Correlation physics from a condensed matter perspective: menu and amuse-bouche

Leon Balents, KITP

serious lecture next week by Cenke Xu

Local resources

How exotic?

1 5 7 8 9 10

(self rated)

Local resources

How exotic?

1 5 7 8 9 10

viewed from outside UCSB

Local resources

How exotic?

1 5 7 8 9 10

viewed from outside UCSB

Today's agenda

- Get to know each other:
  - Offer up a menu of potentially interesting topics to discuss later
  - I will try to offer topics which seem most likely to be fruitful topics to explore
- Apologies if I am ignorant or naive, especially about the cold atom community

Chez KITP

Menu

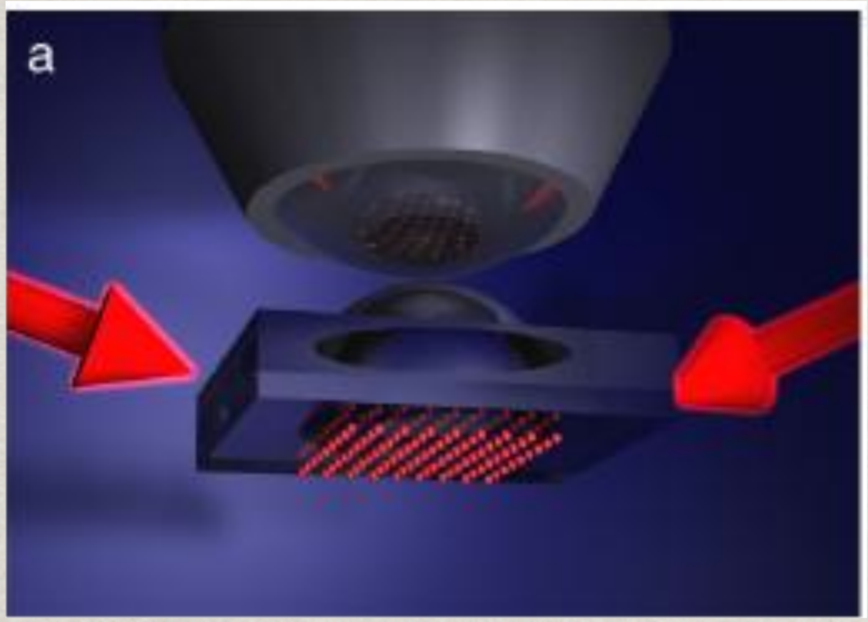
Specials

- High-T_c
- Quantum Spin Liquids
- Mott Transitions
- Spin-Orbit Physics

Classics

- Frustrated Magnetism
- Quantum Criticality

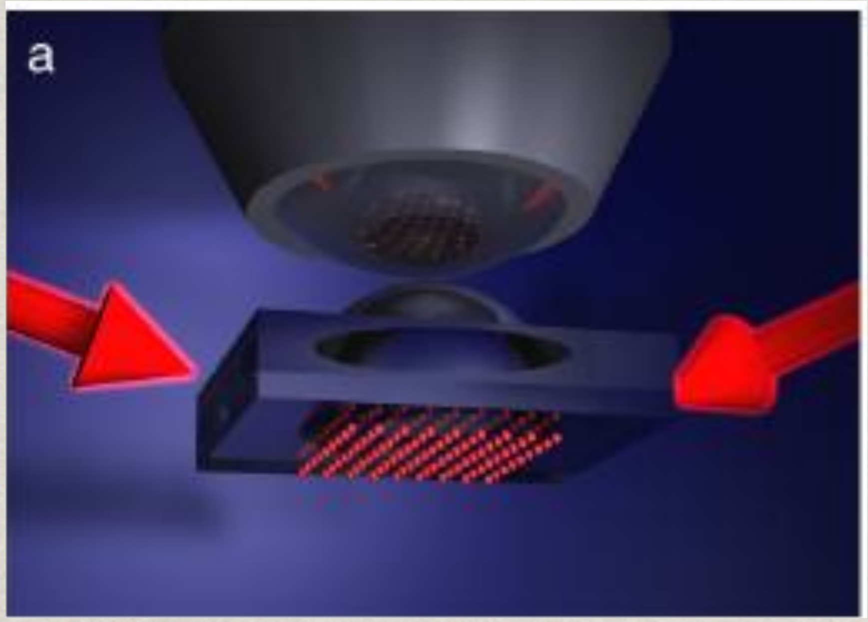
Simulations



quantum

classical

Simulations



quantum

classical

Anything is possible - so what is really interesting?

Motivations in CMT

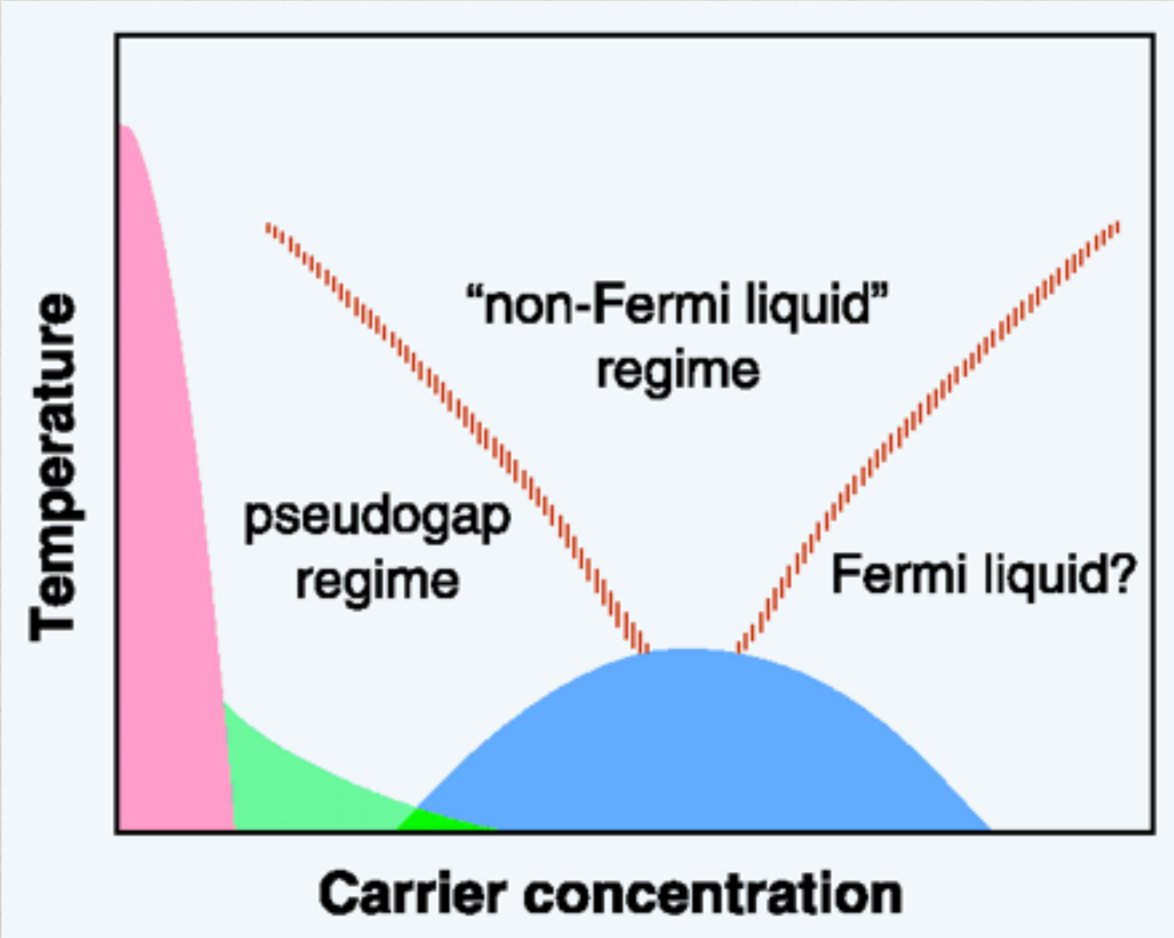
- Understand materials
- Applications
- Expand the boundaries of fundamental theory
  - emergent phenomena - phases, correlations, excitations, topology
  - mechanisms - e.g. of high-T_c, etc.

Topics

- High-T_c - and beyond?
- Quantum spin liquids
- Mott transitions
- Spin orbit physics

High T_c

- "Unsolved" almost 25 years, cuprate superconductivity is probably still considered the most greatest challenge in CMP



High T_c - Questions

- What are the necessary features for high-T_c?
  - 2d?
  - proximity to Mott insulator?
  - antiferromagnetic fluctuations?
  - Single band?
  - Charge transfer material?
  - Is Hubbard model sufficient?

High T_c - Questions

- How do we understand the unusual features of the cuprates?
  - Is there an underlying QCP of importance?
  - What is the nature of the "strange metal"?
  - Is the pseudo-gap region a distinct phase?
  - Is inhomogeneity intrinsic and/or important?
  - Are there "exotic" excitations or phases present or nearby in the phase diagram?

Emulating High-T_c

- Simulate the (fermionic, s=1/2) Hubbard model
- DARPA - "The OLE program will construct an emulator—an artificial material whose behavior is governed by the same underlying mathematical description as the material of interest."

OLE

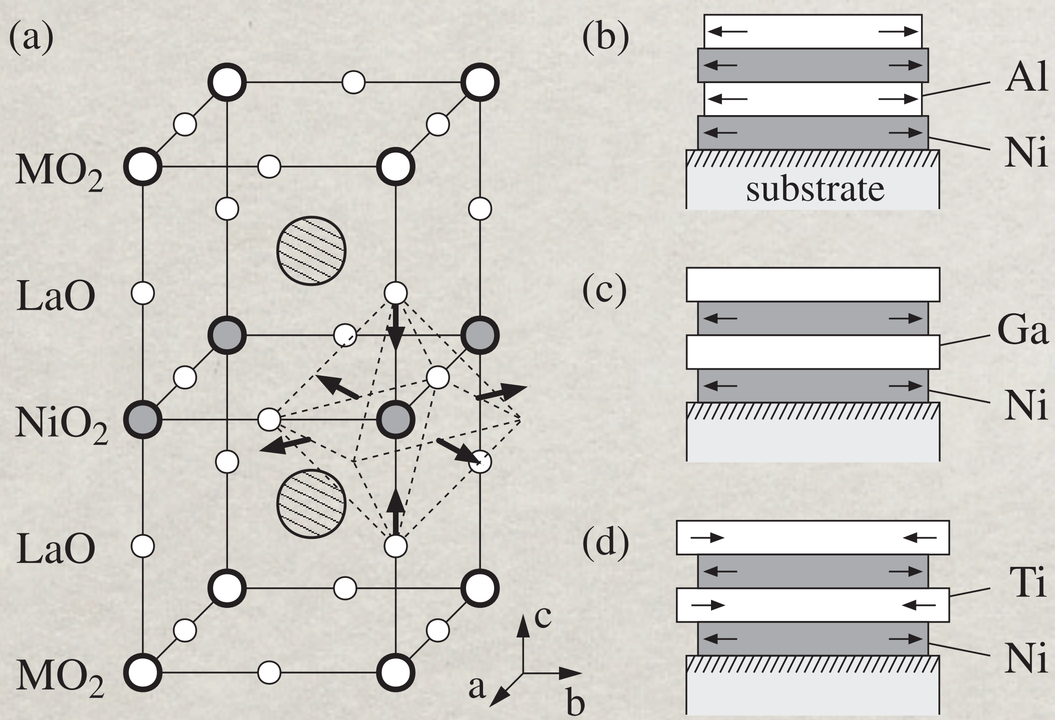
Emulating High T_c

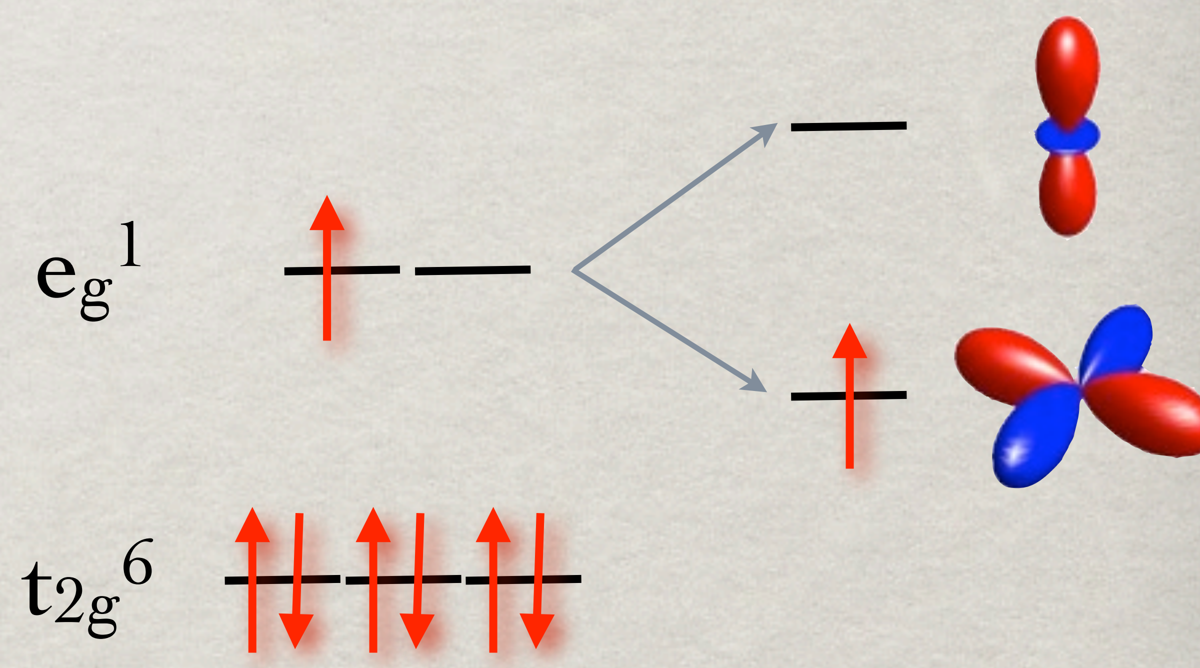
in condensed matter

- There are increasing efforts in condensed matter to grow "designer correlated materials" using layer-by-layer growth of transition metal oxides
  - "Mott interfaces", "Mott heterostructures", "oxide interfaces"
  - There are opportunities for quantum and classical simulation here, and inspiration for new models

Emulating High T_c

in condensed matter

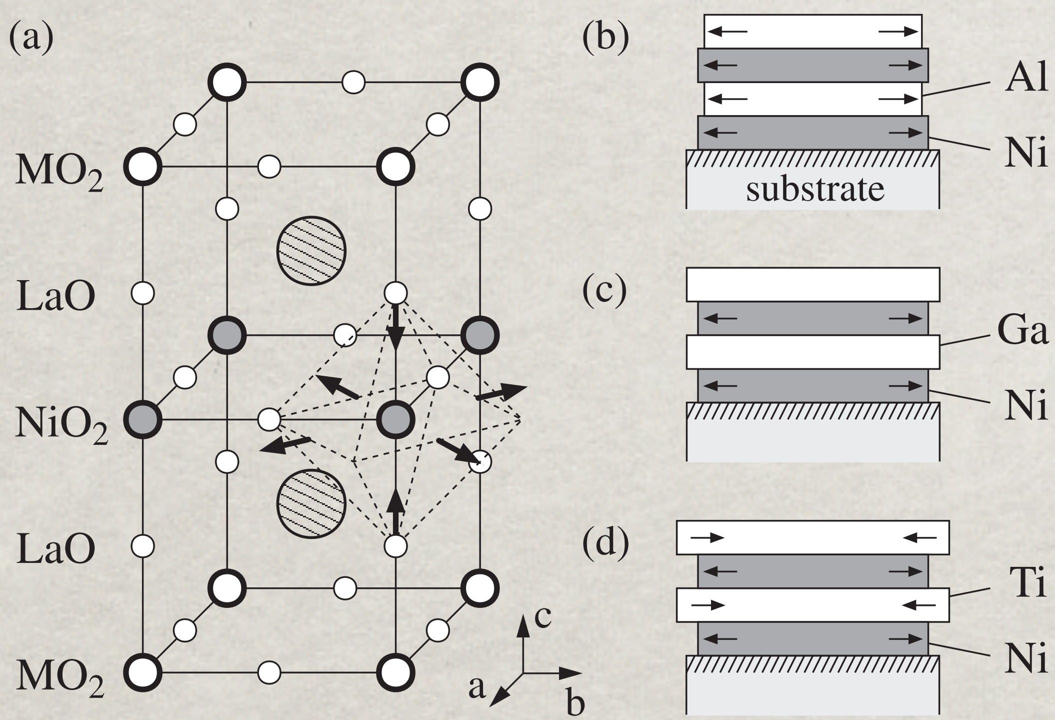




Chaloupka +
Khaliullin, 2008

Emulating High T_c

in condensed matter



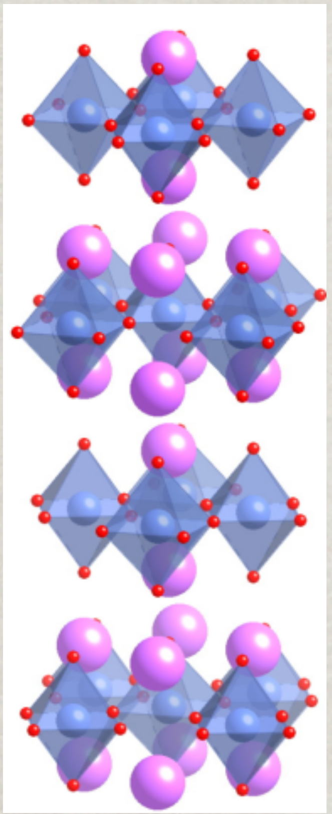
Chaloupka + Khaliullin, 2008

S. Stemmer, unpublished

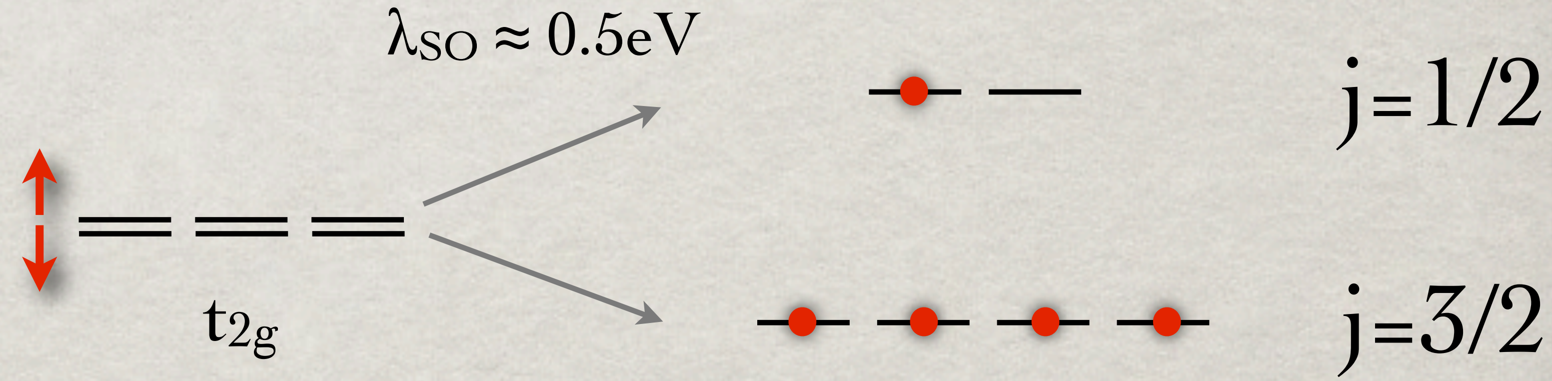
But this doesn't seem to work (so far!)

Emulating High T_c

in condensed matter



Ir^{4+}=$5d^5$

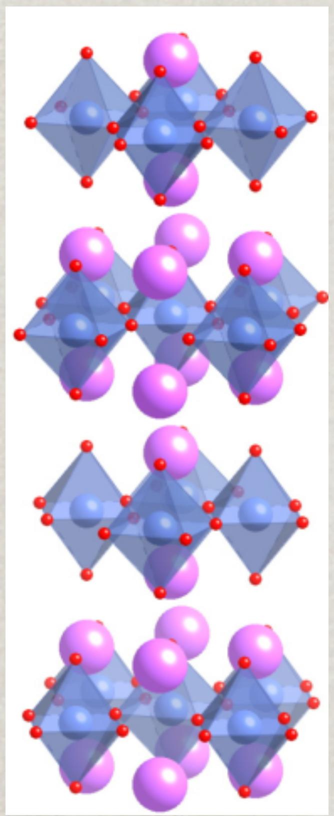


Sr_2IrO_4 - same crystal structure as La_2CuO_4

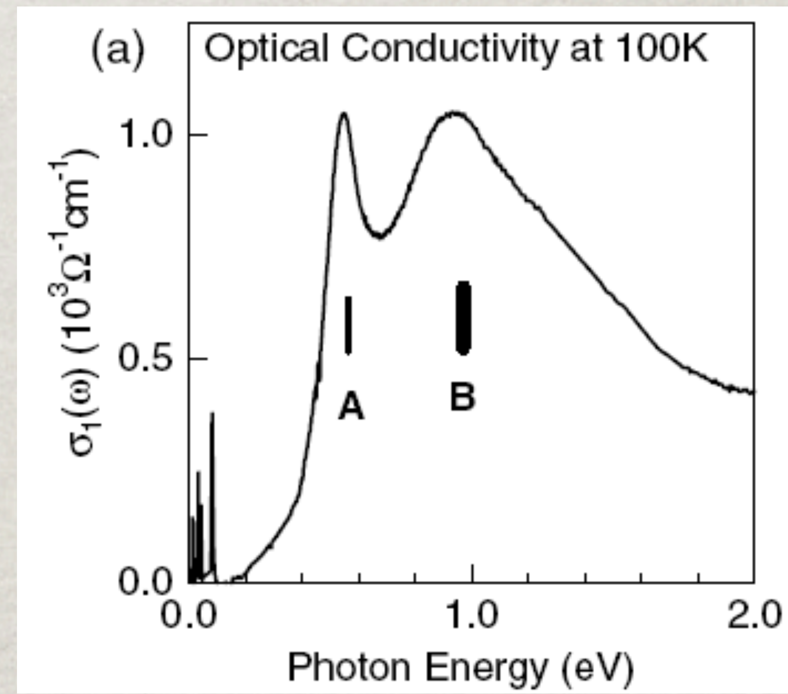
Single j=1/2 Hubbard model on a square lattice

Emulating High T_c

in condensed matter



Sr_2IrO_4 - same crystal structure as La_2CuO_4

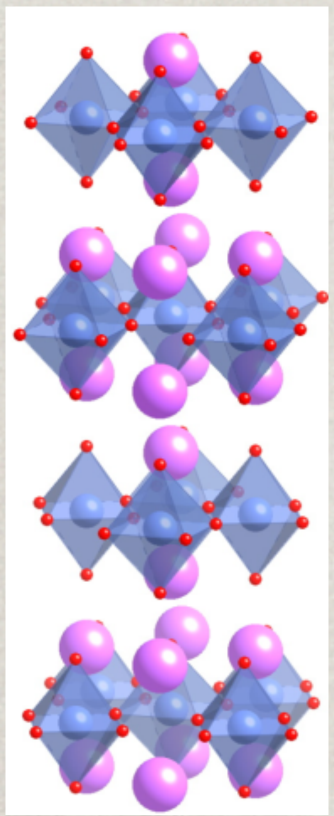


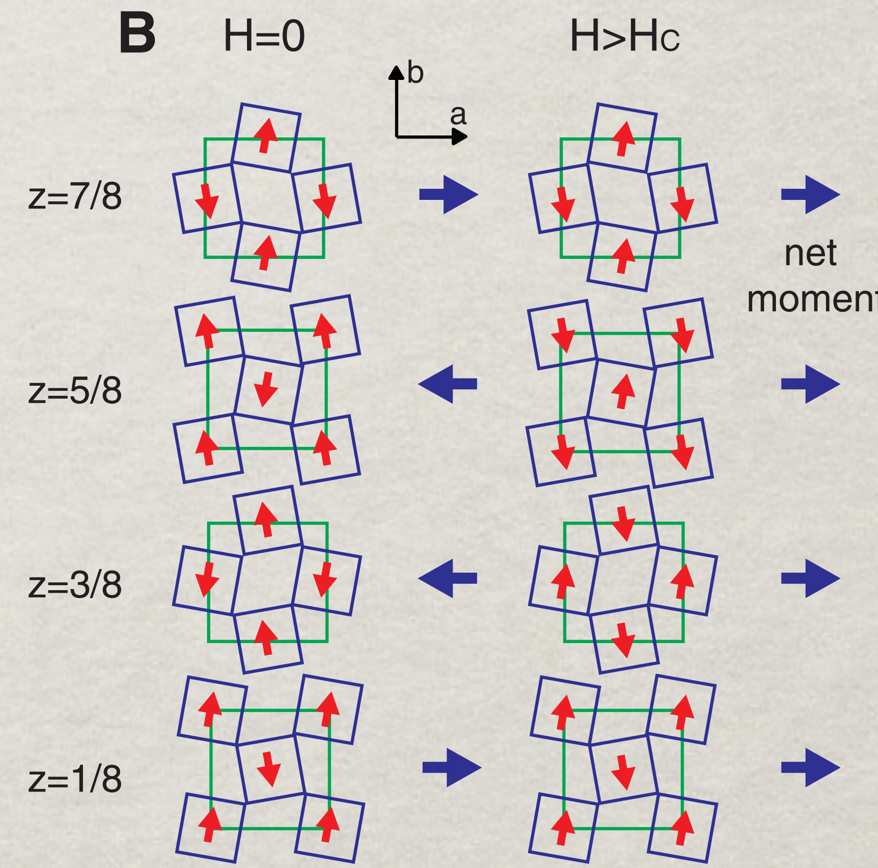
Charge gap = 0.1-0.5 eV

B.J.Kim *et al,* PRL (08)

Emulating High T_c

in condensed matter





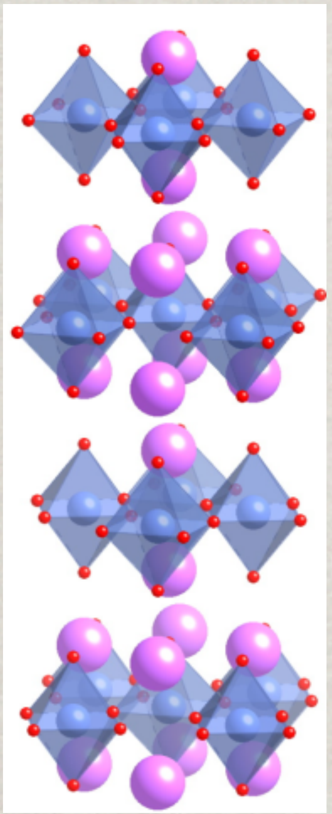
Sr_2IrO_4 - same crystal structure as La_2CuO_4

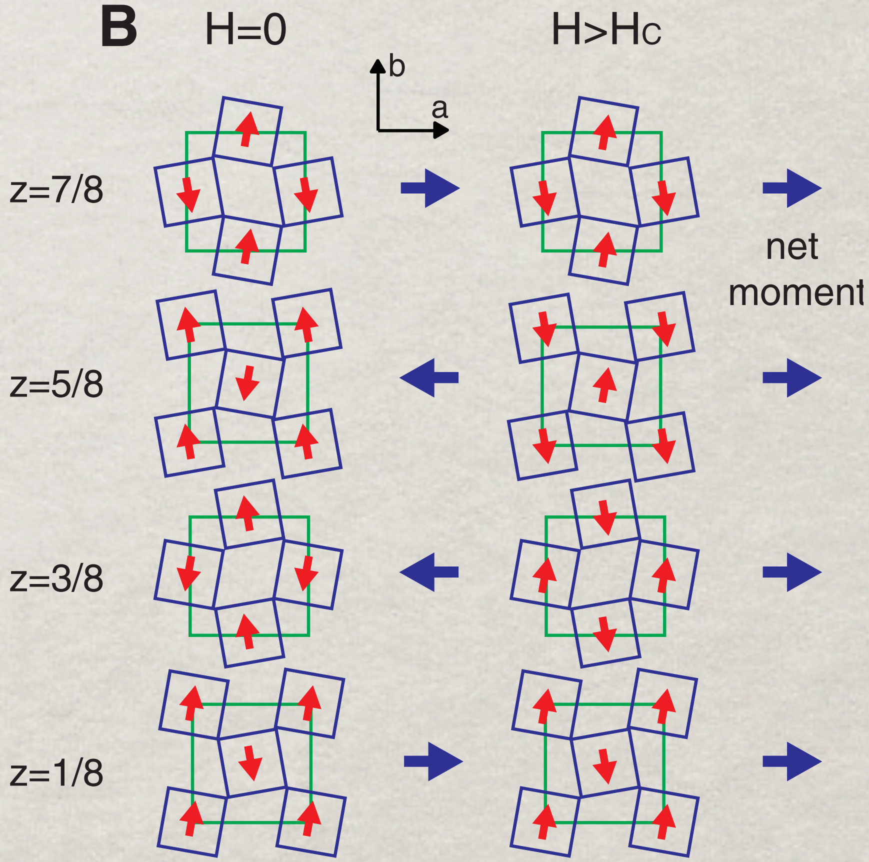
Neel order below T_N = 240K; J ≈1000K

B.J.Kim *et al,* Science (09)

EMULATING HIGH T_C

in condensed matter



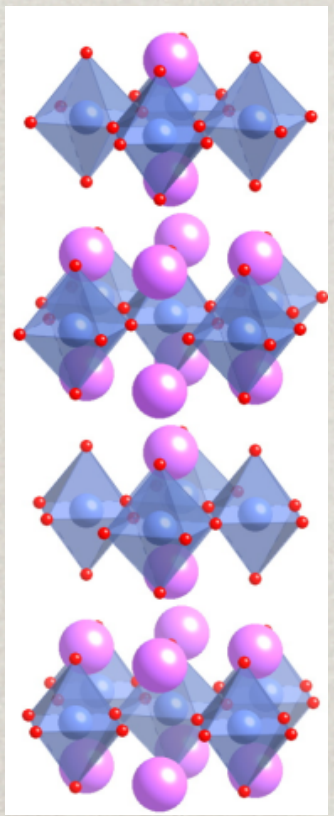


Sr_2IrO_4 - same crystal structure as La_2CuO_4

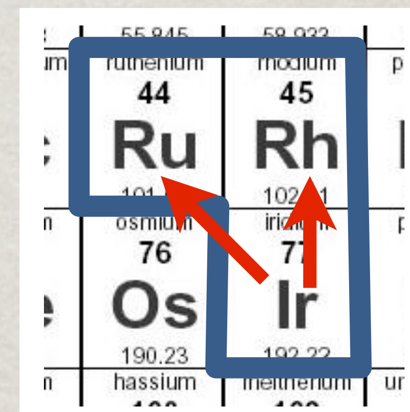
Giant canting angle ≈10°, implies strong Dzyaloshinskii-Moriya D/J ≈0.1

Emulating High T_c

in condensed matter



hole doping



control spin orbit

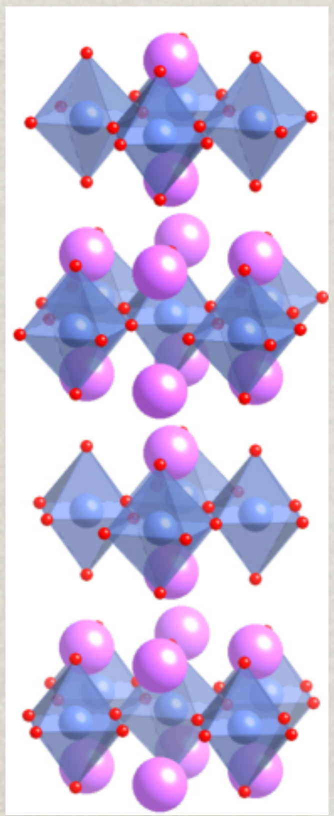
Sr_2IrO_4 - same crystal structure as La_2CuO_4

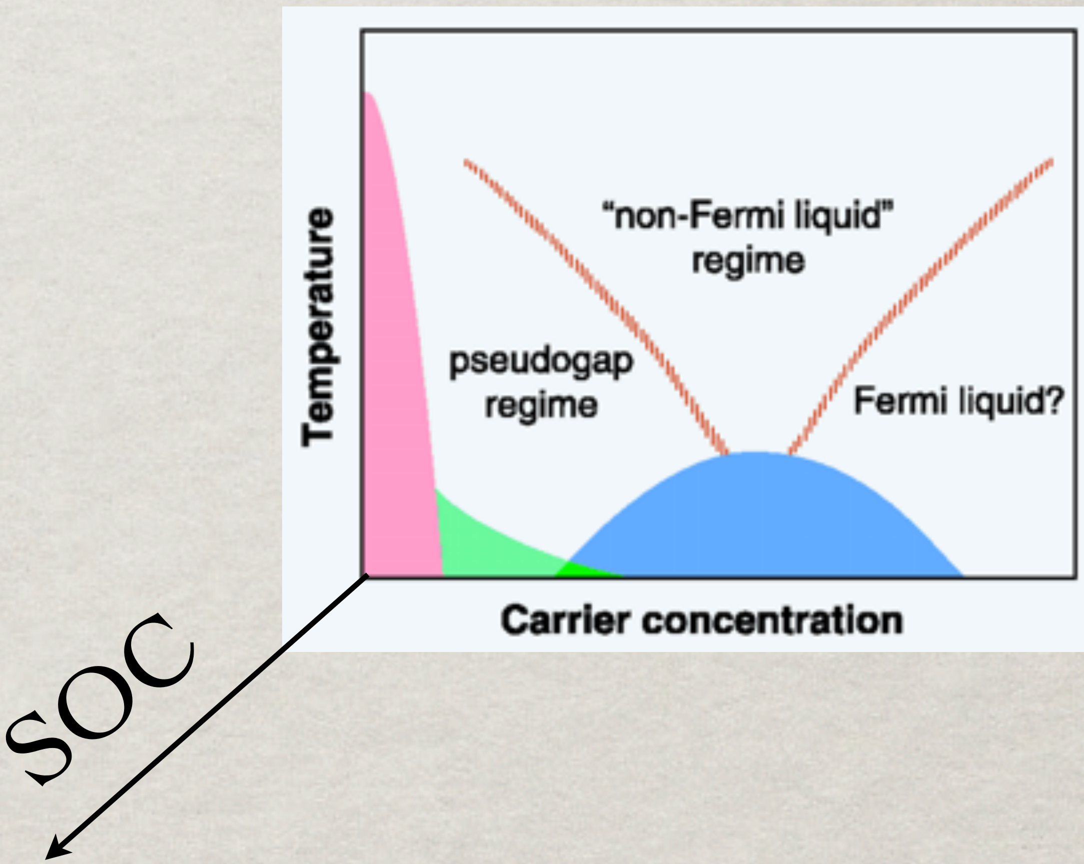
Films of $Sr_2Ir_{1-x}Rh_xO_4$ and $Sr_2Ir_{1-x}Ru_xO_4$ have been grown and show insulator-metal transitions

$La_xSr_{2-x}IrO_4$?

Emulating High T_c

in condensed matter





Sr_2IrO_4 - same crystal structure as La_2CuO_4

Can we fill in this phase diagram?

Quantum Spin Liquids

- QSL = a state in which spins avoid ordering by quantum fluctuations
  - Better: a ground state with "exotic" structure - e.g. emergent gauge structure such as topological order, supporting fractional quasiparticles, etc.
- Main problem:
  - Where to find them?
- Secondary problem:
  - How to distinguish different ones?

Quantum Spin Liquids

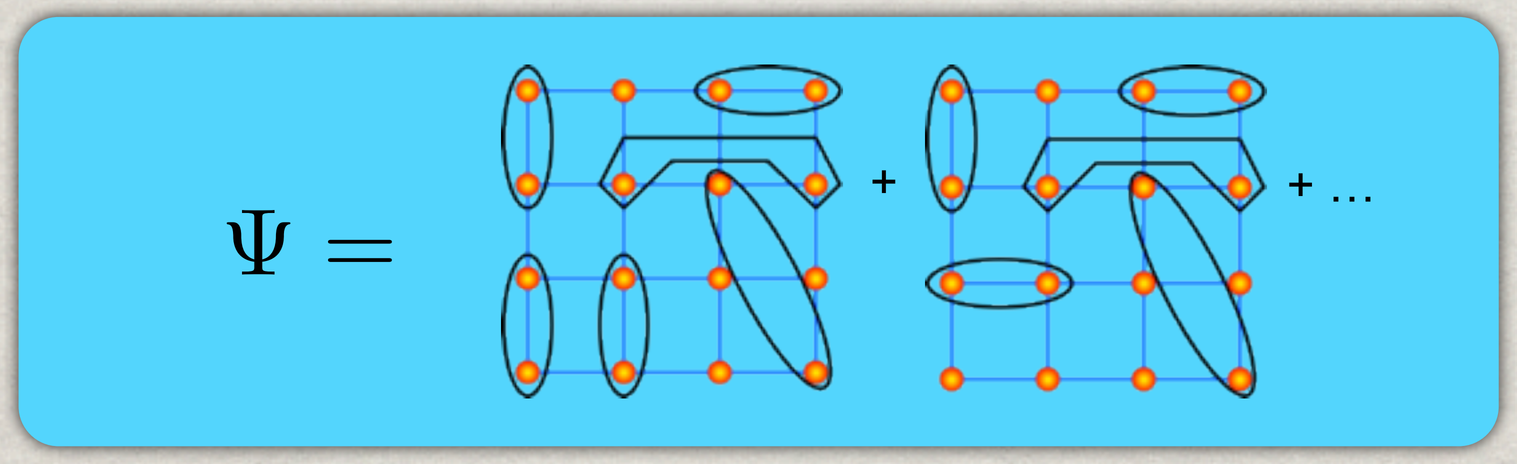
- QSL = a state in which spins avoid ordering by quantum fluctuations
  - Better: a ground state with "exotic" structure - e.g. emergent gauge structure such as topological order, su c.

Advertisement: Rajiv Singh's talk tomorrow, 1:30pm: <u>Experimental Candidates for Quantum Spin-Liquids: Current Status</u>

- Mai
  - W
- Secondary problem:
  - How to distinguish different ones?

RVB States

- Anderson (73): ground states of quantum magnets might be approximated by superpositions of singlet "valence bonds"

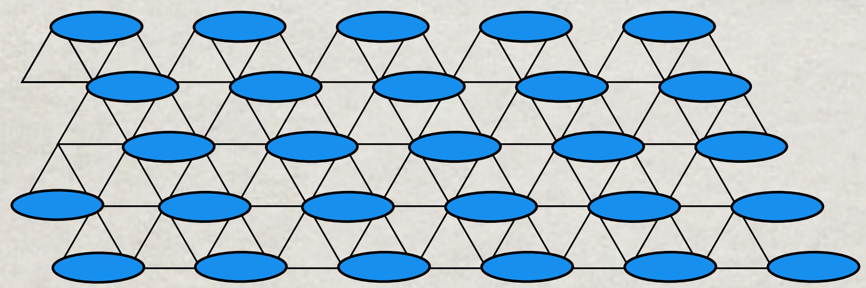


- Valence bond = singlet

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

VB states

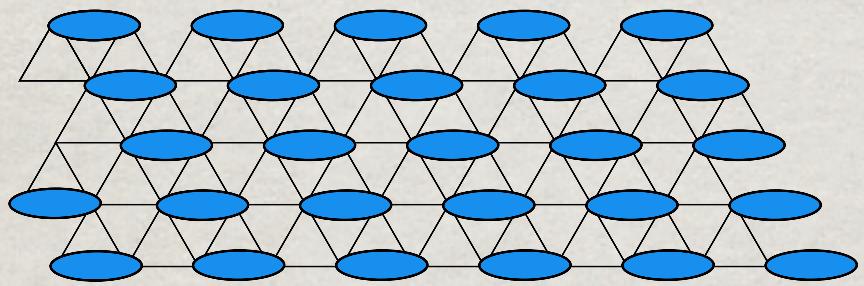
VBS



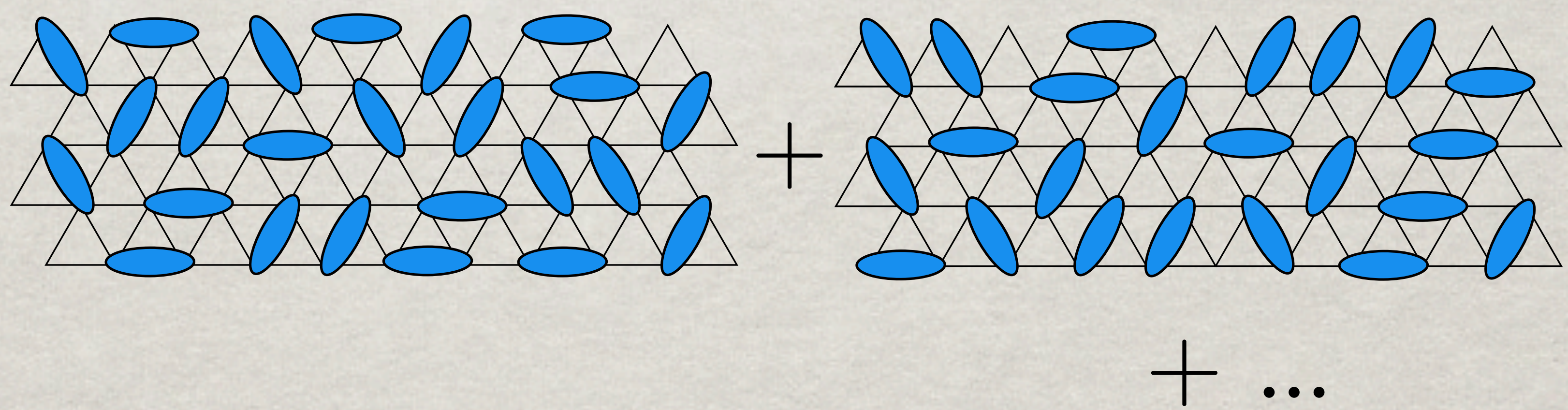
not a spin liquid

VB states

VBS



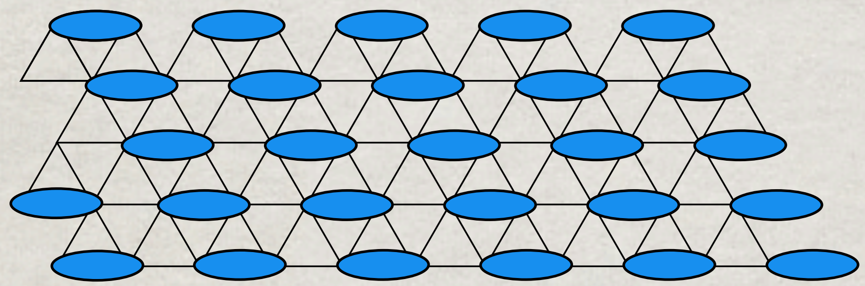
Short-range RVB



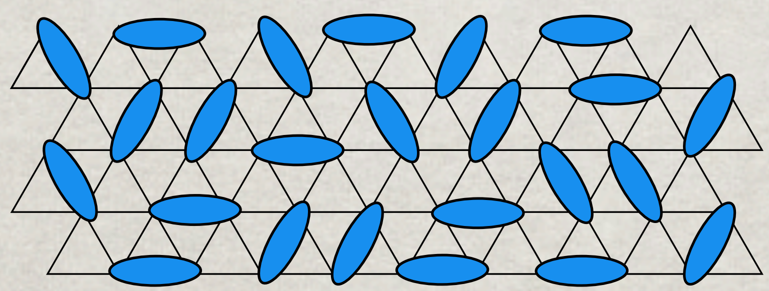
a QSL with an energy gap to break a singlet

VB STATES

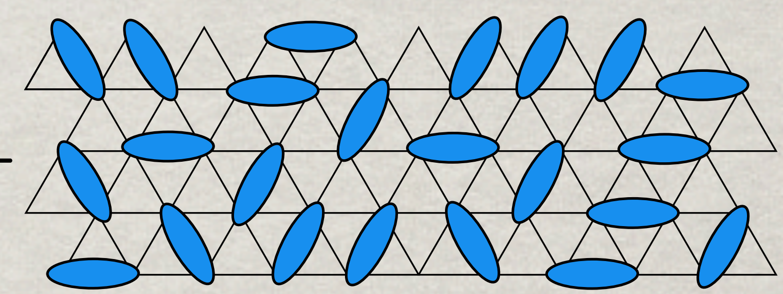
VBS



Short-range RVB

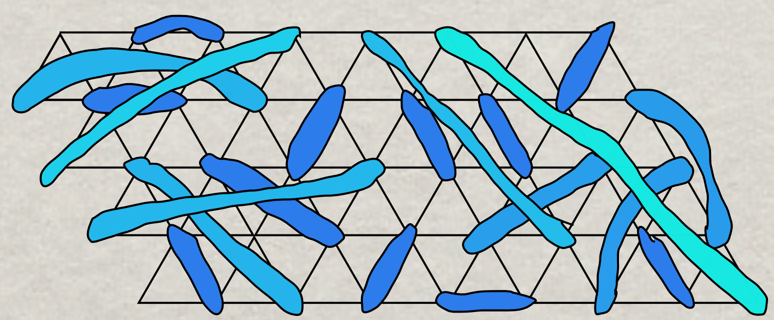


+



+ ...

Long-range RVB

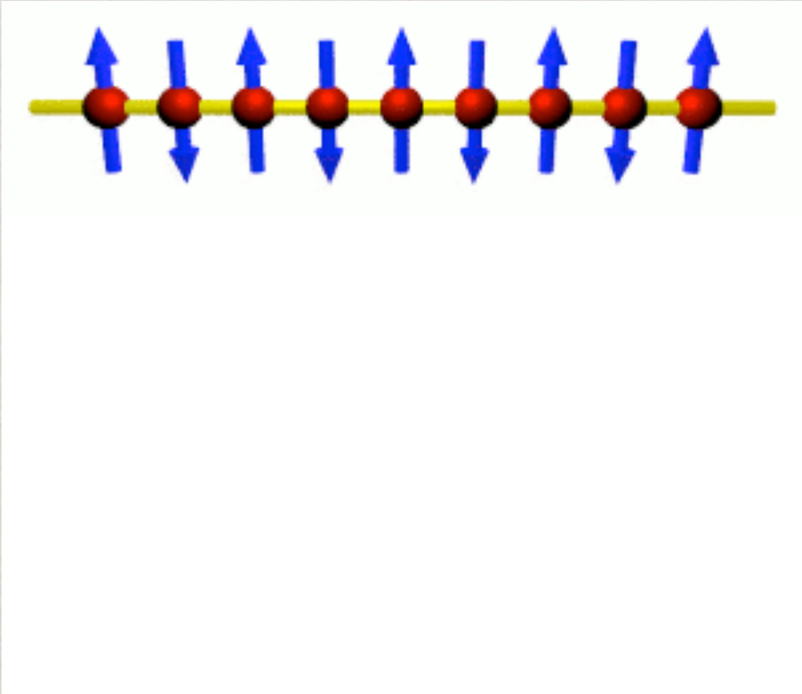


+...

gapless spin excitations

Spinons

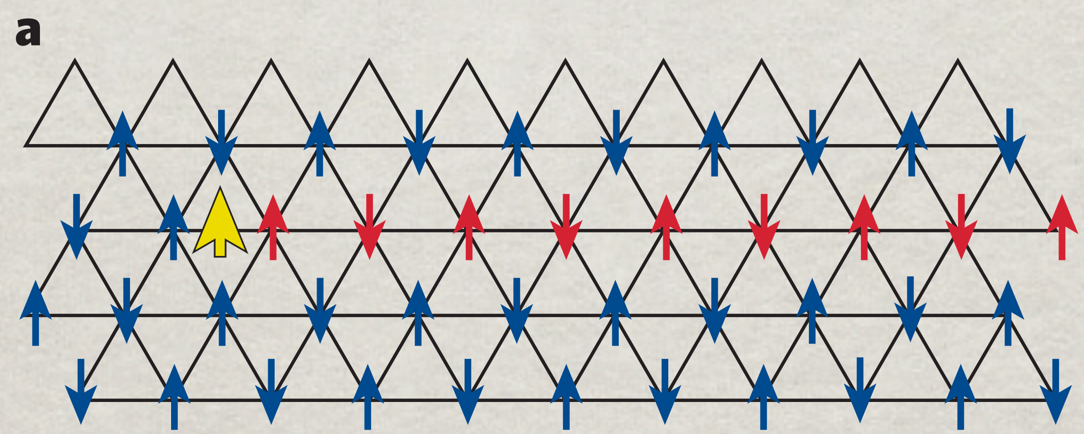
- QSLs generically support "spinons", neutral particles with S=1/2



- In 1d, the spinon is a domain wall or soliton
- It has in this sense a "string", but this does not confine the spinon because the string's boundary is just its endpoint

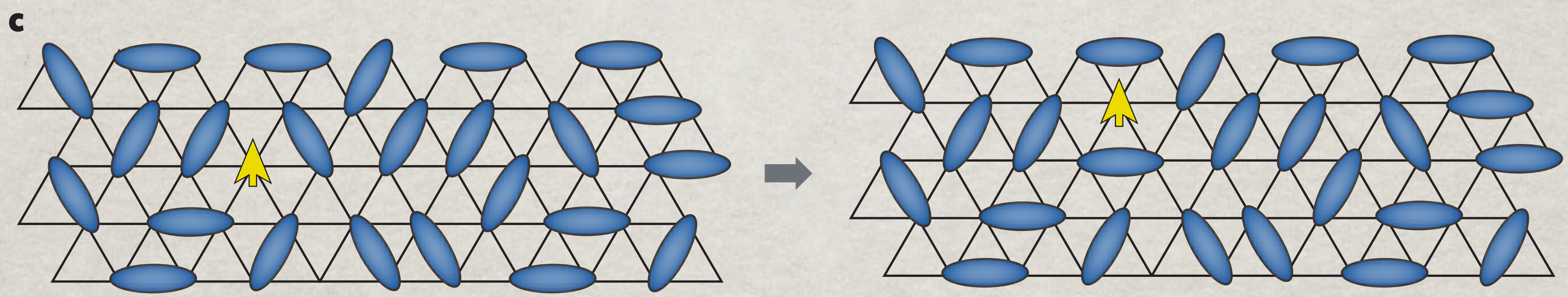
Spinons

- In d>1, any *observable* string costs divergent energy



Spinons

- In d>1, any *observable* string costs divergent energy



- If the ground state is a *superposition* of many states, the string need not be observable, if motion of the string simply reshuffles states in the superposition

Slave particles

- Gutzwiller-type variational wavefunction uses a reference Hamiltonian

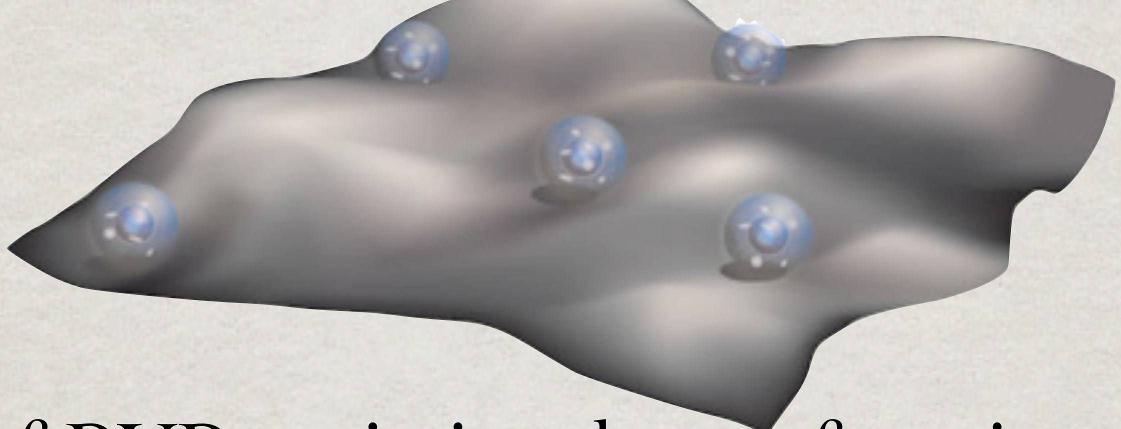
$$H_{ref} = \sum_{ij} \left[t_{ij} c^\dagger_{i\alpha} c_{j\alpha} + \text{h.c.} + \Delta_{ij} c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} + \text{h.c.} \right]$$

- Project

$$|\Psi_{var}\rangle = \prod_i \hat{P}_{n_i=1} |\Psi_{ref}\rangle$$

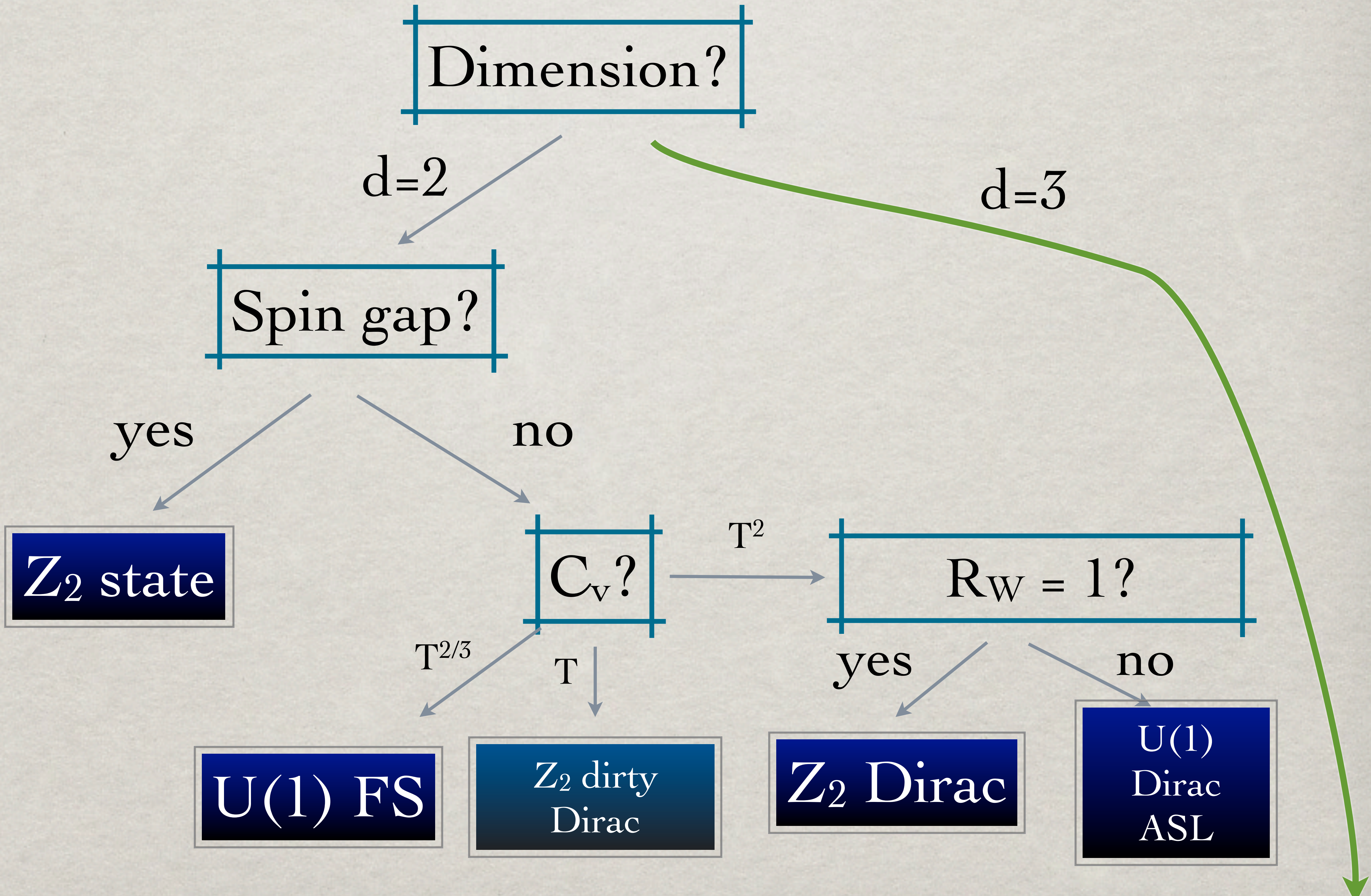
- Gauge transformations of reference state leave physical state invariant
  - this is believed to be reflected in *emergent gauge fields* in the QSL phases: U(1), Z_2, ...

The "landscape"



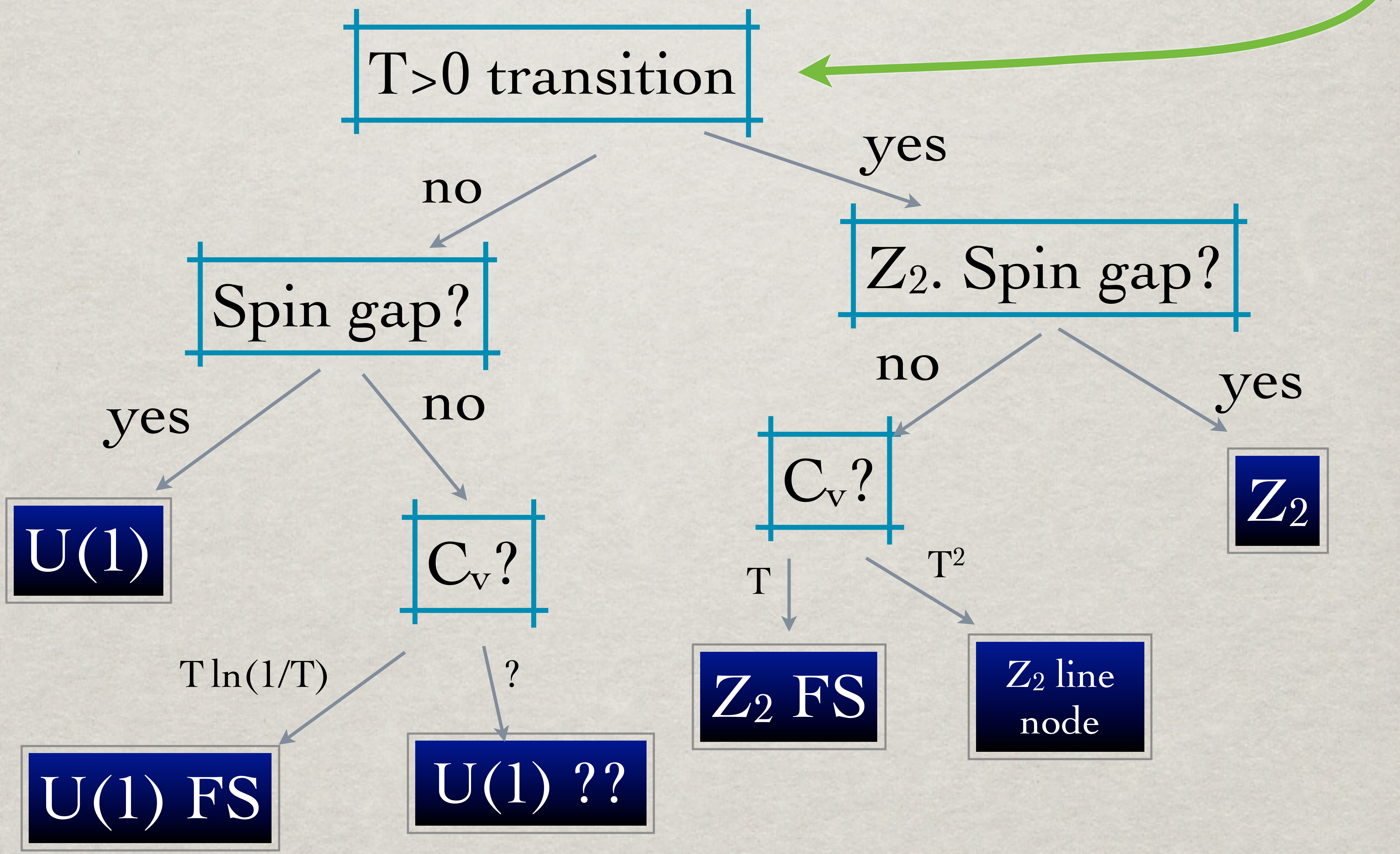
- The space of RVB variational wavefunctions is vast
- The number of distinct Quantum Spin Liquid (QSL) *phases* is also huge
  - e.g. X.G. Wen has classified *hundreds* of different QSL states all with the same symmetry on the square lattice (and this is *not* a complete list!)
  - This makes it difficult to compare all of the states
- Many QSLs are described by non-trivial interacting QFTs, which are themselves not well understood

A diagnostic flowchart



d=3

A diagnostic flowchart



disordered possibilities neglected

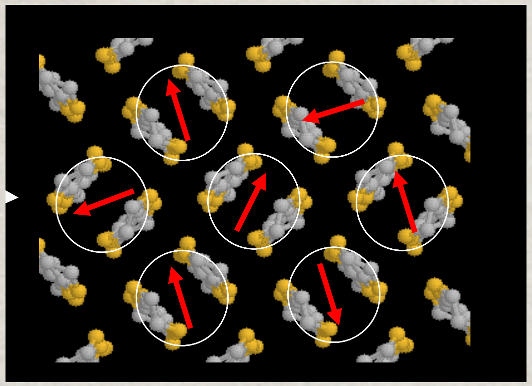
The paradox

- There seem to be so many QSLs in theory
- But *no* clear demonstrations in experiment
  - probably thousands of quantum antiferromagnets have been studied experimentally and nearly all of them order magnetically
  - How to tell? A good subject for discussion.

Where in CMP?

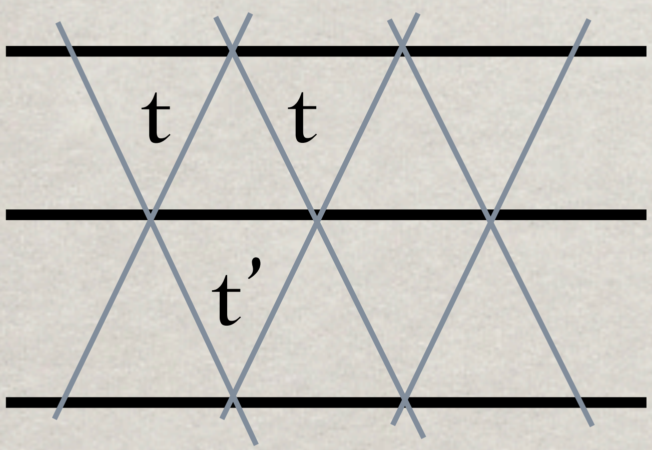
- Materials with
  - S=1/2 spins (necessary?)
  - Frustration
  - Other sources of fluctuations, e.g. proximity to Mott transition (where the electrons become delocalized)
    - e.g. Hubbard rather than Heisenberg

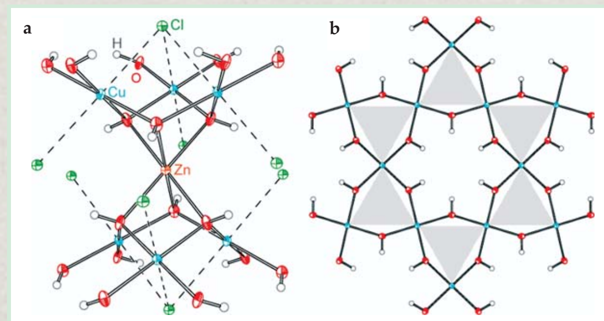
D>1 QSL MATERIALS



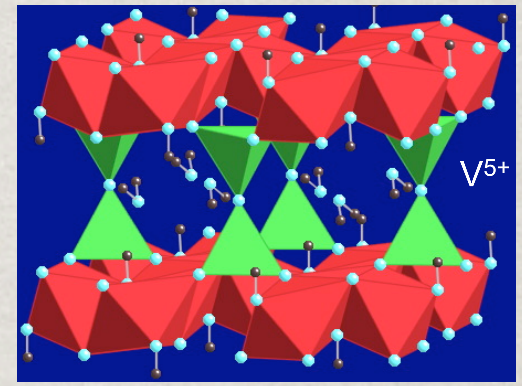
κ-(BEDTTTF)$_2$Cu$_2$(CN)$_3$

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

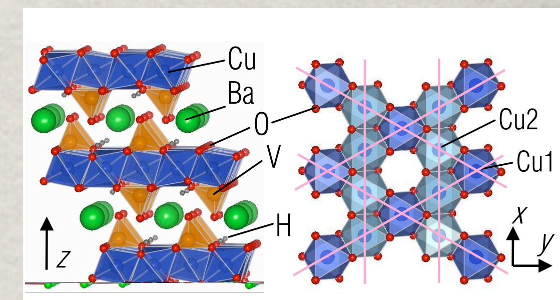




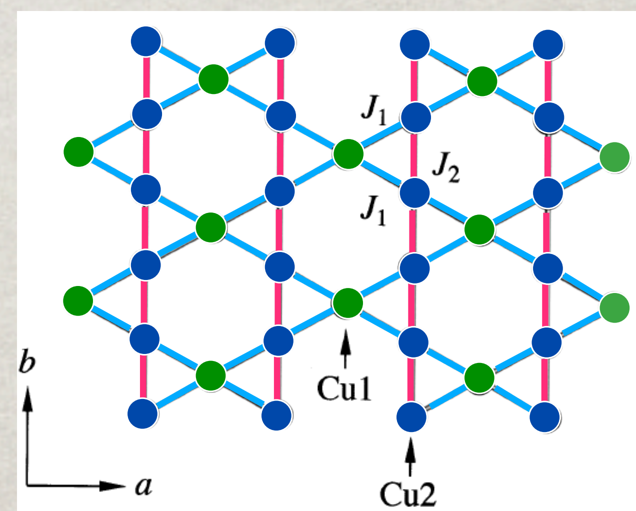
herbertsmithite

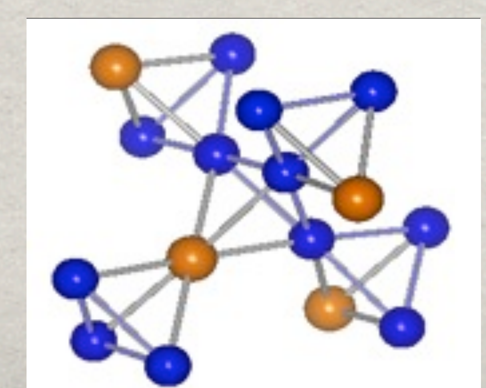


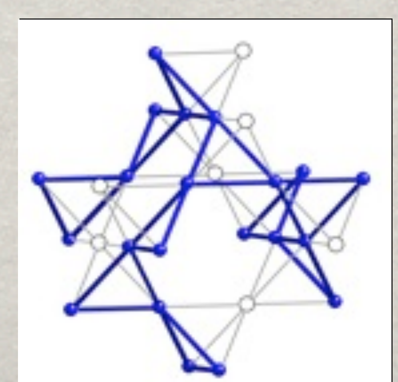
volborthite



vesignieite







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

QSL CANDIDATES

- **Triangular lattice** organics: $\varkappa$-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$, EtMe$_3$Sb[Pd(dmit)$_2$]$_2$
- **Kagome lattices**: herbertsmithite, vesignieite, volborthite
- **Hyperkagome lattice**: $Na_4Ir_3O_8$
- XY **pyrochlore**: $Er_2Ti_2O_7$
- **FCC** double perovskites: A$_2$BB'O$_6$, e.g. Ba_2YMoO_6

recent work in our group

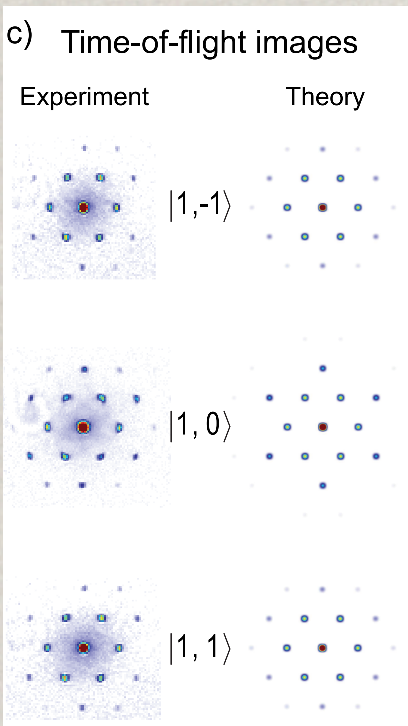
SLs ≠ QSLs

- Classical spin liquids (thermal fluctuations)
  - "spin ice" $Ho_2Ti_2O_7$, $Gd_2Ti_2O_7$
  - Heisenberg pyrochlores ACr_2O_4 , A=Zn, Cd, Hg...
  - "spiral spin liquid" $MnSc_2S_4$,$CoAl_2O_4$?
  - "ring liquid" $Bi_3Mn_4O_{12}(NO_3)$?
- Unconventional partially frozen states (very common)
  - S=1/2 anisotropic kagome: "volborthite" $Cu_3V_2O_7(OH)_2 \cdot 2H_2O$
  - triangular S=1 antiferromagnet: $NiGa_2S_4$
  - FCC antiferromagnet: Sr_2CaReO_6

QSLs in cold atoms?

- Solvable spin models, e.g. Kitaev
  - Difficult: very fine-tuned (might actually exist in CM though!) and must cool deeply
  - Many conserved quantities - hard to equilibrate
- Mimic experimental CM systems
  - e.g. triangular lattice fermionic Hubbard model at 1/2-filling

Triangular lattice



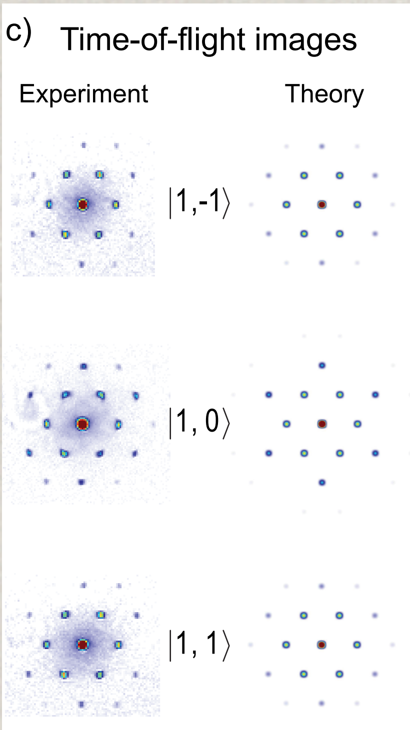
K. Sengstock group

spinon
Fermi
surface

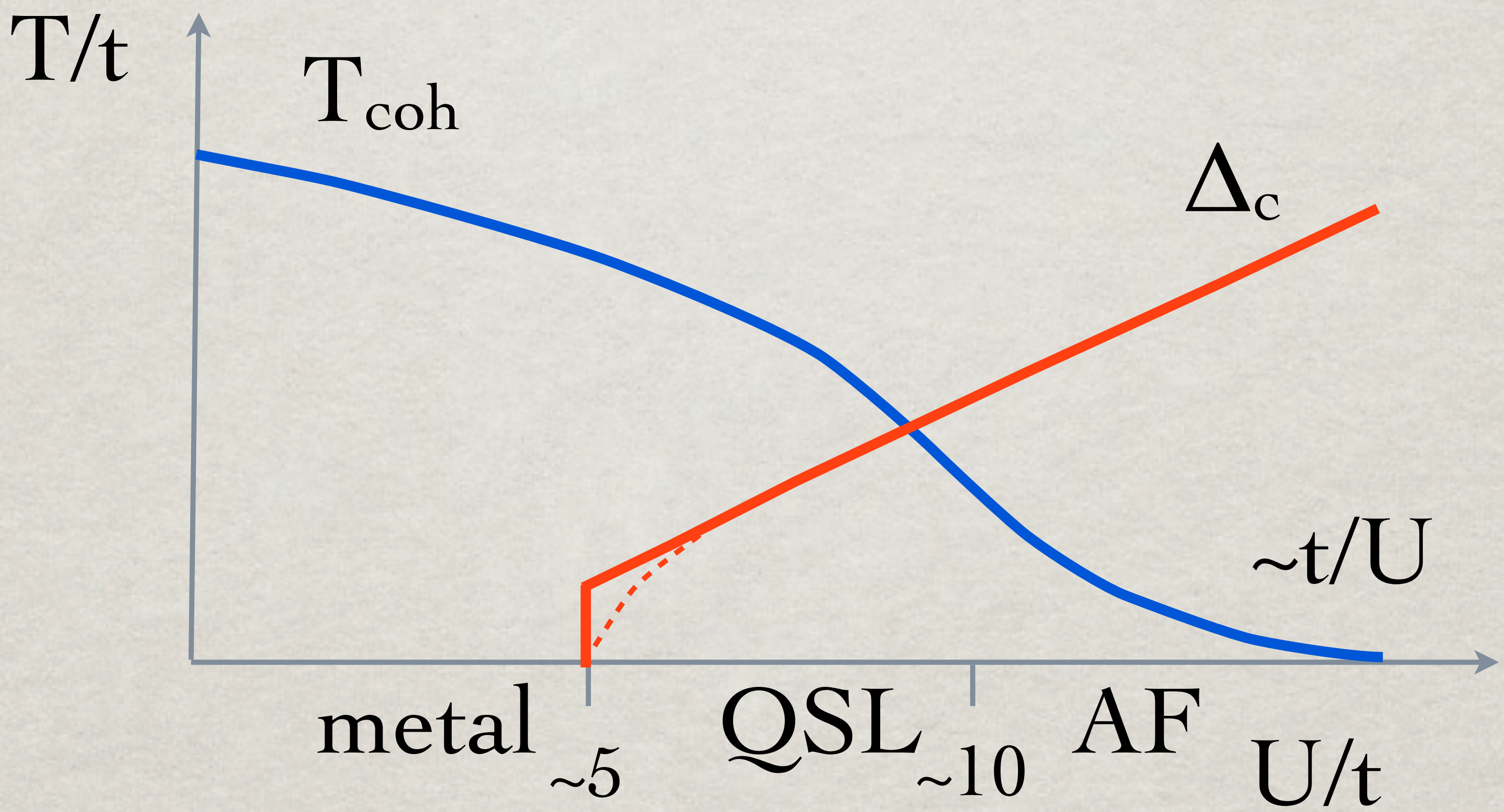
metal ~5 QSL ~10 AF U/t

H. Morita *et al*, 2002
O. Motrunich, 2005
P.A. Lee + S.S. Lee, 2005
B. Kyung + A.M.S. Tremblay, 2006
...
D.N. Sheng *et al*, 2009
H.-Y. Yang *et al*, 2010

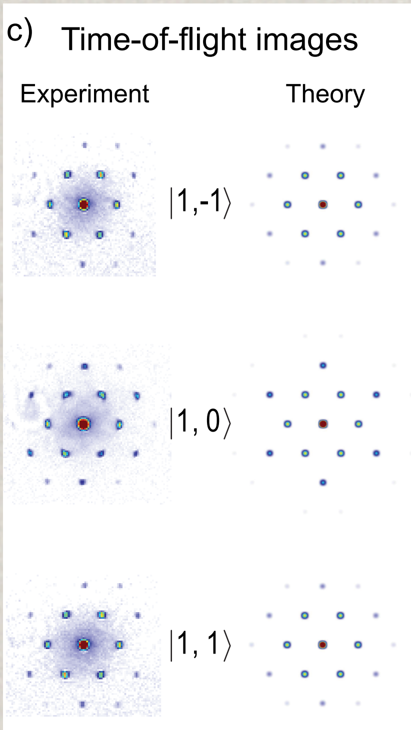
Triangular lattice



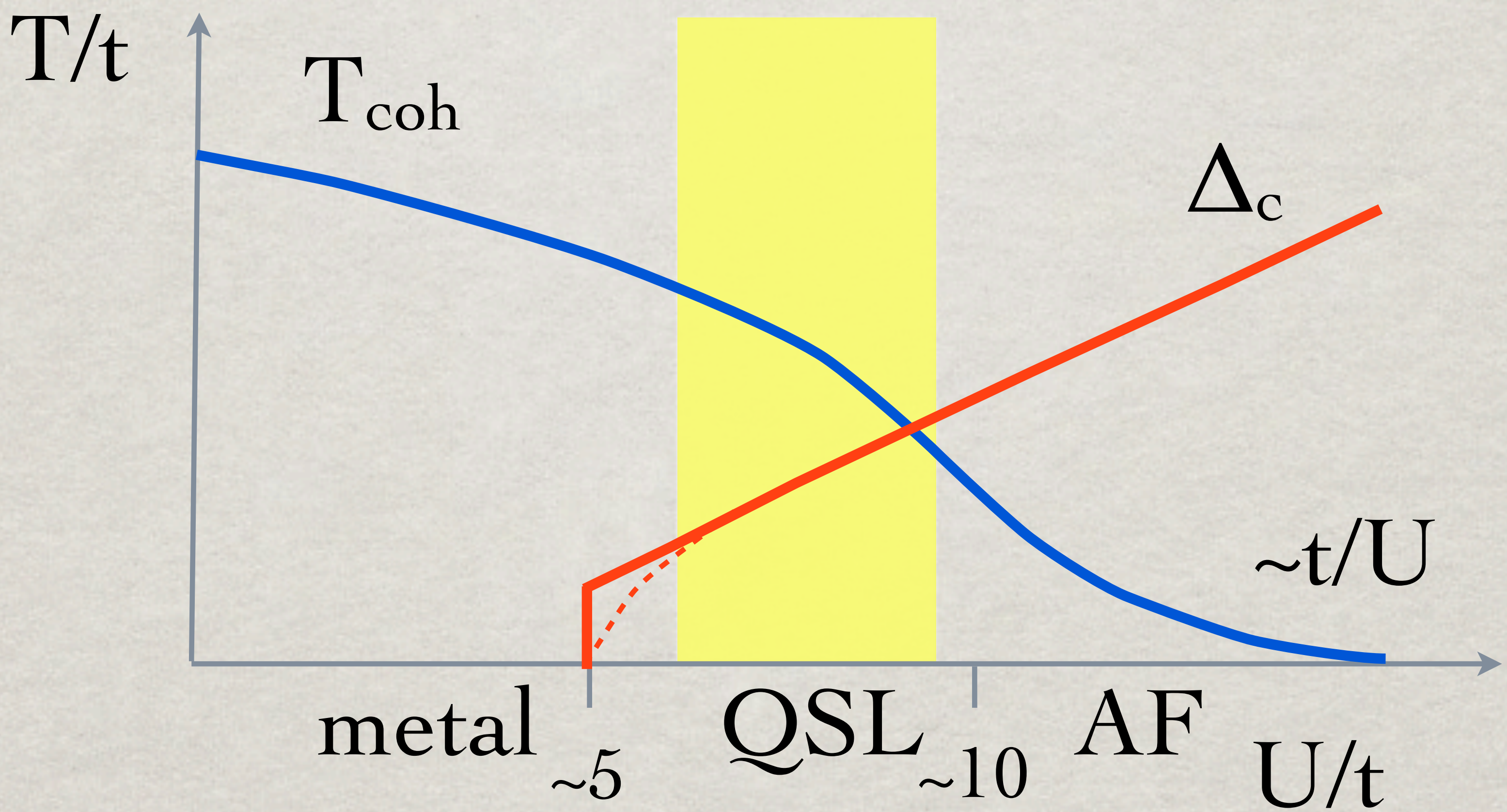
K. Sengstock group



Triangular lattice

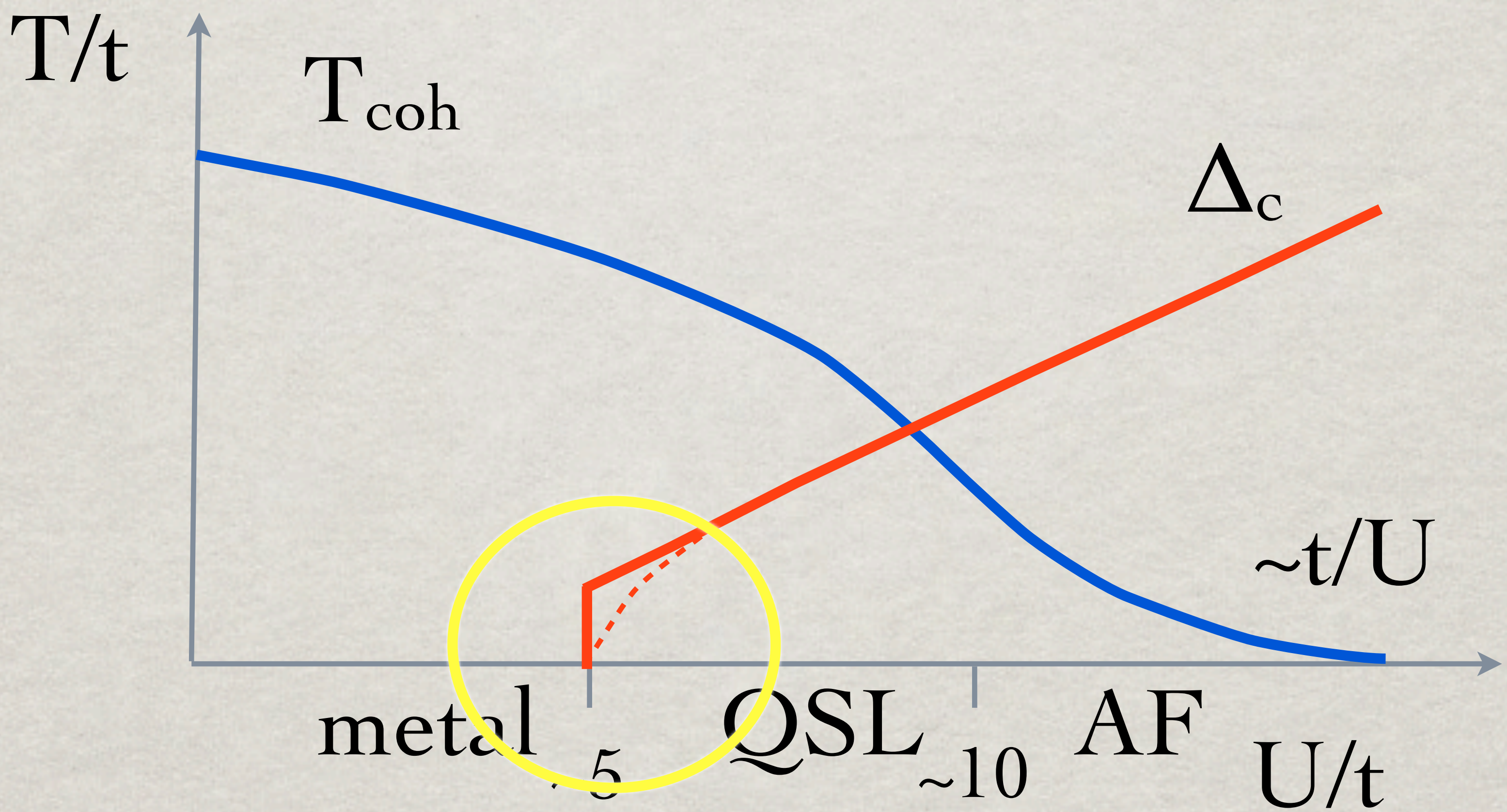


K. Sengstock group



- The "sweet spot" is at intermediate coupling
- One may expect similar things in other frustrated lattices (maybe unfrustrated ones too!)

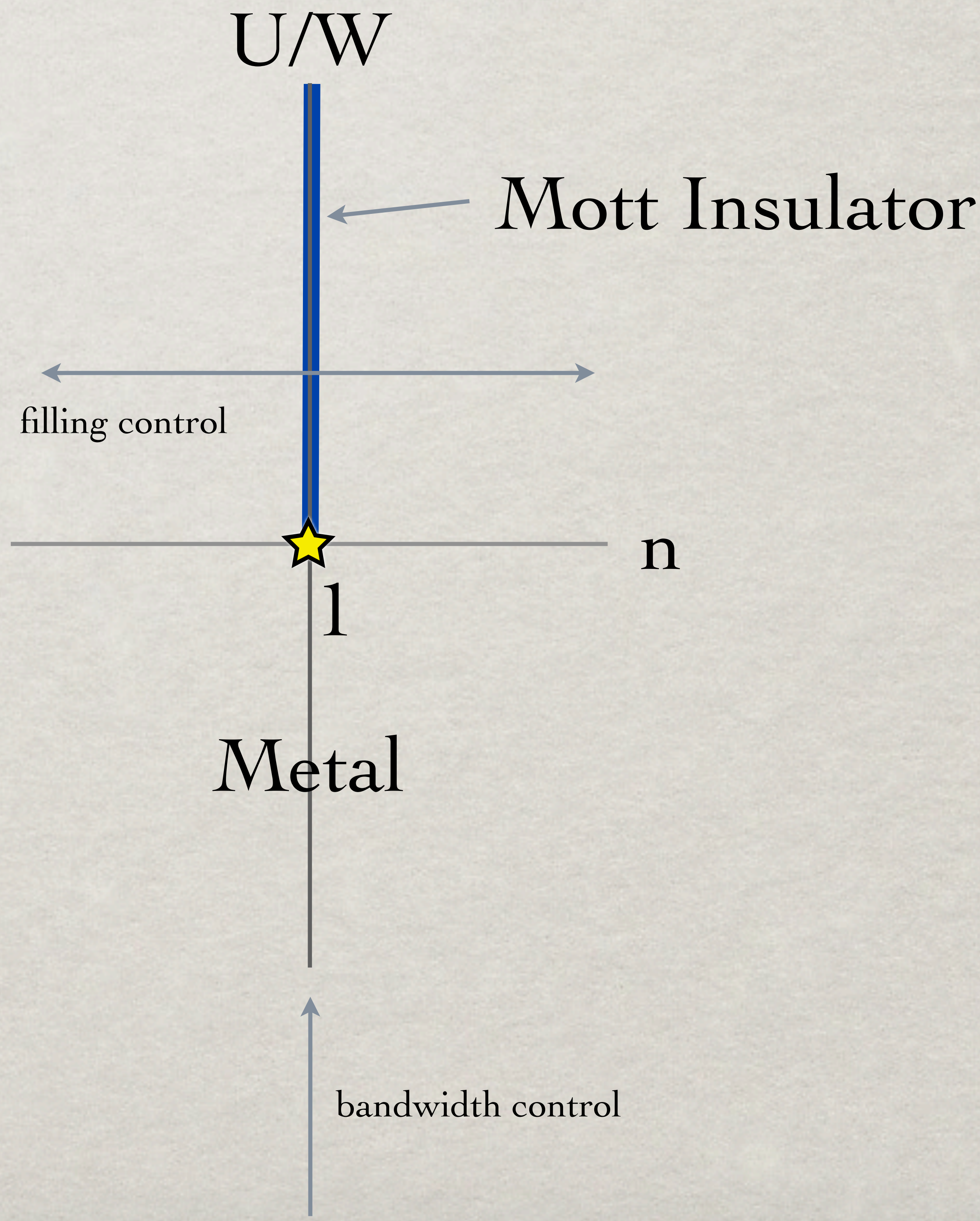
Mott Transitions



- The Mott transition *of fermions* is a storied topic in condensed matter physics

Mott Transition

- Mott state
  - *Single particle* gap
  - insulating
  - local moments
- Metal
  - Fermi surface
  - conducting
  - Pauli paramagnetism



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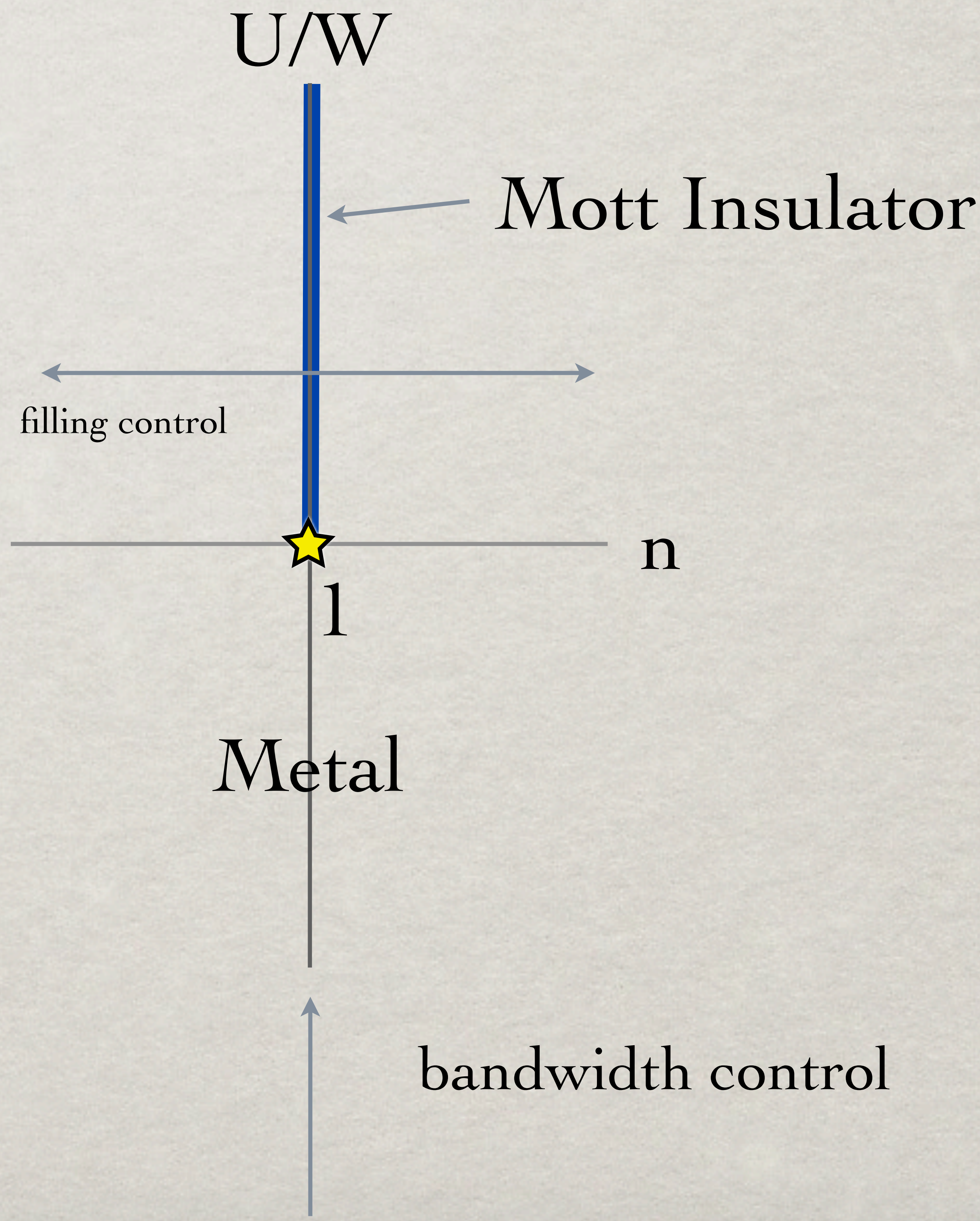


Bandwidth controlled Mott transition

- Mott originally argued for a first order transition
  - But he changed his mind later!
- If it is, a line of first order transitions must exist at T>0
  - this is often seen in experiment

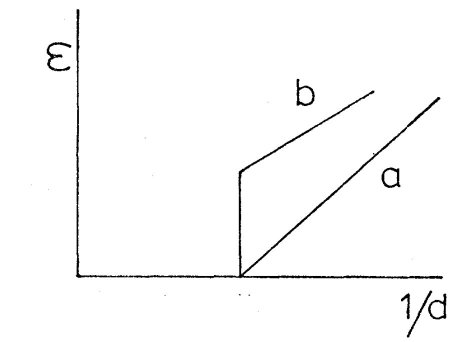
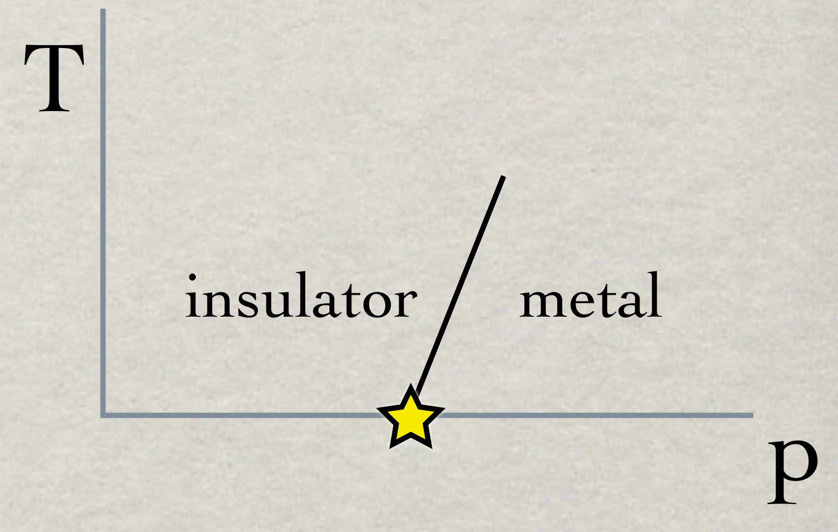


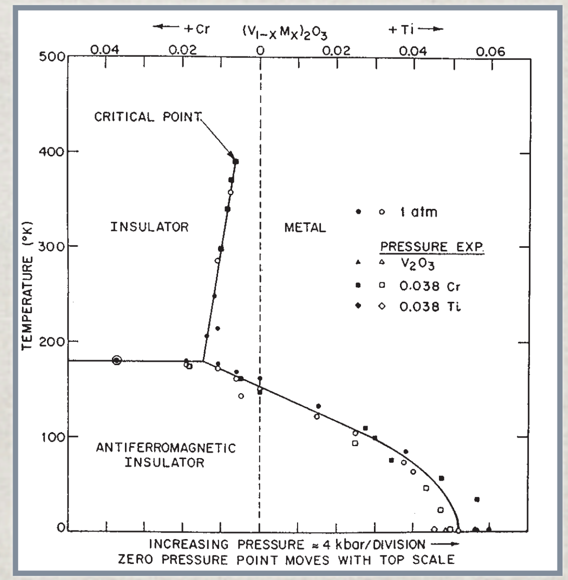
FIG 2. Different predictions about the way the activation energy changes at the transition.



First order Mott transitions

- Vanadates (from Mott's RMP!)
  - V_2O_3 phase diagram

    McWhan, 1971



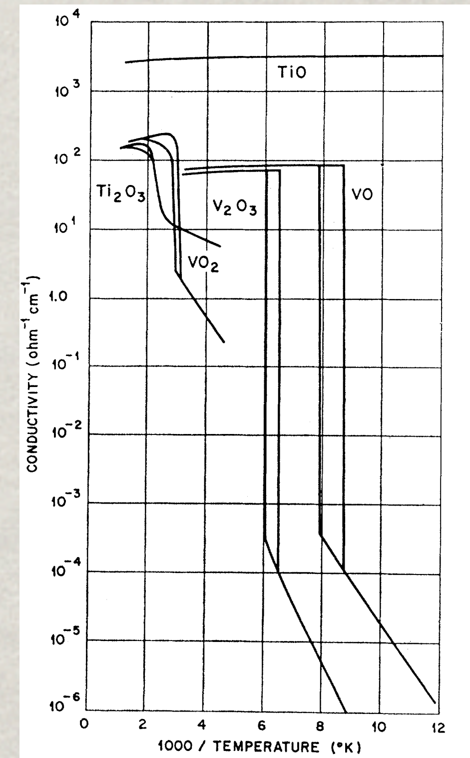
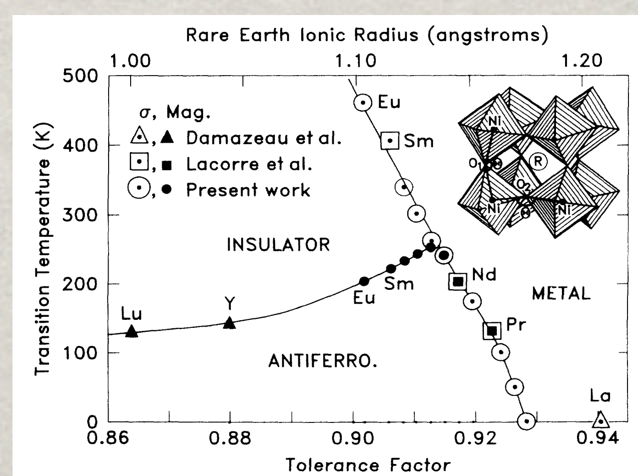
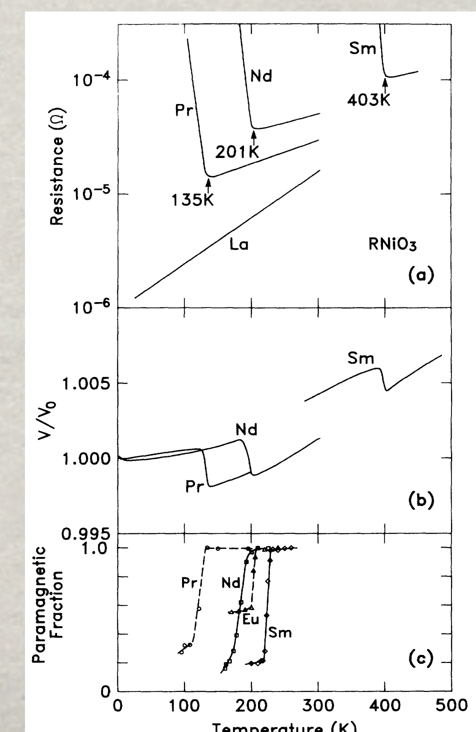


FIG. 7. Conductivities of oxides (Morin[36]).

- Nickelates (perovskites)
  - first order

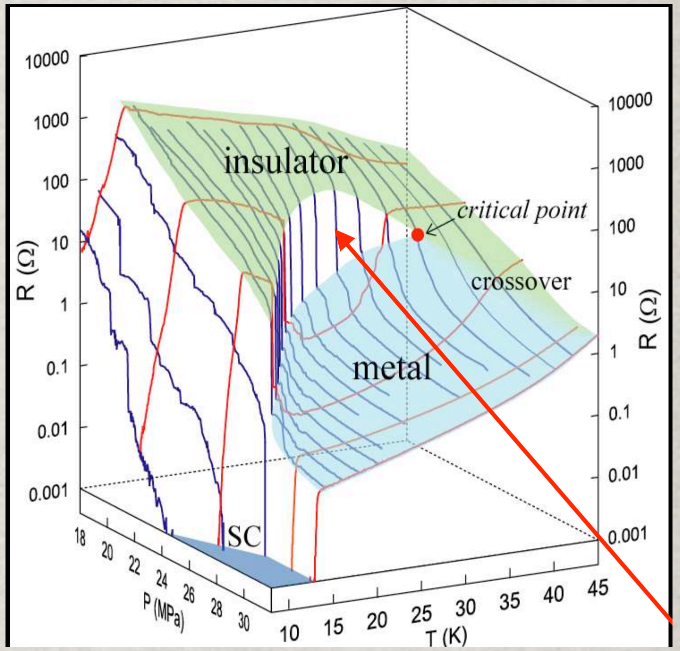




First order Mott transitions

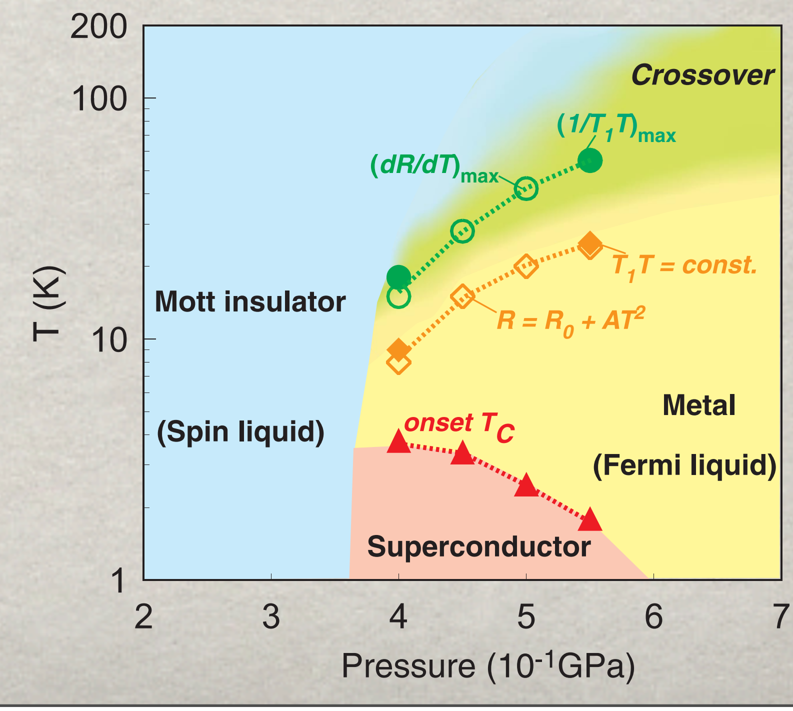
- Seen in several organic quasi-2d conductors

κ-$(ET)_2Cu[N(CN)_2]Cl$



κ-$(ET)_2Cu_2(CN)_3$

K. Kanoda



Recent Activity

- A major focus of method development
    - LDA+U
    - DMFT++
    - Variational wavefunctions, fixed node, etc.
- Many of the most interesting materials may be close to one (e.g. many QSL candidates)
- Study is reinvigorated by Mott heterostructures

$LaNiO_3$ Films

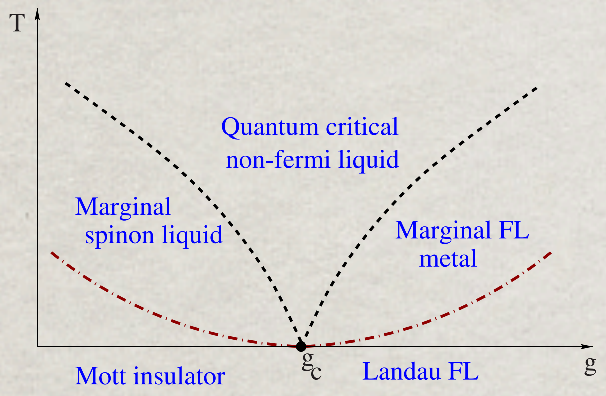
G. Sawatzky, unpublished

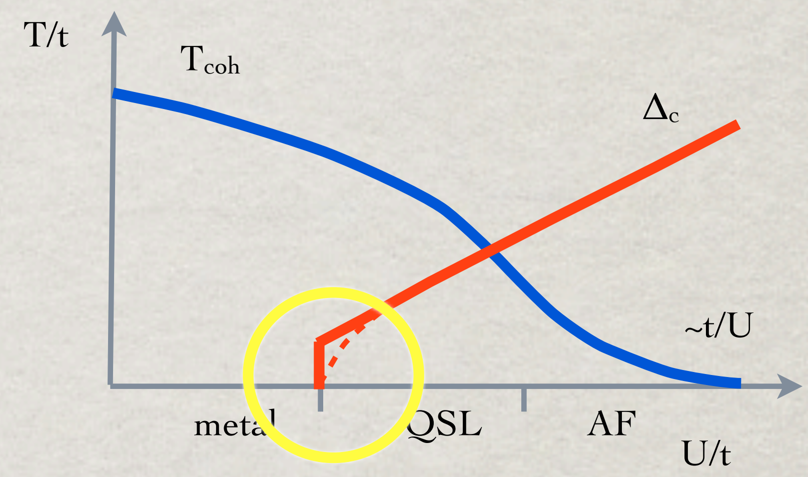
- Numerous groups are now studying $LaNiO_3$ films and superlattices, grown down to thicknesses of a few unit cells

- Strain and interfaces have been shown (experimentally) to alter the electronic structure in a rationalizable way, tuning a metal-insulator transition

Continuous Mott Transitions?

T. Senthil, 2008





- Recently theorists have returned to the idea of a continuous (bandwidth tuned) Mott transition
  - Might occur in frustrated situations
  - Requires "killing" entire Fermi surface at the QCP - very exotic criticality
  - Plausible scenarios based on "slave rotor" approximation

Mott transitions in cold atoms

- In general, the Mott transition occurs with U comparable to bandwidth, so temperature does not need to be too low
- Systems are much more tunable than solid state (lattice depth, symmetry, SU(N))
- Conditions more favorable for continuous transitions:
  - lack of phonons
  - large SU(N) symmetry

Spin orbit physics

$$\lambda \boldsymbol{L} \cdot \boldsymbol{S}$$

λ ↓

fine structure

magnetic anisotropy

spin Hall effect

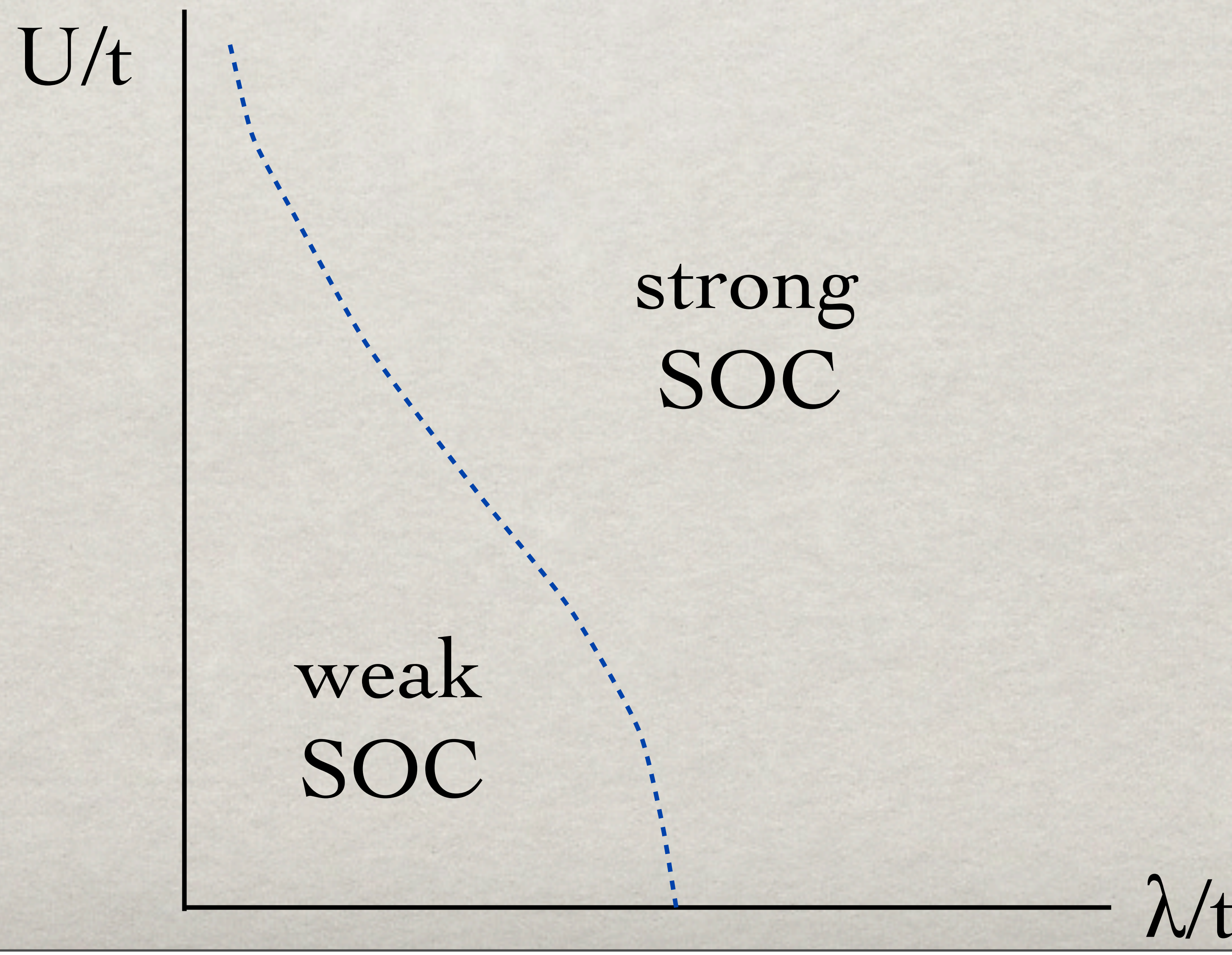
anomalous Hall effect

topological insulators

SOC and Interactions

- Hubbard model:

$$H = t\,H_{\text{hop}} - \lambda \sum_i \boldsymbol{L}\cdot\boldsymbol{S} + U\sum_i n_i(n_i - 1)$$



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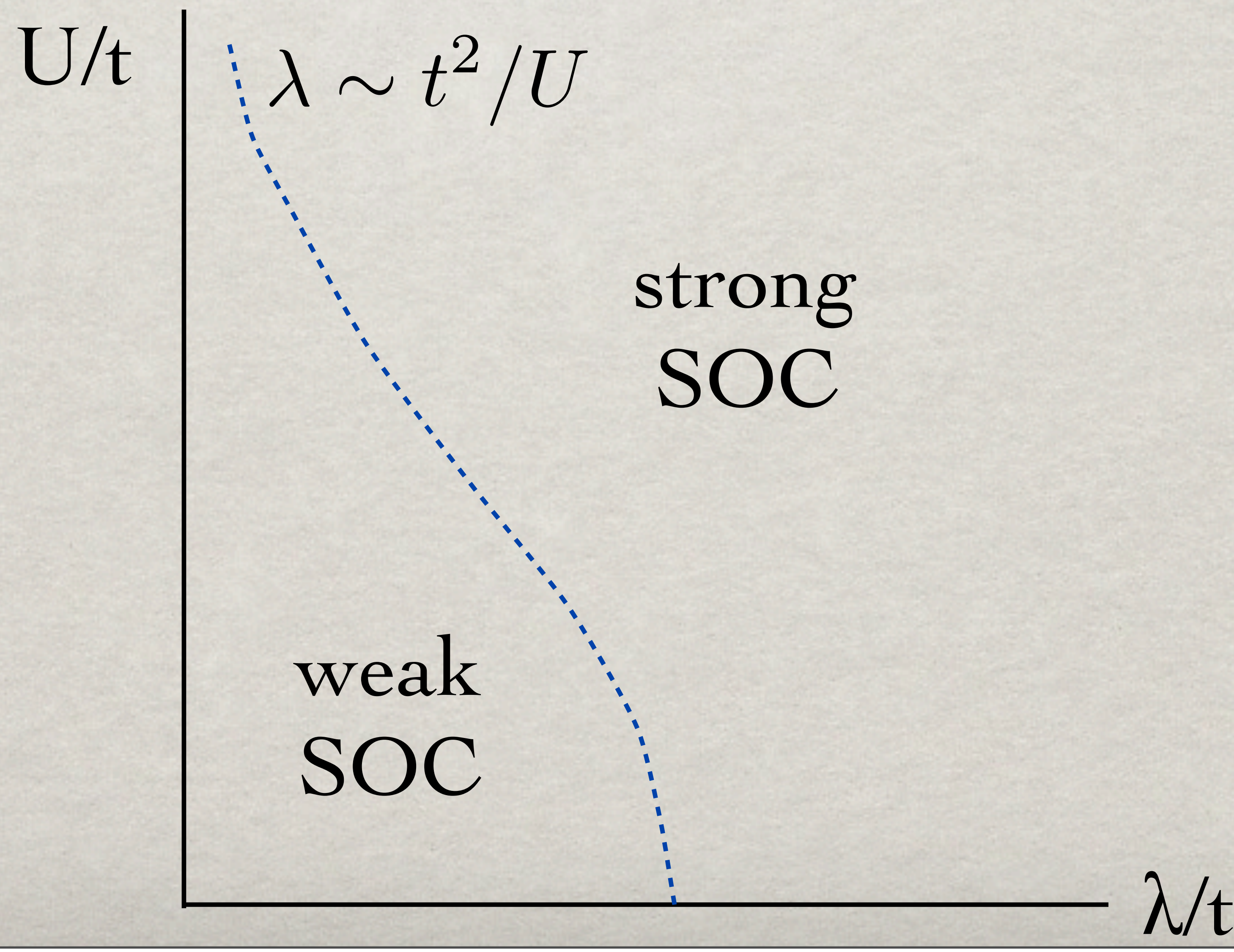

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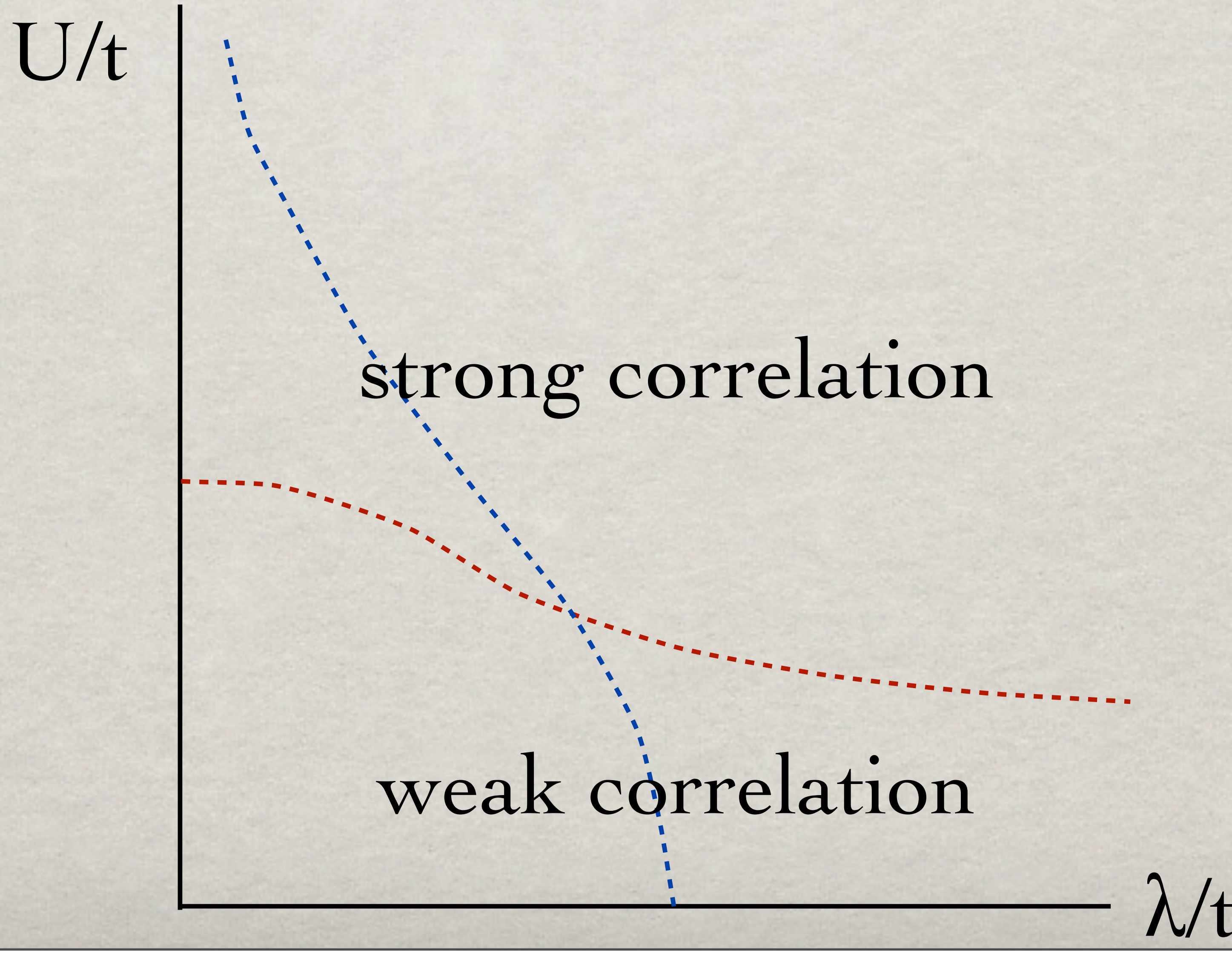

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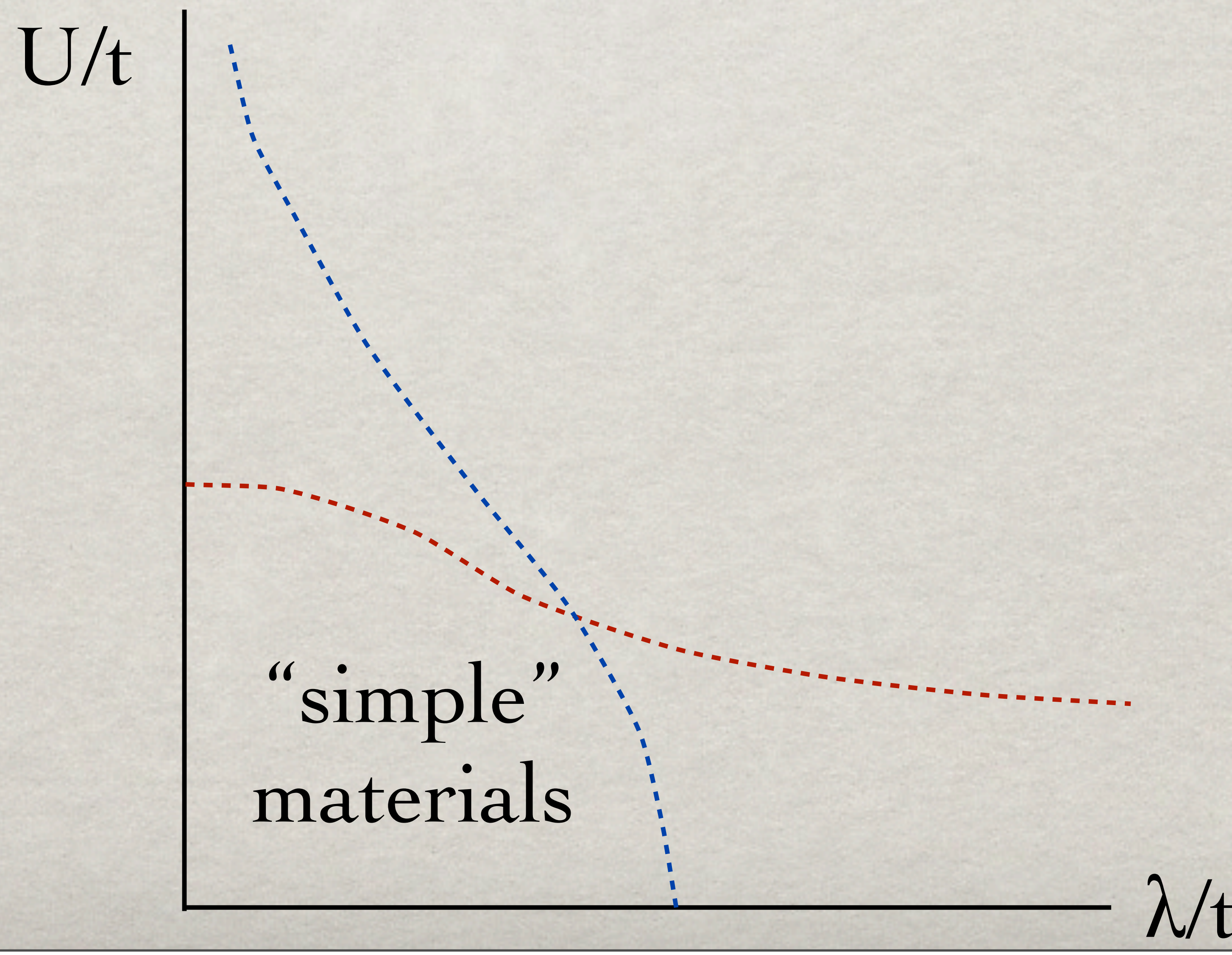

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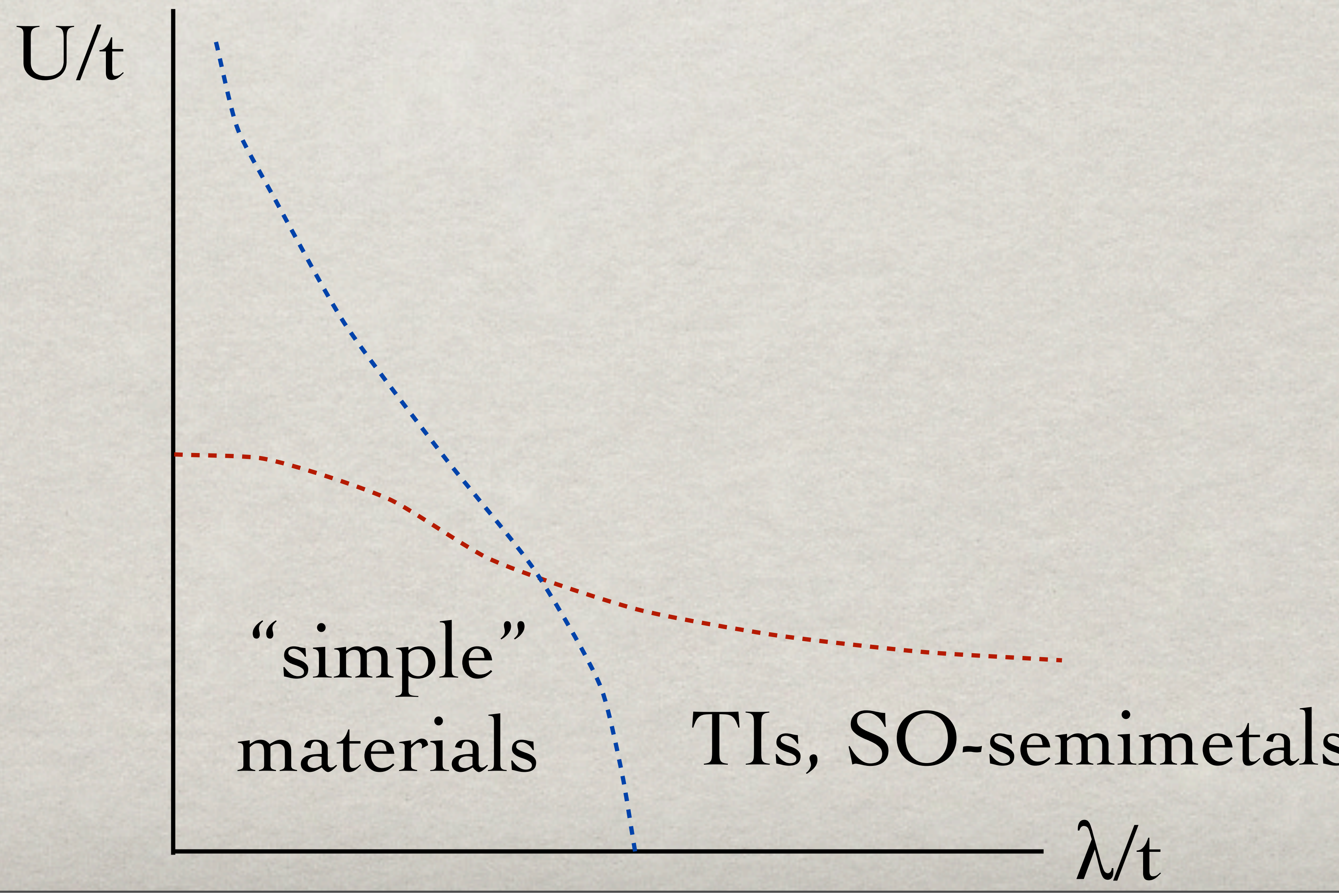

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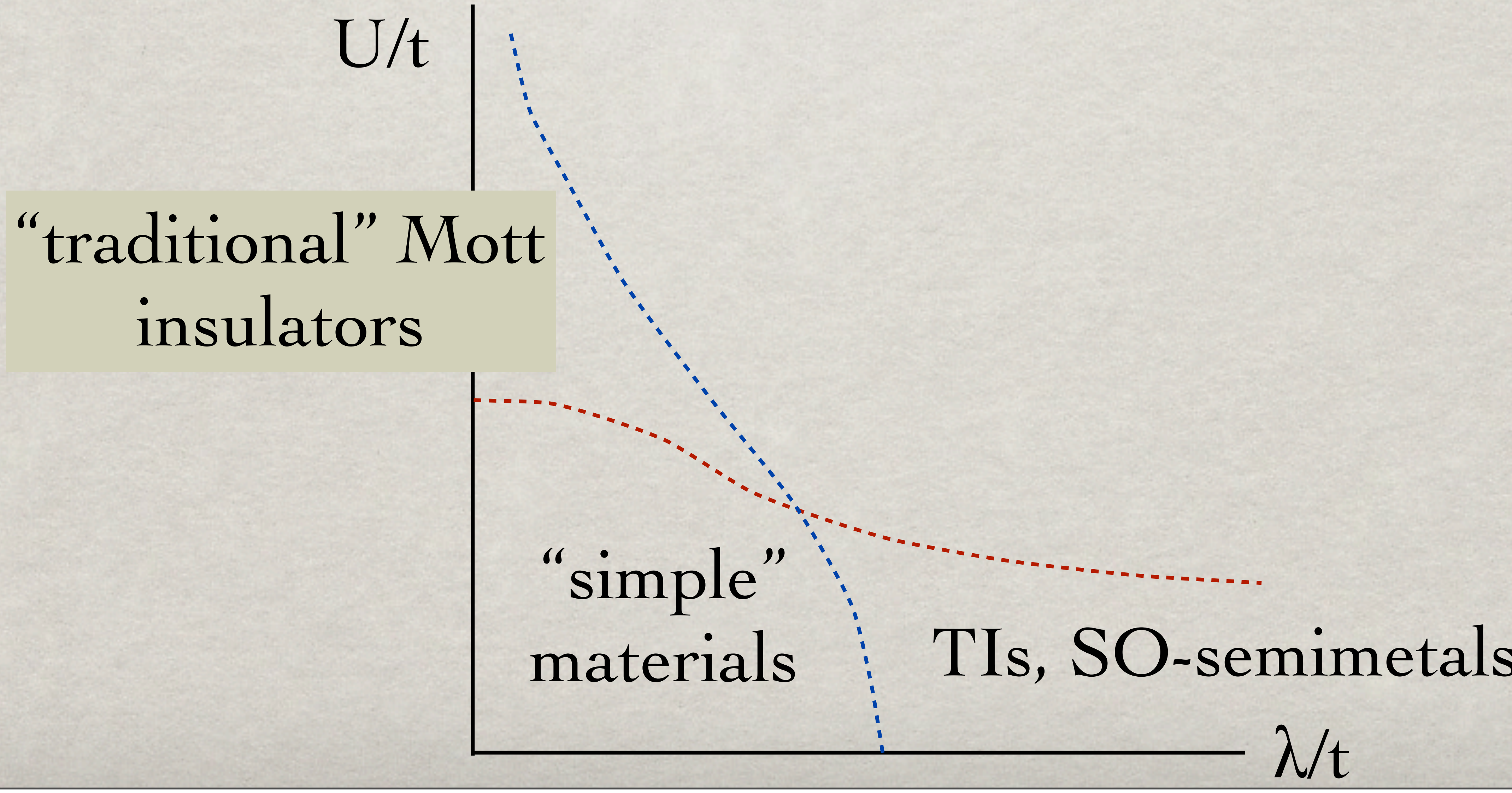
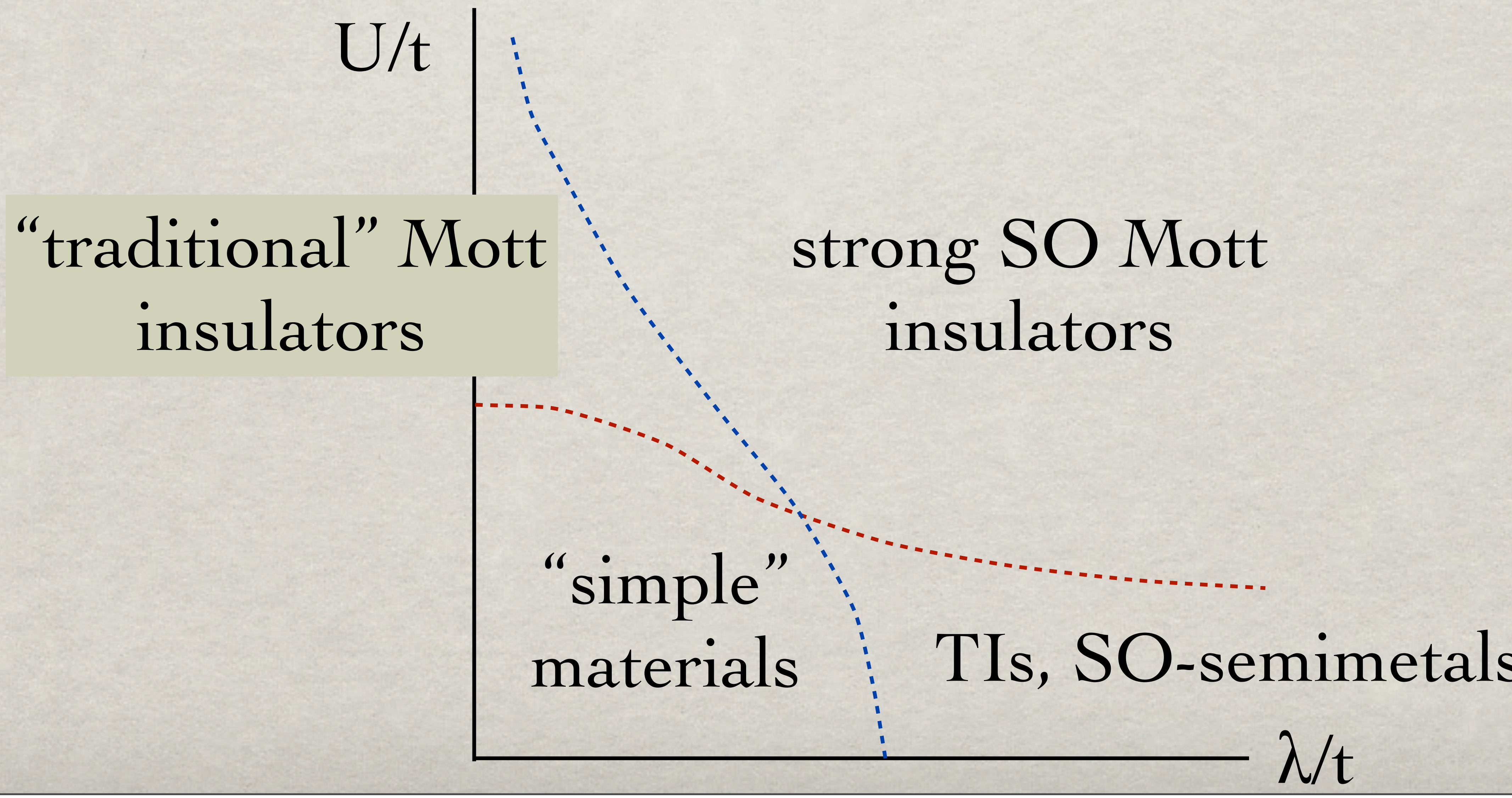


SOC and Interactions

- Hubbard model:

$$H = t\,H_{\rm hop} - \lambda \sum_i \boldsymbol{L}\cdot\boldsymbol{S} + U\sum_i n_i(n_i-1)$$



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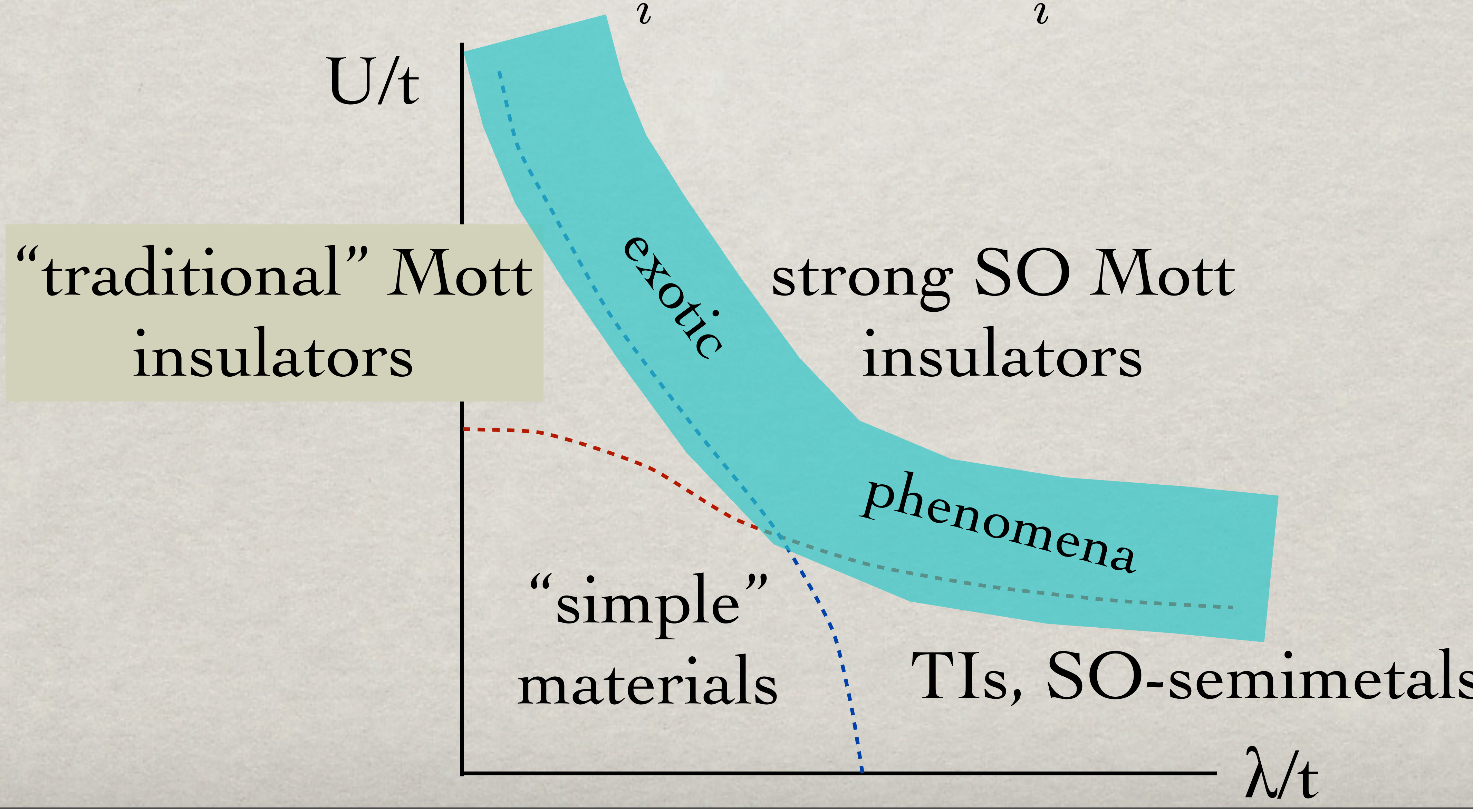
$$H = t\, H_{\text{hop}} - \lambda \sum_i \boldsymbol{L} \cdot \boldsymbol{S} + U \sum_i n_i(n_i - 1)$$



Intermediate regime

- Very common in 5d transition metal oxides:
  - $\lambda \sim U \sim t$ (e.g. Iridates)
- This is a complex regime, with many interesting suggestions:
  - topological Mott insulator — Pesin, Balents 2010; BJ Yang, YB Kim, 2010
  - magnetic topological insulator — Mong, Essin, Moore 2010
  - spin-orbit 3d Dirac semimetal — Wan *et al* 2010

SOC and Interactions

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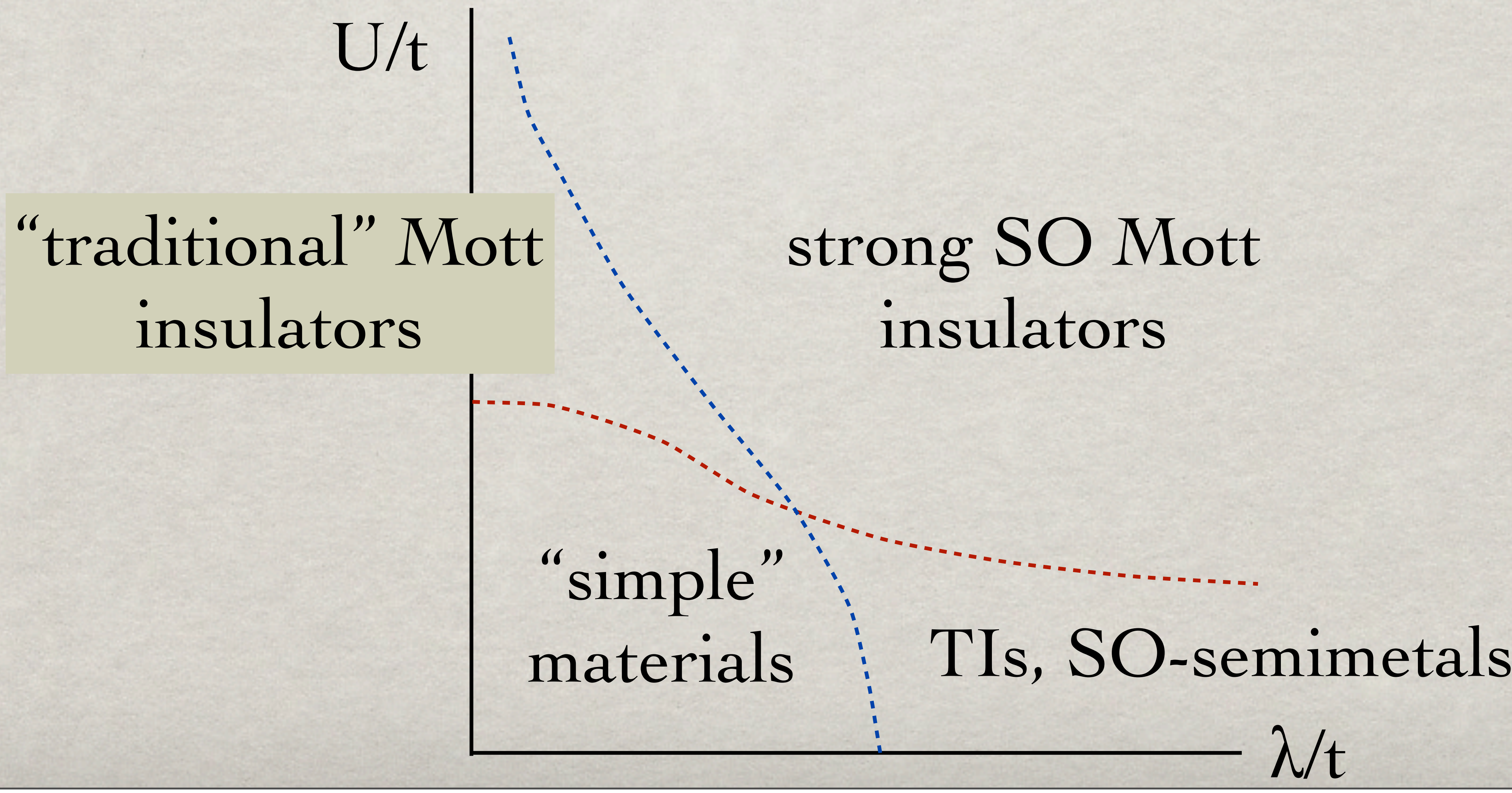
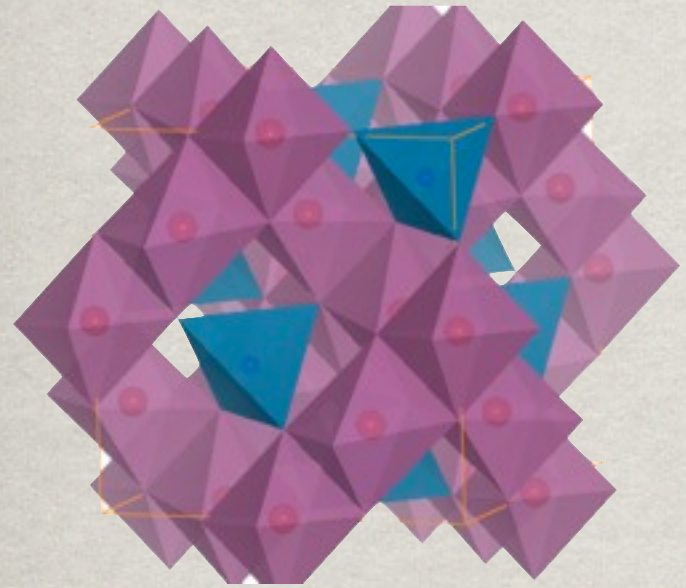
$$H = t\,H_{\text{hop}} - \lambda \sum_i \boldsymbol{L}\cdot\boldsymbol{S} + U\sum_i n_i(n_i-1)$$

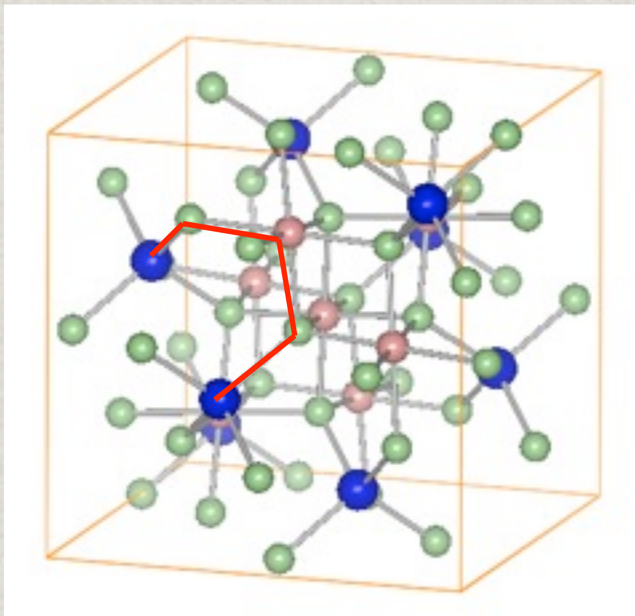


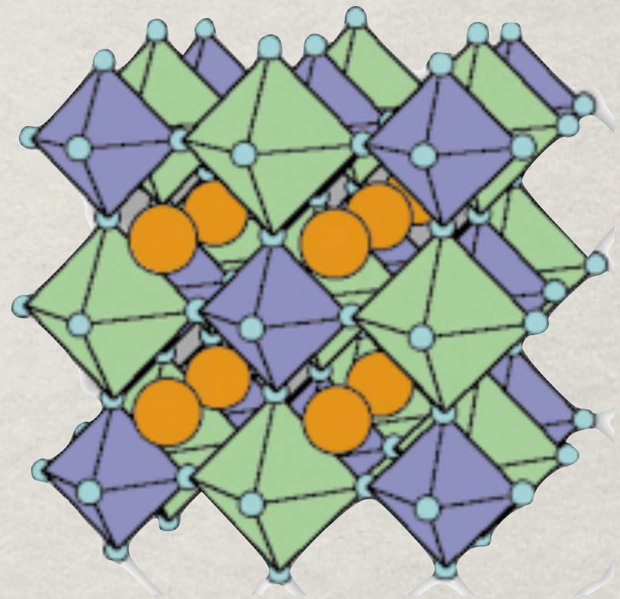
Strong SO + Strong Mott

- Common example: 4f electron systems
  - Here Mott localization is so strong energy scales are very low
- Transition metals: U and λ are anti-correlated, so it is hard to find strong SO Mott insulators
  - Need to seek special situations where bandwidth is unusually low
  - Also need to preserve orbital degeneracy

Strong SO + Strong Mott







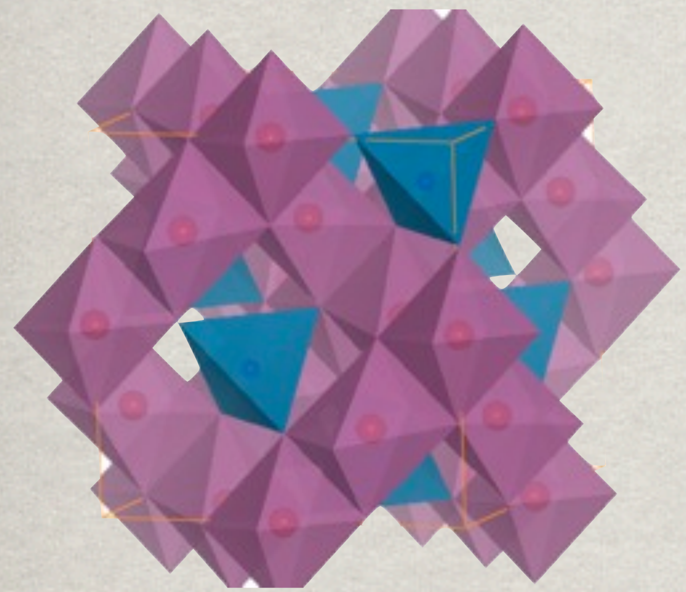
A-site spinels

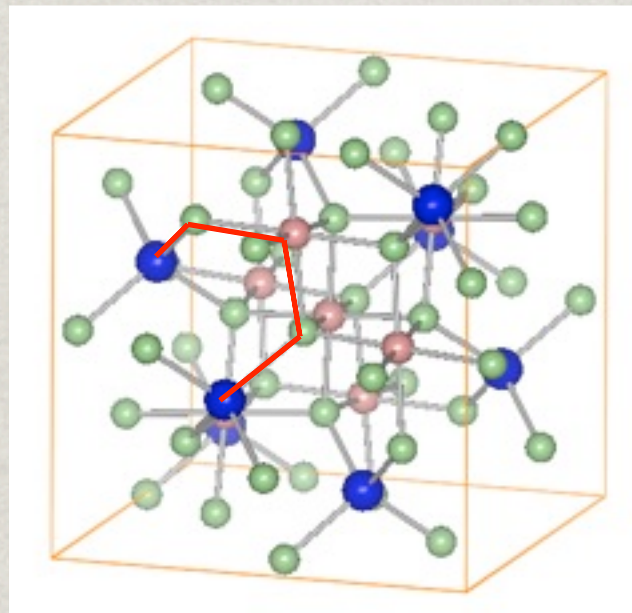
$FeSc_2S_4$

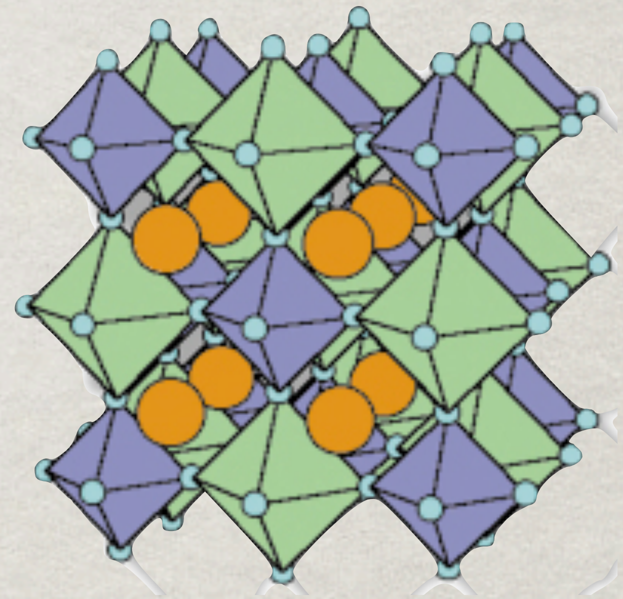
Double perovskites

$A_2BB'O_6$

Strong SO + Strong Mott







A-site spinels

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Double perovskites

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More specifically: insulating rock salt d^0d^1 double perovskites

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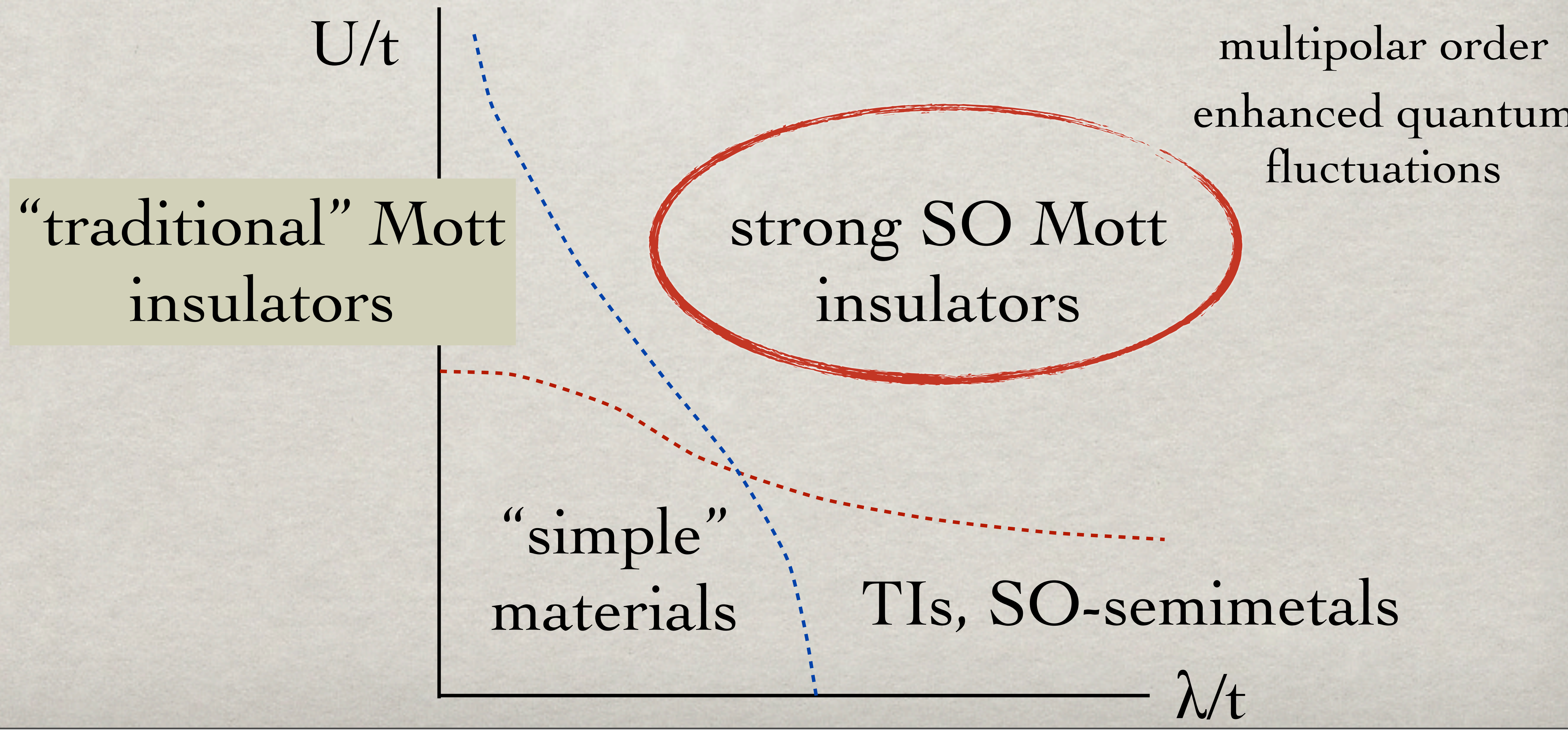

Time for dessert!