Introduction to Quantum Materials

Leon Balents, KITP

QS3 School, June 11, 2018

Quantum Materials

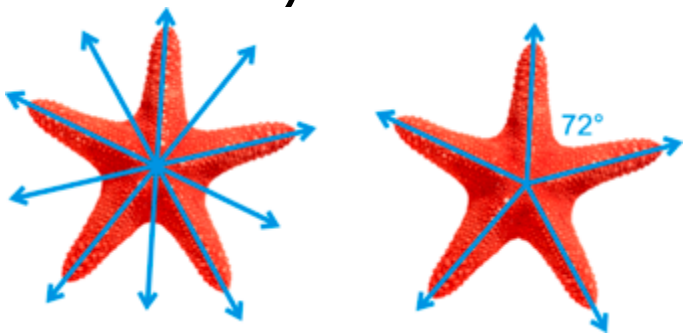
- What are they? Materials where electrons are doing interesting quantum things
- The plan:
  - Lecture 1: Concepts in Quantum Materials
  - Lecture 2: Survey of actual materials

Themes of modern QMs

- Order
- Topology
- Entanglement
- Correlations
- Dynamics

Order: symmetry

- Symmetry: a way to organize matter
- A symmetry is some operation that leaves a system (i.e. a material) invariant (unchanged



- In physics, we usually mean it leaves the Hamiltonian invariant

$$U^\dagger H U = H$$

Order and symmetry

- Why symmetry?
  - It is *persistent*: it only changes through a phase transition
  - It has numerous implications:
    - Quantum numbers and degeneracies
    - Conservation laws
  - Brings powerful mathematics of group theory
    - The set of all symmetries of a system form its symmetry group. Materials with different symmetry groups are in different *phases*

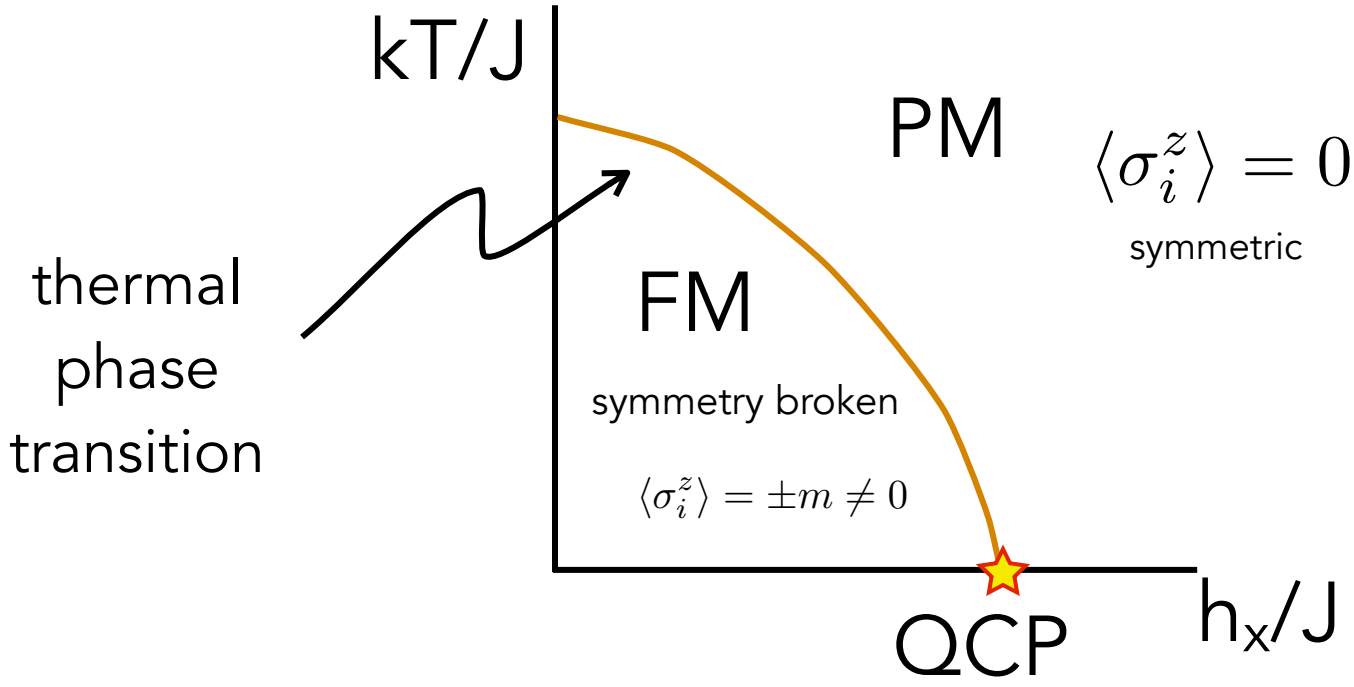
Ising model

- A canonical example

$$H = -J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - h_x \sum_i \sigma_i^x$$

$\sigma^z \to -\sigma^z$

Z_2 symmetry



$\psi = \langle \sigma_i^z \rangle$

"order parameter"

Symmetries in QMs

- Basic symmetries of our world:
  - space-time (Lorentz/Poincare) symmetry
    - spatial isotropy and translations
    - time reversal
  - Charge/particle number conservation
- Approximate symmetries (sometimes)
  - spin-rotation
  - various internal quantum numbers
- These things are broken down to varying degrees in different QMs

Crystallography

- Crystal structure: 230 crystallographic space groups
  - Classifies the arrangements of atoms (which break the symmetries of free space)
- Wallpaper groups in 2d (c.f. 2d materials)
- Basic input to many things
  - Phonons, elasticity, band structure…
  - LOADS of extremely useful stuff on Bilbao crystallographic server…
- Structural phase transition = change of space group.

Structural phase transition

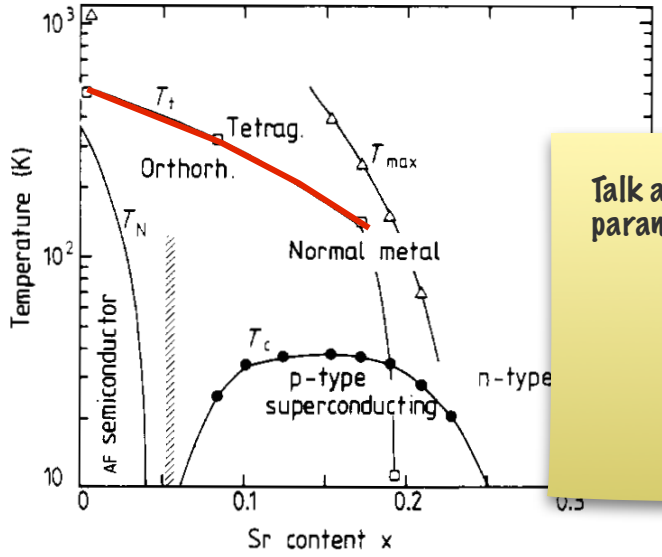
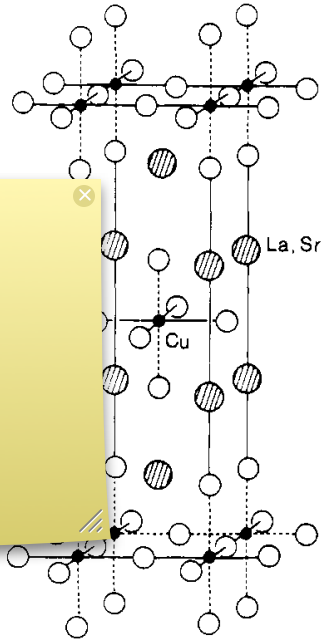
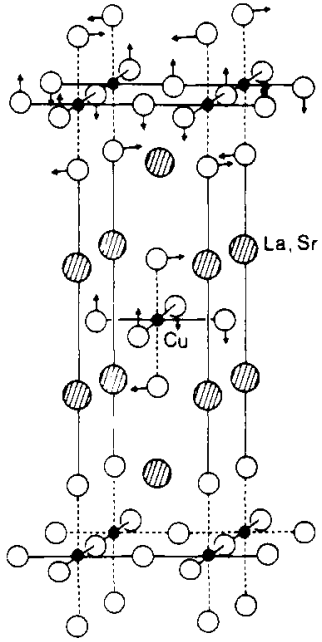


Figure 3. Phase diagram for the system $La_{2-y}Sr_yCuO_{4-\delta}$, $p = y - 2\delta$. Adapted from [15].

Talk about order parameters





tetragonal orthorhombic

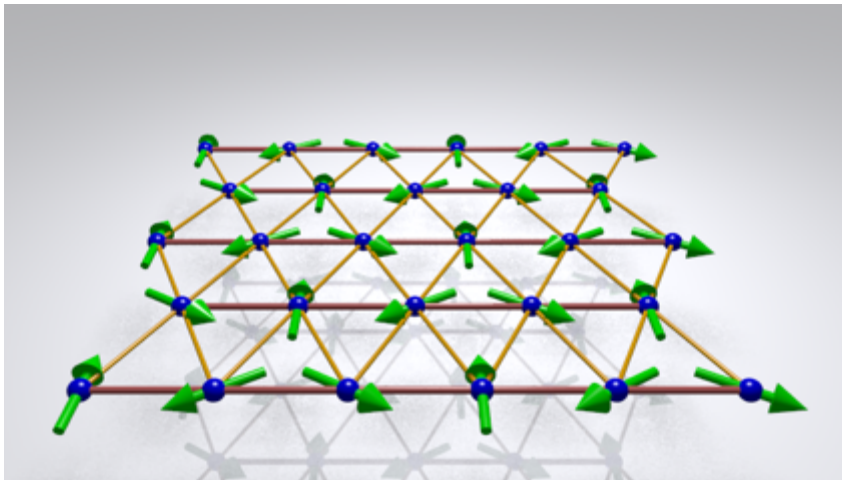
"Order parameters" ~ soft phonon modes

Magnetism

- Fundamental symmetry is *time-reversal*

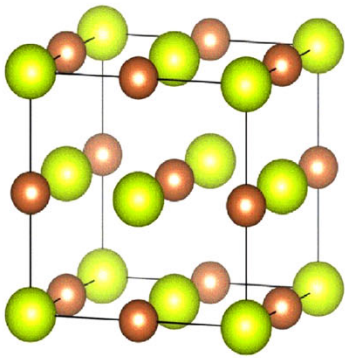
$$\boldsymbol{S}_i \rightarrow -\boldsymbol{S}_i$$

- Any ordering of magnetic moments breaks this symmetry

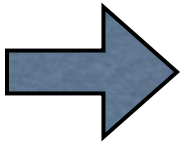


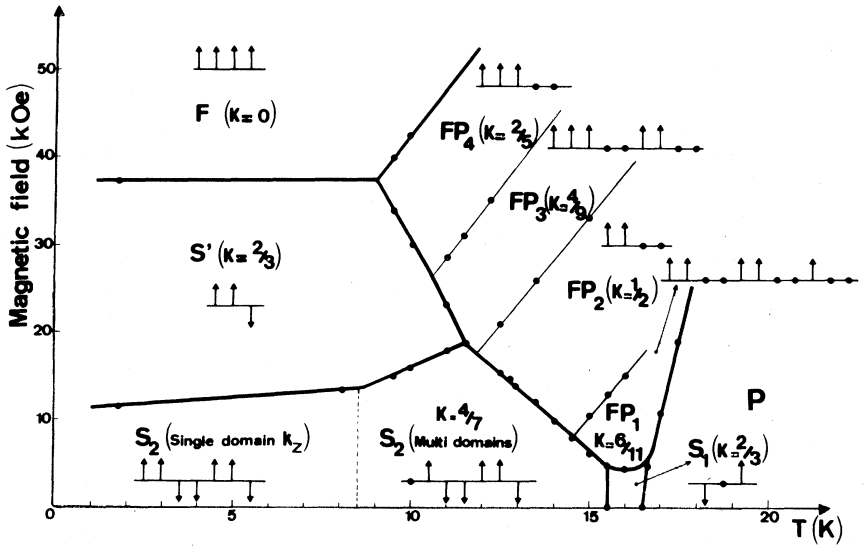
Magnetism

- Broken T-reversal systems are very rich: 1651 magnetic space groups



CeSb





Rossat-Mignod *et al*, 1977

Superconductivity

- Charge conservation symmetry is spontaneously broken in a SC
- Order parameter ~ "pair wavefunction"

$$\Psi_k^{\alpha\beta} = \langle c_{k\alpha} c_{-k\beta} \rangle$$

$$= \Psi_s(k)\epsilon_{\alpha\beta} \qquad \text{singlet}$$

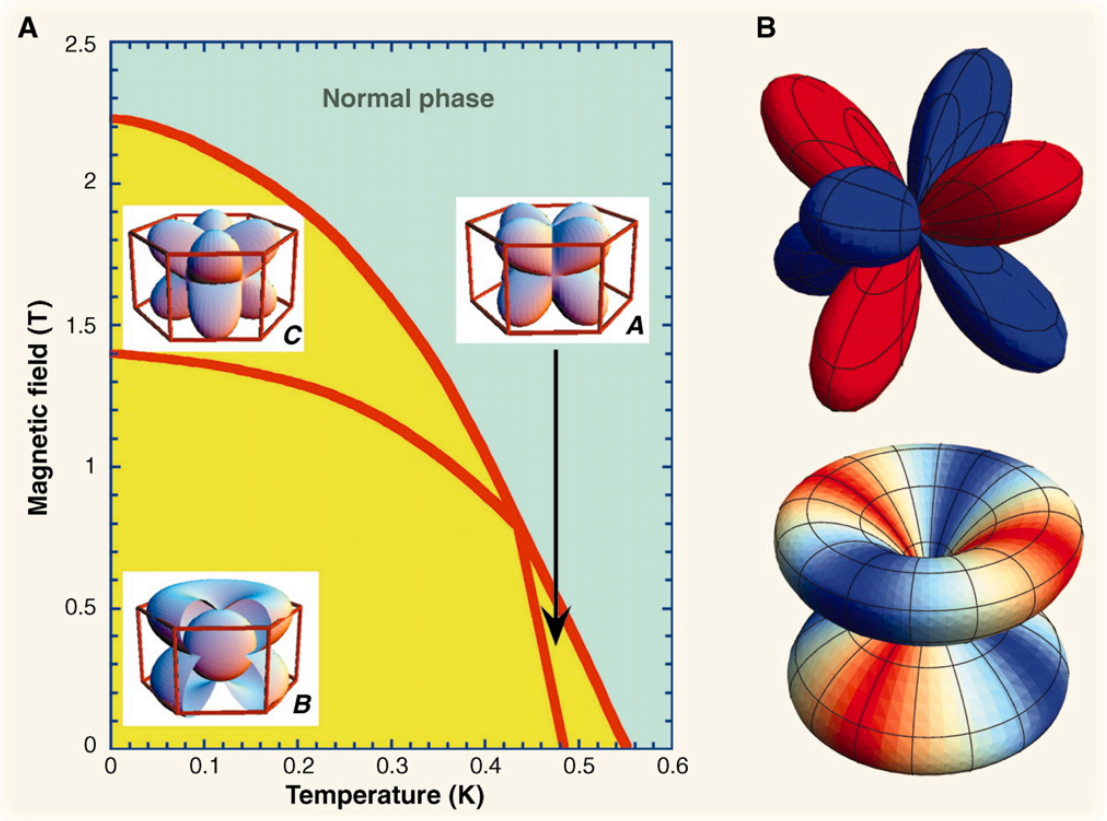
$$= \boldsymbol{\Psi}_t(k) \cdot (\sigma^y \boldsymbol{\sigma})_{\alpha\beta} \qquad \text{triplet}$$

- Many varieties of "orbital" state $\Psi(k)$

s,p,d, p+ip, etc.

UPt_3

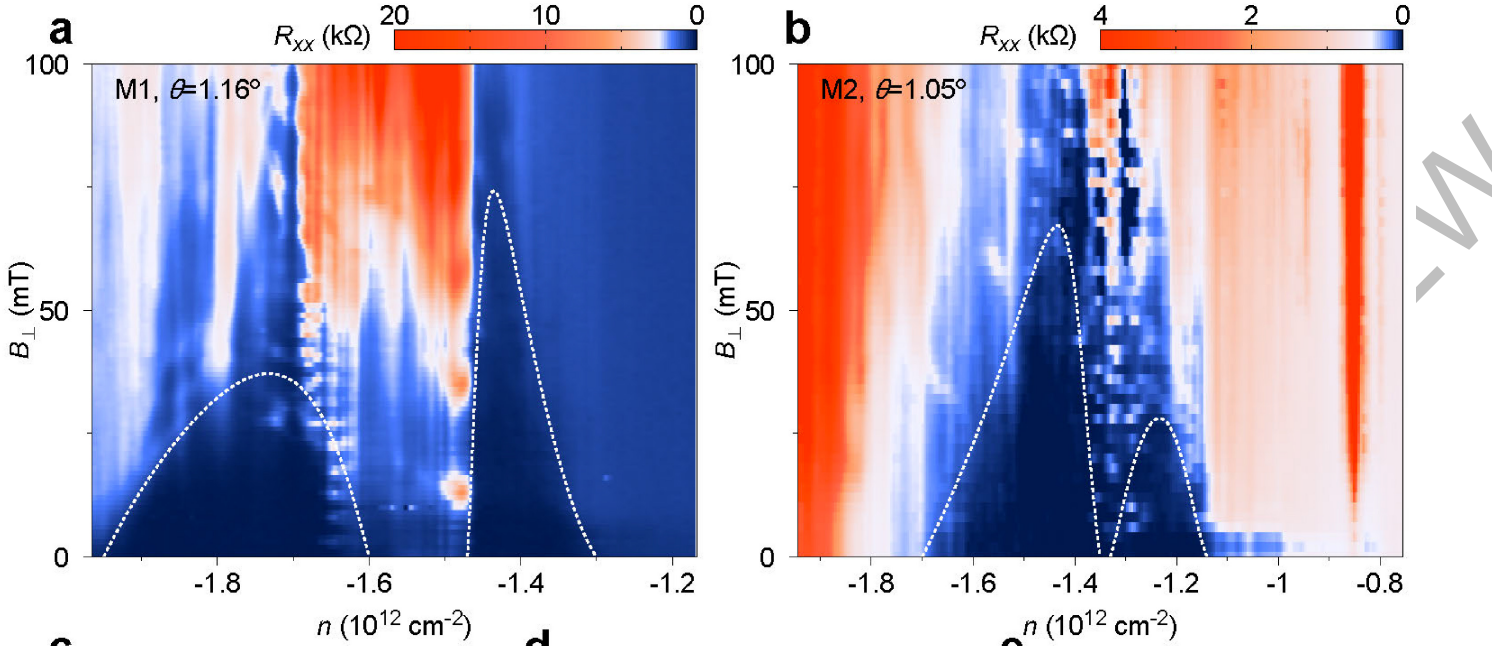
- Several distinct superconducting phases



M. Norman, 2011

Twisted bilayer graphene

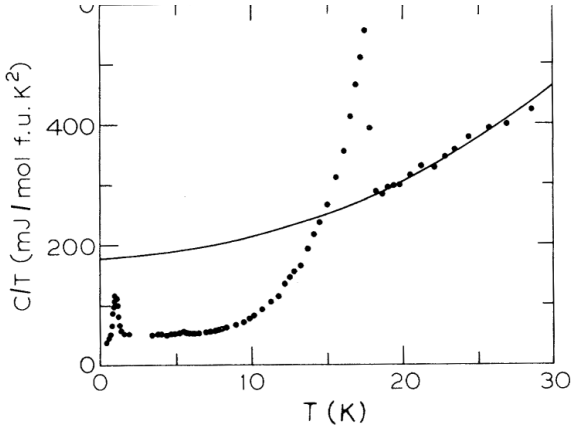
- Recent results (Y. Cao *et al*, 2018)



could be unconventional?

More subtle order

- Classic example: hidden order



URu_2Si_2, Palstra *et al, 1985*

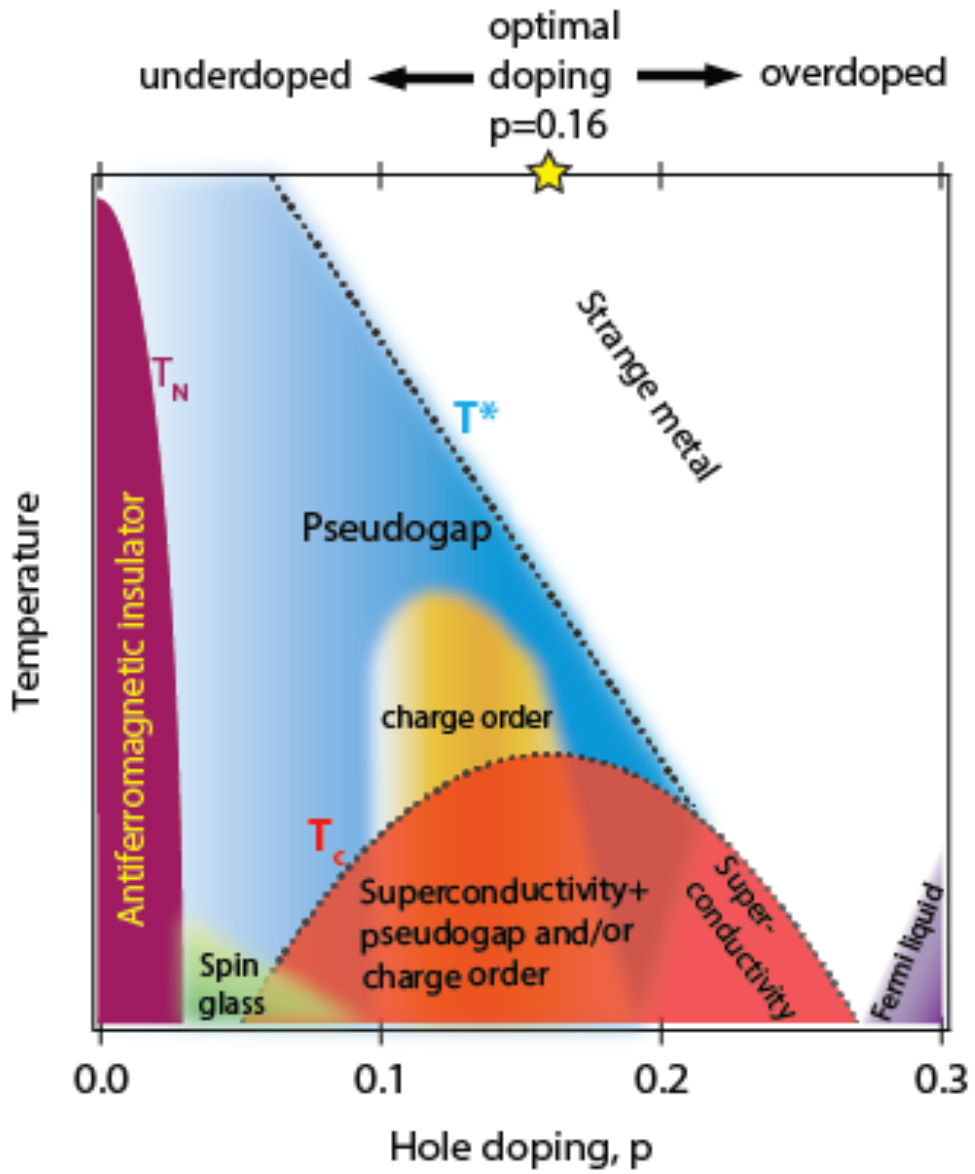
Barzykin and Gorkov (1995)	three-spin correlations [45]
Kasuya (1997)	uranium dimerisation [46]
Ikeda and Ohashi (1998)	*d*-spin density wave [47]
Okuno and Miyake (1998)	CEF and quantum fluctuations [48]
Chandra et al. (2002)	orbital currents [49]
Viroszek et al. (2002)	unconv. spin density wave [50]
Mineev and Zhitomirsky (2005)	staggered spin density wave [51]
Varma and Zhu (2006)	helicity (Pomeranchuk) order [52]
Elgazzar et al. (2009)	dynamical symmetry breaking [53]
Kotetes et al. (2010)	chiral *d*-density wave [54]
Dubi and Balatsky (2011)	hybridization wave [55]
Pepin et al. (2011)	modulated spin liquid [56]
Fujimoto (2011)	spin nematic order [57]
Riseborough et al. (2012)	unconv. spin-orbital density wave [58]
Das (2012)	spin-orbital density wave [59]
Chandra et al. (2013)	hastatic order [60]
Hsu and Chakravarty (2013)	singlet-triplet *d*-density wave [61]

Table 3. Summary of proposals for a specific multipolar magnetic ordering on the uranium ion to explain the HO, with an emphasis on the recent contributions. Note that different symmetries are possible for high-rank multipoles, therefore some kind of multipoles appear more than once.

Nieuwenhuys (1987)	dipole (2^1) order [62]
Santini and Amoretti (1994)	quadrupolar (2^2) order [63]
Kiss and Fazekas (2005)	octupolar (2^3) order [64]
Hanzawa and Watanabe (2005)	octupolar order [65]
Hanzawa (2007)	incommensurate octupole [66]
Haule and Kotliar (2009)	hexadecapolar (2^4) order [67]
Cricchio et al. (2009)	dotriacontapolar (2^5) order [68]
Harima et al. (2010)	antiferro quadrupolar order [69]
Thalmeier and Takimoto (2011)	$E(1, 1)$-type quadrupole [70]
Kusunose and Harima (2011)	antiferro hexadecapole [71]
Ikeda et al. (2012)	E^--type dotriacontapole [72]
Rau and Kee (2012)	E-type dotriacontapole [73]
Ressouche et al. (2012)	dotriacontapolar order [16]

from Mydosh + Openeer, 2014

Pseudo-gap



charge order

loop currents

T-reversal breaking

pair density wave

stripes

nematic

RVB

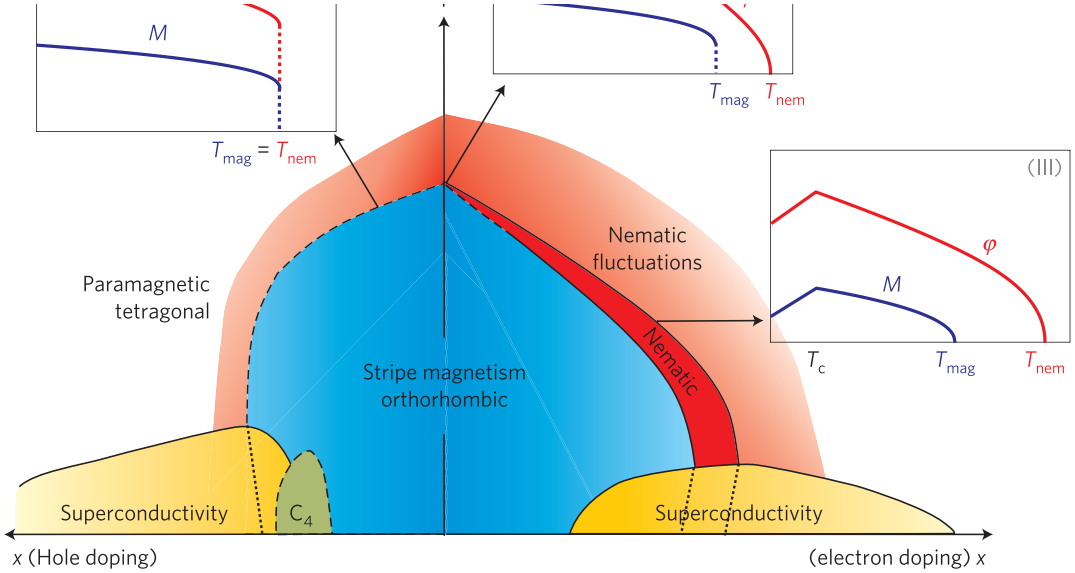
...

competing/intertwined/

hidden/fluctuating orders??

Electron nematic

symmetry is just tetragonal to orthorhombic, but seems to be that electrons, not lattice, are driving the order



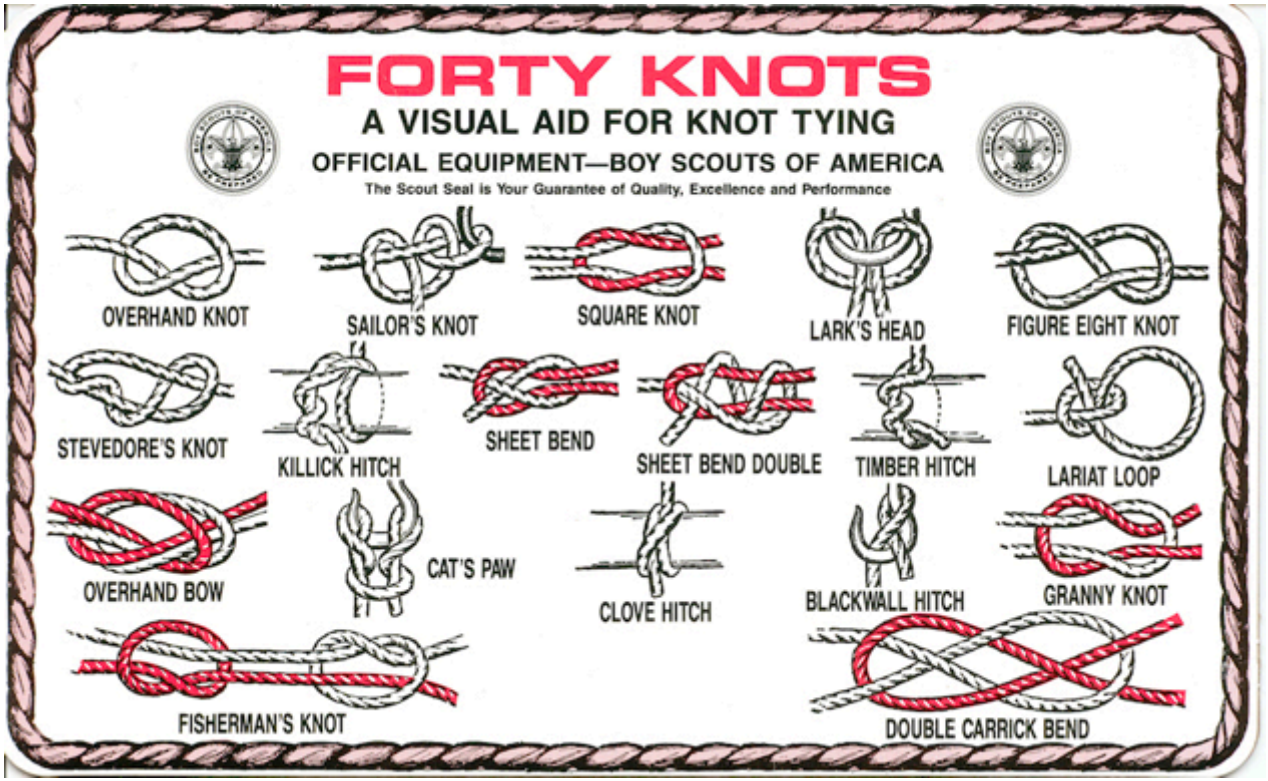
schematic of Fe122 materials from Fernandez *et al*,2014

Order questions

- What is the hidden order in URu_2Si_2?
- Is the pseudo-gap region of the cuprates a consequence of some hidden order?
- Are there mechanisms for unifying different orders in QMs - i.e. can you give a sharp meaning to intertwinement etc.?

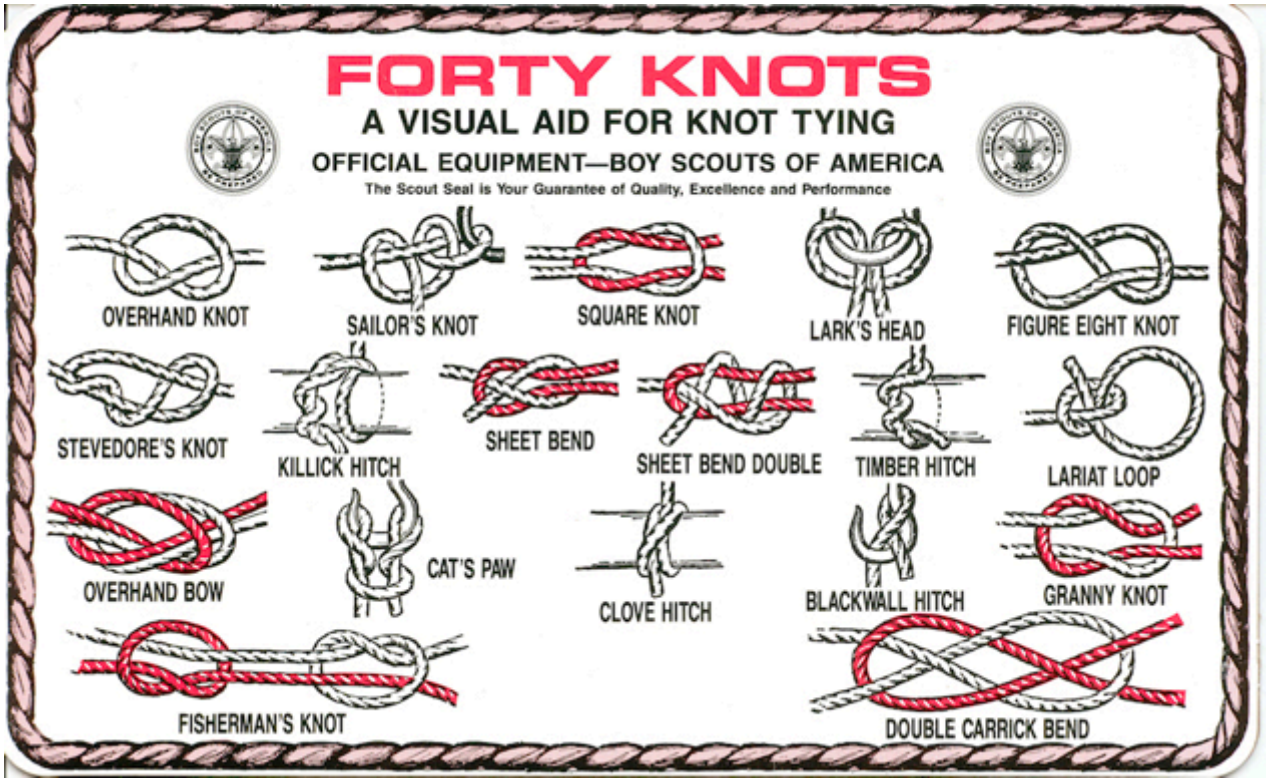
Topology

Mathematical study of objects that can and cannot be smoothly transformed into one another

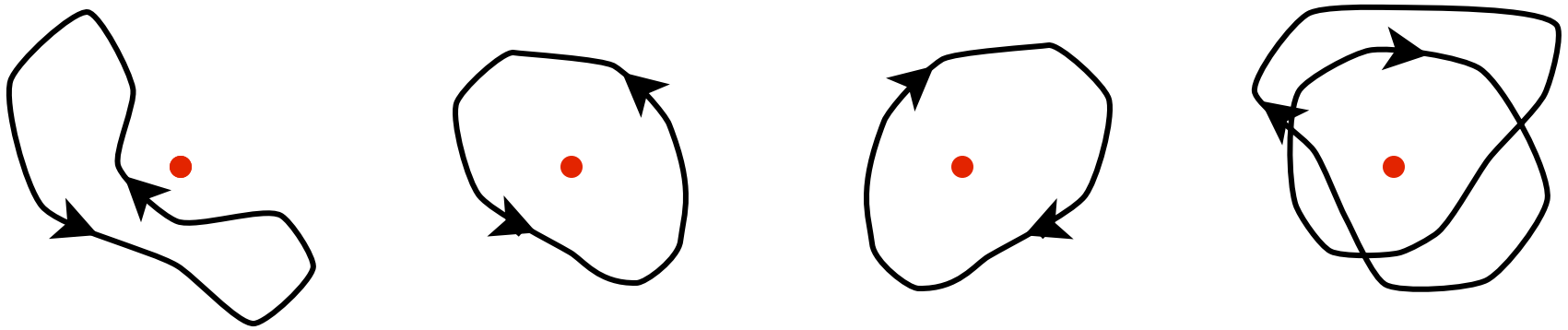


Topology

In physics, “knotted” states can become new phases of matter with robust properties



Topological invariant



W=0 W=1 W=-1 W=-2

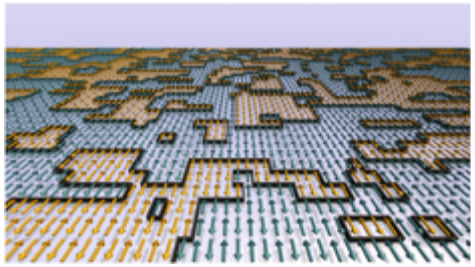
Winding number

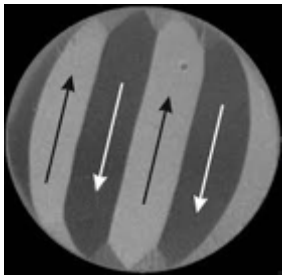
$$W[\mathcal{C}] = \frac{1}{2\pi i}\oint_{\mathcal{C}} \frac{dz}{z} \in \mathbb{Z}$$

$$= \frac{1}{2\pi i}\int ds\, \frac{z'(s)}{z(s)}$$

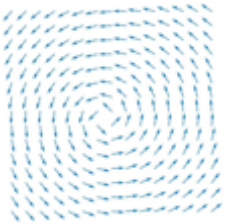
Topology of order

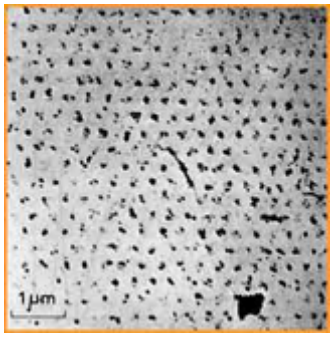
- Spontaneously broken symmetry leads to topological defects: configurations of order parameter that cannot be smoothly "unwound"





discrete order: domain walls





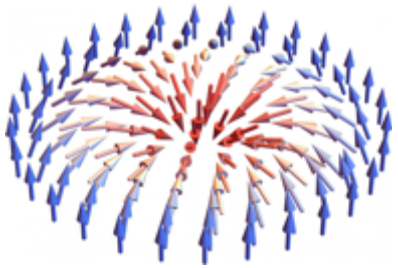
XY/U(1) order: vortices

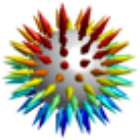
The topological theory of defects in ordered media*†

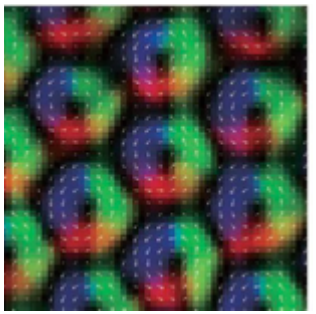
N. D. Mermin

Laboratory of Atomic and Solid State Physics Cornell University, Ithaca, New York 14853

Aspects of the theory of homotopy groups are described in a mathematical style closer to that of condensed matter physics than that of topology. The aim is to make more readily accessible to physicists the recent applications of homotopy theory to the study of defects in ordered media. Although many physical examples are woven into the development of the subject, the focus is on mathematical pedagogy rather than on a systematic review of applications.







vector order: skyrmions/hedgehogs

Topological band theory

Über die Quantenmechanik der Elektronen in Kristallgittern.

Von **Felix Bloch** in Leipzig.

Mit 2 Abbildungen. (Eingegangen am 10. August 1928.)

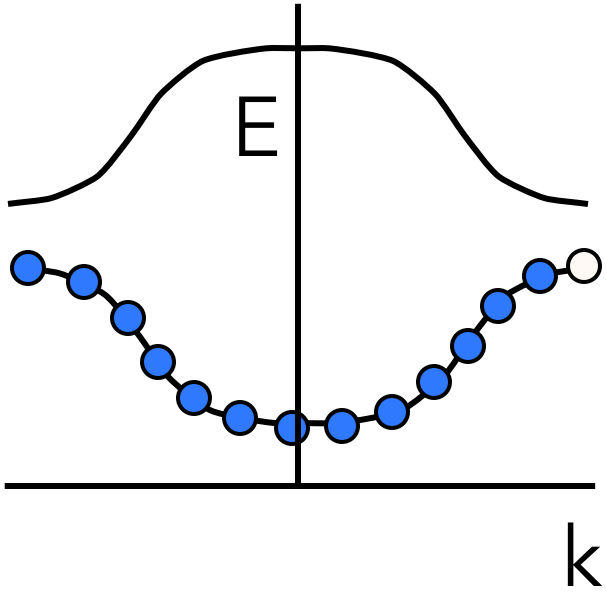
Die Bewegung eines Elektrons im Gitter wird untersucht, indem wir uns dieses durch ein zunächst streng dreifach periodisches Kraftfeld schematisieren. Unter Hinzunahme der Fermischen Statistik auf die Elektronen gestattet unser Modell Aussagen über den von ihnen herrührenden Anteil der spezifischen Wärme des Kristalls. Ferner wird gezeigt, daß die Berücksichtigung der thermischen Gitterschwingungen Größenordnung und Temperaturabhängigkeit der elektrischen Leitfähigkeit von Metallen in qualitativer Übereinstimmung mit der Erfahrung ergibt.

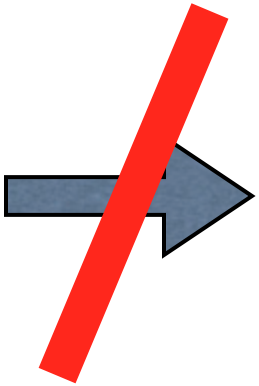
The Structure of Electronic Excitation Levels in Insulating Crystals

GREGORY H. WANNIER
*Princeton University, Princeton, New Jersey**

(Received May 13, 1937)

In this article, a method is devised to study the energy spectrum for an excited electron configuration in an ideal crystal. The configuration studied consists of a single excited electron taken out of a full band of N electrons. The multiplicity of the state is N^2. It is shown that because of the Coulomb attraction between the electron and its hole $N^{8/5}$ states are split off from the bottom of the excited Bloch band; for these states the electron cannot escape its hole completely. The analogy of these levels to the spectrum of an atom or molecule is worked out quantitatively. The bottom of the Bloch band appears as "ionization potential" and the Bloch band itself as the continuum above this threshold energy.



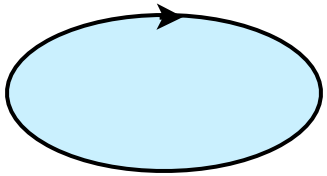


Thouless, 1984

Chern number

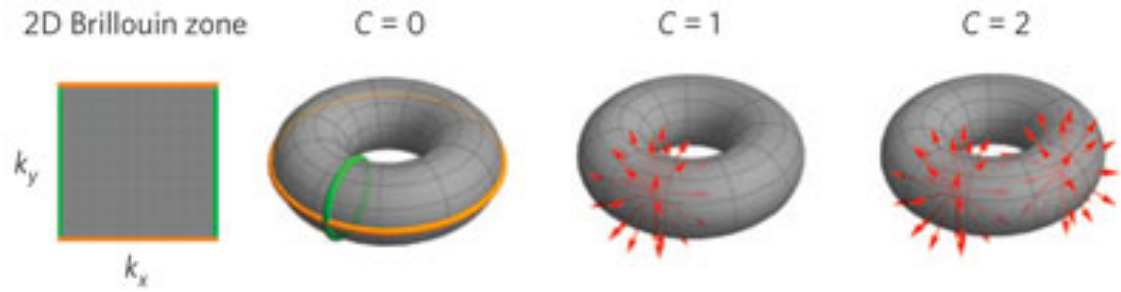
- Bloch states $\psi_n(r) = e^{ik\cdot r} u_{n,k}(r)$
- Berry gauge field $\vec{\mathcal{A}}_n = i\langle u_n | \vec{\nabla}_k | u_n \rangle$

$\vec{\mathcal{B}}_n = \vec{\nabla}_k \times \vec{\mathcal{A}}_n$



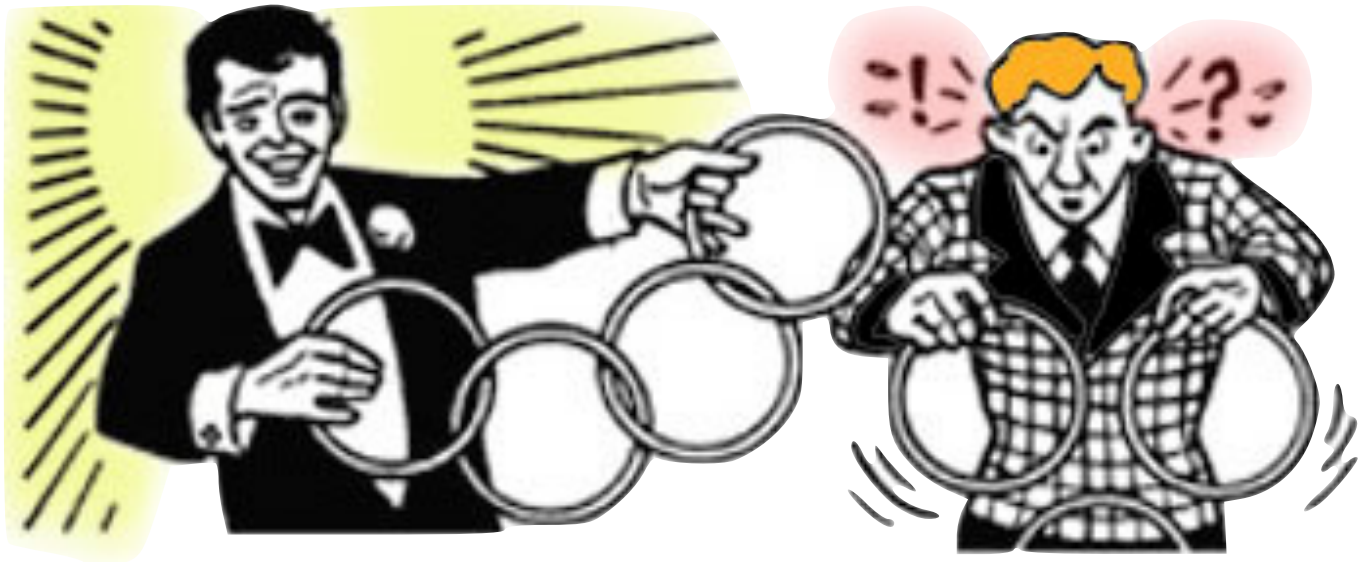
- Net Berry flux gives Chern number

$$q_n = \frac{1}{2\pi} \int d^2k \, \mathcal{B}_n^z \in \mathbb{Z}$$



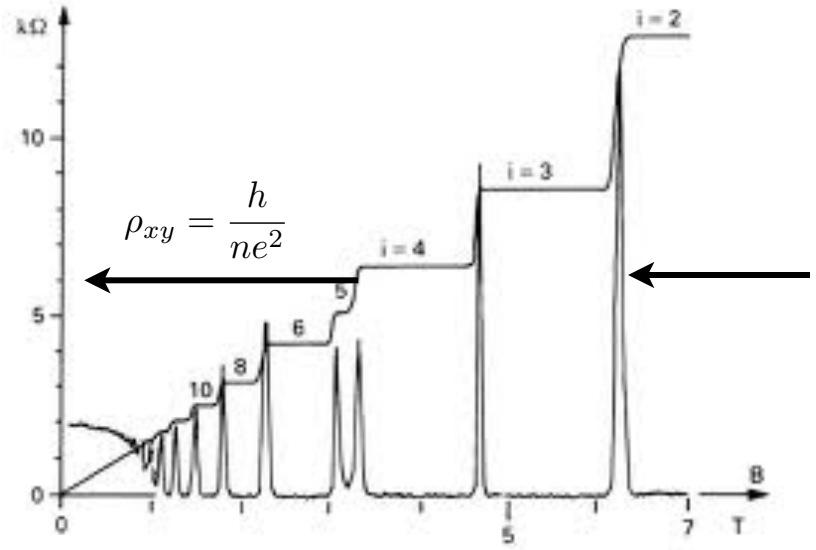
Phase transitions

- There is no *smooth* way to go from one topological sector to another

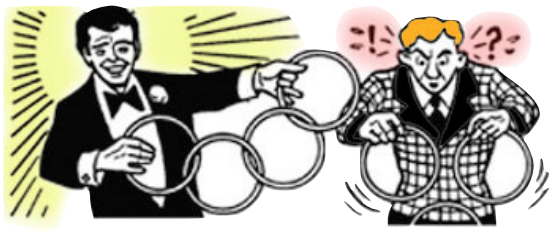


IQHE

- Hall conductance measures Chern number



ρ_{xx} peak signifies gapless quantum critical state

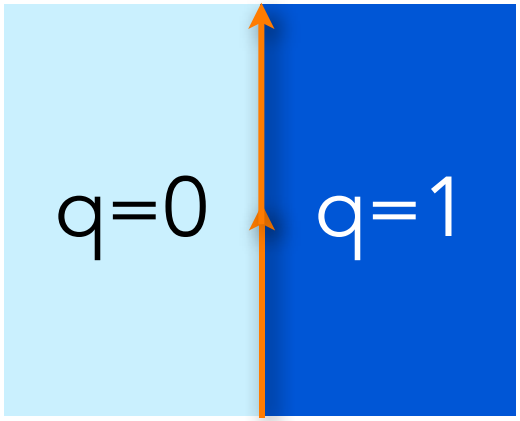


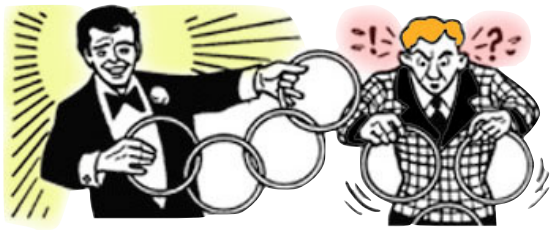
- Passage from one Chern number to another is a <u>quantum phase transition</u>

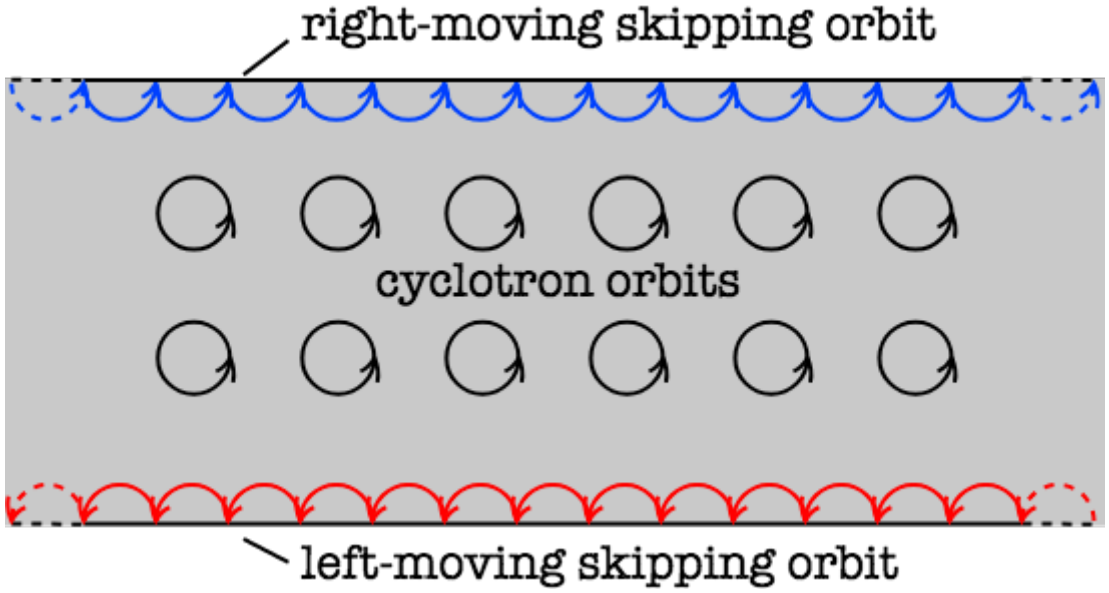
(with no order parameter!)

IQHE

- The boundary between states with different Chern number is gapless



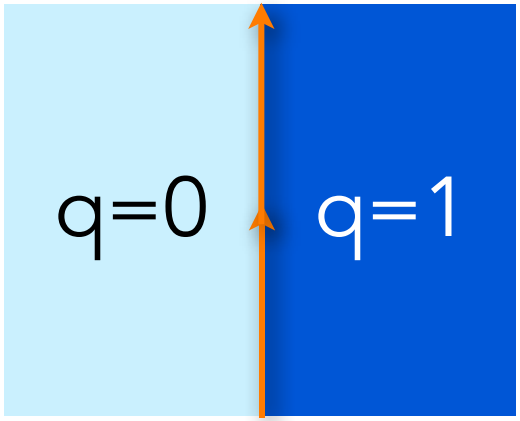


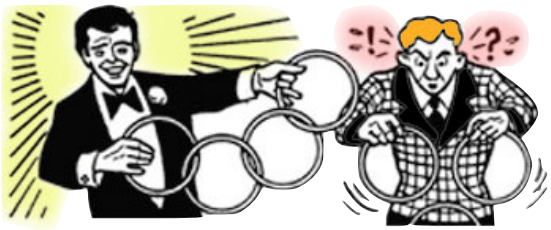


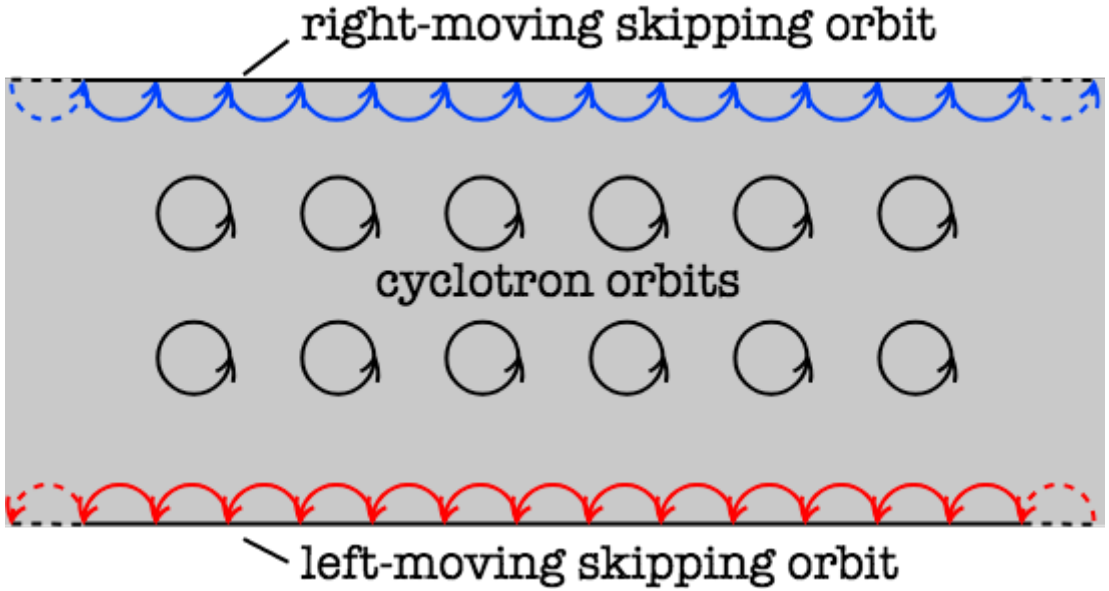
chiral edge states cannot backscatter

IQHE

- The boundary between states with different Chern number is gapless





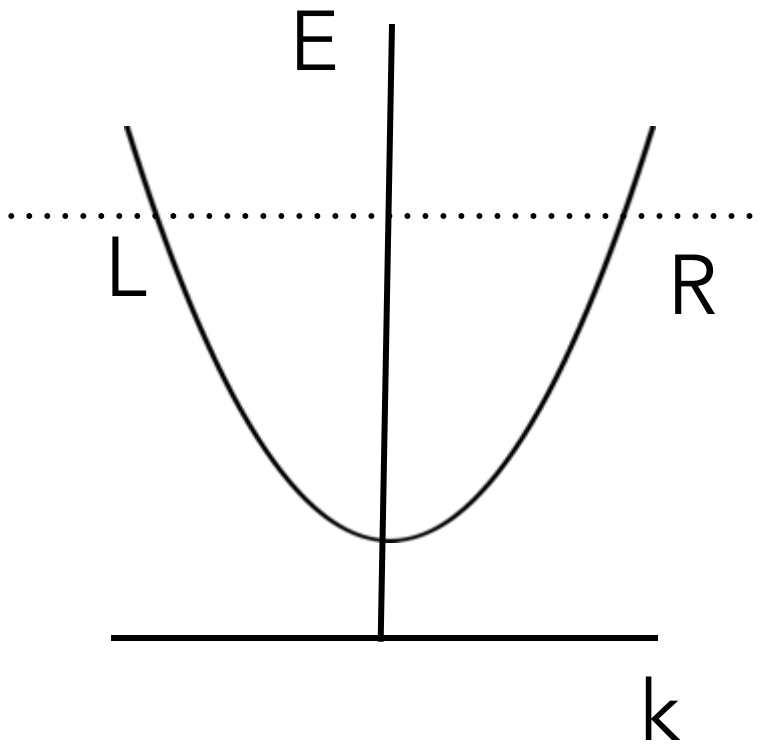


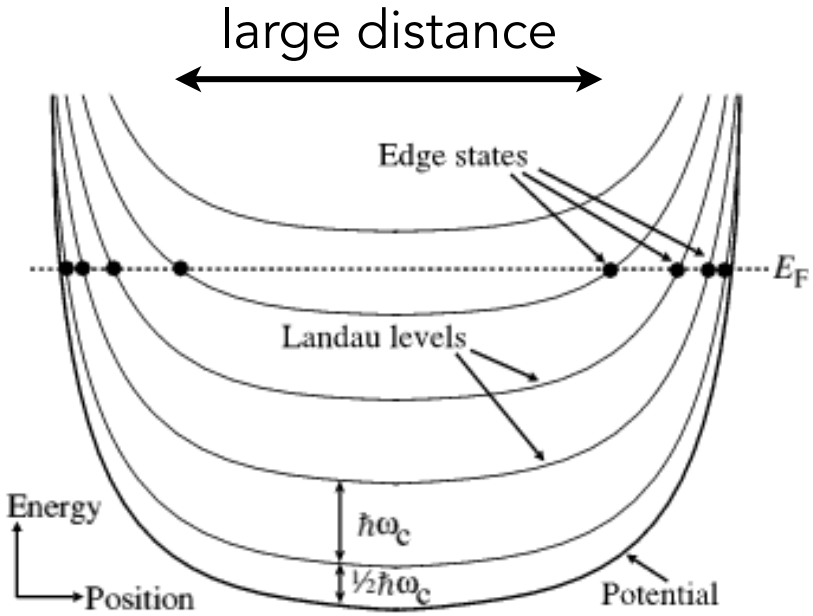
Bulk-boundary correspondence:

Chern Number = N_R-N_L

IQHE

- Edge states are “half” of the low energy excitations of a 1DEG

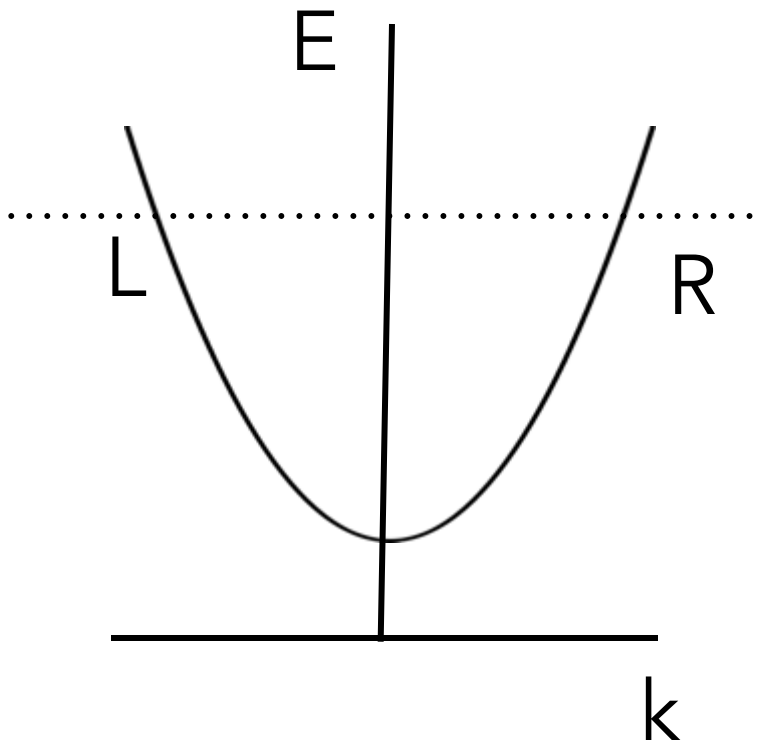


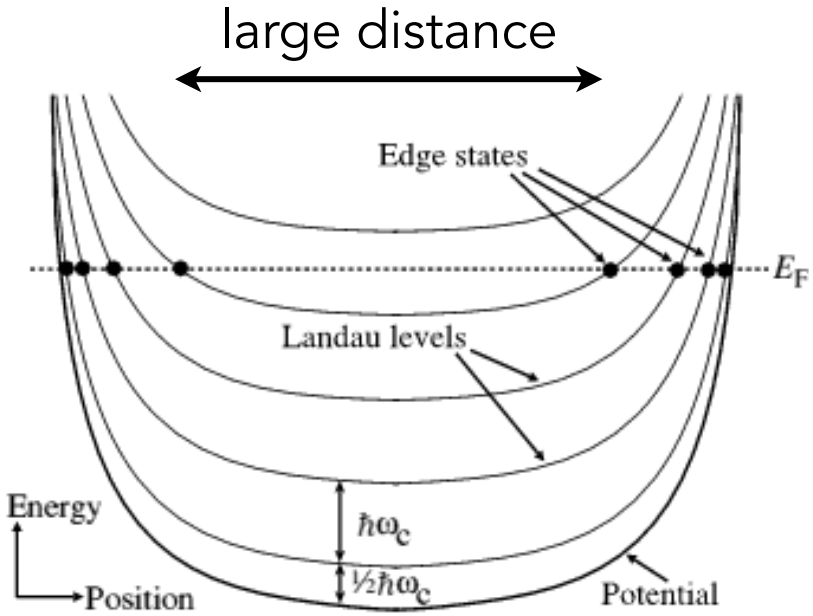


Halperin, 1982

IQHE

- Edge states are “half” of the low energy excitations of a 1DEG





Halperin, 1982

General rule: surface state of a d-dimensional TI cannot be realized in a d-1 dimensional system

Summary - Chern Insulators

- Winding of the one-electron wavefunction over the Brillouin zone
- Quantified by a topological invariant: the Chern number, which coincides with Hall conductance
- States with different values of the topological invariant are different phases
    - Tuning from one to another requires a quantum phase transition
    - The interface between two different values has gapless “protected” edge states, which are “anomalous”: they could not exist in an isolated 1-dimensional system

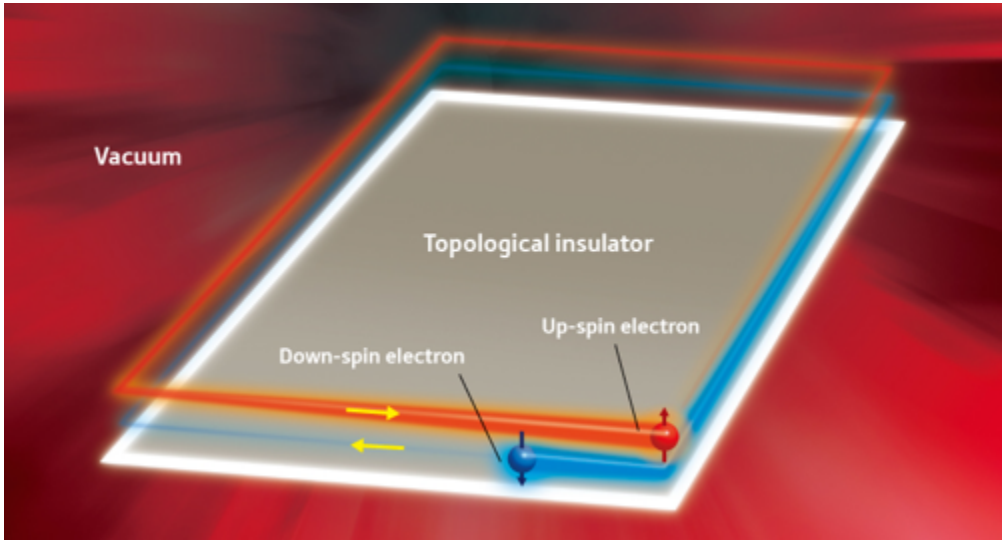
Time-reversal symmetry

- Would be nice to have topological quantization in materials in "natural conditions"
- The Berry curvature is odd under time-reversal $\mathcal{B}(-k) = -\mathcal{B}(k)$
- This implies the Chern number vanishes
- For decades it was believed this meant electronic states are topologically trivial with TRS

Z_2 TIs

2d: Kane, Mele (2005); Bernevig, Hughes, Zhang (2006)
3d: L. Fu, C. Kane, E. Mele (2007); J. Moore, LB (2007)

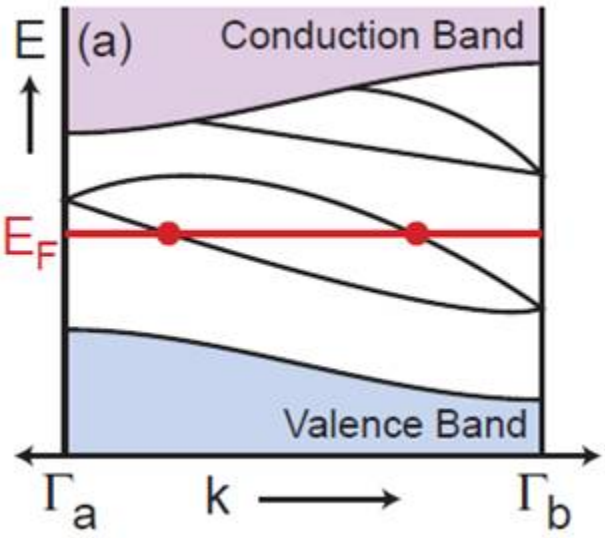
- Even with TR symmetry, a different type of TI is possible (*with spin-orbit coupling)*
- 2d: "QSHE"
- Roughly understood as opposite IQHE's for up and down electrons



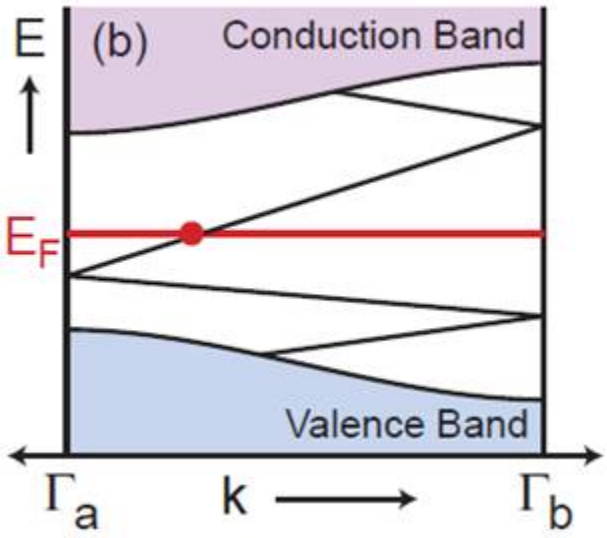
Z_2 TIs

2d: Kane, Mele (2005); Bernevig, Hughes, Zhang (2006)
3d: J. Moore, LB (2007); L. Fu, C. Kane, E. Mele (2007)

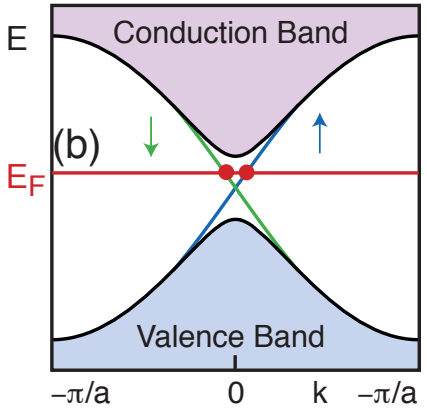
- Q = parity of band crossings between TRI momenta at the surface



"trivial"



"topological"

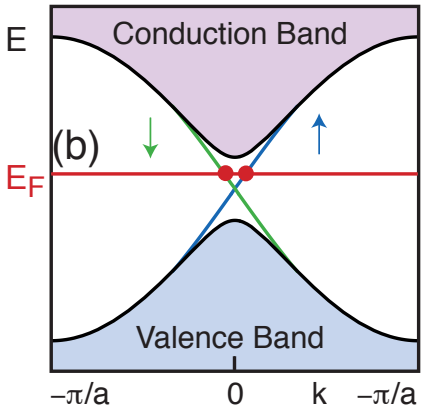


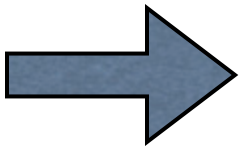
Full zone for TI

Z_2 TIs

J. Moore, LB (2007)
L. Fu, C. Kane, E. Mele (2007)

- In 3d, there are *four* Z_2 parities
  - 3 "weak" parities - describe layered 2d TIs
  - 1 "strong" parity - describes intrinsically 3d physics



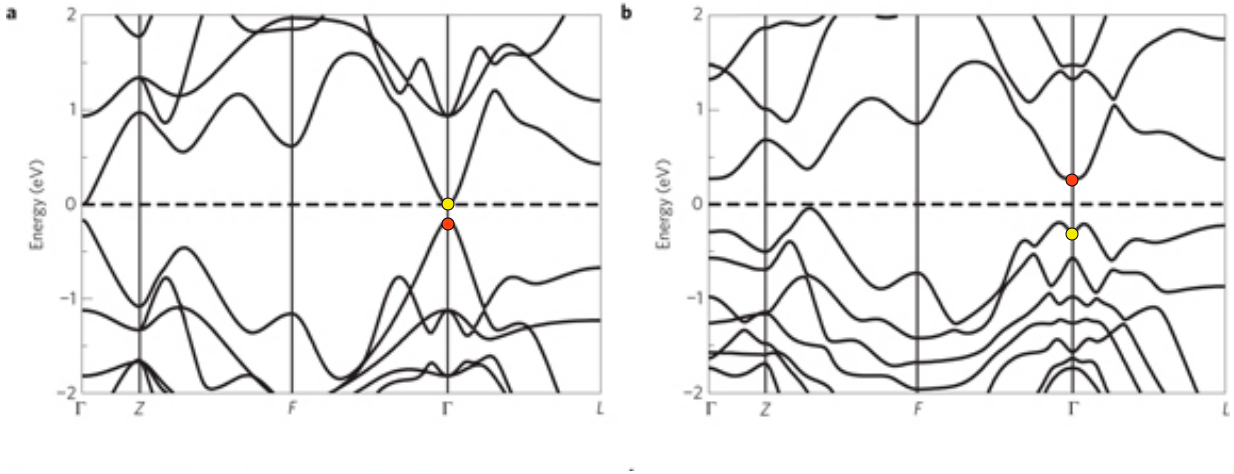


odd number of Dirac cones at any surface

Band inversion

- Different classes of bands cannot be smoothly deformed into one another

Bi_2Se_3



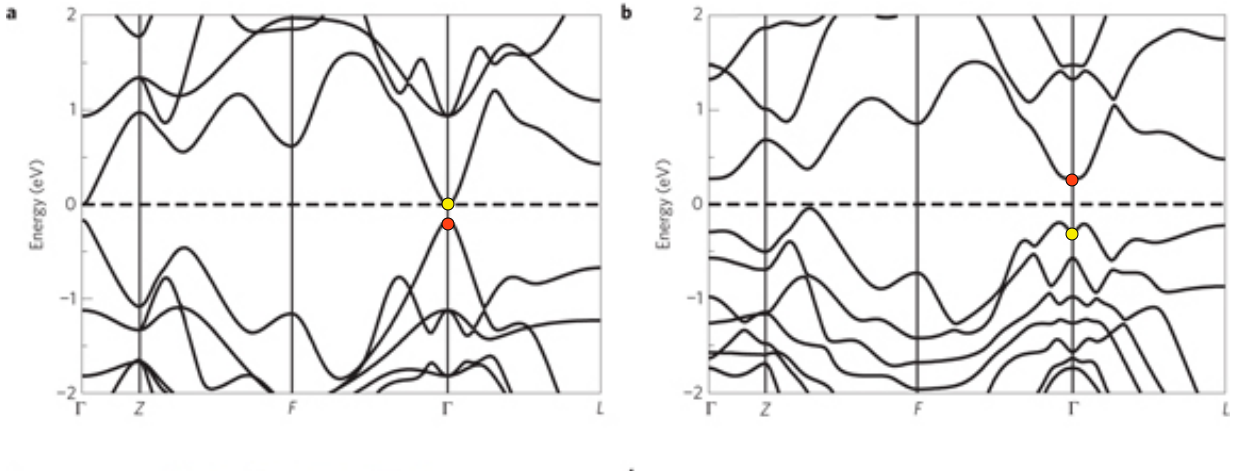
no SOC

w/ SOC

Band inversion

- Different classes of bands cannot be smoothly deformed into one another

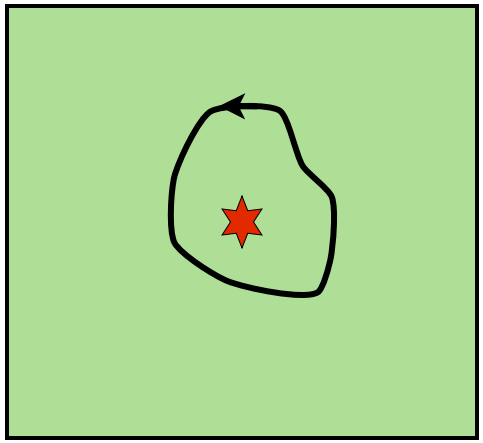
Bi_2Se_3



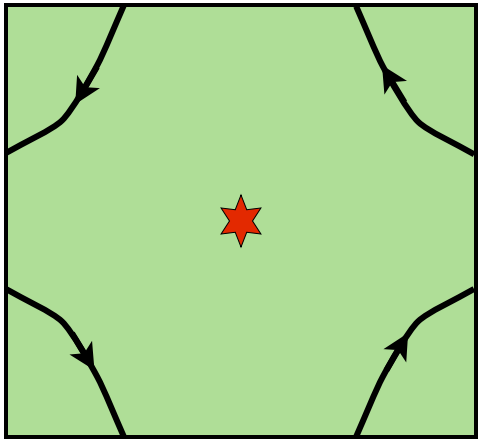
normal insulator topological insulator

Single Dirac cone

- 1/4 Graphene
- 2d Dirac mass breaks TR
- Cannot be found in any 2d model



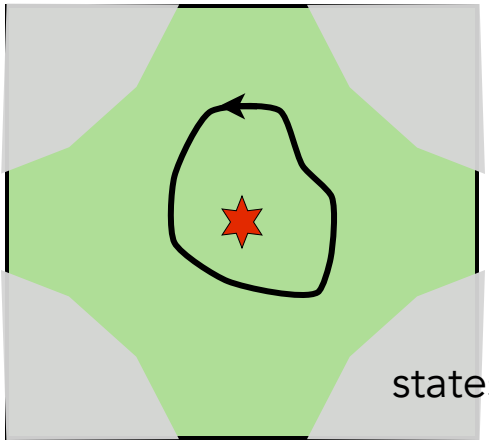
$\Phi = \pi$



$\Phi = 0$

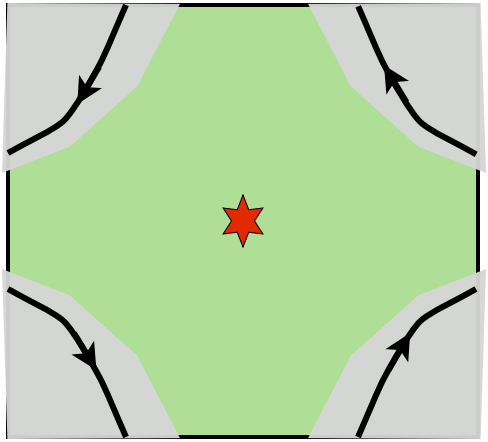
Single Dirac cone

- 1/4 Graphene
- 2d Dirac mass breaks TR
- Cannot be found in any 2d model



$\Phi = \pi$

states decay into bulk

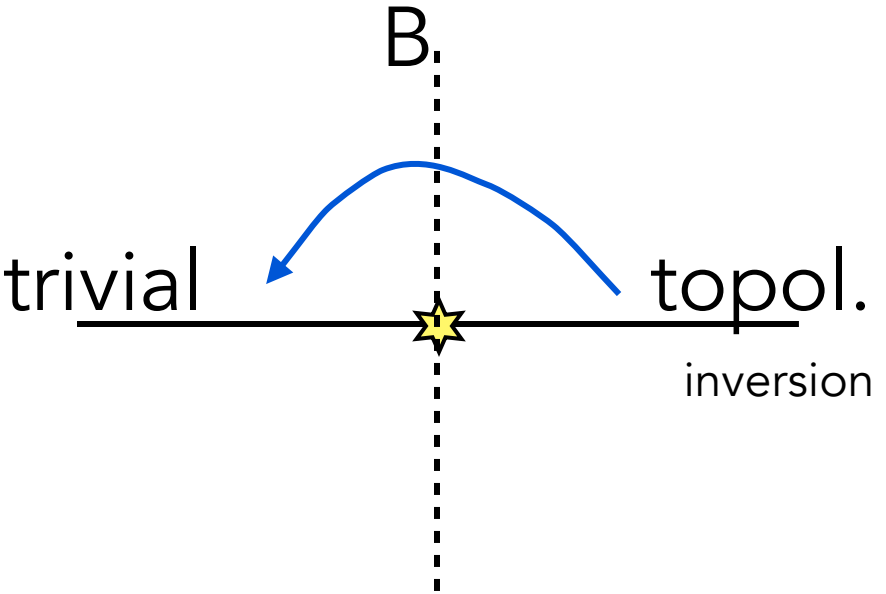


not allowed

Single Dirac cone

- 1/4 Graphene
- 2d Dirac mass breaks TR
- Cannot be found in any 2d model

If time reversal is broken, the Dirac cone is gapped and TI becomes equivalent to trivial insulator



TIs

Broken TRS	with TRS
integer Chern number	Z_2 invariant
= Hall conductance	= magneto-electric polarizability
chiral edge states	helical edge/ surface states

Topological superconductors

"periodic table" of TIs+TSCs

Chern insulator	Z_2 TI
chiral topo. SC	Z_2 Topo. SC

He3B

Name	T	C	S=CT	d=1	d=2	d=3
A	0	0	0	-	$\mathbb{Z}$	-
AIII	0	0	1	$\mathbb{Z}$	-	$\mathbb{Z}$
AI	+1	0	0	-	-	-
BDI	+1	+1	1	$\mathbb{Z}$	-	-
D	0	+1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	-
DIII	-1	+1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
AII	-1	0	0	-	$\mathbb{Z}_2$	$\mathbb{Z}_2$
CII	-1	-1	1	$\mathbb{Z}$	-	$\mathbb{Z}_2$
C	0	-1	0	-	$\mathbb{Z}$	-
CI	+1	-1	1	-	-	$\mathbb{Z}$

IQHE
polyacetylen
chiral p-wave
TRI top. triplet SC (He3 B)
QSHE
3D Z2 top. insulator
chiral d-wave
TRI top. singlet SC

free fermion TIs

A. Schnyder *et al,* 2008

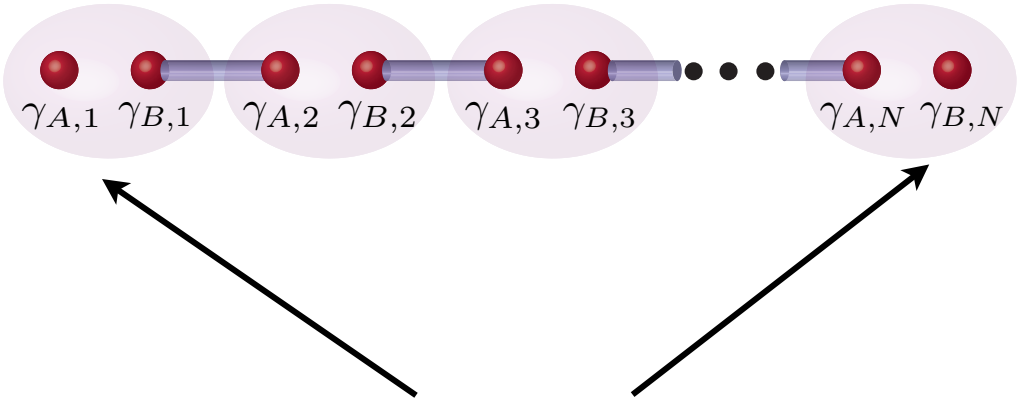
Kitaev, 2009

Kitaev Chain

- 1d spinless "p-wave" superconductor

$$H = -\mu \sum_{x=1}^{N} c_x^\dagger c_x - \sum_{x=1}^{N-1} (t c_x^\dagger c_{x+1} + |\Delta| e^{i\phi} c_x c_{x+1} + h.c.)$$

- Topological for |μ|< 2 t



together these two "Majorana" fermions form *one* two-level system

Topological semi-metals

- Another class of topological states are *semi-metals,* in which band touching is protected by topology
  - Graphene: 2d Dirac fermion
  - TaAs: 3d Weyl fermion
  - Cd_3Se_2: 3d Dirac fermion
  - Mn_3Sn: 3d magnetic Weyl fermions
  - many more!
- In these systems the touching points are like “topological defects”: singularities of Berry curvature
- Near the touching points, electrons have unusual dynamics: lots of potential for interesting physics!

Weyl semimetal

937 PHYSICAL REVIEW

Accidental Degeneracy in the Energy Bands of Crystals

CONYERS HERRING
Princeton University, Princeton, New Jersey
(Received June 16, 1937)

For a crystal without an inversion center, the energy separation $\delta E(\mathbf{k}+\boldsymbol{\kappa})$ in the neigborhood of a point $\mathbf{k}$ where contact of equivalent manifolds occurs may be expected to be of the order of κ as $\kappa \rightarrow 0$, for all directions of $\boldsymbol{\kappa}$.

Weyl semimetal

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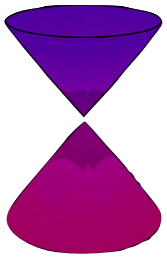
$$H = v\vec{\sigma} \cdot \vec{k}$$



A two-component spinor in three dimensions: "half" of a Dirac fermion. Weyl fermions have a chirality and *must* be massless

(Dirac semimetals also exist)

Weyl semimetal

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Either inversion or time-reversal (or both) must be broken

Weyl semimetal

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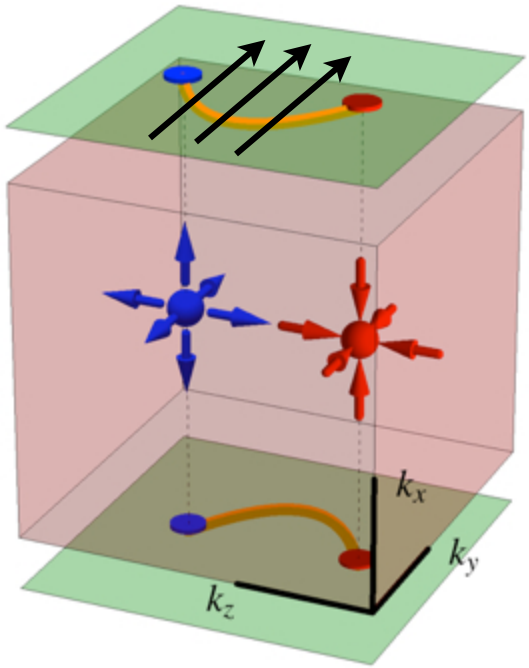
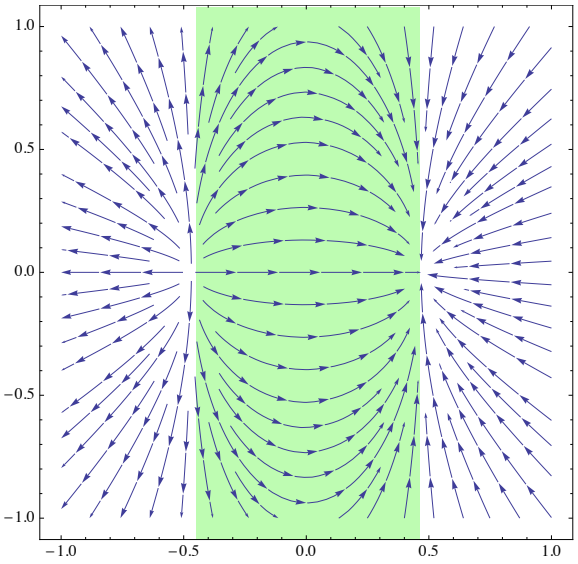
S. Murakami, 2007
X. Wan *et al*, 2011
A. Burkov+LB, 2011

For a crystal without an inversion center, the energy separation $\delta E(\mathbf{k}+\boldsymbol{\kappa})$ in the neigborhood of a point $\mathbf{k}$ where contact of equivalent manifolds occurs may be expected to be of the order of κ as $\kappa \to 0$, for all directions of $\boldsymbol{\kappa}$.





Weyl points are "monopoles" of Berry curvature: topology in k-space!

Review: A.M. Turner, A. Vishwanath, arXiv:1301.0330

Weyl semimetal

937 PHYSICAL REVIEW

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S. Murakami, 2007
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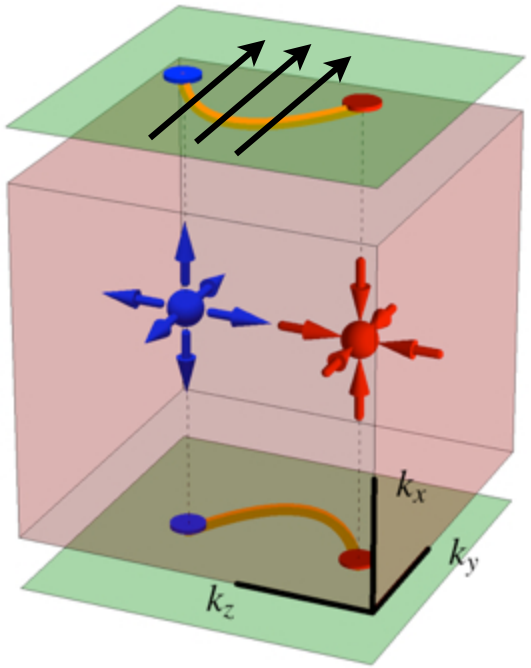
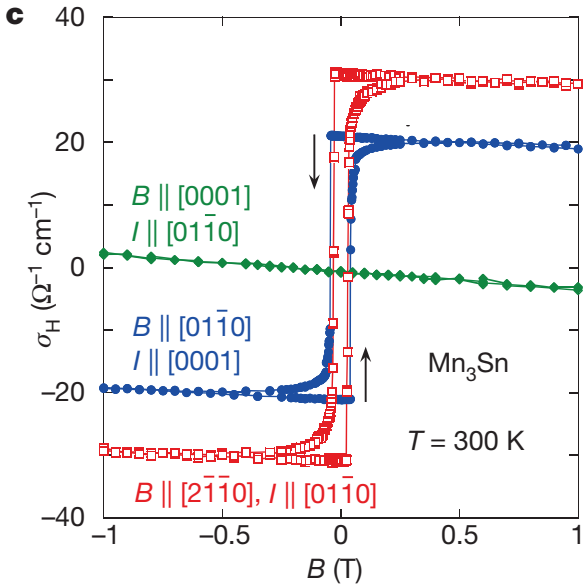


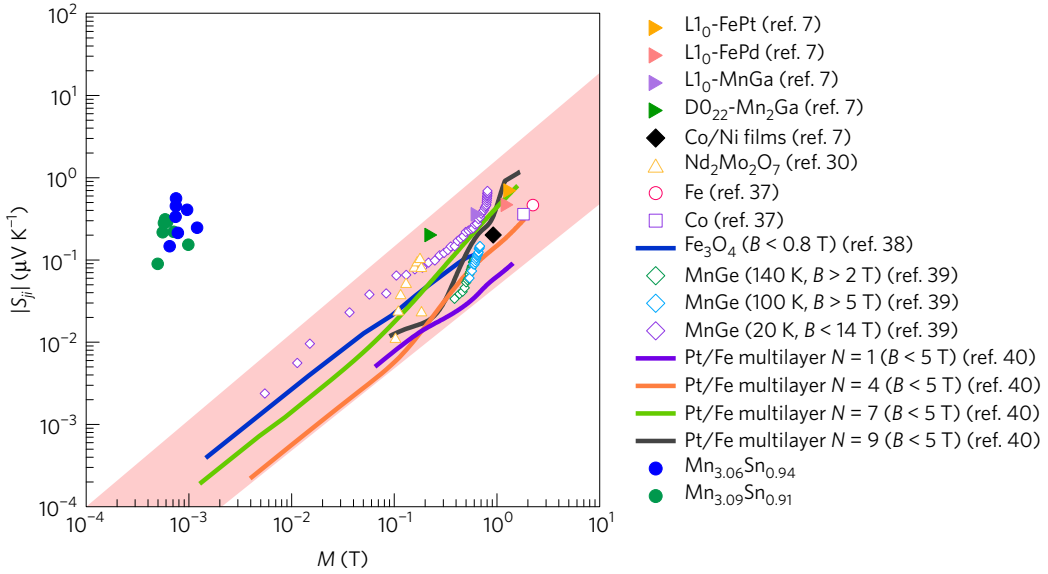
- Striking properties:
  - Anomalous Hall effect
  - ABJ "anomaly": strong negative MR for I ∥ B
  - Surface Fermi arcs

Review: A.M. Turner, A. Vishwanath, arXiv:1301.0330

Mn_3Sn magnetic Weyl



anomalous Hall effect,
Nakatsuji *et al*, 2015



anomalous Nernst effect,
Ikhlas *et al*, 2017

Effects comparable to or exceeding ferromagnetic metals at room temperature

Topological band theory

- Lots more topology if you include all symmetries and atomic structure: "TCIs"

ARTICLE

DOI: 10.1038/s41467-017-00133-2 OPEN

Symmetry-based indicators of band topology in the 230 space groups

Hoi Chun Po[1,2], Ashvin Vishwanath[1,2] & Haruki Watanabe[3]

The interplay between symmetry and topology leads to a rich variety of electronic topological phases, protecting states such as the topological insulators and Dirac semimetals. Previous results, like the Fu-Kane parity criterion for inversion-symmetric topological insulators, demonstrate that symmetry labels can sometimes unambiguously indicate underlying band topology. Here we develop a systematic approach to expose all such symmetry-based indicators of band topology in all the 230 space groups. This is achieved by first developing an efficient way to represent band structures in terms of elementary basis states, and then isolating the topological ones by removing the subset of atomic insulators, defined by the existence of localized symmetric Wannier functions. Aside from encompassing all earlier results on such indicators, including in particular the notion of filling-enforced quantum band insulators, our theory identifies symmetry settings with previously hidden forms of band topology, and can be applied to the search for topological materials.

Topological quantum chemistry

Barry Bradlyn[1]*, L. Elcoro[2]*, Jennifer Cano[1]*, M. G. Vergniory[3,4,5]*, Zhijun Wang[6]*, C. Felser[7], M. I. Aroyo[2] & B. Andrei Bernevig[3,6,8,9]

Since the discovery of topological insulators and semimetals, there has been much research into predicting and experimentally discovering distinct classes of these materials, in which the topology of electronic states leads to robust surface states and electromagnetic responses. This apparent success, however, masks a fundamental shortcoming: topological insulators represent only a few hundred of the 200,000 stoichiometric compounds in material databases. However, it is unclear whether this low number is indicative of the esoteric nature of topological insulators or of a fundamental problem with the current approaches to finding them. Here we propose a complete electronic band theory, which builds on the conventional band theory of electrons, highlighting the link between the topology and local chemical bonding. This theory of topological quantum chemistry provides a description of the universal (across materials), global properties of all possible band structures and (weakly correlated) materials, consisting of a graph-theoretic description of momentum (reciprocal) space and a complementary group-theoretic description in real space. For all 230 crystal symmetry groups, we classify the possible band structures that arise from local atomic orbitals, and show which are topologically non-trivial. Our electronic band theory sheds new light on known topological insulators, and can be used to predict many more.

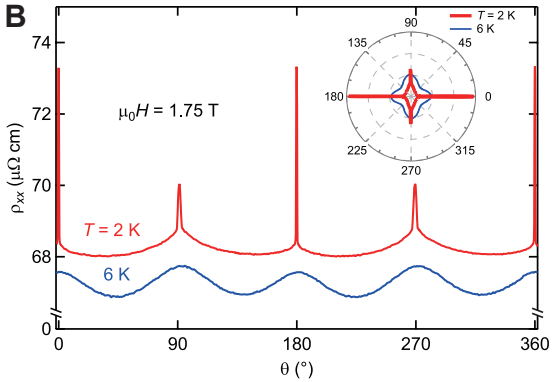
Day 2

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

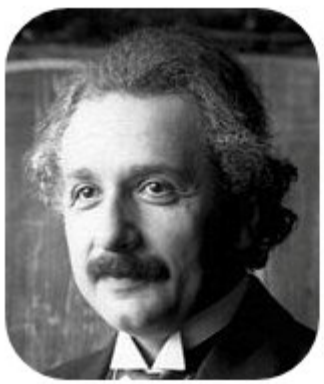
EPR $|\Psi\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$

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??



A. Einstein

B. Podolsky

N. Rosen

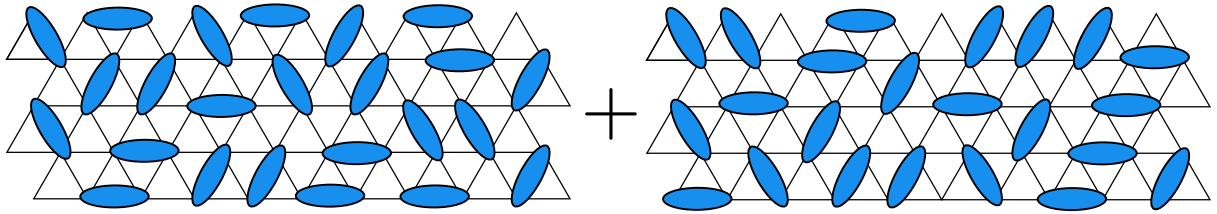
Many Body Entanglement

Phil Anderson, 1973

a "quantum liquid" of spins

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

Ψ =



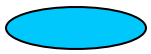
+...

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

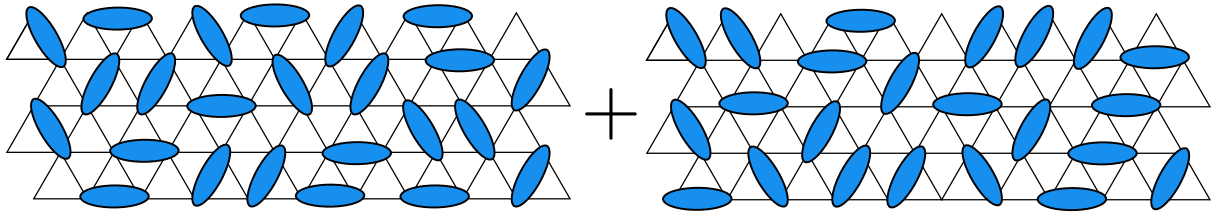
Many Body Entanglement

Phil Anderson, 1973

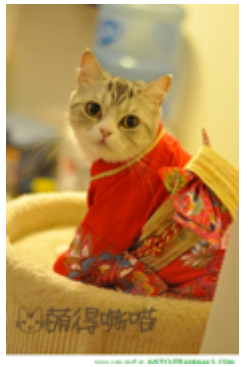
a "quantum liquid" of spins


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

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

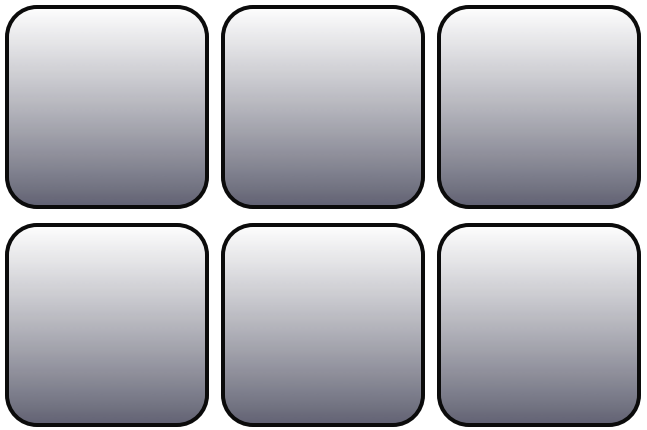
Ordinary (local) Matter

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

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

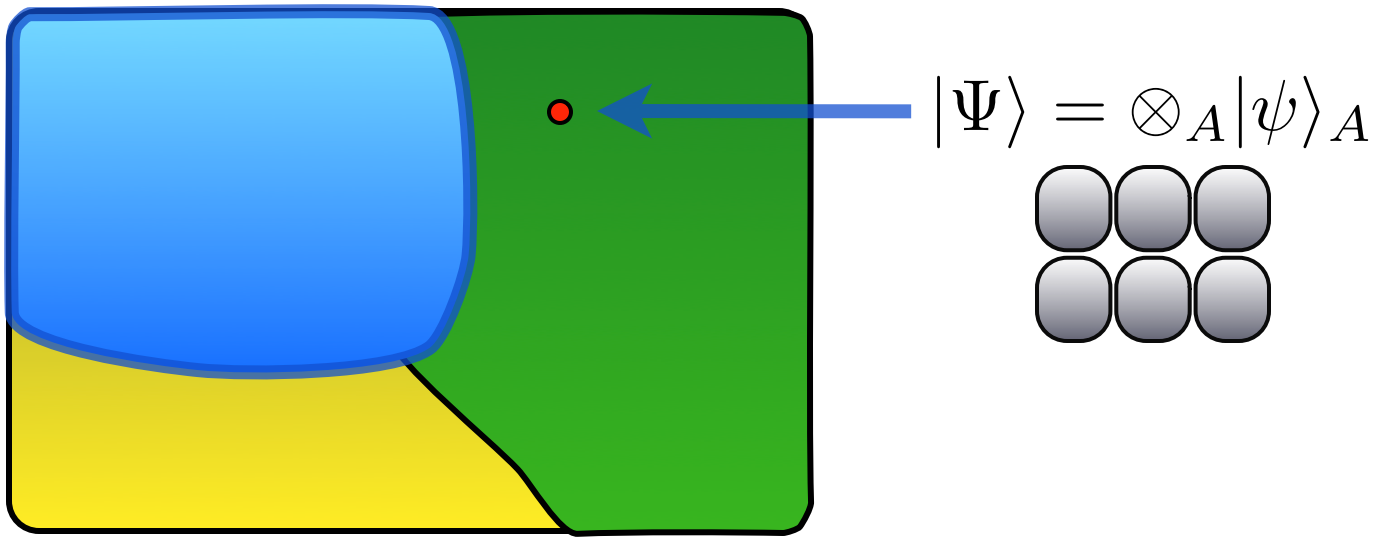


most insulators
are like this

no entanglement
between blocks

"Essentially" a product state?

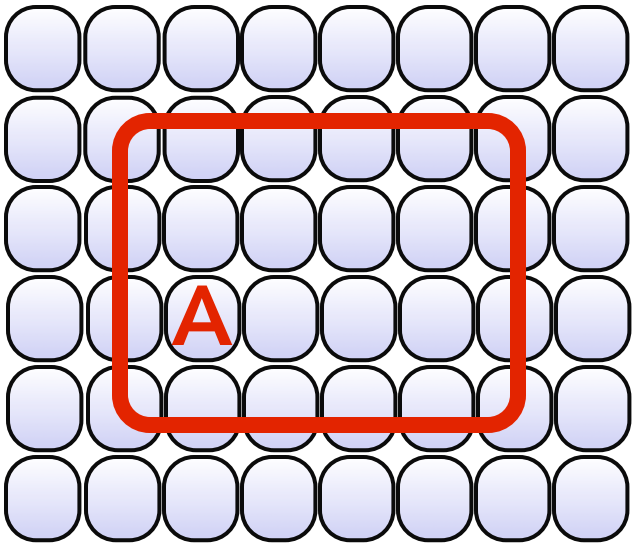
- Adiabatic continuity



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

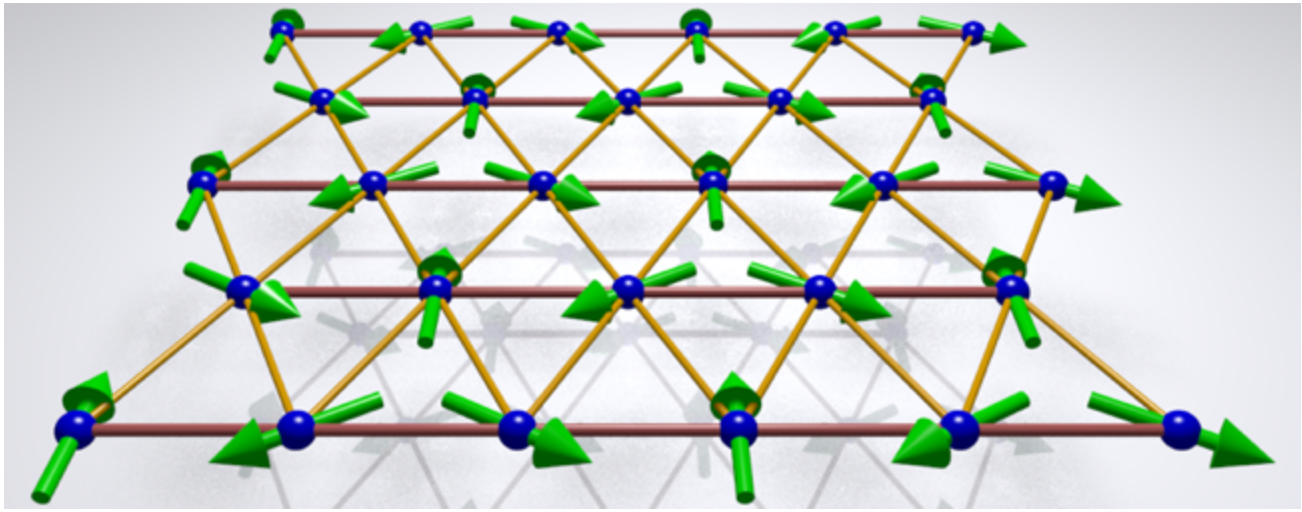
Best example: ordered magnet

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

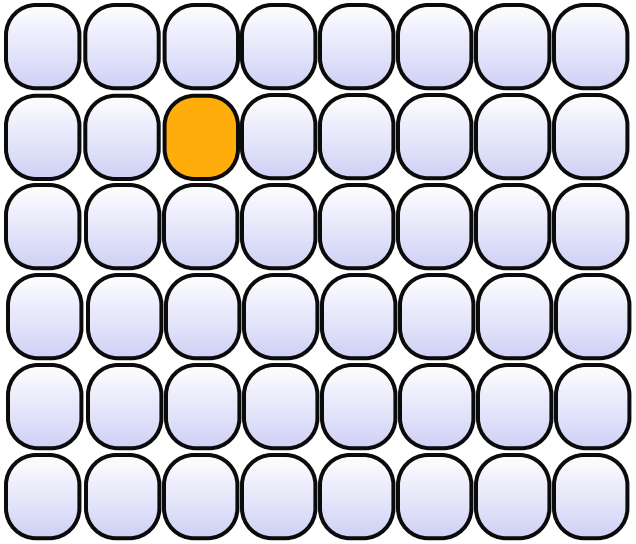
exchange is short-range: local

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

block is a single spin



Quasiparticles

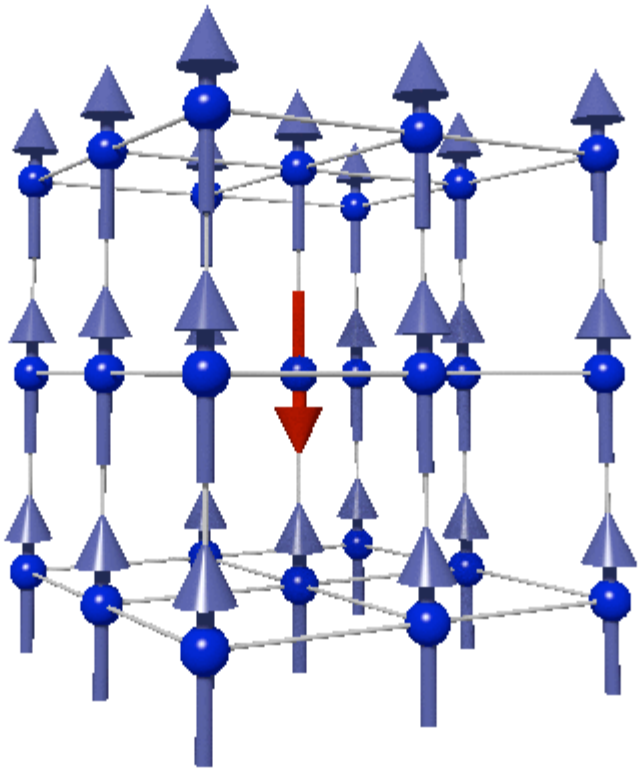


excited states ~ excited levels of one block

- 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

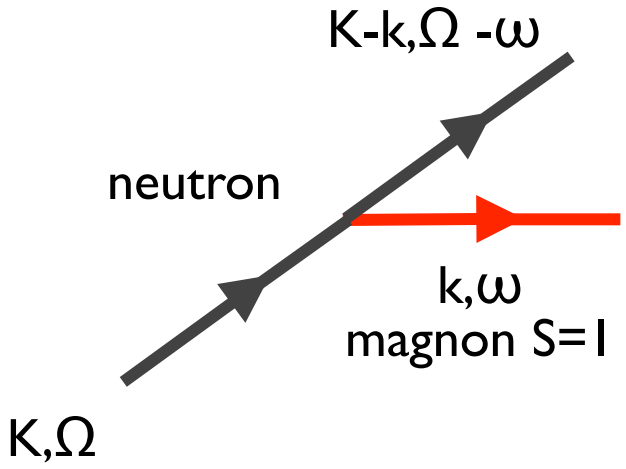
- quantum numbers consistent with finite system: no emergent or fractional quantum numbers

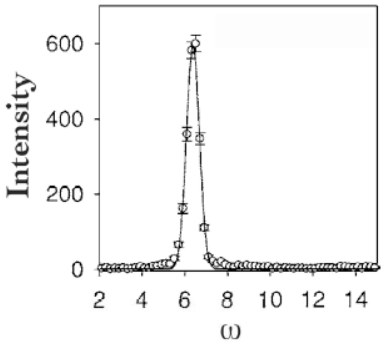
Spin wave



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

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

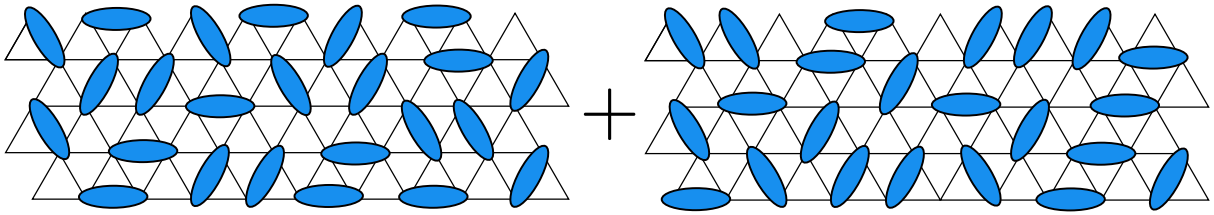


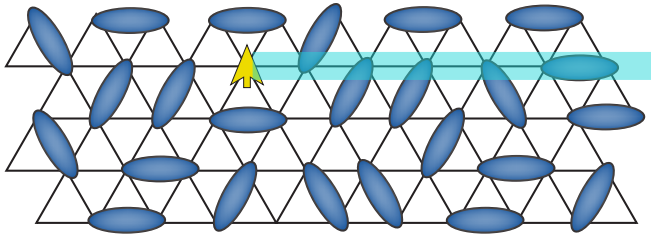


Line shape in Rb_2MnF_4

Quantum spin liquid

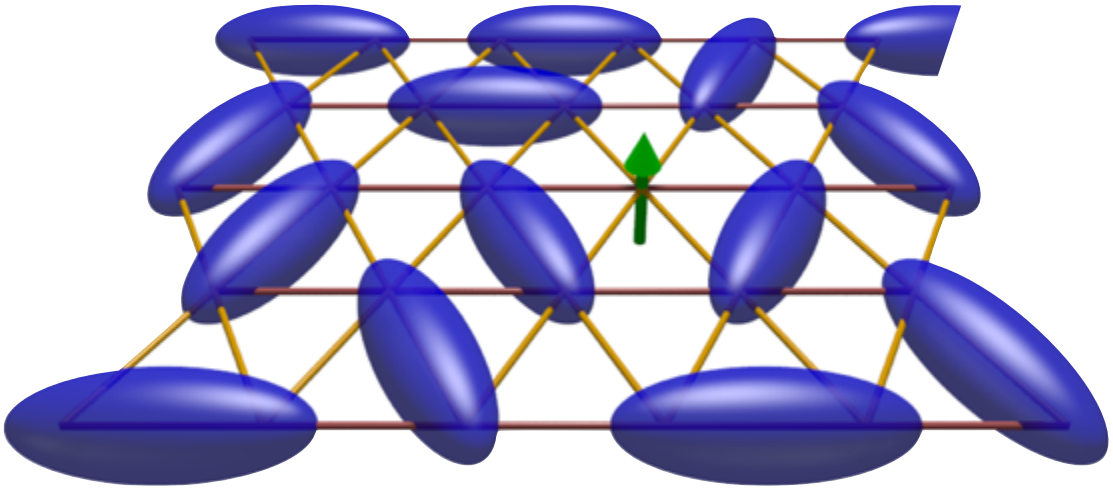
Entanglement -> non-local excitation

Ψ =  +...

Ψ =  +... "spinon"

"quasiparticle" above a non-zero gap

Fractional quantum number

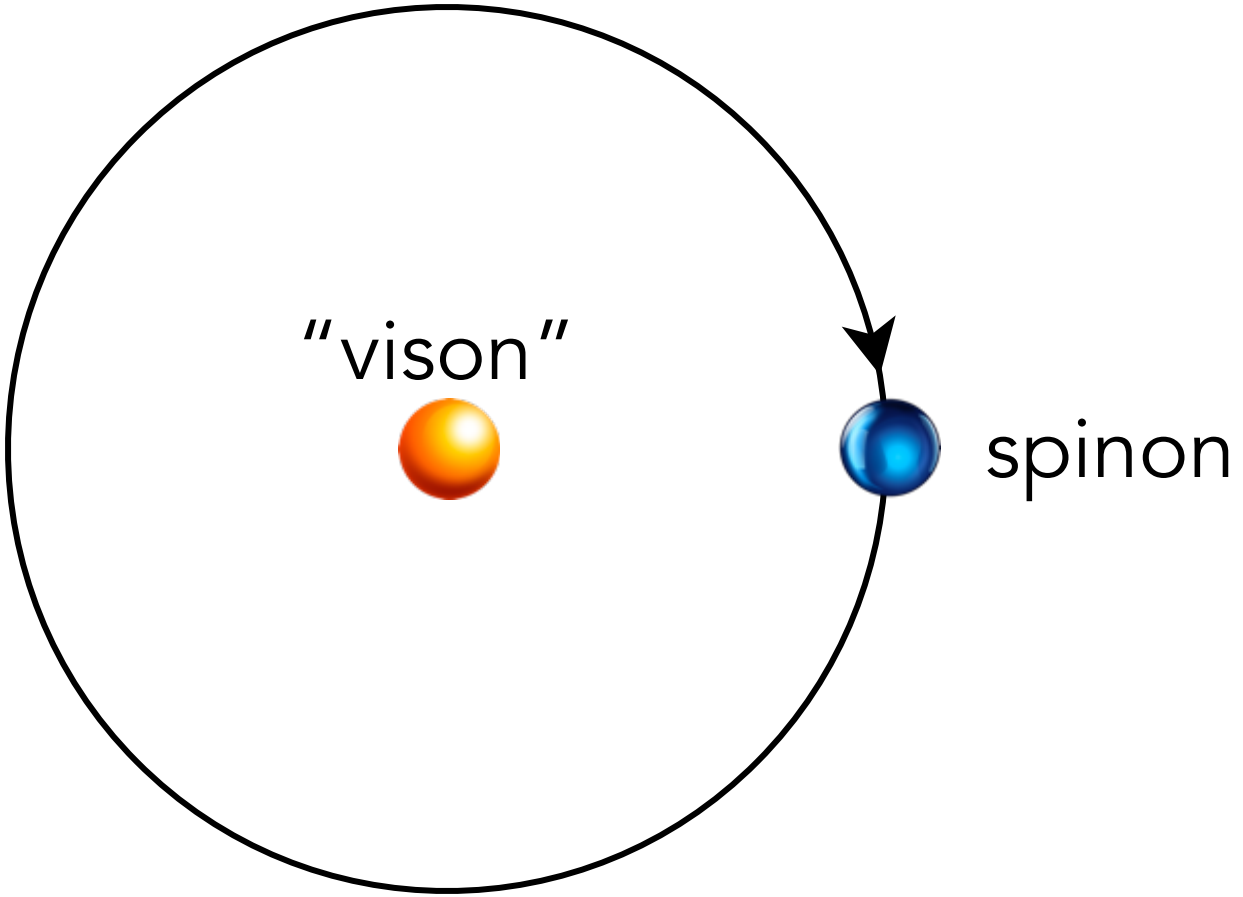


excitation with $\Delta S = 1/2$
not possible for any finite
cluster of spins

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

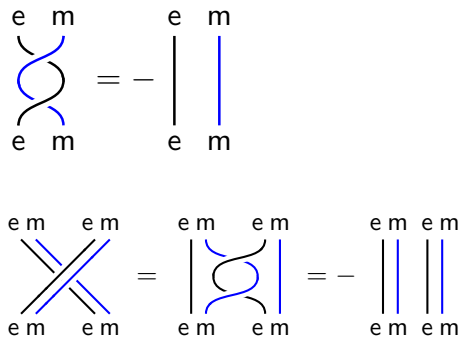
A. Kitaev

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

Warning: this is a different meaning of topological!

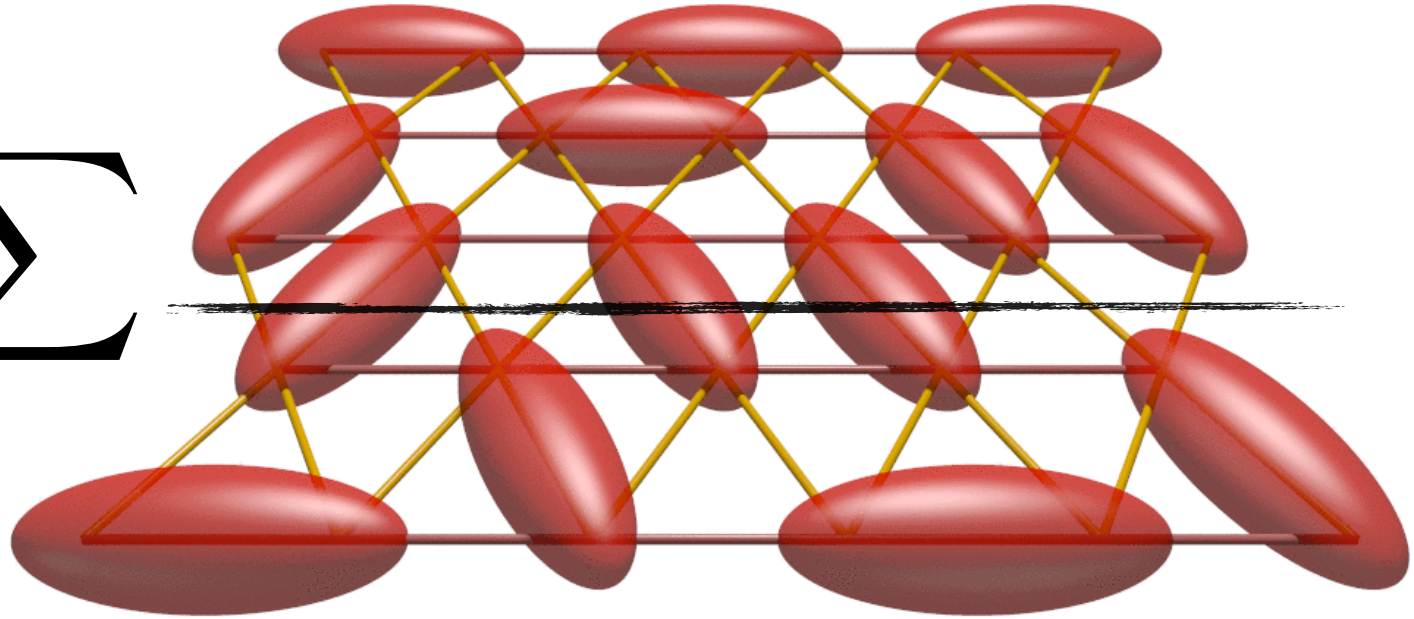
Anderson's RVB state is thus an
nple of a "topological phase" - the
best understood sort of QSL

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

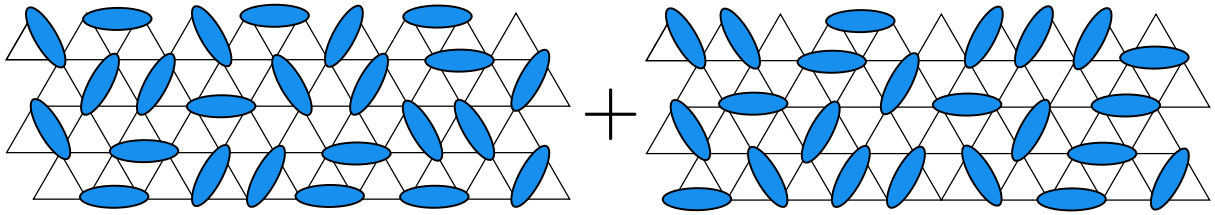
B) Apply a small magnetic field

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

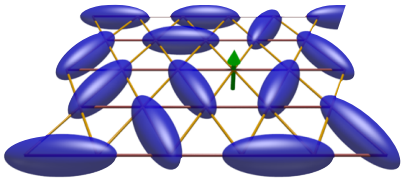
Ψ =  +...

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.

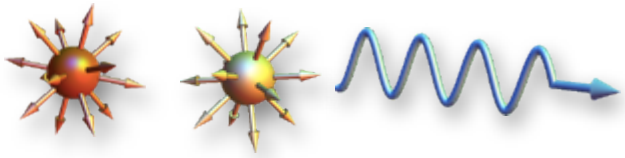
Varieties of QSLs

- Topological QSLs



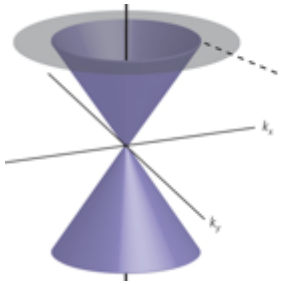
anyonic spinons

- U(1) QSL



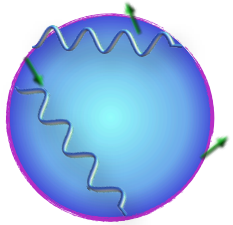
electric+magnetic monopoles, photon

- Dirac QSLs



strongly interacting Dirac fermions

- Spinon Fermi surface

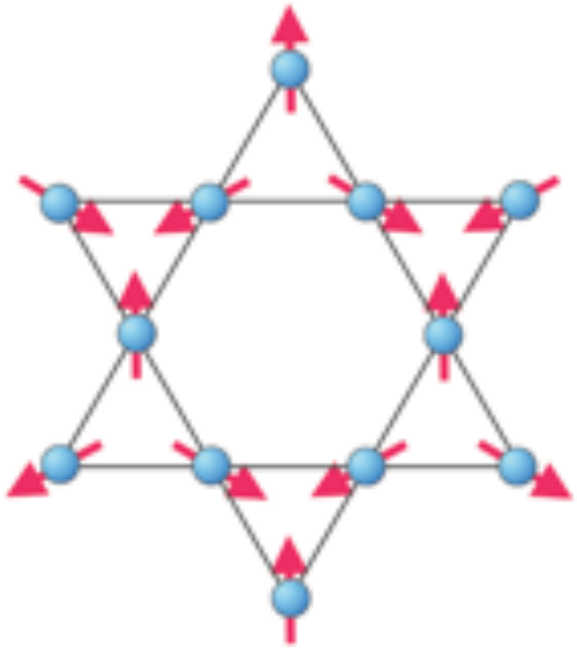


non-Fermi liquid “spin metal”

QSL experiments

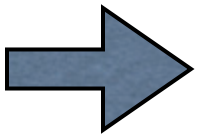
- This is a difficult subject, if you want a challenge!
- Discuss three examples:
  - Kagomé lattice herbertsmithite
  - Organic triangular lattice
  - alpha-$RuCl_3$ Kitaev magnet

Kagomé antiferromagnet



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

Very large classical degeneracy

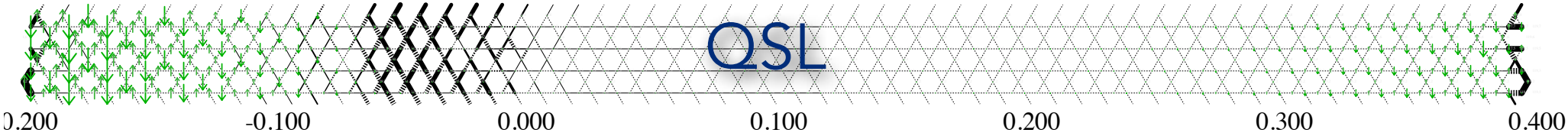


likely to be a QSL

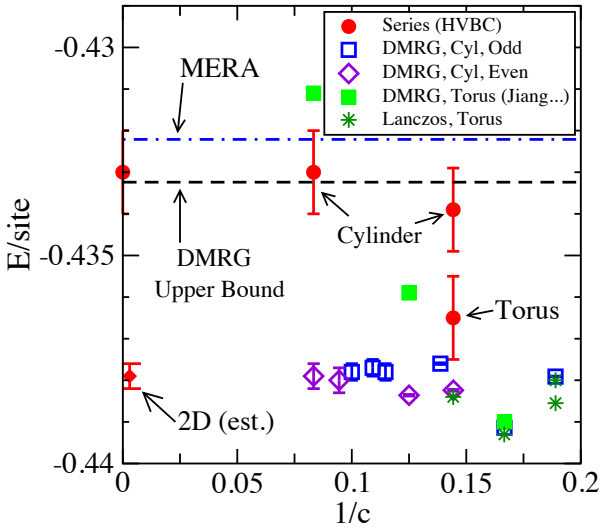
V. Elser, 1989 + many many others

S=1/2 kagomé AF

- Rather definitive evidence for QSL by DMRG



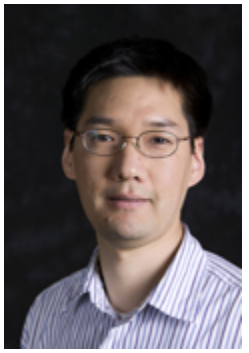
© Steve White



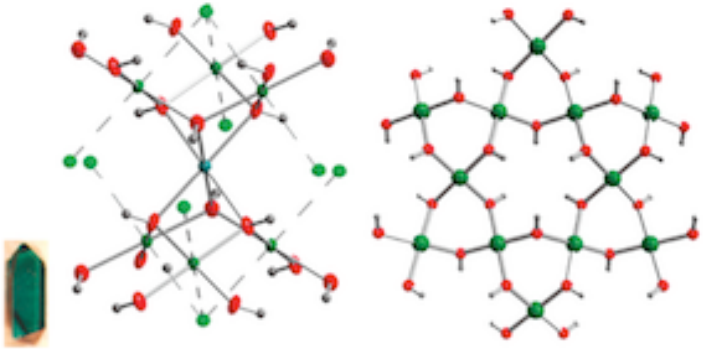
S. Yan *et al*, 2010

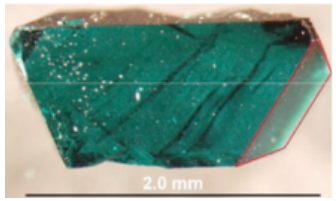
many other studies support existence of some QSL phase

Herbertsmithite



$ZnCu_3(OH)_6Cl_2$

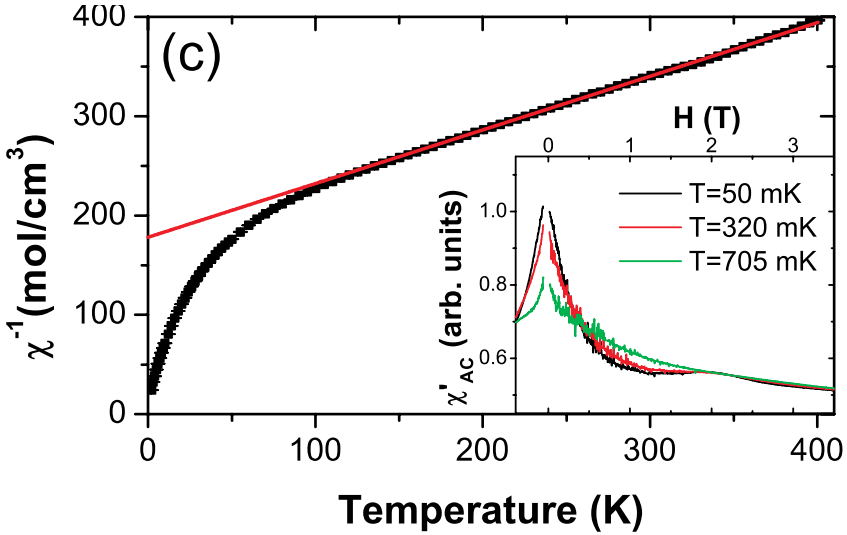




kagomé layers of Cu
S=1/2 spins, separated
by non-magnetic Zn

Heisenberg-like
with J ~ 200K

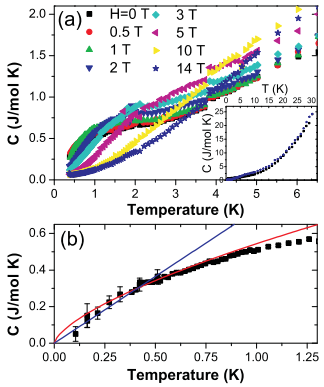
no order down to
50mK



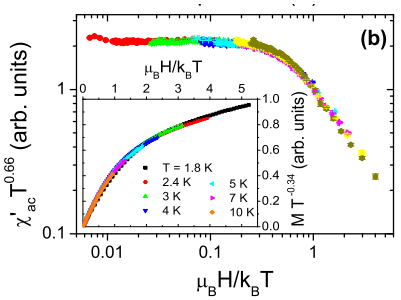
Helton *et al*, 2007

Herbertsmithite

Lots of early evidence for gaplessness



Helton *et al*, *2007*

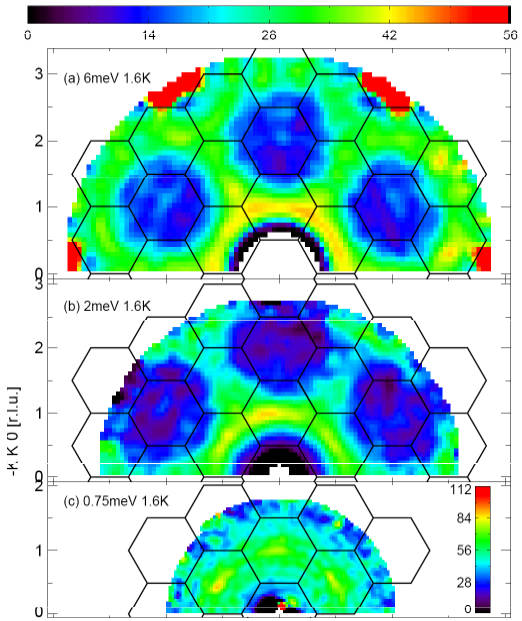


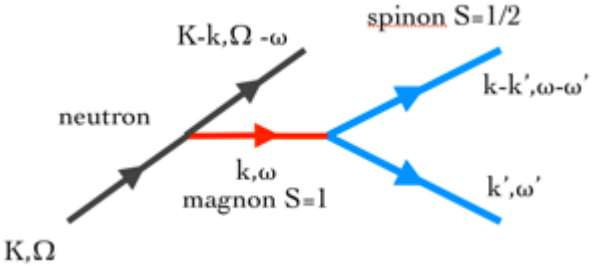
Helton *et al*, *2010*

Single crystal INS

smooth continuum scattering

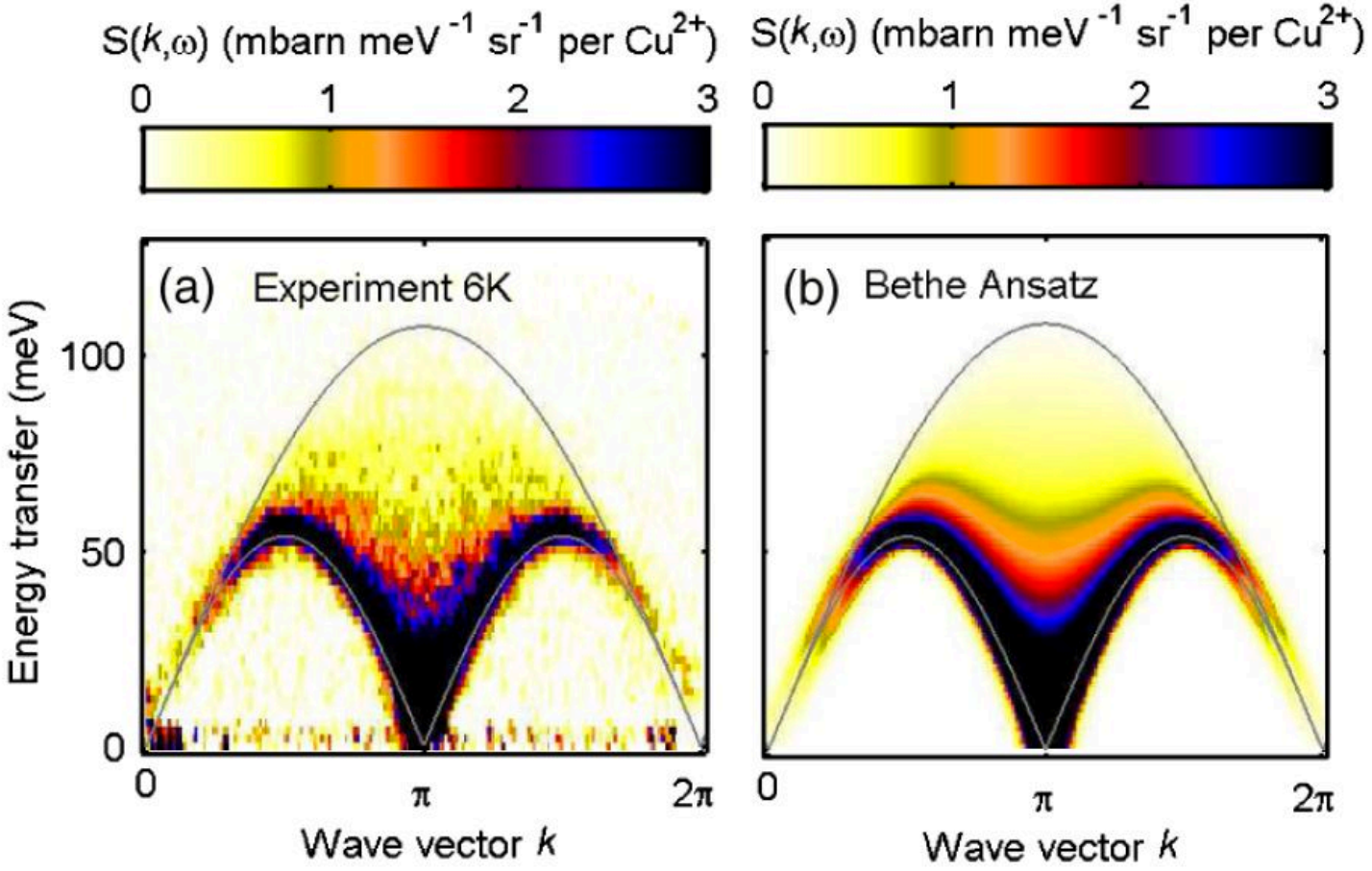
T-H Han *et al*, 2012





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

For comparison: 1d spinons

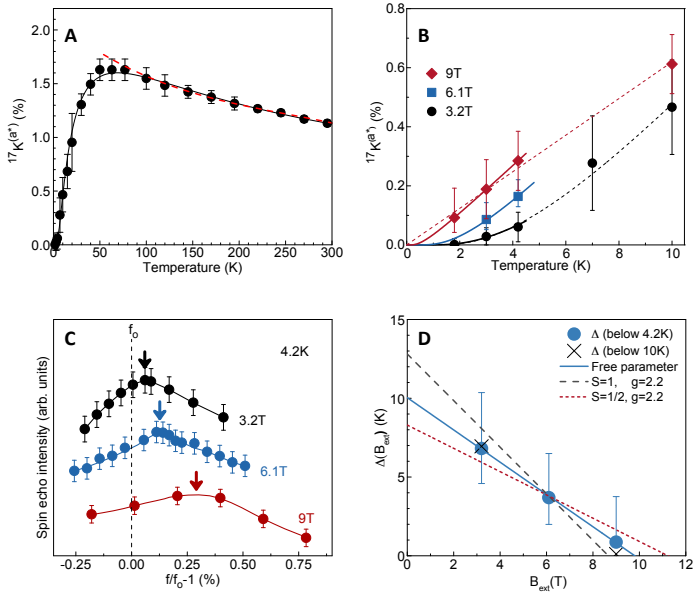


$KCuF_3$ - B. Lake *et al*, 2013

Herbertsmithite

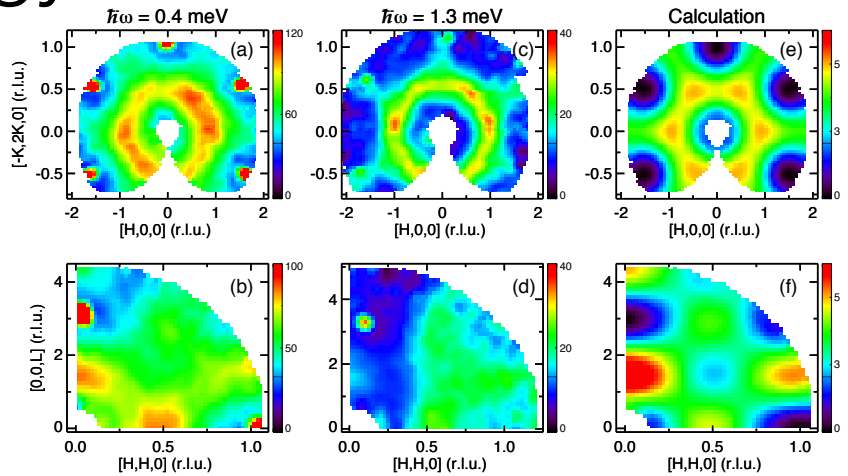
Single crystal NMR

M. Fu *et al*, 2015



estimate gap ~ 10K

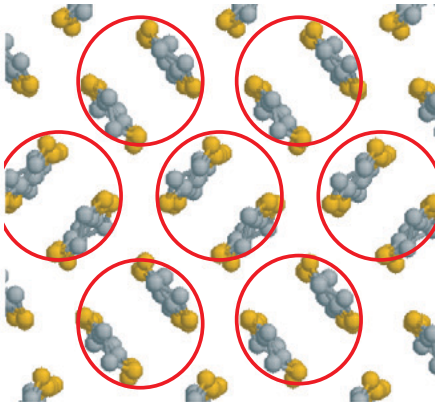
Low energy INS



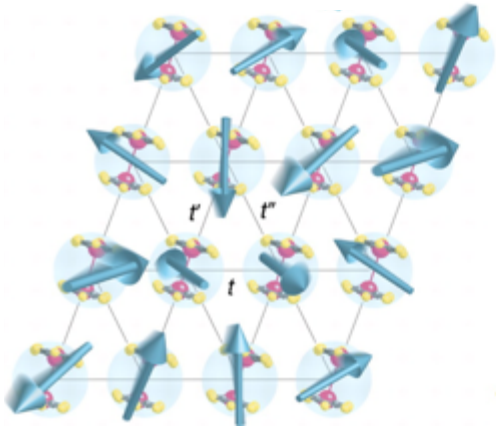
T-H Han *et al*, 2015

claim to separate impurity signal below 0.7meV

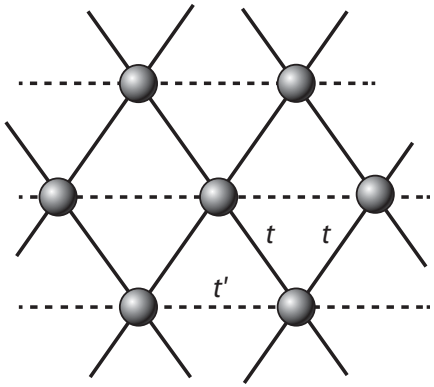
Organics



κ-$(ET)_2X$

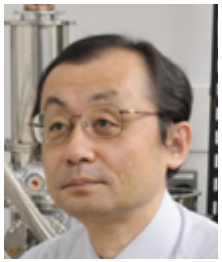


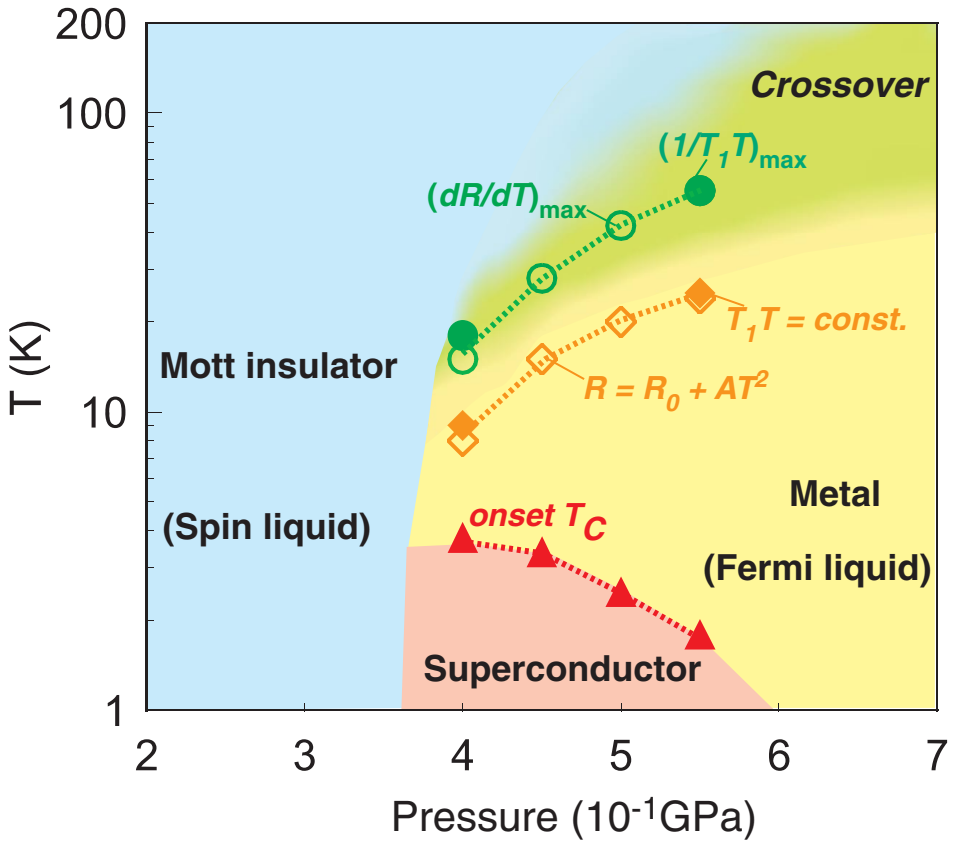
β′-$Pd(dmit)_2$

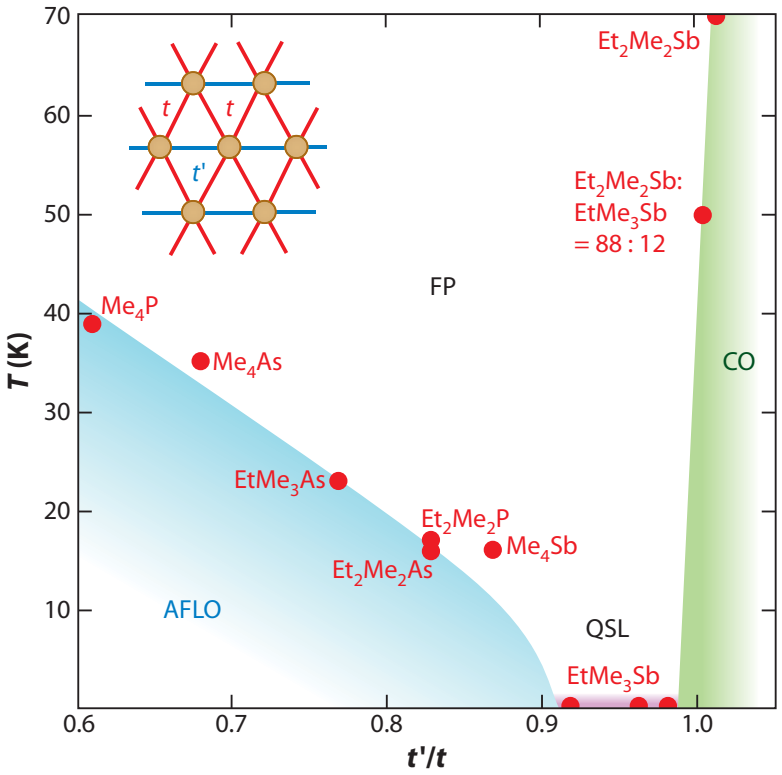


- Molecular materials which behave as effective triangular lattice S=1/2 antiferromagnets with J ~ 250K
- significant charge fluctuations

Organics







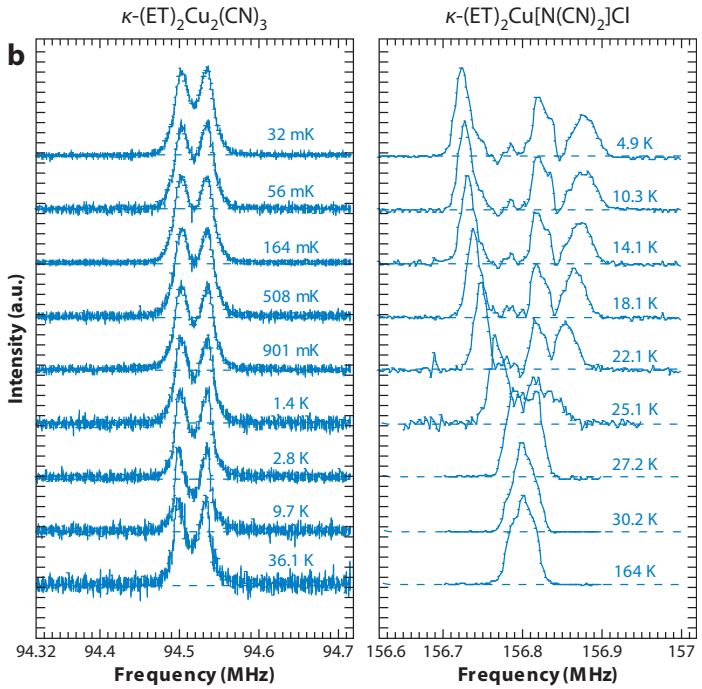
κ-$(ET)_2Cu_2(CN)_3$

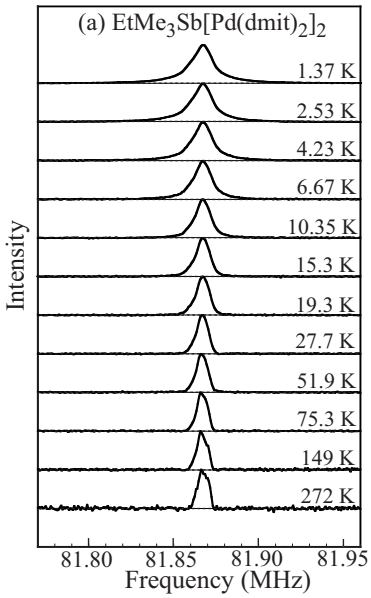
K. Kanoda group (2003-)

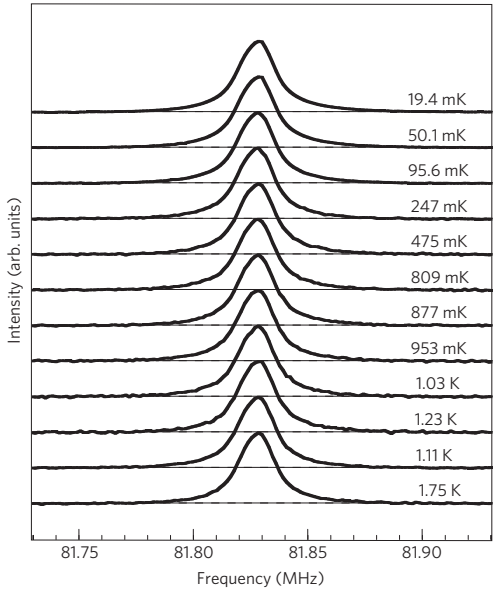
β′-$Pd(dmit)_2$

R. Kato group (2008-)

NMR lineshapes







κ-$(ET)_2Cu_2(CN)_3$

Y. Shimizu *et al*, 2003 ^{1}H NMR

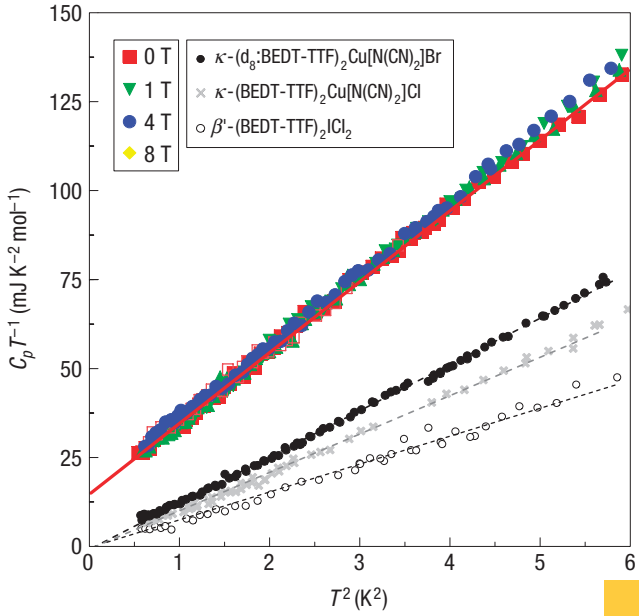
β′-$Pd(dmit)_2$

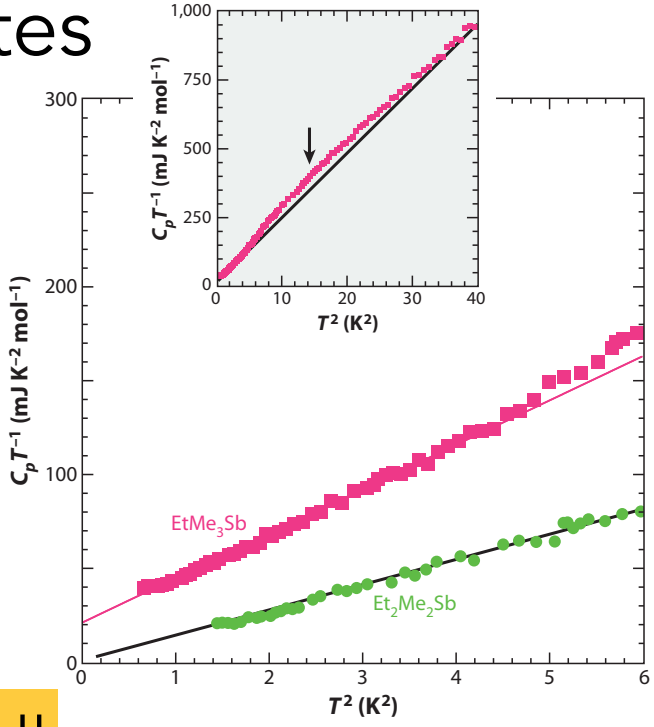
T. Itou *et al*, 2008,2010 ^{13}Cs NMR

Evidence for lack of static moments: f > 1000!

Specific Heat

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





γ_{Cu} ~ 0.7 !!

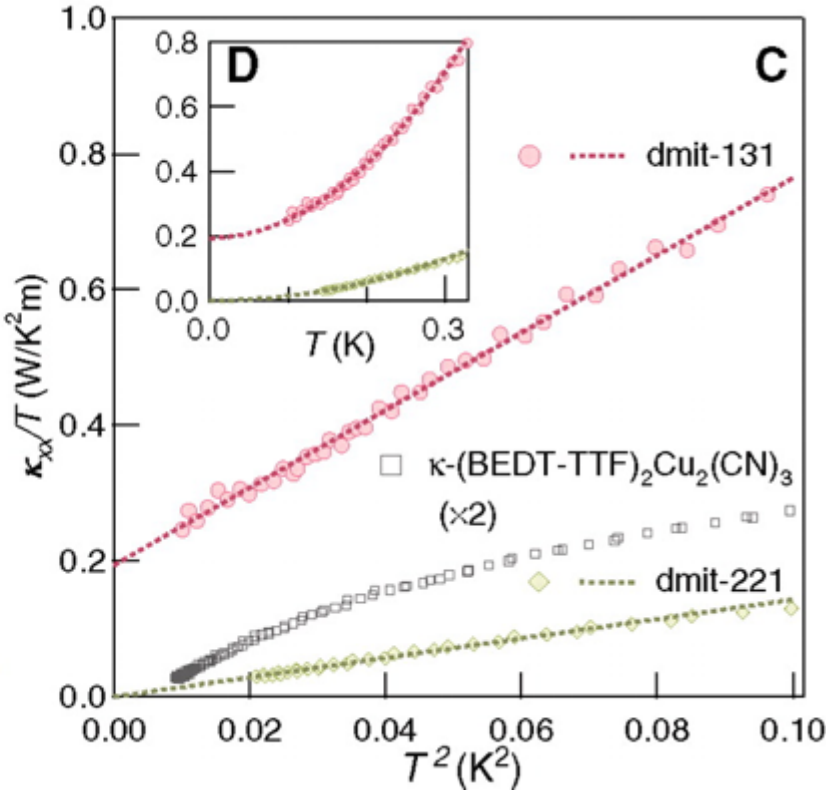
κ-$(ET)_2Cu_2(CN)_3$

β′-$Pd(dmit)_2$

S. Yamashita *et al*, 2008

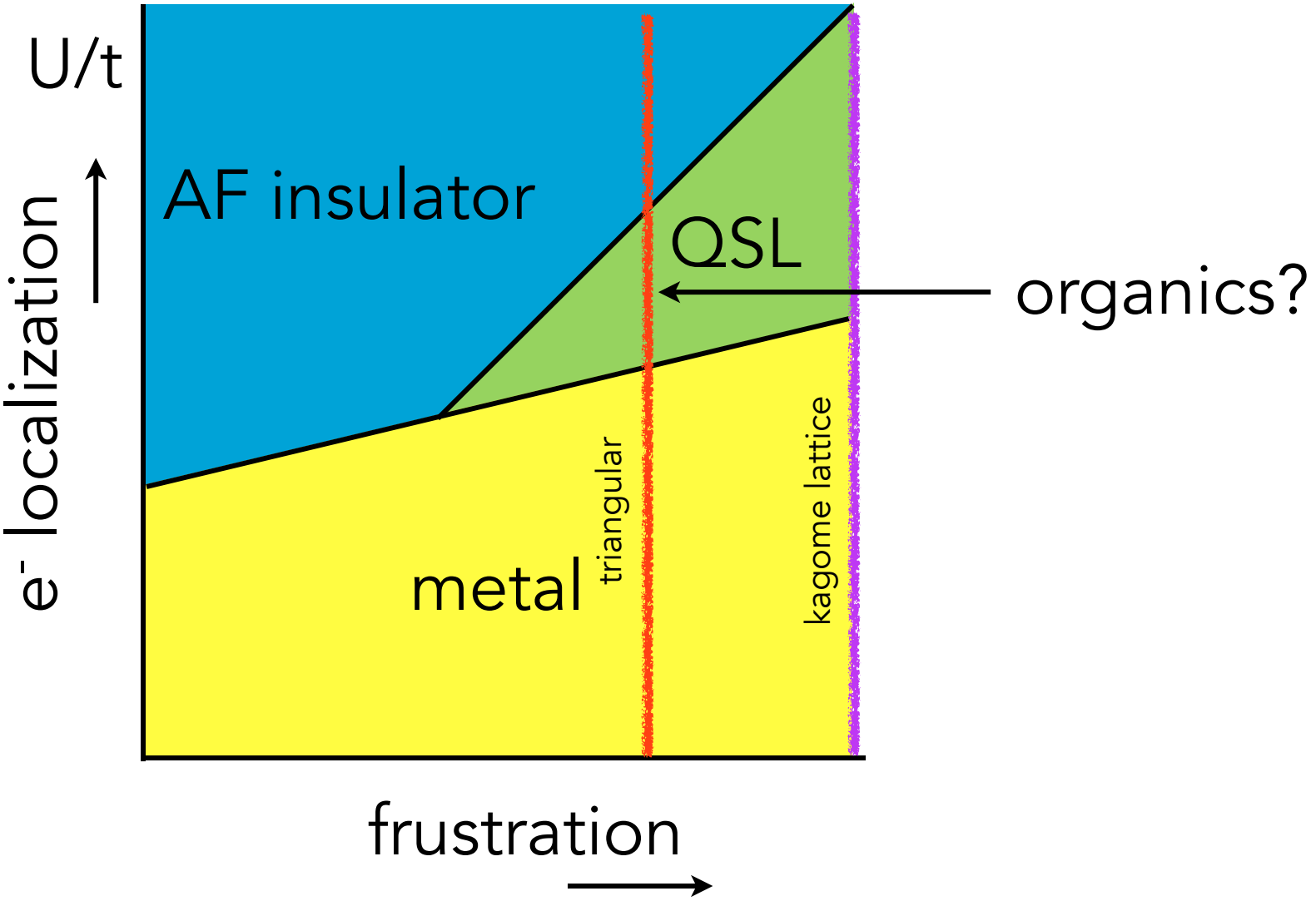
Thermal conductivity

- 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 $l \sim 1$ μm ≈1000 a !



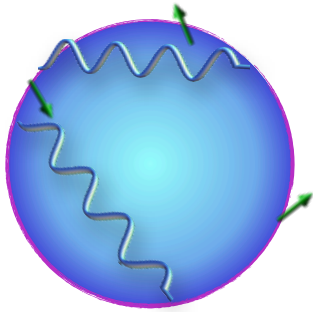
M. Yamashita *et al*, 2010

Charge fluctuations



Organics - Theory

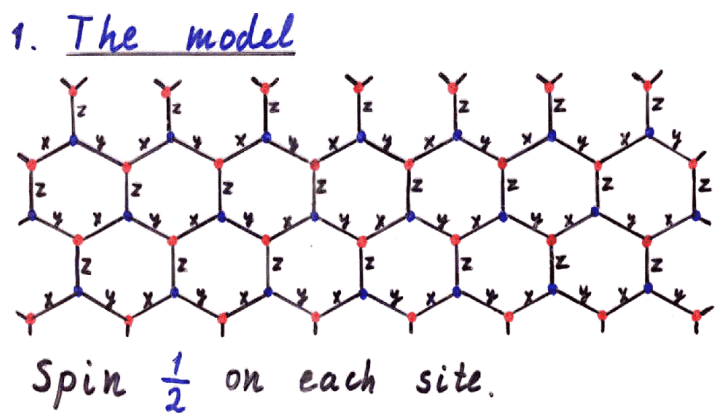
- RVB/QSL state:
  - Motrunich, Lee+Lee: (2005) "uniform RVB"
  - It is described by a **"Fermi sea" of spinons** coupled to a U(1) gauge field
- The anomalous thermal conductivity may be a window into an emergent fermi surface in an insulator!

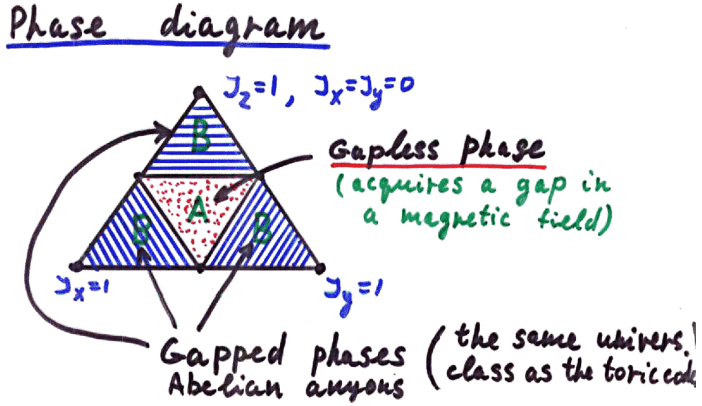


Kitaev model

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

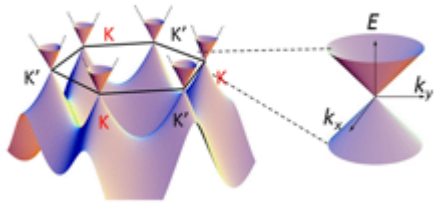
KITP, 2003





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

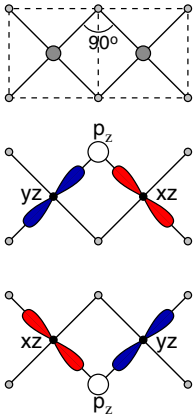
physical Majoranas $H_{\rm m} = K \sum_{\langle ij \rangle} i c_i c_j$

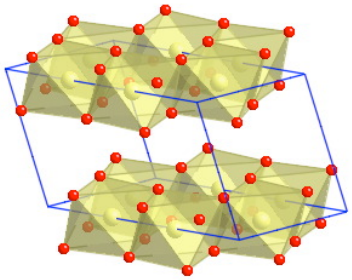


Kitaev Materials

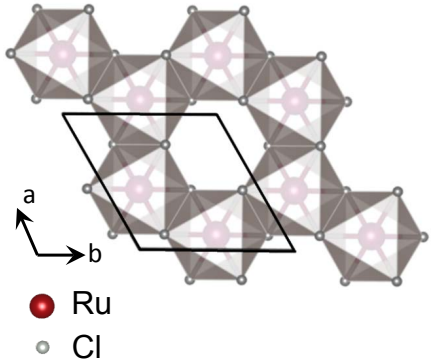
Jackeli, Khaliullin 2009

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



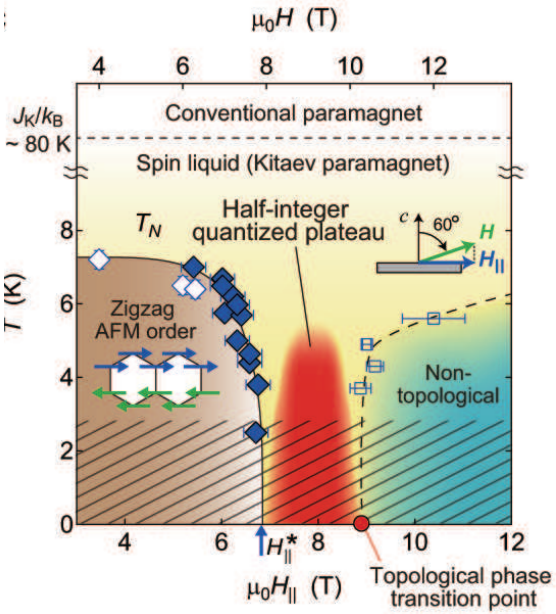
α-$RuCl_3$

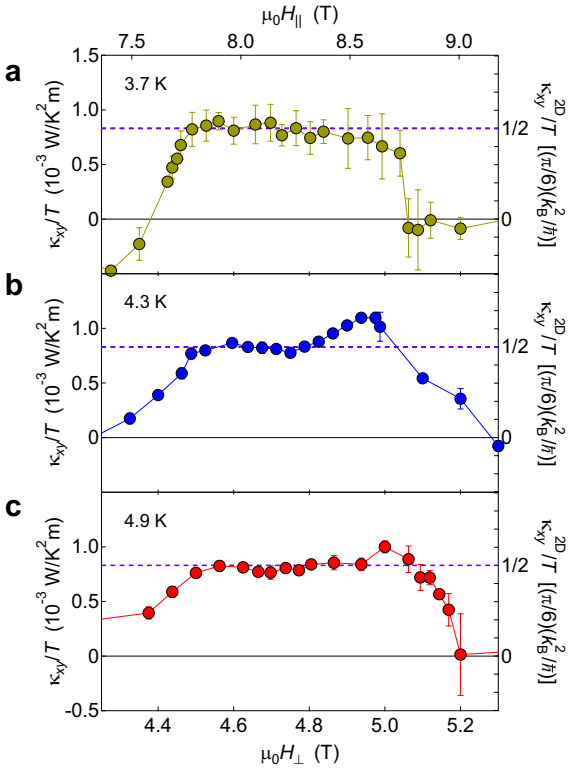
Y.-J. Kim...

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?

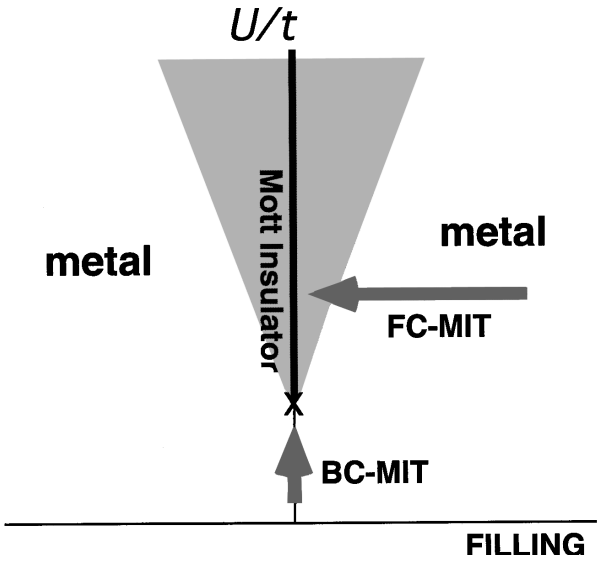
Correlation

- 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

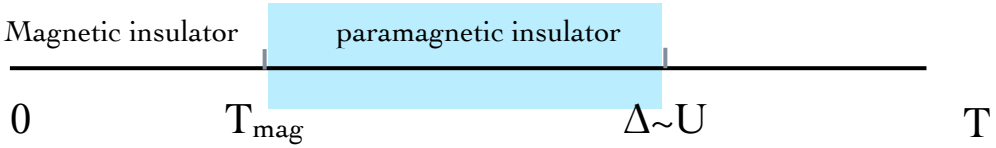
- Hubbard model

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



Imada, Fujimori, Tokura 1998

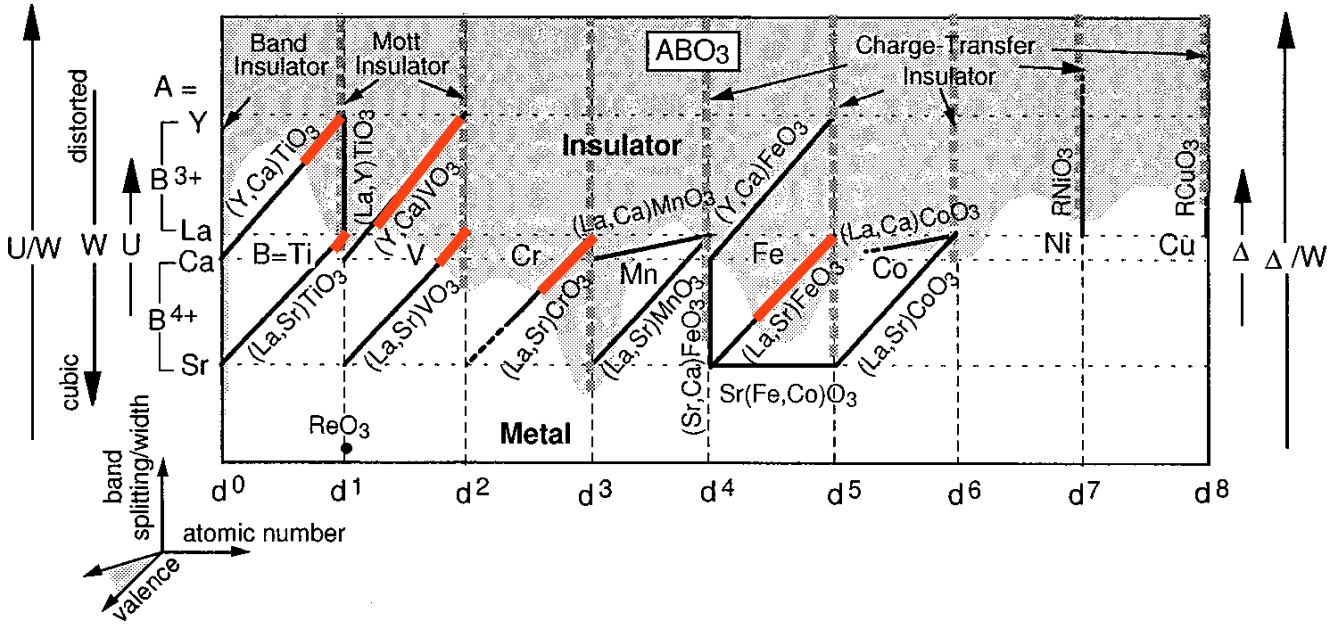
- Physically, a Mott Insulator is one which is insulating due to interaction-induced localization, not due to band physics
  - This is a question of energy scales
  - Deep in the Mott state:



Mott Transition

- And old subject

e.g. perovskites



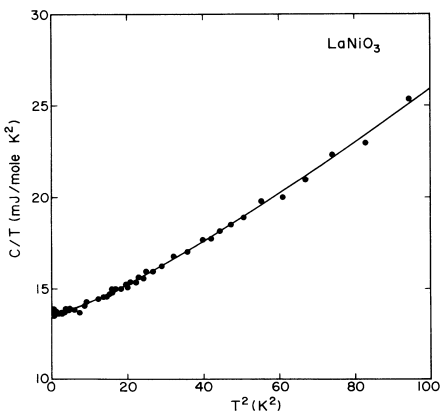
- But still a key theme, and now more accessible in new materials, via new approaches

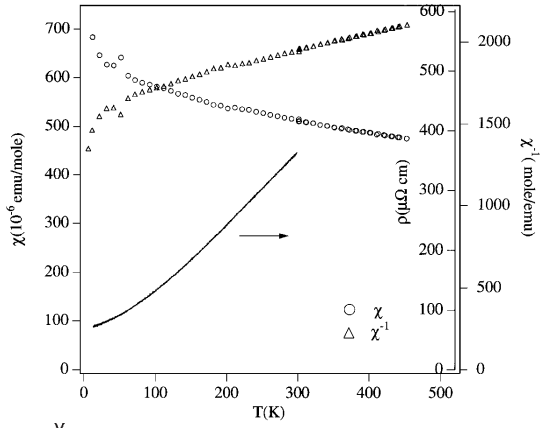
Heavy Electrons

- Mass enhancement near Mott transition

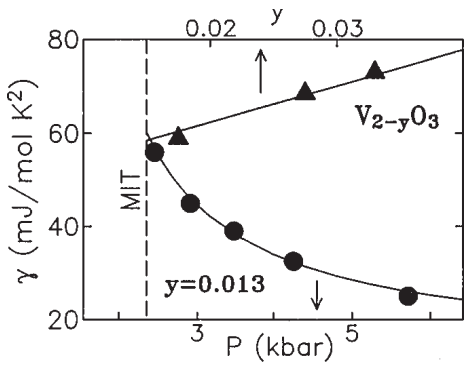
$LaNiO_3$:

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





V_2O_3



Heavy Fermions

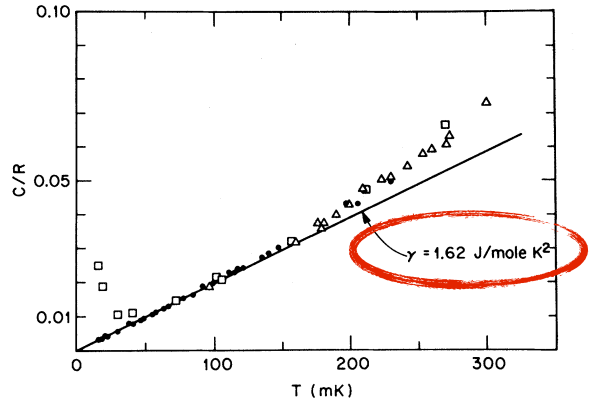


FIG. 1. Specific heat of $CeAl_3$ at very low temperatures in zero field (●, Δ) and in 10 kOe (□).

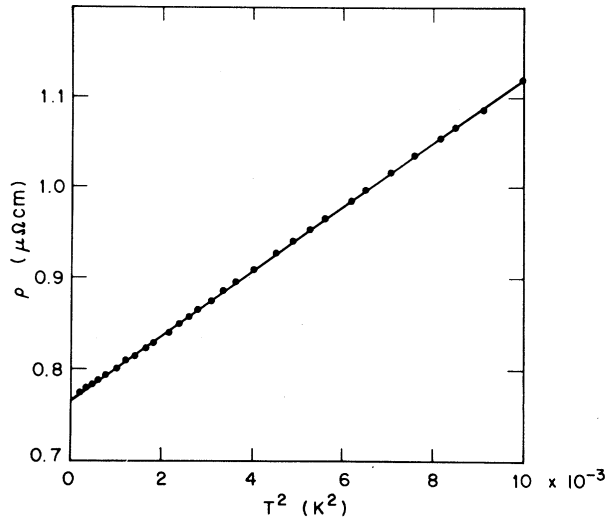


FIG. 3. Electrical resistivity of $CeAl_3$ below 100 mK, plotted against T^2.

$$C \sim \gamma T$$

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

Both γ and A **huge**

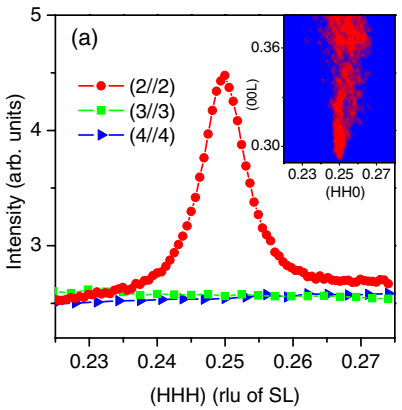
Behave like Fermi liquid with tiny E_F and large electron mass, but only for $T \ll E_F$

Common in "Kondo lattice" materials

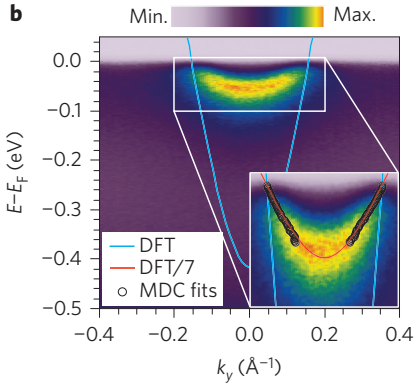
Oxide heterostructures

- New handle on Mott materials from oxide MBE

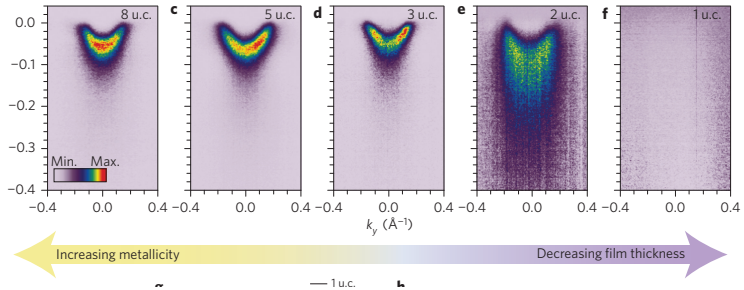
example: $LaNiO_3$ - just on the metallic side of Mott transition <u>in bulk</u>



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



Large mass in 8uc thick films

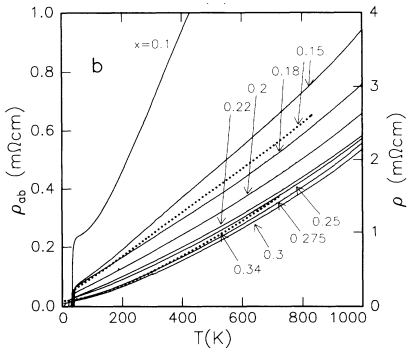


Metal-insulator transition at 2uc thickness

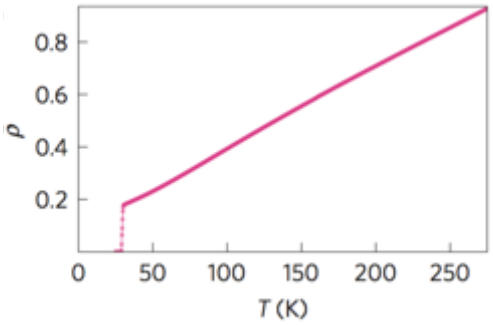
King *et al*, 2014 [Schlom,Shen]

Non-Fermi Liquids

"strange metal"



LSCO Takagi *et al, 1992*



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

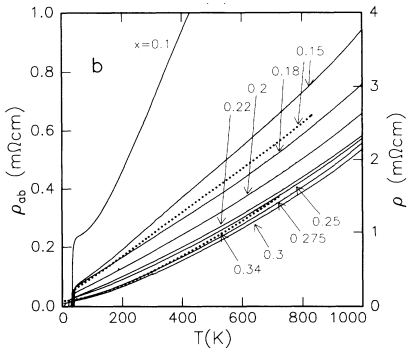
$$\frac{1}{\tau} \sim T \, ?$$

T-linear resistivity/scattering rate:

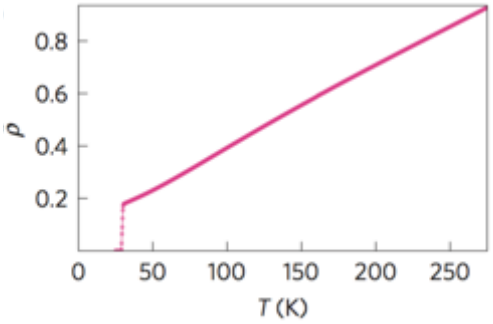
- Many materials
- Often nearby to unconventional superconductivity
- Symptom of a different type of metal? Or of a quantum critical point?

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?

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

self-energy

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

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

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

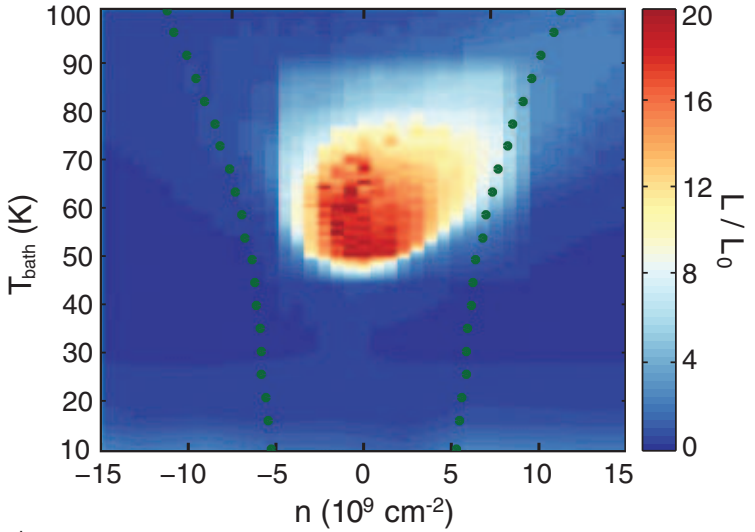
C) Dynamical mean field theory

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*



nple.

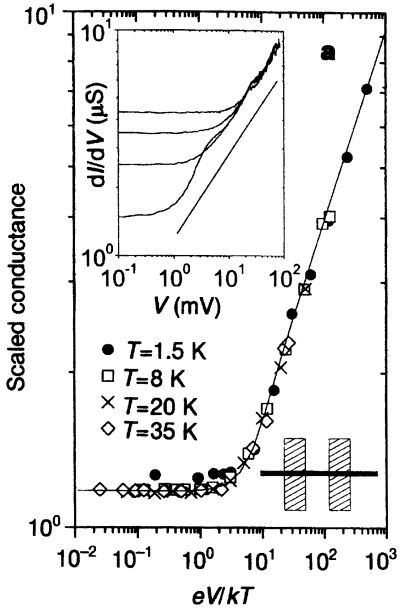
Crossno *et al*, 2016

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

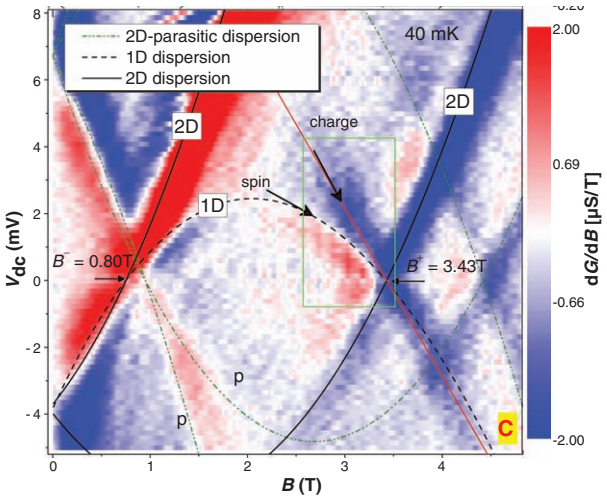
Luttinger liquids

- 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



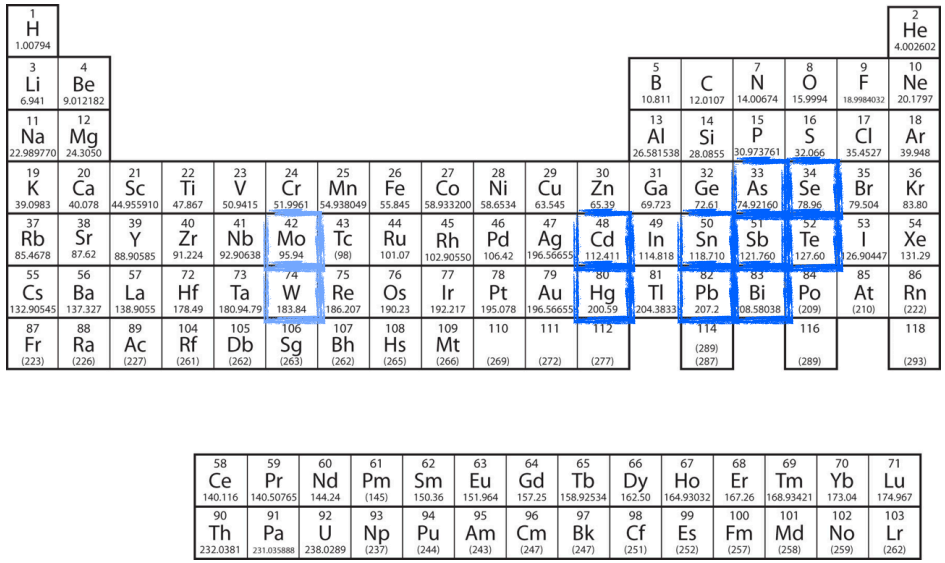
Bockrath *et al*, *nanotubes, 98*



Jompol *et al*, GaAs quantum wires, 2009

QM Materials

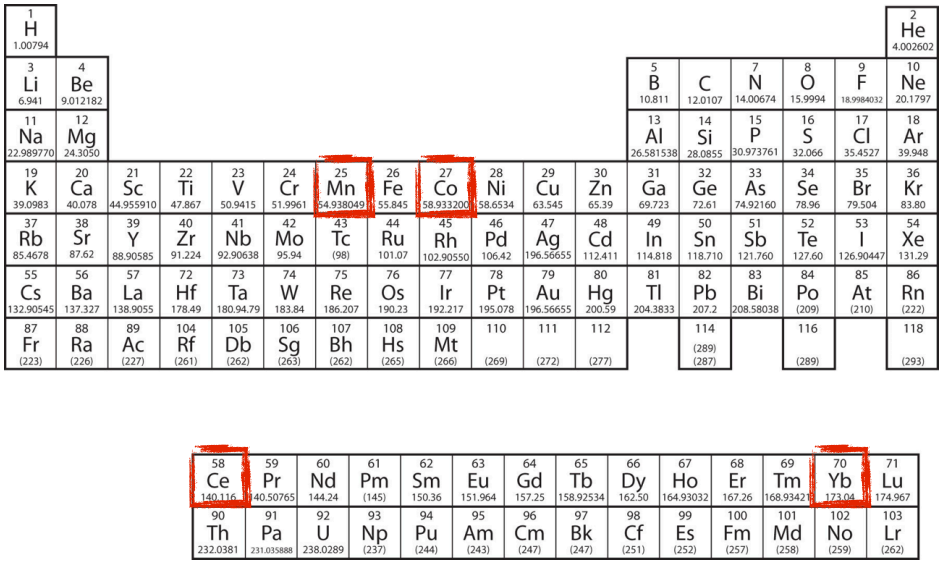
- Topological materials
  - HgTe, Bi_2Se_3, Bi_2Te_3,Sb_2Te_3, TaAs, Cd_2Se_3, WTe_2, $MoTe_2$



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

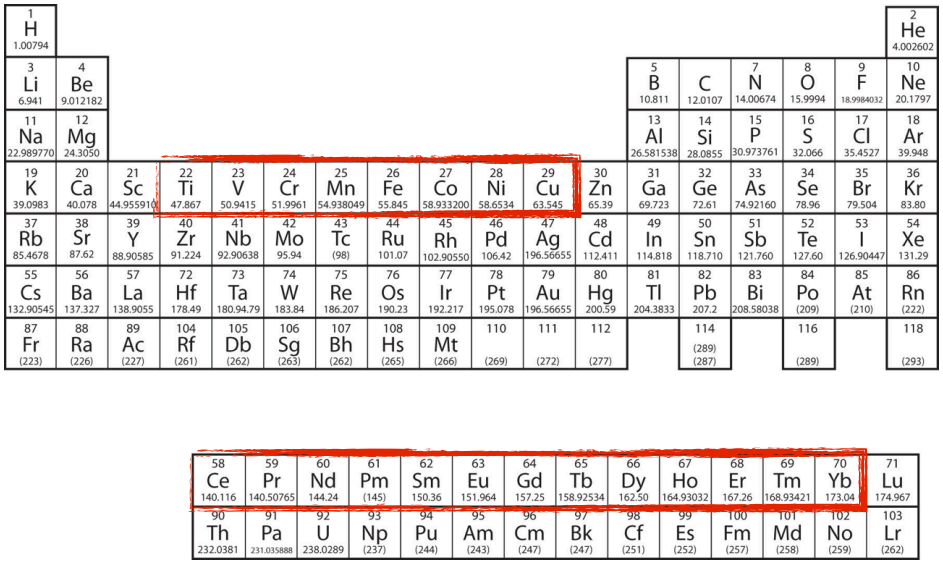


New ingredients in recent materials: partially filled 3d and 4f orbitals: correlations!

Specifically these ions host local moments

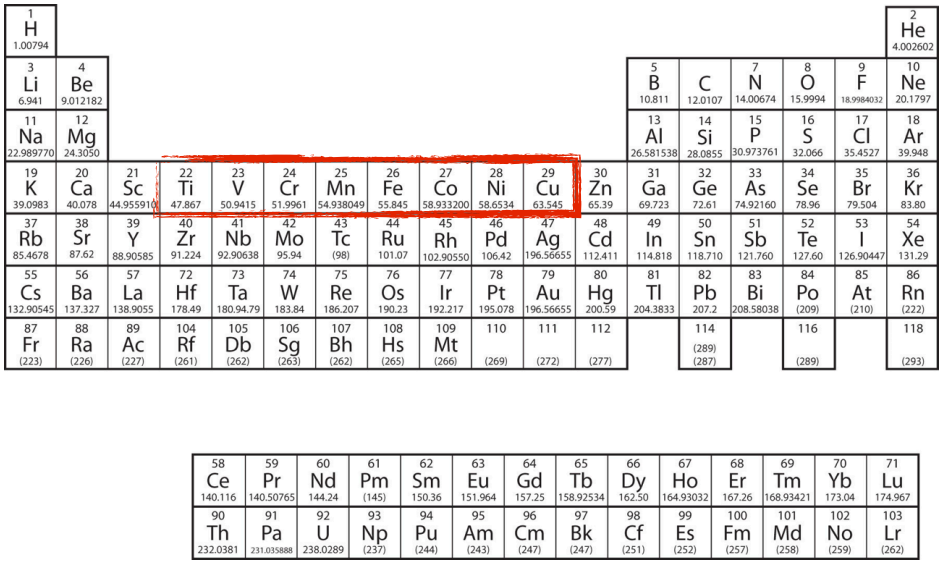
Local moments

- 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.



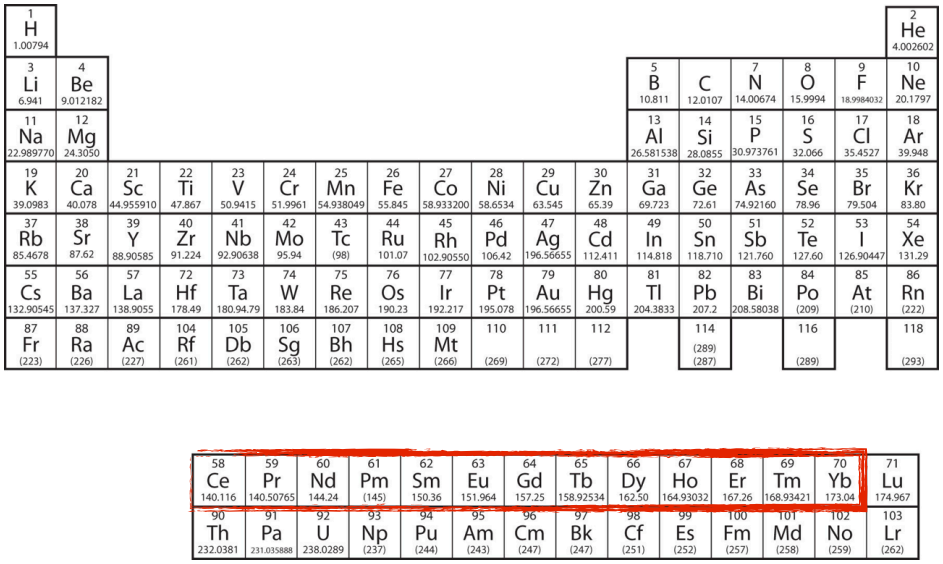
Local moments

- 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).



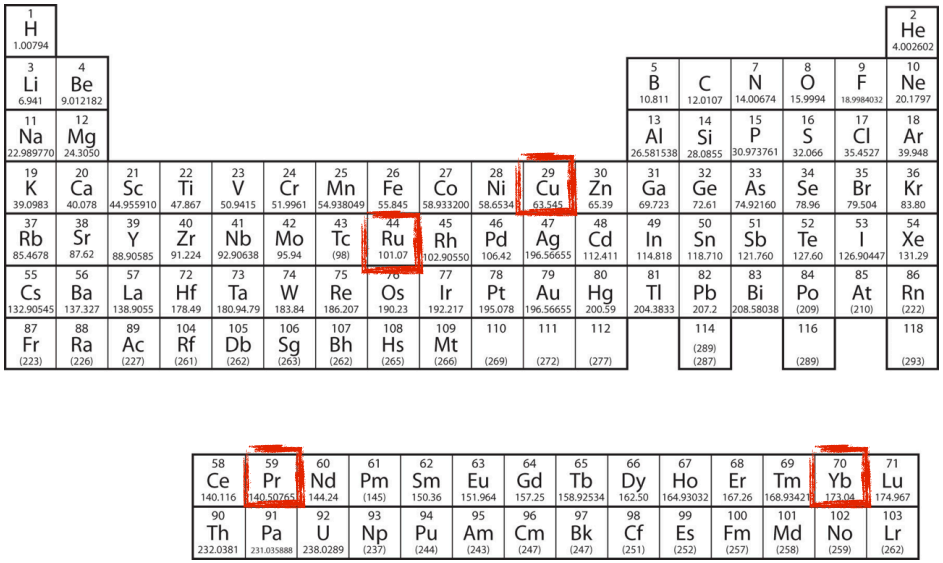
Local moments

- 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.



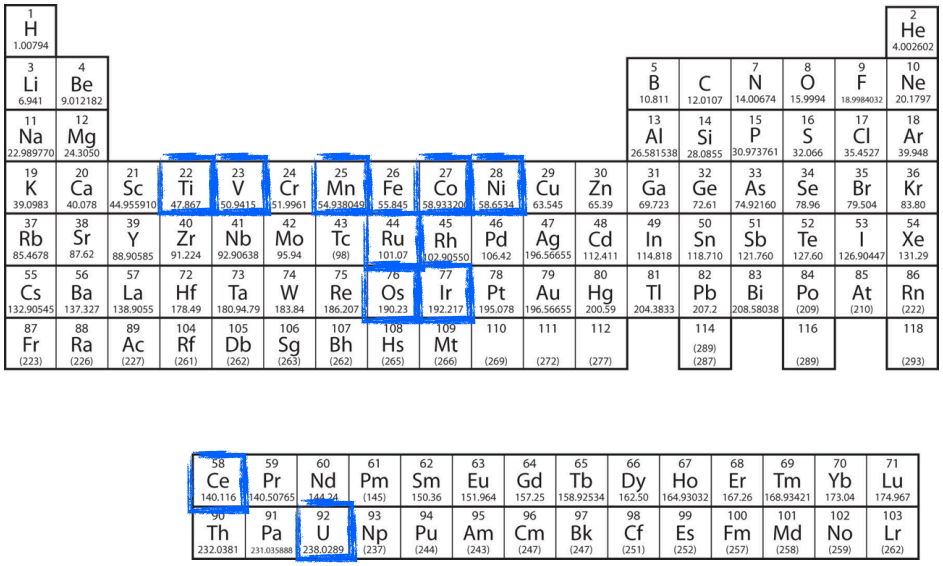
QM Materials

- 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

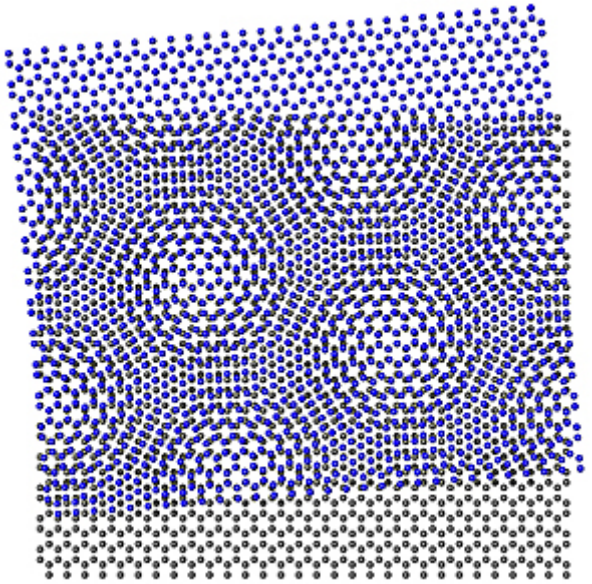
- Correlated metals/ Mott transitions
  - $RTiO_3$,RVO_3,$RNiO_3$, $RMnO_3$,$RCoO_3$,...
  - $Cd_2Os_2O_7$,$Nd_2Ir_2O_7$, Sr_2IrO_4,Sr_2RuO_4,..
  - URu_2Si_2,$CeAl_3$,....

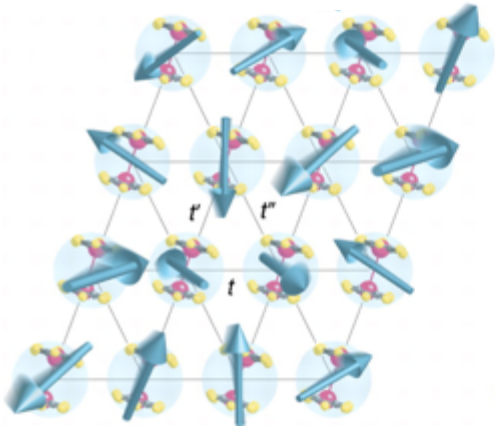


transition metals and rare earths mostly.

QM Materials

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





Thanks