

Introduction to Quantum Materials

Leon Balents, KITP

QS3 School, June 11, 2018

Day 2

Topological frontiers

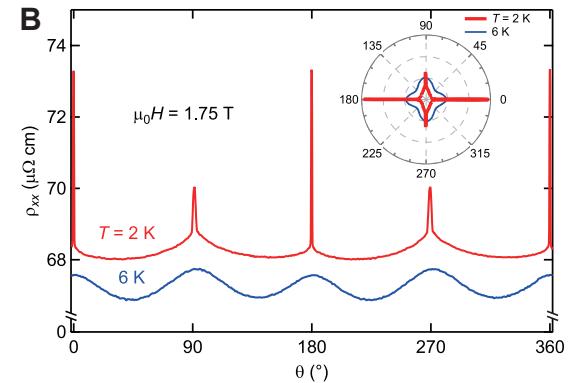
- Can we realize a topological superconductor?
- What is the interplay between topological defects and topological bands?
- What are the robust signatures of topology in transport and other responses?
- Are there strongly interacting topological phases in real materials?

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

entangled: cannot be written as
a product state

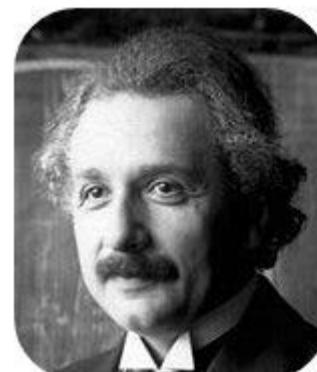
Entanglement

EPR

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



??where is the information??



A. Einstein



B. Podolsky



N. Rosen

Many Body Entanglement



Phil Anderson, 1973

a “quantum liquid” of spins

$$\text{blue oval} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$\Psi = \begin{array}{c} \text{Diagram of a triangular lattice with blue ovals representing spin pairs} \\ + \end{array} \begin{array}{c} \text{Diagram of a triangular lattice with blue ovals representing spin pairs} \\ + \dots \end{array}$$

Resonating Valence Bond state

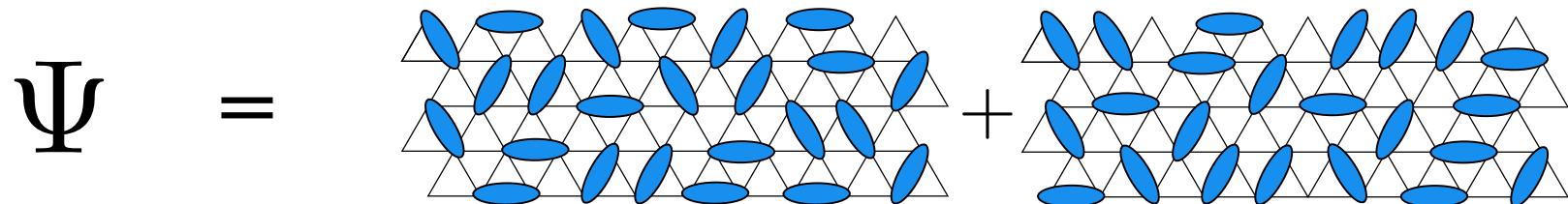
Many Body Entanglement



Phil Anderson, 1973

a “quantum liquid” of spins

$$\text{blue oval} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$



Resonating Valence Bond 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

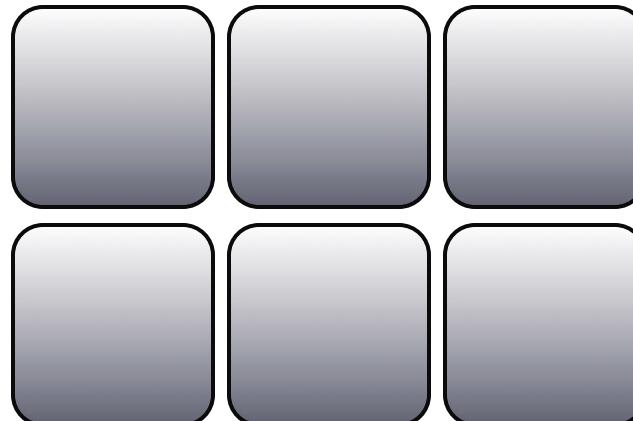
$$H = \sum_x \mathcal{H}(x) \quad \mathcal{H}(x) \text{ has local support near } x$$

Ground state is “essentially”
a product state

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

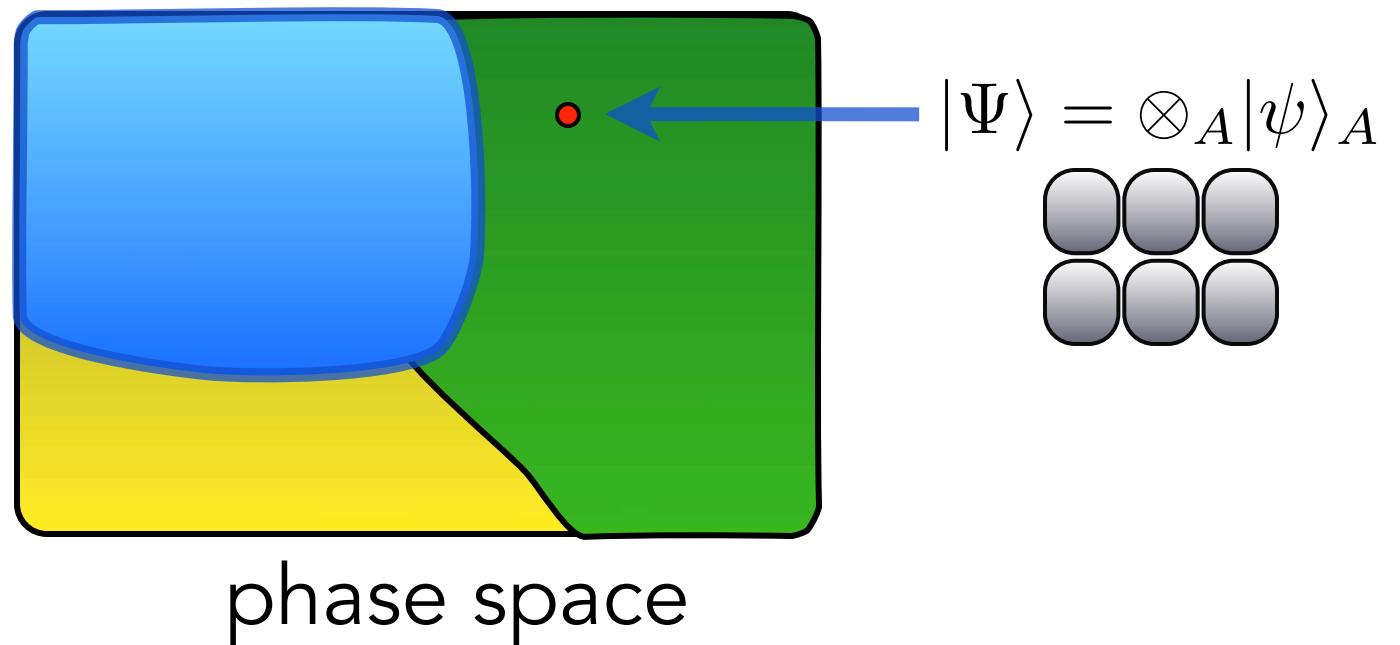
no entanglement
between blocks

most insulators
are like this



“Essentially” a product state?

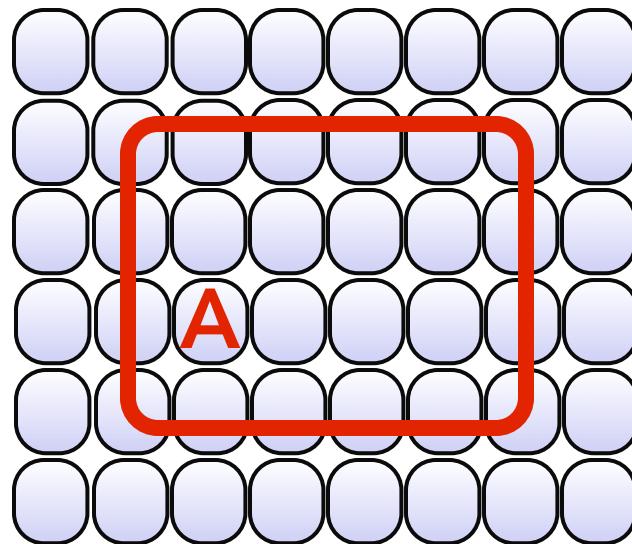
- Adiabatic continuity



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

“Essentially” a product state?

- Entanglement scaling



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

$$S(A) = -\text{Tr}_A (\rho_A \ln \rho_A)$$

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

satisfied with exponentially small corrections

Best example: ordered magnet

Hamiltonian

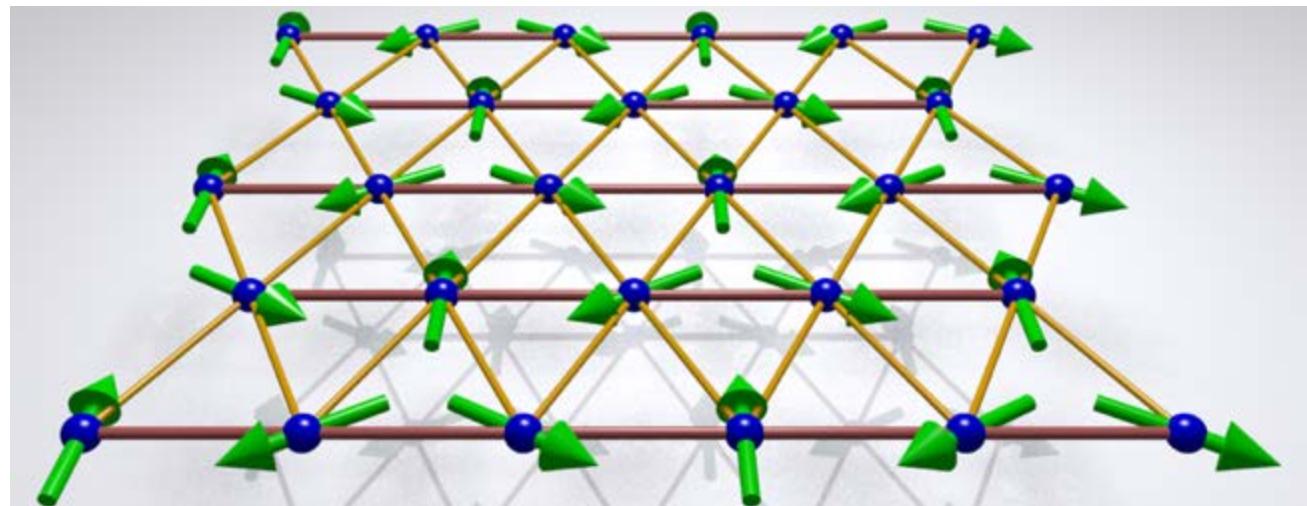
$$H = \sum_{(ij)} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

exchange is short-range: local

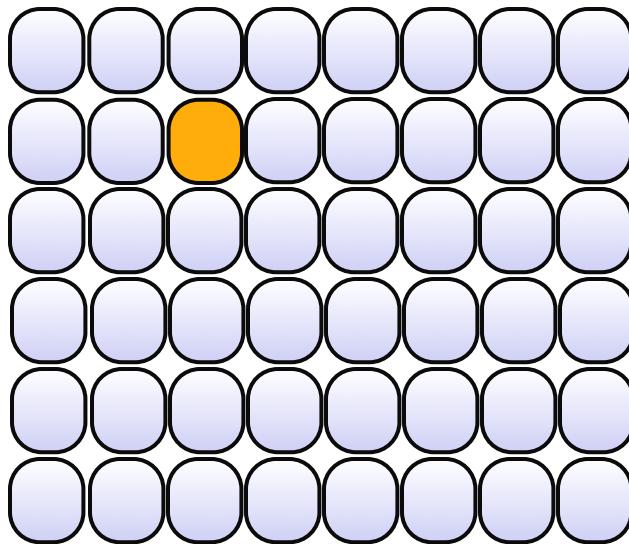
ordered state

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

block is a single spin



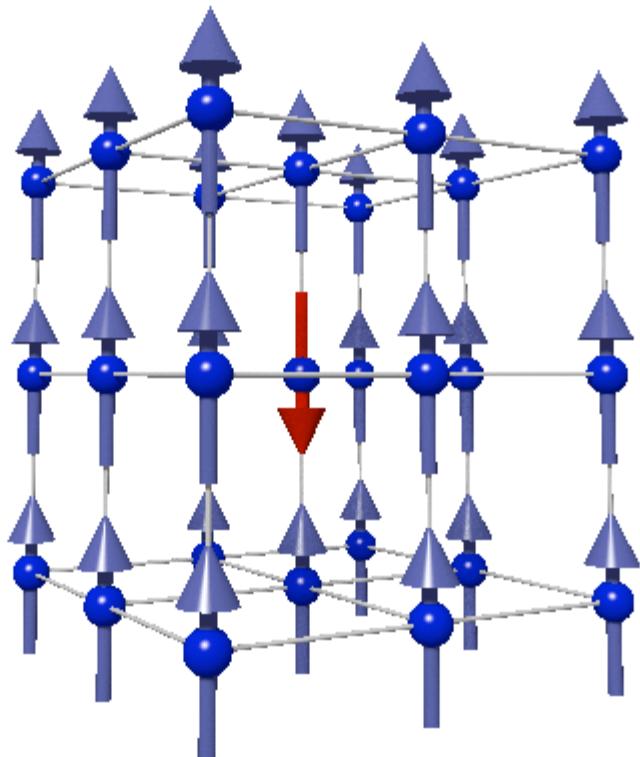
Quasiparticles



excited states ~ excited
levels of one block

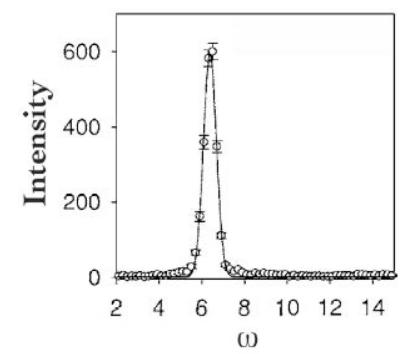
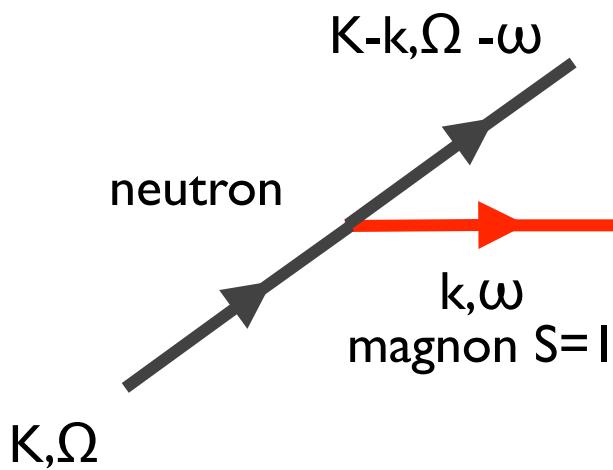
- local excitation can be created with operators in one block
- localized excitation has discrete spectrum with non-zero gap, and plane wave forms sharp band
- quantum numbers consistent with finite system: no emergent or fractional quantum numbers

Spin wave



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

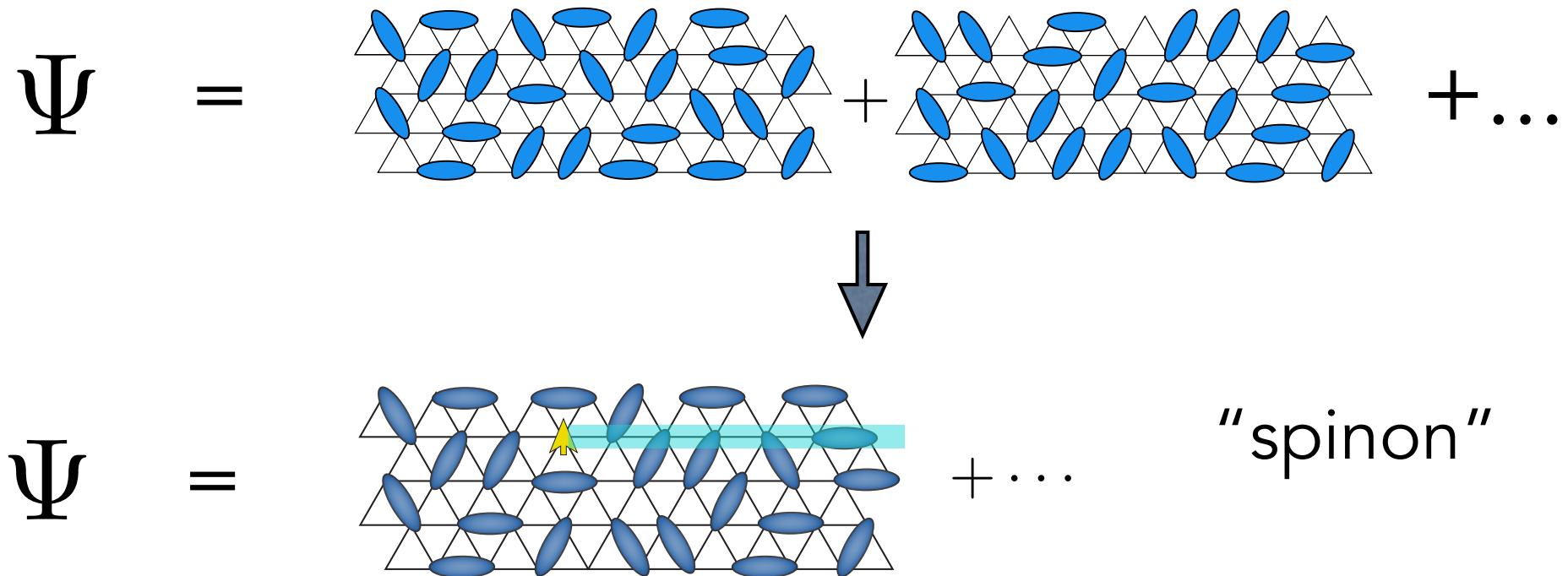
$$|f\rangle = S_k^+ |i\rangle$$



Line shape in Rb_2MnF_4

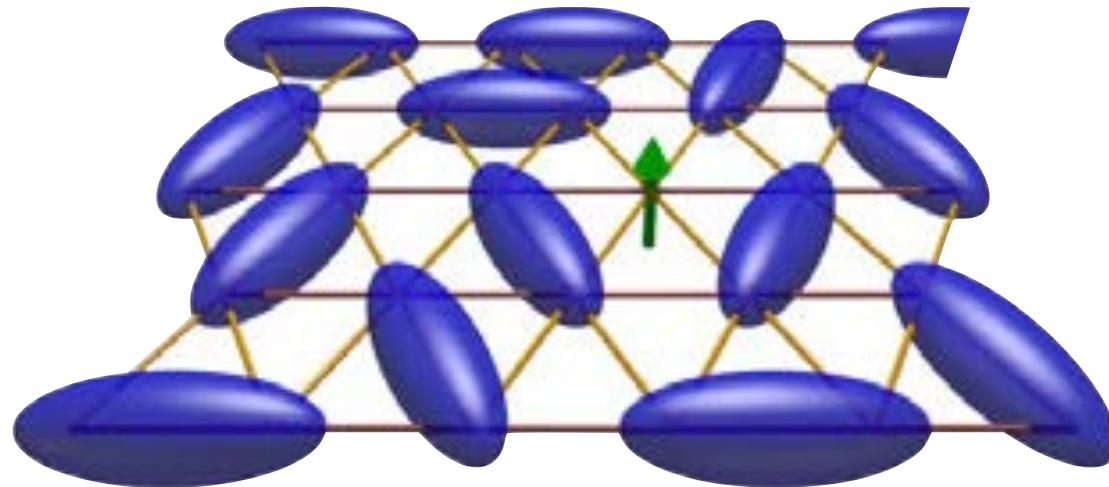
Quantum spin liquid

Entanglement -> non-local excitation



“quasiparticle” above a non-zero gap

Fractional quantum number

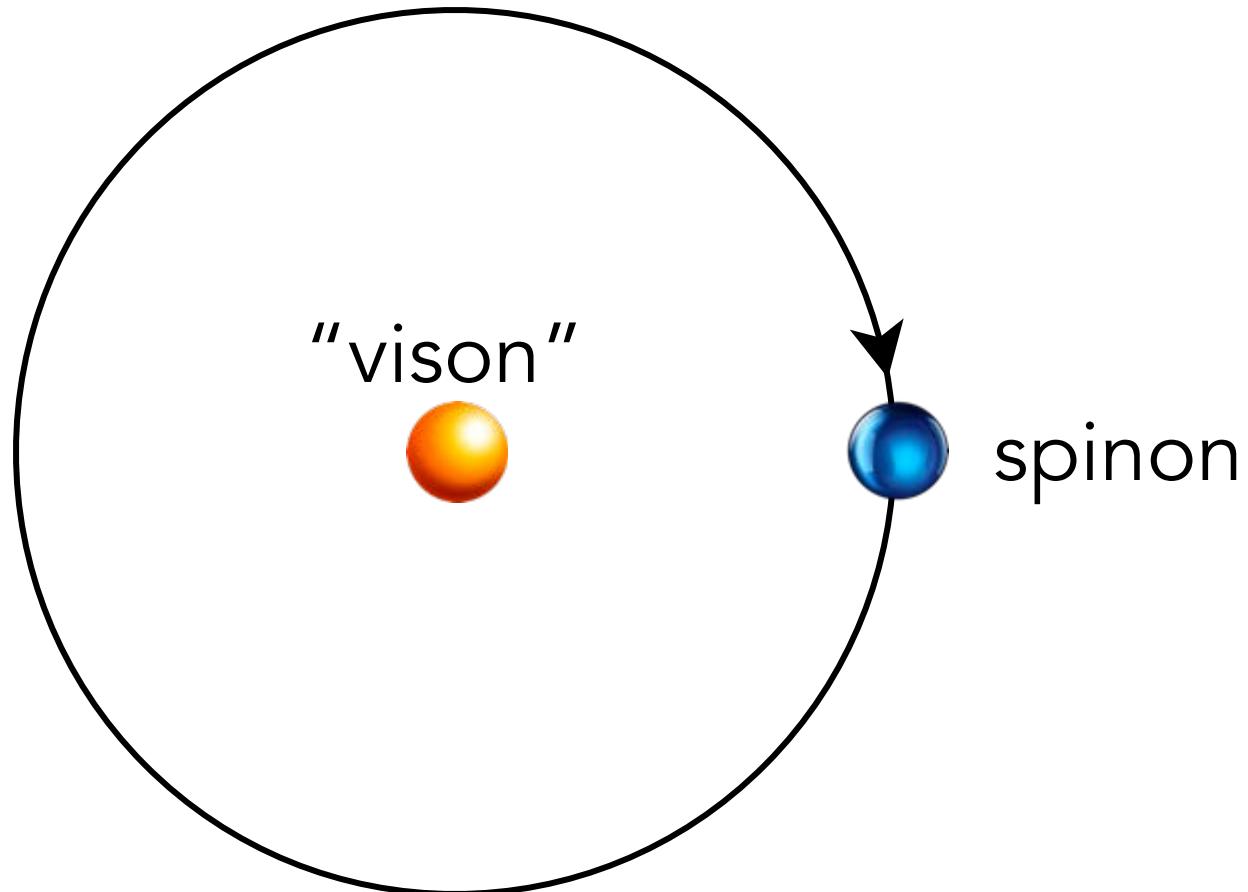


excitation with $\Delta S = 1/2$
not possible for any finite
cluster of spins

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

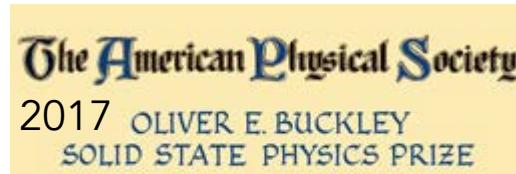


A. Kitaev

(intrinsic)

Topological phases

Warning: this is a
different meaning of
topological!



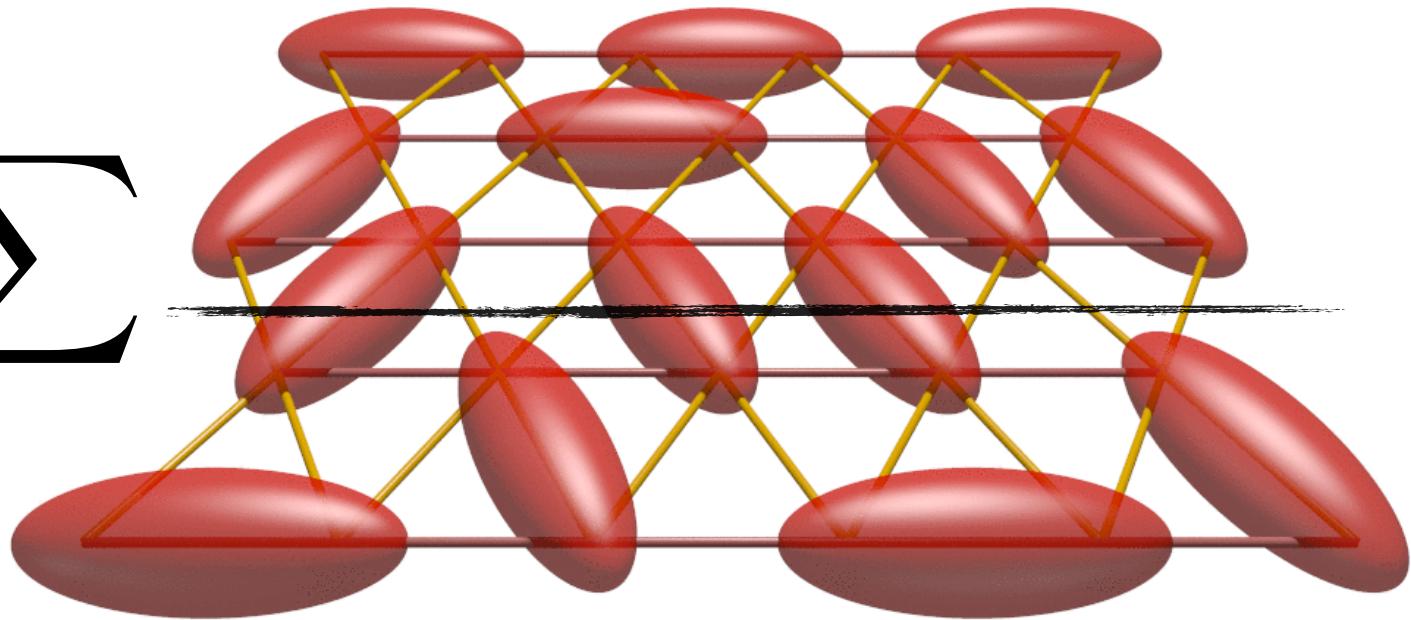
Anderson's RVB state is thus an example of a “topological phase” - the best understood sort of QSL

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

$$\begin{array}{c} e \quad m \\ \diagdown \quad \diagup \\ e \quad m \end{array} = - \begin{array}{c} e \quad m \\ | \quad | \\ e \quad m \end{array}$$
$$\begin{array}{c} e \quad m \quad e \quad m \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \\ e \quad m \quad e \quad m \end{array} = \begin{array}{c} e \quad m \quad e \quad m \\ | \quad | \quad | \quad | \\ e \quad m \quad e \quad m \end{array} = - \begin{array}{c} e \quad m \quad e \quad m \\ || \quad || \quad || \quad || \\ e \quad m \quad e \quad m \end{array}$$

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

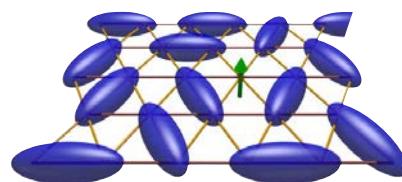
$$\Psi = \begin{array}{c} \text{Diagram of a triangular lattice with blue ovals representing spins, showing two different local arrangements of spins?} \\ + \end{array} \dots$$

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



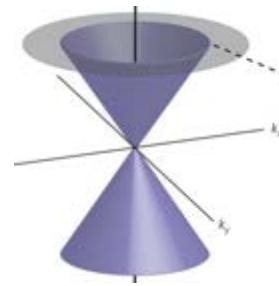
anyonic
spinons

- U(1) QSL



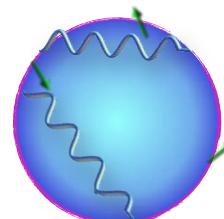
electric+magnetic
monopoles, photon

- Dirac QSLs



strongly
interacting
Dirac fermions

- Spinon Fermi surface

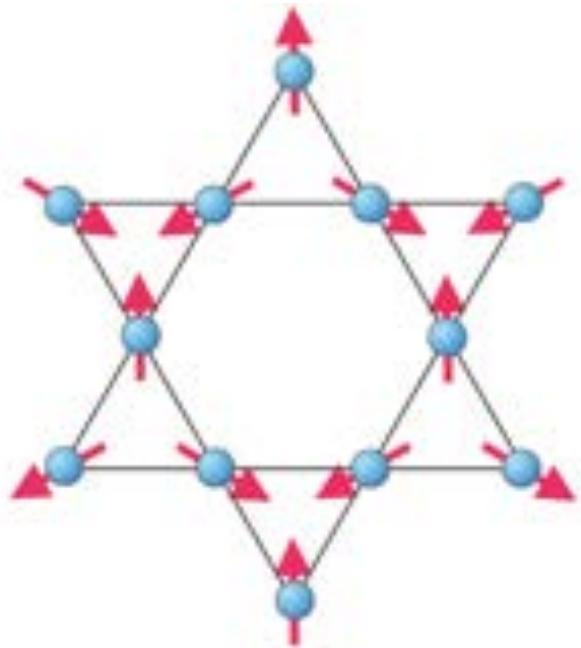


non-Fermi
liquid “spin
metal”

QSL experiments

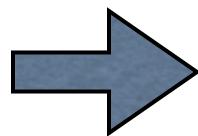
- This is a difficult subject, if you want a challenge!
- Discuss three examples:
 - Kagomé lattice herbertsmithite
 - Organic triangular lattice
 - alpha-RuCl₃ Kitaev magnet

Kagomé antiferromagnet



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

Very large classical
degeneracy

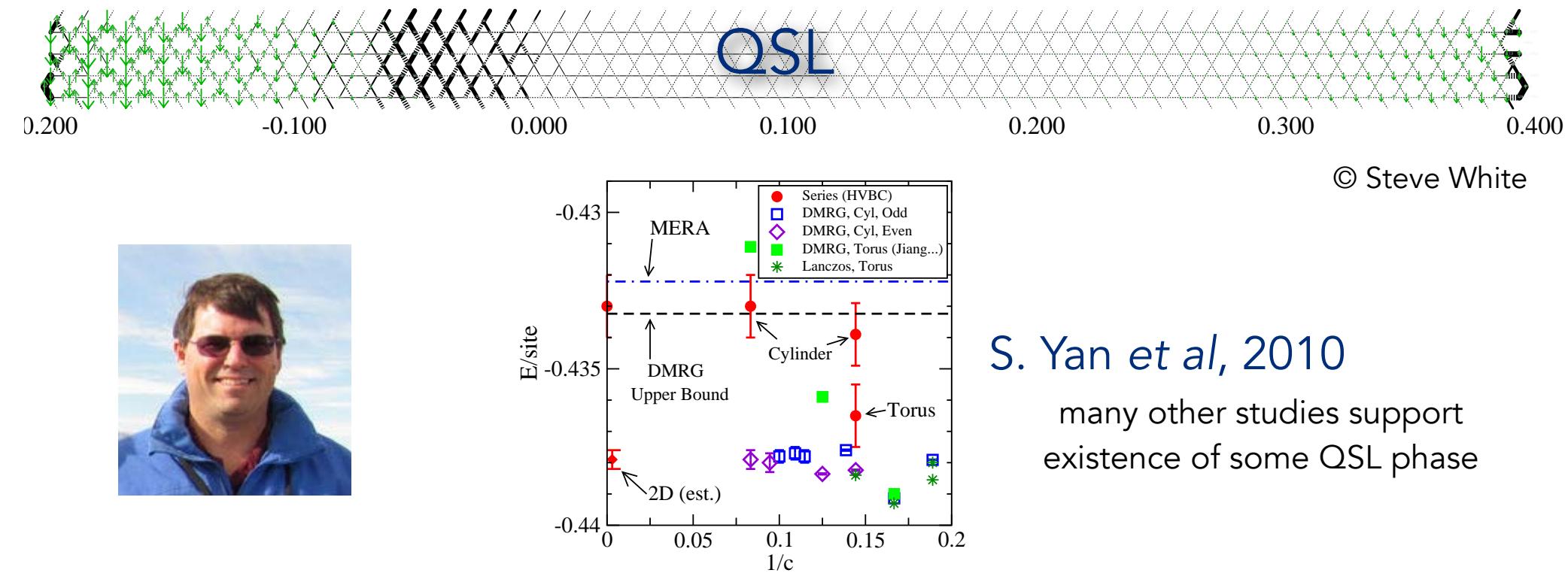


likely to be a QSL

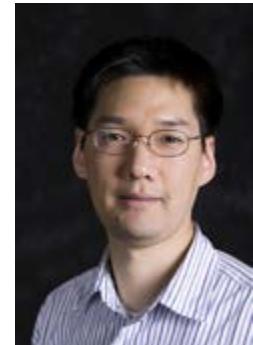
V. Elser, 1989 + many many others

$S=1/2$ kagomé AF

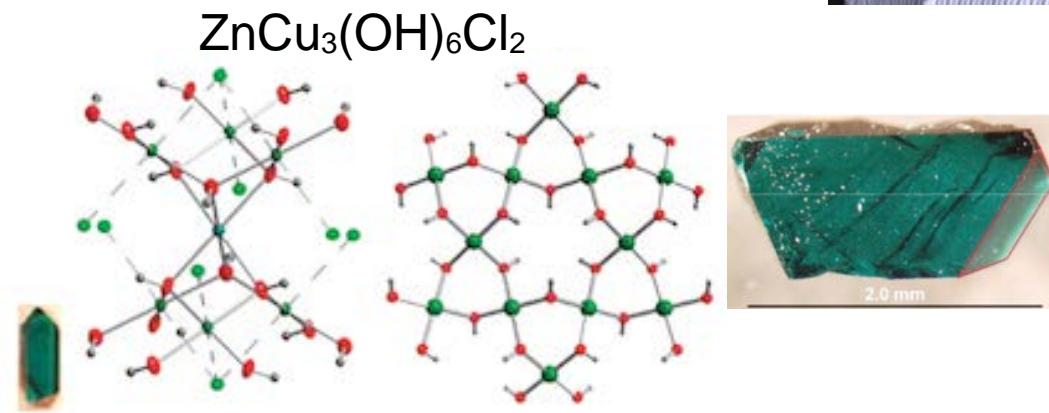
- Rather definitive evidence for QSL by DMRG



Herbertsmithite

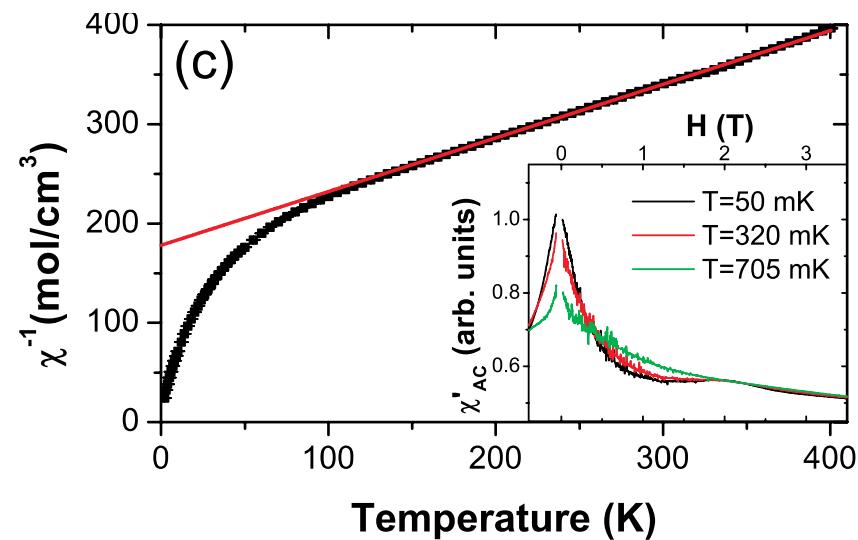


kagomé layers of Cu
 $S=1/2$ spins, separated
by non-magnetic Zn



Heisenberg-like
with $J \sim 200\text{K}$

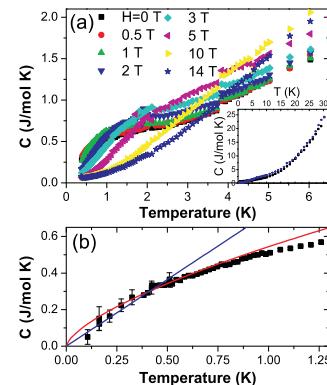
no order down to
50mK



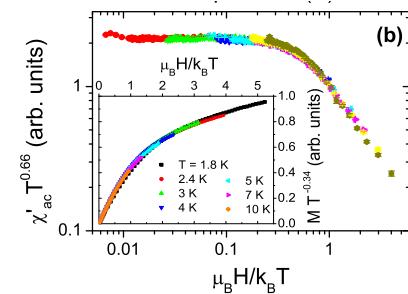
Helton et al, 2007

Herbertsmithite

Lots of early evidence
for gaplessness



Helton et al, 2007

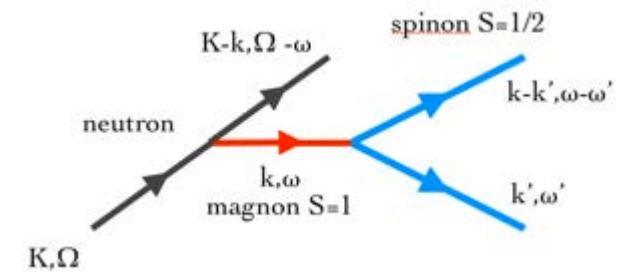
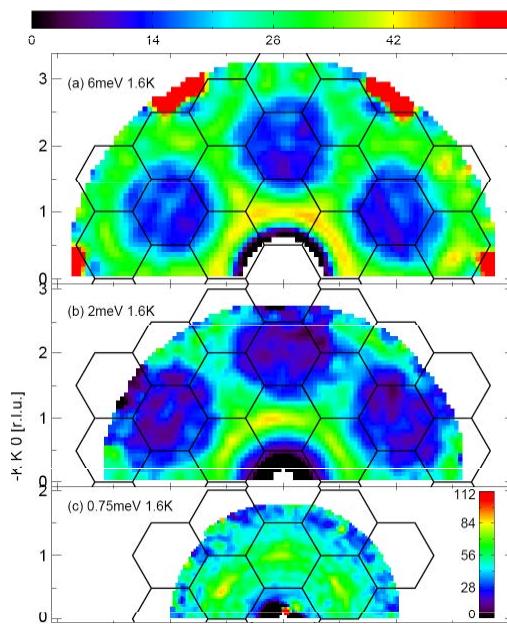


Helton et al, 2010

Single crystal INS

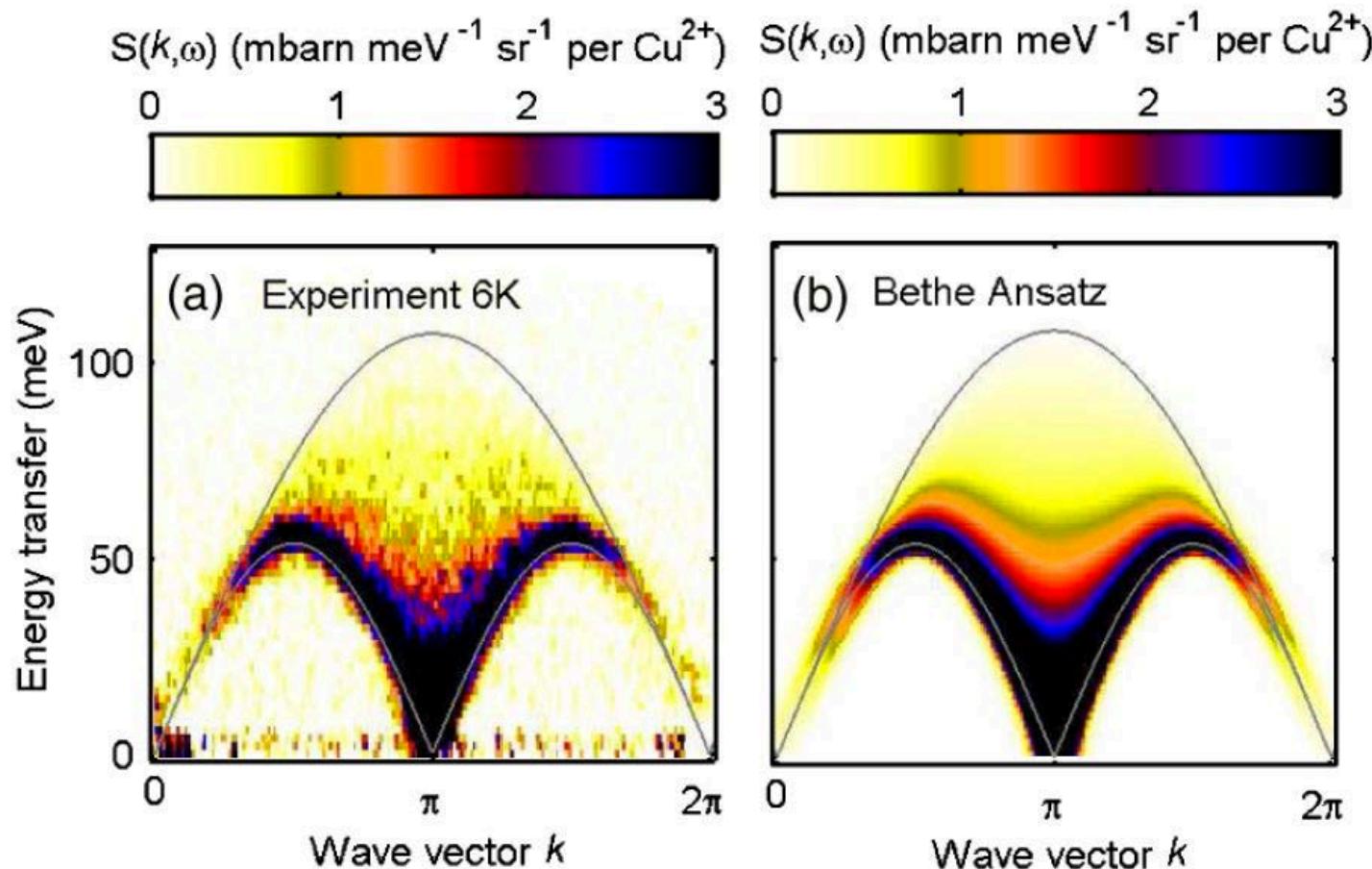
smooth continuum
scattering

T-H Han et al, 2012



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

For comparison: 1d spinons

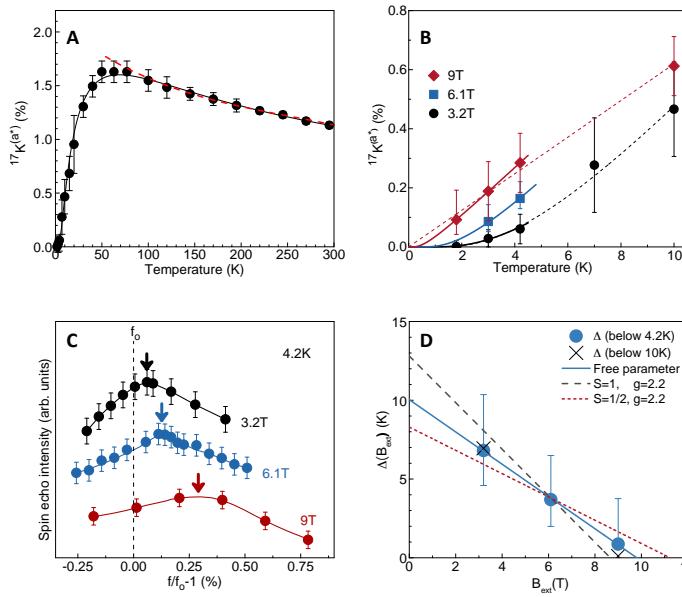


KCuF₃ - B. Lake et al, 2013

Herbertsmithite

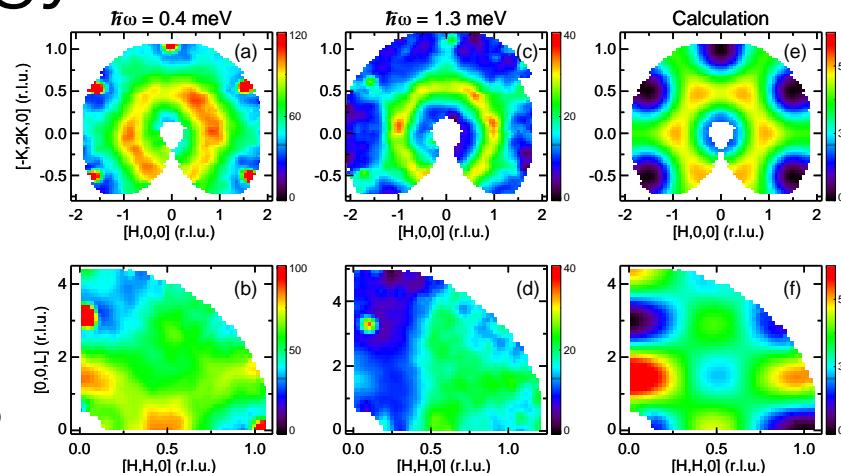
Single crystal NMR

M. Fu *et al*, 2015



estimate gap ~
10K

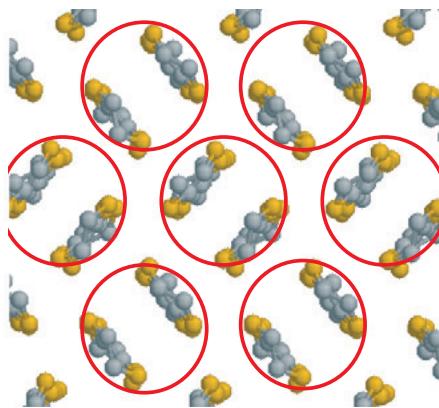
Low energy INS



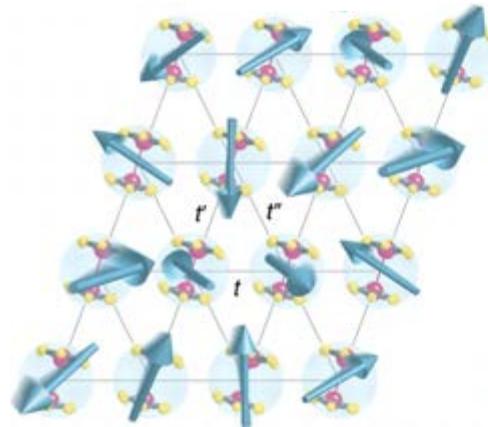
T-H Han *et al*, 2015

claim to separate
impurity signal
below 0.7meV

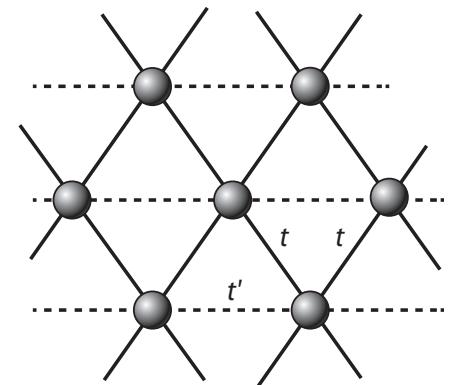
Organics



κ -(ET)₂X

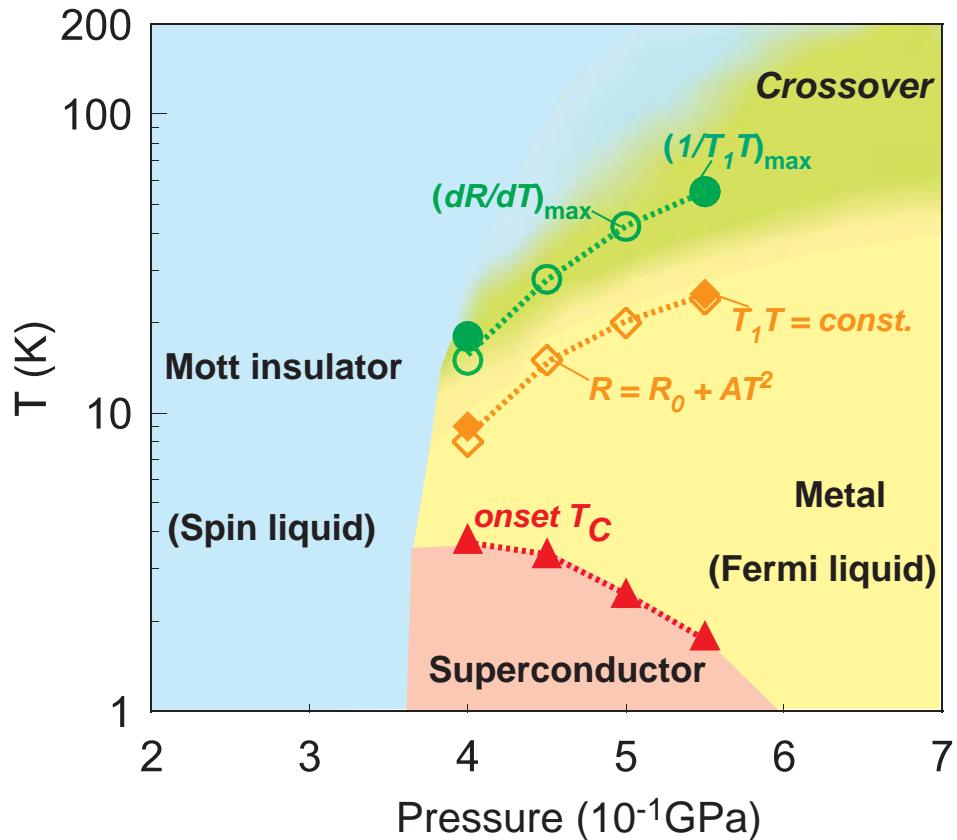


β' -Pd(dmit)₂



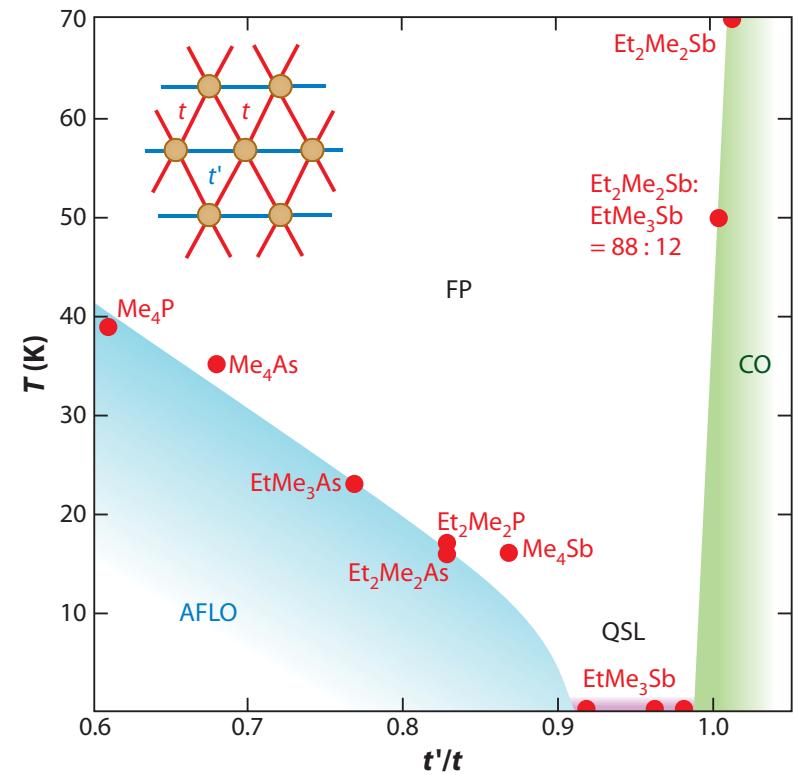
- Molecular materials which behave as effective triangular lattice $S=1/2$ antiferromagnets with $J \sim 250\text{K}$
- significant charge fluctuations

Organics



κ - $(ET)_2Cu_2(CN)_3$

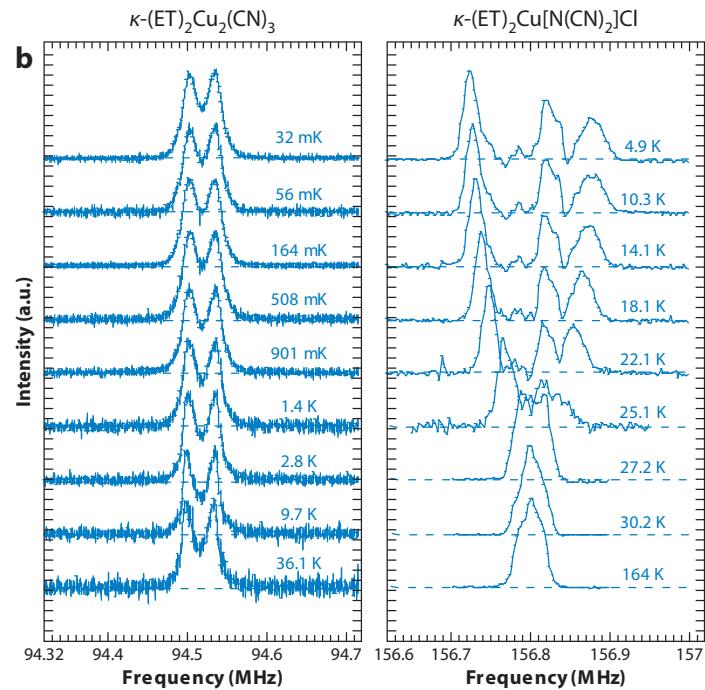
K. Kanoda group (2003-)



β' - $Pd(dmit)_2$

R. Kato group (2008-)

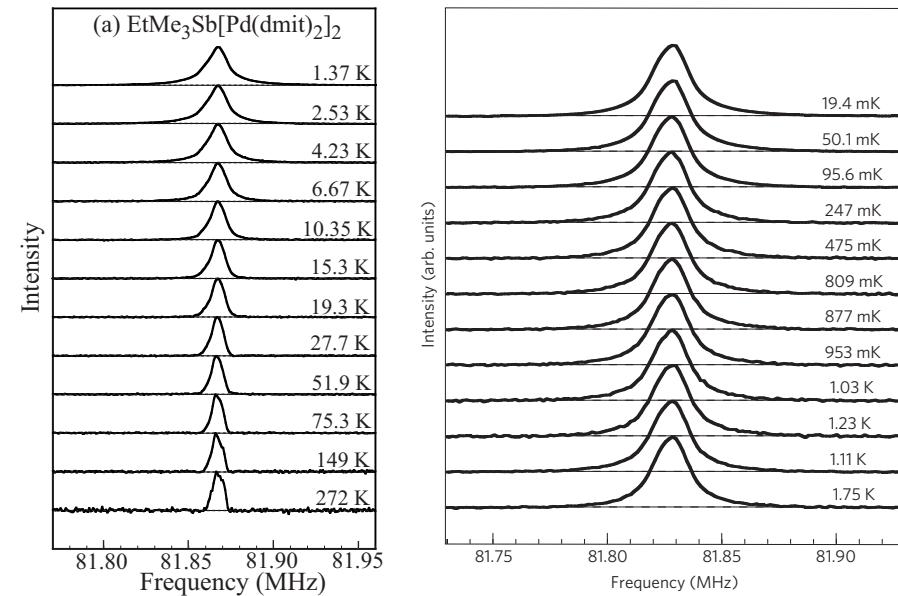
NMR lineshapes



κ -(ET)₂Cu₂(CN)₃

Y. Shimizu
et al, 2003

Evidence for lack of static moments: $f > 1000!$

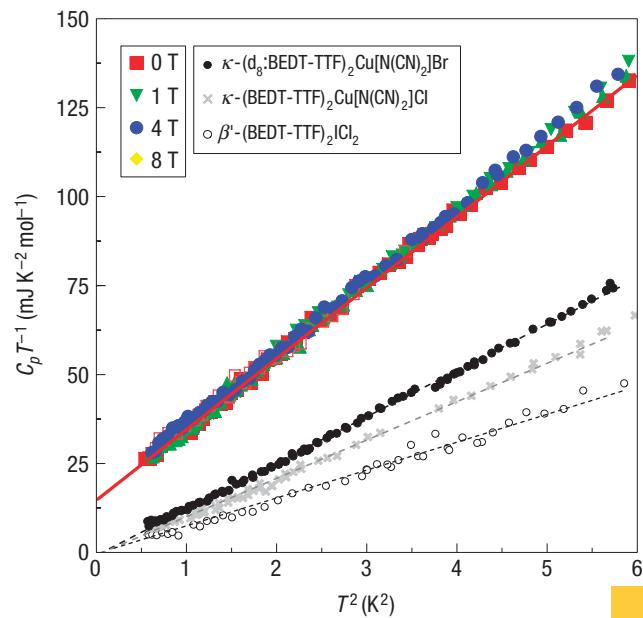


β' -Pd(dmit)₂
T. Itou et
al,
2008,2010

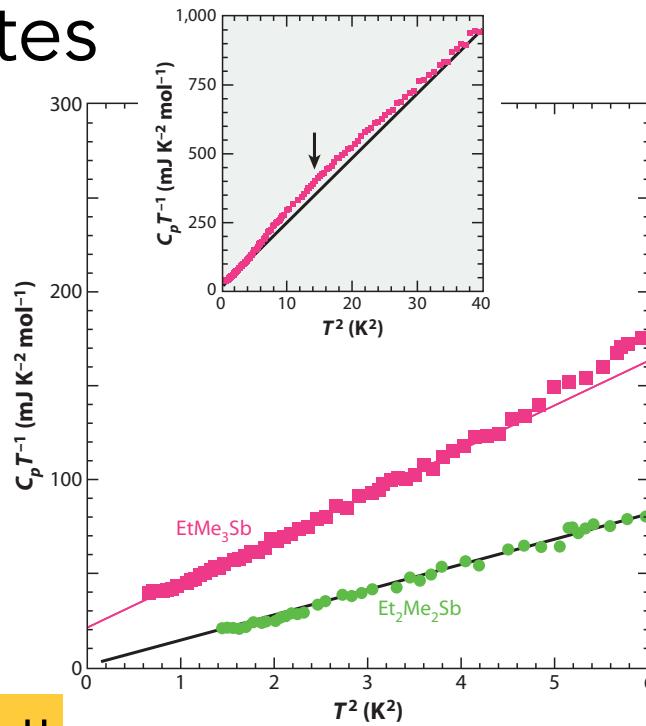
¹³Cs NMR

Specific Heat

- $C \sim \gamma T$ indicates gapless behavior with large density of states



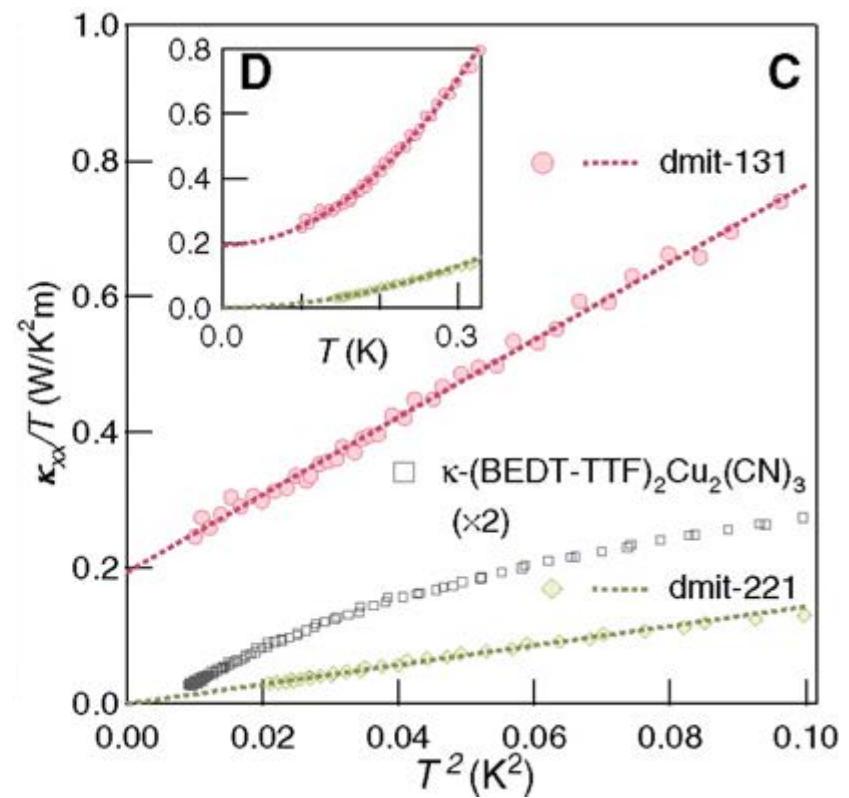
$\gamma_{\text{Cu}} \sim 0.7 !!$



S. Yamashita et al, 2008

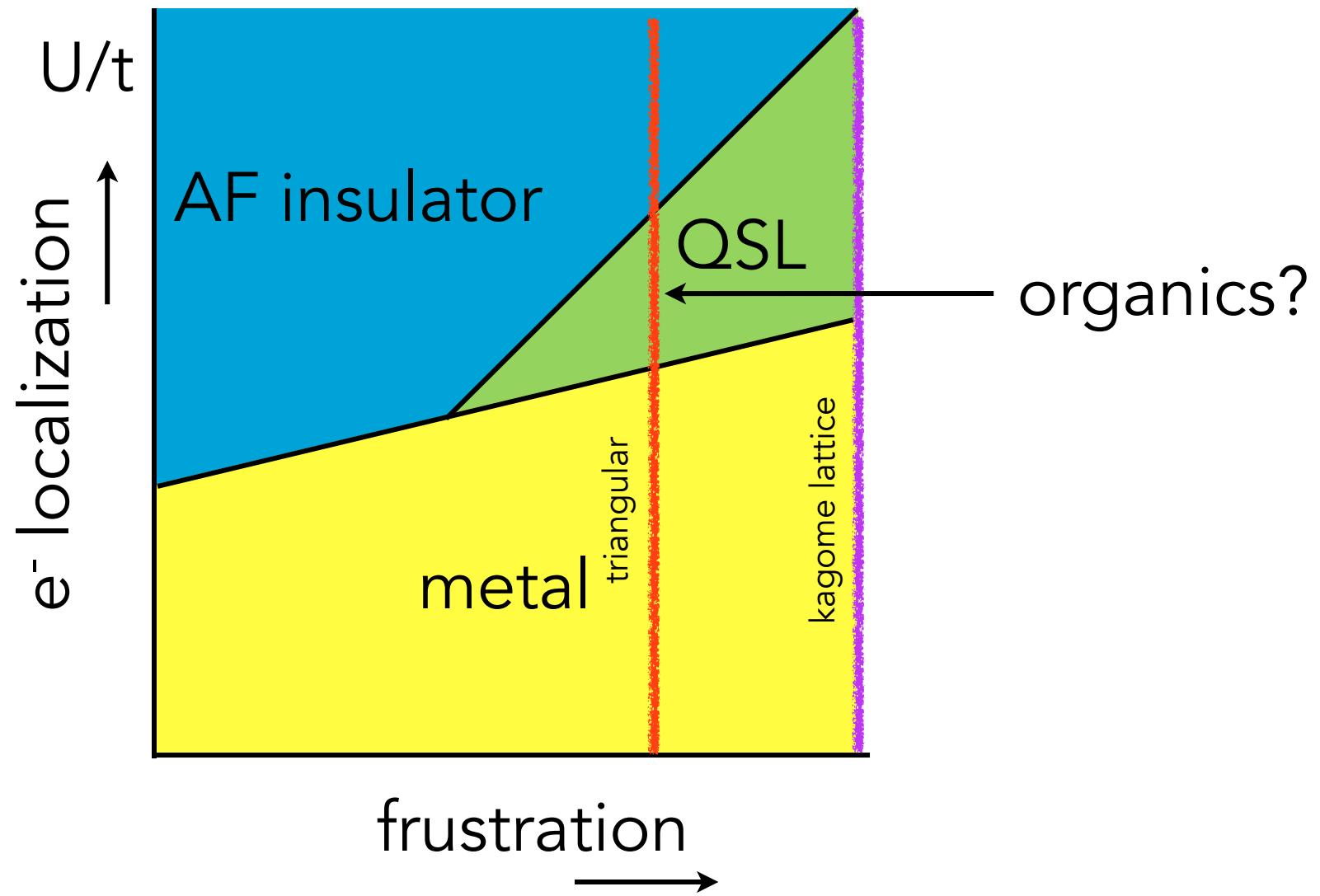
Thermal conductivity

- 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 $l \sim 1 \mu\text{m} \approx 1000 \text{ \AA}$!

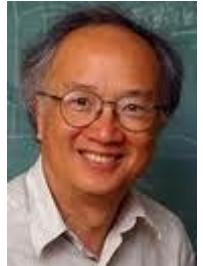


M. Yamashita et al, 2010

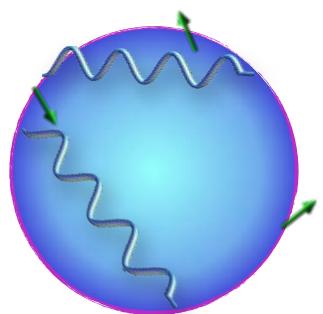
Charge fluctuations



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!





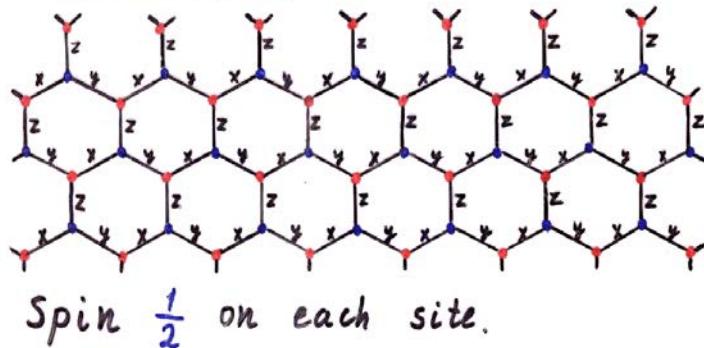
Kitaev model

Kitaev's honeycomb model

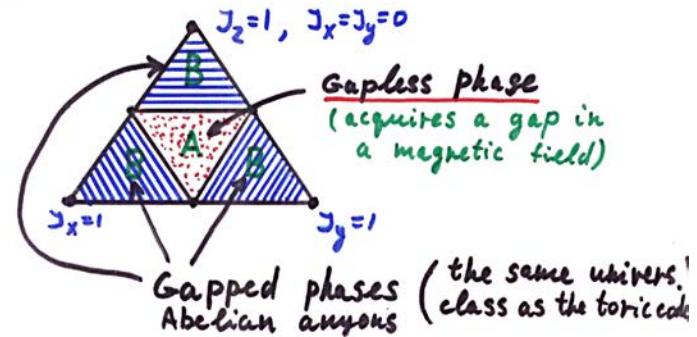
$$H = \sum_{i,\mu} K_\mu \sigma_i^\mu \sigma_{i+\mu}^\mu$$

KITP, 2003

1. The model

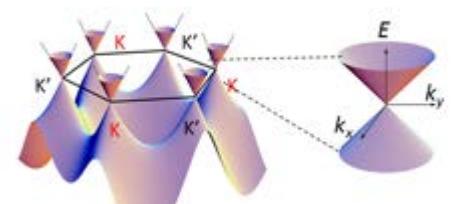


Phase diagram



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

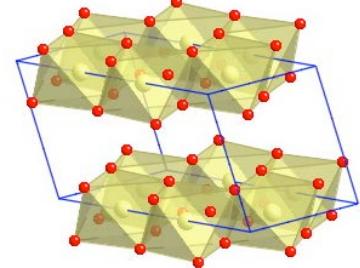
physical Majoranas $H_m = K \sum_{\langle ij \rangle} i c_i c_j$



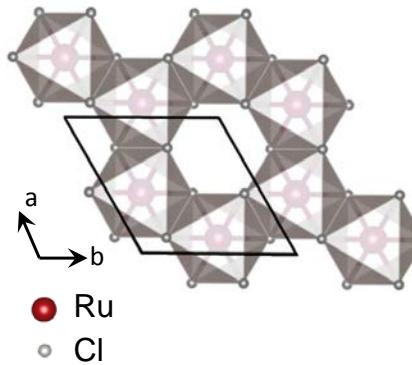
Kitaev Materials

Jackeli, Khaliullin
2009

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



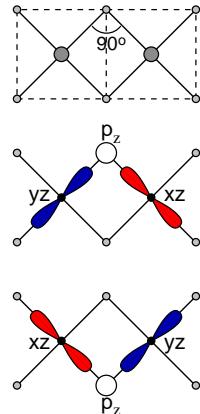
Na_2IrO_3 ,
 (α, β, γ) -
 Li_2IrO_3



$\alpha\text{-RuCl}_3$

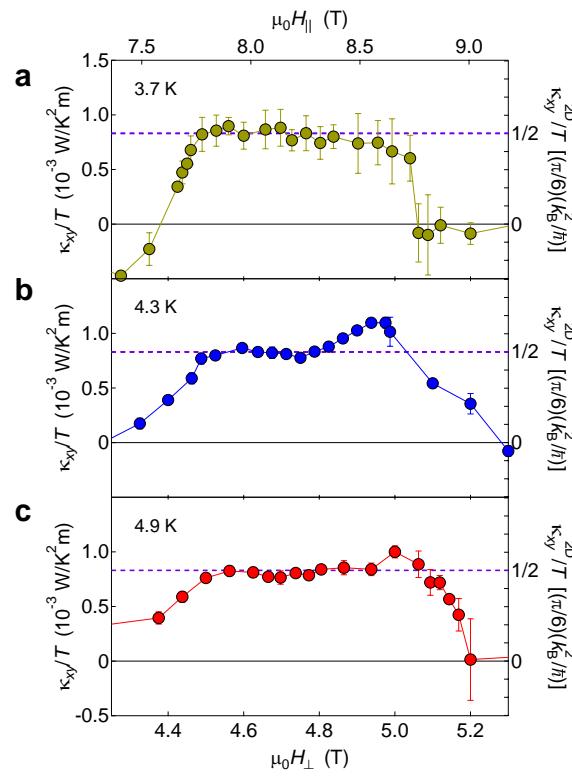
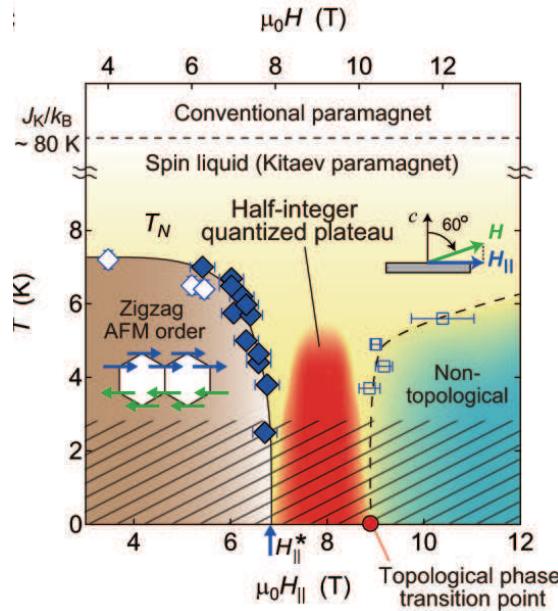
Y.-J. Kim...

Honeycomb and hyper-honeycomb structures



Thermal Hall

- Very recent experiment on a-RuCl₃



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

$c=1/2$ is expected for a chiral Majorana fermion edge, characteristic of “Ising anyons”

Entanglement Issues

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

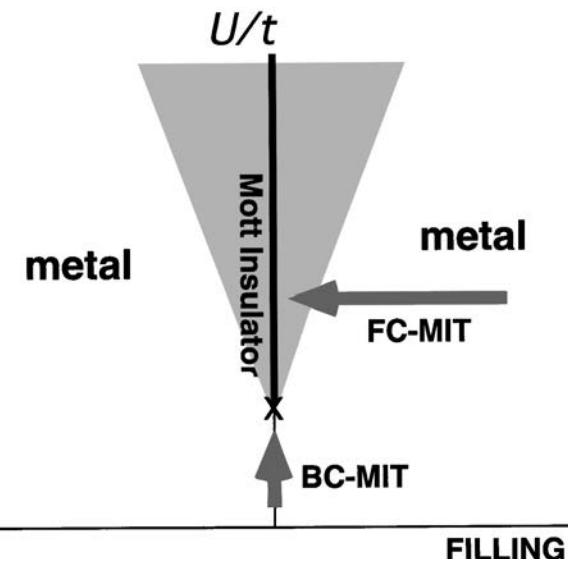
Correlation

- 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

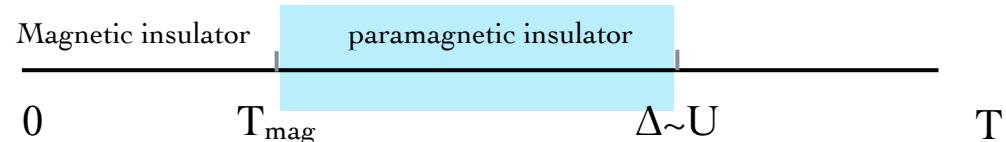
Mott Transition

- Hubbard model

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



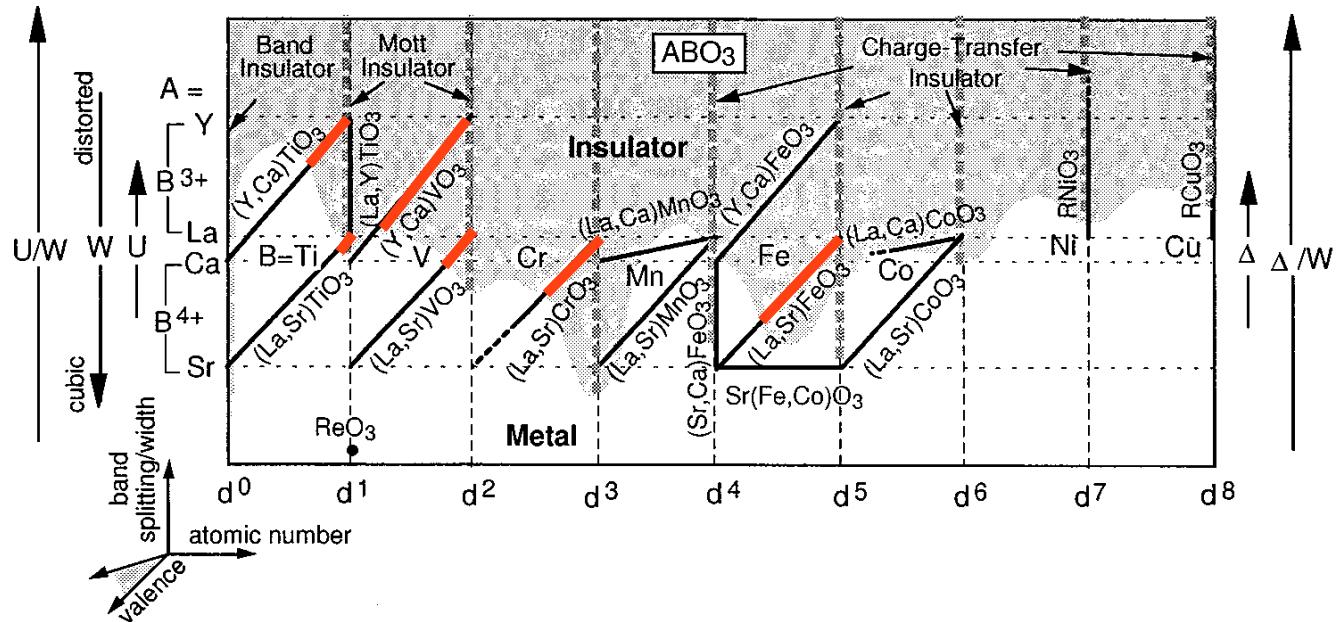
- ✿ Physically, a Mott Insulator is one which is insulating due to interaction-induced localization, not due to band physics
- ✿ This is a question of energy scales
- ✿ Deep in the Mott state:



Mott Transition

- And old subject

e.g.
perovskites



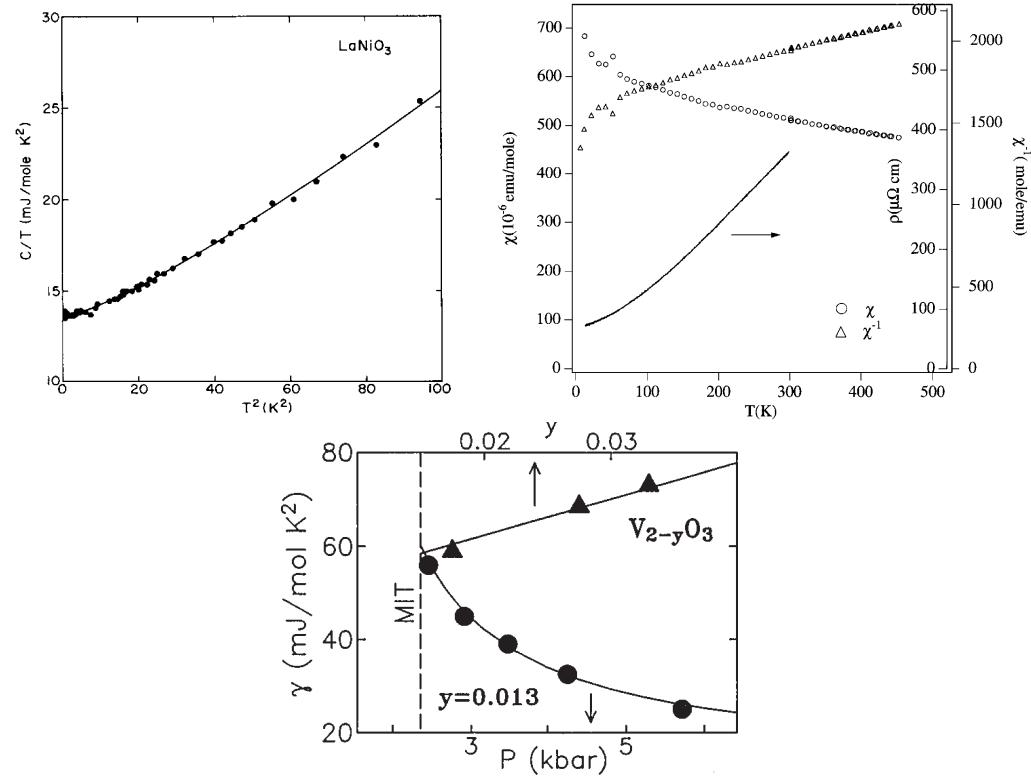
- But still a key theme, and now more accessible in new materials, via new approaches

Heavy Electrons

- Mass enhancement near Mott transition

LaNiO_3 :
 $\gamma/\gamma_{\text{band}} = 10$

V_2O_3



Heavy Fermions

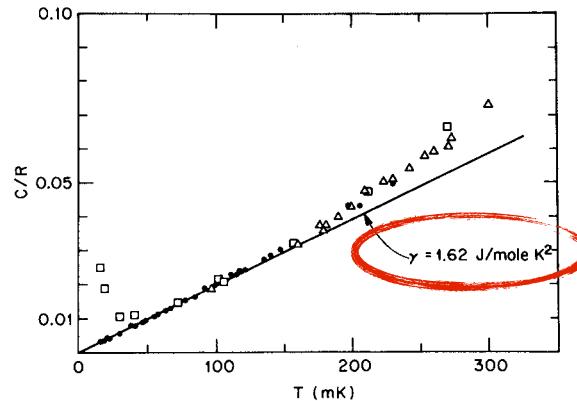


FIG. 1. Specific heat of CeAl_3 at very low temperatures in zero field (\bullet, Δ) and in 10 kOe (\square).

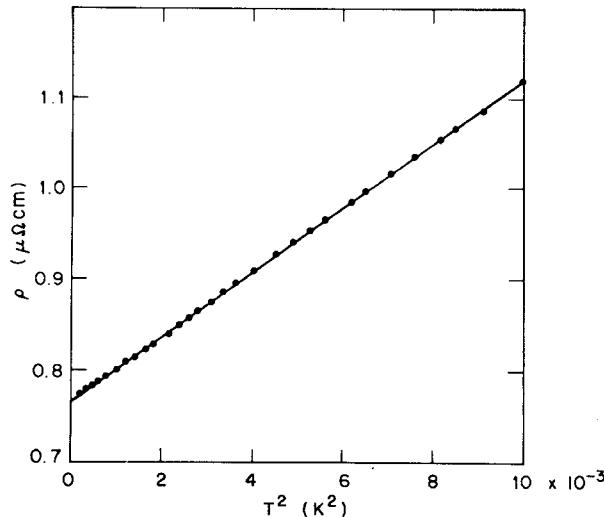


FIG. 3. Electrical resistivity of CeAl_3 below 100 mK, plotted against T^2 .

$$C \sim \gamma T$$

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

Both γ and A huge

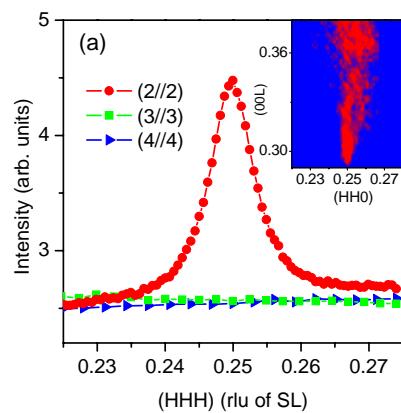
Behave like Fermi liquid with tiny E_F and large electron mass, but only for $T \ll E_F$

Common in "Kondo lattice" materials

Oxide heterostructures

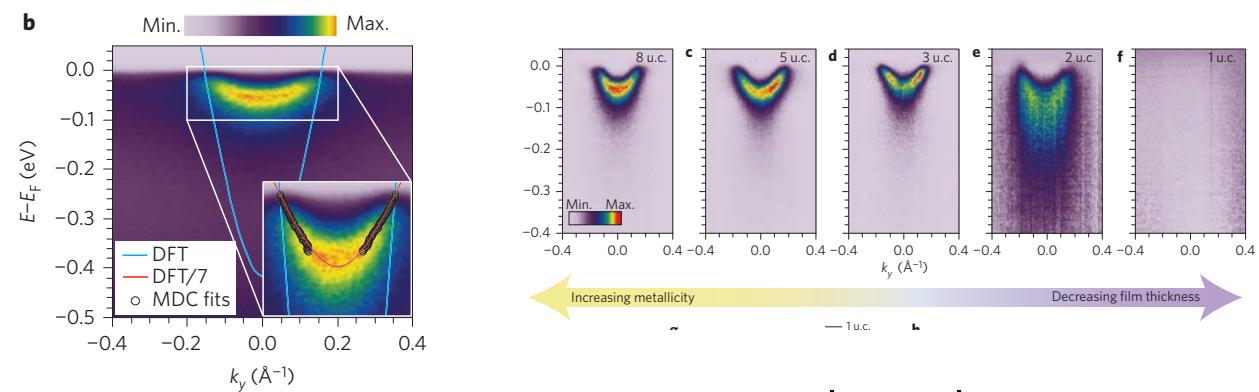
- New handle on Mott materials from oxide MBE

example: LaNiO_3 - just on the metallic side of Mott transition in bulk



AF order for films
<4uc thickness.

Frano et al, 2013



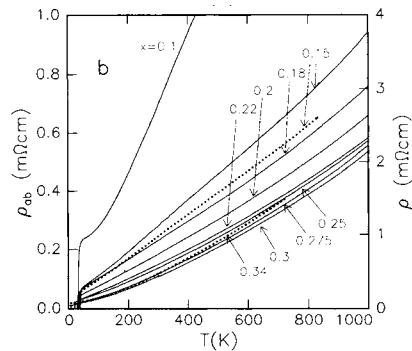
Large mass in 8uc
thick films

Metal-insulator
transition at 2uc
thickness

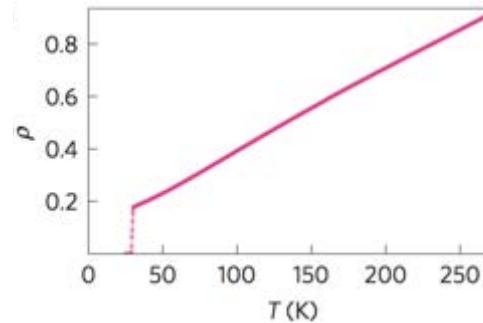
King et al, 2014 [Schlom, Shen]

Non-Fermi Liquids

“strange metal”



LSCO Takagi et al, 1992



BaFe₂(As_{1-x}P_x)₂, Hayes et al, 2016

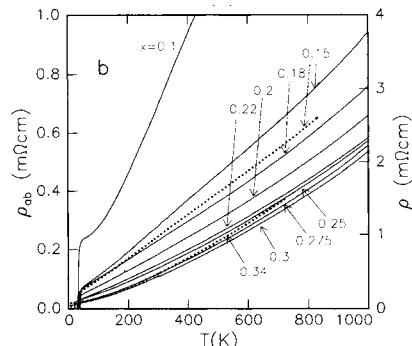
T-linear resistivity/scattering rate:

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

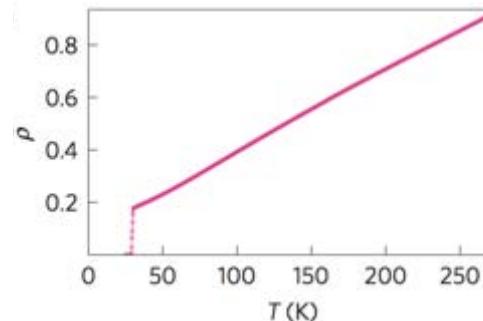
$$\frac{1}{\tau} \sim T ?$$

Non-Fermi Liquids

“strange metal”



LSCO Takagi et al, 1992



BaFe₂(As_{1-x}P_x)₂, Hayes et al, 2016

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

Quasiparticles?

Green's function

$$G_R(k, \omega) = \frac{1}{\omega - \epsilon_k - \Sigma(k, \omega) - i\delta}$$

self-energy

Spectral density

$$\rho(k, \omega) = \frac{-2\Sigma''(k, \omega)}{(\omega - \epsilon_k - \Sigma'(k, \omega))^2 + (\Sigma''(k, \omega))^2}.$$

$$\Sigma_{\text{FL}}'' \sim \omega^2 \sim T^2$$

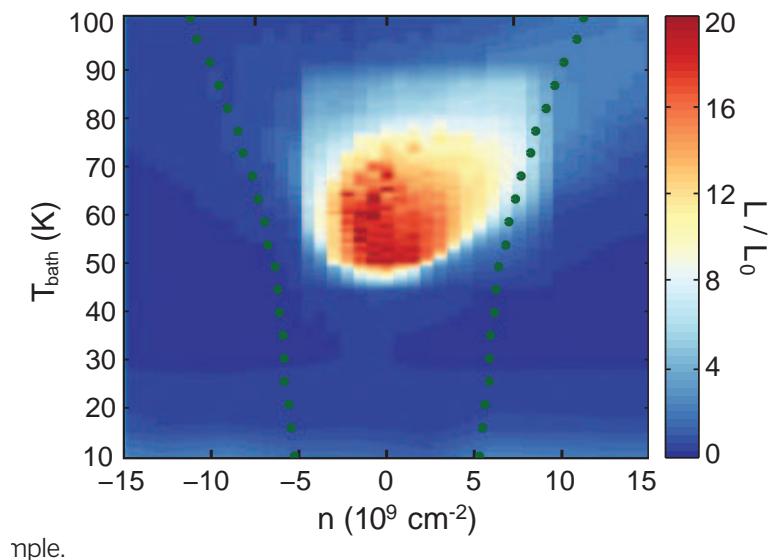
here $\Sigma_{\text{FL}}'' \sim T$

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*



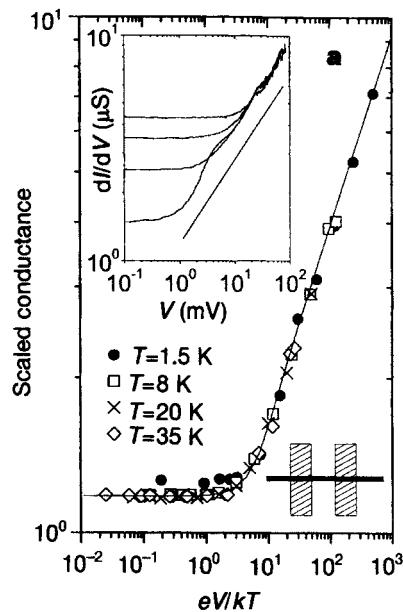
Red region: thermal conductivity much larger than electrical conductivity.
Indicates e-e fluid regime

Crossno et al, 2016

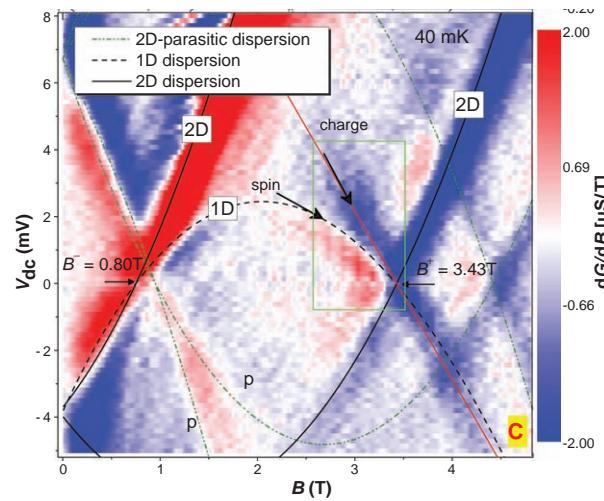
Luttinger liquids

- 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, Bi₂Se₃, Bi₂Te₃, Sb₂Te₃, TaAs, Cd₂Se₃, WTe₂, MoTe₂

1 H 1.00794	2 He 4.002602
3 Li 6.941	4 Be 9.012182
11 Na 22.989770	12 Mg 24.3050
19 K 39.0983	20 Ca 40.078
37 Rb 85.4678	38 Sr 87.62
55 Cs 132.90545	56 Ba 137.327
87 Fr (223)	88 Ra (227)
21 Sc 44.955910	22 Ti 47.867
39 Y 88.90585	40 Zr 91.224
57 La 138.9055	58 Hf 178.49
72 Rf (261)	73 Ta (262)
74 W 180.9479	75 Re 183.84
104 Db (262)	105 Sg (263)
106 Bh (262)	107 Hs (265)
108 Mt (266)	109 Mt (269)
110 Mt (272)	111 Mt (277)
111 Mt (277)	112 Mt (277)
31 Ga 69.723	32 Ge 72.61
49 In 114.818	50 As 112.411
51 Sn 118.710	52 Sb 121.760
53 I 127.60	54 Te 126.90447
55 Br 79.504	56 Kr 83.80
57 As 78.96	58 Se 79.504
59 Se 79.504	60 Br 83.80
61 Pm 140.116	62 Sm 140.50765
63 Eu 144.24	64 Gd 150.36
65 Tb 151.964	66 Dy 157.25
67 Ho 158.92534	68 Er 162.50
69 Tm 164.93022	70 Yb 167.26
71 Lu 173.04	72 At (210)
73 No (259)	74 Rn (222)
75 Po (209)	76 At (210)
77 Te (209)	78 Rn (223)
79 Te (209)	80 Po (209)
81 Tl 204.3833	82 Pb 207.2
83 Bi 208.59038	84 Po 209.59038
85 At (210)	86 Rn (223)
87 Rn (223)	88 Lr (262)

58 Ce 140.116	59 Pr 140.50765	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.964	64 Gd 157.25	65 Tb 158.92534	66 Dy 162.50	67 Ho 164.93022	68 Er 167.26	69 Tm 168.93421	70 Yb 173.04	71 Lu 174.967
90 Th 232.0381	91 Pa 231.035688	92 U 238.0289	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

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

QM Materials

- Topological materials
- HgTe, Bi₂Se₃, Bi₂Te₃, Sb₂Te₃, TaAs, Cd₂Se₃, WTe₂, MoTe₂
- Mn₃Sn, Mn₃Ge, YbPtBi, CeAlGe, Co₂MnGa

1 H 1.00794	2 He 4.002602
3 Li 6.941 9.012182	4 Be 9.012182
11 Na 22.989770 24.3050	12 Mg 24.3050
19 K 39.0983 40.078	20 Ca 44.955910
37 Rb 85.4678 87.62	38 Sr 88.90585 89.0585
55 Cs 132.90545 137.327	56 Ba 138.9055 138.9055
87 Fr (223)	88 Ra (226)
89 Ac (227)	104 Rf (261)
106 Db (262)	105 Sg (263)
107 Bh (262)	108 Hs (265)
109 Mt (266)	110 Nh (269)
111 (272)	111 (272)
112 (277)	112 (277)
114 (289)	116 (289)
116 (289)	118 (293)

5 B 10.811	6 C 12.0107	7 N 14.00674	8 O 15.9994 18.9984032	9 F 20.1797 35.4527	10 Ne 39.948
13 Al 26.581538	14 Si 28.0855	15 P 30.973761	16 S 32.066	17 Cl 35.4527	18 Ar 39.948
19 K 39.0983 40.078	21 Sc 44.955910	22 Ti 47.867	23 V 50.9415	24 Cr 51.9961	25 Mn 54.938049
37 Rb 85.4678 87.62	39 Y 91.224	41 Nb 92.90638	42 Mo 95.94	43 Tc (98)	44 Fe 55.845
55 Cs 132.90545 137.327	57 La 138.9055 138.9055	72 Hf 178.49	73 Ta 180.9479	74 W 183.84	75 Re 186.207
87 Fr (223)	89 Ac (227)	90 Rf (261)	91 Db (262)	92 Sg (263)	93 Bh (262)
94 Pu (244)	105 Nh (237)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)
99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)	104 Lu 174.967

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.

¹ H 1.00794																			² He 4.002602
3 Li 6.941	4 Be 9.012182																		
11 Na 22.989770	12 Mg 24.3050																		
19 K 39.0983	20 Ca 40.078	21 Sc 44.955910	22 Ti 47.867	23 V 50.9415	24 Cr 51.9961	25 Mn 54.938049	26 Fe 55.845	27 Co 58.933200	28 Ni 58.6534	29 Cu 63.545	30 Zn 65.39	31 Ga 69.723	32 Ge 72.61	33 As 74.92160	34 Se 78.96	35 Br 79.504	36 Kr 83.80		
37 Rb 85.4678	38 Sr 87.62	39 Y 88.90585	40 Zr 91.224	41 Nb 92.90638	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.90550	46 Pd 106.42	47 Ag 106.56655	48 Cd 112.411	49 In 114.818	50 Sn 118.710	51 Sb 121.760	52 Te 127.60	53 I 126.90447	54 Xe 131.29		
55 Cs 132.90545	56 Ba 137.327	57 La 138.9055	72 Hf 178.49	73 Ta 180.9479	74 W 183.84	75 Re 186.207	76 Os 190.23	77 Ir 192.217	78 Pt 195.078	79 Au 196.56655	80 Hg 200.59	81 Tl 204.3833	82 Pb 207.2	83 Bi 208.58038	84 Po (209)	85 At (210)	86 Rn (222)		
87 Fr (223)	88 Ra (226)	89 Ac (227)	104 Rf (261)	105 Db (262)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (266)	110 Mt (269)	111 Mt (272)	112 Mt (277)		114 (289)	116 (289)			118 (293)		

58 Ce 140.116	59 Pr 140.50765	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.964	64 Gd 157.25	65 Tb 158.92534	66 Dy 162.50	67 Ho 164.93022	68 Er 167.26	69 Tm 168.93421	70 Yb 173.04	71 Lu 174.967
90 Th 232.0381	91 Pa 231.035688	92 U 238.0289	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

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).

¹ H 1.00794																			² He 4.002602	
³ Li 6.941	⁴ Be 9.012182																			
¹¹ Na 22.989770	¹² Mg 24.3050																			
¹⁹ K 39.0983	²⁰ Ca 40.078	²¹ Sc 44.955910	²² Ti 47.867	²³ V 50.9415	²⁴ Cr 51.9961	²⁵ Mn 54.938049	²⁶ Fe 55.845	²⁷ Co 58.933200	²⁸ Ni 58.6534	²⁹ Cu 63.545	³⁰ Zn 65.39	³¹ Ga 69.723	³² Ge 72.61	³³ As 74.92160	³⁴ Se 78.96	³⁵ Br 79.504	³⁶ Kr 83.80			
³⁷ Rb 85.4678	³⁸ Sr 87.62	³⁹ Y 88.90585	⁴⁰ Zr 91.224	⁴¹ Nb 92.90638	⁴² Mo 95.94	⁴³ Tc (98)	⁴⁴ Ru 101.07	⁴⁵ Rh 102.90550	⁴⁶ Pd 106.42	⁴⁷ Ag 106.56655	⁴⁸ Cd 112.411	⁴⁹ In 114.818	⁵⁰ Sb 118.710	⁵¹ Te 121.760	⁵² I 127.60	⁵³ Xe 126.90447	⁵⁴ Kr 131.29			
⁵⁵ Cs 132.90545	⁵⁶ Ba 137.327	⁵⁷ La 138.9055	⁷² Hf 178.49	⁷³ Ta 180.9479	⁷⁴ W 183.84	⁷⁵ Re 186.207	⁷⁶ Os 190.23	⁷⁷ Ir 192.217	⁷⁸ Pt 195.078	⁷⁹ Au 196.56655	⁸⁰ Hg 200.59	⁸¹ Tl 204.3833	⁸² Pb 208.58038	⁸³ Bi (209)	⁸⁴ Po (210)	⁸⁵ At (222)	⁸⁶ Rn (223)			
⁸⁷ Fr (223)	⁸⁸ Ra (226)	⁸⁹ Ac (227)	¹⁰⁴ Rf (261)	¹⁰⁵ Db (262)	¹⁰⁶ Sg (263)	¹⁰⁷ Bh (262)	¹⁰⁸ Hs (265)	¹⁰⁹ Mt (266)	¹¹⁰ Ho (269)	¹¹¹ Cm (272)	¹¹² Dy (277)		¹¹⁴ Ho (289)	¹¹⁶ Fm (289)						

⁵⁸ Ce 140.116	⁵⁹ Pr 140.50765	⁶⁰ Nd 144.24	⁶¹ Pm (145)	⁶² Sm 150.36	⁶³ Eu 151.964	⁶⁴ Gd 157.25	⁶⁵ Tb 158.92534	⁶⁶ Dy 162.50	⁶⁷ Ho 164.93032	⁶⁸ Er 167.26	⁶⁹ Tm 168.93421	⁷⁰ Yb 173.04	⁷¹ Lu 174.967				
⁹⁰ Th 232.0381	⁹¹ Pa 231.035688	⁹² U 238.0289	⁹³ Np (237)	⁹⁴ Pu (244)	⁹⁵ Am (243)	⁹⁶ Cm (247)	⁹⁷ Bk (247)	⁹⁸ Cf (251)	⁹⁹ Es (252)	¹⁰⁰ Fm (257)	¹⁰¹ Md (258)	¹⁰² No (259)	¹⁰³ Lr (262)				

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.

¹ H 1.00794																				² He 4.002602	
³ Li 6.941	⁴ Be 9.012182																				
¹¹ Na 22.989770	¹² Mg 24.3050																				
¹⁹ K 39.0983	²⁰ Ca 40.078	²¹ Sc 44.955910	²² Ti 47.867	²³ V 50.9415	²⁴ Cr 51.9961	²⁵ Mn 54.938049	²⁶ Fe 55.845	²⁷ Co 58.933200	²⁸ Ni 58.6534	²⁹ Cu 63.545	³⁰ Zn 65.39	³¹ Ga 69.723	³² Ge 72.61	³³ As 74.92160	³⁴ Se 78.96	³⁵ Br 79.504	³⁶ Kr 83.80				
³⁷ Rb 85.4678	³⁸ Sr 87.62	³⁹ Y 88.90585	⁴⁰ Zr 91.224	⁴¹ Nb 92.90638	⁴² Mo 95.94	⁴³ Tc (98)	⁴⁴ Ru 101.07	⁴⁵ Rh 102.90550	⁴⁶ Pd 106.42	⁴⁷ Ag 106.50655	⁴⁸ Cd 112.411	⁴⁹ In 114.818	⁵⁰ Sn 118.710	⁵¹ Sb 121.760	⁵² Te 127.60	⁵³ I 126.90447	⁵⁴ Xe 131.29				
⁵⁵ Cs 132.90545	⁵⁶ Ba 137.327	⁵⁷ La 138.9055	⁷² Hf 178.49	⁷³ Ta 180.9479	⁷⁴ W 183.84	⁷⁵ Re 186.207	⁷⁶ Os 190.23	⁷⁷ Ir 192.217	⁷⁸ Pt 195.078	⁷⁹ Au 196.56655	⁸⁰ Hg 200.59	⁸¹ Tl 204.3833	⁸² Pb 207.2	⁸³ Bi 208.58038	⁸⁴ Po (209)	⁸⁵ At (210)	⁸⁶ Rn (222)				
⁸⁷ Fr (223)	⁸⁸ Ra (226)	⁸⁹ Ac (227)	¹⁰⁴ Rf (261)	¹⁰⁵ Db (262)	¹⁰⁶ Sg (263)	¹⁰⁷ Bh (262)	¹⁰⁸ Hs (265)	¹⁰⁹ Mt (266)	¹¹⁰ Nt (269)	¹¹¹ (272)	¹¹² (277)		¹¹⁴ (289)	¹¹⁶ (289)						¹¹⁸ (293)	

⁵⁸ Ce 140.116	⁵⁹ Pr 140.50765	⁶⁰ Nd 144.24	⁶¹ Pm (145)	⁶² Sm 150.36	⁶³ Eu 151.964	⁶⁴ Gd 157.25	⁶⁵ Tb 158.92534	⁶⁶ Dy 162.50	⁶⁷ Ho 164.93022	⁶⁸ Er 167.26	⁶⁹ Tm 168.93421	⁷⁰ Yb 173.04	⁷¹ Lu 174.967
⁹⁰ Th 232.0381	⁹¹ Pa 231.035688	⁹² U 238.0289	⁹³ Np (237)	⁹⁴ Pu (244)	⁹⁵ Am (243)	⁹⁶ Cm (247)	⁹⁷ Bk (247)	⁹⁸ Cf (251)	⁹⁹ Es (252)	¹⁰⁰ Fm (257)	¹⁰¹ Md (258)	¹⁰² No (259)	¹⁰³ Lr (262)

QM Materials

- Quantum spin liquids and interesting insulating antiferromagnets

¹ H 1.00794	² He 4.002602
³ Li 6.941 9.012182	⁴ Be
¹¹ Na 22.989770	¹² Mg 24.3056
¹⁹ K 39.0983	²⁰ Ca 40.078
³⁷ Rb 85.4678	³⁸ Sr 87.62
⁵⁵ Cs 132.9045	⁵⁶ Ba 137.327
⁸⁷ Fr (223)	⁸⁸ Ra (226)
²¹ Sc 44.955910	²² Ti 47.867
²³ V 50.9415	²⁴ Cr 51.9961
²⁵ Mn 54.938049	²⁶ Fe 55.845
²⁷ Co 58.933200	²⁸ Ni 58.6534
²⁹ Cu 63.545	³⁰ Zn 65.39
³¹ Ga 69.723	³² Ge 72.61
³³ As 74.92160	³⁴ Se 78.96
³⁵ Br 79.504	³⁶ Kr 83.80
³⁷ Rb 85.4678	³⁸ Sr 87.62
³⁹ Y 88.90585	⁴⁰ Zr 91.224
⁴¹ Nb 92.90638	⁴² Mo 95.94
⁴³ Tc (98)	⁴⁴ Ru 101.07
⁴⁵ Rh 102.90550	⁴⁶ Pd 106.42
⁴⁷ Ag 106.56655	⁴⁸ Cd 112.411
⁴⁹ In 114.818	⁵⁰ Sn 121.760
⁵¹ Sb 127.60	⁵² Te 126.9045
⁵³ I 131.29	⁵⁴ Xe 131.29
⁵⁵ Cs 132.9045	⁵⁶ Ba 138.9055
⁵⁷ La 138.9055	⁷² Hf 178.49
⁷³ Ta 180.9479	⁷⁴ W 183.84
⁷⁵ Re 186.207	⁷⁶ Os 190.23
⁷⁷ Ir 192.217	⁷⁸ Pt 195.078
⁷⁹ Hg 200.59	⁸⁰ Bi 204.3833
⁸¹ Tl 207.3	⁸² Pb 208.58038
⁸³ Bi (209)	⁸⁴ Po (210)
⁸⁵ At (222)	⁸⁶ Rn (222)

- $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$, a-
 RuCl_3 , $\text{Pr}_2\text{Zr}_2\text{O}_7$,
 Cs_2CuCl_4 , $\text{Yb}_2\text{Ti}_2\text{O}_7$

QM Materials

- Correlated metals/
Mott transitions
- $\text{RTiO}_3, \text{RVO}_3, \text{RNiO}_3,$
 $\text{RMnO}_3, \text{RCoO}_3, \dots$
- $\text{Cd}_2\text{Os}_2\text{O}_7, \text{Nd}_2\text{Ir}_2\text{O}_7,$
 $\text{Sr}_2\text{IrO}_4, \text{Sr}_2\text{RuO}_4, \dots$
- $\text{URu}_2\text{Si}_2, \text{CeAl}_3, \dots$

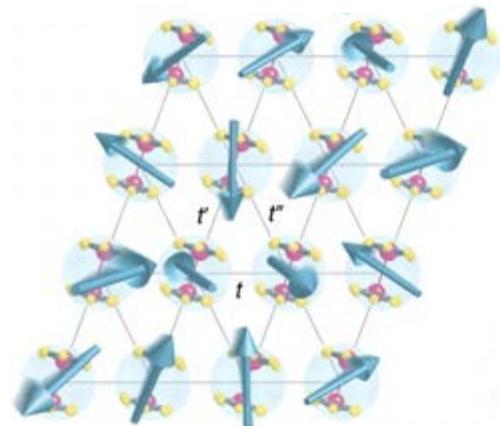
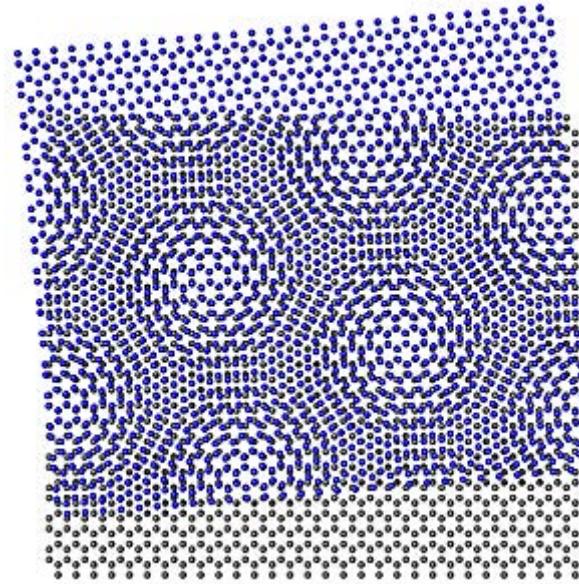
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³ Li 6.941	⁴ Be 9.012182
¹¹ Na 22.989770	¹² Mg 24.3050
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³⁷ Rb 85.4678	³⁸ Sr 87.62
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⁸⁷ Fr (223)	⁸⁸ Ra (227)
²¹ Sc 44.955910	²² Ti 47.867
³⁹ Y 88.90585	⁴⁰ Zr 91.224
⁵⁷ La 138.9055	⁷² Hf 178.49
⁸⁹ Ac (261)	⁷³ Ta 180.9479
¹⁰⁴ Rf (262)	⁷⁴ W 183.84
¹⁰⁵ Db (263)	⁷⁵ Re 186.207
¹⁰⁶ Sg (262)	⁷⁶ Os 190.23
¹⁰⁷ Bh (265)	⁷⁷ Ir 192.217
¹⁰⁸ Hs (266)	⁷⁸ Pt 195.078
¹⁰⁹ Mt (269)	⁷⁹ Au 196.56655
¹¹⁰ Dy (272)	⁸⁰ Hg 200.59
¹¹¹ Tb (277)	⁸¹ Ag 196.92534
¹¹² Ho (277)	⁸² Cd 112.411
	⁸³ In 114.818
	⁸⁴ Sn 118.710
	⁸⁵ Pb 121.760
	⁸⁶ Bi 127.60
	⁸⁷ Po (209)
	⁸⁸ At (210)
	⁸⁹ Rn (222)
	⁹⁰ Te 126.90447
	⁹¹ I 131.29
	⁹² Xe 131.29
⁵⁸ Ce 140.116	⁵⁹ Pr 140.50765
⁶⁰ Nd 144.24	⁶¹ Pm (145)
⁶² Sm 150.36	⁶³ Eu 151.964
⁶⁴ Gd 157.25	⁶⁵ Tb 162.50
⁶⁶ Dy 164.93022	⁶⁷ Ho 167.26
⁶⁸ Er 168.93421	⁶⁹ Tm 173.04
⁷⁰ Yb 173.04	⁷¹ Lu 174.967
⁹³ U (237)	⁹⁴ Pu (244)
⁹⁵ Np (237)	⁹⁶ Am (243)
⁹⁶ Cm (247)	⁹⁷ Bk (247)
⁹⁸ Cf (251)	⁹⁹ Es (252)
¹⁰⁰ Fm (257)	¹⁰¹ Md (258)
¹⁰¹ No (259)	¹⁰² Lr (262)

⁵⁸ Ce 140.116	⁵⁹ Pr 140.50765	⁶⁰ Nd 144.24	⁶¹ Pm (145)	⁶² Sm 150.36	⁶³ Eu 151.964	⁶⁴ Gd 157.25	⁶⁵ Tb 162.50	⁶⁶ Dy 164.93022	⁶⁷ Ho 167.26	⁶⁸ Er 168.93421	⁶⁹ Tm 173.04	⁷⁰ Yb 173.04	⁷¹ Lu 174.967
⁹⁰ Th 232.0381	⁹¹ Pa 231.035688	⁹² U (237)	⁹³ Np (237)	⁹⁴ Pu (244)	⁹⁵ Am (243)	⁹⁶ Cm (247)	⁹⁷ Bk (247)	⁹⁸ Cf (251)	⁹⁹ Es (252)	¹⁰⁰ Fm (257)	¹⁰¹ Md (258)	¹⁰² No (259)	¹⁰³ Lr (262)

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