Quantum spin liquids and the Mott transition

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D. Mross and T. Senthil, PRB 10; PRB 11;
T. Grover, N. Trivedi, T. Senthil, P.A. Lee, PR B 10.

T. Senthil, PR B 08
D. Podolsky, A. Paramekanti, Y.B. Kim, T. Senthil, PRL 09

Potter,Barkeshli, McGreevy, TS, forthcoming.

States of quantum magnetism

Ferromagnetism: May be 600 BC

$$|\uparrow\uparrow\uparrow\uparrow \ldots\ldots\ldots\rangle$$

Antiferromagnetism: 1930s

$$|\uparrow\downarrow\uparrow\downarrow \ldots\ldots\ldots\rangle$$

Key concept of broken symmetry.

Prototypical ground state wavefunction:
direct product of local degrees of freedom

Short range quantum entanglement.

1930s- present: elaboration of broken symmetry and other
states with short range entanglement

Last ≈ 10 years

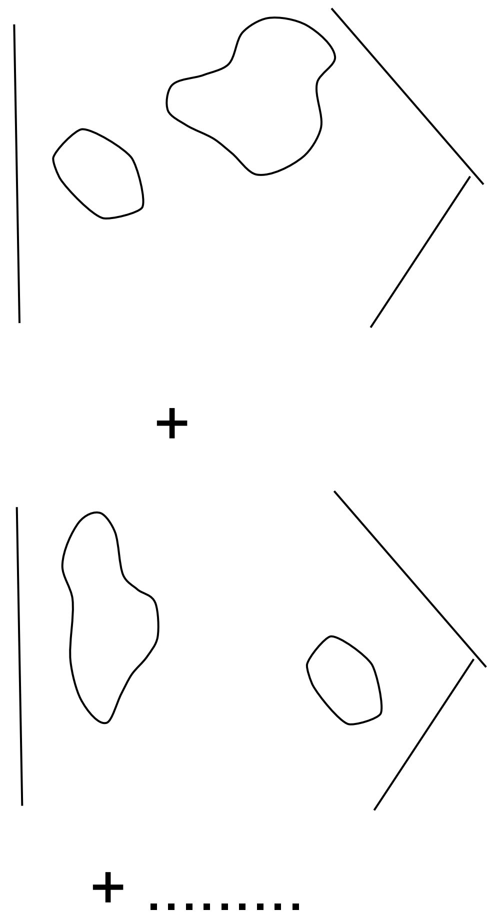
Experimental discovery of quantum spin liquid state*.

Qualitatively new kind of state of matter.

Prototypical ground state wavefunction

Not a direct product of local degrees of freedom.

Long range quantum entanglement



* In d > 1

Long Range Entangled Phases

Phases with Long Range Entanglement (LRE): new chapter in condensed matter physics at least as rich as previous chapter (LRO phases)

Many new phenomena - emergence of fractional quantum numbers.

New conceptual and technical theoretical tools to understand.

May be also new kinds of experimental probes will be most useful.

Other examples: fractional quantum Hall phases, Fermi and non-Fermi liquids,.......

Some candidate materials

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

$EtMe_3Sb[Pd(dmit)_2]_2$

Quasi-2d, approximately isotropic triangular lattice; best studied candidate spin liquids

$Na_4Ir_3O_8$

Three dimensional `hyperkagome' lattice

$ZnCu_3(OH)_6Cl_2$

Volborthtite, ...

2d Kagome lattice (`strong' Mott insulator)

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Three dimensional `hyperkagome' lattice

Close to pressure driven Mott transition: `weak' Mott insulators

$ZnCu_3(OH)_6Cl_2$

Volborthtite, ...

2d Kagome lattice (`strong' Mott insulator)

Some phenomena in experiments

ALL candidate materials:

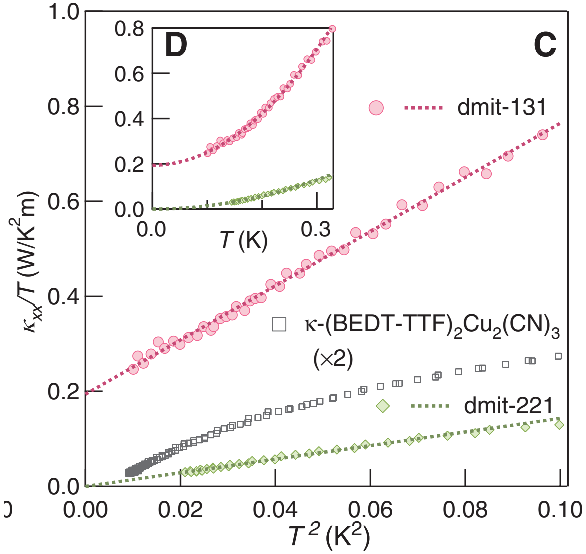
No magnetic ordering down to lowest measured T (<< natural exchange scales J)

BUT

Gapless excitations down to T << J.

Most extensively studied in organic spin liquids with J ≈ 250 K.

Example: Thermal transport
in dmit SL.
M. Yamashita et al, Science 2010.



Plan for talk

1. Quantum spin liquids in weak Mott insulators

Key idea: Gapless fermionic ``spinons" with a Fermi surface at intermediate scales. (Baskaran, Anderson'87; ....**Motrunich**, 2005, S.S. Lee, P.A. Lee, 05)

2. Detecting the spinon Fermi surface

3. Quantum spin liquids and metal-insulator transitions

Theoretical approaches to quantum spin liquids in a weak Mott insulator

Approach from insulator

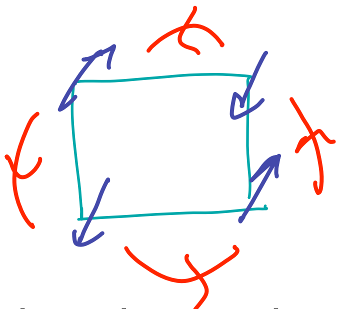
$t/U \nearrow \Rightarrow$ Build in more virtual charge fluctuations in ground state wave function

$$H_{eff}[\{\vec{S}_i\}] = \sum_{ij} J_{ij}\, \vec{S}_i \cdot \vec{S}_j + K \sum_{\square} \left(P_{1234} + P^{-1}_{1234}\right) + \cdots$$

longer range exchange

Motrunich, 2005

P_{1234} =



= 4-particle ring exchange, etc

Various numerics: ring exchange promotes spin liquids (LiMing et al 00, Motrunich 05, H.-Y. Yang et al, 2010)

Alternate: approach from the metal

Interacting Fermi fluid: Incorporate correlations with Jastrow factor

$$\psi_F(\mathbf{r}_1\sigma_1, ...\mathbf{r}_N\sigma_N) = \prod_{ij} f(\mathbf{r}_i - \mathbf{r}_j)\psi_{Slater}(\mathbf{r}_1\sigma_1, ...\mathbf{r}_N\sigma_N) \quad (1)$$

Special case: Gutzwiller approximation to lattice Hubbard model; choose

$$f_{ij} = g\delta_{ij} \quad (2)$$

with $g < 1$ to weigh down double occupancy of any site.

An interesting point of view

Can think of $\psi_F = (\text{Jastrow}) \times \psi_{slater}$

as $\psi_F = \psi_b(\vec{r}_1, \ldots, \vec{r}_N)\, \psi_{slater}(\vec{r}_1\sigma_1, \ldots, \vec{r}_N\sigma_N)$

(where $\psi_b(\vec{r}_1, \ldots, \vec{r}_N)$ is the Boson wave fn)

Clearly any choice of ψ_b will give a legitimate fermion wavefunction

Choosing ψ_b as wavefunction of superfluid leads to the Fermi liquid wavefunction ψ_F.

Obtaining a Mott insulator from the metal

Start with wavefunction of correlated metal

$$\Psi_f(\vec{r}_1\sigma_1, \cdots, \vec{r}_N\sigma_N) = \underbrace{\Psi_b(\vec{r}_1, \cdots, \vec{r}_N)}_{\text{superfluid}}\,\Psi_{slater}(\{\vec{r}_\ell\sigma_\ell\})$$

How to get a Mott insulator?

Let $\Psi_b \rightarrow$ wavefunction of localized solid of bosons

$\Rightarrow$ freeze out charge motion

$\Psi_f = \Psi_b^{solid}\,\Psi_{slater}$ is wavefunction for fermionic Mott insulator!

Comments

$\psi_F = \psi_b^{solid}\psi_{Slater}$ is a spin singlet wavefunction. Expect spin correlations similar to a metal?

Extreme limit: Completely freeze out all charge fluctuations

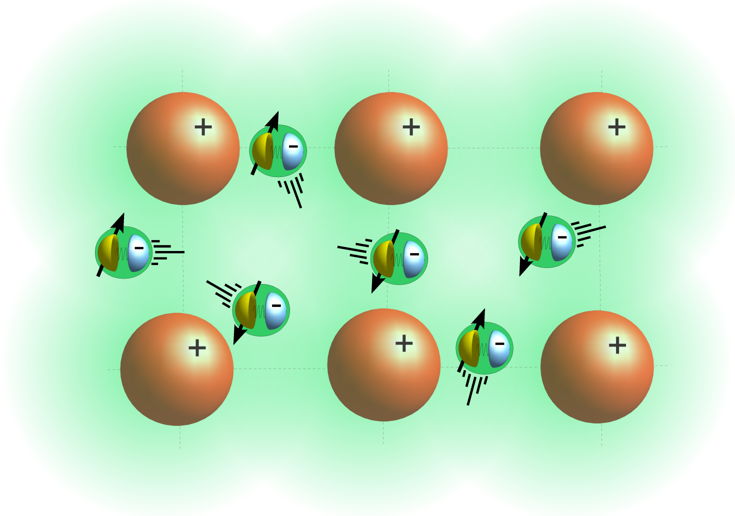
$$\psi_b^{solid} \to P_G \tag{1}$$

Gutzwiller projector $P_G = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$

Result: Pure spin wavefunction; can be tested variationally on ring exchange spin models derived in t/U expansion.

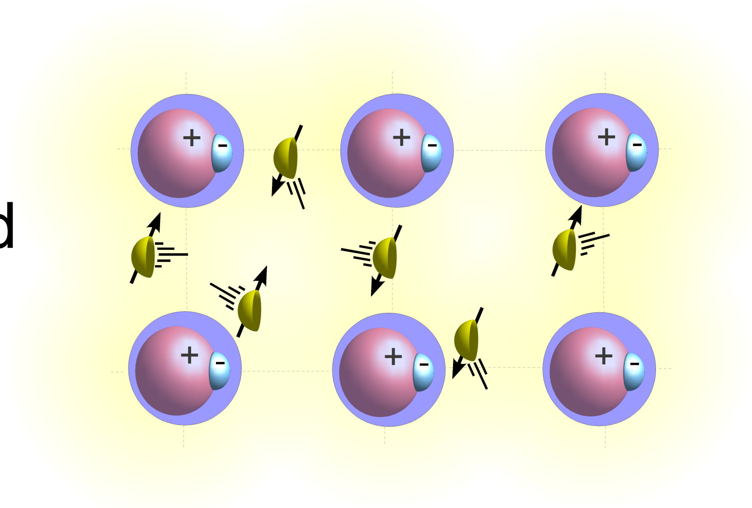
Picture of Mott transition

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.

Formal theory

Slave particle representation:

$$c_\alpha = b f_\alpha$$

b: charge-e spin-0 boson (chargon/holon)

f: charge-0 spin-1/2 fermion (spinon)

Slave boson mean field theory:

$$H_{mf} = H_b + H_f \quad (1)$$

$$H_b = -t_c \sum_{<ij>} \left(b_i^\dagger b_j \right) + U \sum_i \frac{n_i(n_i - 1)}{2} \quad (2)$$

$$H_f = - \sum_{<ij>} t_{ij}^s \left(f_i^\dagger f_j + h.c \right) \quad (3)$$

Correlated metal: $t_c \gg U$, $< b > \neq 0$.

Mott insulator: $U \gg t_c$, bosons from a Mott insulator while fermions form a Fermi surface (i.e, a quantum spin liquid with spinon Fermi surface).

Readily generalize to other distinct quantum spin liquid states (eg BCS pairing of spinons).

Fluctuations: gauge theory

Slave particle representation $c_{i\alpha} = b_i f_{i\alpha}$

invariant under $b_i \to b_i e^{i\theta_i}$, $f_{i\alpha} \to f_{i\alpha} e^{-i\theta_i}$

$\Rightarrow$ $U(1)$ "gauge" redundancy

$\therefore$ True low energy physics below charge gap

$$H = -\sum_{ij} t_{ij} \left(e^{i a_{ij}} f^\dagger_{i\alpha} f_{j\alpha} + h.c \right)$$

(+ constraint $\nabla \cdot E = f^\dagger f$)

Properties of this spin liquid (cont'd) (in d = 2)

RPA theory: many papers in the 90s;
Recent controlled calculation beyond RPA: Mross, McGreevy, Liu, and TS, 2010.

Specific heat $C_v \sim T^{\frac{2}{3}}$

Spin susceptibility $\chi \sim const$

Thermal conductivity $\kappa \sim T^{\frac{1}{3}}$.

Sharp $2K_f$ singularities in both spin density $f^\dagger \sigma f$ and *spinon density* $f^\dagger f$.

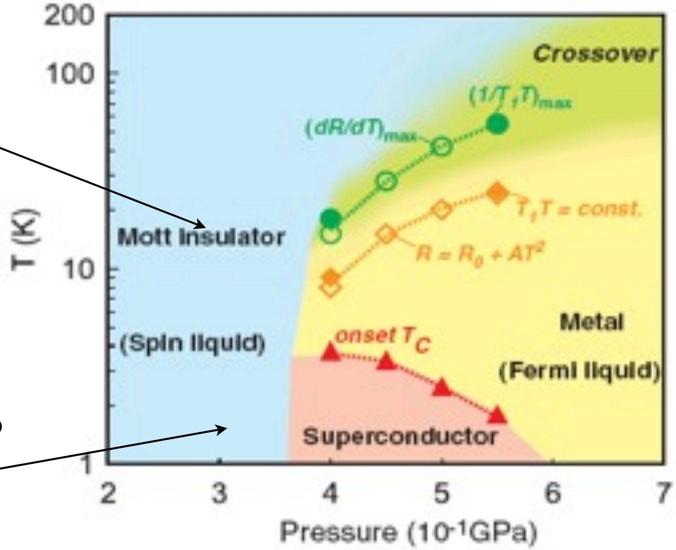
Application to experiment: Spinon FS as a universal intermediate temperature `mother' state

Spinon FS?

(Motrunich, 05)

Pairing instability?

(Lee, Lee, TS, 06)



Low T instability in kappa-ET at ambient pressure at same temperature scale as SC instability under pressure

In dmit SL, no SC under pressure down to 1 K => weaker pairing tendency

Instability scale at ambient pressure also suppressed compared to kappa-ET

Fundamental theoretical concept: Spinon Fermi surface at intermediate-T.

Basic framework for thinking about low-T physics (instability of spinon fermi surface).

Crucial question

What experiments can reveal a `ghost' Fermi surface of spinons in the Mott insulator?

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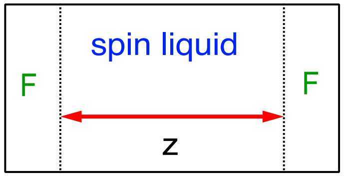
What experiments can reveal a `ghost' Fermi surface of spinons in the Mott insulator?
A few proposals

1. Possible quantum oscillations in applied B-field (Motrunich 2006)
Problems: Unusual orbital response; low-T instability.

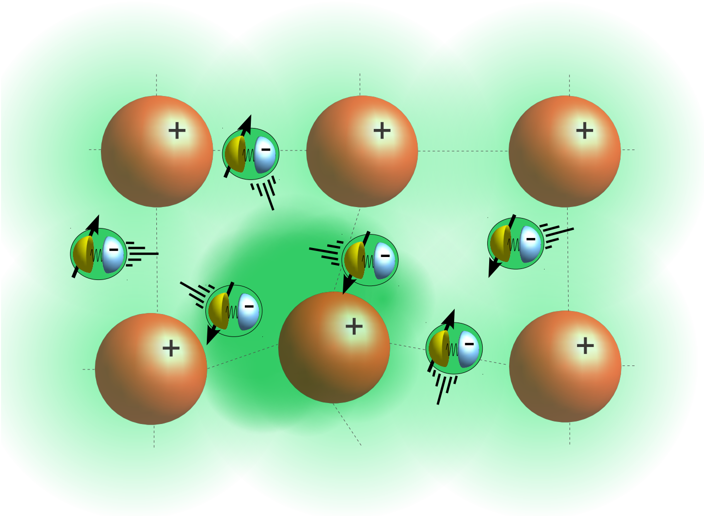
2. Oscillatory magnetic coupling between two ferromagnets separated by spin liquid buffer (Micklitz, Norman, 2009)



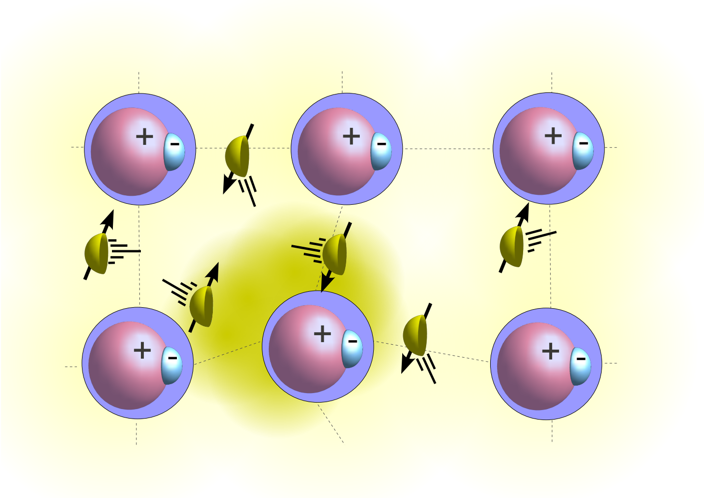
3. Kohn anomaly in phonon spectrum (Mross, TS, 2010)

4. Standing wave patterns in STM for tunneling above the Mott gap (Mross, TS 2010)

Kohn anomaly in phonon spectrum



Normal metal:
Ion motion screened by electron fluid;
Kohn anomaly due to change in screening at 2Kf wavevector



Spin liquid Mott insulator:
Ion bound to electron charge while electron spin stays mobile.

Ion-chargon motion carries gauge charge which is screened by spinon fluid => Kohn anomaly due to spinon FS.

Comments

1. 2Kf wavevectors known (approximately) for both organics, hyperkagome iridate.

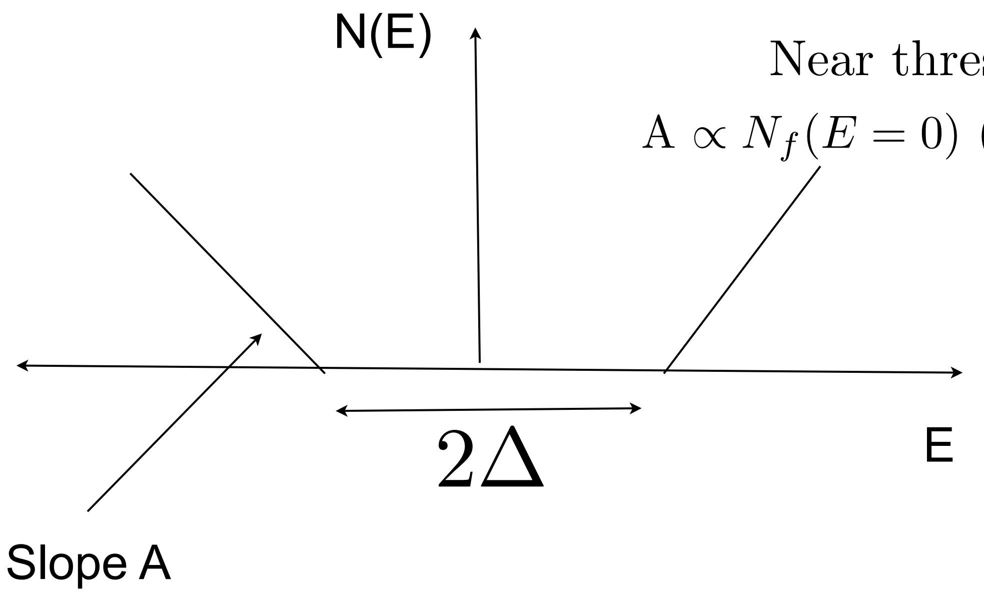
Obtain phonon spectrum thru inelastic X-ray?

2. Kohn anomaly survives even in strong Mott insulator if it has a spinon FS.

May be useful to look in Kagome magnets (Herbertsmithite, Volborthite, etc).

3. Phonon dynamics potentially useful probe of spinon physics in a gapless spin liquid Mott insulator.

STM to detect spinon Fermi surface in weak Mott insulators?



Near threshold $N(E) \approx A(|E| - \Delta)\theta(|E| - \Delta)$.

$A \propto N_f(E = 0)$ (= spinon d.o.s at spinon Fermi surface)

Near defects A = A(x) has spatial modulation at 2Kf wavevectors of spinon FS due to standing wave pattern of spinon d.o.s

=> study spatial modulation of A to determine 2Kf wavevectors.

Very low-T state: many theoretical ideas but all have problems with some aspect of experiments.

Establishing existence of spinon Fermi surface will set the stage for progress in theory of very low-T state.

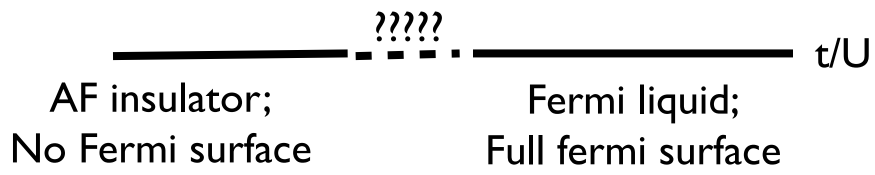
Quantum spin liquids and metal-insulator transitions

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

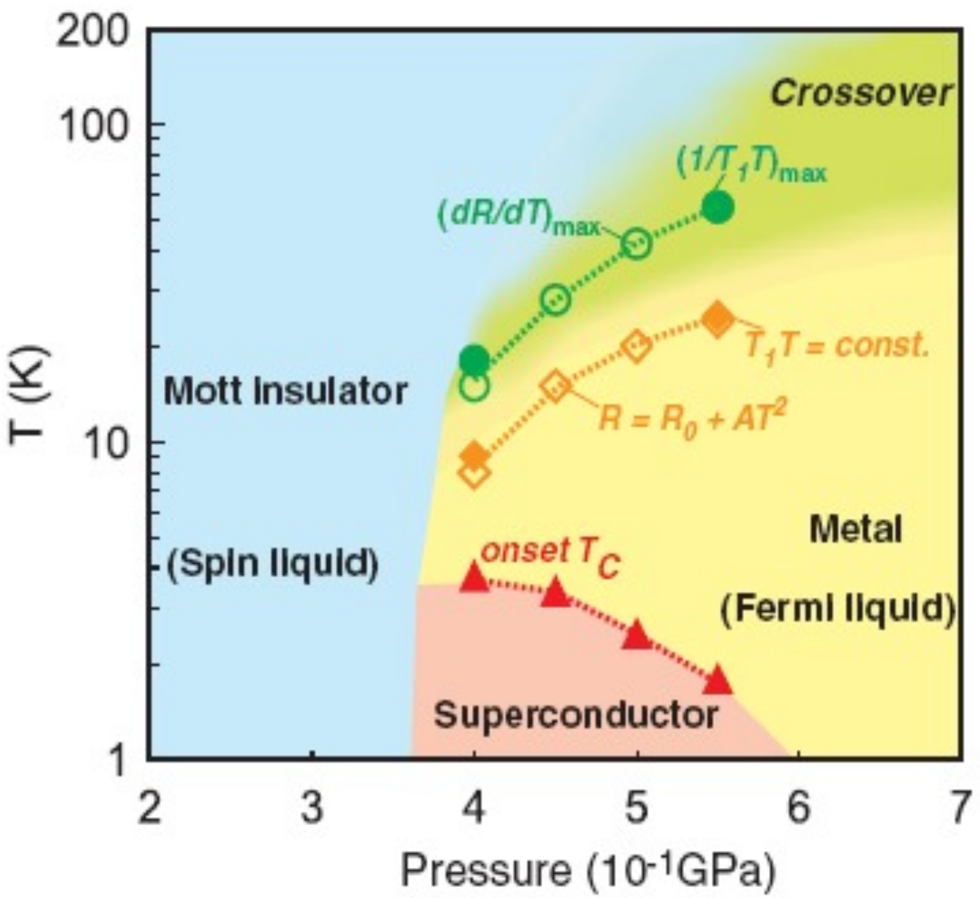
Typically in most materials the Mott transition is first order.

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 - '08



κ-$(ET)_2Cu_2(CN)_3$

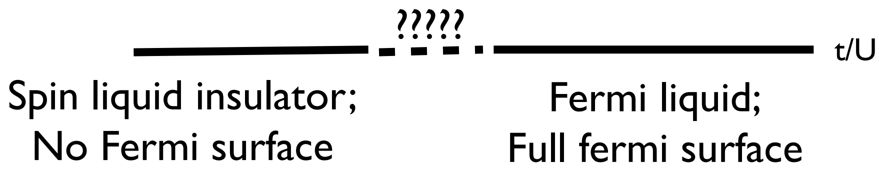
under pressure

Quantum spin liquids and the Mott transition

Some questions:

1. Can the Mott transition be continuous?

2. Fate of the electronic Fermi surface?



Slave particle framework

Split electron operator

$$c^{\dagger}_{r\sigma} = b^{\dagger}_{r} f_{r\alpha}$$

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.

Quantum spin liquids and the Mott transition

1. Can the Mott transition be continuous?

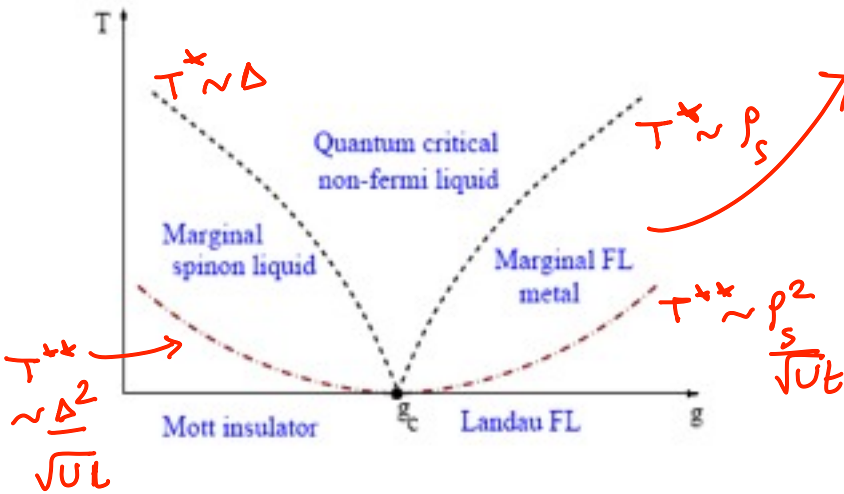
2. Fate of the electronic Fermi surface?

Concrete tractable theory of a continuous Mott transition;
demonstrate critical Fermi surface at Mott transition;
definite predictions for many quantities (TS, 2008).

Example: universal jump of residual resistivity on approaching from metal.

Finite-T crossovers

TS, 2008



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

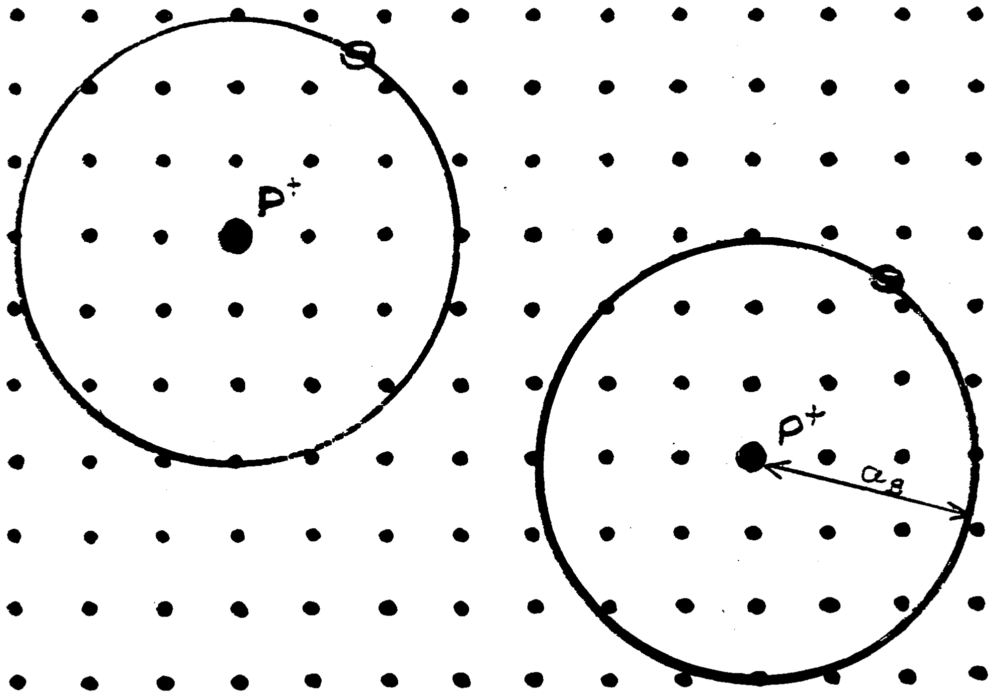
Metal-insulator transitions in doped semiconductors

Eg: Si:P, Si:B

Subject of many studies over last 3 decades.

Is there a quantum spin liquid?
(Potter, Barkeshli, McGreevy, TS, forthcoming)

Basic picture

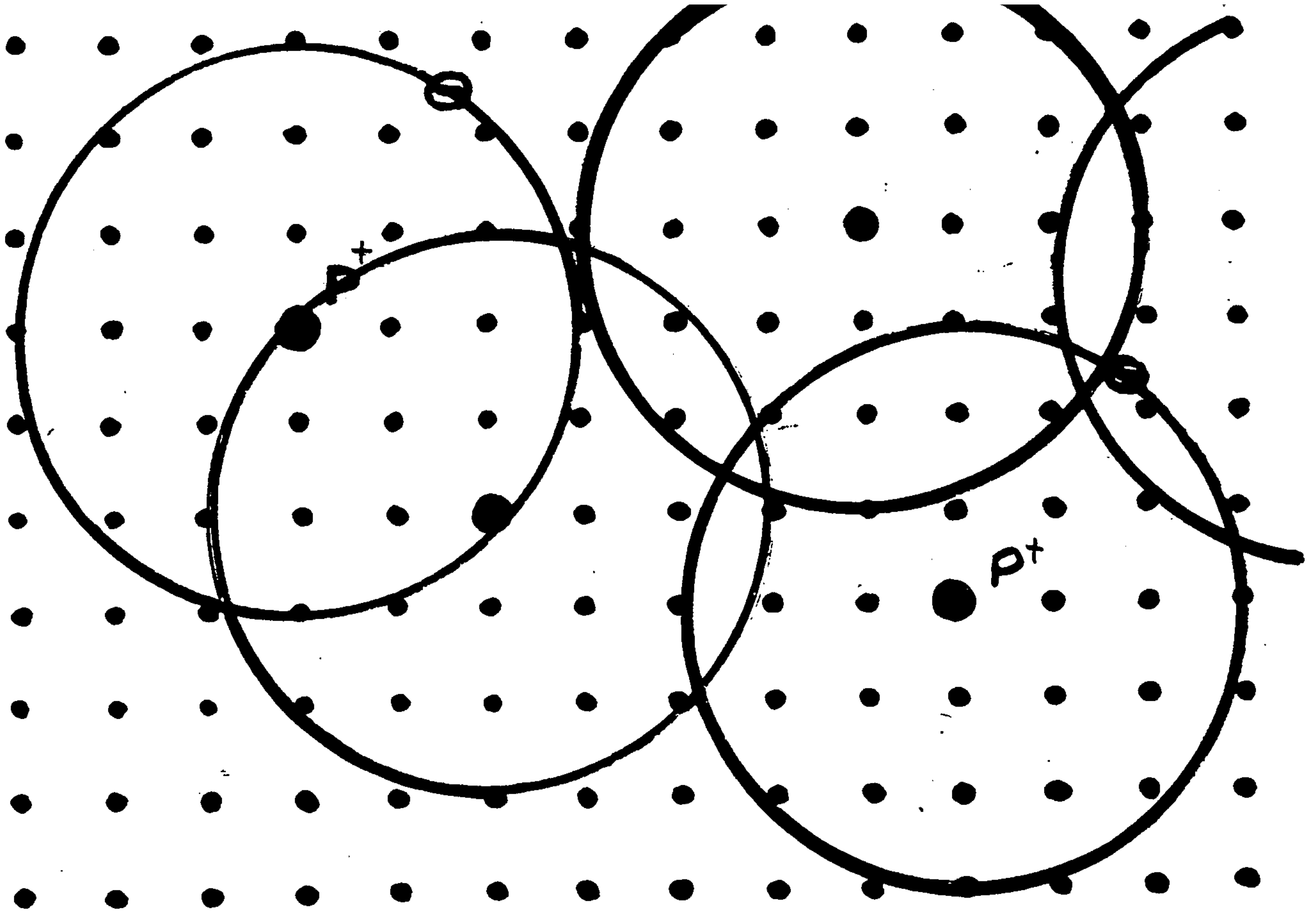


Extra electron of P forms a hydrogen-like state.

$$a_B \approx 20A$$

Simple model: Randomly placed ``Hydrogen atoms''.
Half-filled Hubbard model on random lattice.

Increase P concentration to get metal



Local moments in insulator: Random singlets

Bhatt, Lee, 1982

Each local moment forms a singlet bond with a fixed partner.

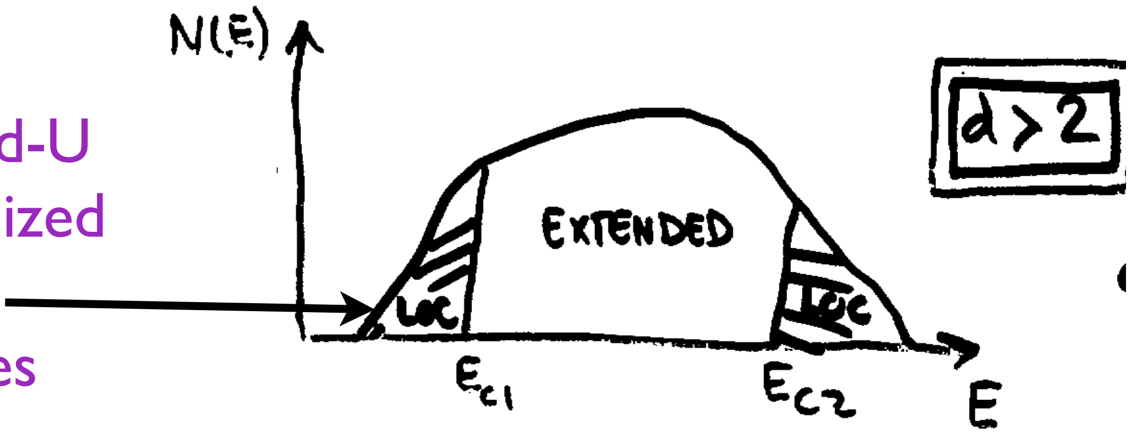
Broad distribution of singlet bond energies.

Anomalous low-T thermodynamics: diverging spin susceptibility, C/T (dominated by rare weakly coupled spin pairs).

Metallic phase: persistence of some local moments

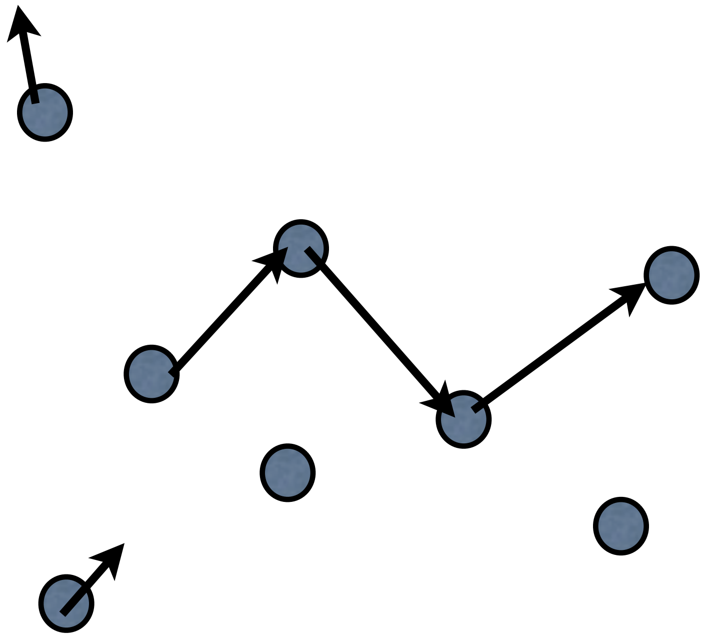
Near transition, some rare fraction of sites retain local moments which then dominate low-T thermodynamics.

Picture: Hubbard-U on localized states produces local moments.



Two fluid phenomenology of metal

Paalanen et al, 1988; Gan, Lee, 86;
Milovanovic, Sachdev, Bhatt, 1989;
Bhatt, Fisher, 1992



Itinerant electron fluid coexisting with small fraction of local moments.

Near transition, fraction of local moment sites about 15%.

Thermodynamics: independent contribution from both fluids.

Evolution across Metal-Insulator Transition (MIT)

What is fate of conducting fluid?

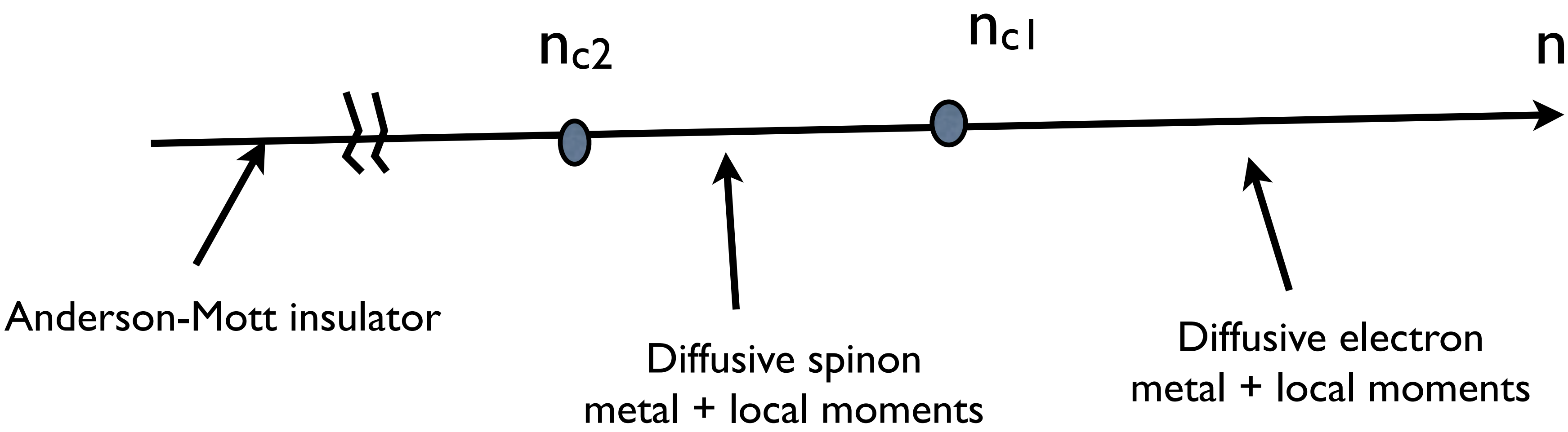
Three possibilities:

1. ``Conventional wisdom"
Itinerant electrons -------> Anderson insulator

2. Fraction of sites with local moments increases to approach 1 at MIT (generically unlikely).

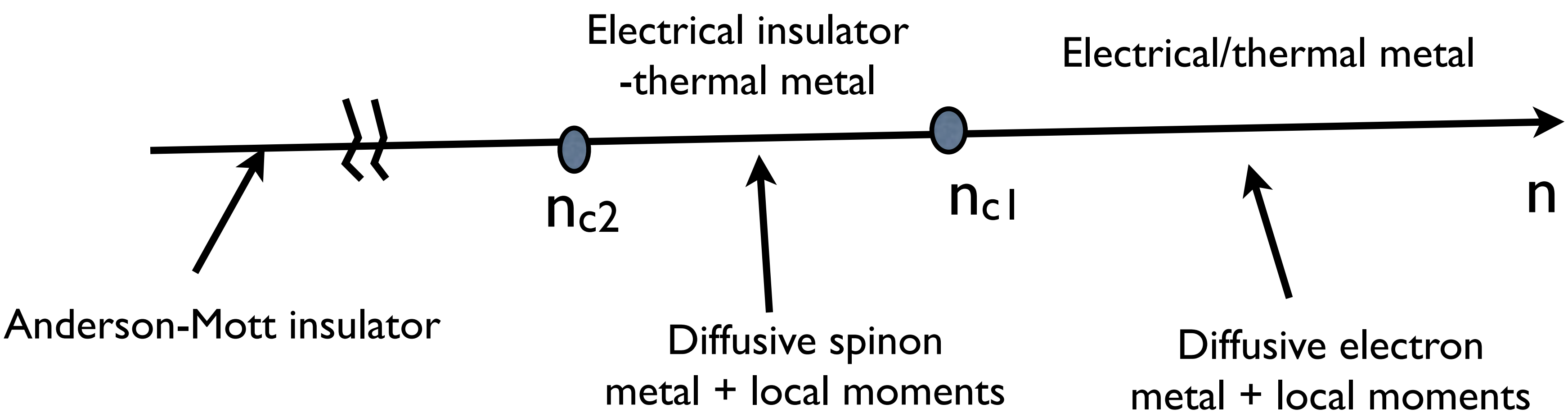
3. New possibility: Conducting fluid Mott localizes into a quantum spin liquid with diffusive spinons (Potter, Barkeshli, McGreevy, TS)

Possible route to metal-insulator transition



Some consequences-I

Diffusive spinon metal is electrical insulator but a thermal conductor.
=> electrical metal-insulator transition separated from thermal metal-insulator transition.



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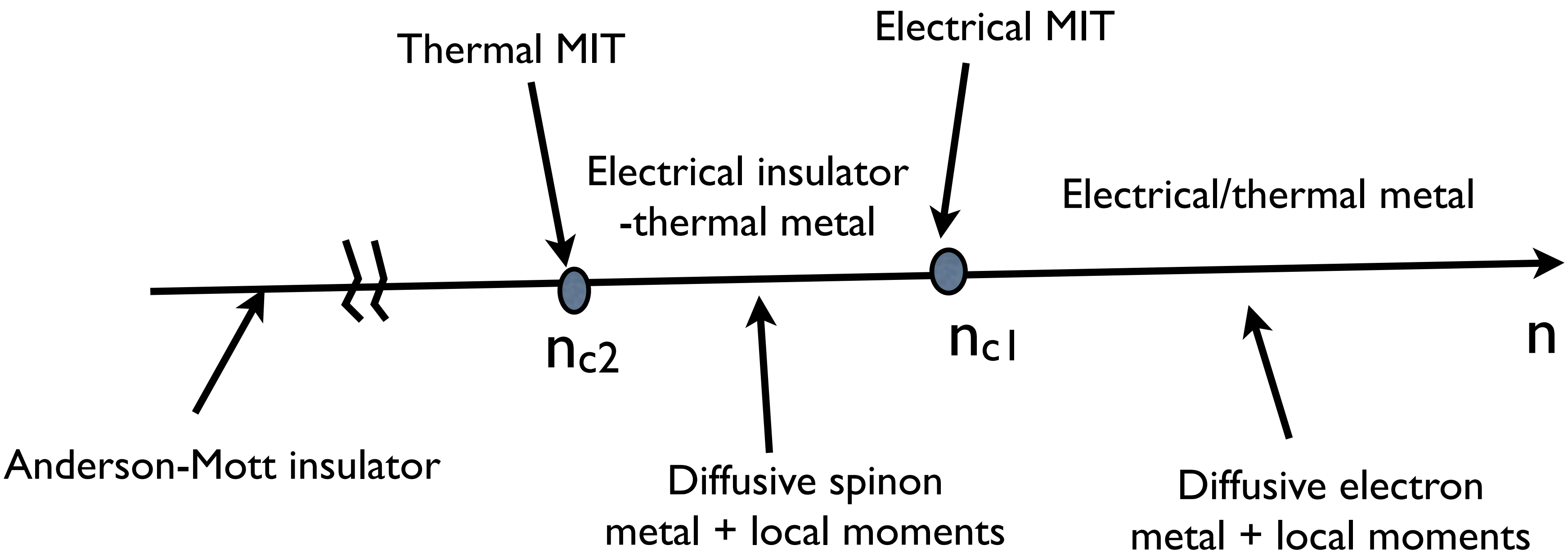
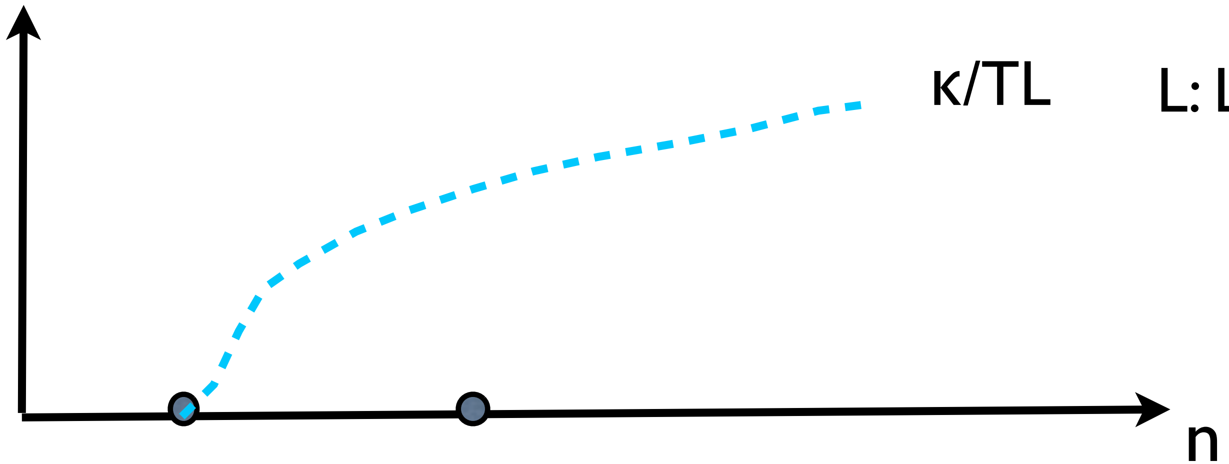
Crucial test: measure thermal transport in insulator.



Some consequences -II

Existence of diffusive spinon metal will impact critical behavior of electrical conductivity near electrical MIT.

Jump of residual conductivity at MIT; non-monotonic T-dependence.



L: Lorentz number

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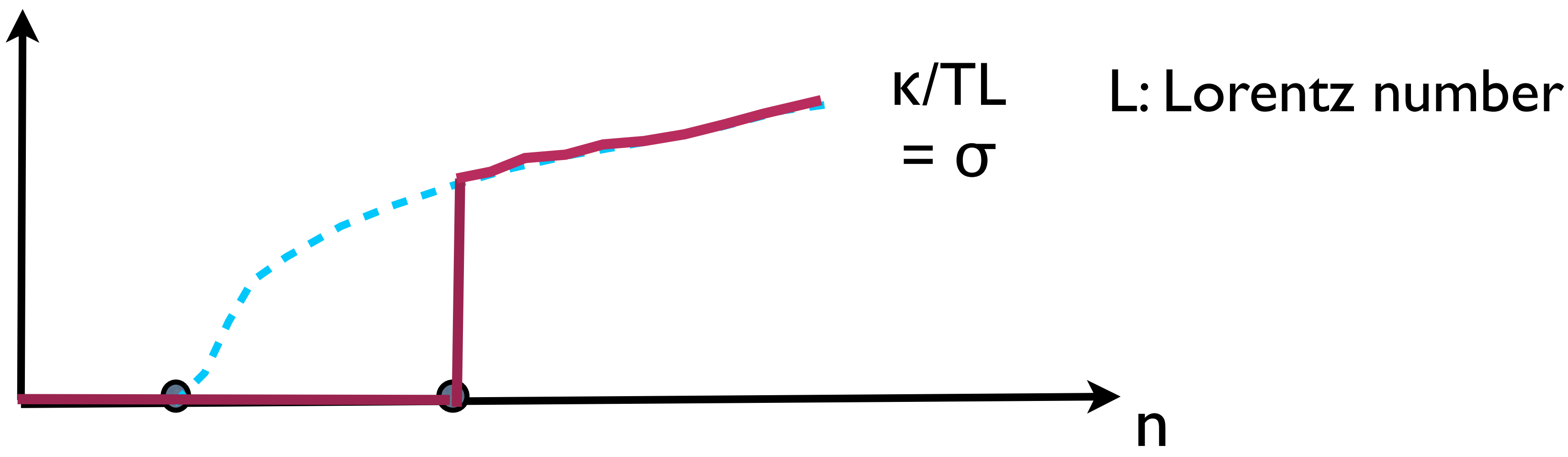

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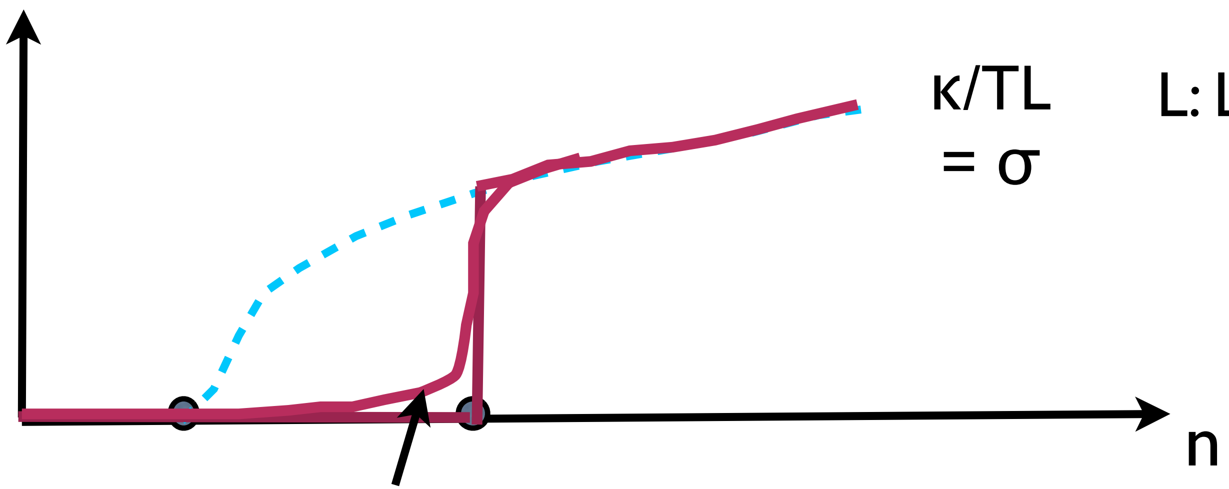

L: Lorentz number

Thermal rounding of jump; complicates extrapolation to T=0 conductivity.

Summary

Growing number of candidate quantum spin liquid materials - many dramatic phenomena.

Theoretical framework: Spinon FS at intermediate temperature, instability (pairing?) at very low T.

Needed: experimental detection of spinon FS, gauge field effects, theoretical clarification of very low-T physics.

Opportunity for progress on classic old problems: Mott and other metal-insulator transitions.