Quantum spin liquids and the Mott transition

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Band versus Mott insulators

Band insulators: even number of electrons per unit cell; completely filled bands

Mott insulators: odd number of electrons per unit cell; charges localize due to Coulomb interaction.

Physics of electronic Mott insulators

Prototype: ½-filled Hubbard model at large-U

$$H = -\sum t_{ij} \left(c^{\dagger}_{i\alpha} c_{j\alpha} + h.c \right) + U \sum_i \frac{n_i (n_i - 1)}{2}$$

Large-U : Charges localize below some temperature $\sim o(U)$

Active low energy degree of freedom is electron spin

Describe by $H_{eff} \approx J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + \cdots$

$\left(J \sim t^2/U > 0 \right)$ - the problem of "quantum magnetism"

Spin liquids and other exotica in quantum magnets

- Traditional quantum magnetism: Ordered ground states

(Neel, spin Peierls, ……)

Concept of broken symmetry

Modern theory (last 2 decades): Possibility of `spin liquid' states in any dimension d.

Eg: Mott insulators with 1 electron/unit cell with no broken symmetry

Maturing theoretical understanding -

extensive developments in last few years

What is a quantum spin liquid?

Rough description: Quantum paramagnet that does not break any symmetries of microscopic Hamiltonian.

More precise: Mott insulator with ground state <u>NOT</u> smoothly connected to band insulator.

Well known in $d=1$ spin chains

Some natural questions

Can quantum spin liquids exist in d > 1? (Anderson '73)

Do quantum spin liquids exist in d > 1?

Some natural questions

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Theoretical question

Do quantum spin liquids exist in d > 1?

Experimental question

Some natural questions

Can quantum spin liquids exist in d > 1? (Anderson '73)

Theoretical question: YES!!

Do quantum spin liquids exist in d > 1?

Experimental question: Remarkable new materials possibly in spin liquid phases

Organics κ-$(ET)_2Cu(CN)_3$; Kagome $ZnCu(OH)_2Cl_2$,

$EtMe_3Sb[Pd(dmit)_2]_2$; Hyper Kagome $Na_4Ir_3O_8$

2d solid He-3

Why are quantum spin liquids interesting?

1. Exotic excitations

Excitations with fractional spin (spinons),

non-local emergent interactions described through gauge fields

As rich in possibility if not richer than the fractional quantum Hall systems…….but requires less extreme conditions (eg: no strong B-fields)

Why are quantum spin liquids interesting?

2. Ordering not captured by concept of broken symmetry

- new concepts of `topological order' and generalizations

Order is a global property of ground state wavefunction

Possibility of encoding information non-locally.

?? Useful for computing?? (Kitaev)

Why are quantum spin liquids interesting?

3. Platform for onset of many unusual phenomena

Eg: (i) Superconductivity in doped Mott insulators

?? Relevant to cuprates ??

(Anderson '87; Kivelson, Rokhsar, Sethna '88)

(ii) Non-fermi liquid phenomena in correlated d or f-electron metals.

Why are quantum spin liquids interesting?

4. Excellent experimental setting for exploration of violation of long cherished notions of condensed matter physics

-quasiparticles with fractional quantum numbers and unusual statistics

- the very existence of a quasiparticle description

- inadequacy of Landau order parameter to describe phases and phase transitions of correlated matter

Stability of quantum spin liquids

1. Solution of concrete quantum spin models within 1/N expansions
   (Read, Sachdev '91)

2. Effective field theory descriptions (Wen '91; Balents,Fisher,Nayak, '99; TS, Fisher'00,…..)

3. Solution of effective models of quantum dimers (Moessner,Sondhi'01; Misguich,Serban,Pasquier'02;….)

4. Solution of various quantum spin/boson models
   (Kitaev'97,'06;Balents,Fisher,Girvin '02, Motrunich, TS'02, ……)

5. Numerical calculations on simpler models
   (Misguich,Lhuillier'98; Sheng, Balents, '05; Isakov,Paramekanti,Kim,Sen,Damle'07)

Where might we find quantum spin liquids?

- Geometrically frustrated quantum magnets

- ``Intermediate'' correlation regime

Eg: Mott insulators that are not too deeply into the insulating regime

Where might we find quantum spin liquids?

- Geometrically frustrated quantum magnets

Kagome magnets ?

- ``Intermediate'' correlation regime

Eg: Mott insulators that are not too deeply into the insulating regime

Perhaps more promising in experiments ?

Organics $\kappa(ET)_2Cu_2(CN)_3$; solid He-3 ? Hyperkagome $Na_4Ir_3O_8$?
$EtMe_3Sb[Pd(dmit)_2]_2$

Wavefunctions

An example

Anderson '87

Ground state : $|\Psi_{gd}\rangle = P_G \, |\text{s-wave gapped BCS}\rangle$

P_G : Gutzwiller projection to 1 electron/site ;

yields RVB spin wave function

Spinon excitations $|\text{spinon}\rangle = P_G \, |\text{BCS quasiparticle}\rangle$

Projection "neutralizes" the charge to leave behind a spinon.

Other excitations

Excitations of a superconductor - (i) quasiparticles

(ii) $hc/2e$ vortices

$$P_G \, |BCS\rangle \longrightarrow |\text{spin liquid}\rangle$$

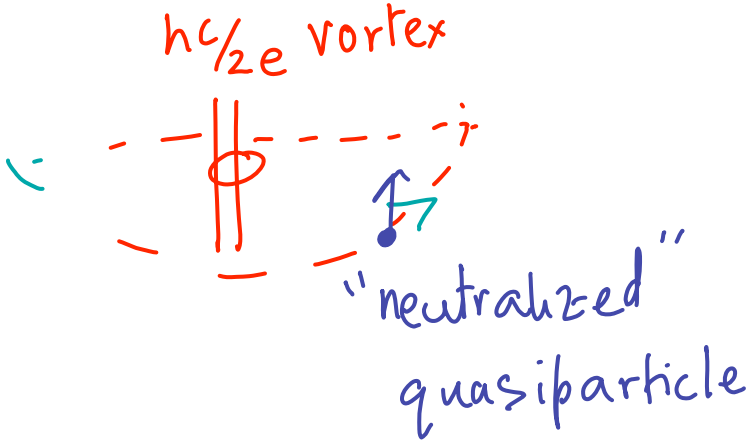
$$P_G \, |\text{quasiparticle}\rangle \longrightarrow |\text{spinon}\rangle$$

$$P_G \, |hc/2e \text{ vortex}\rangle = |v\rangle = ??$$

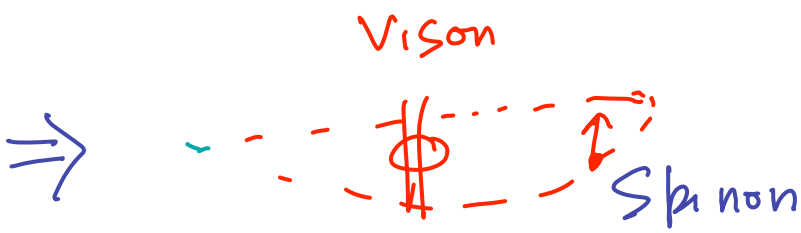
$|v\rangle$: a "topological" excitation of the spin liquid

("vison": TS, Fisher '00)

Full description of excitation spectrum



: Phase of π



: Phase of π

Full excitation spectrum: Spin-$\frac{1}{2}$ spinons, spin-0 visons with infinitely non-local "statistical" interaction

Utility of gauge theory

Convenient mathematical formulation of non-local interaction:

Spinons – Ising "electric charge"

Visons – Ising "magnetic flux"

Non-locality: Aharanov-Bohm interaction

Gauge theory forced upon us as natural language for describing spin liquids

Varieties of spin liquids

Different kinds of spin liquids with different "emergent" gauge structure

Eg: U(1) spin liquids in $d=3$ quantum magnets

- spinons with emergent Coulomb interaction mediated by emergent photon.

(Wen, Motrunich, TS, Hermele, Fisher, Balents, ...)

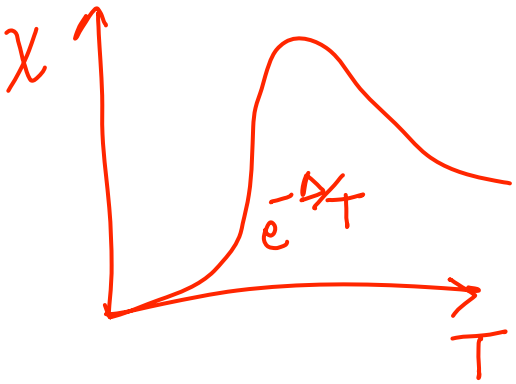
Numerical confirmation: Bannerjee et. al. '07

A useful distinction:

Gapped versus gapless spin spectrum

(i) Spin liquids with spin gap

Best understood theoretically

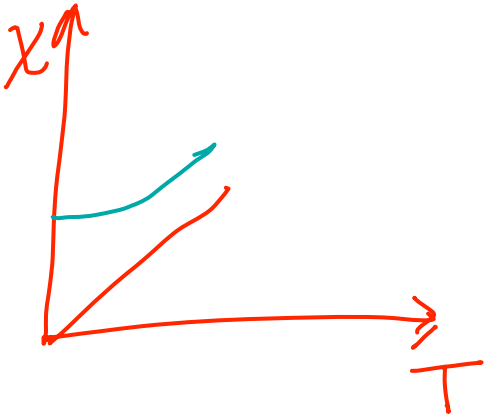


(ii) Spin spectrum may be gapless

Spinons with Fermi statistics

that have Fermi points or

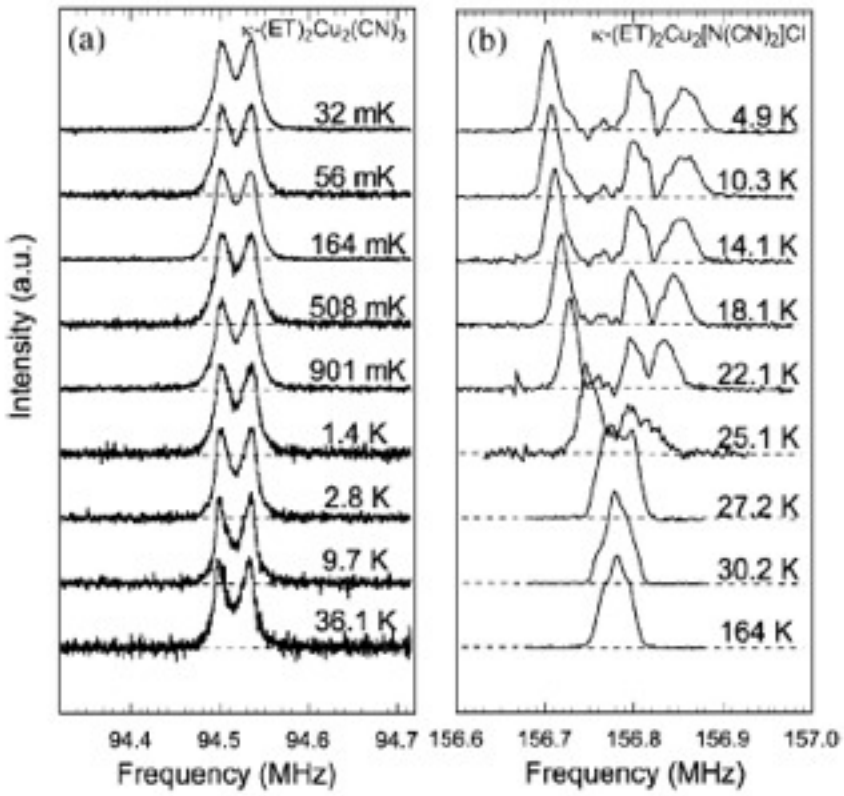
Fermi surfaces ($\Rightarrow$ Nontrivial low-T thermal transport)



Best experimental candidate

(Expt : Kanoda , 2002 - present) κ-$(ET)_2Cu_2(CN_3)_2$

Weak Mott insulator close to Mott transition



$\approx$ Isotropic Δ lattice

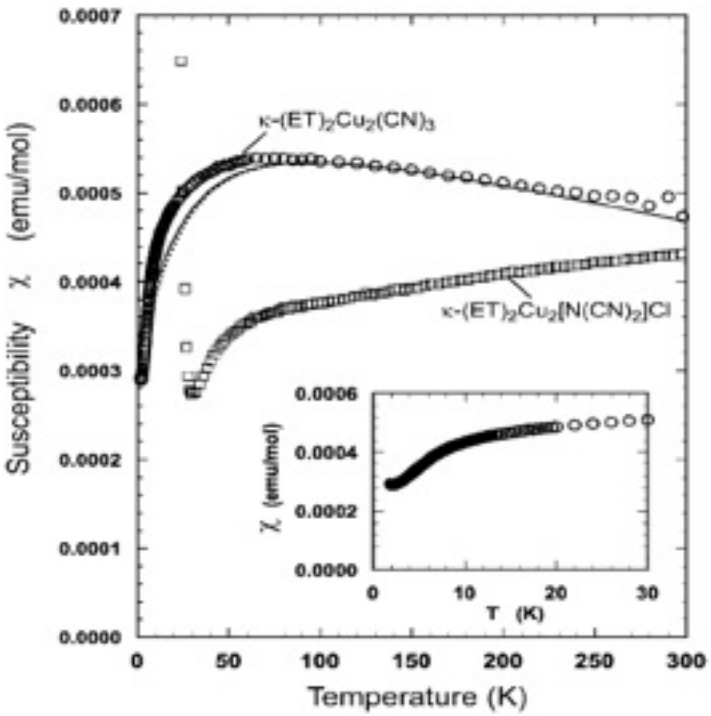
No ordering to 32 mK

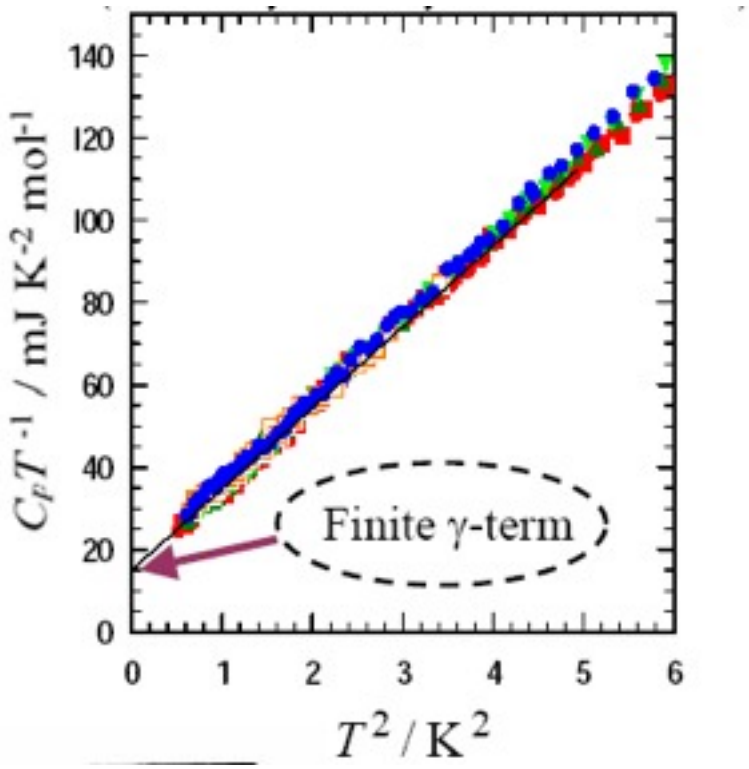
$\ll J \approx 250$ K

but $\chi \to$ const.

$\frac{1}{T_1 T} \to \frac{1}{\sqrt{T}}$ (above 10 K)

A gapless spin liquid



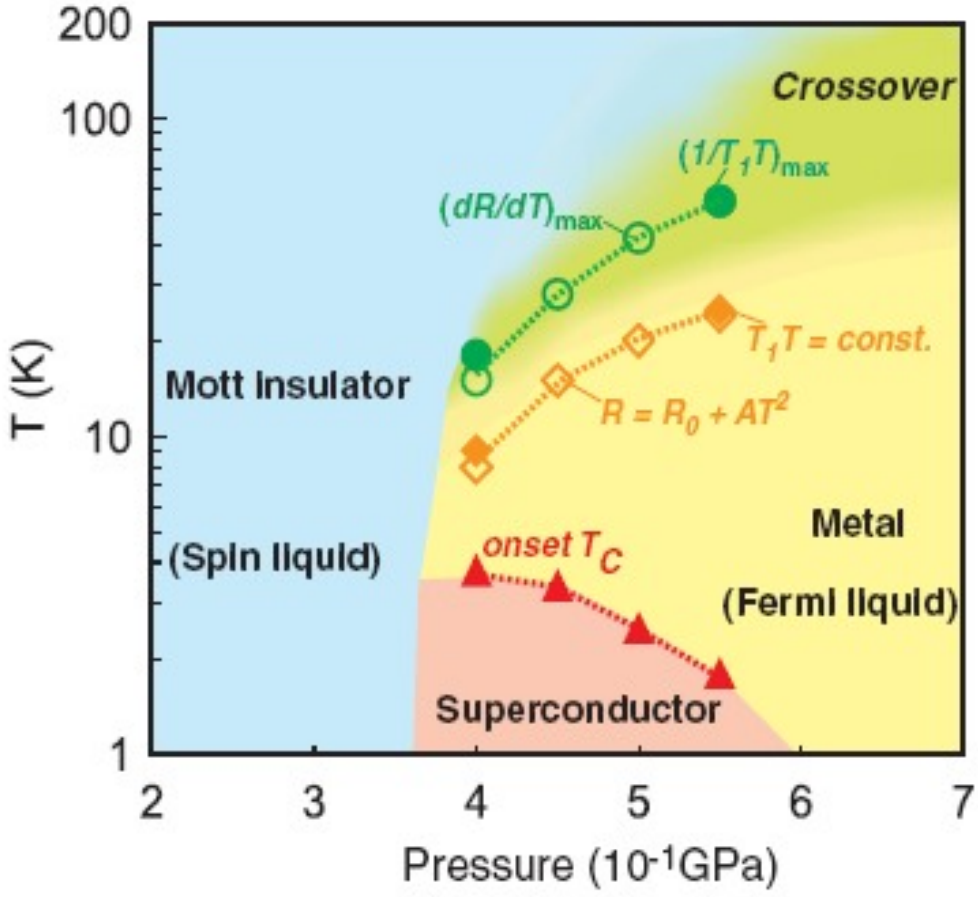


$\chi(T \to 0) \to$ const.
$C_p(T \to 0) \to$ const.

Wilson ratio $\frac{\chi T}{C}$ = const. $\sim O(1)$

Phase diagram

Proximity to Mott transition



Summary of quantum spin liquid review

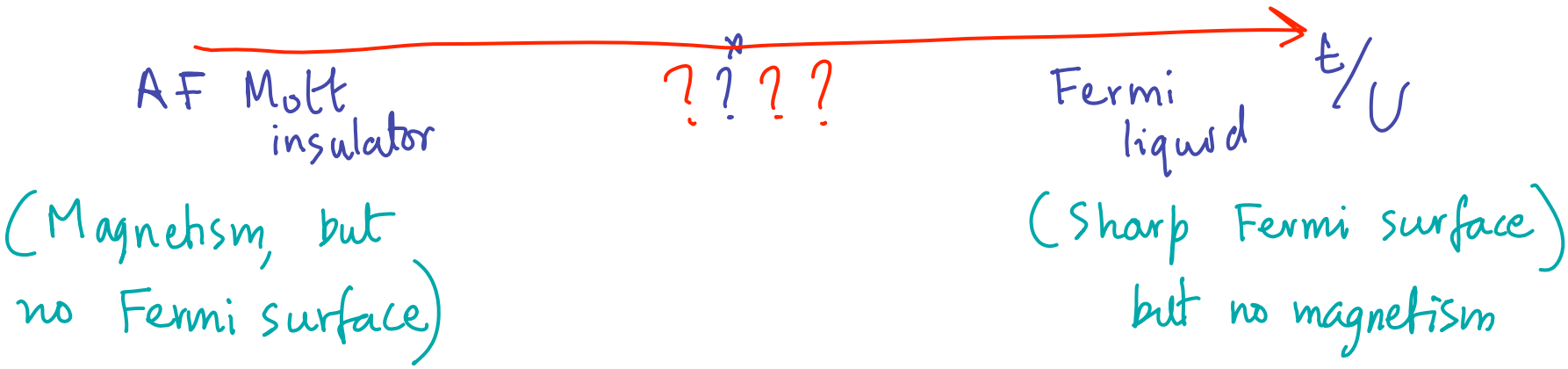
- Maturing theoretical understanding of quantum spin liquid phases in d > 1
- Theoretically demonstrable violations of long cherished notions of condensed matter physics
- Interesting candidate materials exist – exciting times ahead!
- Important general lessons for correlated metallic systems

The Mott metal-insulator transition

Difficult old problem in condensed matter physics

Simple example: Mott transition of one band systems

$\frac{1}{2}$-filled Hubbard model on non-bipartite lattice in $d=2$ or 3



Fermi surface of metal needs to disappear at Mott transition.

Some difficulties

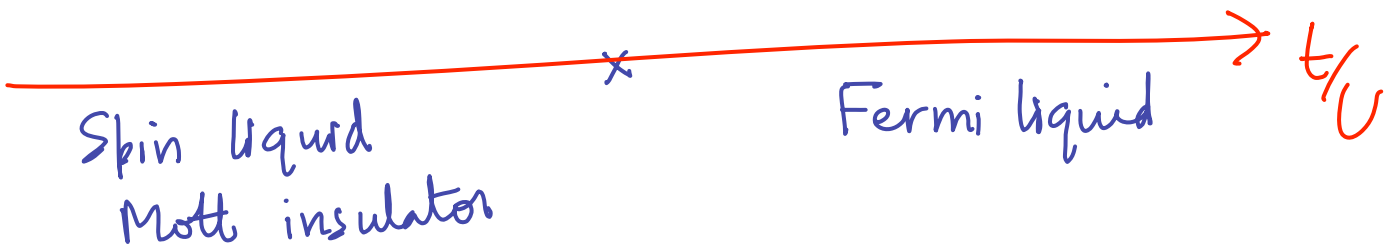
1. No order parameter for the metal-insulator transition

2. Need to deal with a sharp Fermi surface on metallic side

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

Quantum spin liquids to a (partial) rescue

Mott transition between metal and a quantum spin liquid

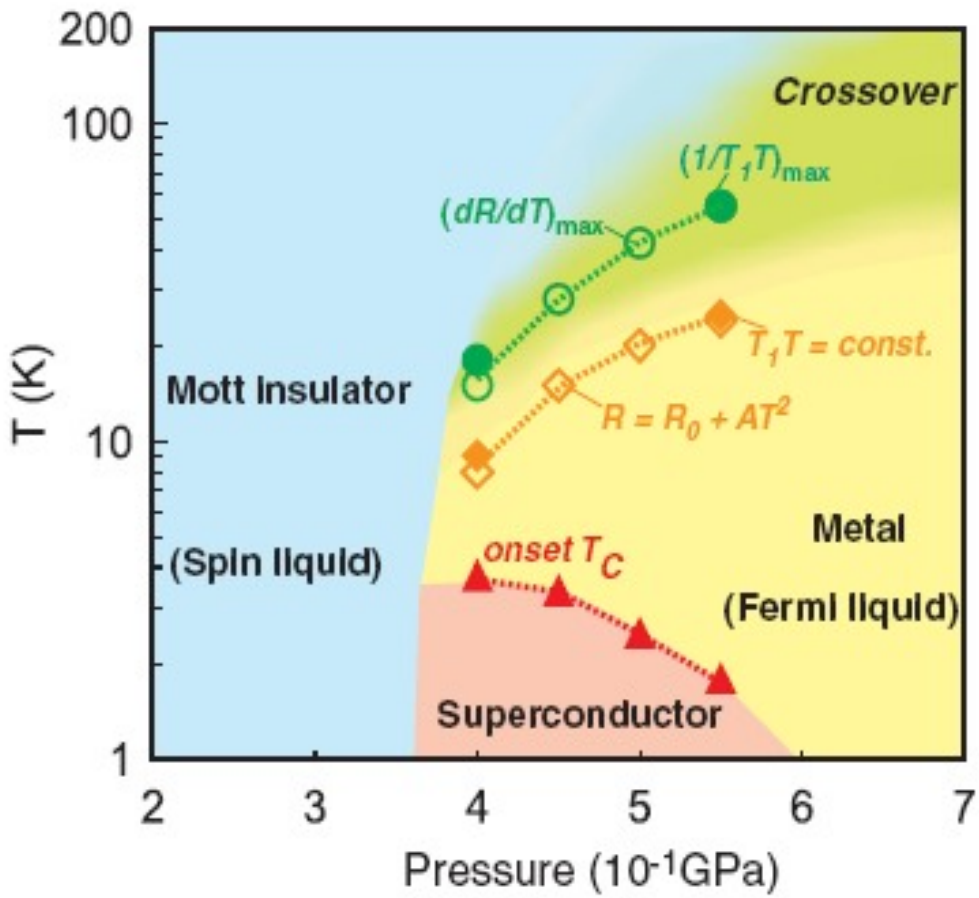


Mott transition without complications of magnetism

Can study issues of loss of Fermi surface, metallic conduction, etc; possibly even 2nd order

Possible experimental realization of a second order Mott transition

Kanoda et al '03 - '08



κ-$(ET)_2Cu_2(CN)_3$

under pressure

One band Hubbard model on isotropic Δ lattice

No magnetic order in insulator!

Spinon Fermi surface? (Motrunich '05, Lee & Lee '05)

How might a Fermi surface disappear?

Can a Fermi surface disappear continuously through a 2nd order transition?

One route – quasiparticle weight Z vanishes continuously and everywhere on Fermi surface!

(a la Brinckman-Rice '71)

Concrete example in other contexts: "Kondo breakdown" model (TS, Vojta, Sachdev '04)

Electronic structure at criticality: ``Critical Fermi surface"

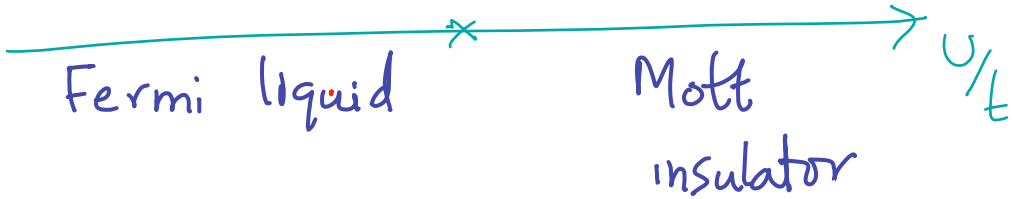
Crucial question : Nature of electronic excitations right at quantum critical point when $Z=0$?

Claim : At critical point, Fermi surface remains sharply defined even though there is no Landau quasiparticle (TS, '08)

"Critical Fermi surface"

Why a critical Fermi surface?

Mott transition example:



What is gap $\Delta(\vec{k})$ in electron spectral function $A(\vec{k},\omega)$?

Fermi liquid : $\Delta(\vec{k} \in FS) = 0$

Mott insulator : Sharp gap $\Delta(\vec{k}) \neq 0$ for all $\vec{k}$

Evolution of single particle gap

Approach from Mott

2nd order transition to metal $\Rightarrow$ expect Mott gap

$\Delta(\vec{k})$ will close continuously

To match to Fermi surface in metal, $\Delta(\vec{k}) \to 0$ for all $\vec{k} \in FS$.

$\Rightarrow$ Fermi surface sharp at critical point.

But as $Z = 0$ no sharp quasiparticle

$\Rightarrow$ Non-Fermi liquid with sharp "critical" Fermi surface!

Why a critical Fermi surface?

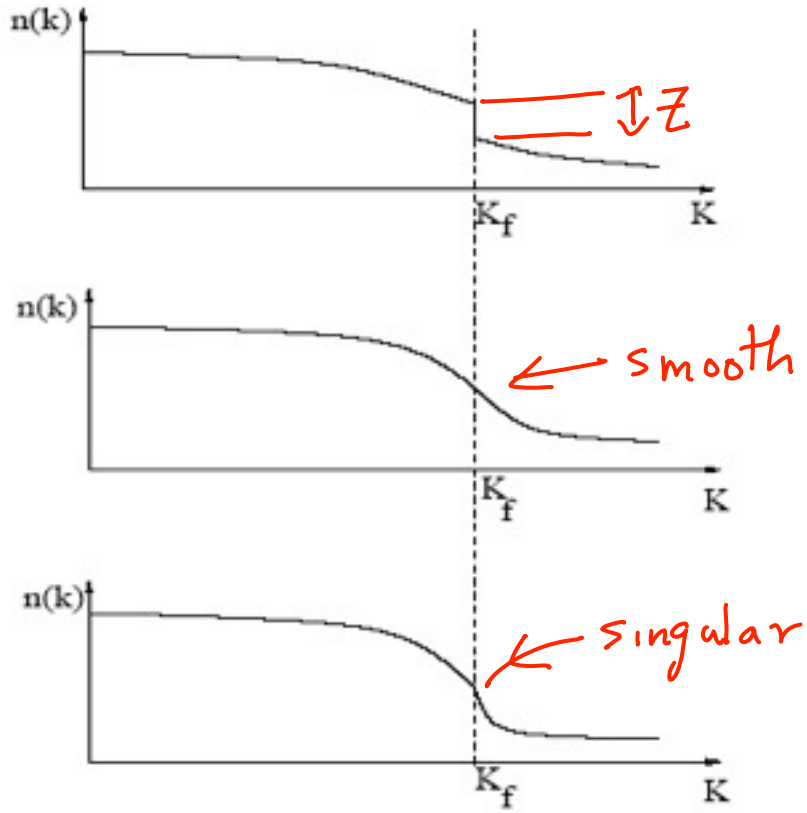
Evolution of momentum distribution

Metal with Fermi surface

Phase where Fermi surface has disappeared

Critical point

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



Killing a Fermi surface

Disappearance of Fermi surface through a continuous transition

At critical point

(a) $Z = 0$

(b) Fermi surface sharp

(Similar argument for heavy fermion critical points, hiTc, Mott critical point, etc)

Some obvious consequences/questions

Critical Fermi surface $\Rightarrow$ unusual criticality with phenomena different from familiar critical points

1. Structure of universal singularities/scaling phenomena ?

2. Calculational framework ?

Some obvious consequences/questions

Critical Fermi surface ⇒ unusual criticality with phenomena different from familiar critical points

1. Structure of universal singularities/scaling phenomena ?

General scaling theory - TS '08

2. Calculational framework ?

Focus of this talk : concrete theory of a continuous Mott transition - TS '08

Theoretical framework

Slave rotor description: $c_{i\alpha} \sim e^{i\phi_i} f_{i\alpha}$

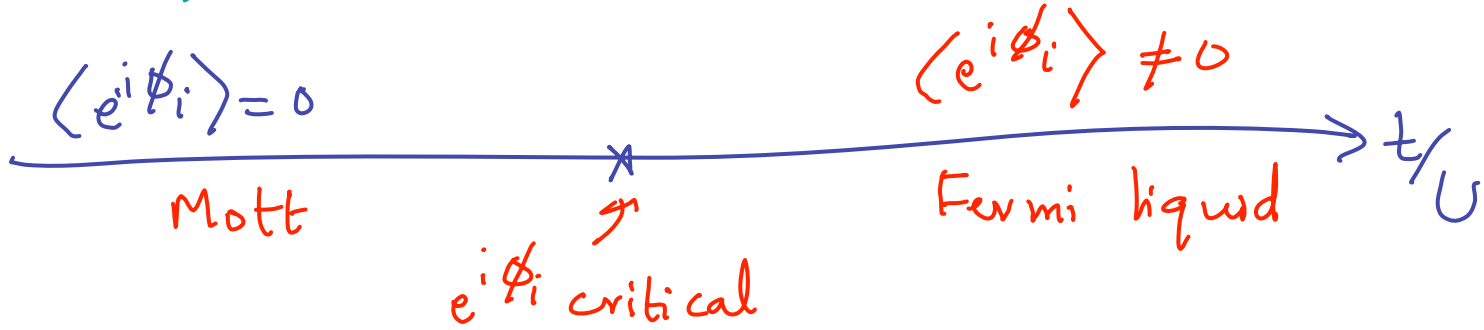
charge-e spinless boson

neutral spin-½ fermion ("spinon")

U(1) gauge redundancy: local phase rotations of $e^{i\phi_i}$ & $f_{i\alpha}$

Mean field theory: Florens, Georges '04

Fluctuations: TS '08



Structure of critical theory in d = 2

$$S_{eff} = \underbrace{S[e^{i\phi}, a]}_{\text{3D XY coupled to U(1) gauge field } a_\mu} + \underbrace{S[f, a]}_{\text{spinon Fermi surface coupled to } a_\mu}$$

RPA analysis : Effective action for transverse gauge field

$$S_{eff} \simeq \int_{q,\omega} \left(\frac{|\omega|}{q} + \sqrt{q^2+\omega^2} \right) |a|^2$$

$$\simeq \int_{q,\omega} \left(\frac{|\omega|}{q} + |q| \right) |a|^2$$

Coupling to bosons: a_μ decouples due to Landau damping term

$\Rightarrow$ Bosons in 3D XY class

Fermions :

Same as "Coulomb" interaction case of HLR theory of $\frac{1}{2}$-filled Landau level

$$S = \underbrace{S[b]}_{\text{bosons in 3D XY universality class}} + \underbrace{S[f,a]}_{\text{strongly coupled spinon-gauge system (same as HLR with Coulomb)}}$$

Critical Fermi surface at Mott criticality

Electron spectral function

$$A_c(\vec{k}, \omega) \sim \frac{|\omega|^{\eta}}{\ln \frac{1}{\omega}} F\left(\frac{\omega \ln \frac{1}{|\omega|}}{k_{\parallel}} \right)$$

Sharp critical Fermi surface but no Landau quasiparticle.

"Scaling form" with $\alpha = -\eta$, $z = 1^+$

(η = anamolous exponent in 3D XY model)

Approach from Fermi liquid

Vanishing quasiparticle residue $Z \sim \dfrac{|\delta g|^{2\beta}}{\ln \frac{1}{|\delta g|}}$

Diverging effective mass $\dfrac{m^*}{m} \sim \ln \dfrac{1}{|\delta g|}$

(but $Z \neq \dfrac{m}{m^*}$)

Diverging Landau parameters $F_0^a \sim \dfrac{m^*}{m} \to \infty$ $(\chi_0 \to \text{const.})$

$F_0^s \sim |\delta g|^{-\nu} \to \infty$

Compressibility $\kappa \to 0$ (and zero sound speed $\to \infty$)

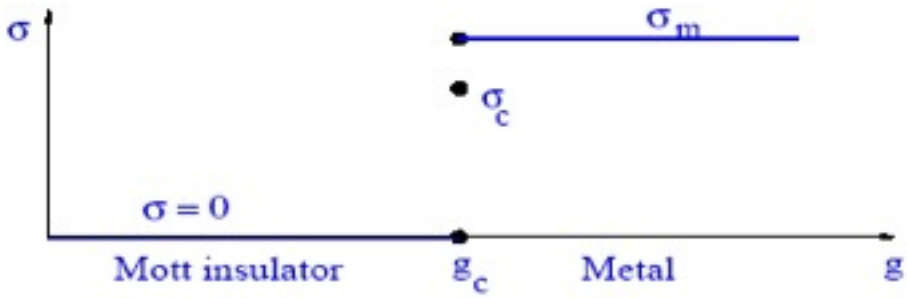
Critical thermodynamics/transport

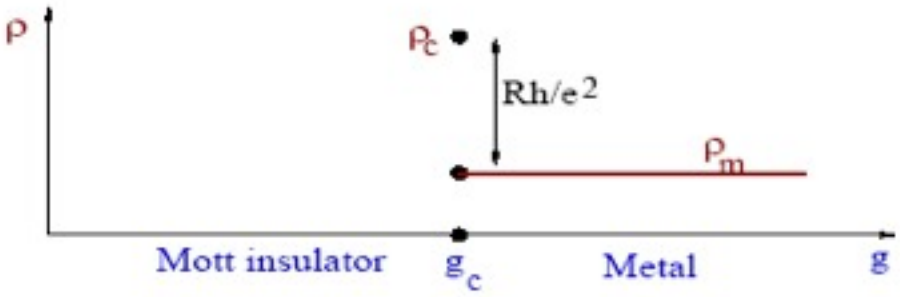
$$C_V \sim T \ln \frac{1}{T} \quad , \quad \chi_0 \to \text{const.}$$

Resistivity $\rho = \underbrace{\rho_b}_{\text{boson}} + \underbrace{\rho_f}_{\text{fermion}}$ (Ioffe-Larkin rule)

$$\rho_b = Rh/e^2 = \text{universal}, \quad \rho_f \sim \rho_0 + o\left(T^2 \ln \frac{1}{T}\right)$$

Universal resistivity jump





$$\rho = \rho_b + \rho_f$$

Metal: $\rho_b = 0 \Rightarrow \rho = \rho_f$

Insulator: $\rho_b = \infty \Rightarrow \rho = \infty$

Mott critical point

$$\rho_b = Rh/e^2$$

$\Rightarrow$ Residual resistivity jumps at Mott transition.

On approaching from metal, jump $= Rh/e^2 =$ <u>universal</u>.

Crossover out of criticality: Anderson is different (from Higgs)

Move from critical point to Fermi liquid:

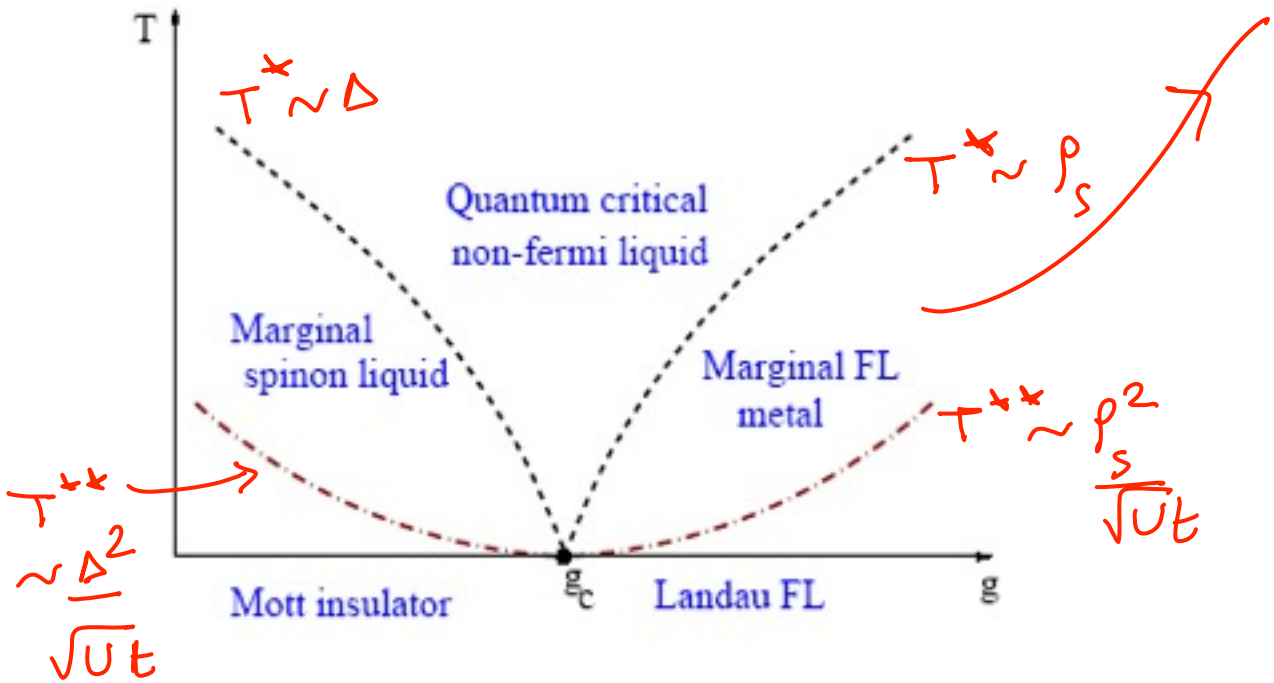
Boson condensation scale $\sim \rho_s$ = boson stiffness

Modified gauge action $S_{eff} \sim \int_{q,\omega} \left(\frac{|\omega|}{q} + q f(\rho_s/q) \right) |a|^2$

Gauge fluctuations quenched at scale $\sim \rho_s^2 \ll \rho_s$

$\Rightarrow$ Charge & spin sectors emerge out of criticality at different scales

Finite T crossovers: Marginal Fermi liquids



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

Same Mott transition in three dimensions

(Podolsky, Paramekanti, Kim, Senthil '08)

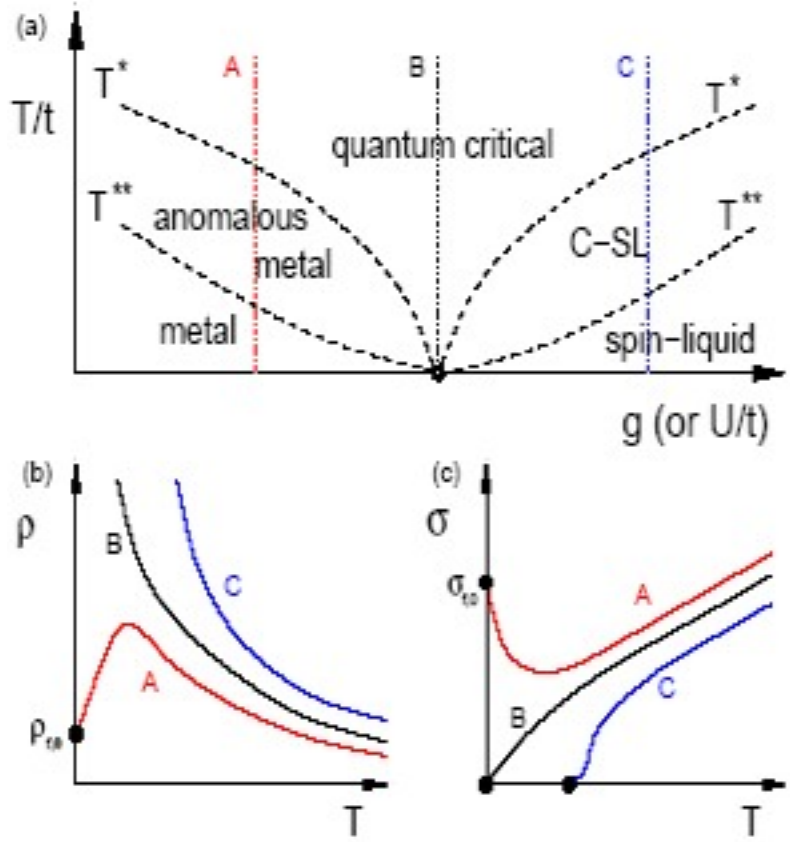
Second order Mott transition possible also in 3d.

Weaker singularities compared to 2d

Eg: At QCP, $C_v \sim T \ln \ln 1/T$

Most interesting prediction:

Resistivity maximum in metallic phase close to Mott transitions



Experiments: $Na_4Ir_3O_8$ near pressure-tuned Mott transition?

Summary-II

- Concrete theory of a continuous Mott transition in two dimensions

- demonstrate critical Fermi surface

- predict universal resistivity jump, emergence of marginal Fermi liquids

- filling controlled transition tuned by chemical potential can also be studied.

Future: Lots of challenges !