
Introduction to
Quantum Materials
Leon Balents, KITP
QS3 School, June 11, 2018

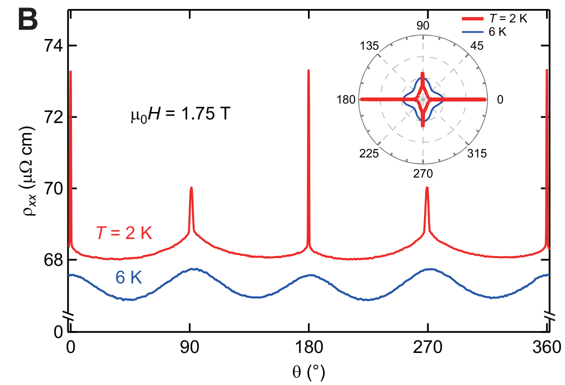
Day 2

Topological frontiers

- Can we realize a topological superconductor?
- What is the interplay between topological defects and topological bands?
- What are the robust signatures of topology in transport and other responses?
- Are there strongly interacting topological phases in real materials?

Ask Professor Joe

SAMR in CeAlGe, a magnetic Weyl material



What's going on??

A) Device is sensing magnetic poles

B) It's the chiral anomaly

C) Protection from backscattering leads to low resistance away from high symmetry directions

D) The field is sweeping across Ising ordered "nematic"-like phases resulting in domain wall resistance

E) Joe's cell phone interfered with the signal from the cryostat

Themes of modern QMs

- Order
- Topology
- Entanglement
- Correlations

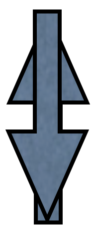
Entanglement

EPR $$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|{\uparrow\downarrow}\rangle - |{\downarrow\uparrow}\rangle\right)$$

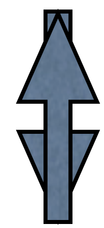
entangled: cannot be written as a product state

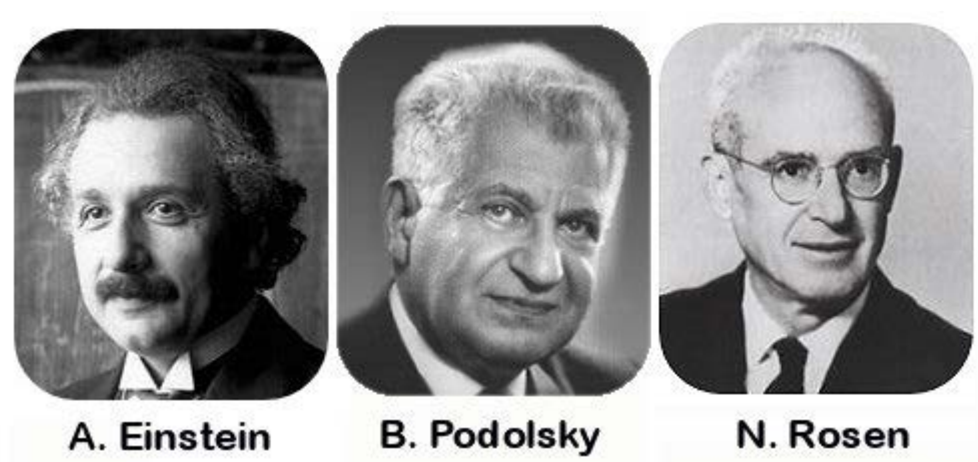
Entanglement

EPR $$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$



??where is the information??

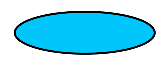


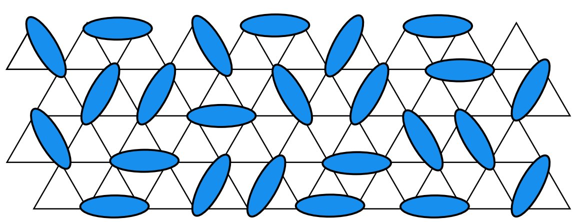
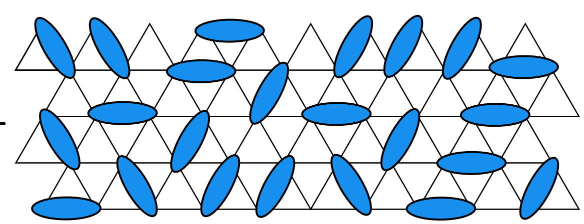


Many Body Entanglement

Phil Anderson, 1973

a "quantum liquid" of spins

 $= \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$

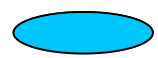
Ψ =  $+$  $+ \ldots$

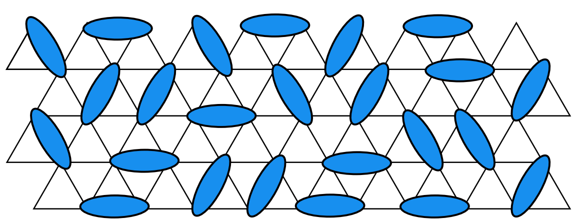
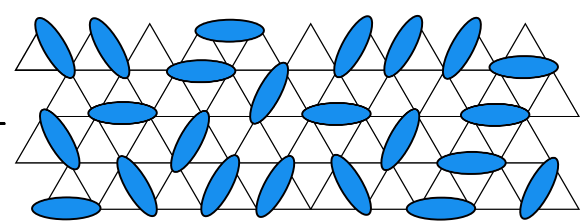
Resonating **V**alence **B**ond state

Many Body Entanglement

Phil Anderson, 1973

a "quantum liquid" of spins

 $= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$

Ψ =  +  + ...

Resonating **V**alence **B**ond state

Ordinary (local) Matter

We can consistently assign local properties (elastic moduli, etc.) and obtain all large-scale properties

- Measurements far away do not affect one another
- From local measurements we can deduce the global state

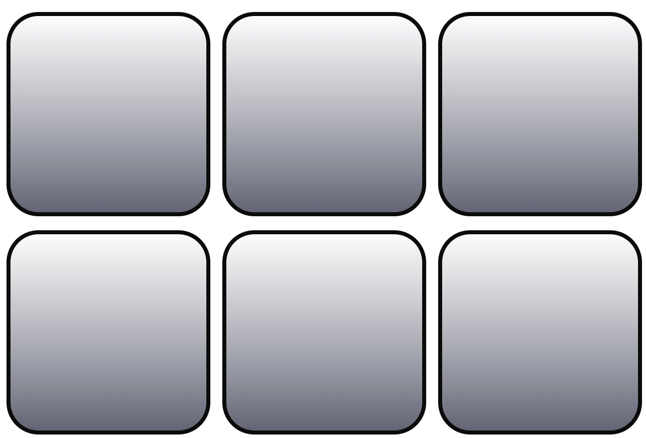
Ordinary (local) Matter

Hamiltonian is local

$$H = \sum_{\mathbf{x}} \mathcal{H}(x) \qquad \mathcal{H}(x) \text{ has local support near x}$$

Ground state is "essentially" a product state

$$|\Psi\rangle = \otimes_A |\psi\rangle_A$$

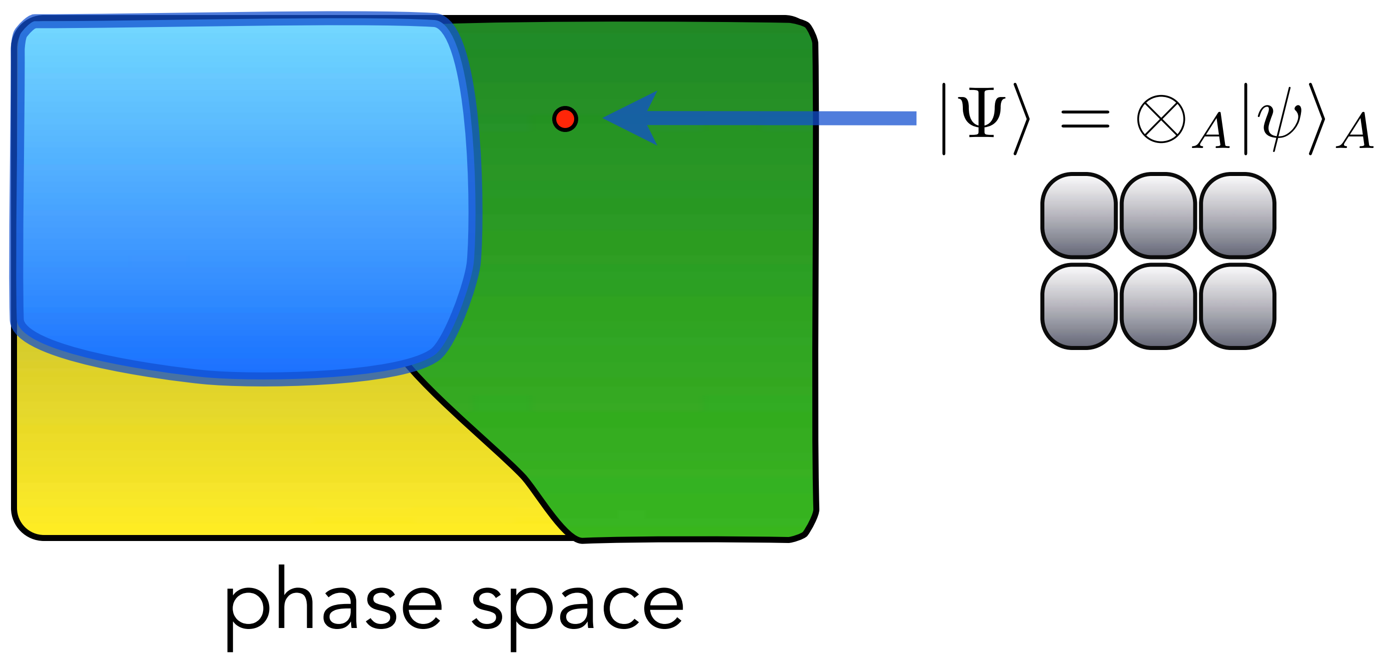


no entanglement between blocks

most insulators are like this

“Essentially” a product state?

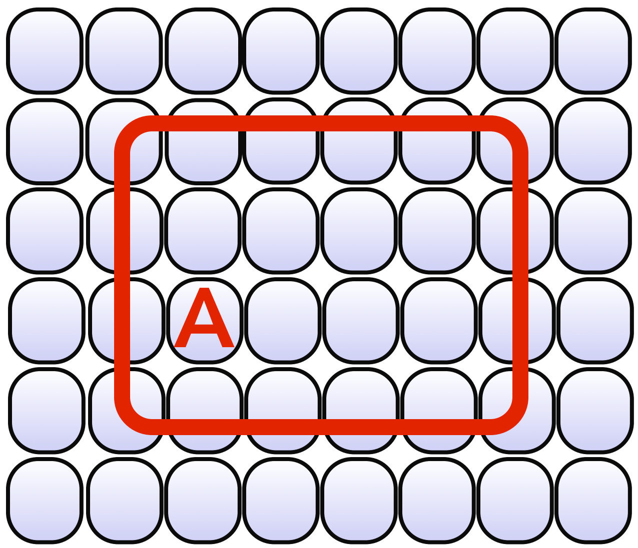
- Adiabatic continuity



n.b. This is not true for gapless fermi systems

"Essentially" a product state?

- Entanglement scaling



$$\rho_A = \mathrm{Tr}_{\bar{A}} |\Psi\rangle\langle\Psi|$$

$$S(A) = -\mathrm{Tr}_A \left(\rho_A \ln \rho_A\right)$$

$S(A) \sim \sigma L^{d-1}$ area law

satisfied with exponentially small corrections

Best example: ordered magnet

Hamiltonian

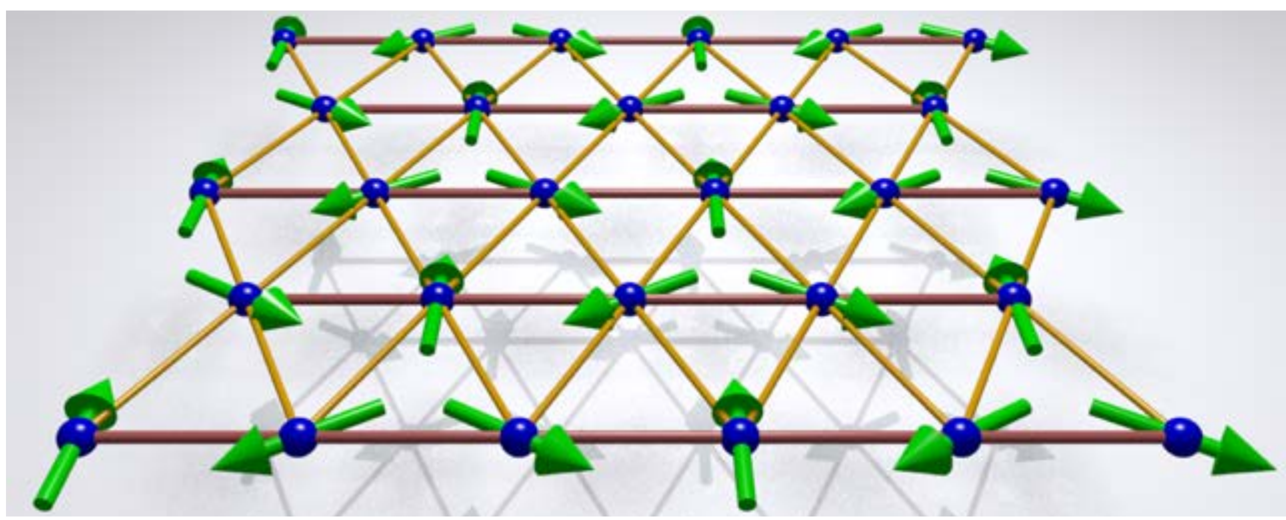
$$H = \sum_{(ij)} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

exchange is short-range: local

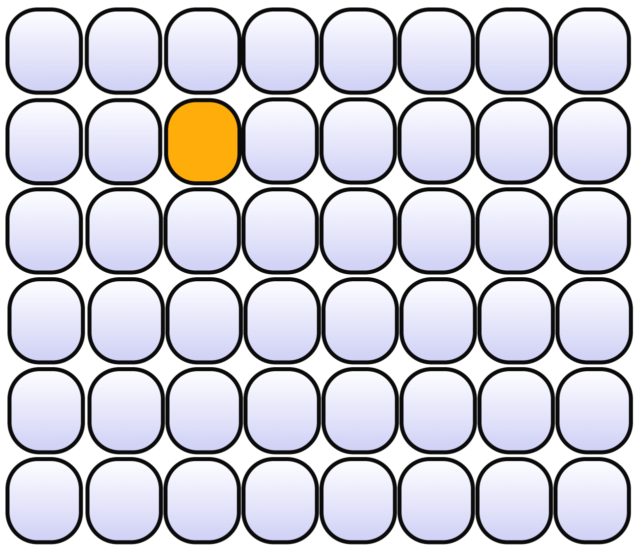
ordered state

$$|\Psi\rangle \approx \bigotimes_i |\boldsymbol{S}_i \cdot \hat{n}_i = +S\rangle$$

block is a single spin



Quasiparticles

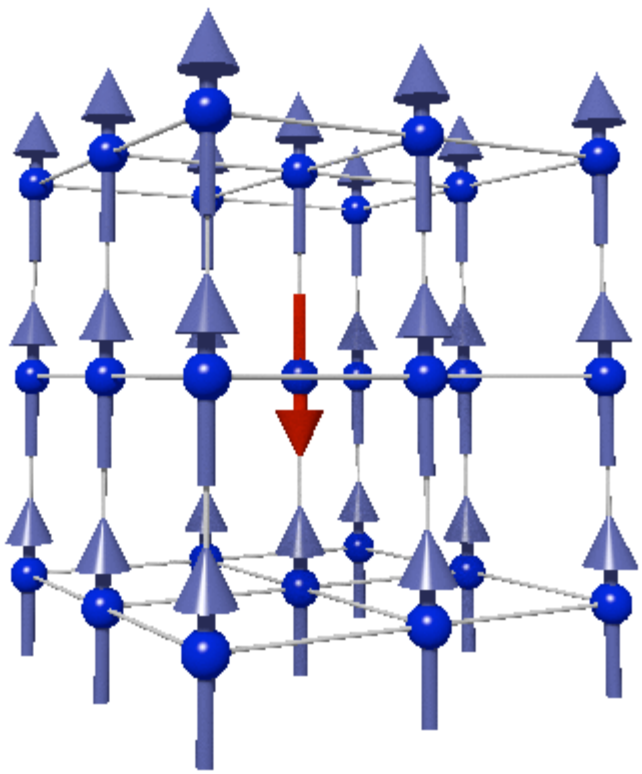


excited states ~ excited levels of one block

- local excitation can be created with operators in one block
- localized excitation has discrete spectrum with non-zero gap, and plane wave forms sharp band

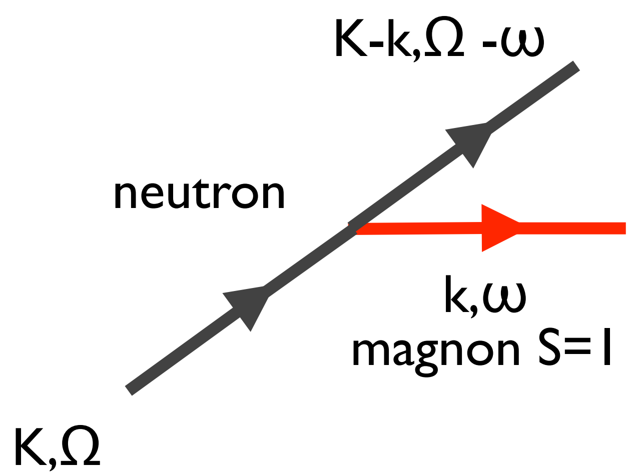
- quantum numbers consistent with finite system: no emergent or fractional quantum numbers

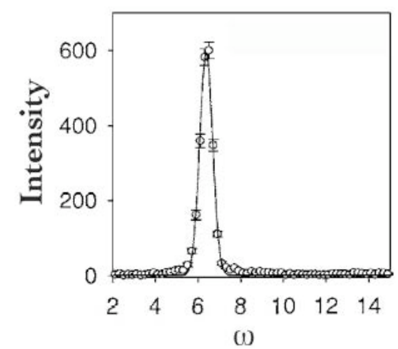
Spin wave



$$\omega(k) \approx \Delta - 2t \cos k_x a - \cdots$$

$$|f\rangle = S_k^+ |i\rangle$$

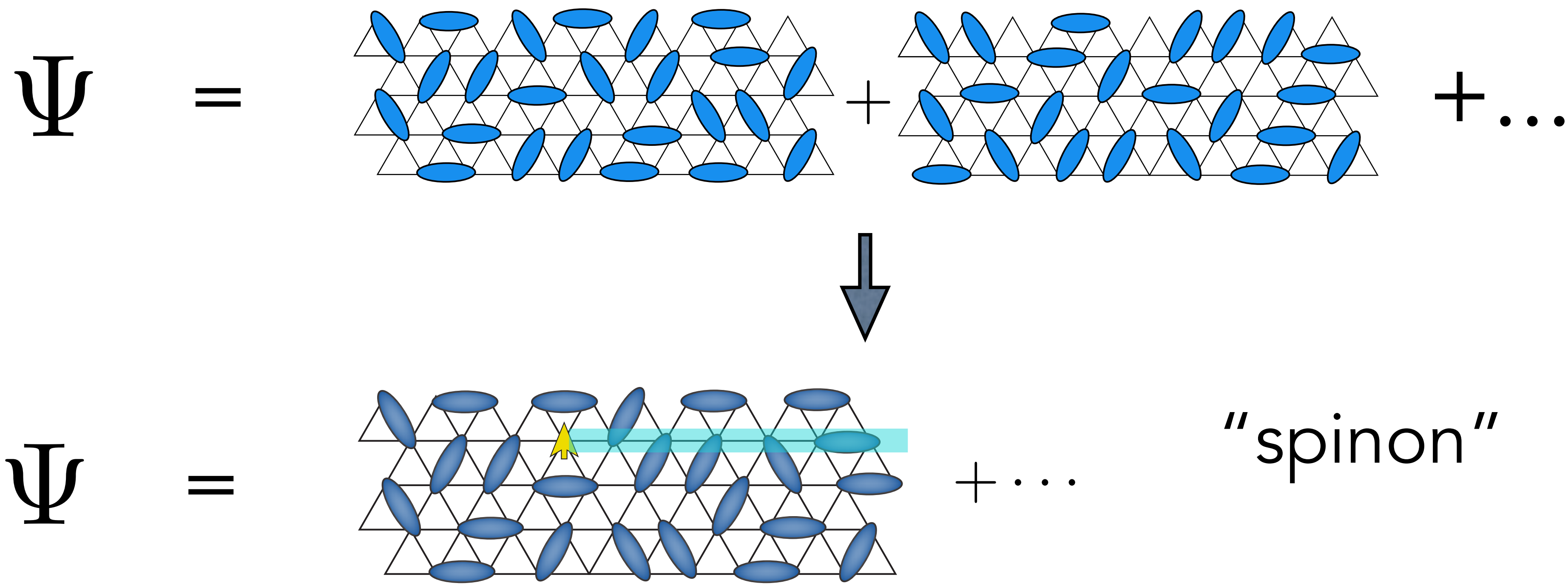




Line shape in Rb_2MnF_4

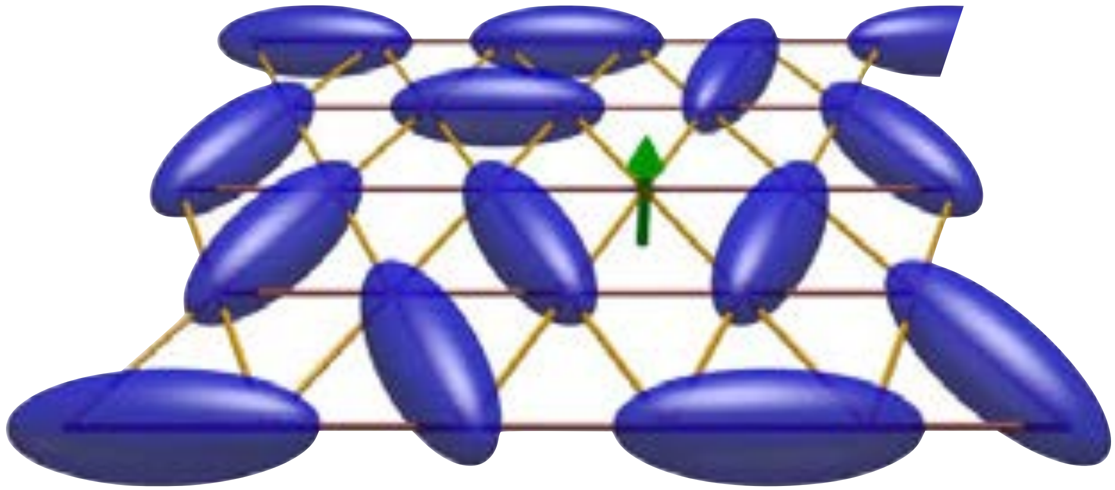
Quantum spin liquid

Entanglement -> non-local excitation



“quasiparticle” above a non-zero gap

Fractional quantum number

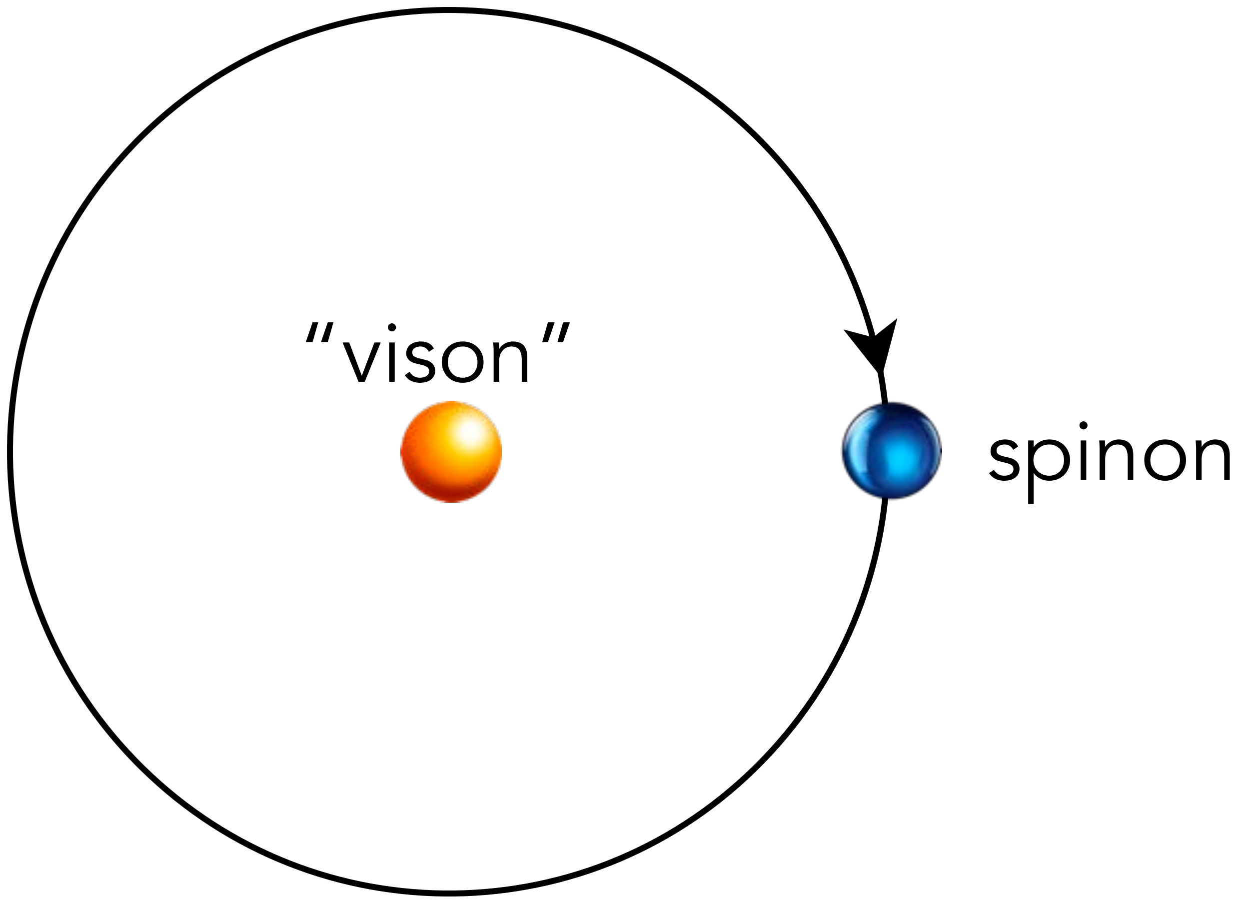


excitation with $\Delta S = 1/2$
not possible for any finite
cluster of spins

always created in pairs by any
local operator

Anyons

A characteristic of
"intrinsic
Topological Order"



$$\Psi \rightarrow -\Psi$$

"mutual semions"

Where does this name vison come from?

A) Because they occur at high pressures like in a vise

B) Vision was taken by the Marvel character

C) Vortex+Ising = vison

D) Named after the zoological name for the mink, because their long-range statistical interaction extends like the famous fur

E) I don't know but why do people keep naming particles that don't exist?

X.-G. Wen

(intrinsic)

Topological phases

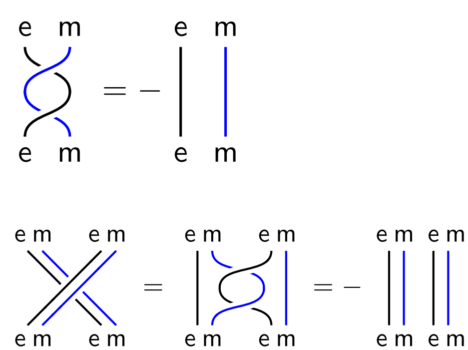
A. Kitaev

The American Physical Society
2017 OLIVER E. BUCKLEY
SOLID STATE PHYSICS PRIZE

Warning: this is a different meaning of topological!

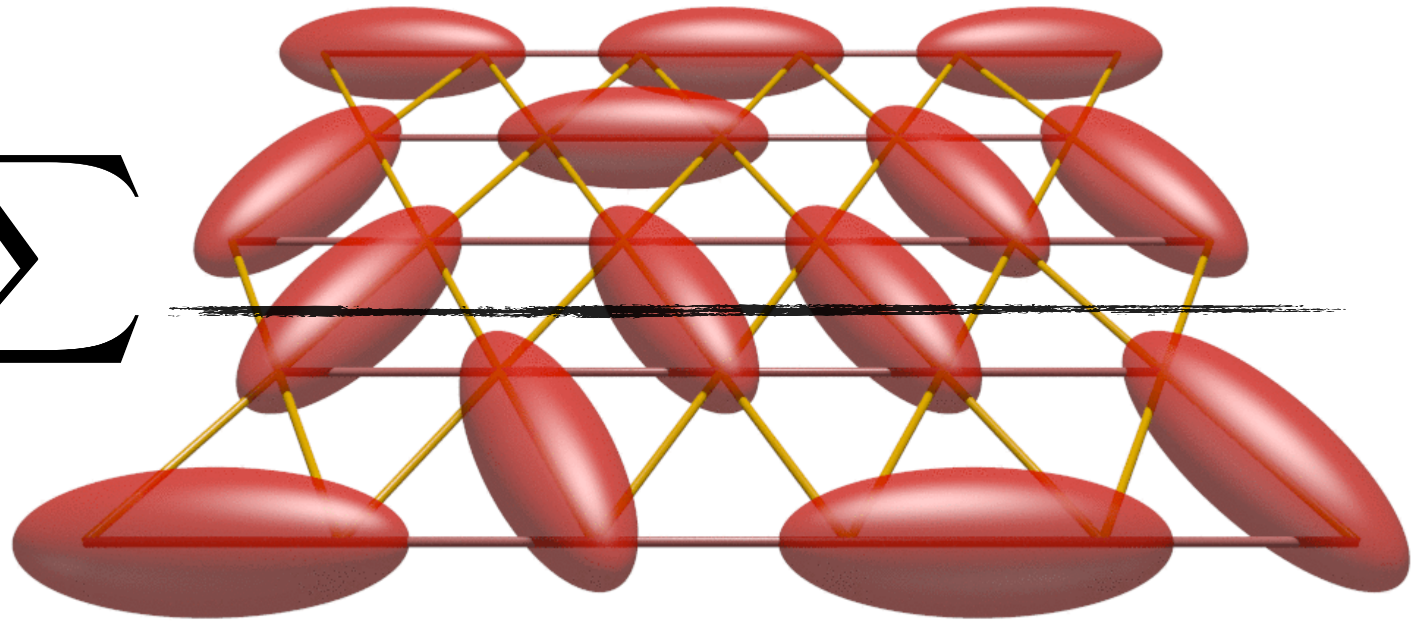
Anderson's RVB state is thus an
mple of a “topological phase” - the
best understood sort of QSL

Understood and classified by anyons and their braiding rules in 2d



Stability

$$\Psi = \sum$$



Robustness arises from topology: a QSL is a stable *phase* of matter (at T=0)

How stable is a topological QSL? Which of the choices below will make a 2d QSL become the same as a paramagnet?

A) Apply some weak strain

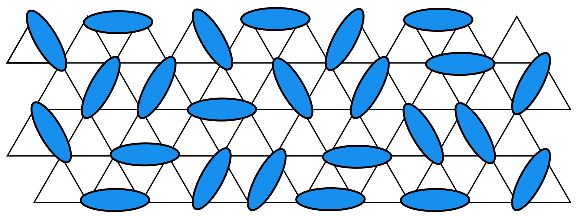
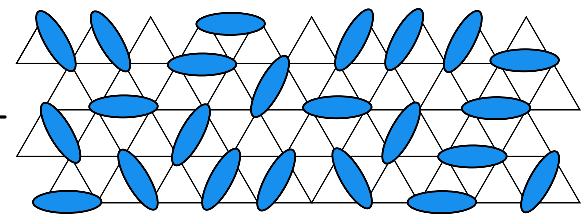
B) Apply a small magnetic field

C) Add some weak randomness to the bonds

D) Beat the heck out of it with a hammer

E) Warm it up

Quantum spin liquid

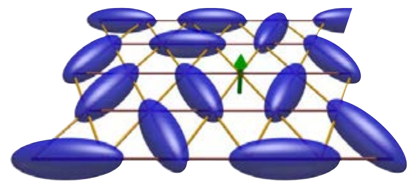
$\Psi =$  $+$  $+ \ldots$

For ~500 spins, there are more amplitudes than there are atoms in the visible universe!

Different choices of amplitudes can realize different QSL phases of matter.

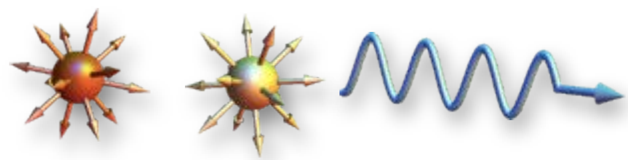
Varieties of QSLs

- Topological QSLs



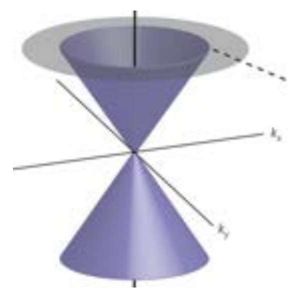
anyonic
spinons

- U(1) QSL



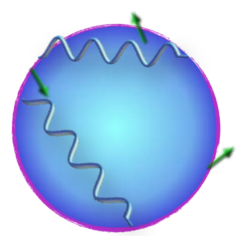
electric+magnetic
monopoles, photon

- Dirac QSLs



strongly
interacting
Dirac fermions

- Spinon Fermi surface

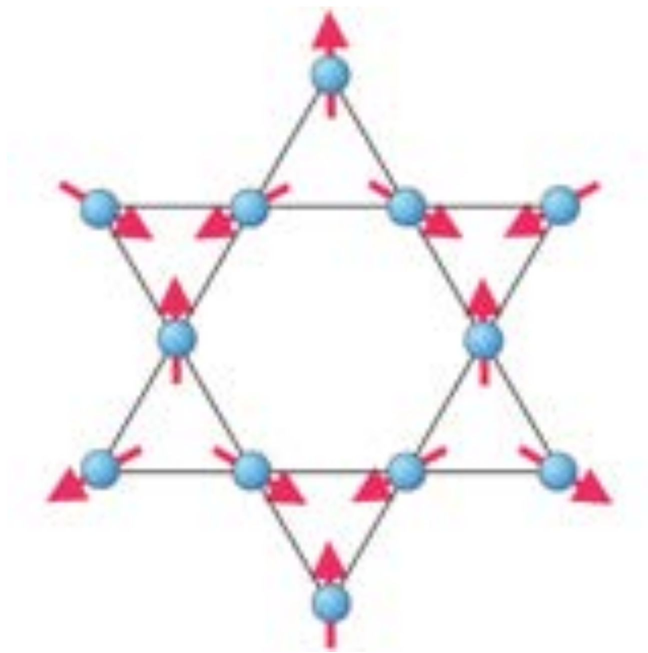


non-Fermi
liquid "spin
metal"

QSL experiments

- This is a difficult subject, if you want a challenge!
- Discuss three examples:
  - Kagomé lattice herbertsmithite
  - Organic triangular lattice
  - alpha-$RuCl_3$ Kitaev magnet

Kagomé antiferromagnet



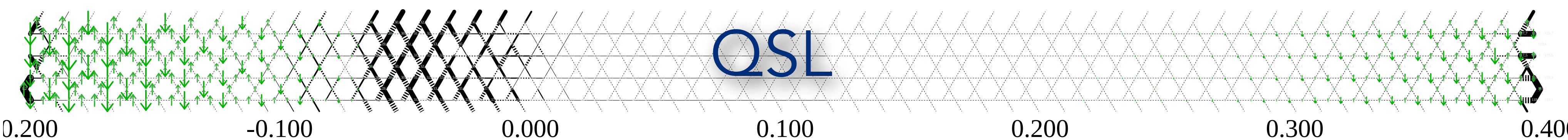
$$H = J \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \ldots$$

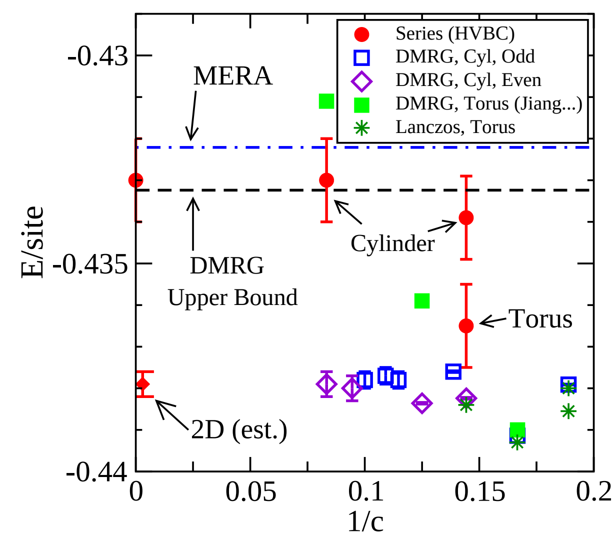
Very large classical degeneracy → likely to be a QSL

V. Elser, 1989 + many many others

S=1/2 kagomé AF

- Rather definitive evidence for QSL by DMRG

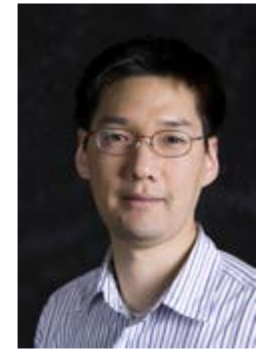




S. Yan *et al*, 2010

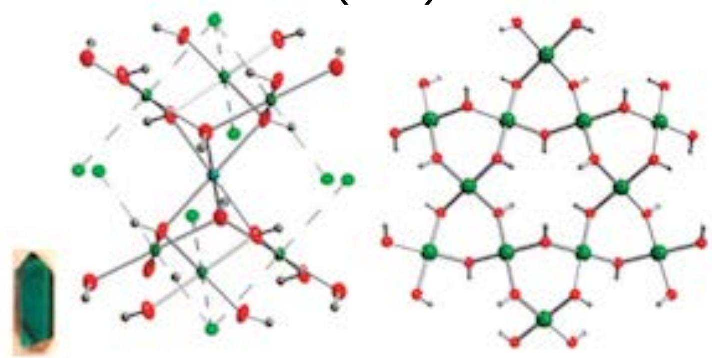
many other studies support existence of some QSL phase

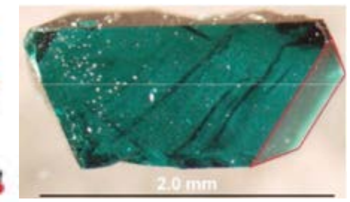
Herbertsmithite



kagomé layers of Cu S=1/2 spins, separated by non-magnetic Zn

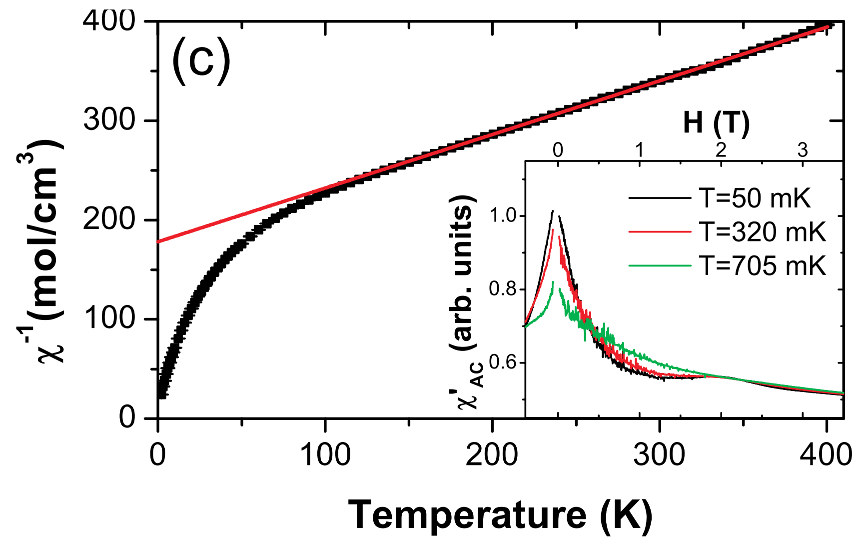
$ZnCu_3(OH)_6Cl_2$





Heisenberg-like with J ~ 200K

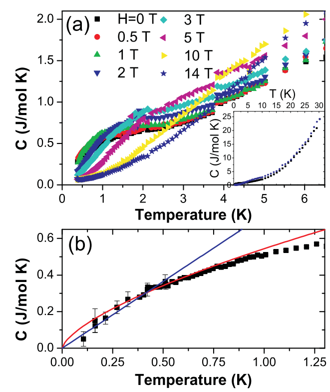
no order down to 50mK



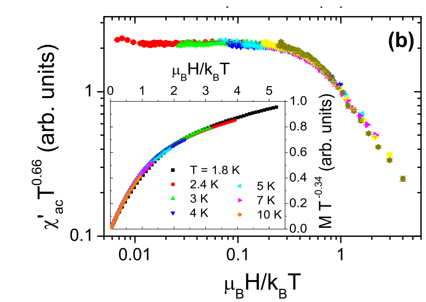
Helton *et al*, 2007

Herbertsmithite

Lots of early evidence
for gaplessness



Helton *et al*, *2007*

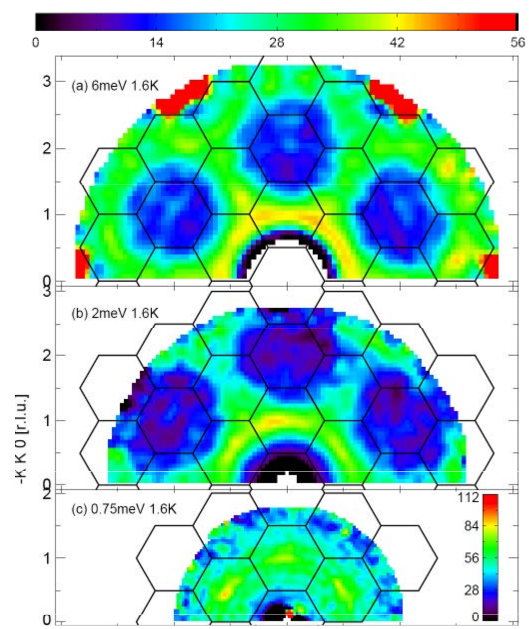


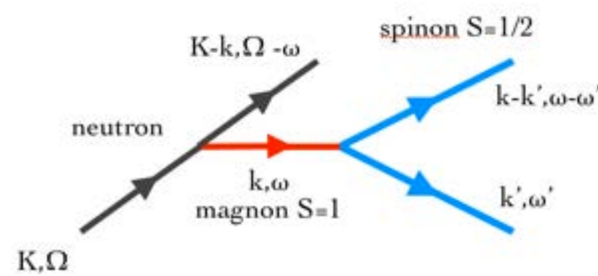
Helton *et al*, *2010*

Single crystal INS

smooth continuum
scattering

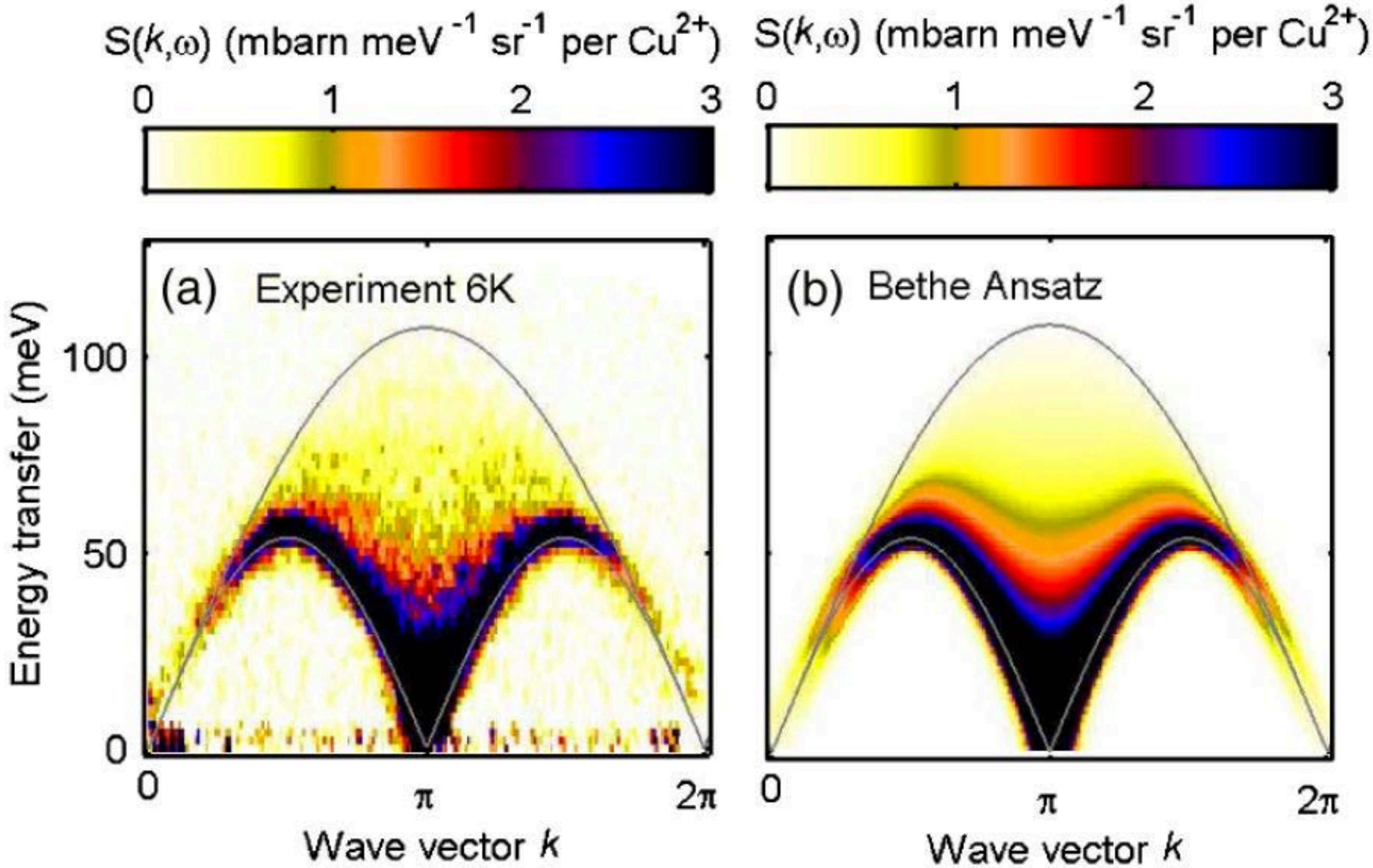
T-H Han *et al*, 2012





continuum scattering
expected
...but probably with more
structure?

For comparison: 1d spinons

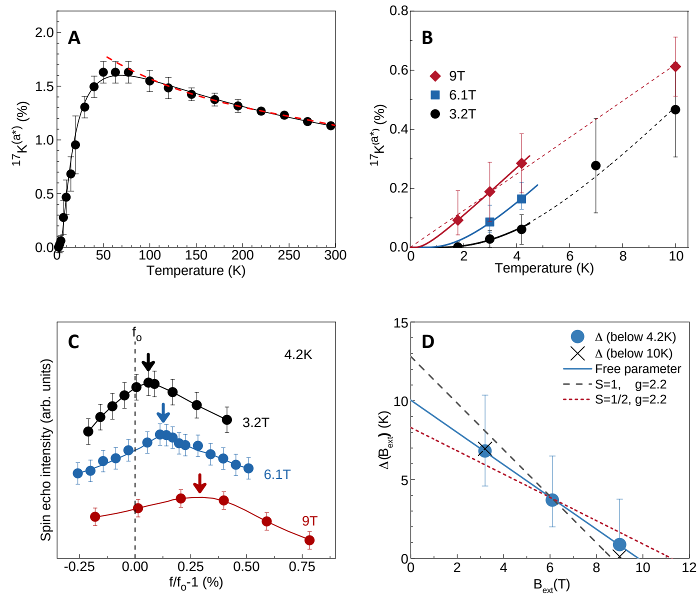


$KCuF_3$ - B. Lake *et al*, 2013

Herbertsmithite

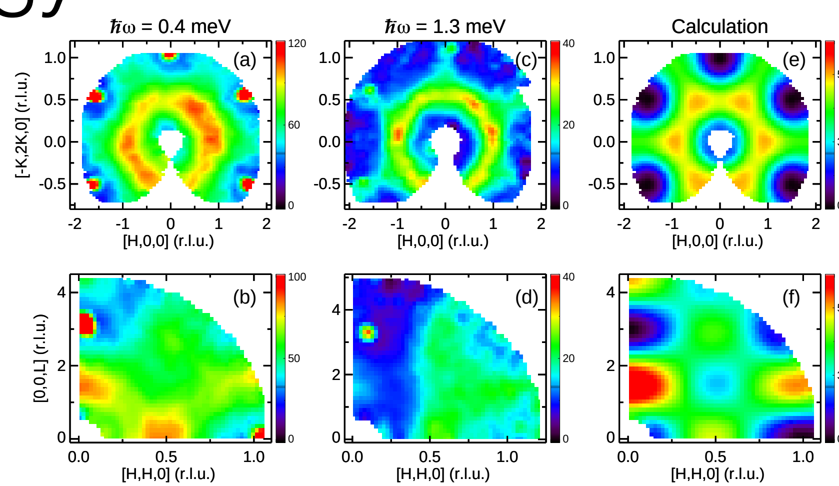
Single crystal NMR

M. Fu *et al*, 2015



estimate gap ~ 10K

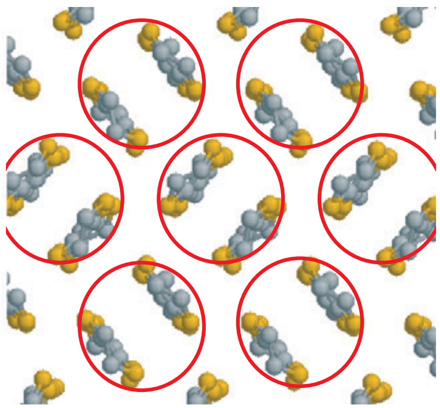
Low energy INS



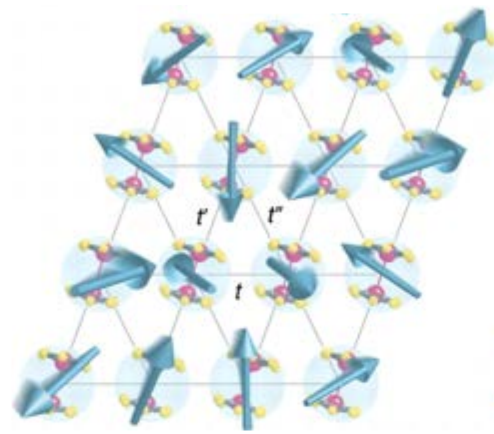
T-H Han *et al*, 2015

claim to separate impurity signal below 0.7meV

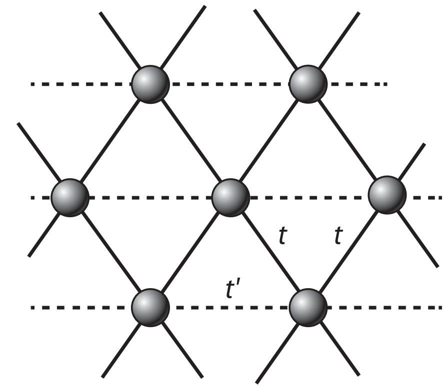
Organics



κ-$(ET)_2X$

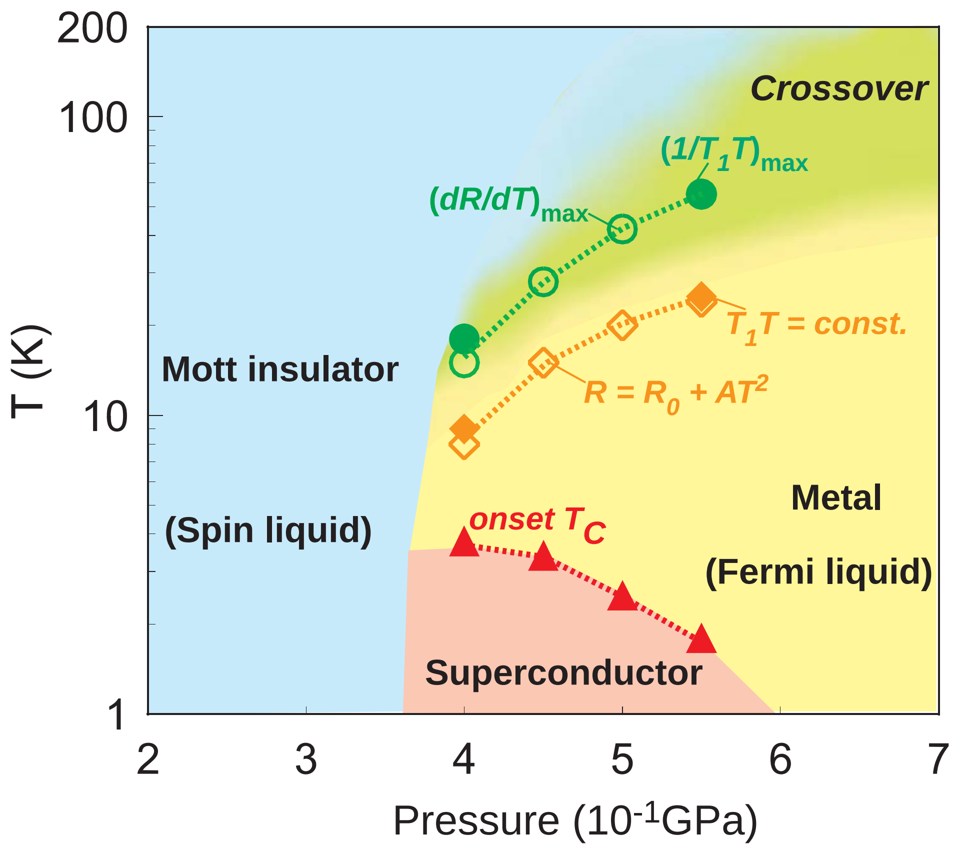


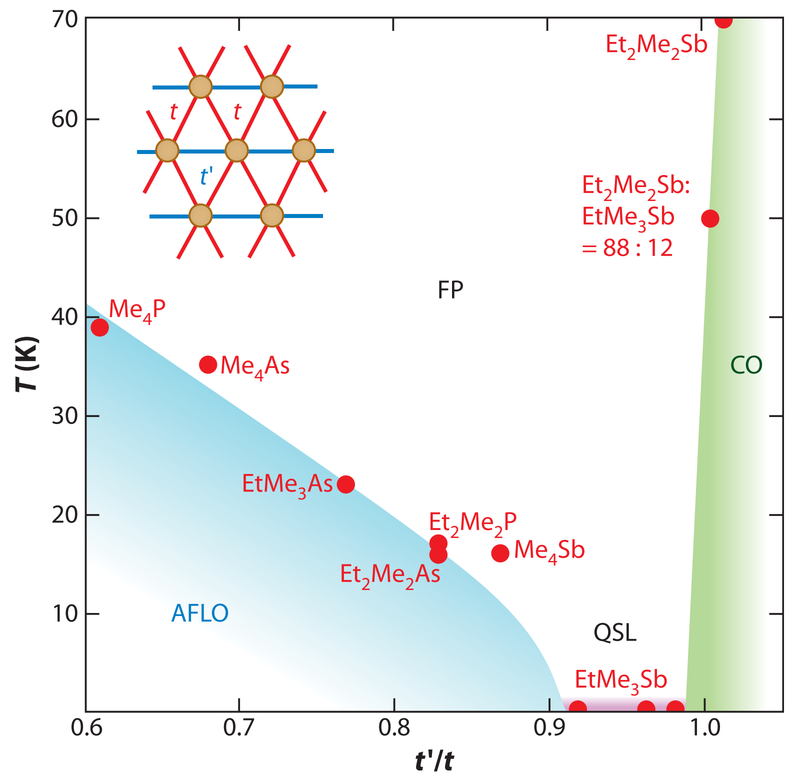
β′-$Pd(dmit)_2$



- Molecular materials which behave as effective triangular lattice S=1/2 antiferromagnets with J ~ 250K
    - significant charge fluctuations

Organics





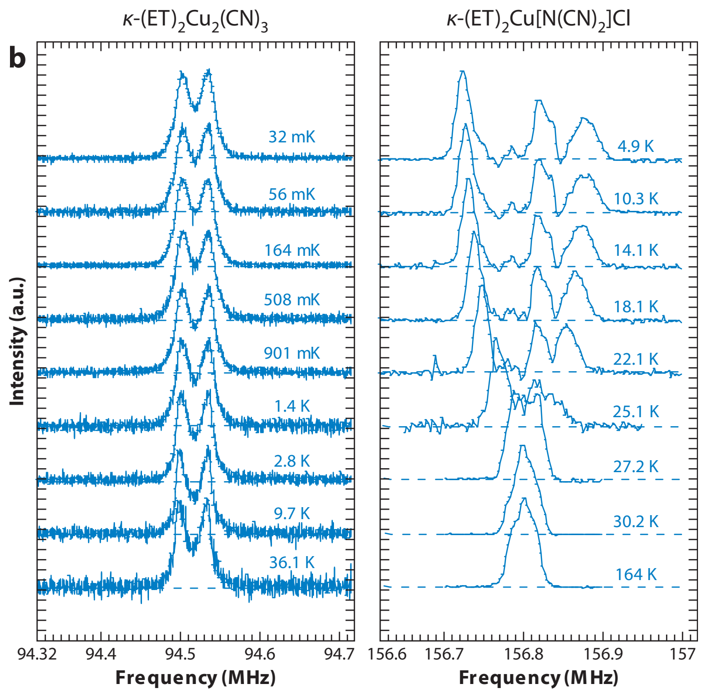
κ-$(ET)_2Cu_2(CN)_3$

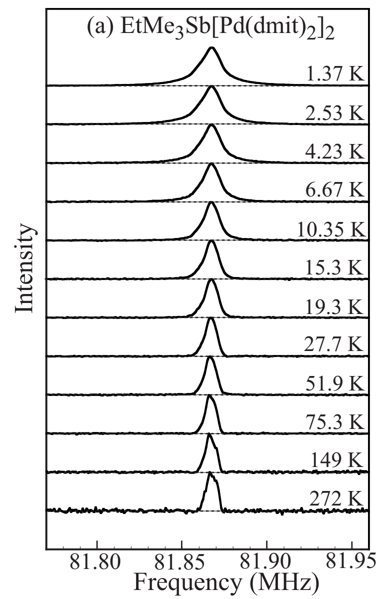
β′-$Pd(dmit)_2$

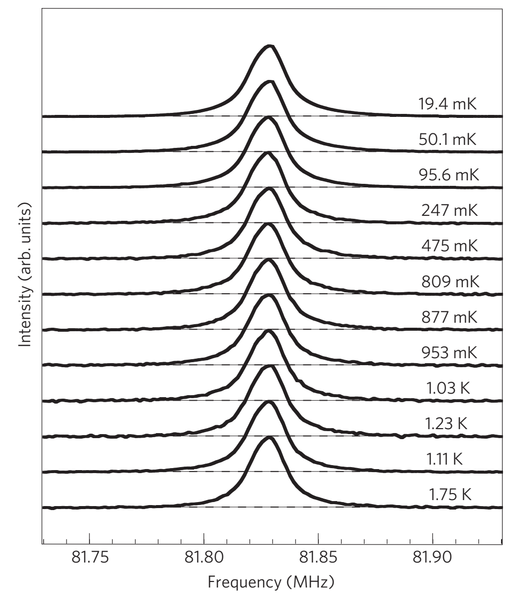
K. Kanoda group (2003-)

R. Kato group (2008-)

NMR lineshapes







κ-$(ET)_2Cu_2(CN)_3$

β′-$Pd(dmit)_2$

Y. Shimizu *et al*, 2003

^{1}H NMR

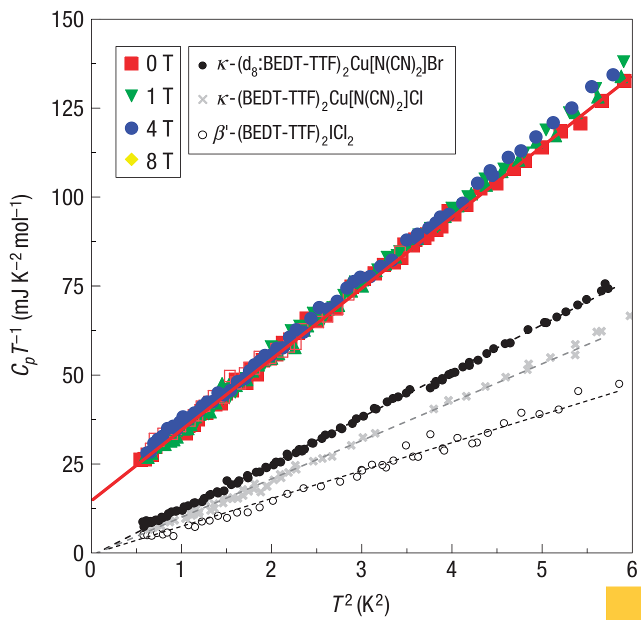
T. Itou *et al*, 2008,2010

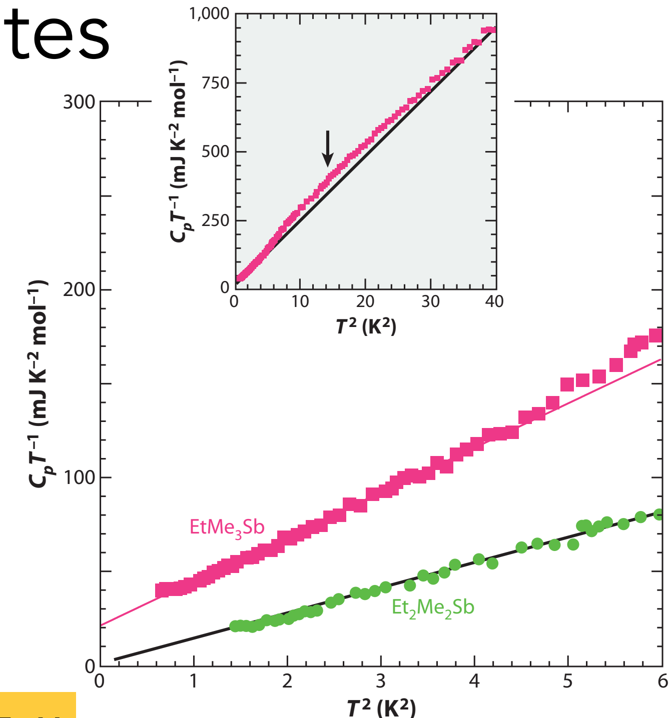
^{13}Cs NMR

Evidence for lack of static moments: f > 1000!

Specific Heat

- C ~ γT indicates gapless behavior with large density of states





γ_{Cu} ~ 0.7 !!

κ-$(ET)_2Cu_2(CN)_3$

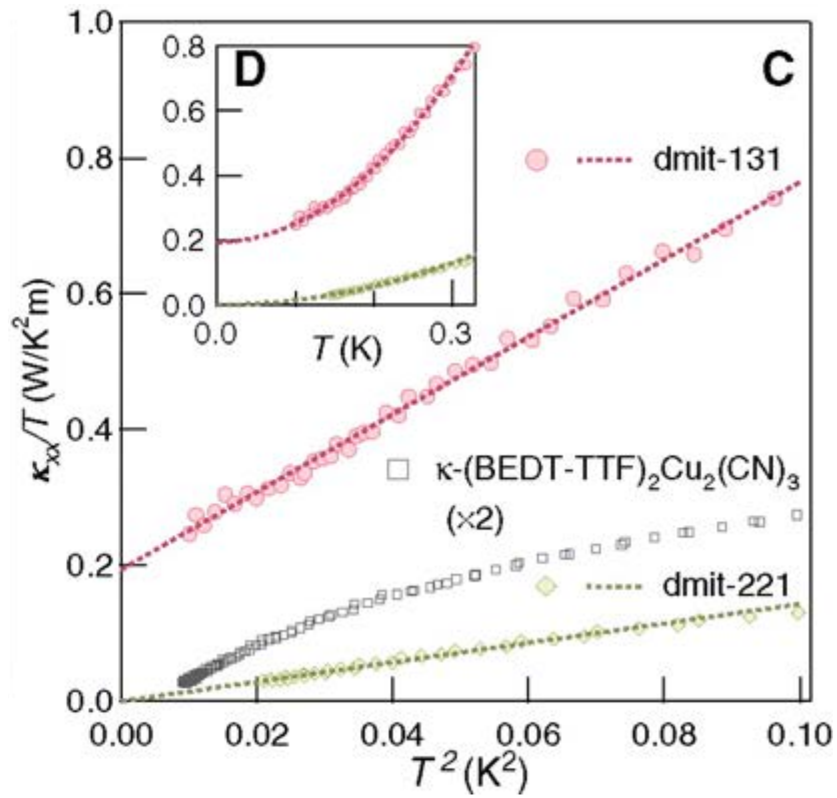
β′-$Pd(dmit)_2$

S. Yamashita *et al*, 2008

Thermal conductivity

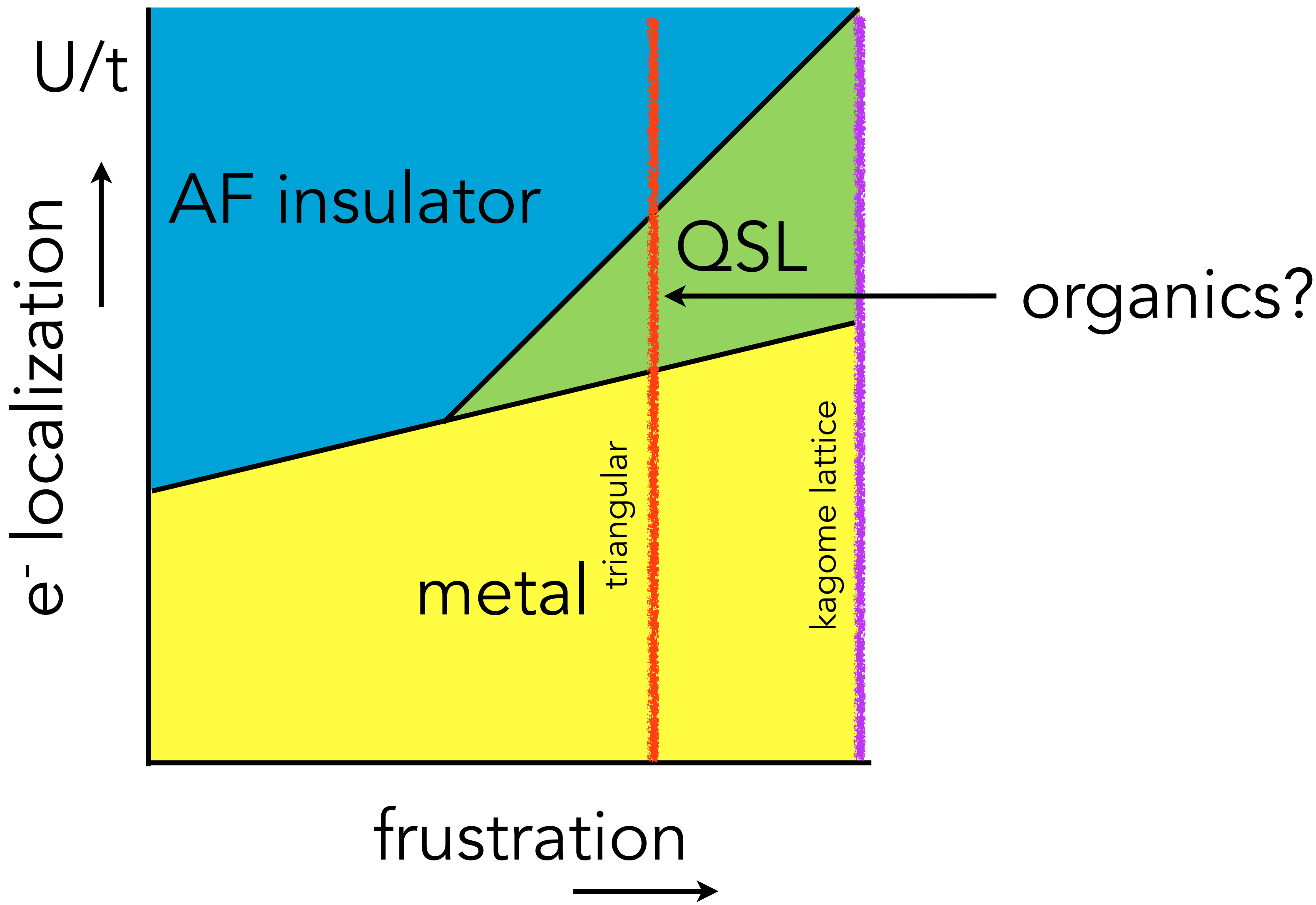
- Huge linear thermal conductivity indicates the gapless excitations are propagating, at least in dmit

- Estimate for a *metal* would correspond to a mean free path l ~ 1 μm ≈1000 a !



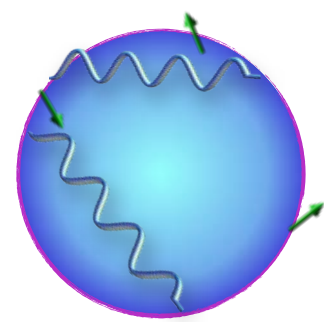
M. Yamashita *et al*, 2010

Charge fluctuations



Organics - Theory

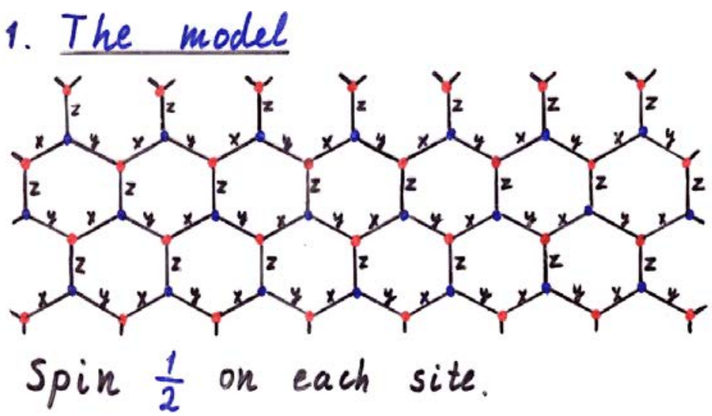
- RVB/QSL state:
  - Motrunich, Lee+Lee: (2005) “uniform RVB”
  - It is described by a **“Fermi sea” of spinons** coupled to a U(1) gauge field
- The anomalous thermal conductivity may be a window into an emergent fermi surface in an insulator!

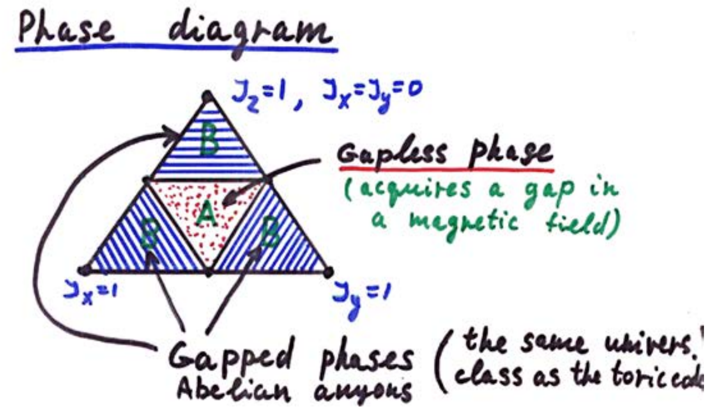


Kitaev model

Kitaev's honeycomb model $H = \sum_{i,\mu} K_\mu \sigma_i^\mu \sigma_{i+\mu}^\mu$

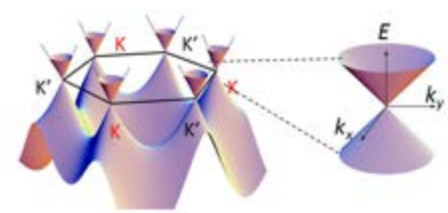
KITP, 2003





exact parton construction $\sigma_i^\mu = i c_i c_i^\mu \quad c_i c_i^x c_i^y c_i^z = 1$

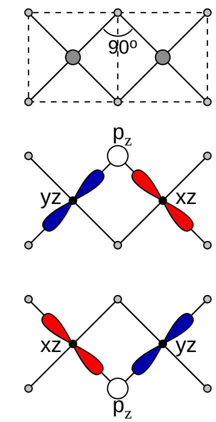
physical Majoranas $H_\mathrm{m} = K \sum_{\langle ij \rangle} i c_i c_j$

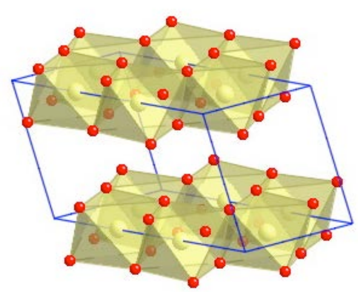


Kitaev Materials

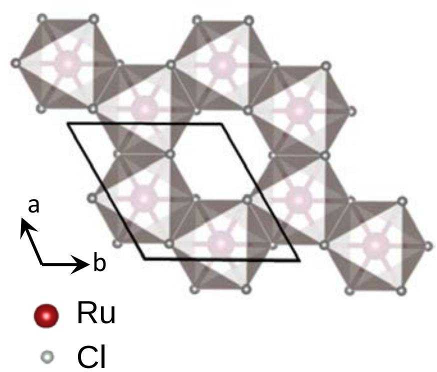
Jackeli, Khaliullin
2009

Showed that Kitaev interaction can be large in edge-sharing octahedra with large spin-orbit-coupling





Na_2IrO_3, (α,β,γ)-Li_2IrO_3



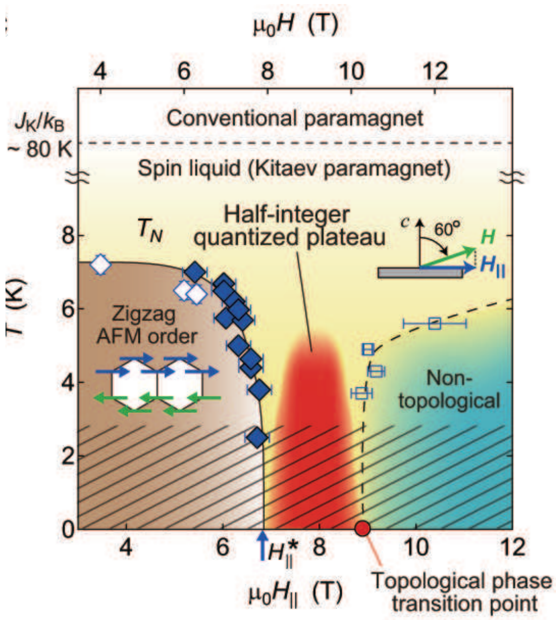
α-$RuCl_3$

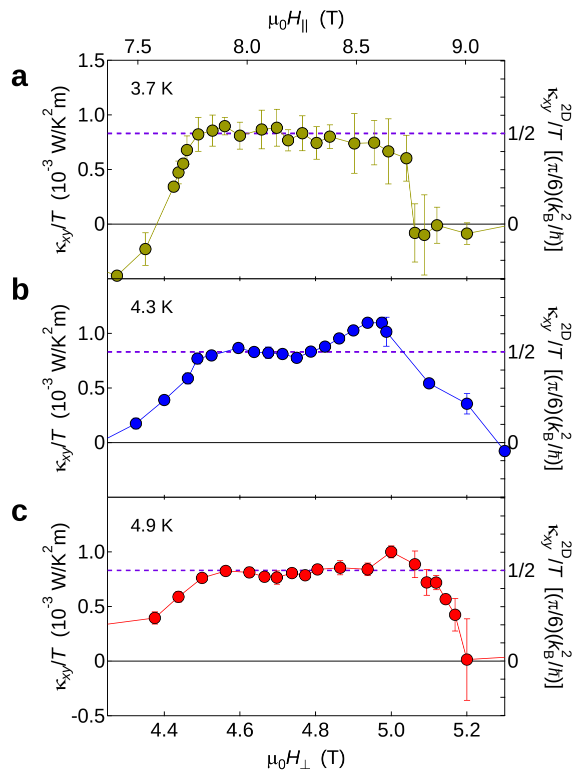
Y.-J. Kim...

Honeycomb and hyper-honeycomb structures

Thermal Hall

- Very recent experiment on a-RuCl$_3$





$$\frac{\kappa_{xy}}{T} = c\frac{\pi}{6}\frac{k_B^2}{\hbar}$$

c=1/2 is expected for a *chiral Majorana fermion edge*, characteristic of "Ising anyons"

Y. Kasahara *et al*, arXiv:1805.05022

Entanglement Issues

- Can you definitively identify highly entangled phases? How?
- Can you measure entanglement?
- What are the links between entanglement, thermalization, and hydrodynamics?

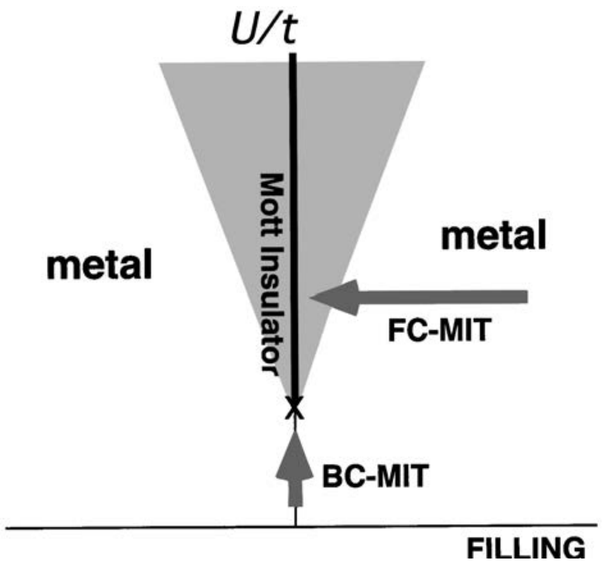
Correlation

- Many phenomena result from interactions that are neither topological nor simply described in terms of entanglement (which can be thought of as a particular type of correlation)
  - Mott metal-insulator transition
  - Heavy electrons and non-Fermi liquids
  - Fluctuating orders and pseudogaps
  - Low dimensional systems

Mott Transition

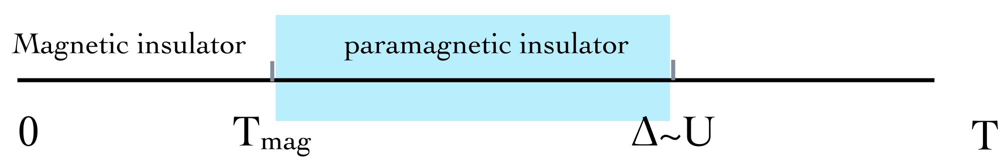
- Hubbard model

$$H = -t \sum_{\langle ij \rangle} c^\dagger_{i\alpha} c_{j\alpha} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



Imada, Fujimori, Tokura 1998

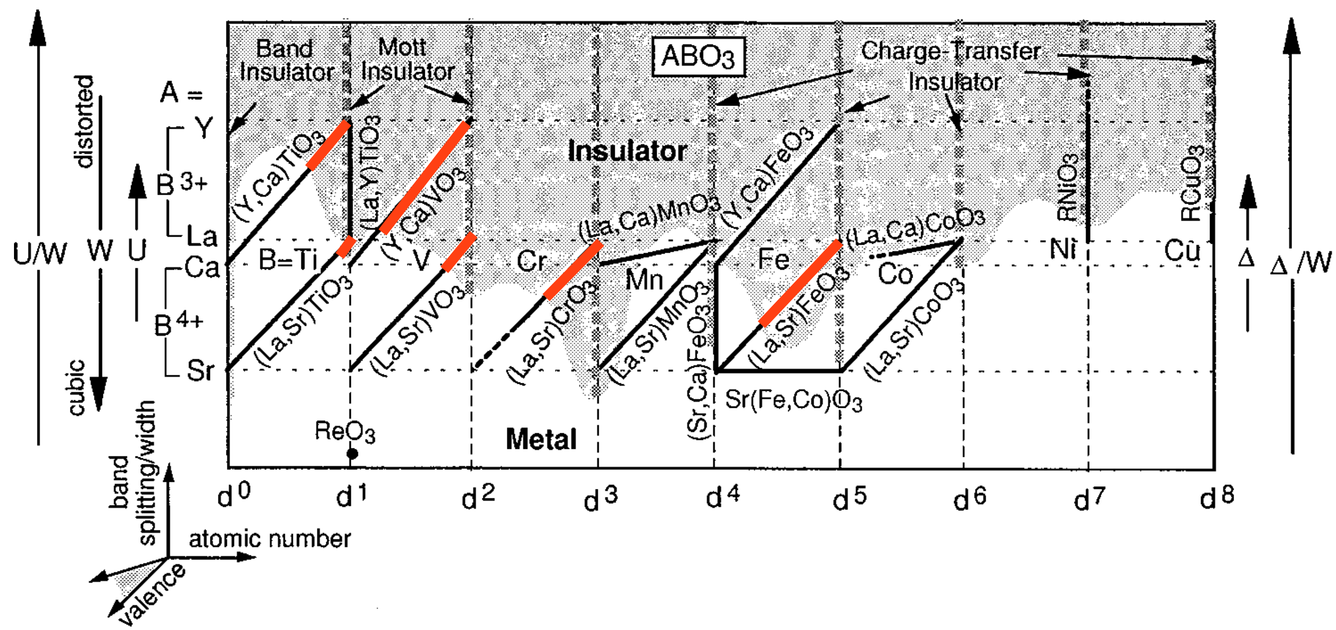
- Physically, a Mott Insulator is one which is insulating due to interaction-induced localization, not due to band physics
  - This is a question of energy scales
  - Deep in the Mott state:



Mott Transition

- And old subject

e.g. perovskites



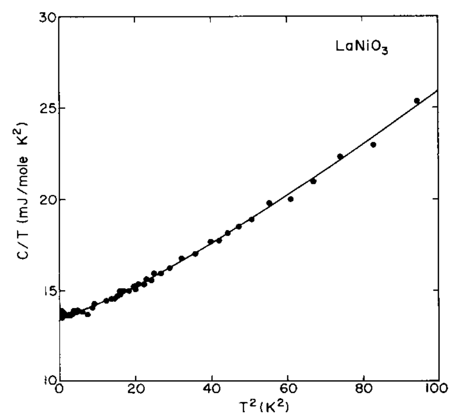
- But still a key theme, and now more accessible in new materials, via new approaches

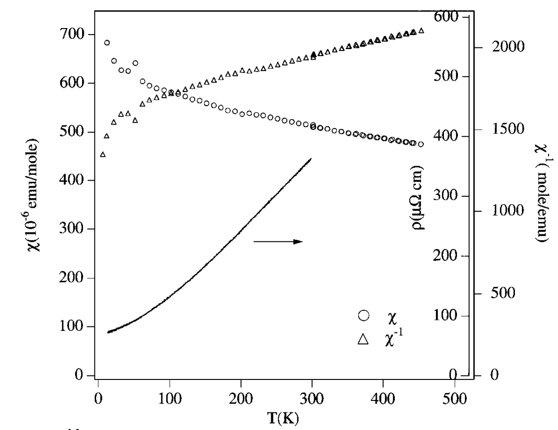
Heavy Electrons

- Mass enhancement near Mott transition

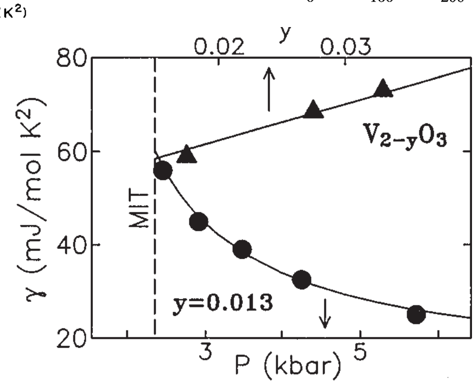
$LaNiO_3$:

$\gamma/\gamma_{\mathrm{band}} = 10$





V_2O_3



Heavy Fermions

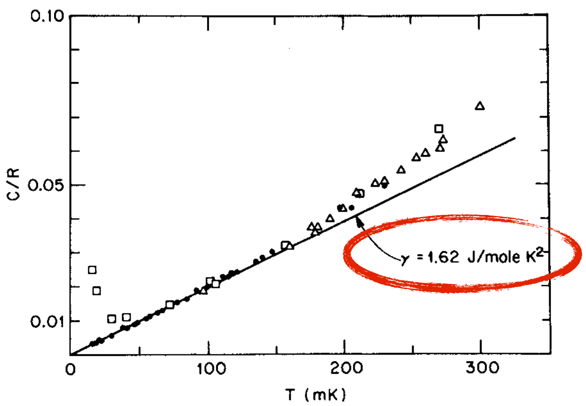


FIG. 1. Specific heat of $CeAl_3$ at very low temperatures in zero field (●, Δ) and in 10 kOe (□).

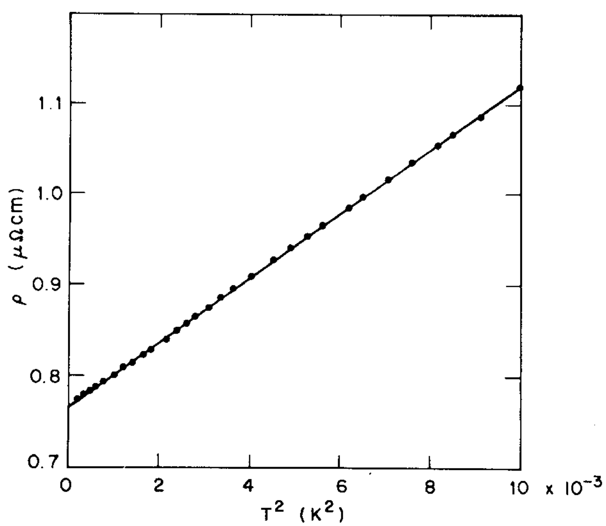


FIG. 3. Electrical resistivity of $CeAl_3$ below 100 mK, plotted against T^2.

$$C \sim \gamma T$$

$$\rho(T) - \rho(0) \sim AT^2$$

Both γ and A **huge**

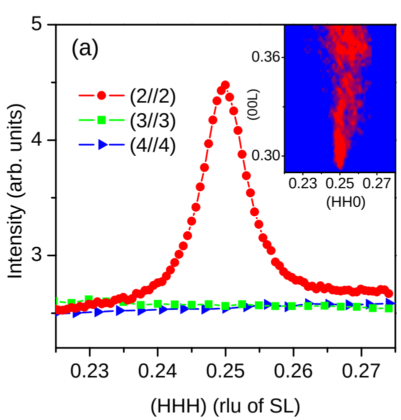
Behave like Fermi liquid with tiny E_F and large electron mass, but only for $T \ll E_F$

Common in “Kondo lattice” materials

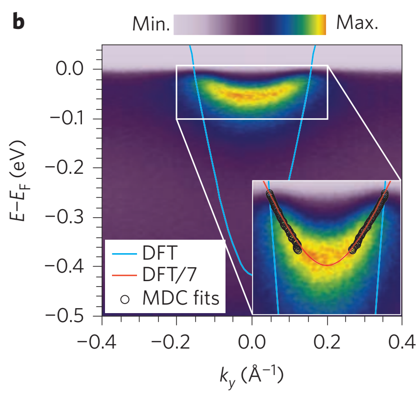
Oxide heterostructures

- New handle on Mott materials from oxide MBE

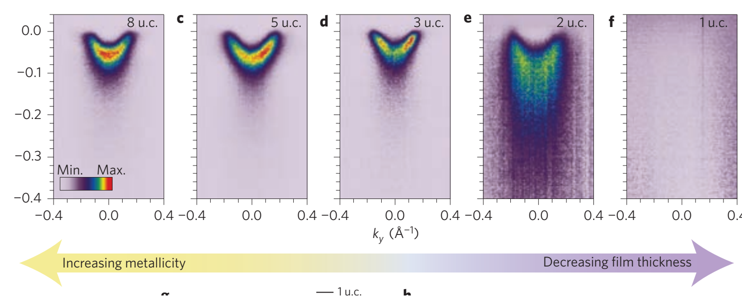
example: $LaNiO_3$ - just on the metallic side of Mott transition <u>in bulk</u>



AF order for films <4uc thickness. Frano *et al*, 2013



Large mass in 8uc thick films

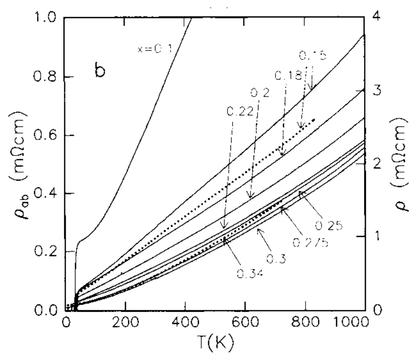


Metal-insulator transition at 2uc thickness

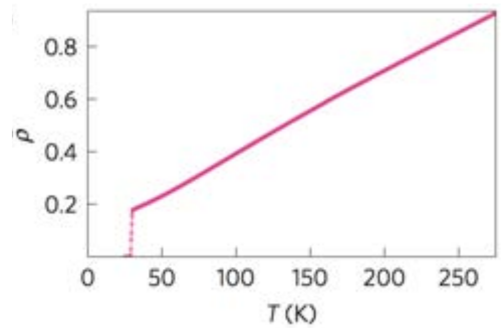
King *et al*, 2014 [Schlom,Shen]

Non-Fermi Liquids

"strange metal"



LSCO Takagi *et al, 1992*



$BaFe_2(As_{1-x}P_x)_2$, Hayes *et al, 2016*

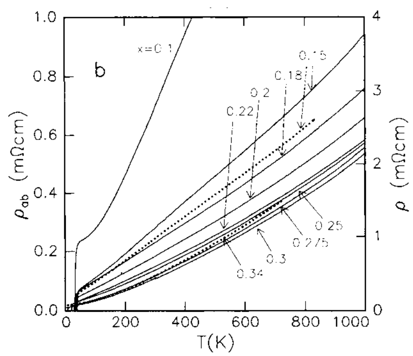
$$\frac{1}{\tau} \sim T\,?$$

T-linear resistivity/scattering rate:

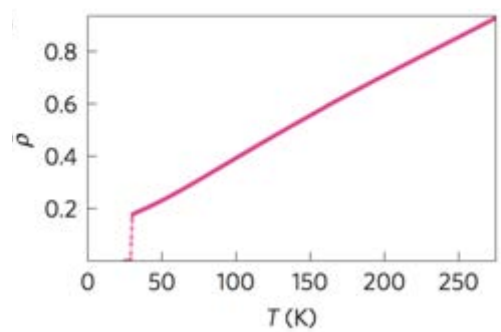
- Many materials
- Often nearby to unconventional superconductivity
- Symptom of a different type of metal? Or of a quantum critical point?

Non-Fermi Liquids

"strange metal"



LSCO Takagi *et al, 1992*



$BaFe_2(As_{1-x}P_x)_2$, Hayes *et al, 2016*

$$\frac{1}{\tau} \sim T\,?$$

Quasiparticles?

self-energy

Green's function $$G_R(\boldsymbol{k},\omega) = \frac{1}{\omega - \epsilon_{\boldsymbol{k}} - \Sigma(\boldsymbol{k},\omega) - i\delta}$$

Spectral density $$\rho(\boldsymbol{k},\omega) = \frac{-2\Sigma''(\boldsymbol{k},\omega)}{(\omega - \epsilon_{\boldsymbol{k}} - \Sigma'(\boldsymbol{k},\omega))^2 + (\Sigma''(\boldsymbol{k},\omega))^2}.$$

$$\Sigma''_{\mathrm{FL}} \sim \omega^2 \sim T^2$$

here $\Sigma''_{\mathrm{FL}} \sim T$

What is the mechanism of the strange metal?

A) Electron nematic quantum criticality

B) It’s dual to a black hole in anti-de-Sitter space

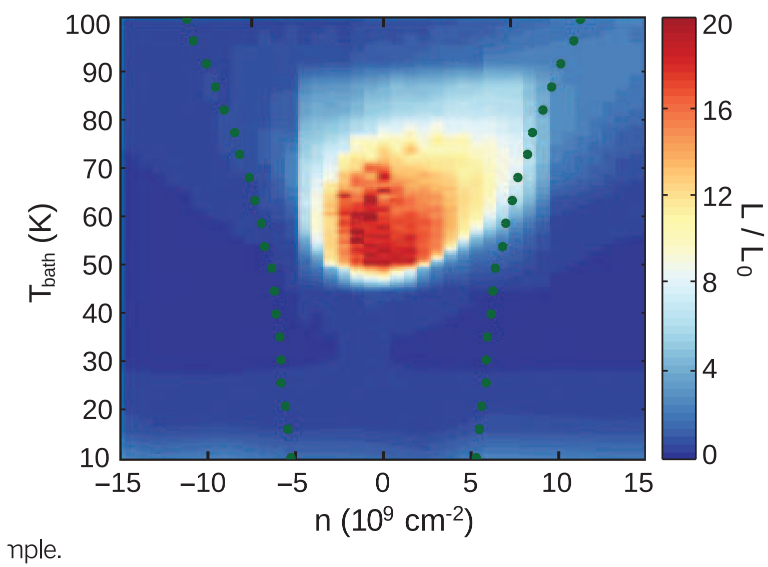
C) Dynamical mean field theory

D) Interaction with an emergent gauge field

E) Measurement error

Hydrodynamic flow

- Low density, ultra-clean fluids - here graphene: e-e scattering creates *viscous flow*



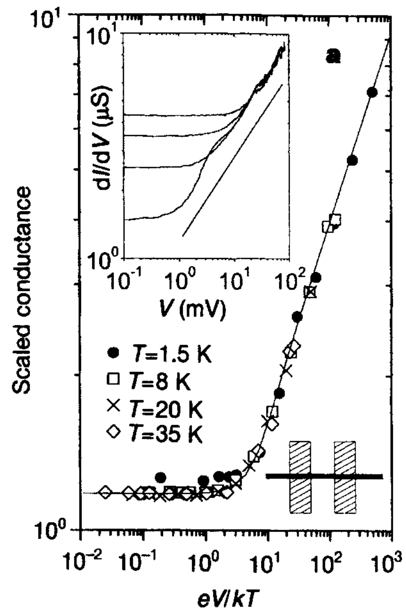
Crossno *et al*, 2016

Red region: thermal conductivity much larger than electrical conductivity. Indicates e-e fluid regime

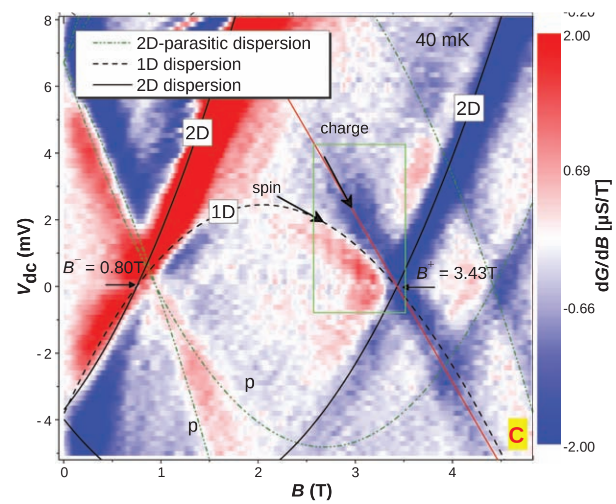
Luttinger liquids

- One dimension: it is known that all metals are "strange"

electron spectral function develops *power-law* singularities instead of quasiparticle pole: many manifestations in spectroscopy, transport



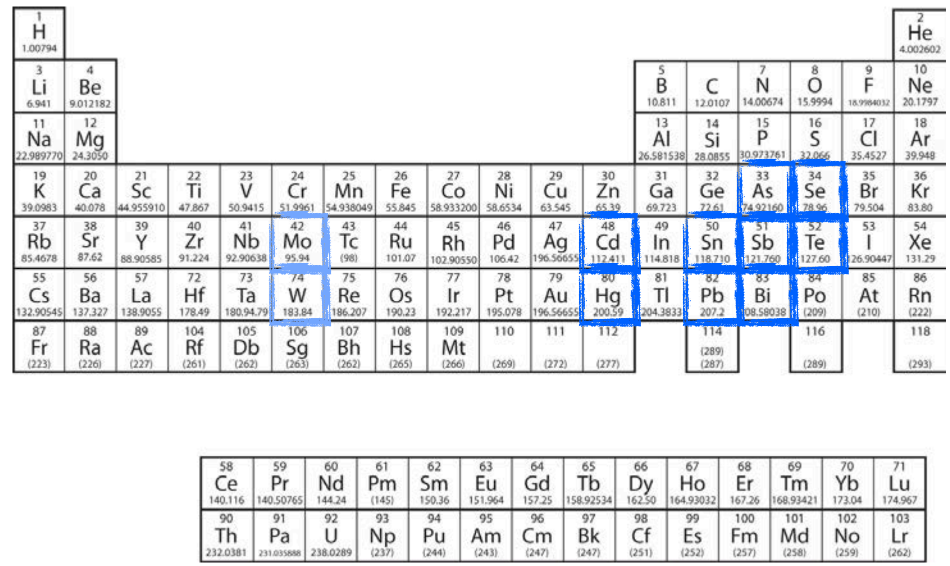
Bockrath *et al*, *nanotubes, 98*



Jompol *et al*, GaAs quantum wires, 2009

QM Materials

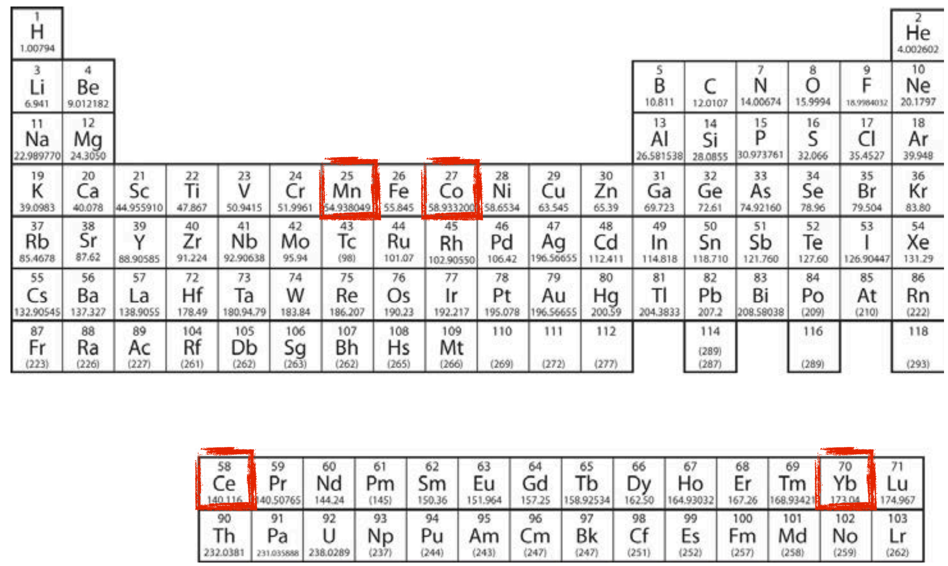
- Topological materials
  - HgTe, Bi_2Se_3, Bi_2Te_3,Sb_2Te_3, TaAs, Cd_2Se_3, WTe_2, $MoTe_2$



mostly s+p electron materials. Very extended, highly overlapping orbitals. Weak correlations. Heavy for strong SOC.

QM Materials

- Topological materials
  - HgTe, Bi_2Se_3, Bi_2Te_3,Sb_2Te_3, TaAs, Cd_2Se_3, WTe_2, $MoTe_2$
  - Mn_3Sn, Mn_3Ge, YbPtBi, CeAlGe, Co_2MnGa

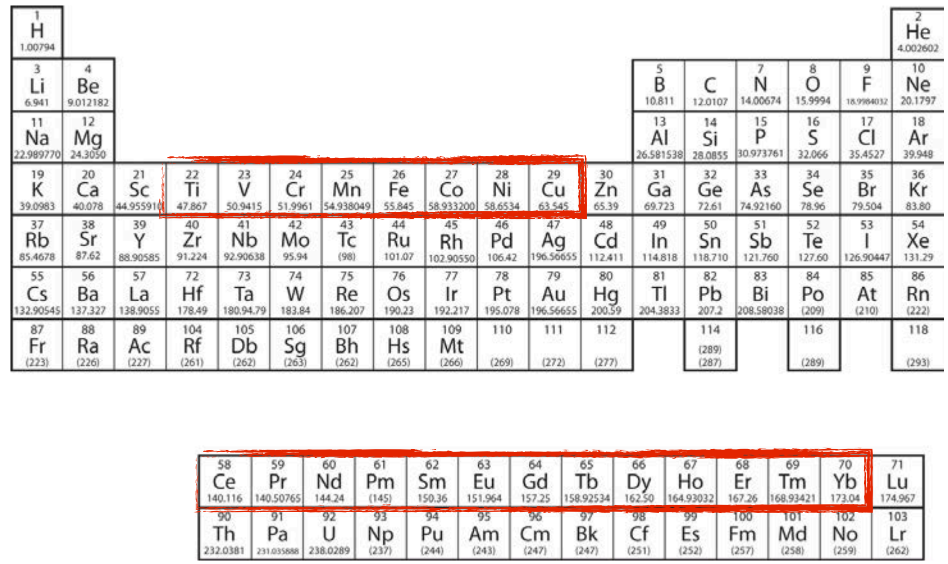


New ingredients in recent materials: partially filled 3d and 4f orbitals: correlations!

Specifically these ions host local moments

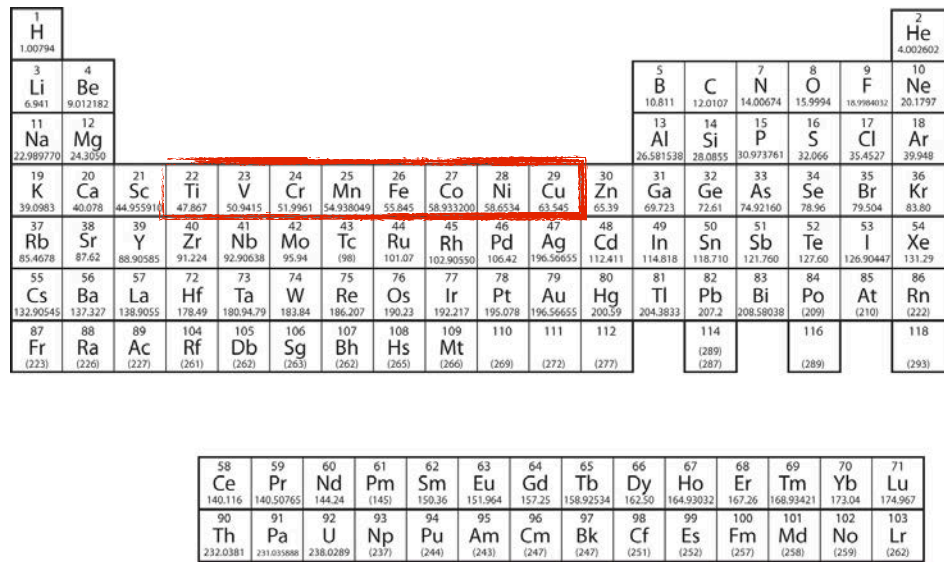
Local moments

- Most magnetism in QMs comes from either 3d transition metal ions or 4f rare earths. These have relatively localized orbitals which don't overlap strongly with neighbors and have strong Coulomb repulsion, which localizes electrons best.



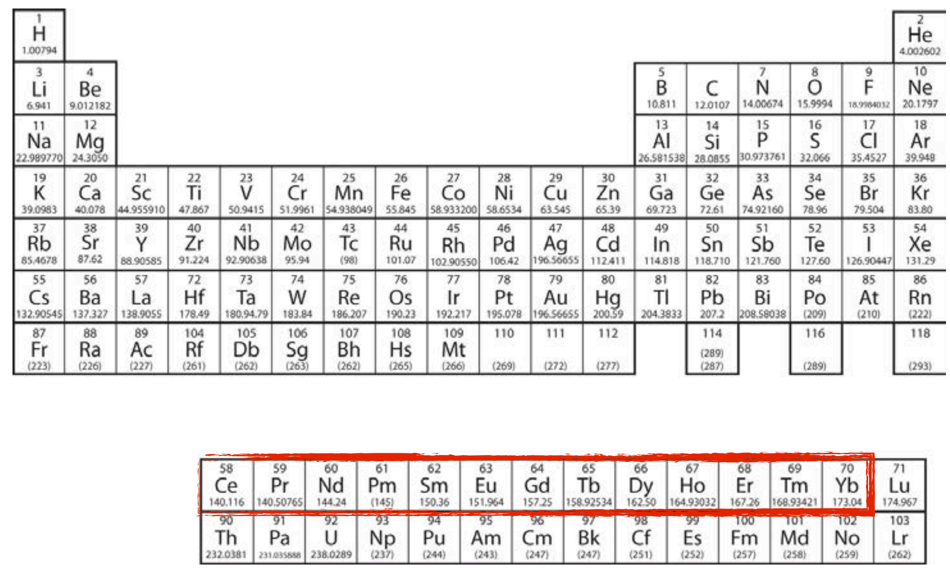
Local moments

- In 3d transition metals, *usually* magnetism is fairly isotropic, i.e. spins are “Heisenberg like”, because crystal fields split the d orbitals and spin-orbit coupling is relatively weak (Co is most common exception, when very localized). Exchange interactions between spins vary from quite strong (1000K) to quite weak (1K).



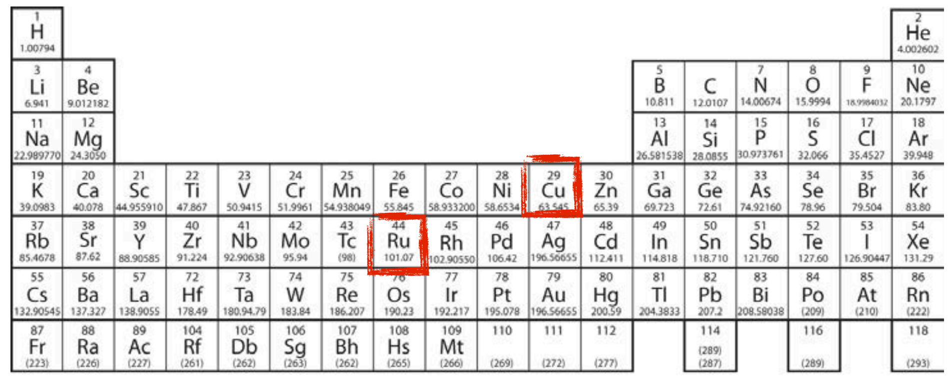
Local moments

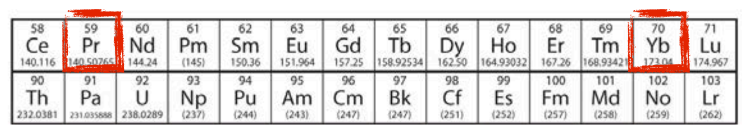
- In 4f lanthanides, spin-orbit coupling is dominant over crystal fields and so magnetic moments become large (incorporating orbital moment) and often very anisotropic (due to large SOC). They have complex multiplet structures, and weak exchange interactions.



QM Materials

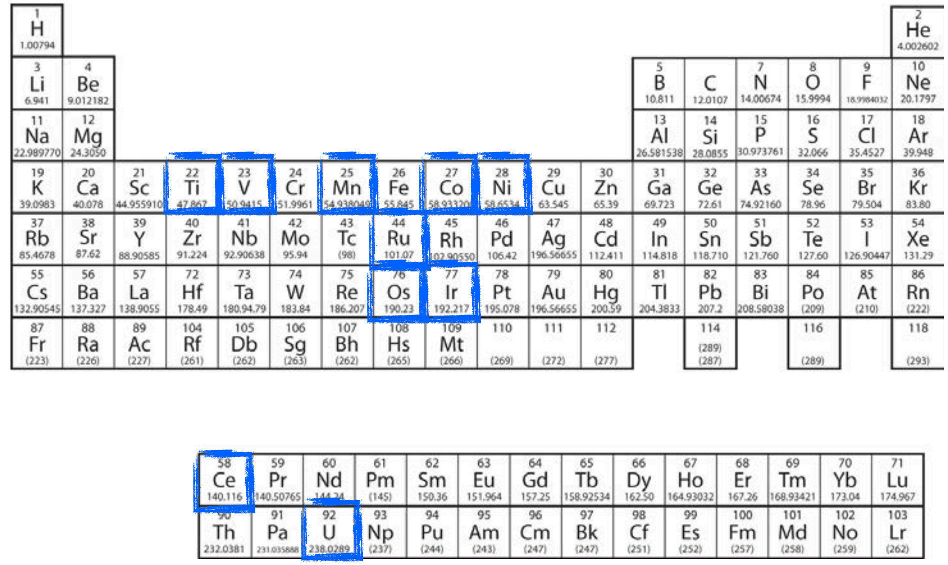
- Quantum spin liquids and interesting insulating antiferromagnets
    - $ZnCu_3(OH)_6Cl_2$, a-$RuCl_3$, $Pr_2Zr_2O_7$, Cs_2CuCl_4, $Yb_2Ti_2O_7$





QM Materials

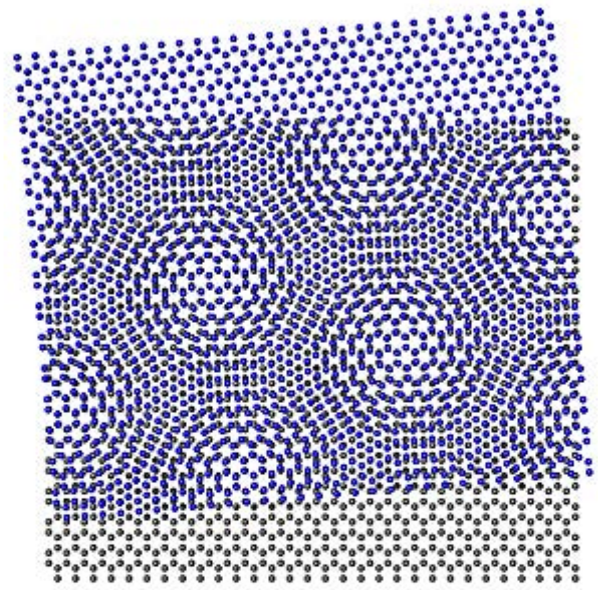
- Correlated metals/ Mott transitions
  - $RTiO_3$,RVO_3,$RNiO_3$, $RMnO_3$,$RCoO_3$,...
  - $Cd_2Os_2O_7$,$Nd_2Ir_2O_7$, Sr_2IrO_4,Sr_2RuO_4,..
  - URu_2Si_2,$CeAl_3$,....

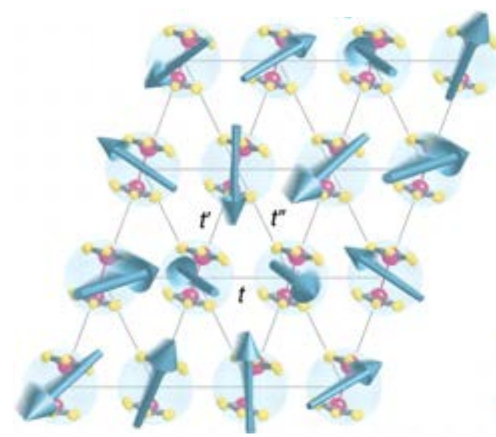


transition metals and rare earths mostly.

QM Materials

- Twisted graphene, organics "break the mold"
  - Become correlated because large unit cell suppresses hopping/bandwidth
  - "designed" QMs





Thanks