The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

2253-11

Workshop on Synergies between Field Theory and Exact Computational Methods in Strongly Correlated Quantum Matter

24 - 29 July 2011

General, realistic, and interesting models of correlated quantum systems

L. Balents

Kavli Institute for Theoretical Physics
University of California Santa Barbara
Santa Barbara, CA
U.S.A.

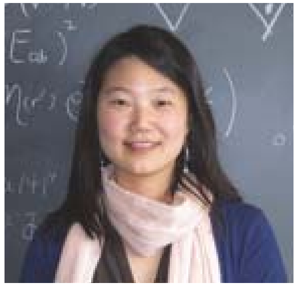
General, realistic, and interesting models of correlated quantum systems

Leon Balents, KITP, UCSB

Synergies between Field Theory and Exact Computational Methods in Strongly Correlated Quantum Matter, Trieste, July 2011

Collaborators

Lucile Savary
UCSB/ENS Lyon



SungBin Lee
UCSB

Shigeki Onoda
RIKEN

Gang Chen
U. Colorado

Kate Ross

Bruce Gaulin

McMaster

Theory institute

Models!

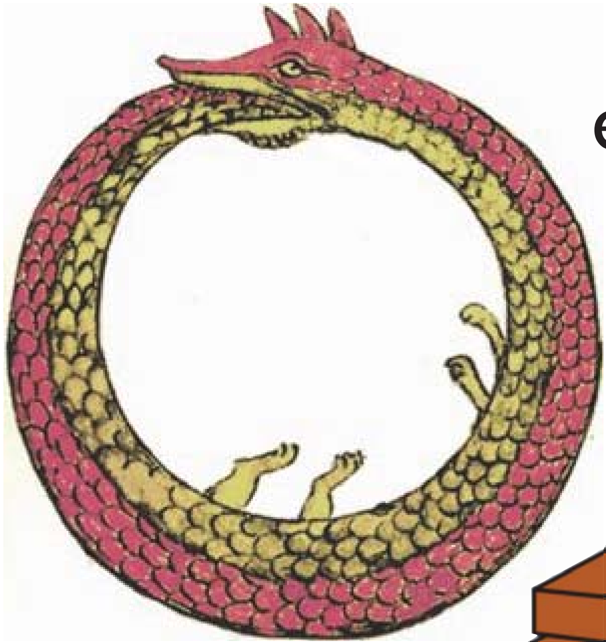
- Def for this talk: "model" = a Hamiltonian significantly simpler than realistic electrons +atoms

Models!

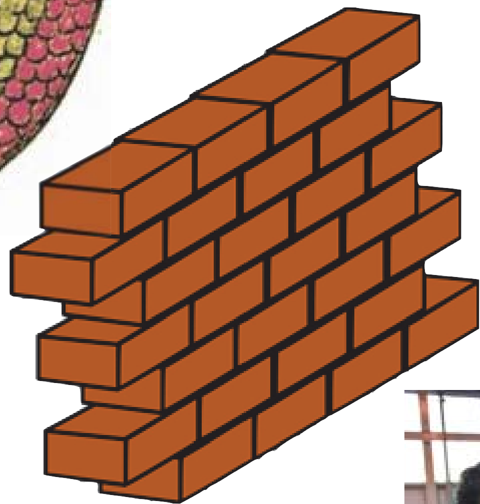
- Models are wonderful:
  - Glorious history: Ising model, Bethe chain, O(n) model...
  - Enable our primitive classical brains to understand something
  - Less degrees of freedom means more chance of successful simulation
  - Not shackled by the constraints of the real world

Just playing around

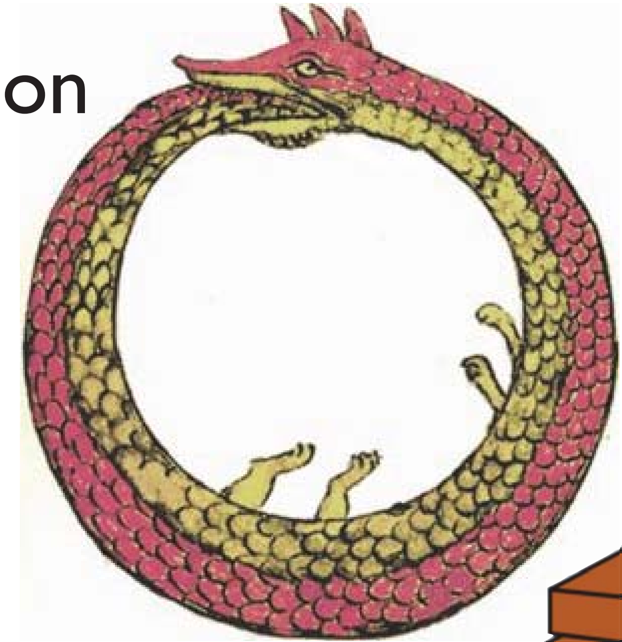
field theory



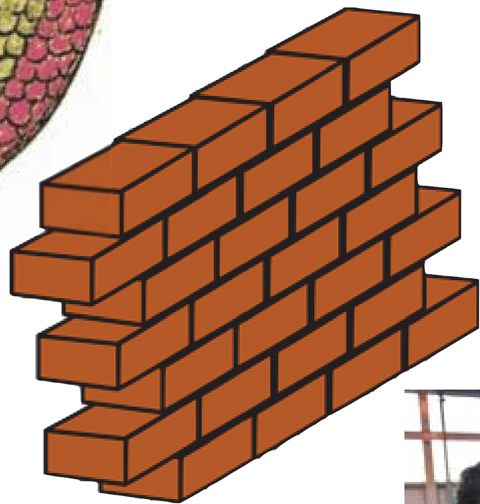
exact computation



exact computation

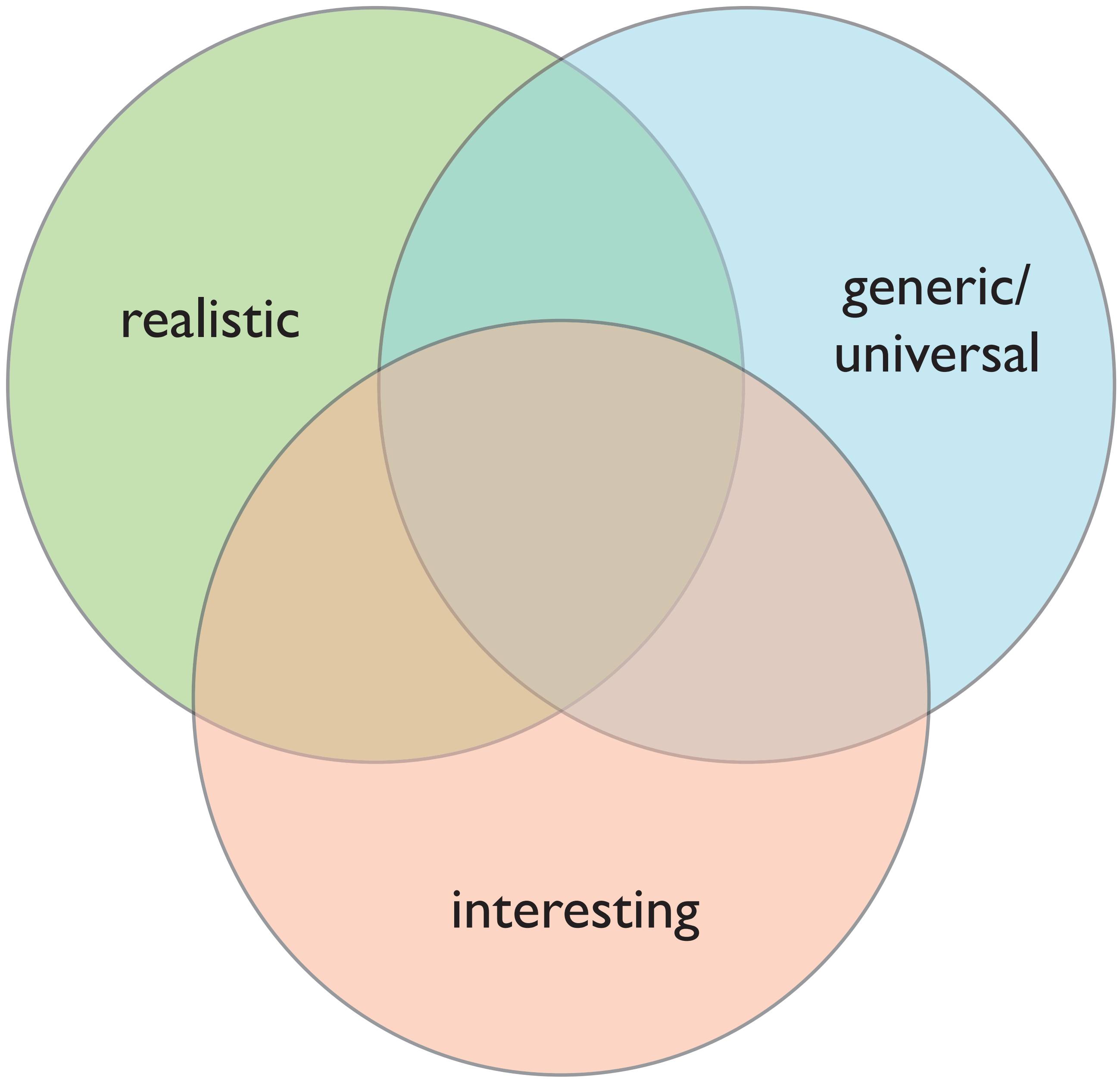


field theory



How to choose?

- Some criteria
  - universal
  - realistic
  - interesting


realistic
generic/
universal
interesting

How to choose?

- Some criteria
  - universal
  - realistic
  - interesting
- Better: addresses a significant scientific problem

Problems

- QCPs in itinerant fermi systems
  - Learning to simulate these is an important goal for numerics
  - c.f. F. Assaad's talk this afternoon

Problems

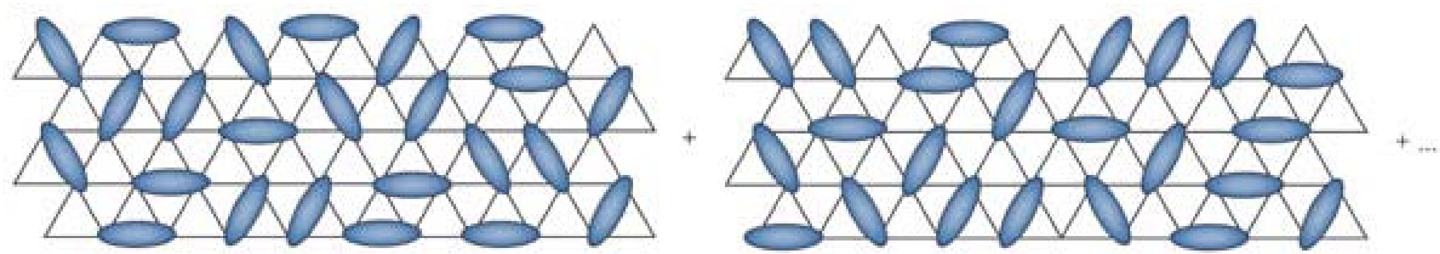
- QCPs in itinerant fermi systems
- Quantum spin liquids (QSLs)
- Mott insulators with strong spin-orbit coupling

Quantum Spin Liquid

- A system of interacting local moments with a non-magnetic ground state breaking no symmetries
- A ground state exhibiting an emergent gauge structure that supports exotic excitations with fractional quantum numbers and/or non-local emergent statistical interactions

Theoretical phenomenology

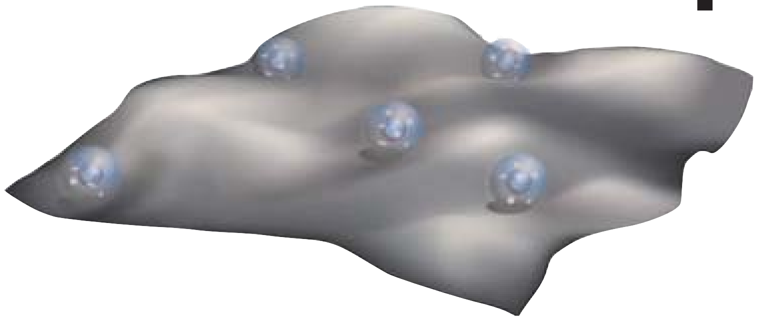
- Resonating valence bonds: singlet pairs

$\Psi =$ 

  - "long range entanglement"

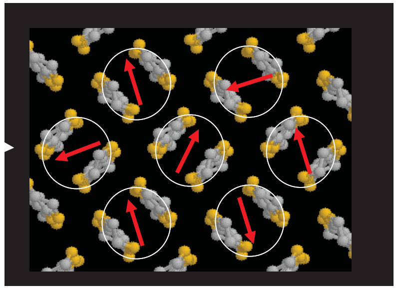
- Effective field theories of many such states can be constructed from slave particle methods, and constitute a large family of lattice gauge theories

The "landscape"



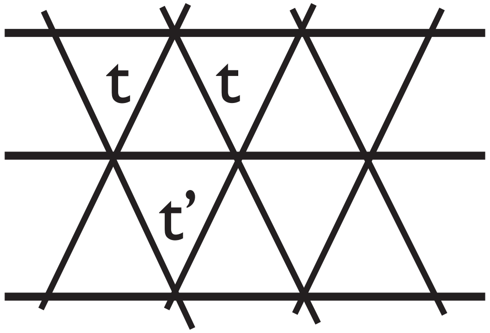
- The number of distinct Quantum Spin Liquid (QSL) *phases* is huge
  - e.g. X.G. Wen has classified *hundreds* of different QSL states all with the same symmetry on the square lattice (and this is *not* a complete list!)
  - In principle we should have lots of states to compare with experiment
  - most of these states are "understood" at least as far as their qualitative low temperature thermodynamics

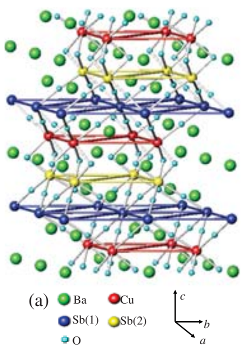
d>1 QSL materials



κ-(BEDTTTF)$_2$Cu$_2$(CN)$_3$

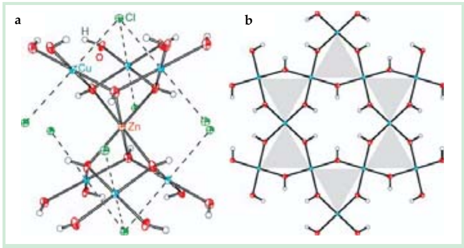
EtMe$_3$Sb[Pd(dmit)$_2$]$_2$



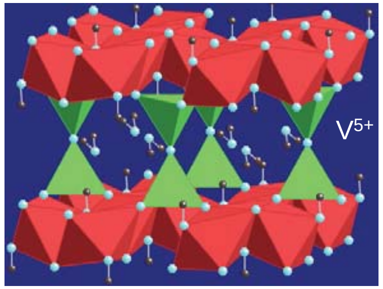


Ba$_3$CuSb$_2$O$_9$

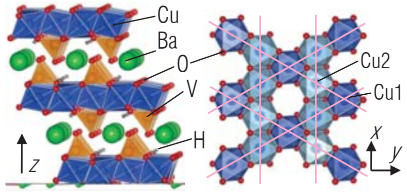
...



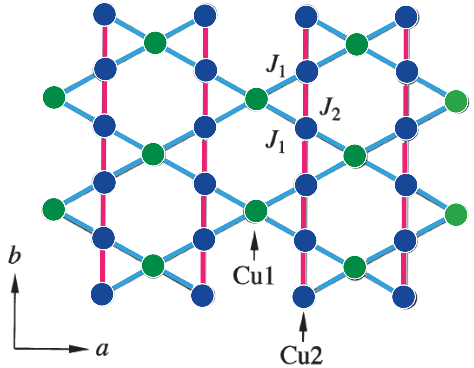
herbertsmithite

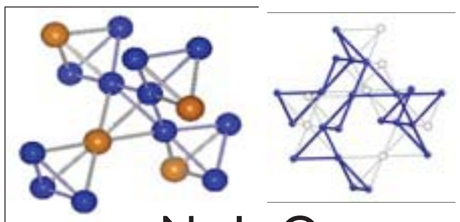


volborthite

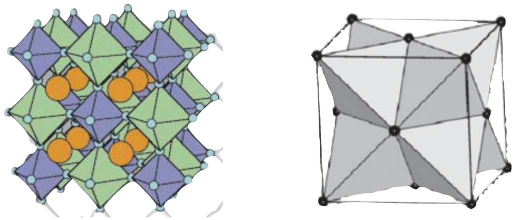


vesignieite

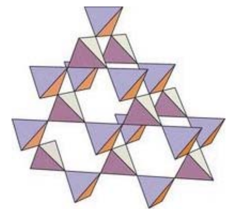




Na$_4$Ir$_3$O$_8$



Ba$_2$YMoO$_6$



A$_2$B$_2$O$_7$

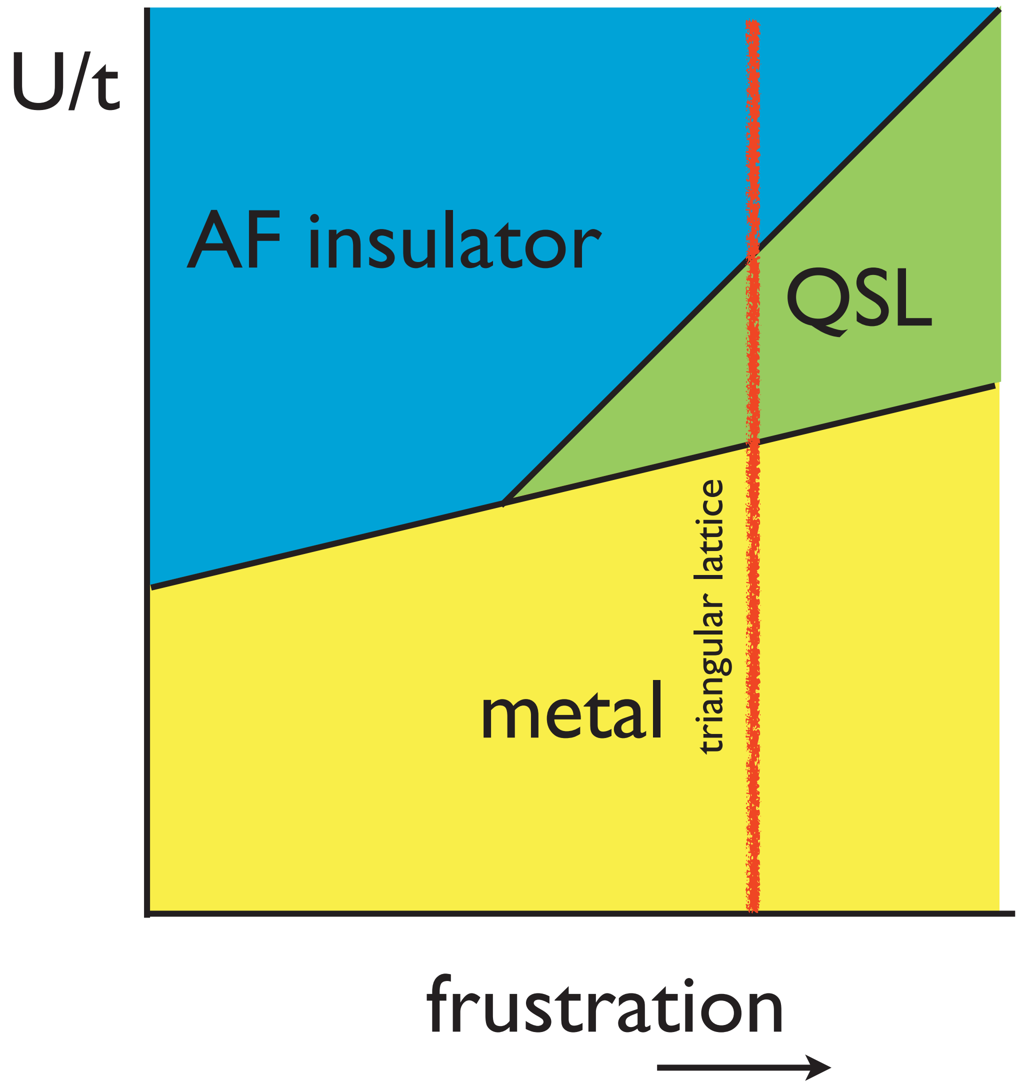
QSL Models

- Proof of principle examples
  - dimers (Moessner/Sondhi, ...)
  - XXZ (BFG, Melko *et al*, ...)
  - bosons (Motrunich/Senthil, ...)

QSL Models

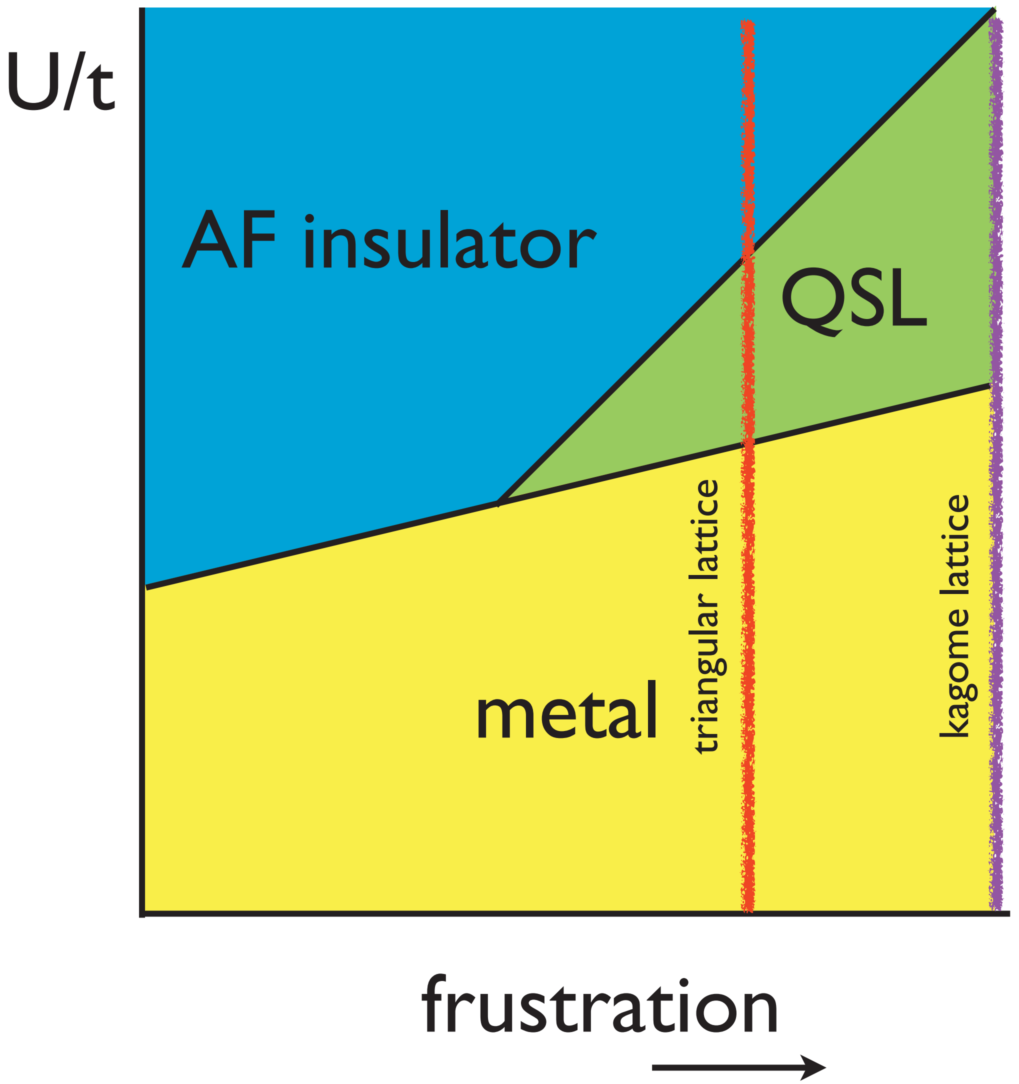
- More realistic
    - Heisenberg antiferromagnet
        - popular theories for kagome lattice: predicts gapped Z_2 or gapless Dirac "algebraic spin liquid" state
    - Hubbard/ring exchange models
        - popular theory associates spinon Fermi surface state with semi-itinerant regime near the Mott transition on the triangular lattice

“Standard” view



c.f. Thursday morning talks

“Standard” view



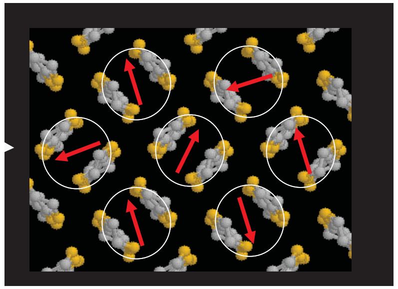
Status

- *None* of the theoretical QSLs is a compelling match to experiment, e.g:
  - little connection to intermediate to high energy physics of experiment
  - problems with aspects of low energy response
  - recent experiments on strong insulator $Ba_3CuSb_2O_9$ suggest behavior previously linked to itinerancy may not be

Status

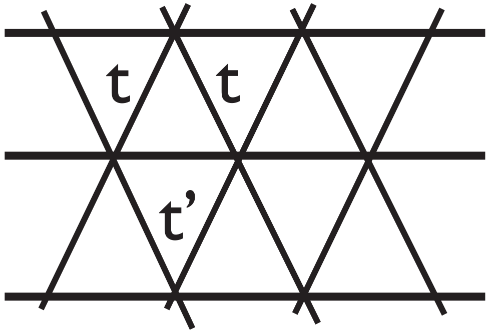
- Role for numerics+field theory:
  - *Relevant* models of QSLs and/or QSL candidate materials
  - *Quantitative* comparisons to experiment to sharpen the questions

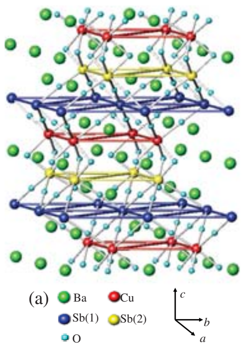
d>1 QSL materials



κ-$(BEDTTTF)_2Cu_2(CN)_3$

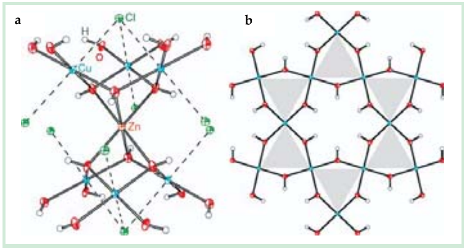
$EtMe_3Sb[Pd(dmit)_2]_2$



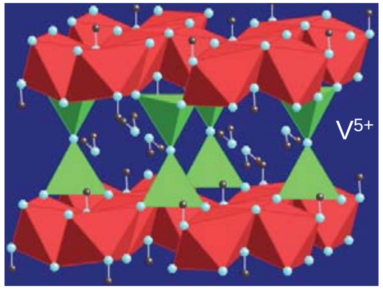


$Ba_3CuSb_2O_9$

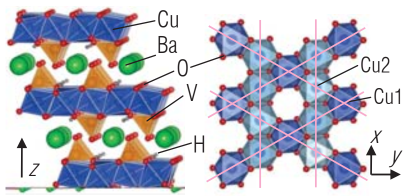
...



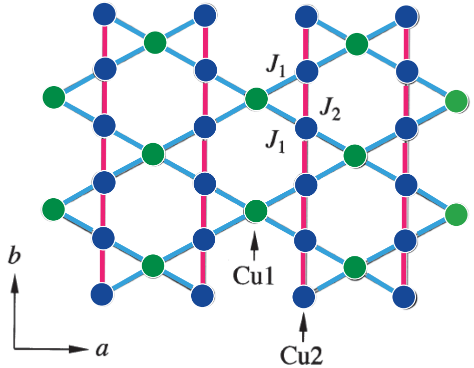
herbertsmithite



volborthite



vesignieite



Do we really understand the models and materials?

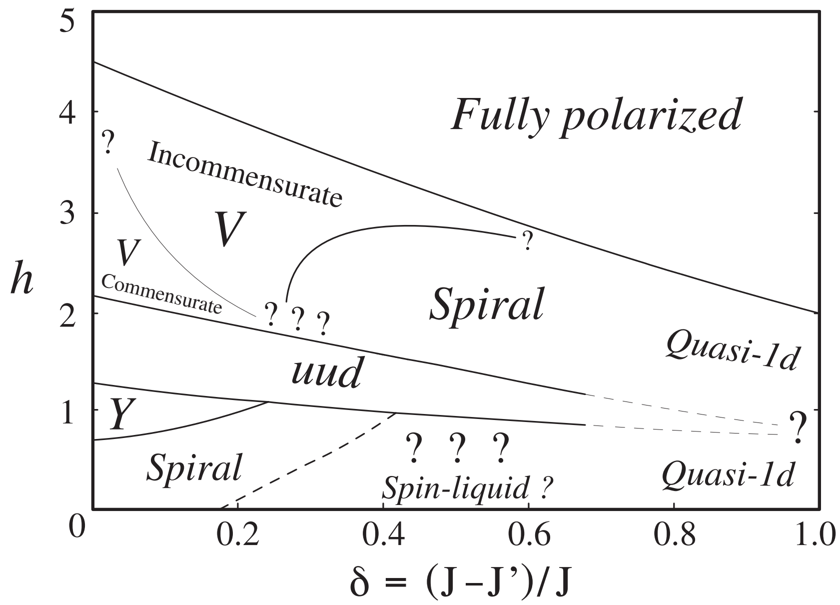
Model Issues

- Unknowns:
  - spatial anisotropy
  - 3d coupling
  - Dzyaloshinskii-Moriya
  - itinerancy
  - disorder
- Dialog between theory and experiment is necessary to sharpen the comparison

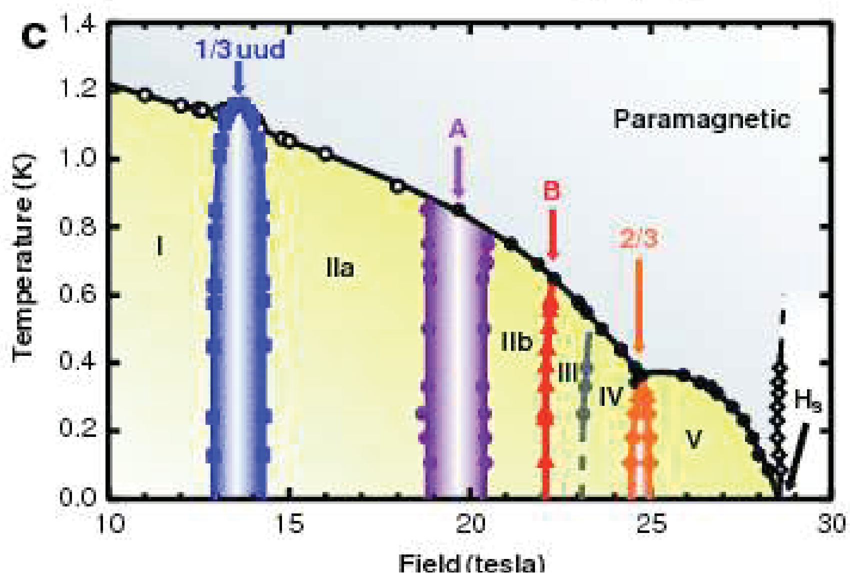
Connecting to experiment

- Apart from obviously trying to search for and study QSL ground states, one can try to make other very useful comparisons
  - Magnetization process
  - Neutron scattering (here we are mostly lacking experimental data)

Triangular



Tay, Motrunich 2010

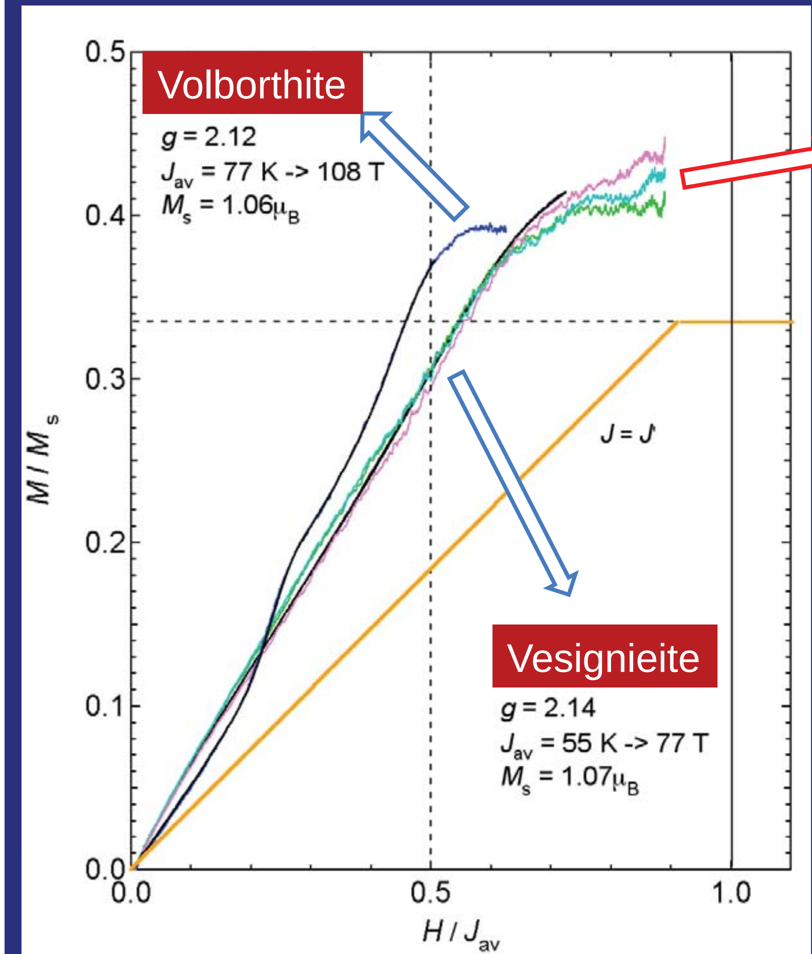


Cs_2CuBr_4: Fortune *et al*, 2009

Rich intermediate field features put strong constraints on anisotropy, DM

Kagome

Magnetization plateau at over 1/3



Commonly to two kagomes:

- Plateau or a vicinal slope at ~$0.4M_s$ above $M_s/3$
- Small plateau fields

Probably not due to spatial anisotropy but ...

Intrinsic for the *S*-1/2 KAFM?

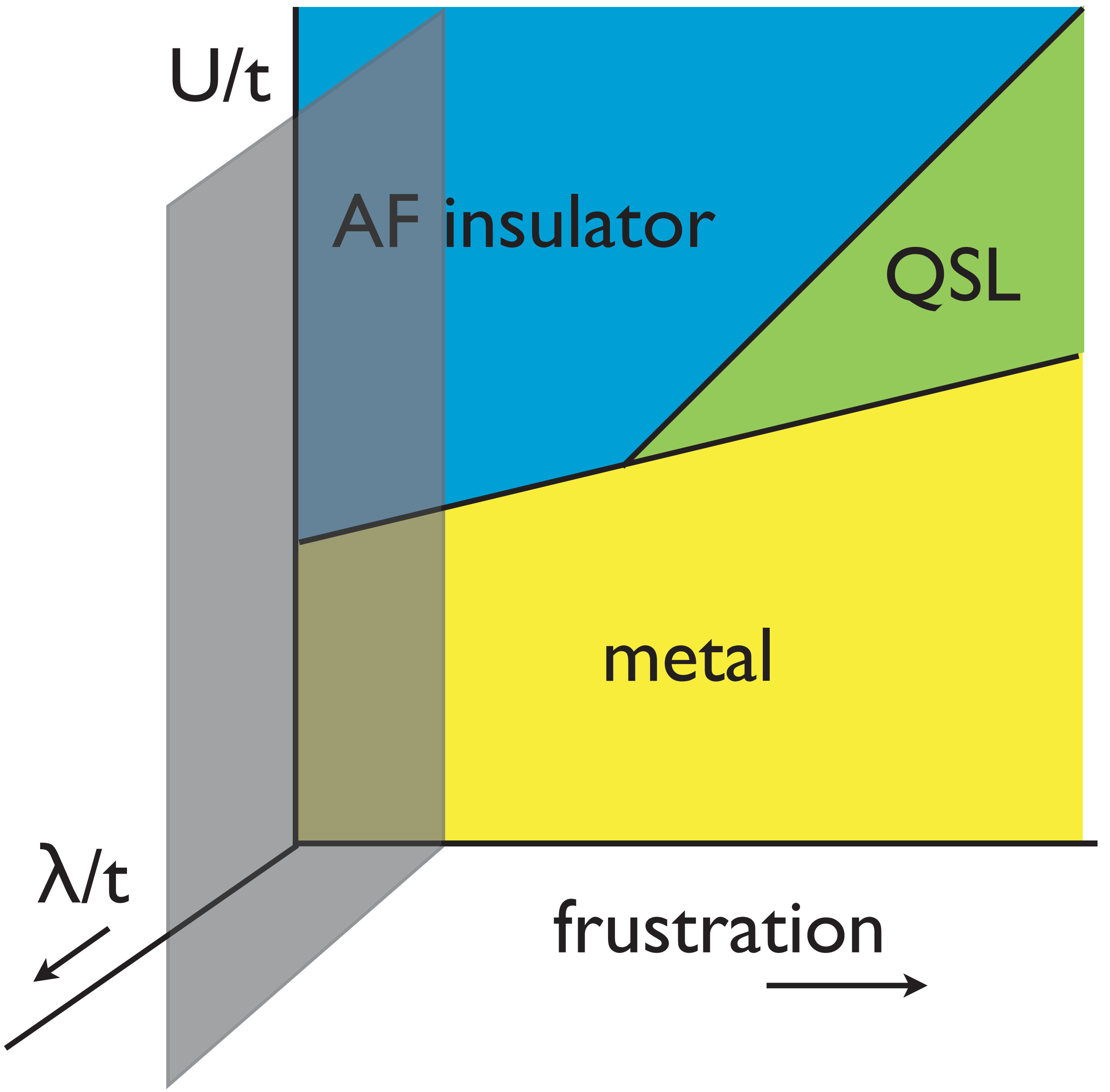
Z. Hiroi

H<70T

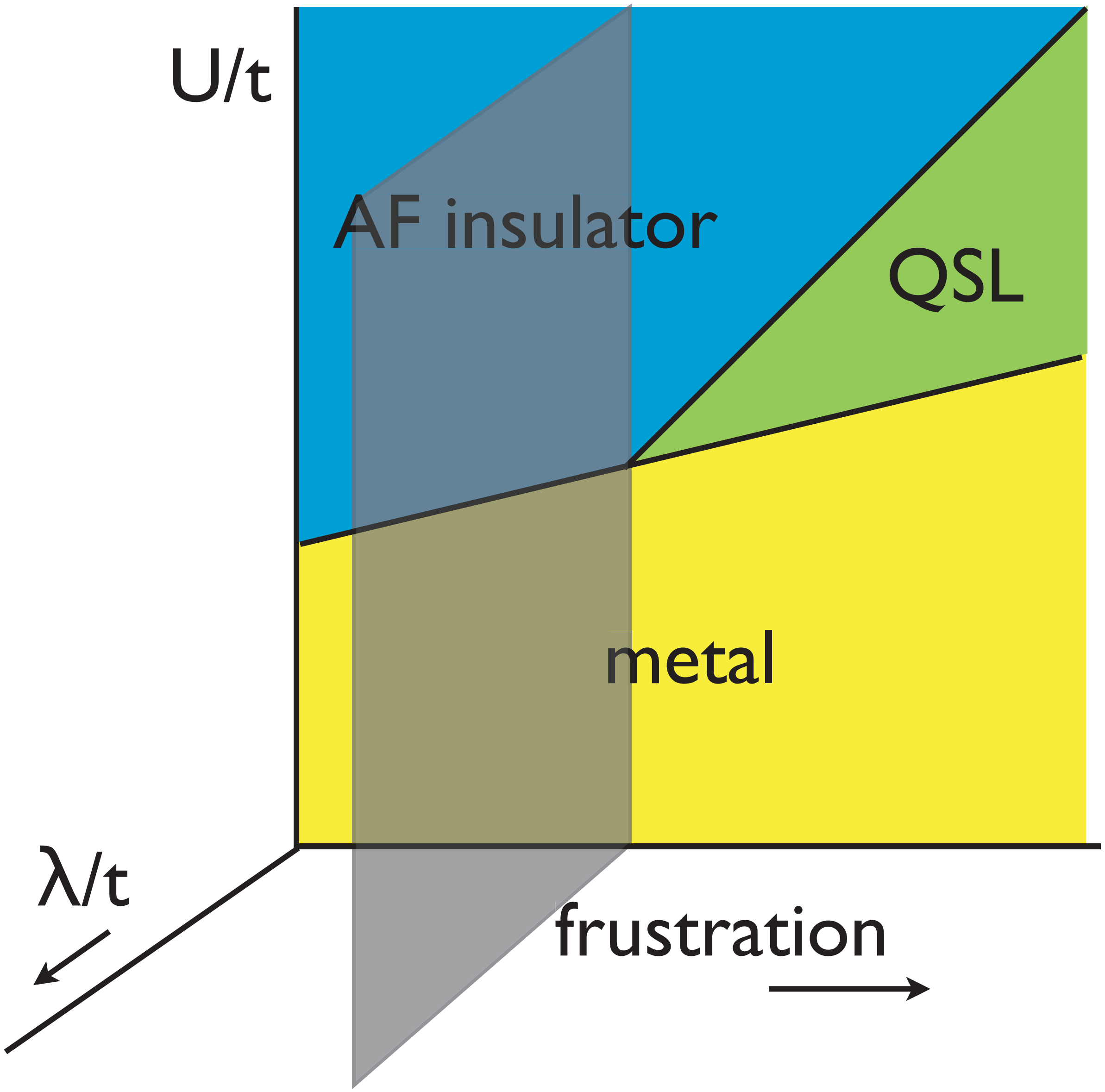
Problems

- QCPs in itinerant fermi systems
- Quantum spin liquids (QSLs)
- Mott insulators with strong spin-orbit coupling

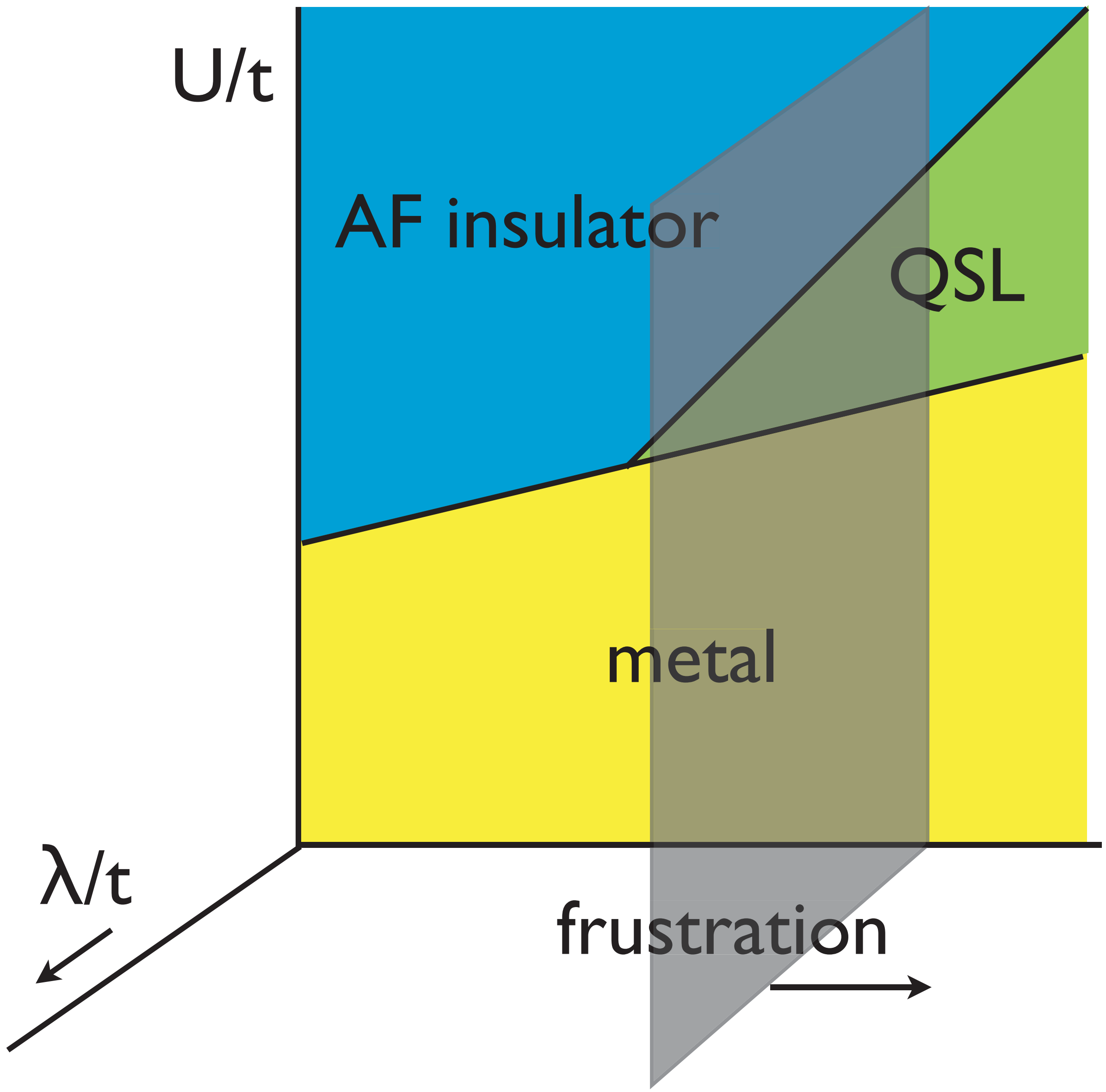
Another axis



Another axis

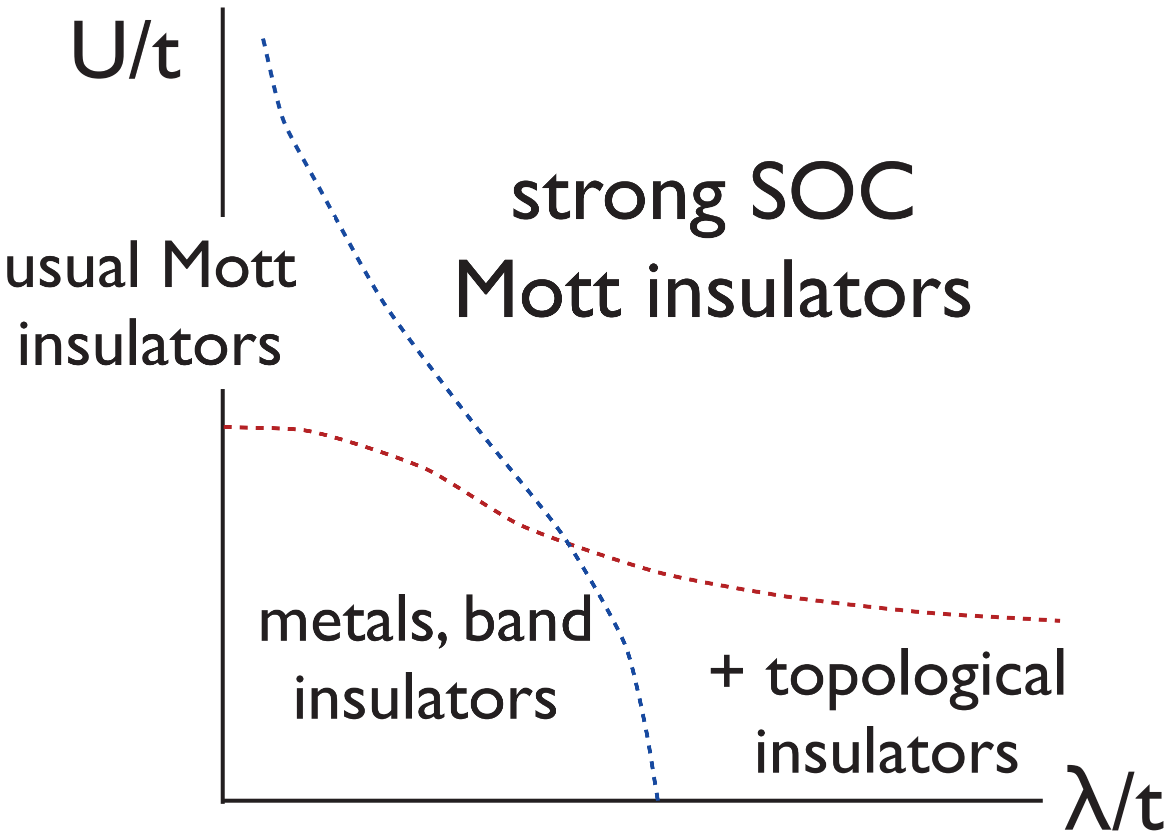


Another axis



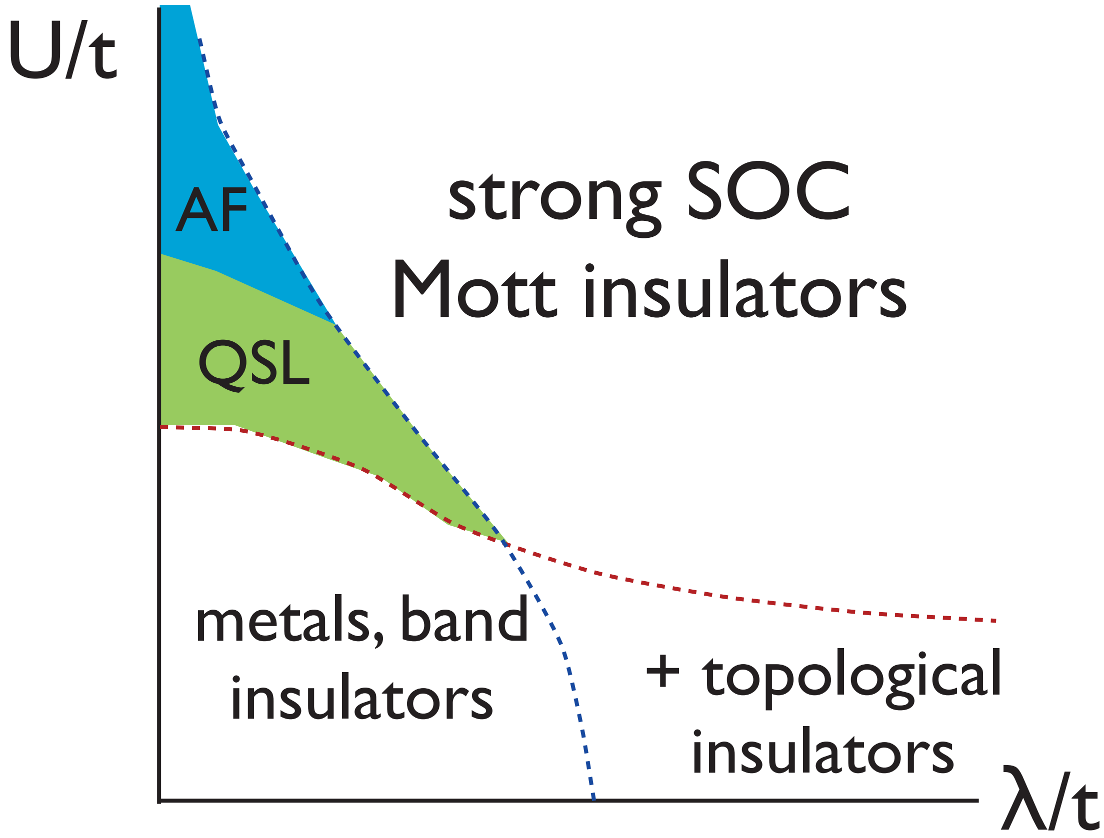
Another axis

- Schematic phase diagram from Pesin +Balents, 2010



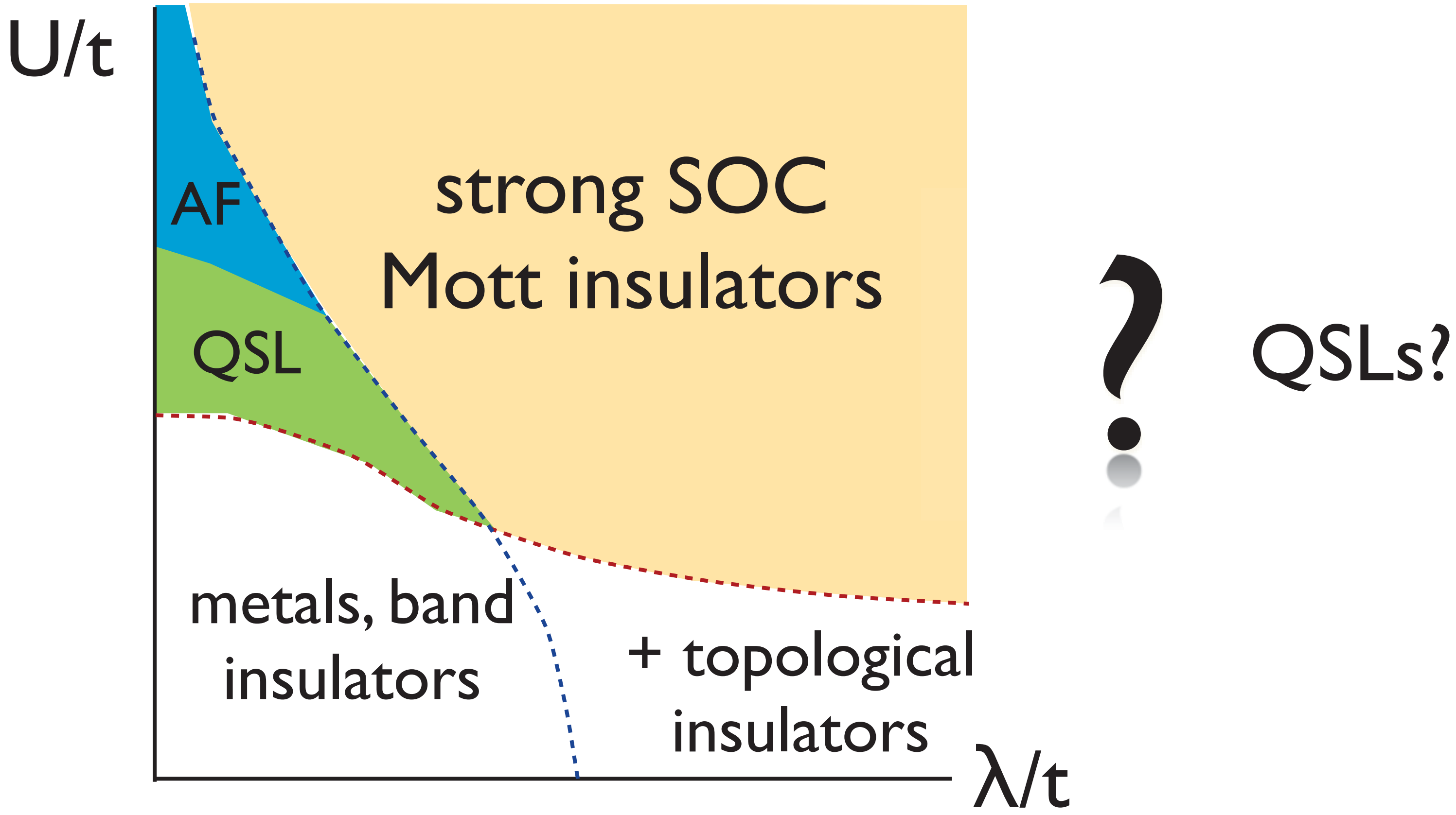
Another axis

- Schematic phase diagram from Pesin +Balents, 2010



Another axis

- Schematic phase diagram from Pesin +Balents, 2010

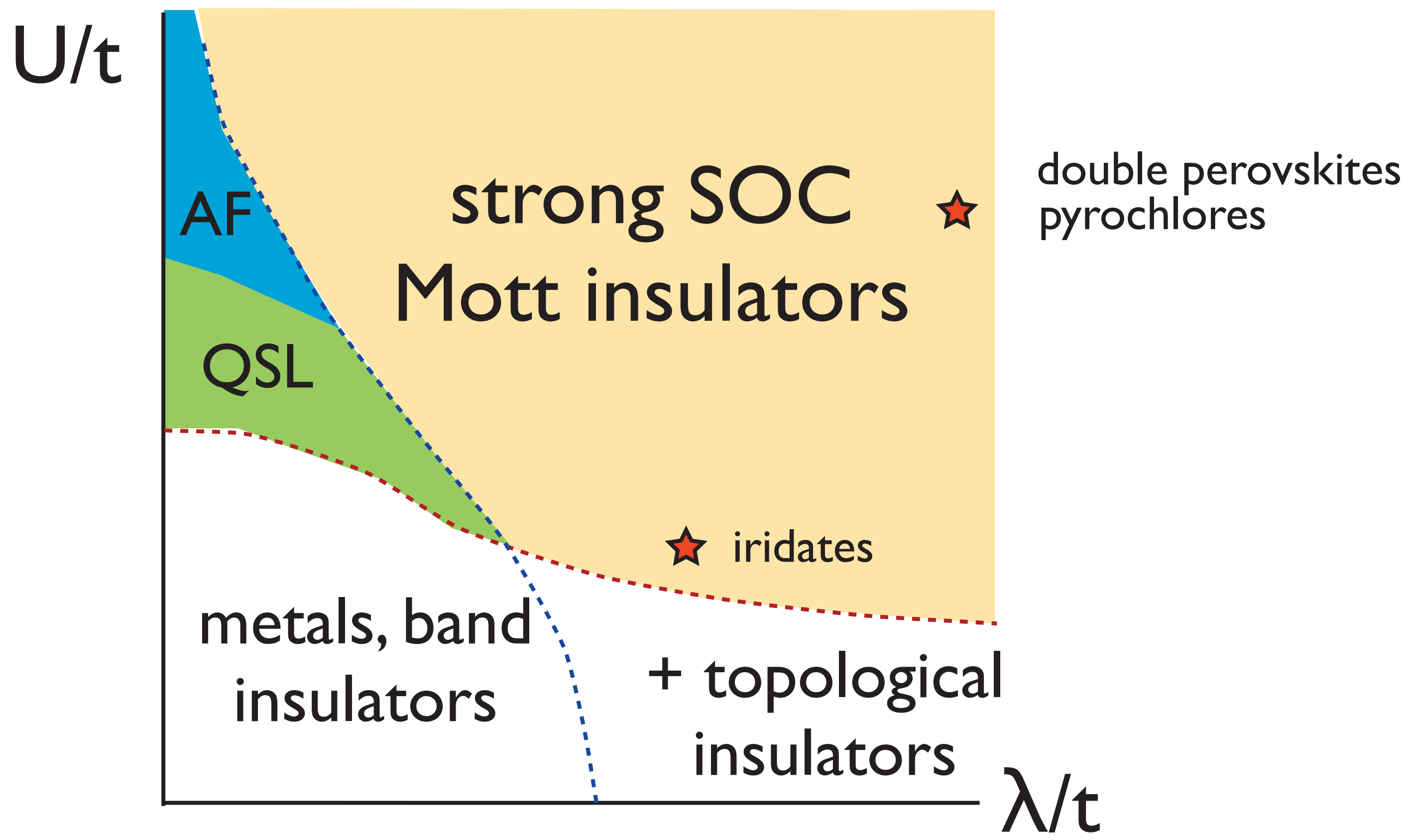


Strong SOC

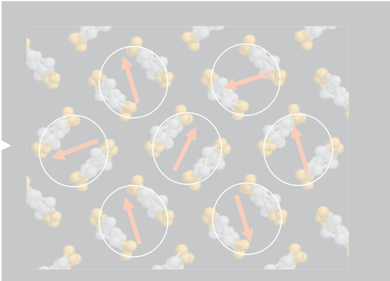
- Strong SOC may sometimes encourage quantum spin liquid behavior by
  - inducing strong multipolar interactions that enhance quantum fluctuations
  - creating specific Ising-like couplings that are extremely frustrated
- Even more novel spin-orbit coupled states are possible in the intermediate correlation regime, near the Mott transition

Another axis

- Schematic phase diagram from Pesin +Balents, 2010

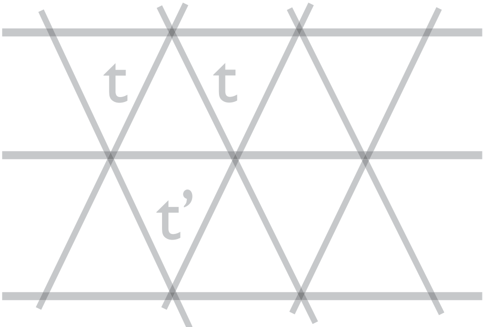


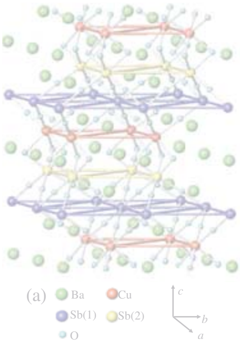
d>1 QSL materials



κ-(BEDTTTF)$_2$Cu$_2$(CN)$_3$

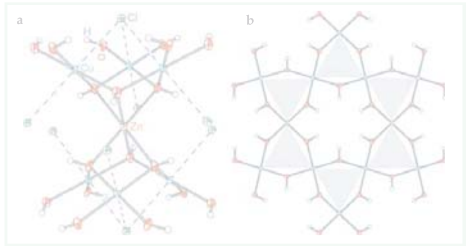
EtMe$_3$Sb[Pd(dmit)$_2$]$_2$



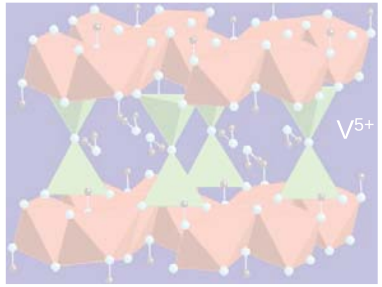


Ba$_3$CuSb$_2$O$_9$

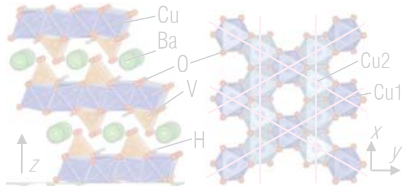
...



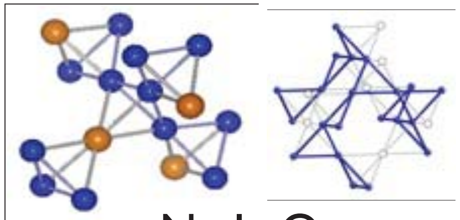
herbertsmithite



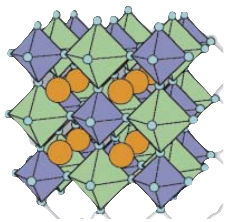
volborthite

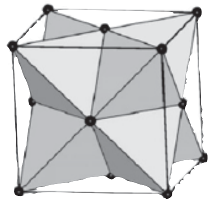


vesignieite

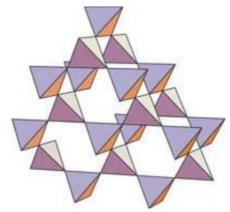


Na$_4$Ir$_3$O$_8$





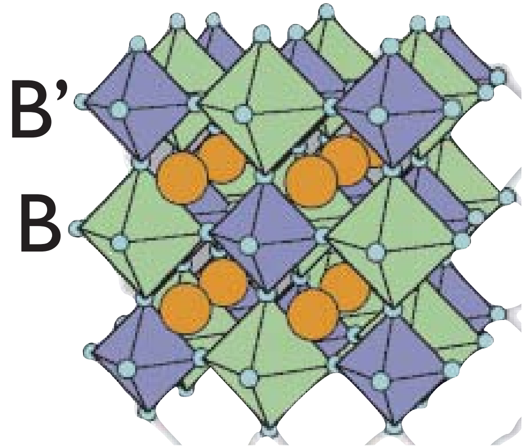
Ba$_2$YMoO$_6$



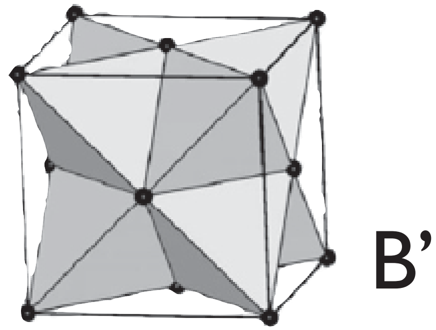
A$_2$B$_2$O$_7$

Rock salt double perovskites

$A_2BB'O_6$



fcc lattice

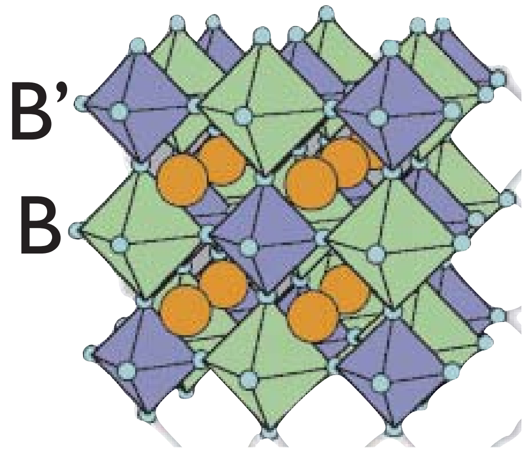


Material	B'	Θ_{CW}
Ba_2YMoO_6	Mo^{5+} ($4d^1$)	-90K to -219K
La_2LiMoO_6	Mo^{5+} ($4d^1$)	-45K
Sr_2MgReO_6	Re^{6+} ($5d^1$)	-426K
Sr_2CaReO_6	Re^{6+} ($5d^1$)	-443K
Ba_2CaReO_6	Re^{6+} ($5d^1$)	-40K
Ba_2LiOsO_6	Os^{7+} ($5d^1$)	-40K
Ba_2NaOsO_6	Os^{7+} ($5d^1$)	-10K to -32K

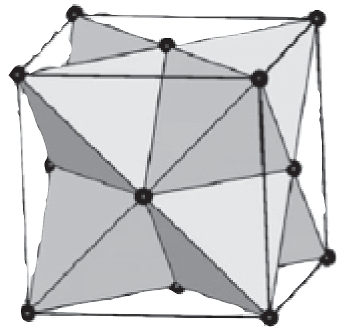
Cussen *et al* (2006)
de Vries *et al* (2010)
Aharen *et al* (2010)
Wiebe *et al* (2003)
Wiebe *et al* (2002)
Yamamura *et al* (2006)
Stitzer *et al* (2002)
Erickson *et al* (2007)

Rock salt double perovskites

$A_2BB'O_6$



fcc lattice



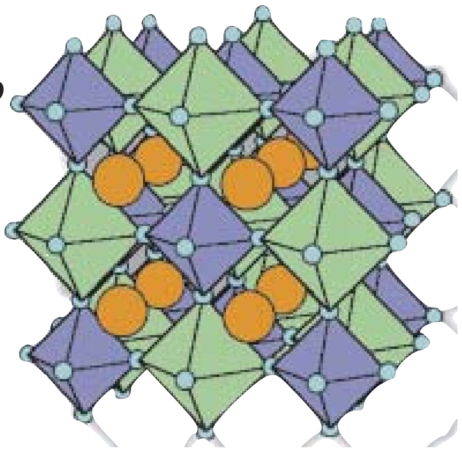
Material	B'	Θ_{CW}
Ba_2YMoO_6	Mo^{5+} ($4d^1$)	-90K to -219K
La_2LiMoO_6	Mo^{5+} ($4d^1$)	-45K
Sr_2MgReO_6	Re^{6+} ($5d^1$)	-426K
Sr_2CaReO_6	Re^{6+} ($5d^1$)	-443K
Ba_2CaReO_6	Re^{6+} ($5d^1$)	-40K
Ba_2LiOsO_6	Os^{7+} ($5d^1$)	-40K
Ba_2NaOsO_6	Os^{7+} ($5d^1$)	-10K to -32K

λ~100meV

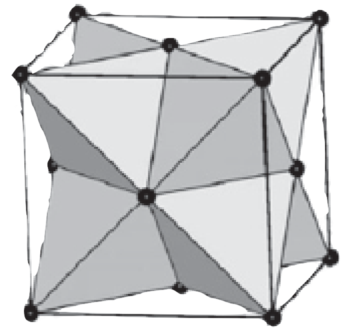
λ~400meV

Rock salt double perovskites

$A_2BB'O_6$



fcc lattice



Material	B'	Θ_{CW}
Ba_2YMoO_6	Mo^{5+} ($4d^1$)	-90K to -219K
La_2LiMoO_6	Mo^{5+} ($4d^1$)	-45K
Sr_2MgReO_6	Re^{6+} ($5d^1$)	-426K
Sr_2CaReO_6	Re^{6+} ($5d^1$)	-443K
Ba_2CaReO_6	Re^{6+} ($5d^1$)	-40K
Ba_2LiOsO_6	Os^{7+} ($5d^1$)	-40K
Ba_2NaOsO_6	Os^{7+} ($5d^1$)	-10K to -32K

no order down to 2K

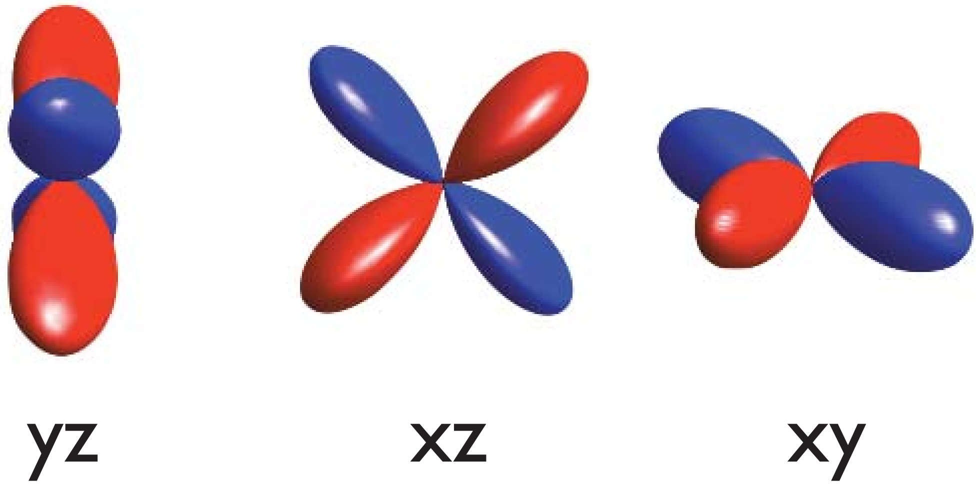
λ~400meV

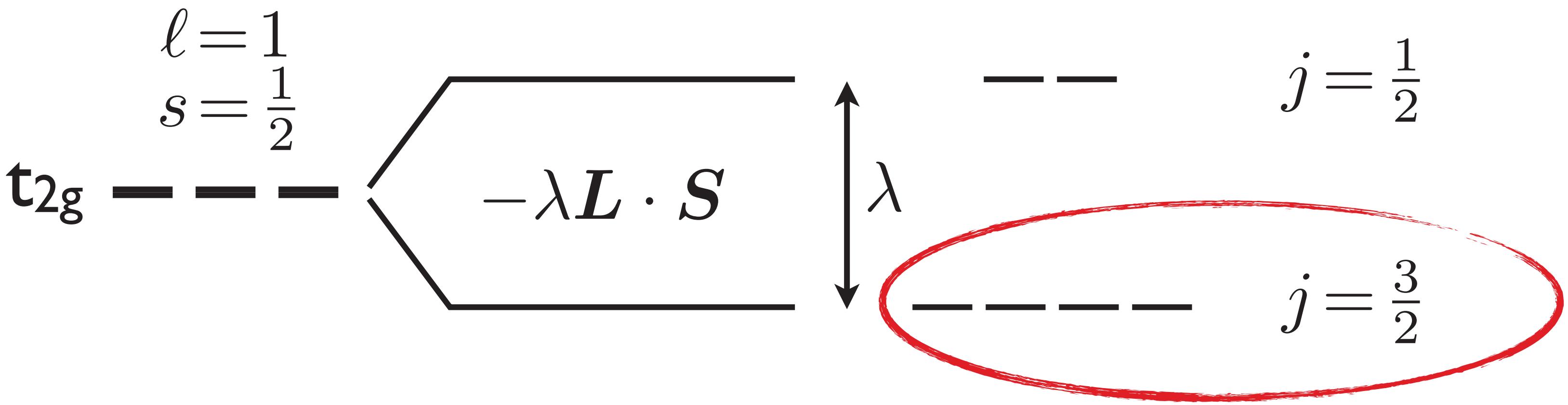
Single ion physics

t_{2g} orbitals

= effective l=1 orbital angular momentum

$$P_{t_{2g}} \boldsymbol{L}_{\ell=2} P_{t_{2g}} = -\boldsymbol{L}_{\ell=1}$$





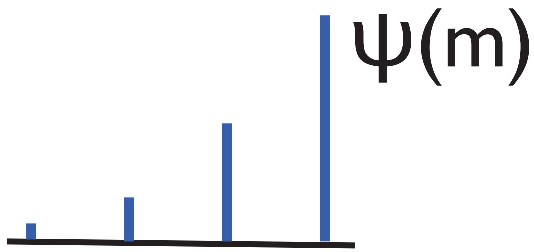
Quantum fluctuations

- Usually s>1 spins are expected to be rather classical - why?

$$\boldsymbol{j}_i \cdot \boldsymbol{j}_j = j_i^z j_j^z + \frac{1}{2}(j_i^+ j_j^- + j_i^- j_j^+)$$

- Exchange induces only $j^z = \pm 1$ transitions

m = $-\frac{3}{2}$ $-\frac{1}{2}$ $\frac{1}{2}$ $\frac{3}{2}$



Spin wavefunction is peaked around classical state

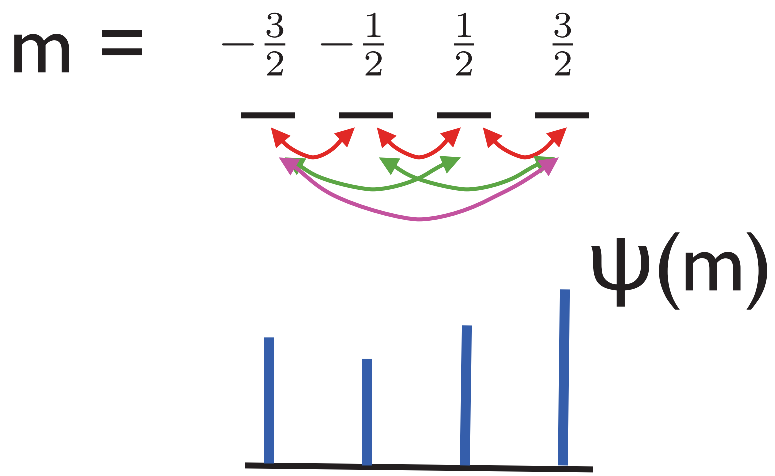
Quantum fluctuations

- Higher order exchange

c.f. G. Chen *et al*, PRB **80**,174440 (2010).

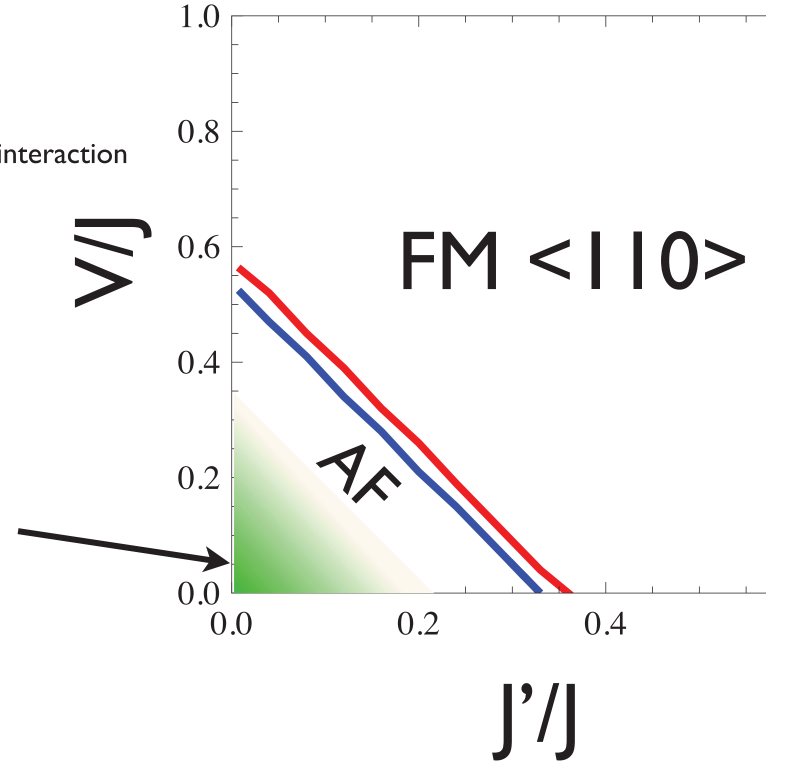
$$H \sim j_i^+ j_j^- + (j_i^+)^2 (j_j^-)^2 + (j_i^+)^3 (j_j^-)^3 + \cdots$$

- Exchange induces $\Delta j^z = \pm 1, \pm 2, \pm 3$ transitions

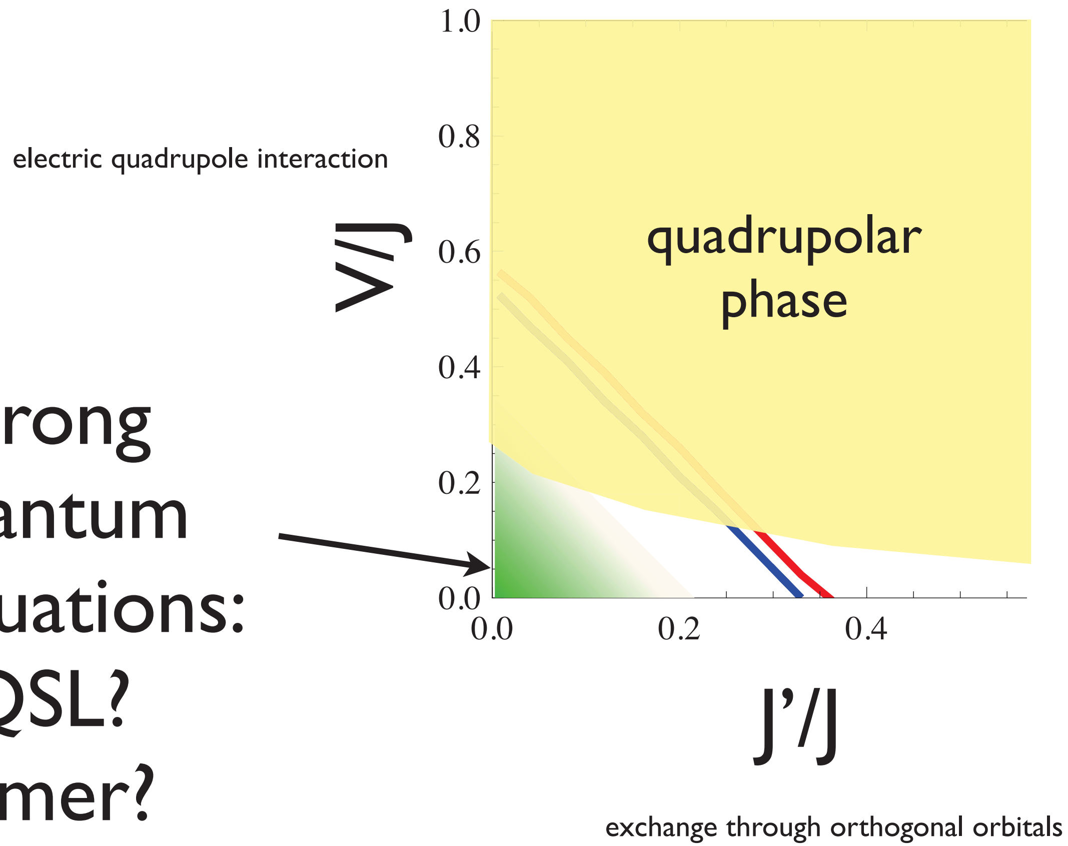


May have much less classical state

T=0 Phase diagram



T>0 Phase diagram

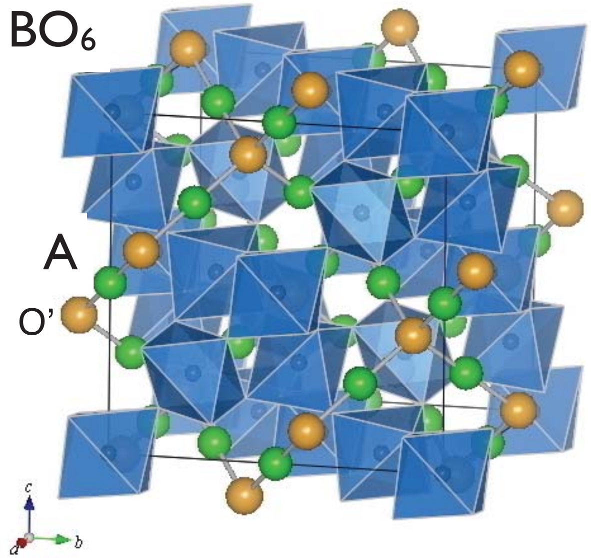


strong quantum fluctuations: QSL? dimer?

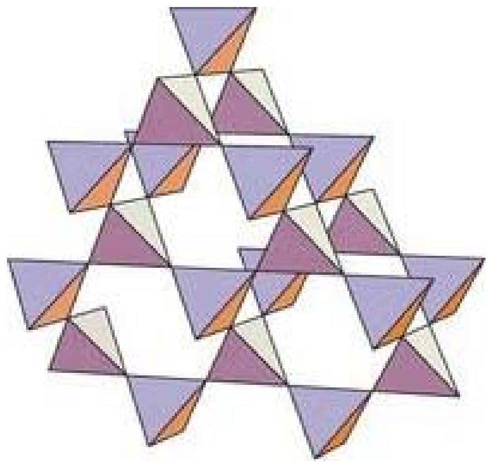
Experiments

- Ba_2YMoO_6 appears the best candidate for a QSL in these materials, but the situation is unclear at present
- Very recent experiments [JP Carlo *et al*, arXiv:1105.3457] claim to have observed a singlet-triplet gap of 29meV suggesting some sort of singlet "RVB" ground state

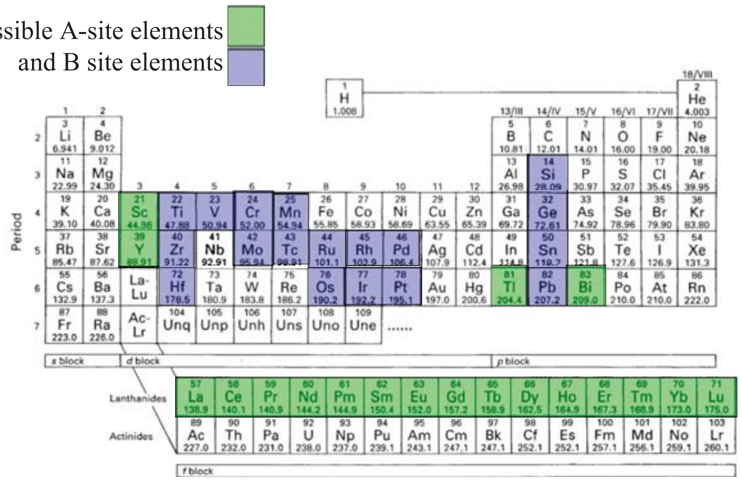
Rare earth pyrochlores



$A_2B_2O_7$



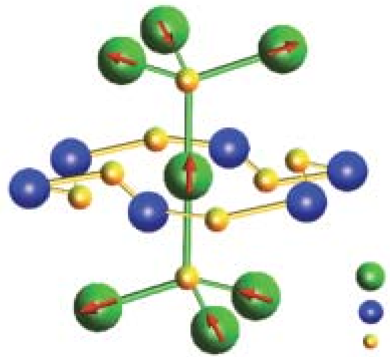
A (B) sublattice



$(A^{3+})_2(B^{4+})_2(O^{2-})_7$

From Gardner, Gingras, Greedan, RMP 2010.

Local Physics



- 4f electrons are well localized: textbook example of Hund's rules
  - Strong SOC: local J eigenstates split by crystal fields
  - Result: typically the ground state is a doublet
- So there is typically an effective S=1/2 description - with natural local quantization axis

S. Curnoe, 2008
S. Onoda, 2010

Hamiltonian

$$H = J_{zz} \sum_{\langle i,j \rangle} S_i^z S_j^z$$

classical NN spin ice

$$-J_{\pm} \sum_{\langle i,j \rangle} \left(S_i^+ S_j^- + S_i^- S_j^+ \right)$$

$$+ J_{z\pm} \sum_{\langle i,j \rangle} \left[S_i^z \left(\zeta_{ij} S_j^+ + \zeta_{ij}^* S_j^- \right) + i \leftrightarrow j \right]$$

$$+ J_{\pm\pm} \sum_{\langle i,j \rangle} \left(\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^- \right)$$

+ quantum fluctuations

= "quantum spin ice"

+ dipolar

Hamiltonian

S. Curnoe, 2008
S. Onoda, 2010

$$H = J_{zz} \sum_{\langle i,j \rangle} S_i^z S_j^z$$

classical NN spin ice

$$-J_{\pm} \sum_{\langle i,j \rangle} \left(S_i^+ S_j^- + S_i^- S_j^+ \right)$$

$$+ J_{z\pm} \sum_{\langle i,j \rangle} \left[S_i^z \left(\zeta_{ij} S_j^+ + \zeta_{ij}^* S_j^- \right) + i \leftrightarrow j \right]$$

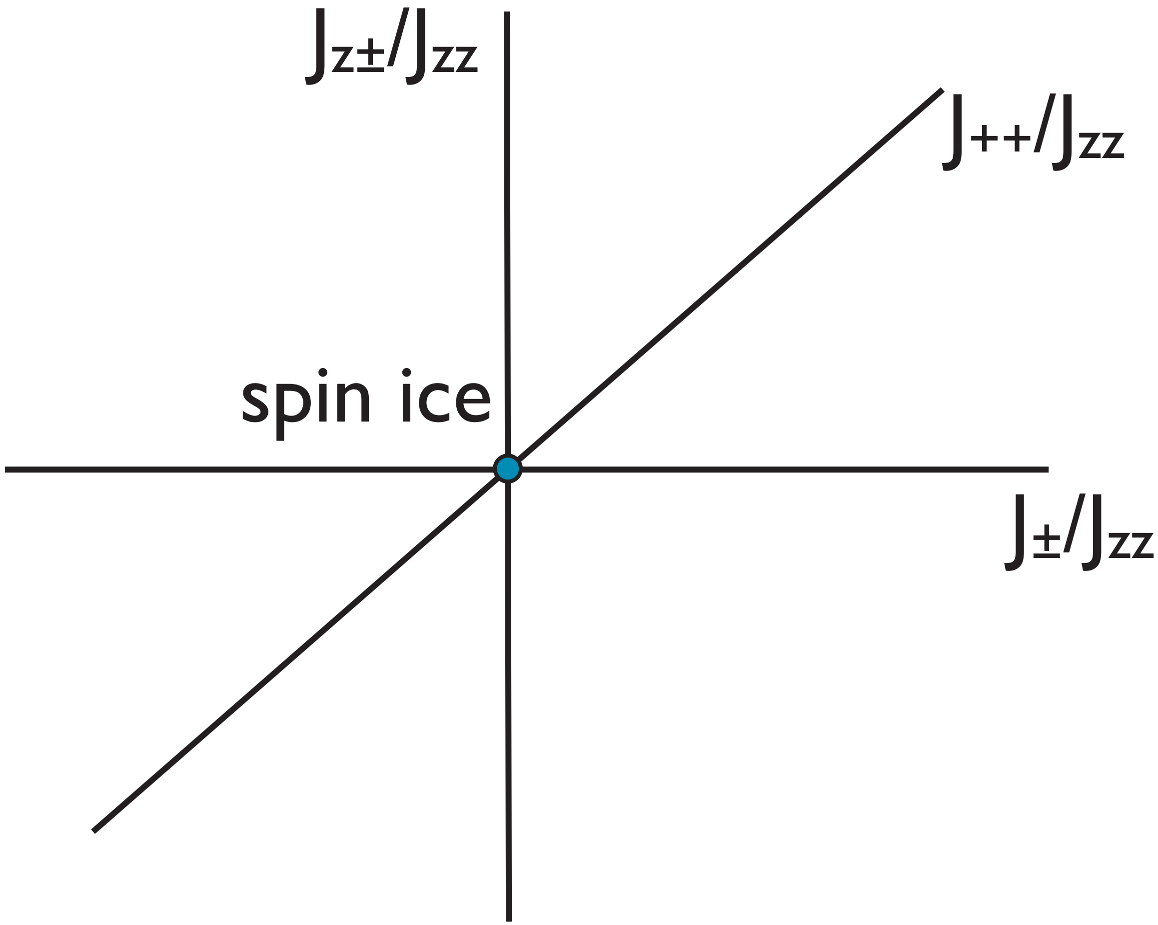
+ quantum fluctuations

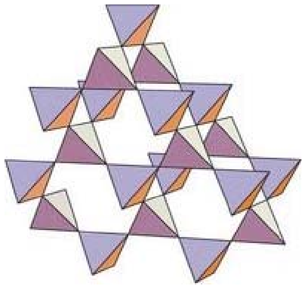
$$+ J_{\pm\pm} \sum_{\langle i,j \rangle} \left(\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^- \right)$$

= "quantum spin ice"

exchange terms dominate in $Yb_2Ti_2O_7$, $Er_2Ti_2O_7$, $Tb_2Ti_2O_7$, $Pr_2Sn_2O_7$ + ???

T=0 Phase Diagram?

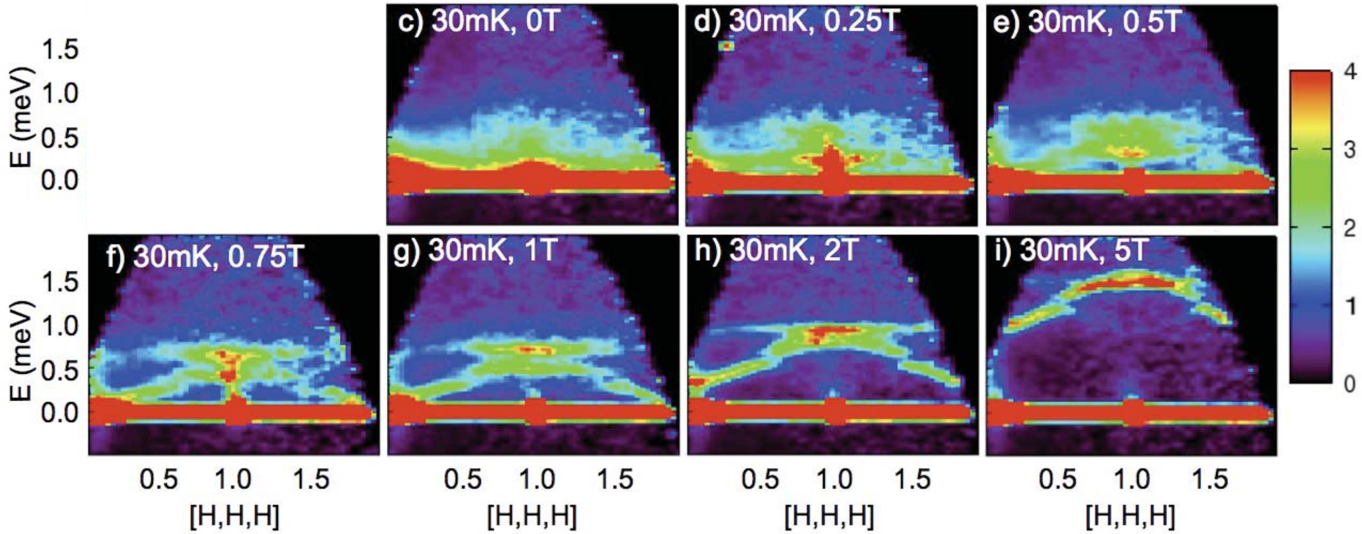




$Yb_2Ti_2O_7$

pyrochlore lattice

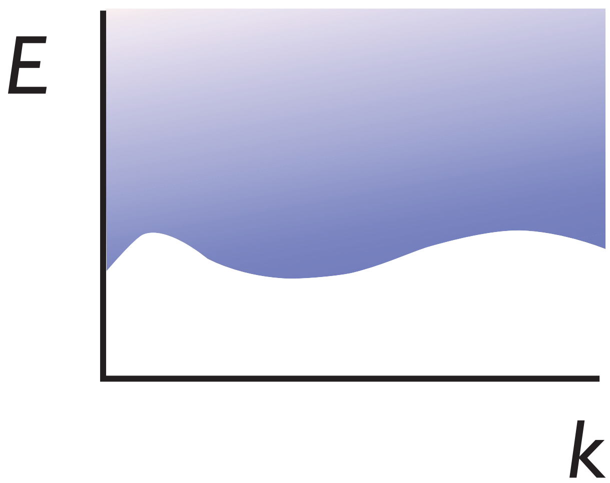
K.A. Ross *et al* (2009)



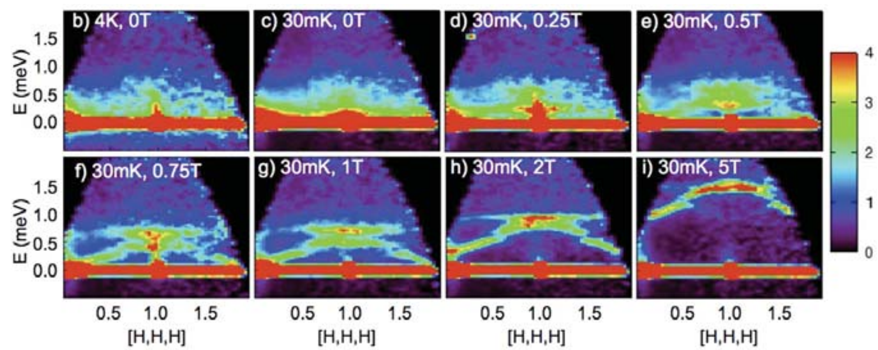
- Spin waves appear absent in low field, but emerge for B>0.5T
  - a low field spin liquid state?

Fractionalization

- Generally, a neutron excites *two* monopoles/spinons in the QSL
  - This results in two-particle continuum scattering, rather than sharp magnons or triplons

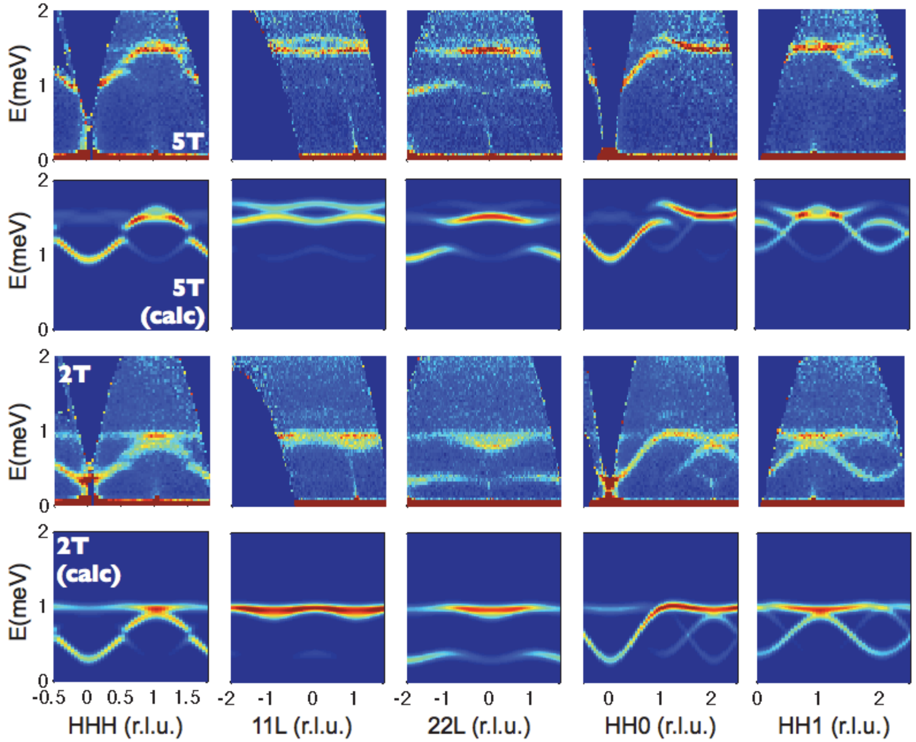


c.f. diffuse scattering in $Yb_2Ti_2O_7$?



Spin interactions

- Complete phenomenological Hamiltonian extracted from INS with B=5T



K. Ross, L. Savary, B. Gaulin, and LB

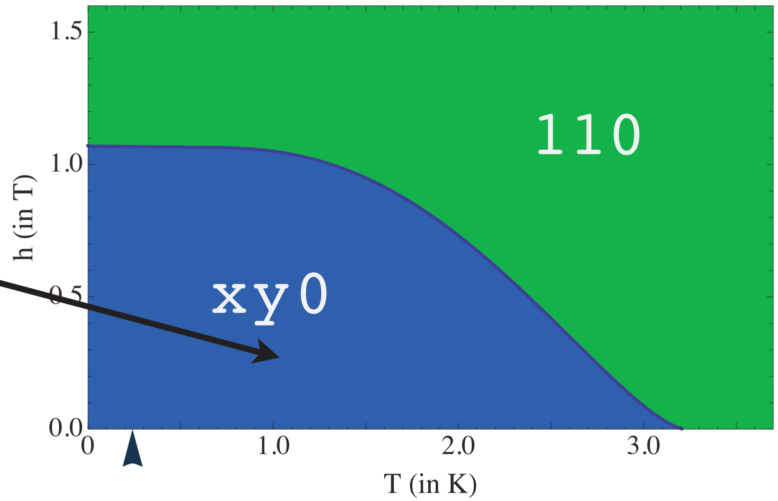
J_{zz} = 0.17±0.04 meV

$J_{\pm}$ = 0.05±0.01 meV $J_{z\pm}$ = 0.14±0.01 meV $J_{\pm\pm}$ = 0.05±0.01 meV

Fluctuations

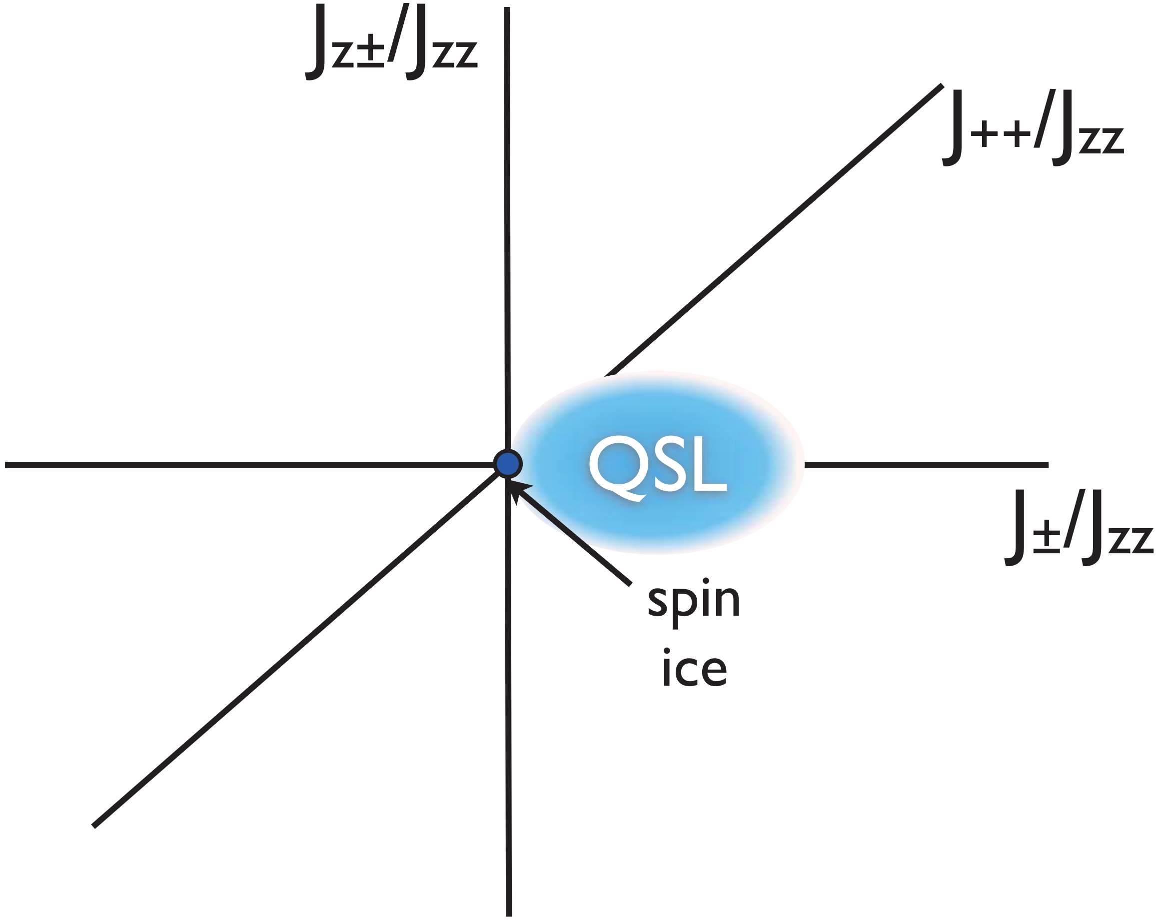
- Comparison with mean field theory *fails badly* at low field

MFT predicts an ordered ferromagnet here



thermodynamic phase transition observed here: 14 times lower temperature than mean field T_c

T=0 Phase Diagram



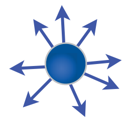
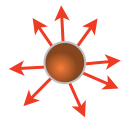
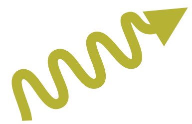
U(1) QSL = emergent compact QED

M. Hermele, MPA Fisher, L. Balents, 2004


ICE AGE 2
THE QUANTUM

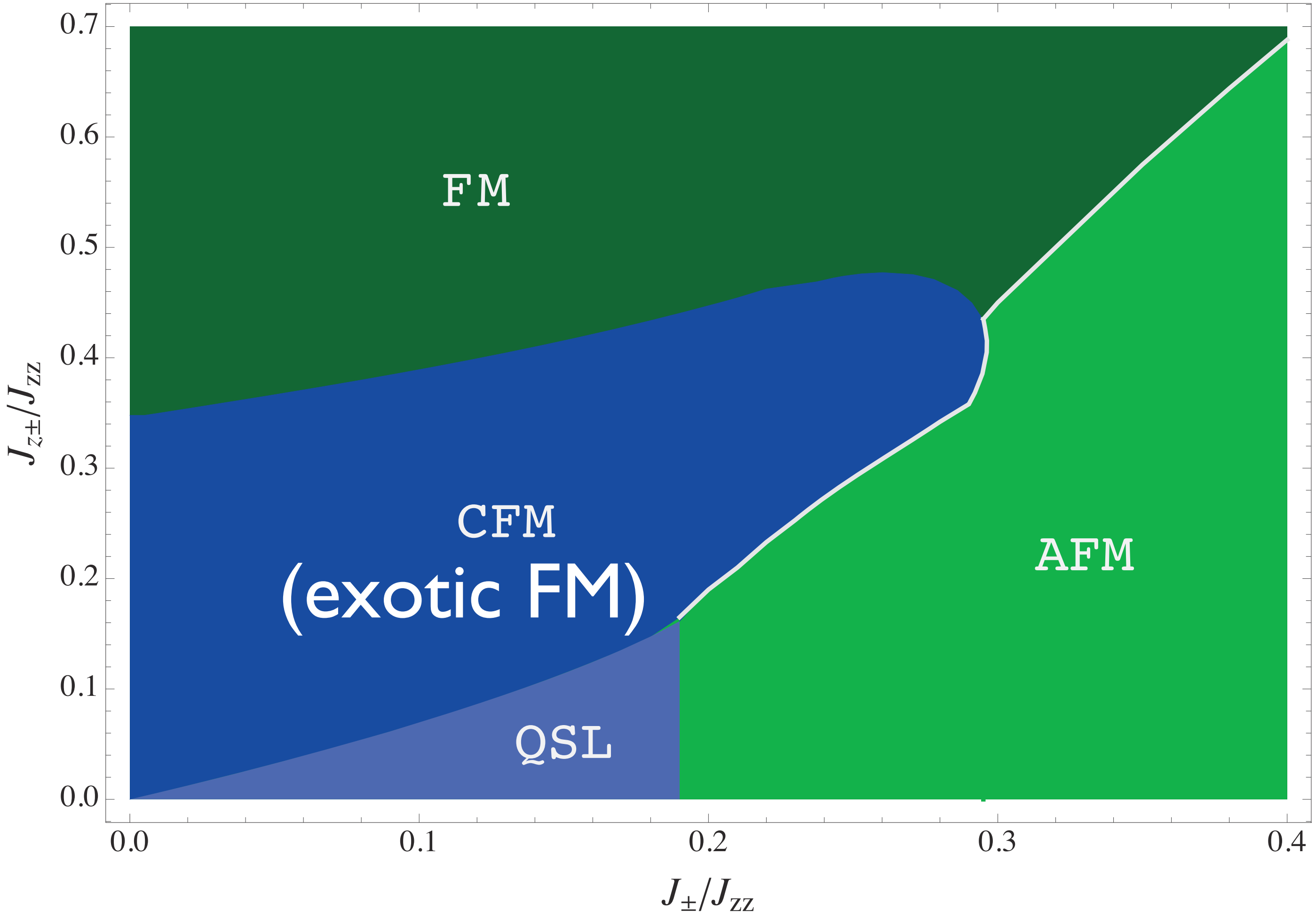
Hermele *et al*, 2004

Excitations

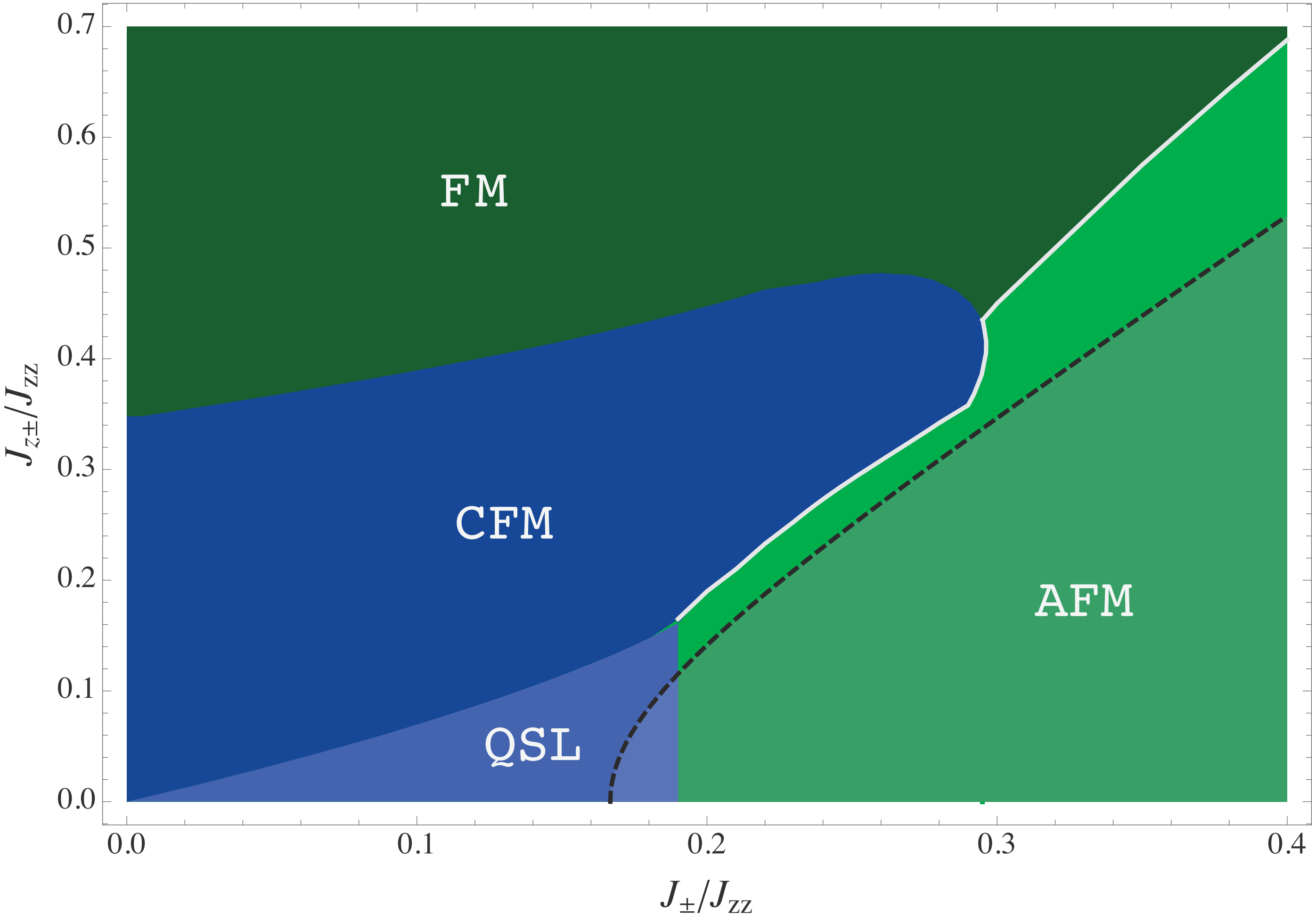
- Where spin ice realizes "emergent magnetostatics", the QSL is "emergent compact quantum electrodynamics"
  - *coherent propagating* monopoles = "spinons"
    
  - dual (electric) monopoles
    
  - artificial photon
    

Phase Diagram

(gauge MFT)

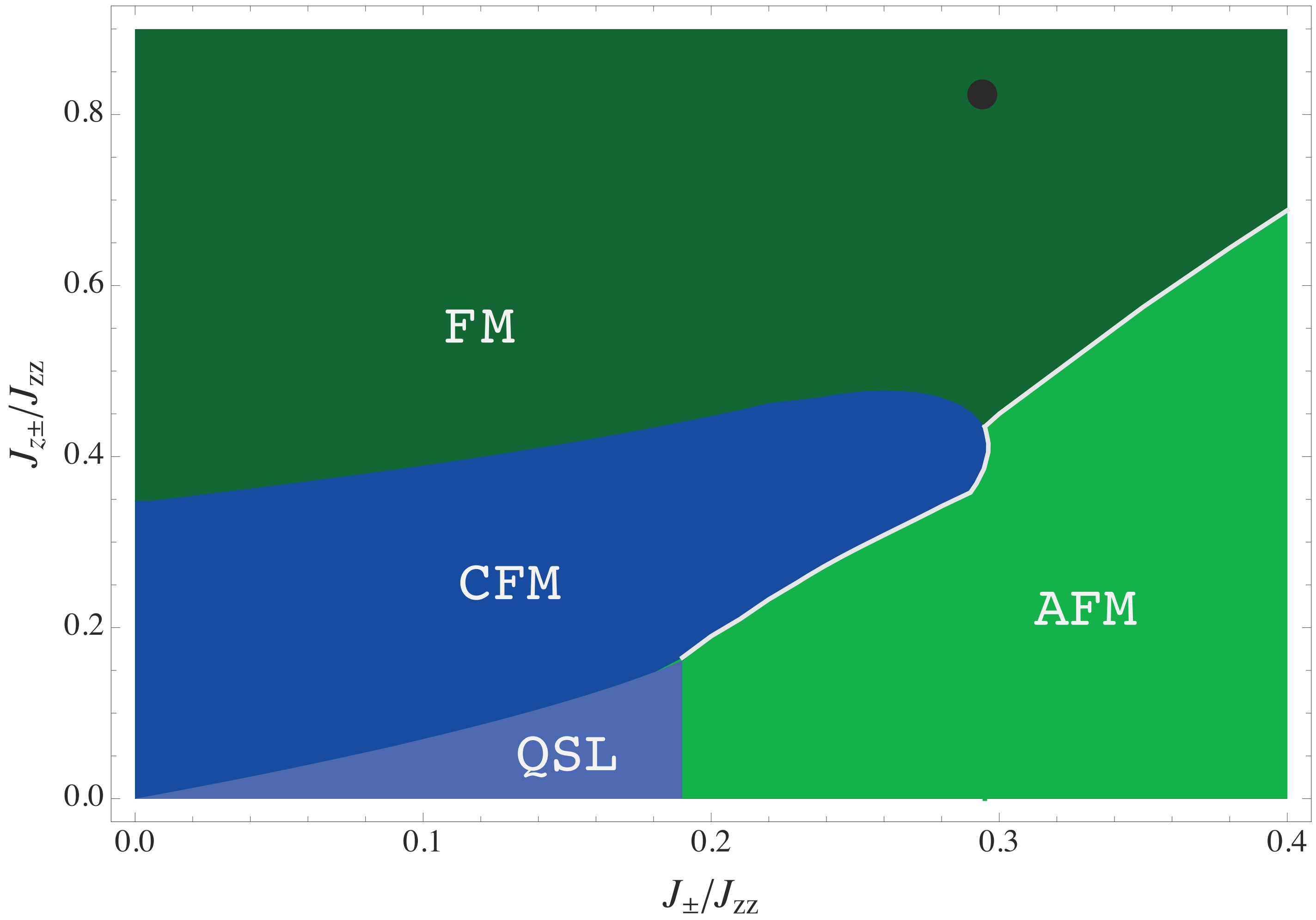


Phase Diagram

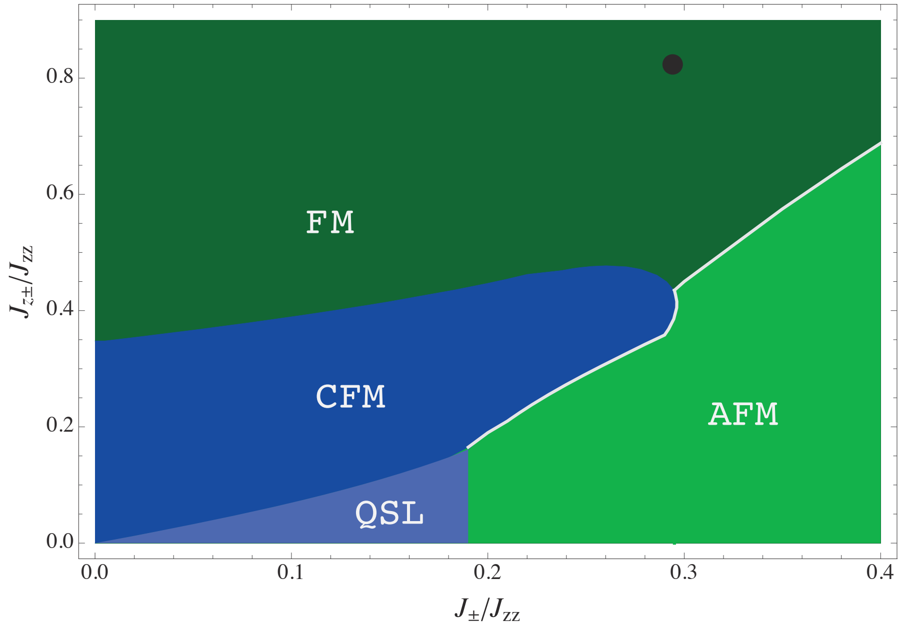


classical boundary

Phase Diagram



Phase Diagram

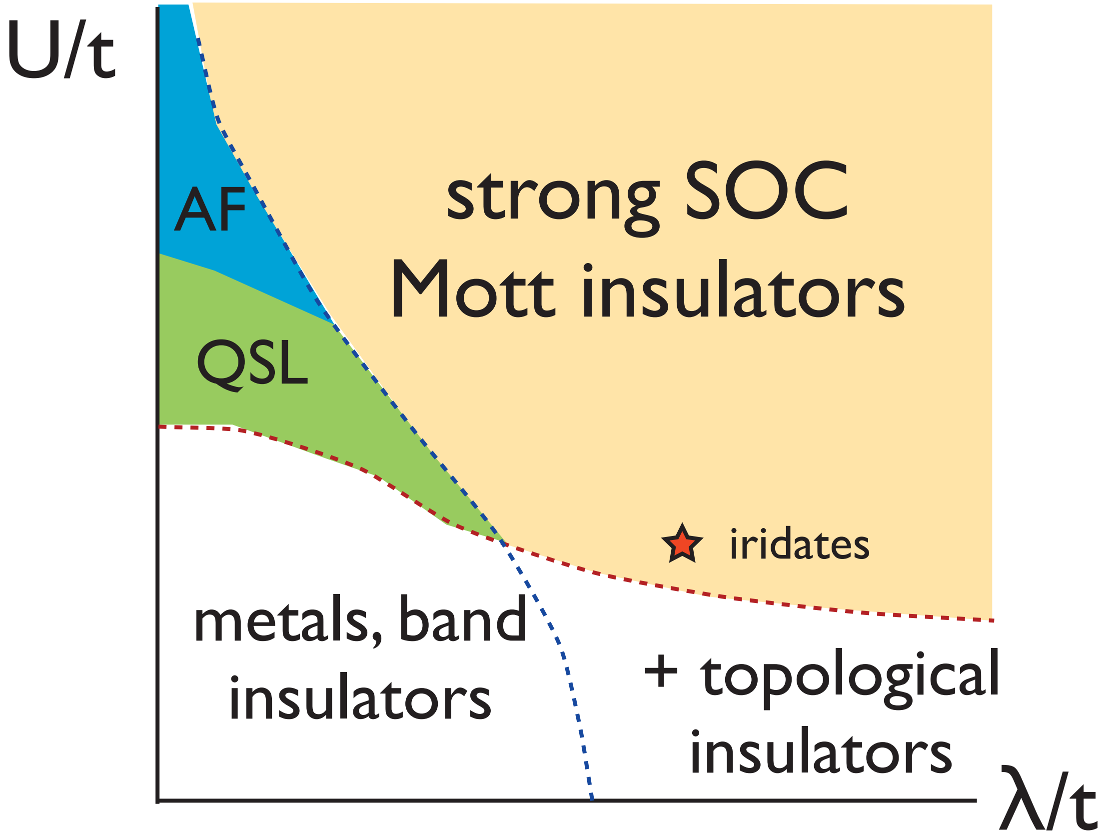


- Interesting to place other pyrochlores on this phase diagram
- And to *check* it by numerics!

Intermediate Correlation

- Many 5d transition metal compounds are close to Mott transitions, where U~t~λ

$Ln_2Ir_2O_7$
Sr_2IrO_4
Na_2IrO_3
...

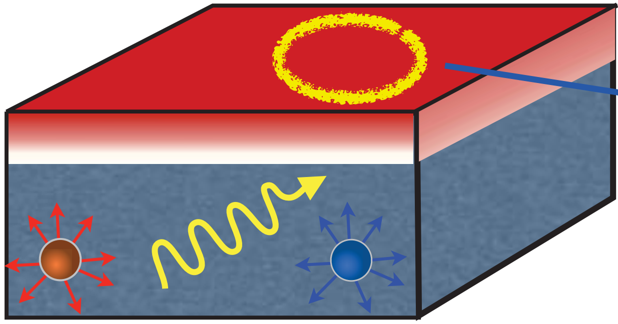


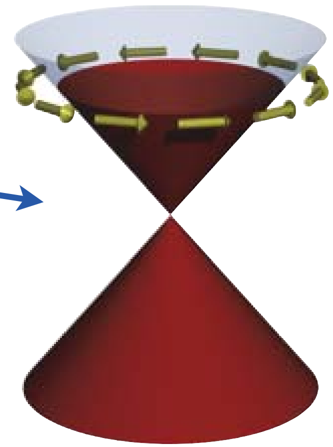
From TBI to MI

- How does a topological insulator evolve into a Mott insulator with increasing correlations?
  - Might a QSL still be favored for intermediate correlations?
  - If so, it could share some of the character of the topological insulator
- One such state is a "topological Mott insulator" [Pesin + Balents, (2010)]

Topological Mott Insulator

$c_{ia}^{\dagger} \sim b_i^{\dagger} f_{ia}$ neutral fermionic "spinon" inherits band topology



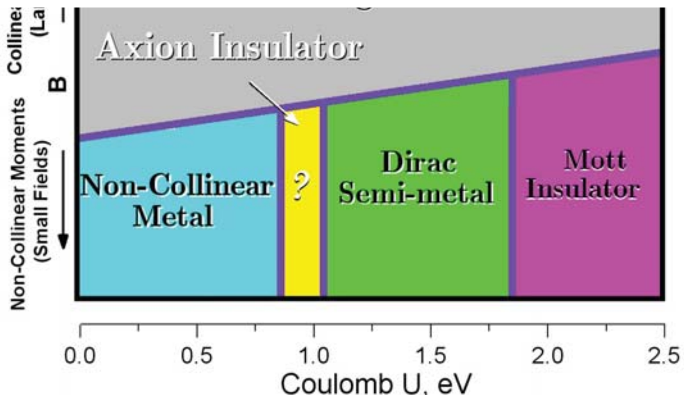


gapless surface states are *neutral*: an insulating surface with metal-like spin transport

From TBI to MI

- Many scenarios are possible, and will depend upon the details

TBI		AF MI	Hartree-Fock
TBI	TBI w/ AF surface	AF MI	
TBI	TMI	AF MI	slave rotor



LDA+U

X. Wan *et al* (2010)


Thank you for your attention