# Quantum spin liquids near the Mott transition

T. Senthil (MIT)

Liujun Zou, TS, arXiv (2016)

TS, PR B 78, 045109 (2008)
TS, PR B 78, 035103 (2008)

W. Witczak-Krempa, P. Ghaemi, Y.B. Kim, TS, PR B 2012

# Quantum spin liquids near the Mott transition

Questions:

1. What is a quantum spin liquid? Why is it interesting?

2. Why does it show up near the Mott transition?

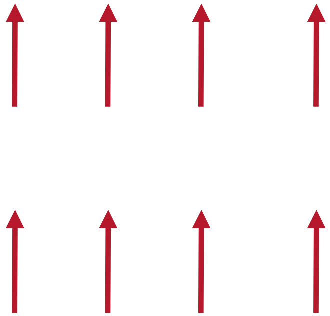
3. What does it teach us about the Mott transition?

# Magnetism in solids

Most familiar form of magnetism: ferromagnetism.

Discovered may be around 600 BC.

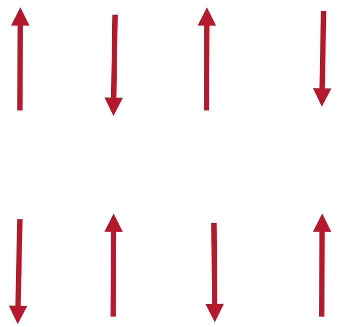
Microscopic picture: Electron spins inside magnet are all pointed in same direction.



Example of broken symmetry: Microscopic interactions do not pick direction for spin but macroscopic magnetized state has specific spin orientation.

# Antiferromagnetism: The more common magnetism

Actually the more common form of magnetism is not the familiar ferromagnetism but is ``antiferromagnetism''.



Also a broken symmetry state -
spin orientation frozen in time but oscillates in space
Microscopic interactions allow any orientation.

Despite being more common antiferromagnetism was discovered only in the 1930s!

Ferromagnetism: easily detected.

Antiferromagnetism: need microscopic probes that sense spin orientation with atomic spatial resolution.

# Quantum description of magnetism

The essential properties of these magnetic states of matter is contained in their ground state wavefunction.

Example: Prototypical wavefunctions

Ferromagnet $\left| \uparrow\uparrow\uparrow\uparrow \cdots\cdots\cdots \right\rangle$

Antiferromagnet $\left| \uparrow\downarrow\uparrow\downarrow \cdots\cdots\cdots \right\rangle$

Prototypical wavefunctions capture the pattern of broken symmetry which holds the key to many macroscopic properties of these phases.

# Crucial feature: short range entanglement

For familiar magnetic states,
prototypical ground state wavefunction factorizes as
**direct product of local degrees of freedom**

$$\left| \uparrow\uparrow\uparrow\uparrow \ldots\ldots\ldots \right\rangle$$

$$\left| \uparrow\downarrow\uparrow\downarrow \ldots\ldots\ldots \right\rangle$$

**Quantum entanglement short ranged in space.**

1930s- present: elaboration of broken symmetry and other states with Short Range Entanglement (SRE).

# Modern times

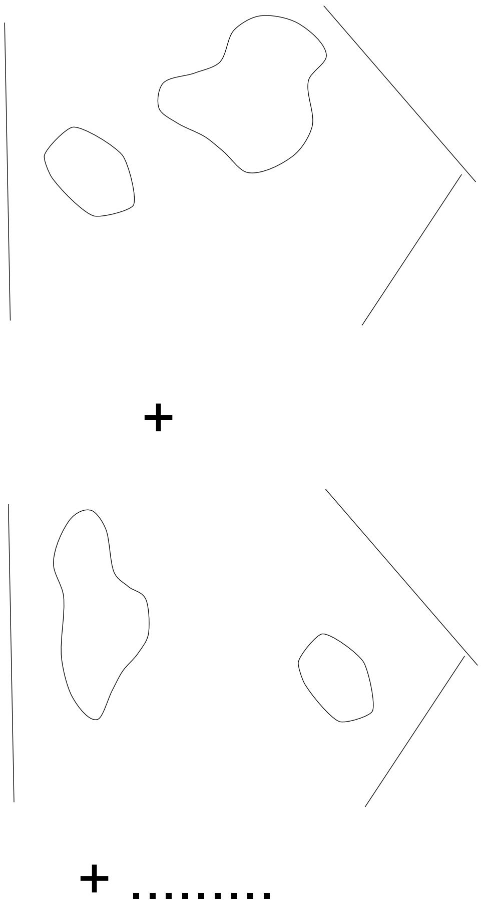
**Experimental discovery of a *qualitatively* new kind of magnetic matter.**

**Popular name: ``quantum spin liquid”**

Prototypical ground state wavefunction

**Not a direct product of local degrees of freedom**.

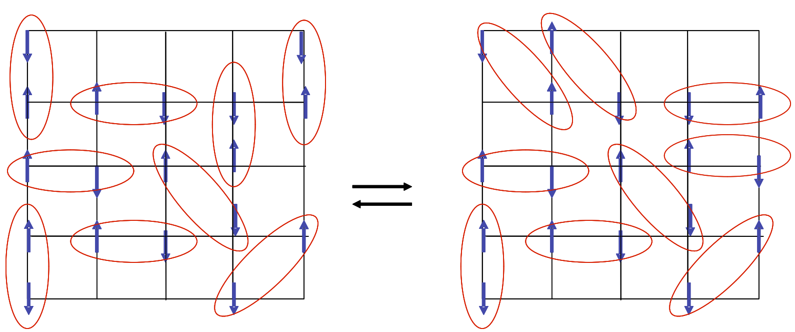
**Quantum entanglement is long ranged in space.**




* In d > 1

# What is a quantum spin liquid?

**Rough(*) description: ``Quantum paramagnet" - Spins do not freeze but fluctuate in time and space due to quantum zero point motion.**
***(*) Caveat: Not all quantum paramagnets (eg, valence bond solids) are quantum spin liquids***



Resonance between many different configurations (like in benzene)
In each configuration each spin forms an ***entangled pair*** with one other partner spin.

Envisaged by P.W. Anderson (1973, 1987); older suggestion of Pauling (1950s)

# Long Range Entangled (LRE) phases

**Universal information about state not visible by looking only at small part of system.**

**Older very famous example: Fractional quantum Hall states.**

**Other fascinating examples: metallic ground state of electrons.**

**Conventional metals: ``Fermi Liquid" state (oldest familiar Long Range Entangled state)**

**Many new metals: ``Non-fermi liquids"**

# Can quantum spin liquid phases exist?
# Question for theory

Yes!!! (work of many people over last 20 years)

Many dramatic phenomena seen to be theoretically possible.

Examples:

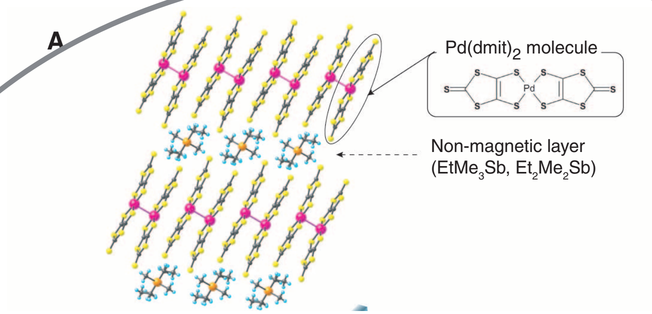
1. Electron can break apart into fractions

2. Emergence of long range quantum mechanical interactions between fractional pieces of electron.

Similar phenomena established in FQHE in two dimensions but now are known to be possible in much less restrictive situations.

# Do quantum spin liquid phases exist?
# Question for experiment

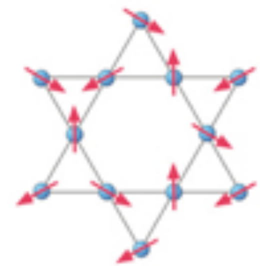
Yes - many interesting candidate materials in last few years!!




Layered organic crystals

$\kappa-(ET)_2Cu_2(CN)_3$ Kanoda et al, 2003-now

$EtMe_3Sb[Pd(dmit)_2]_2$ Kato et al, 2008



Some layered inorganic minerals

$ZnCu_3(OH)_6Cl_2$ (Y. Lee, Nocera et al, 2007)

Herbertsmithite

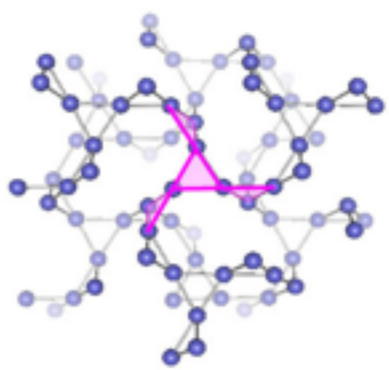
$Cu_3V_2O_7(OH)_2\cdot 2H_2O$ (Z. Hiroi et al, 2010)

Volborthite

Three dimensional transition metal oxide

$Na_4Ir_3O_8$

(H. Takagi et al, 2008)



# Some phenomena in experiments

Quantum spin liquid materials are all electrical insulators.

Despite this (in some candidate materials) many properties other than electrical conduction are very similar to that of a metal.

Two examples at low temperature:

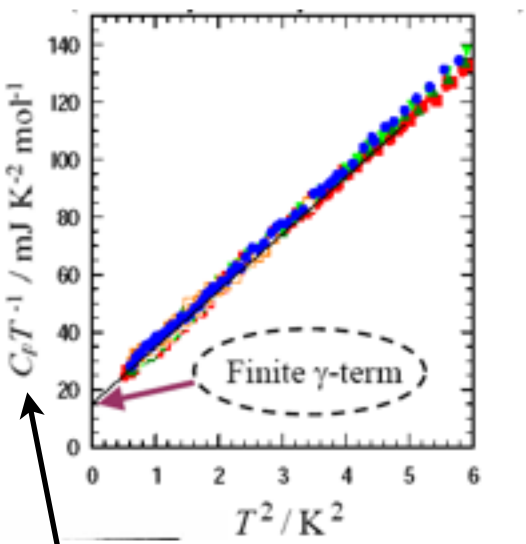
1. Entropy very similar to that of a metal at low temperature

2. Conduct heat just like a metal even though they are electrical insulators.

Very strange......not known to happen in any ordinary insulator.

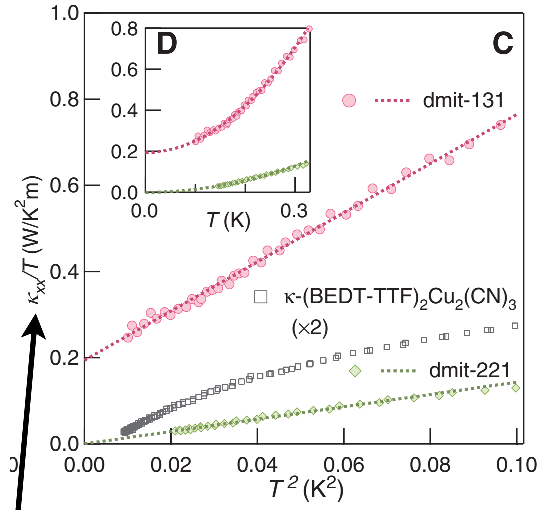
# Some phenomena in experiments

S. Yamashita et al, Nat Phys, 2008




Heat capacity

M.Yamashita et al, Science 2010




Thermal conductivity

These are both exactly like in a metal but were measured in an insulator.

# Towards understanding experiments

Low-T properties of metals are determined by mobile electrons obeying Pauli exclusion principle.

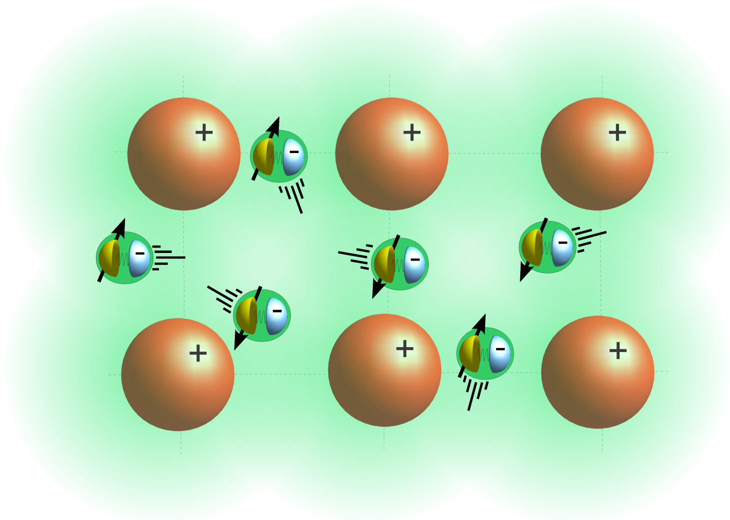
In an insulator there cannot be mobile electrons.

A promising idea: perhaps there are emergent particles obeying Pauli exclusion that carry the electron spin but not its charge inside these materials.

Such phenomena are known to be theoretically possible in quantum spin liquid phases (but are prohibited in more conventional phases)

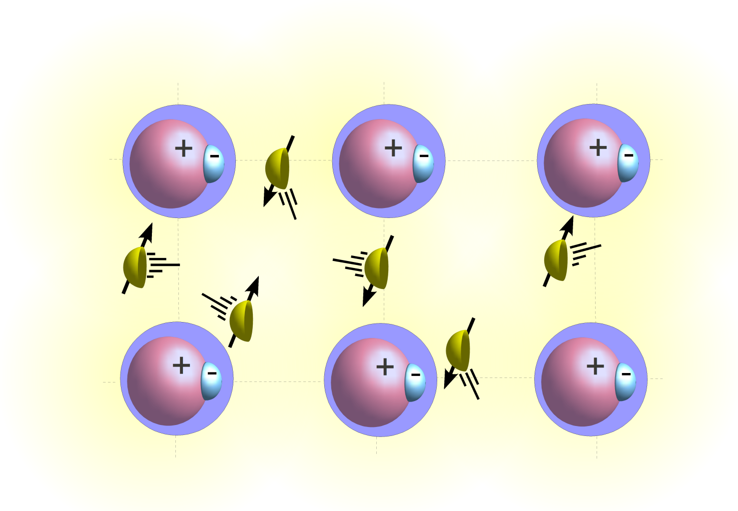
# Picture of (one example of) a quantum spin liquid

Metal



Electrons swimming in sea of +vely charged ions

A quantum spin liquid



Electron charge gets pinned to ionic lattice while spins continue to swim freely.

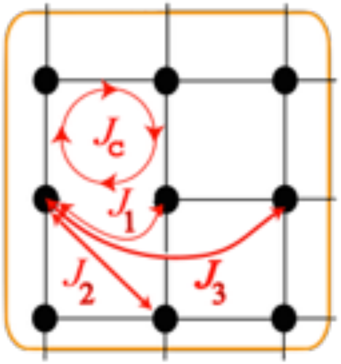
# Why near Mott transition?

Vicinity of Mott transition

- Large virtual charge fluctuations frustrate magnetic ordering; short distance physics is that of a metal even if insulating at long distances.

Approach from insulator:

Must supplement Heisenberg exchange with multi-particle ``ring exchange''.




Such ring exchange promotes spin spin liquids
Many kinds of numerics: Exact diagonalization (Li Ming et al, 2000; H.-Y. Yang et al, 2010), Variational wave functions (Motrunich, 05, …..), Density Matrix Renormalization Group on strips (Sheng et al, 09).

# Why organic materials?

Easy to tune through the Mott transition with pressure.

Layered frustrated geometry increases quantum fluctuations (of local moments) => weaken magnetic ordering allowing the spin liquid to successfully compete.

Discovery of quantum spin liquids in organics and other materials is one of the most exciting chapters in condensed matter physics!

- ``long range quantum entanglement” in magnetic systems

- fractional quantum numbers, emergent gauge forces
- .........

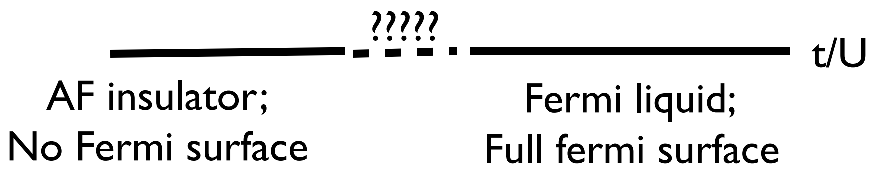
Rest of this talk: lessons from quantum spin liquids for the Mott transition.

# The electronic Mott transition

Difficult old problem in quantum many body physics

How does a metal evolve into a Mott insulator?

Prototype: One band Hubbard model at half-filling on non-bipartite lattice



# Why hard?

1. No order parameter for the metal-insulator transition

2. Need to deal with gapless Fermi surface on metallic side

3. Complicated interplay between metal-insulator transition and magnetic phase transition

Typically in most materials the Mott transition is first order.

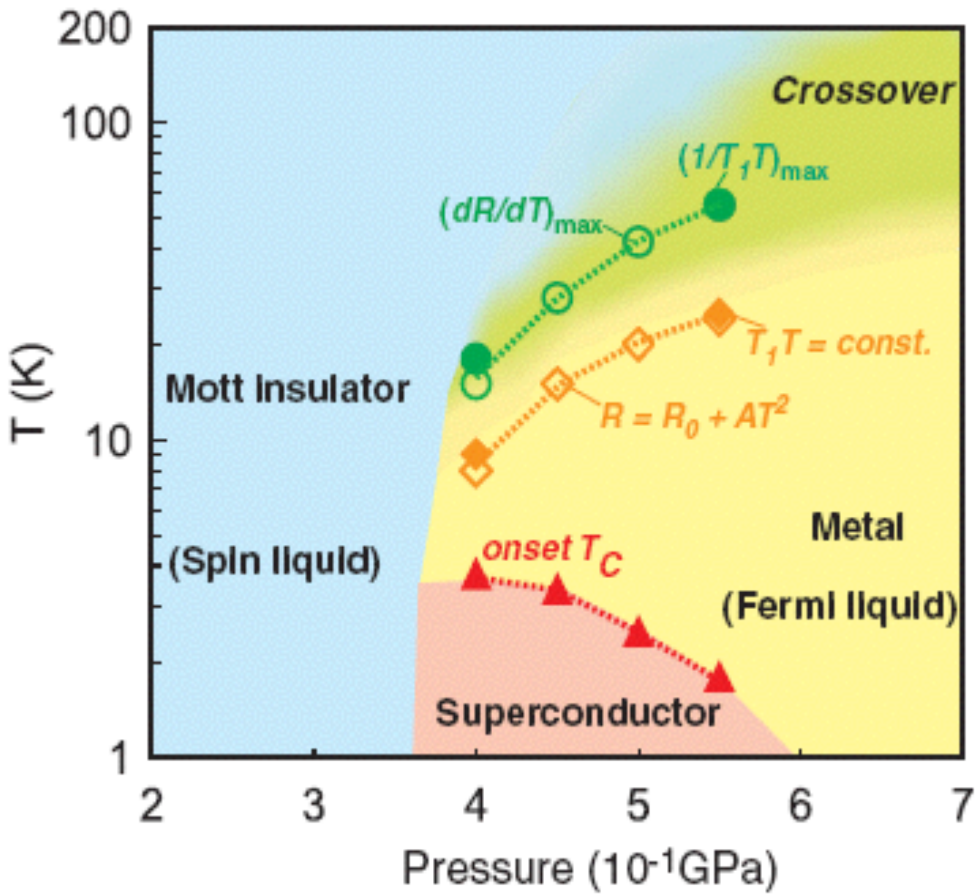
But (at least on frustrated lattices) transition is sometimes only weakly first order
- fluctuation effects visible in approach to Mott insulator from metal.

Quantum spin liquid Mott insulators:

Opportunity for progress on the Mott transition -
study metal-insulator transition without complications of magnetism.

# Possible experimental realization of a second order(?) Mott transition

Kanoda et al, 03- now



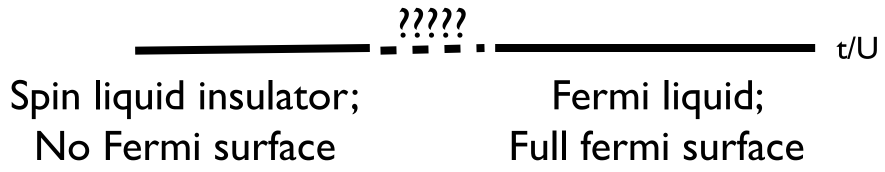

$\kappa-(ET)_2Cu_2(CN)_3$ under pressure

# Quantum spin liquids and the Mott transition

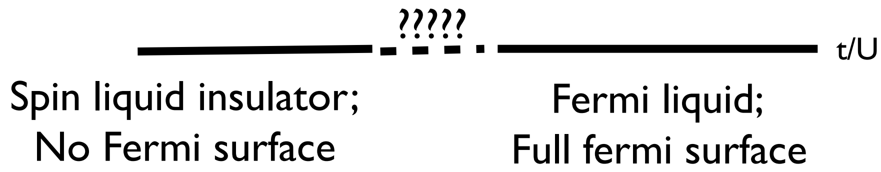
Some questions:

1. Can the Mott transition be continuous?

2. Fate of the electronic Fermi surface?



# Killing the Fermi surface




At half-filling, through out metallic phase,
Luttinger theorem => size of Fermi surface is fixed.

Approach to Mott insulator: entire Fermi surface must
die while maintaining size (cannot shrink to zero).

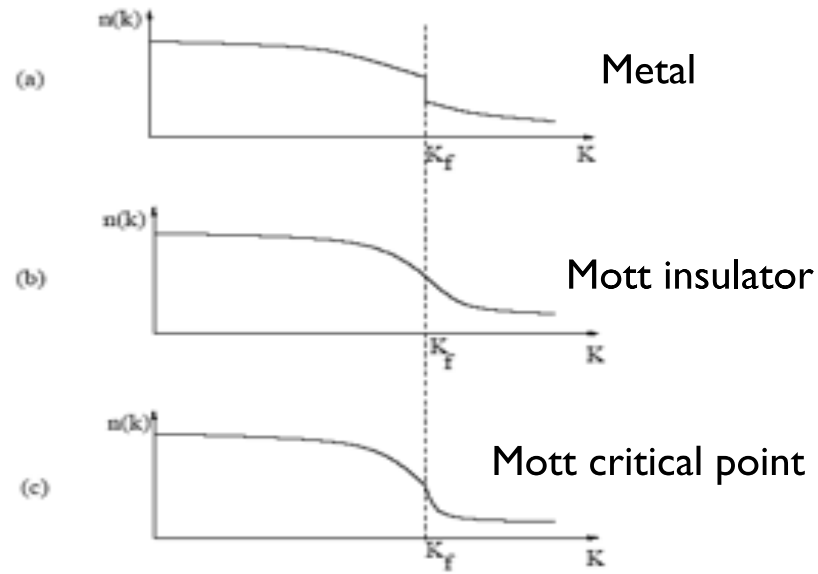
If Mott transition is second order, critical point necessarily very unusual.

``Fermi surface on brink of disappearing" - expect non-Fermi liquid physics.

Similar ``killing of Fermi surface" also at Kondo breakdown transition
in heavy fermion metals, and may be also around optimal doping in cuprates.

# How can a Fermi surface die continuously?

Continuous disappearance of Fermi surface if quasiparticle weight Z vanishes continuously everywhere on the Fermi surface (Brinkman, Rice, 1970).




Concrete examples: Slave particle theories in d = 2, d = 3 (TS, Vojta, Sachdev 2003, TS 2008); DMFT in infinite d (Vollhardt, Metzner, Kotliar, Georges 1990s),

# Basic question for theory

Crucial question: Nature of electronic excitations right at quantum critical point when Z = 0.

Claim: At critical point, Fermi surface remains sharply defined even though there is no Landau quasiparticle.

TS, 2008

``Critical Fermi surface”.

# Why a critical Fermi surface?

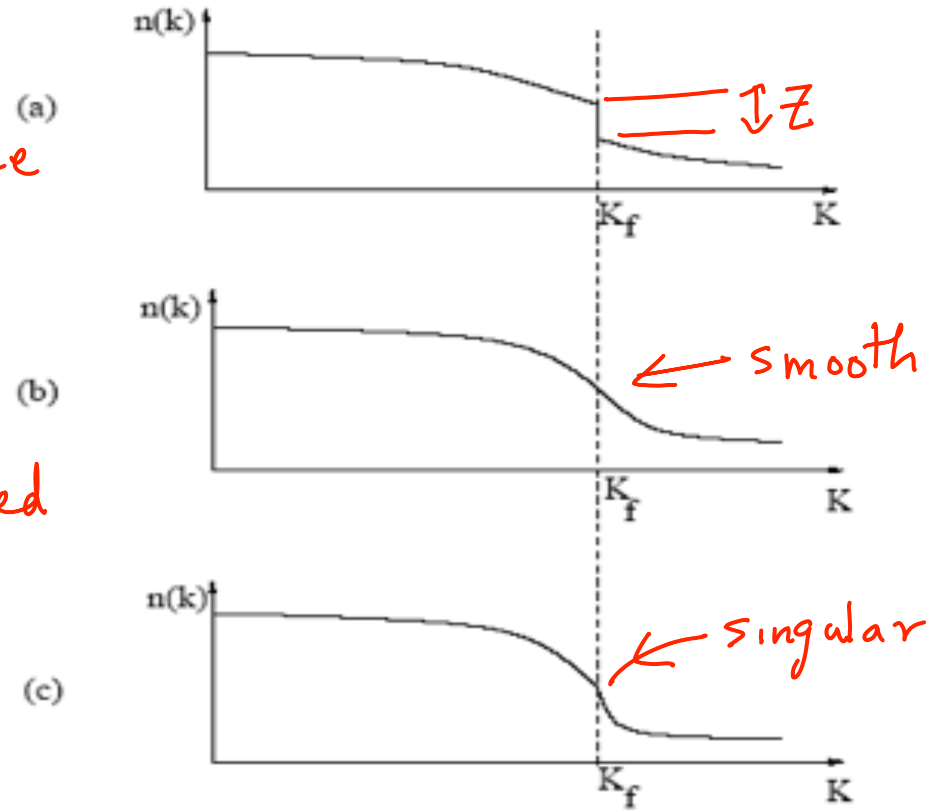
## Evolution of momentum distribution

Metal with Fermi surface

Phase where Fermi surface has disappeared

Critical point

n (K) continuous at $K_F$ but is singular

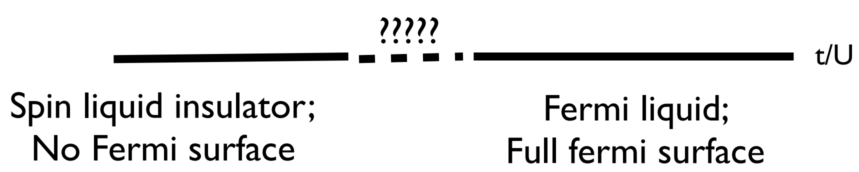


# Quantum spin liquids and the Mott transition

Some questions:

1. Can the Mott transition be continuous at T = 0?

2. Fate of the electronic Fermi surface?




Only currently available theoretical framework to answer these questions is slave particle gauge theory.

(Mean field: Florens, Georges 2005;
Spin liquid phase: Motrunich, 05, S.S. Lee, P.A. Lee, 05)

# Slave particle framework

Split electron operator

$$c_{r\sigma} = b_r f_{r\alpha}$$

Fermi liquid: $\langle b \rangle \neq 0$

Mott insulator: $b_r$ gapped

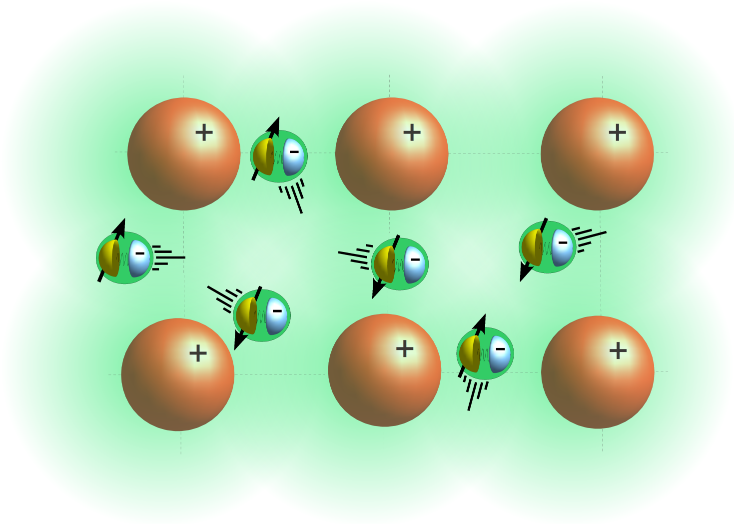
Mott transition: $b_r$ critical

In all three cases $f_{r\alpha}$ form a Fermi surface.

Low energy effective theory: Couple $b, f$ to fluctuating $U(1)$ gauge field.

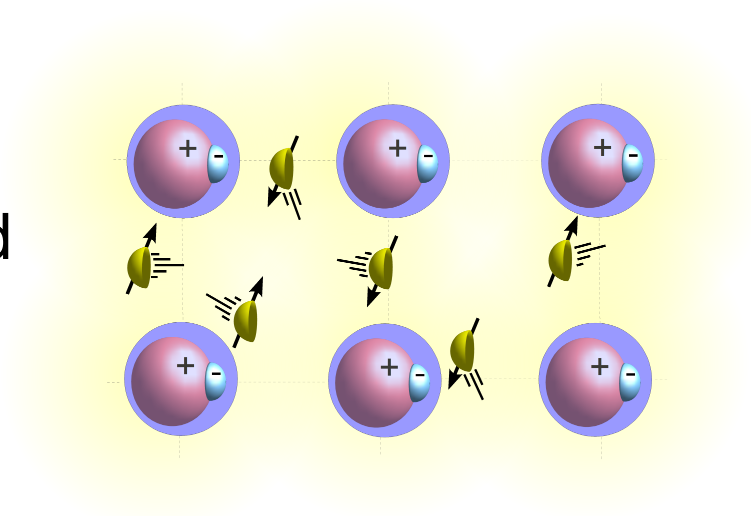
# Picture of Mott transition

Metal



Electrons swimming in sea of +vely charged ions

Mott spin liquid near metal



Electron charge gets pinned to ionic lattice while spins continue to swim freely.

# Quantum spin liquids and the Mott transition

1. Can the Mott transition be continuous?

2. Fate of the electronic Fermi surface?

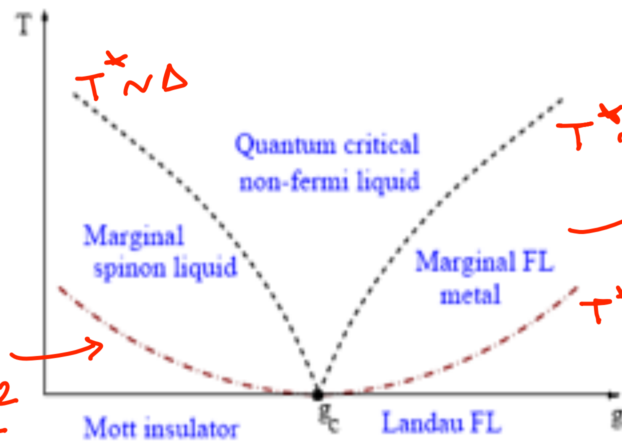
Analyse fluctuations: Concrete tractable theory of a continuous Mott transition (TS 2008); demonstrate critical Fermi surface at Mott transition;

Definite predictions for many quantities (TS, 2008, Witczak-Krempa, Ghaemi, Kim, TS, 2012).

- Universal jump of residual resistivity on approaching from metal
- Log divergent effective mass
- Two diverging time/length scales near transition
- Emergence of marginal fermi liquids

# Finite-T crossovers: emergence of a Marginal Fermi Liquid

TS, 2008




$T^* \sim \Delta$

$T^{**} \sim \frac{\Delta^2}{\sqrt{Ut}}$

$T^* \sim \rho_s$

$T^{**} \sim \frac{\rho_s^2}{\sqrt{Ut}}$

In this regime electron Greens function

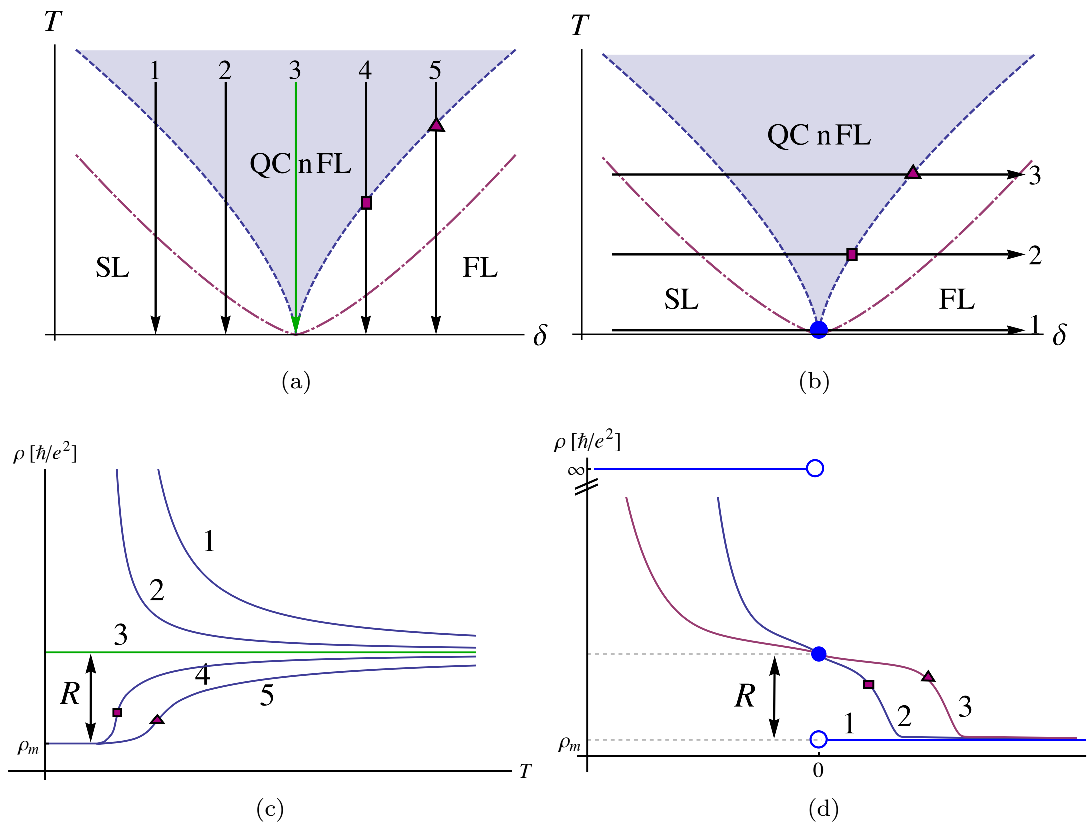
$$G(\vec{k}, i\omega) \sim \frac{|\langle b \rangle|^2}{i\omega\left(1 + a \ln \frac{1}{|\omega|}\right) - \epsilon_k}$$

= Marginal FL form proposed for hiTc by Varma et al '89

# Low temperature electrical transport

TS 08; Witczak-Krempa, Ghaemi, TS,Kim, 12

Universal jump of residual resistivity on approaching from metal




$$\rho - \rho_m = \frac{\hbar}{e^2} G\left(\frac{\delta^{z\nu}}{T}\right)$$

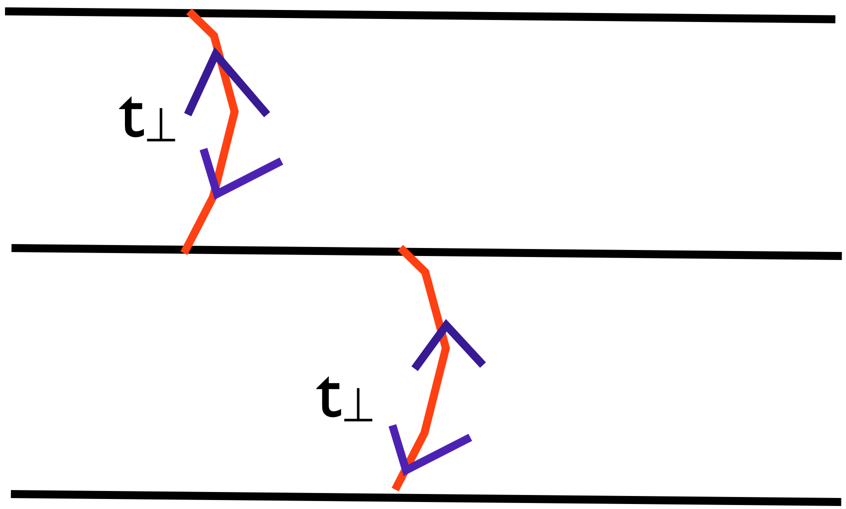
$$z = 1,\ \nu \approx 0.672$$

# Some new results: The continuous Mott transition in a layered system

Real materials: Layered 3d with weak interlayer tunneling of electrons.

Fermi liquid regime: Interlayer tunneling coherent => 3d metal.

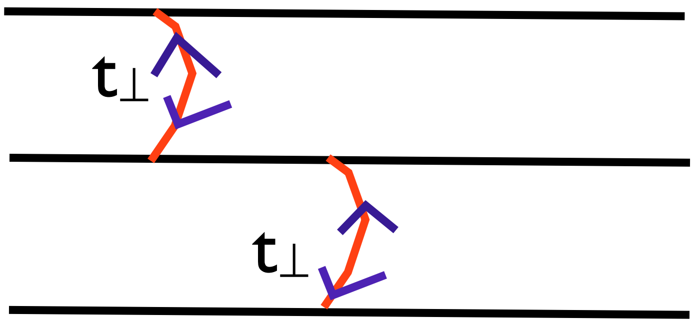
Spin liquid Mott insulator: Spinons cannot tunnel coherently => different layers dynamically decouple (in-plane spinon metal but interlayer spinon insulator).

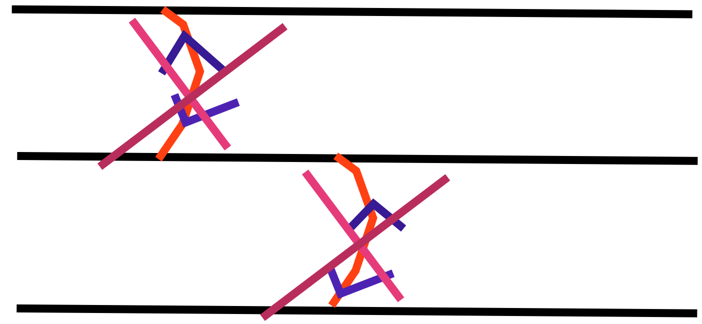



Liujun Zou, TS, 16

Liujun Zou, TS, 16

# Interlayer coherence: Metal vs spin liquid Mott insulator



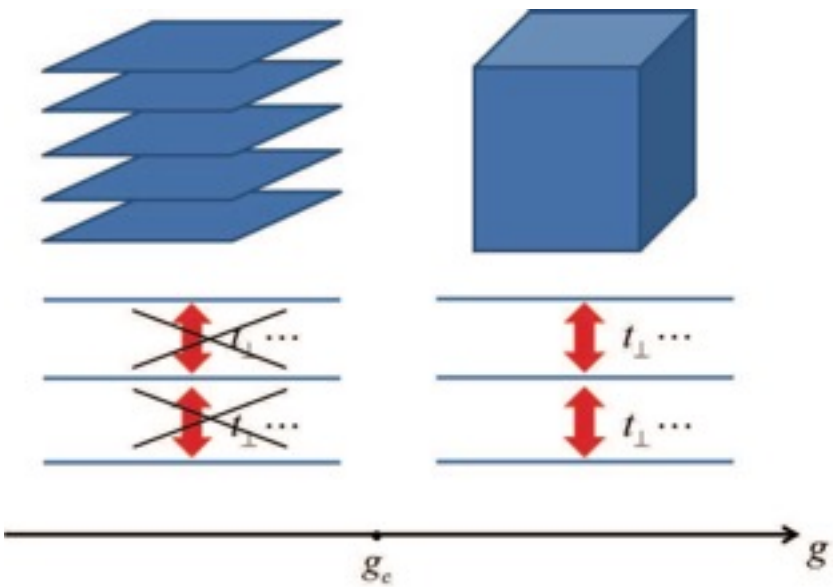



Metal: coherent 3d metal at T = 0.

Spin liquid: interlayer hopping of spinons is blocked; interlayer thermal insulator at T = 0 (but in-plane thermal conductor).

What happens to Mott quantum crtical point?

# Dimensionality-change at the Mott transition



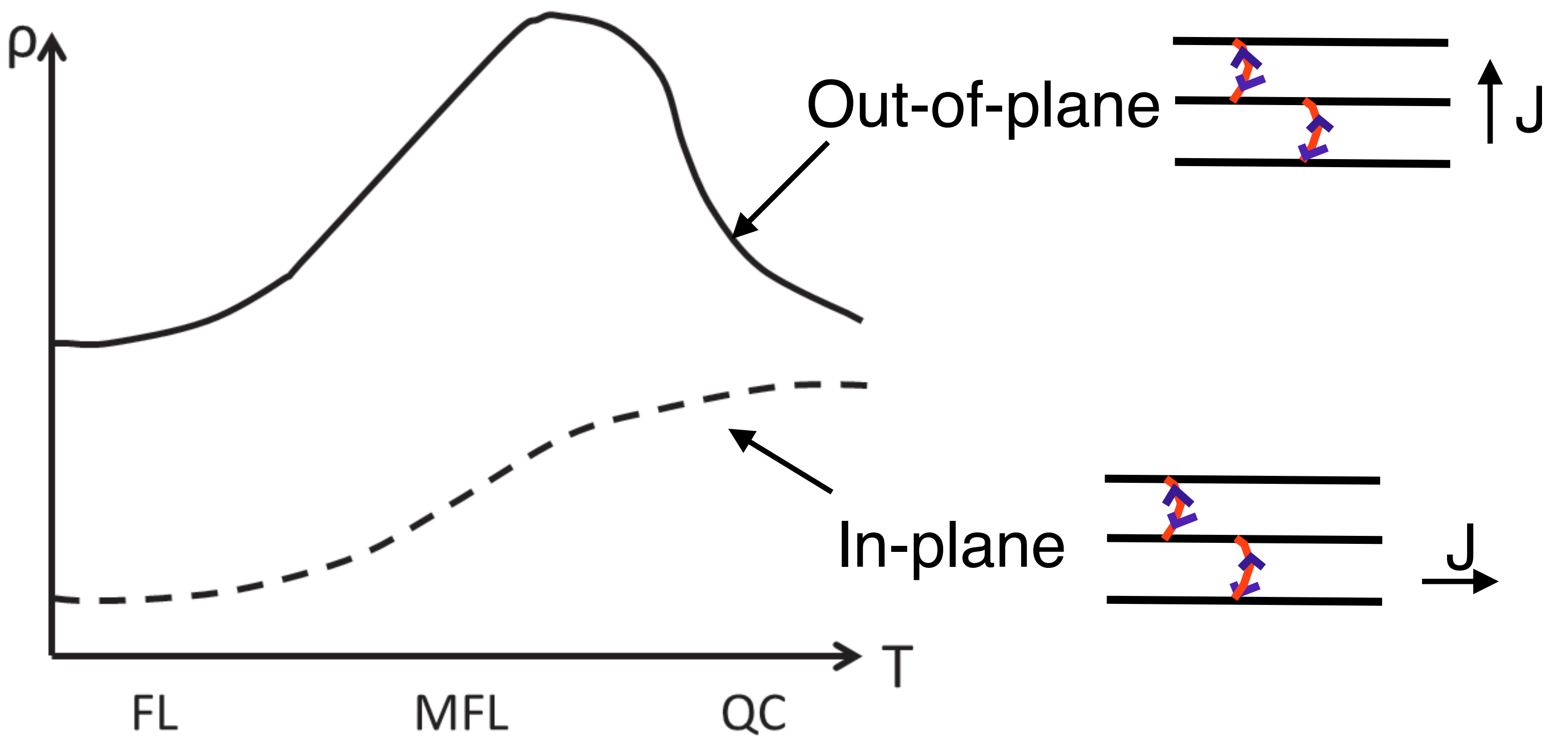

Results (Zou, TS, 2016)
Dimensional decoupling occurs already at quantum critical point (QCP).

Electrical transport at bandwidth tuned QCP:
Metallic in-plane resistivity $\rho$ = const.
Insulating out-of-plane $\rho \approx 1/T$.

Nearly critical metal:
``Coherence peak" in interlayer resistivity:

Liujun Zou, TS, 16

# Nearly critical metal: Interplane versus in-plane transport




- Similar phenomena near chemical potential tuned continuous Mott transition (applications to doped organics, cuprates?)

# Summary

Quantum spin liquids - exciting new chapter in old field of magnetism.

Quantum spin liquids in organic materials provide an opportunity for progress on classic old problems: Mott and other metal-insulator transitions.

Continuous Mott transition possible; several predictions for experiment (eg: universal resistivity jump in d = 2 plus incoherent interlayer insulator)

Lessons for cuprates, heavy fermions, and other central problems in modern condensed matter physics.