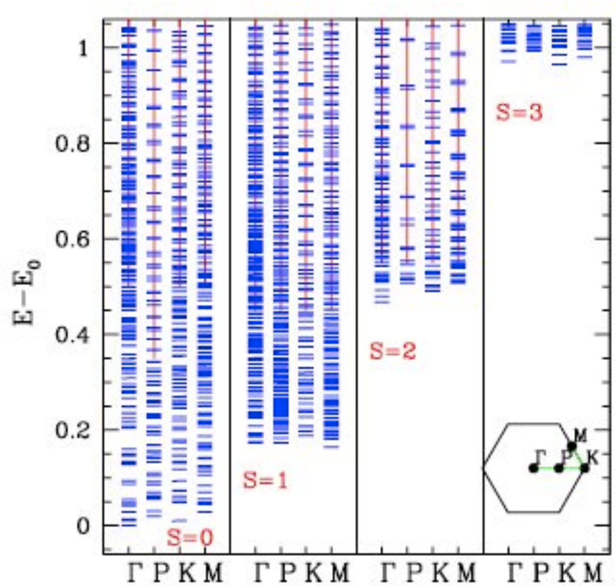
Exact Diagonalization (36 sites)



square



triangular



Kagome

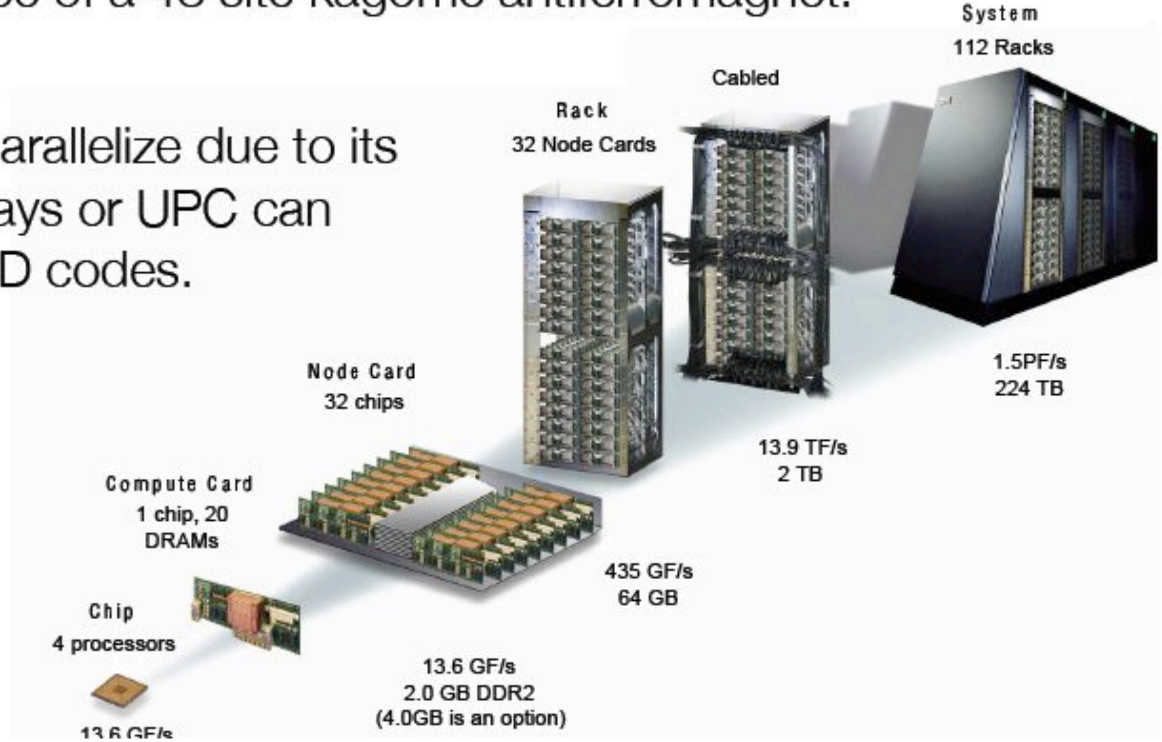
Sindzingre & Lhuillier, EPL 88, 27009 (2009)

Parallelization:
How to harness the petaflop computers ?

- Cutting edge petaflop systems have a huge number of core, but only a moderate amount of node-local memory.

- Next generation ED codes need to be developed in order to attack e.g. the 80 billion Hilbert space of a 48 site kagome antiferromagnet.

- Problem remains difficult to parallelize due to its all-to-all structure. Global Arrays or UPC can help developing distributed ED codes.



Andreas Lauchli, QS2009 Workshop

$Na_4Ir_3O_8$

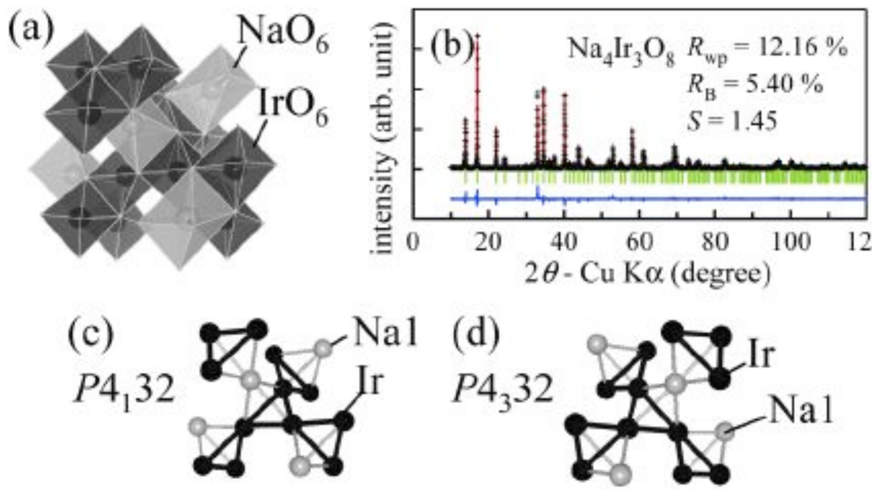
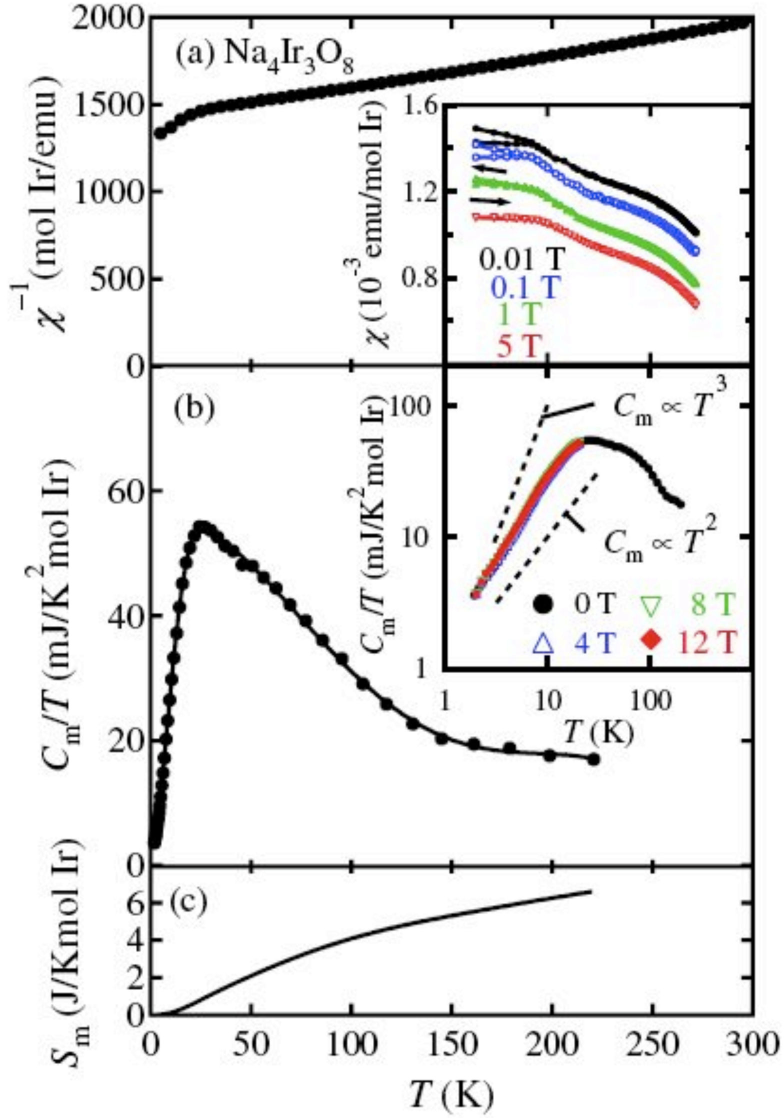


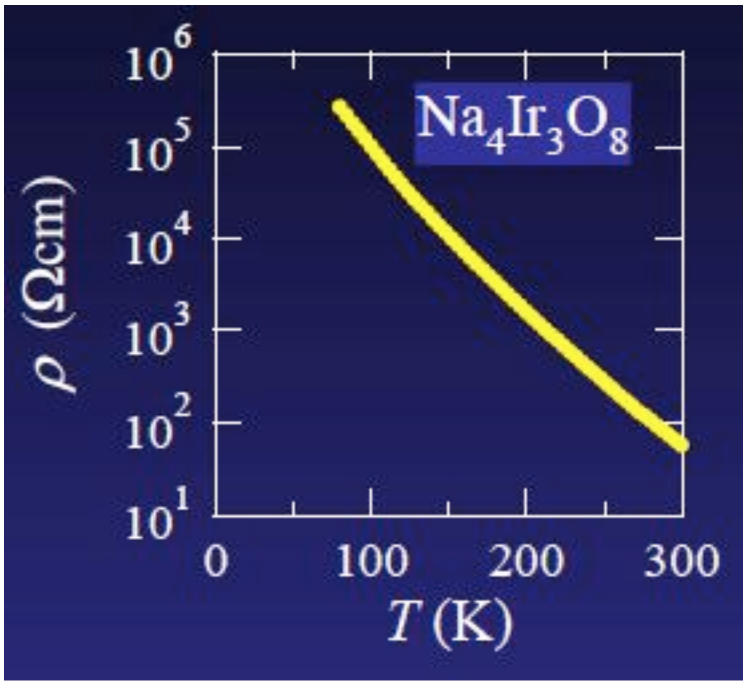
FIG. 1 (color online). (a) Crystal structure of $Na_4Ir_3O_8$

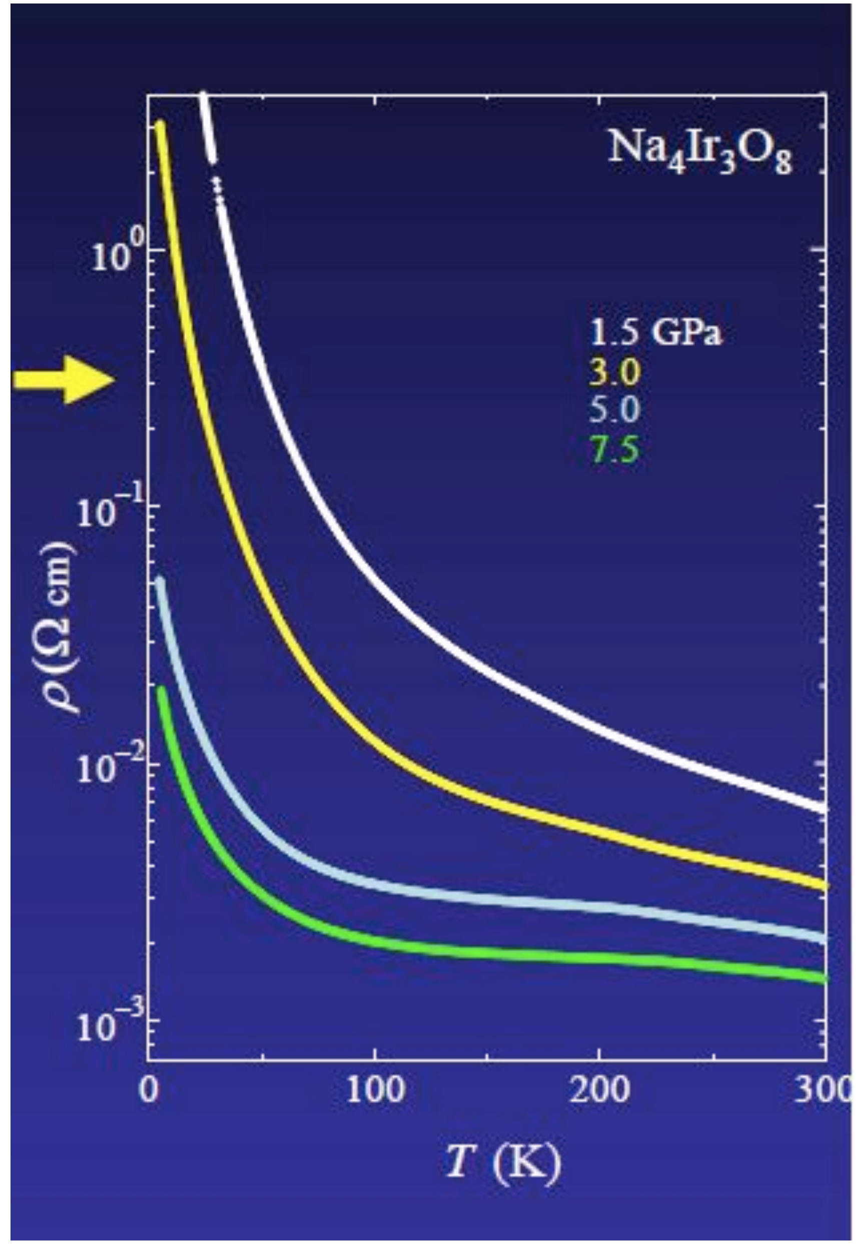


$\Theta_{CW} \sim -650$ K, $\mu_{eff} \sim 2\ \mu_B$

Okamoto *et al.*, PRL 99, 137207 (2007)

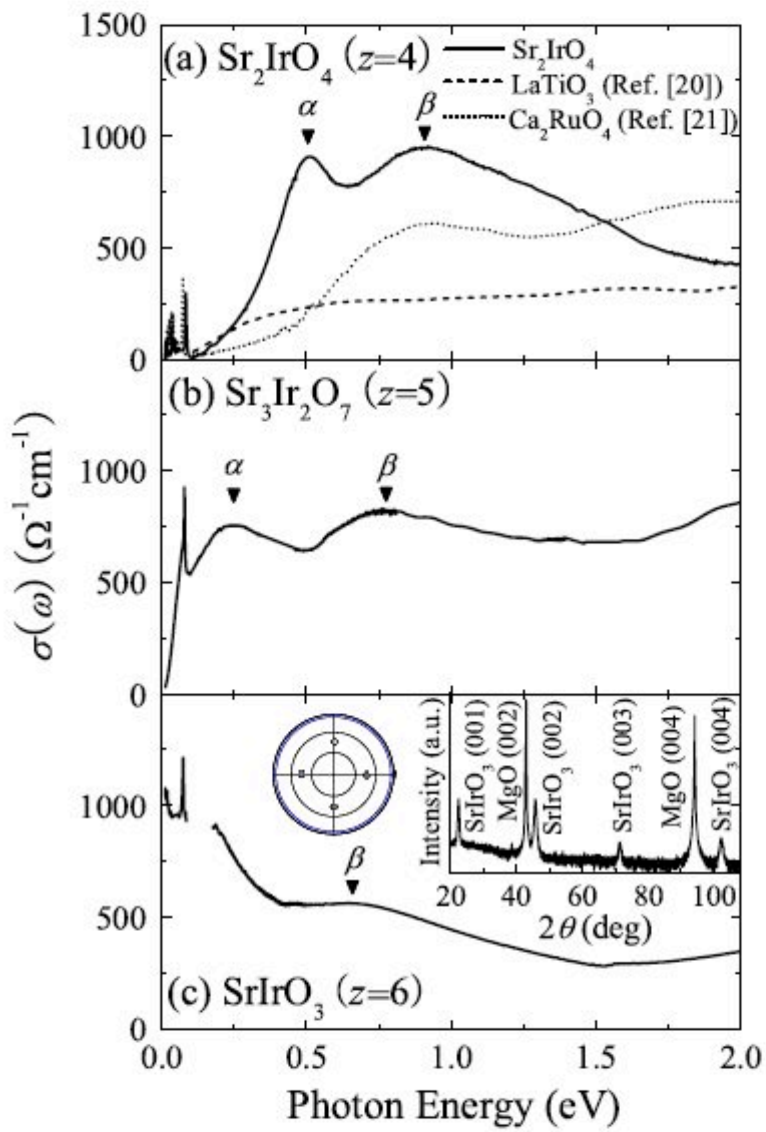
Mott Insulator?





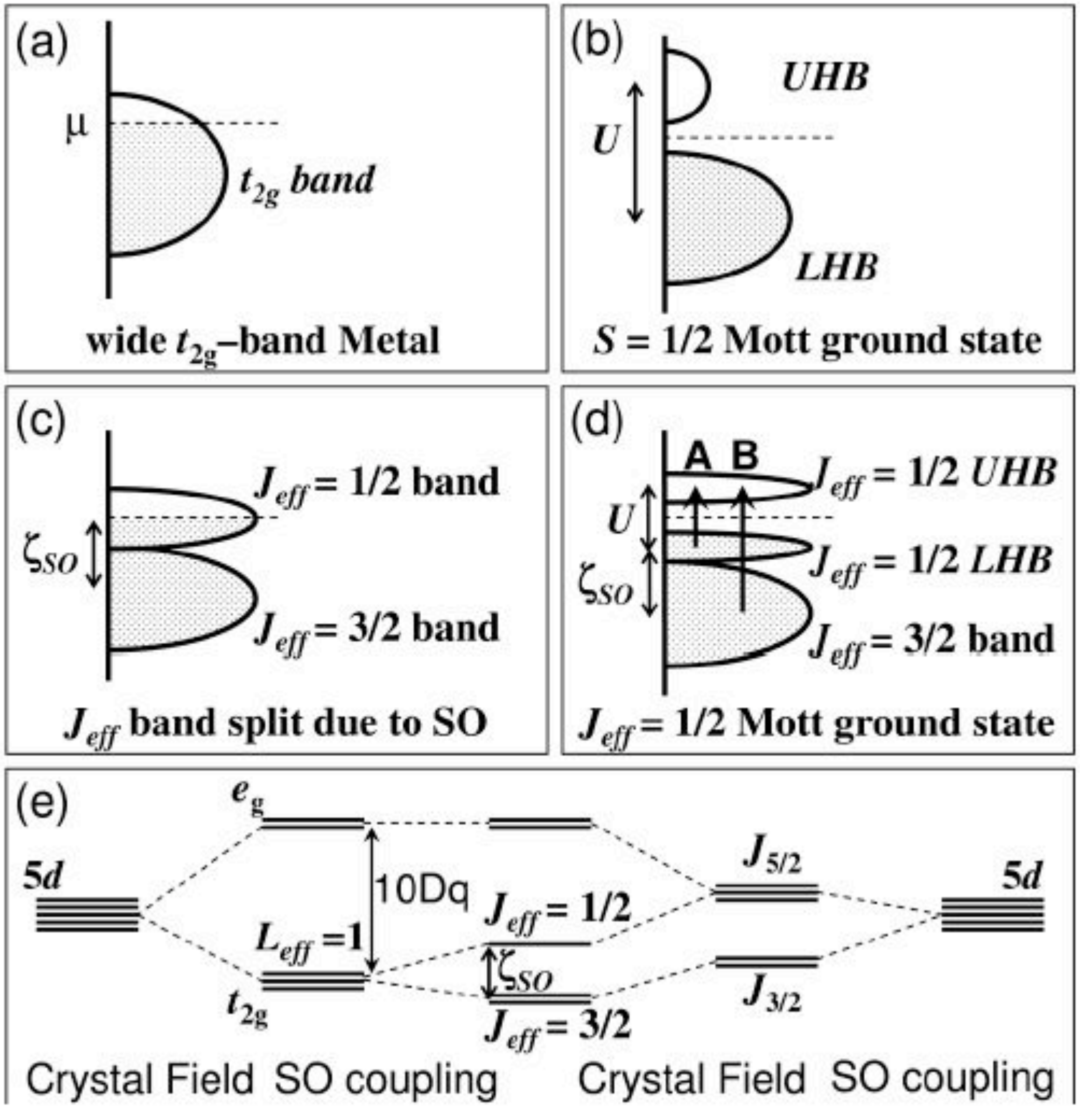
H. Takagi, unpublished

Sr_2IrO_4 (La_2CuO_4 analogue) appears to be a Mott insulator



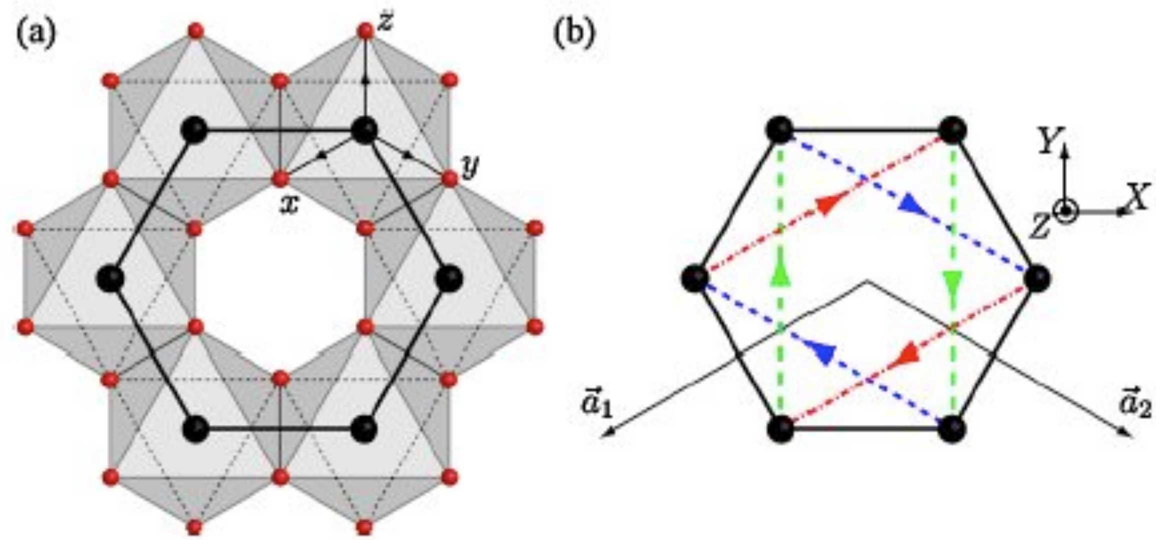
Moon *et al.*, PRL 101, 206402 (2008)

Spin-orbit plus d^5 configuration leads to a half filled doublet



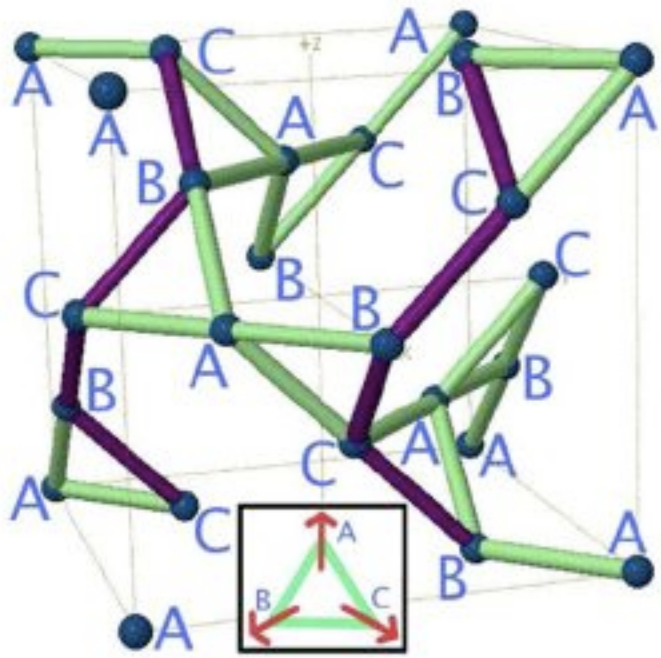
Kim *et al*., PRL 101, 076402 (2009)

Quantum Spin Hall Effect in Na_2IrO_3?



Shitade *et al*., PRL 102, 256403 (2009)

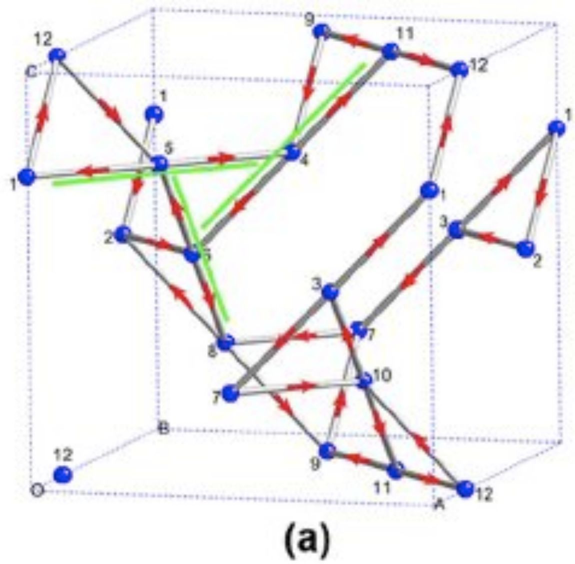
$Na_4Ir_3O_8$ - Ir ions form a network of corner sharing triangles



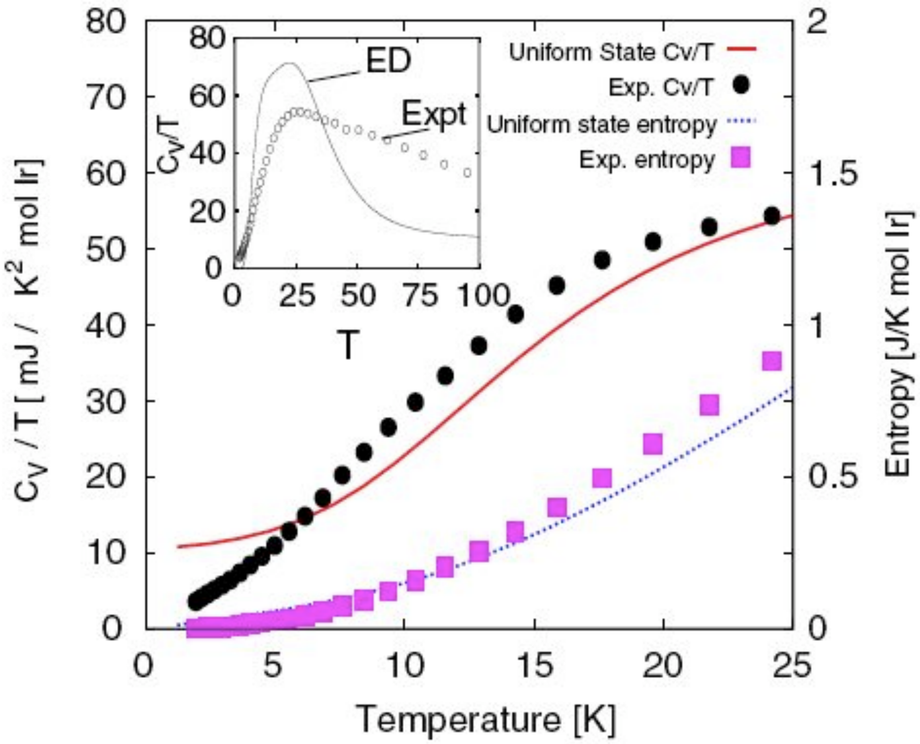
Semiclassical - J S·S

Lawler *et al.*, PRL 100, 227201 (2008)

10 site loops



Zhou *et al*., PRL 101, 197201 (2008)



Lawler *et al*., PRL 101, 197202 (2008)

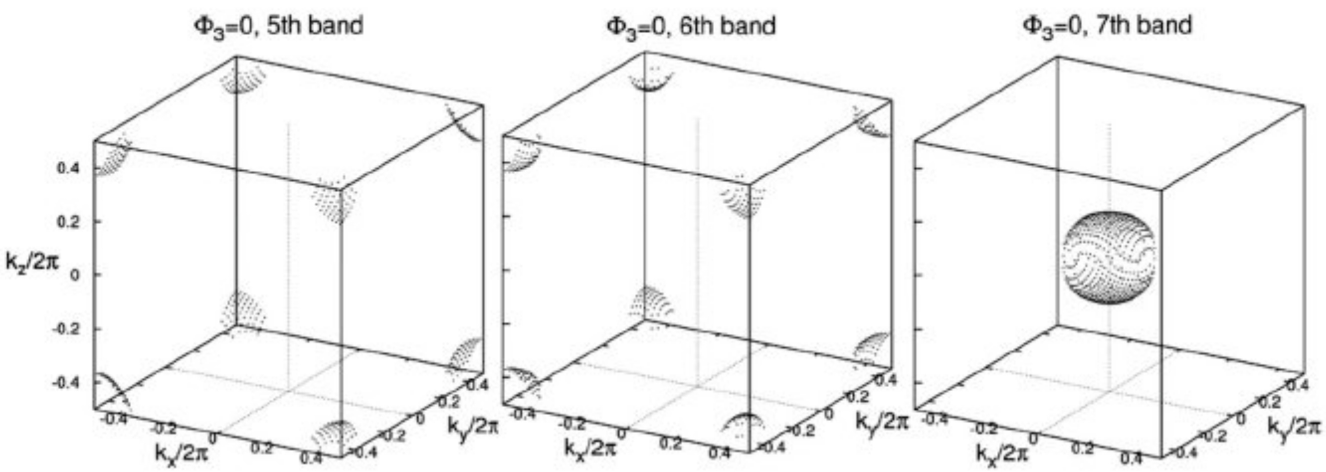
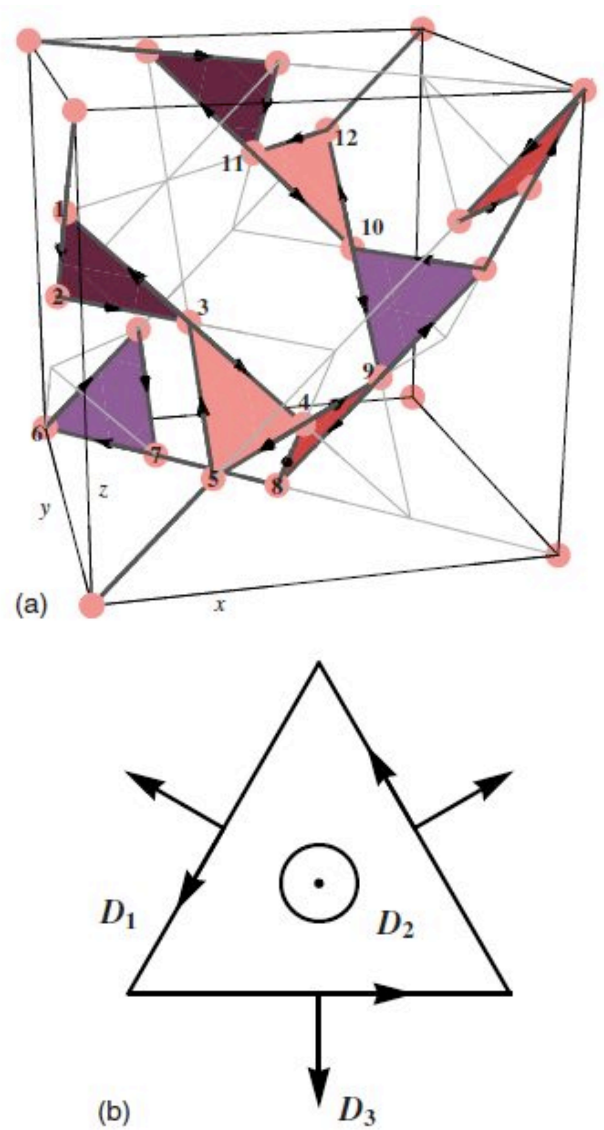


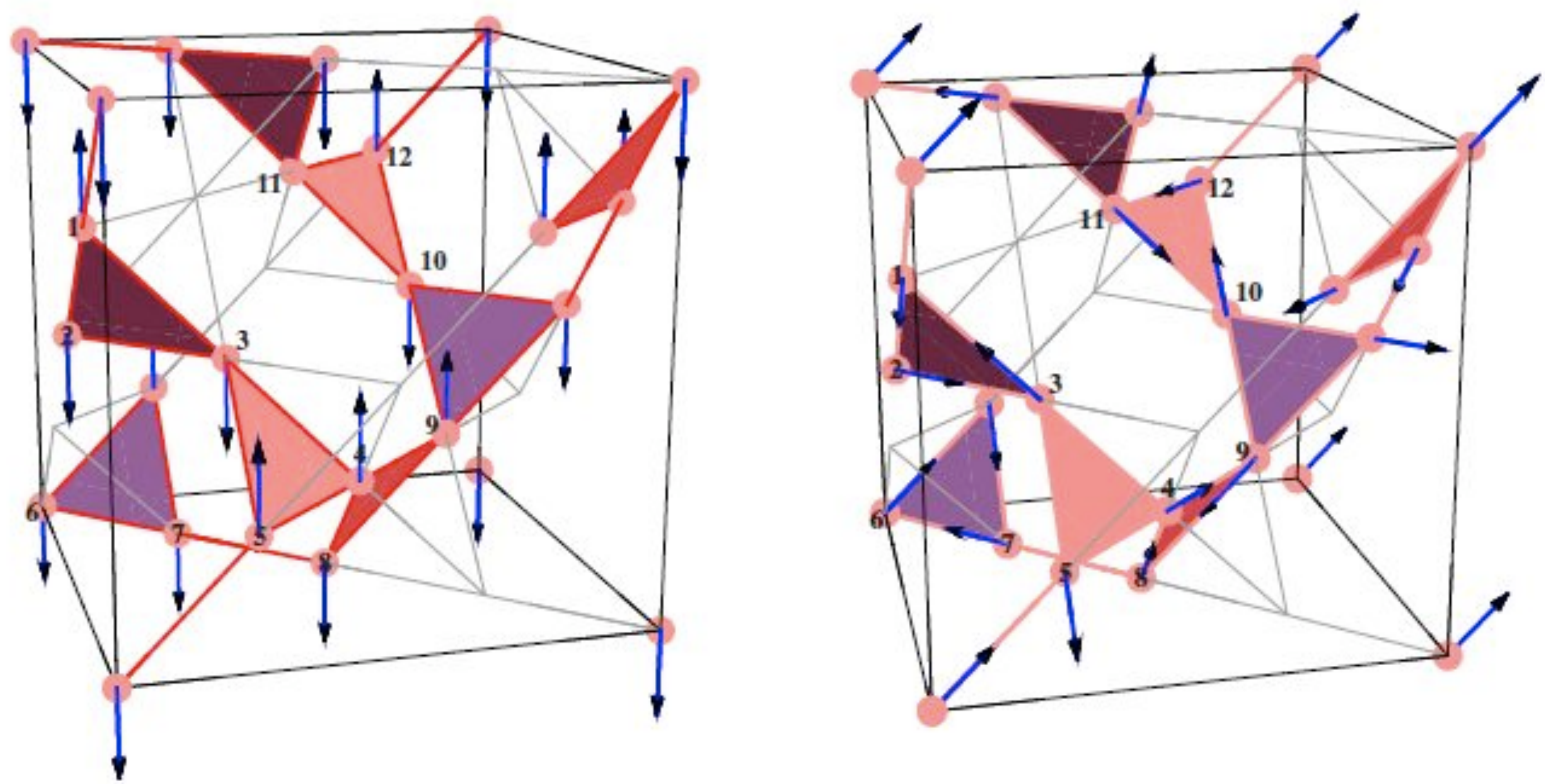
FIG. 2. Fermi surfaces of the zero flux state at half-filling.

$Na_4Ir_3O_8$ - anisotropy important due to spin-orbit coupling



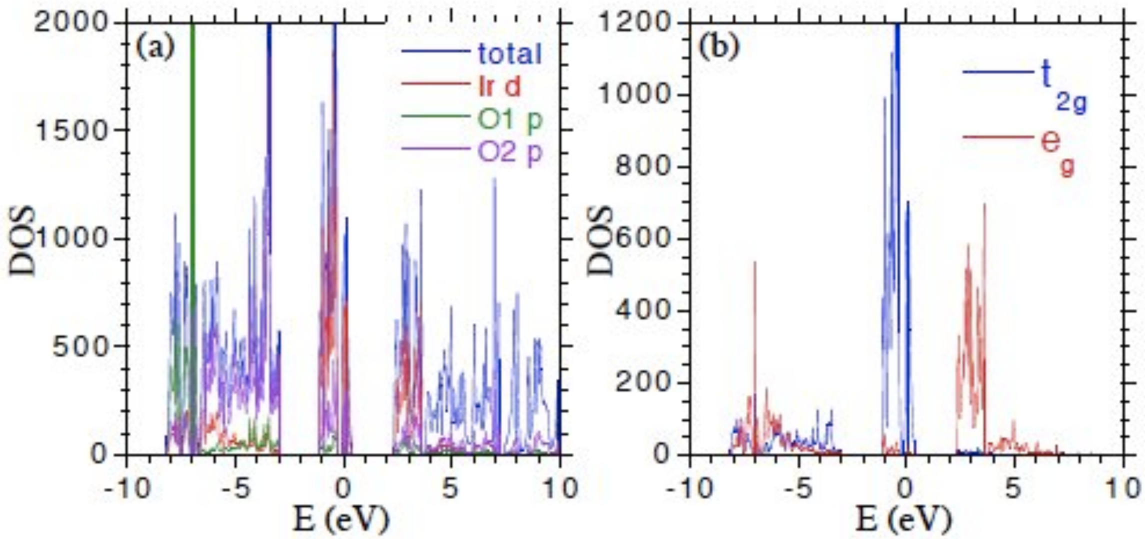
Chen & Balents, PRB 78, 094403 (2008)

Possible ground states in the presence of anisotropy

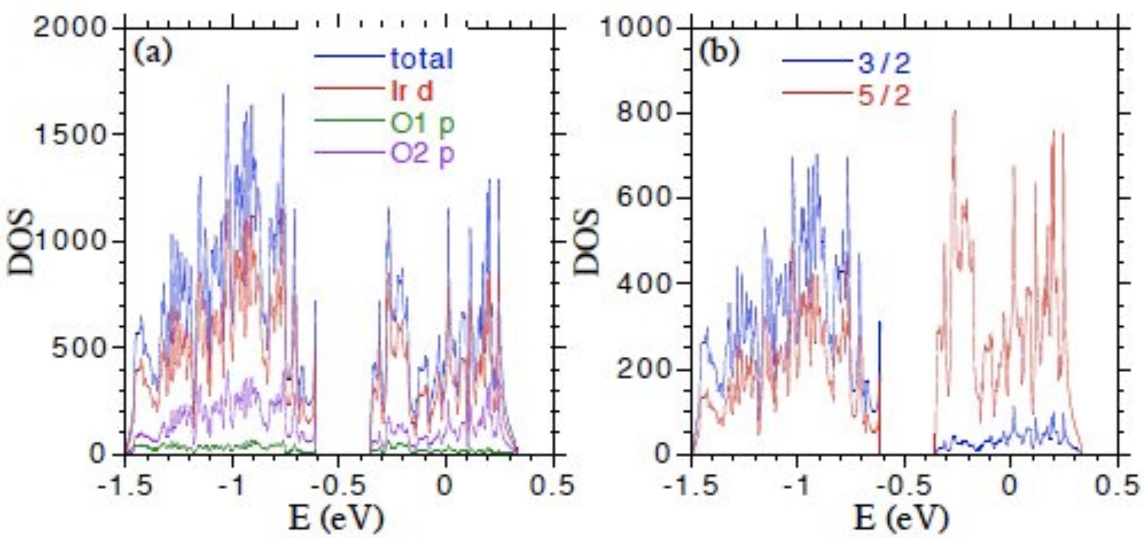


Chen & Balents, PRB 78, 094403 (2008)

LDA



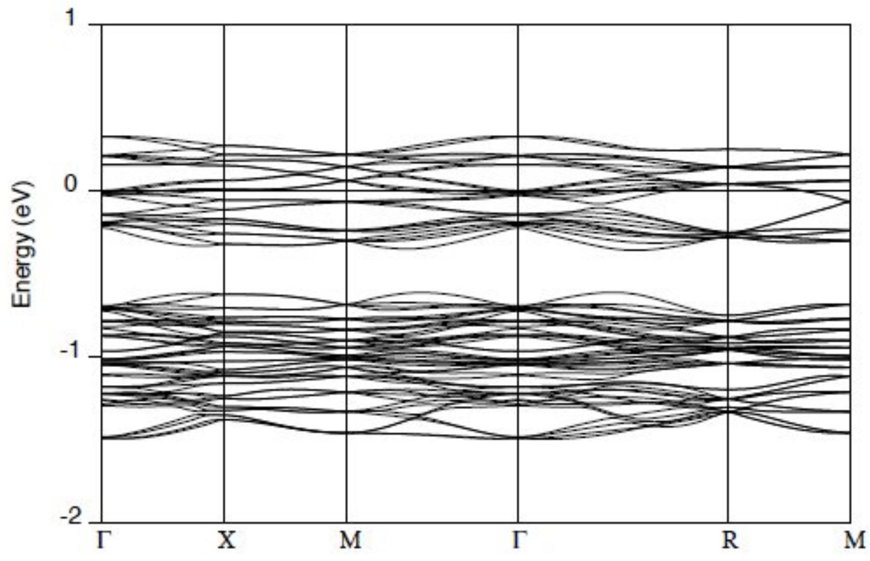
No spin-orbit



Spin-orbit

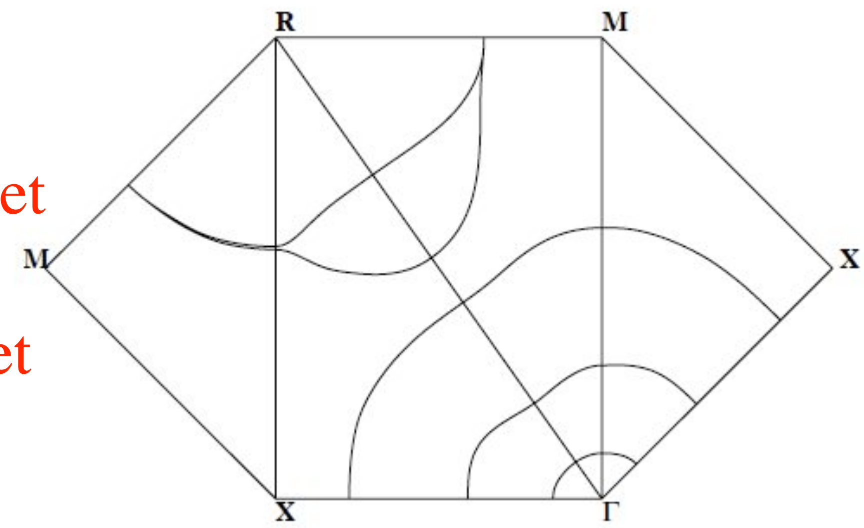
Norman & Micklitz, PRB 81, 024428 (2010)

LDA (spin-orbit)

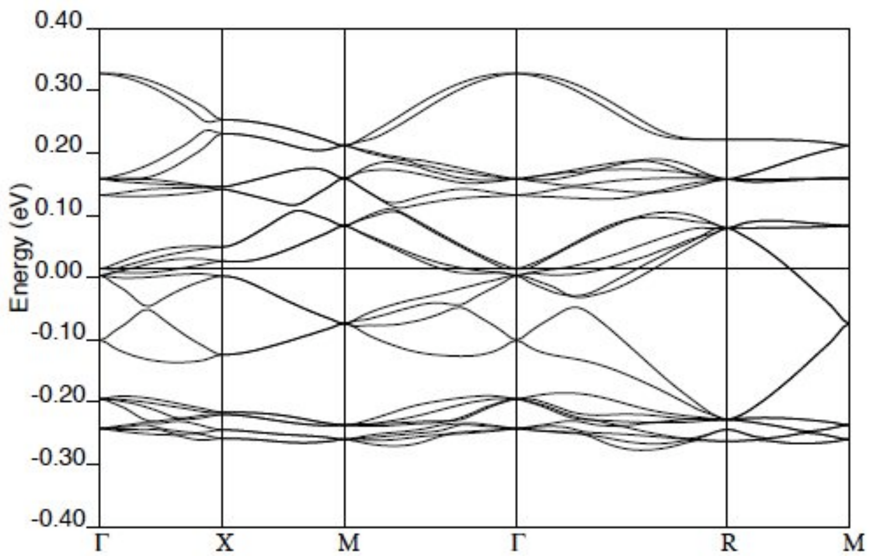


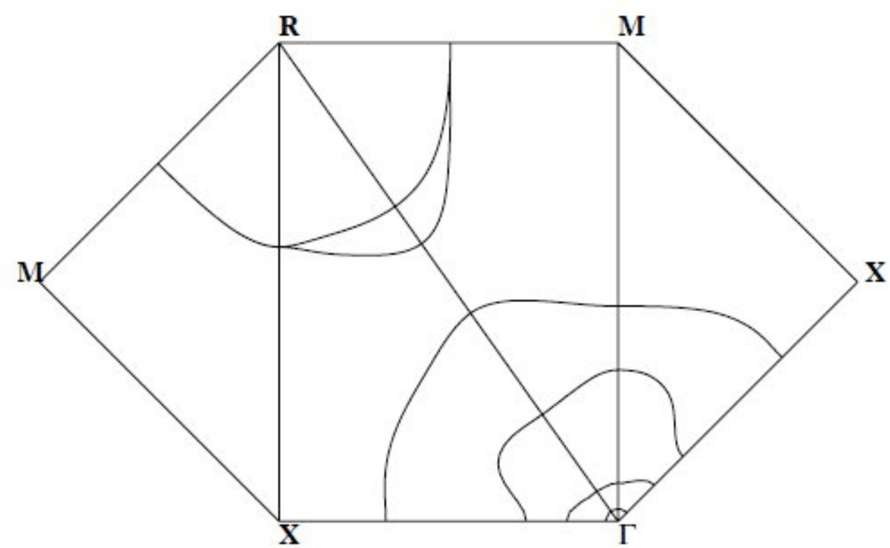
doublet

quartet



Tight Binding Fit





Direct Ir-Ir Exchange is Isotropic!

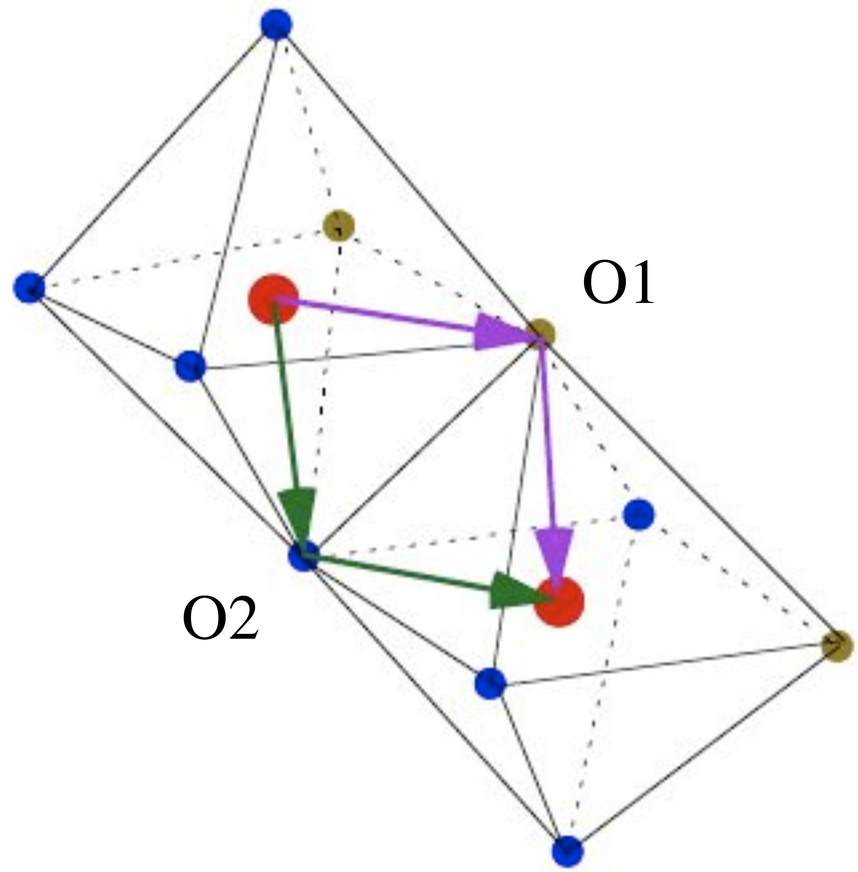
J = 4 t^2/U

where

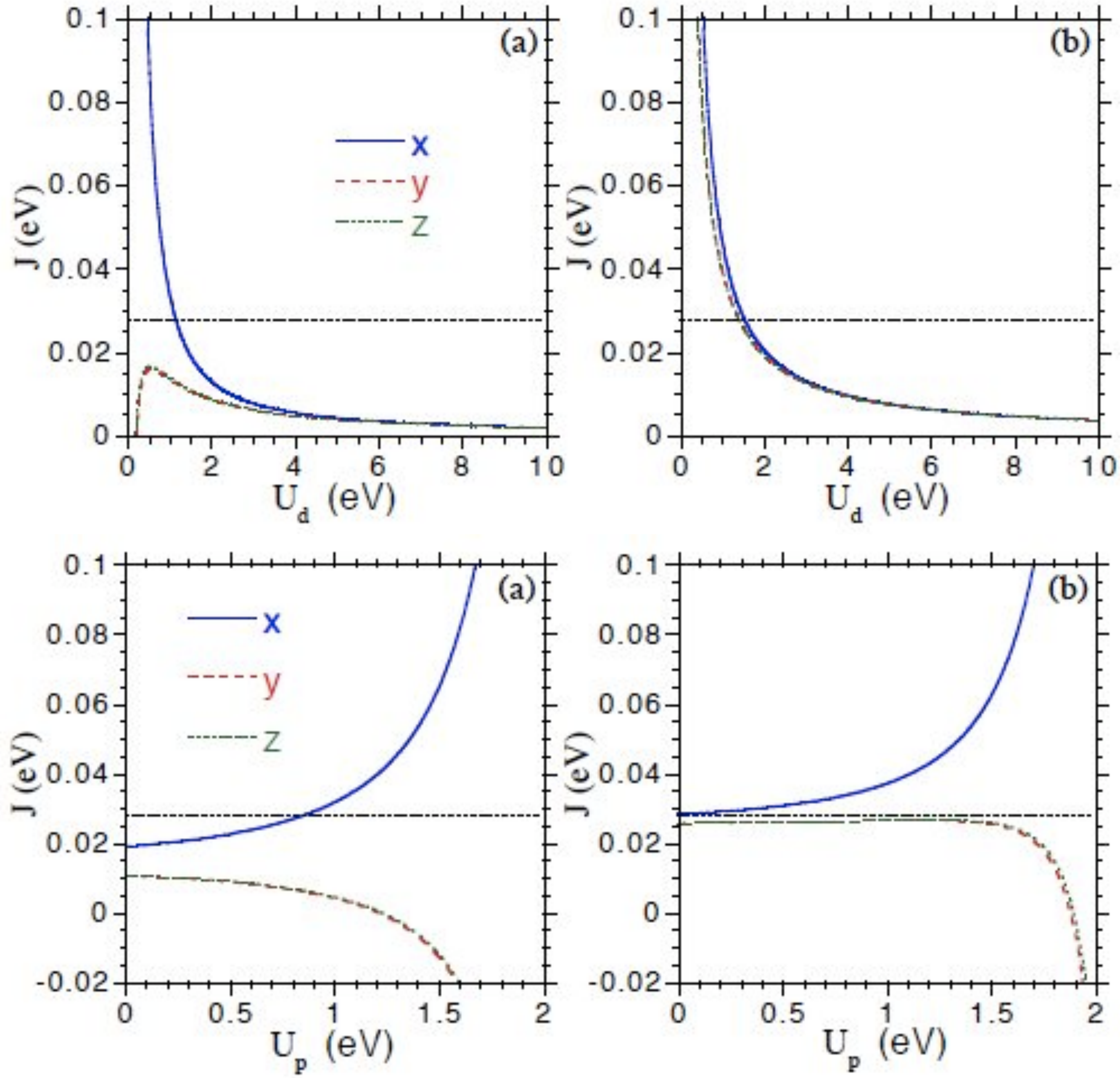
$$t = \frac{1}{4}t^{\sigma}_{dd} + \frac{1}{3}t^{\pi}_{dd} + \frac{5}{12}t^{\delta}_{dd}$$

But superexchange is present which should gives rise to anisotropic exchange plus Dzyaloshinskii-Moriya

Superexchange



Total Exchange versus U_d and U_p for two tight binding fits



<- exp.

How to Detect a Spinon Fermi Surface

Norman & Micklitz, PRL 102, 067204 (2009)

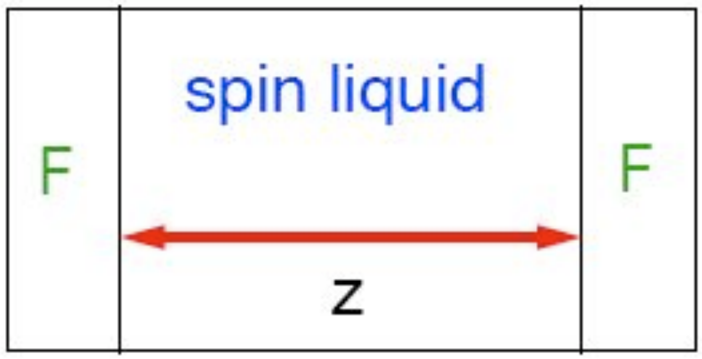


FIG. 1: (Color online) The proposed experiment involves two ferromagnetic layers (F) with a spin liquid spacer of variable thickness, z. Depending on the sign of the oscillatory coupling, the two ferromagnets will be aligned or anti-aligned.

Parkin *et al.*, PRL 64, 2304 (1990)

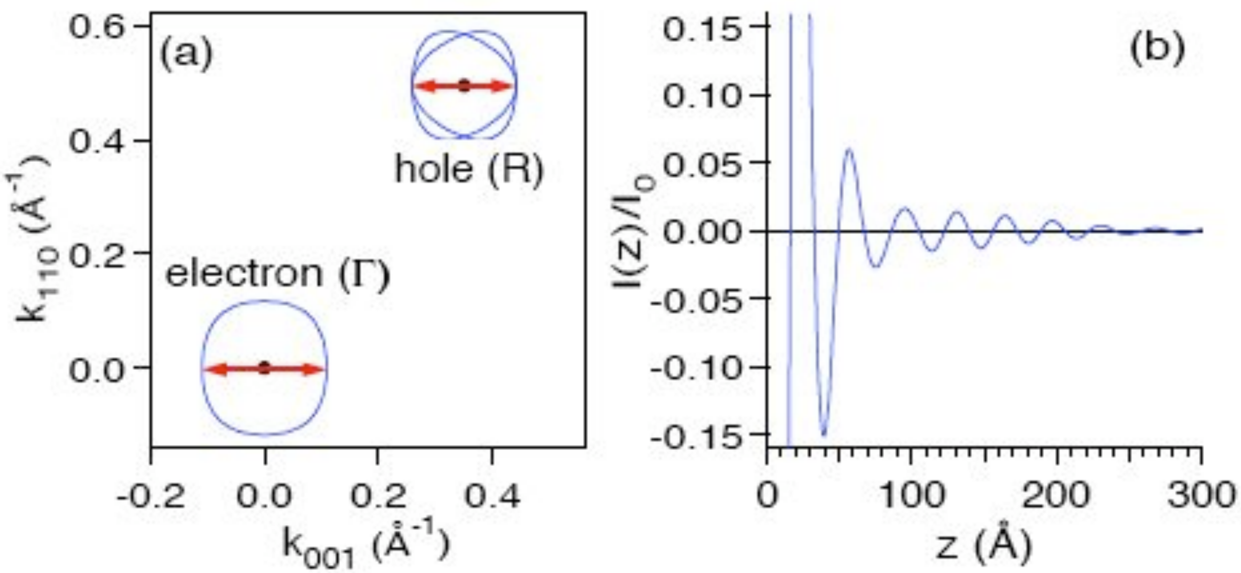


FIG. 3: (Color online) (a) Spinon Fermi surface for $Na_4Ir_3O_8$ (a=8.985Å). Spanning vectors are indicated by arrows. (b) Calculated oscillatory response from Eq. 7.

$$I(z) = I_0(\frac{d}{z})^2 \sum_n \frac{m_n^*}{m} \sin(2k_{Fn}z)$$

Bruno & Chappert, PRB 46, 261 (1992)

Cuprates are Mott insulators characterized by a half filled band and have a large J

So are iridates!

Can iridates be doped, and if so, will they become high temperature superconductors?