Novel continuous quantum Mott transitions

T. Senthil (MIT)

TS, in progress

TS, PR B 08.

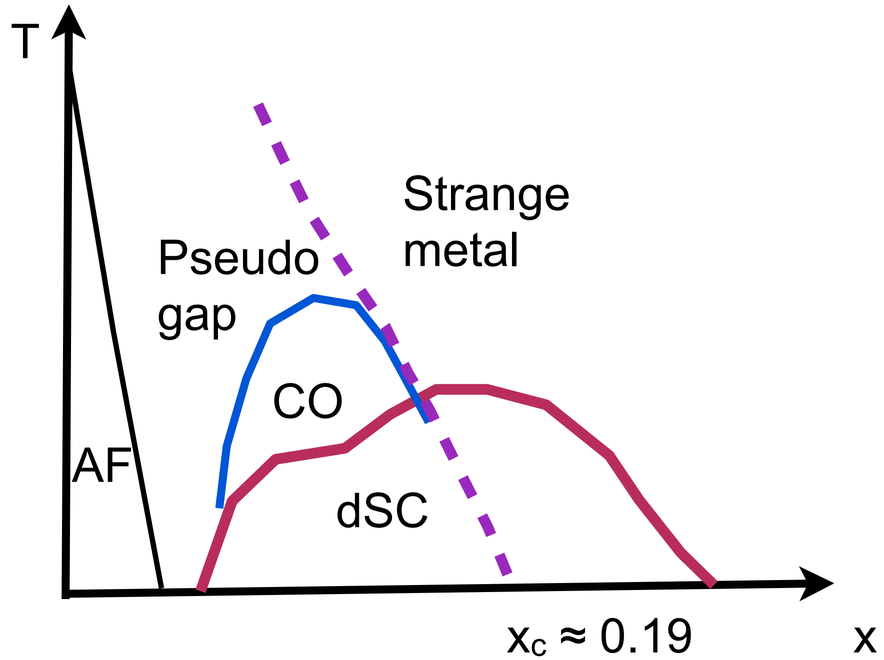
D. Podolsky, A. Paramekanti, Y.B. Kim, TS, PRL 09.

D. Mross and TS, PRB 11.

A. Potter, M. Barkeshli, J. McGreevy, TS, PRL 2012 .

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

Cuprate phase diagram



CO: charge order

Most mysterious: strange metal regime

Ideas on strange metal

Strange metal plausibly linked to quantum criticality

Increasing evidence for a quantum critical point around xc ≈ 0.19 in ``normal'' state:

1. Termination of pseudogap crossover at T = 0 (Tallon, Loram 2000)

2. Onset of charge order at T = 0 (Keimer et al, 14).

Some (likely) properties of the strange metal

1. Sharp gapless Fermi surface but no Landau quasiparticles

2. Critical charge order correlations.

Some (likely) properties of the strange metal

1. Sharp gapless Fermi surface but no Landau quasiparticles
2. Critical charge order correlations.

A (lowly) theoretical challenge:

Construct examples of such strange metal fixed points at finite density.

A route to some examples

Focus on commensurate density x = 1/4 or x = 1/5 and study continuous Mott transitions from Fermi liquid to Mott insulator.

?Corresponding critical point - an example strange metal fixed point with a critical Fermi surface and critical charge order correlations ?

Plan of talk

1. Theory of a continuous Mott metal-insulator transition in $d = 2$ at $x = 0$

Evolution from Fermi liquid to quantum spin liquid insulator: Predictions for transport experiments

2. Electronic Mott transition at filling $1/q$: Formulation

3. Warm-up: Superfluid-insulator transitions of bosons at commensurate filling $1/q$ (a review)

Plan of talk

1. Theory of a continuous Mott metal-insulator transition in $d = 2$ at $x = 0$

Evolution from Fermi liquid to quantum spin liquid insulator: Predictions for transport experiments

2. Electronic Mott transition at filling 1/q : Formulation

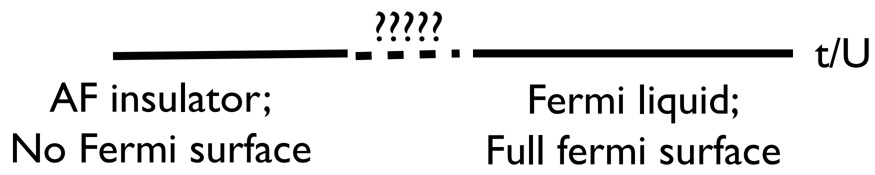
3. Warm-up: Superfluid-insulator transitions of bosons at commensurate filling 1/q (a review)

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.

Some candidate spin liquid 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)

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

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

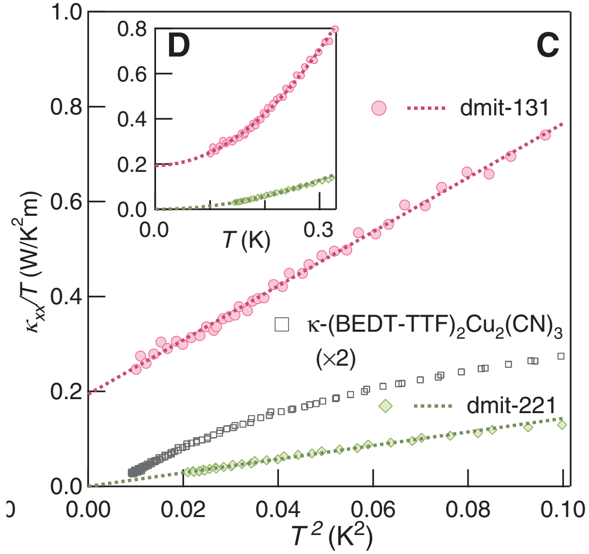
ALL candidate quantum spin liquid materials:

<u>Gapless</u> excitations down to T << J.

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

Example: Thermal transport in dmit SL.

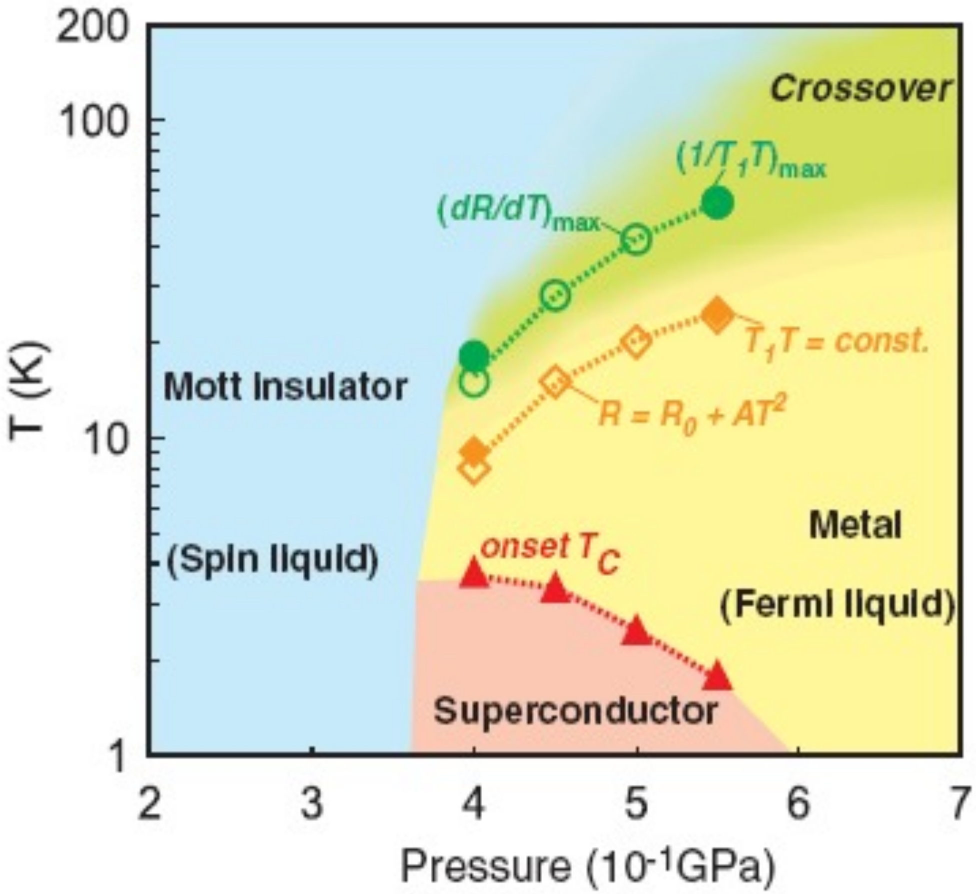
Electrical Mott insulator but thermal metal!



M. Yamashita et al, Science 2010.

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

Kanoda et al '03 - '08



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

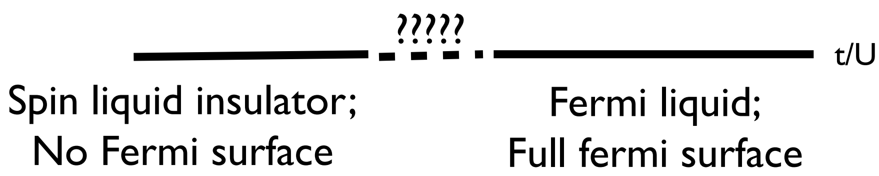
under pressure

Quantum spin liquids and the Mott transition

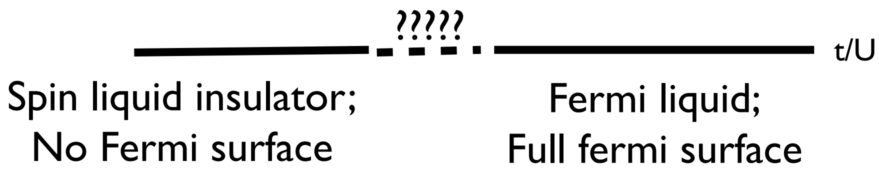
Some questions:

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).

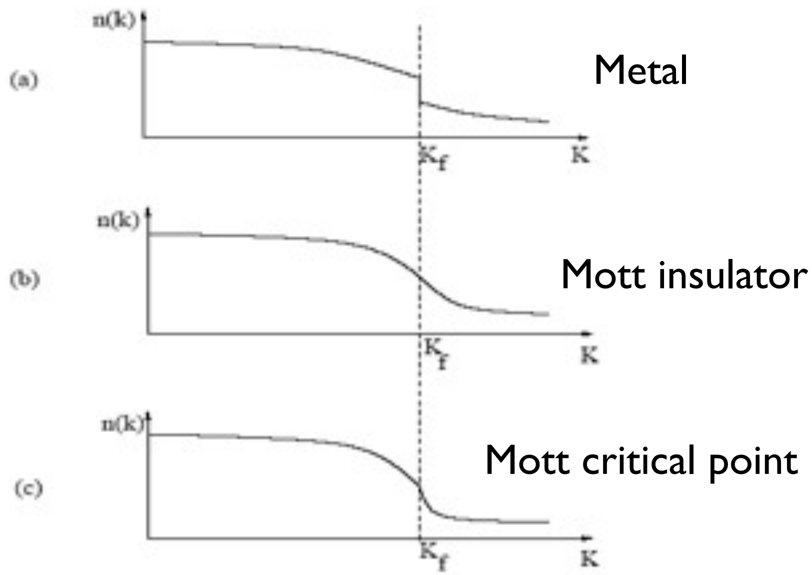
If Mott transition is second order, critical point necessarily very unusual.

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

Basic question for theory

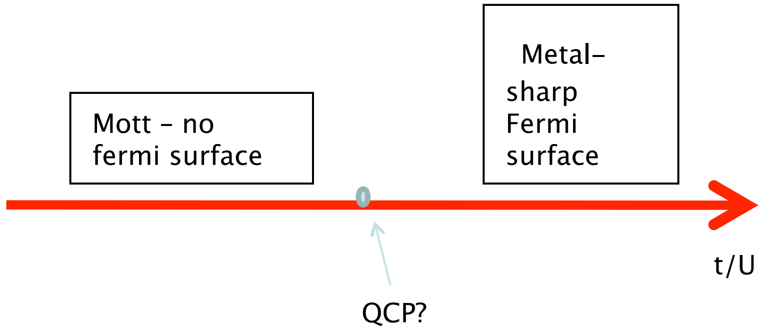
Crucial question: Nature of electronic excitations right at quantum critical point when $Z = 0$.

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?



What is gap $\Delta(\mathbf{K})$ to add electron at momentum $\mathbf{K}$?

Fermi liquid: $\Delta(\mathbf{K}) \in FS = 0.$
Mott insulator: Sharp gap $\Delta(\mathbf{K}) \neq 0$ for all $\mathbf{K}$

Evolution of single particle gap

Approach from Mott:
Second order transition to metal => $\Delta(\mathbf{K})$ will close continuously.

Match to Fermi surface (FS) in metal => $\Delta(\mathbf{K}) \rightarrow 0$ for all $\mathbf{K} \in FS$.

=> Fermi surface sharp at critical point.
But as $Z = 0$ no sharp quasiparticle.

Non-fermi liquid with sharp critical Fermi surface.

Why a critical Fermi surface?

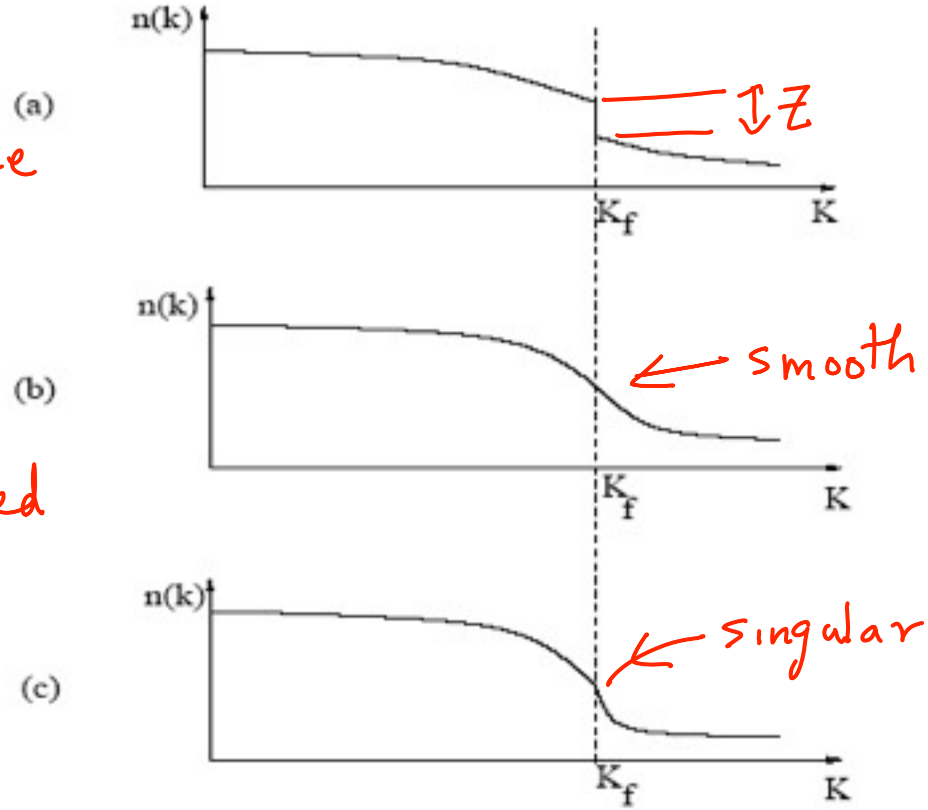
Evolution of momentum distribution

Metal with Fermi surface

Phase where Fermi surface has disappeared

Critical point

n(K) continuous at K_F but is singular

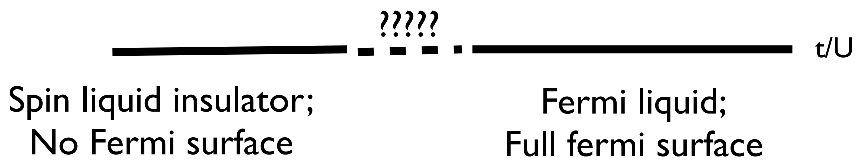


Quantum spin liquids and the Mott transition

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

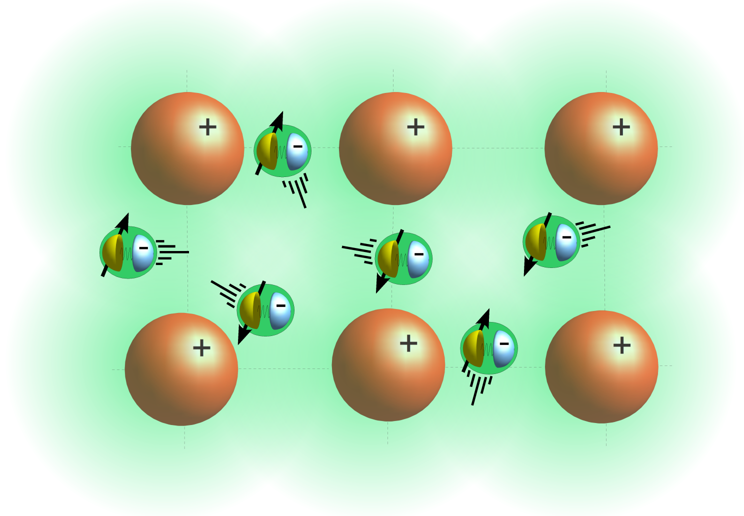
Mott transition: b_r critical

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

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

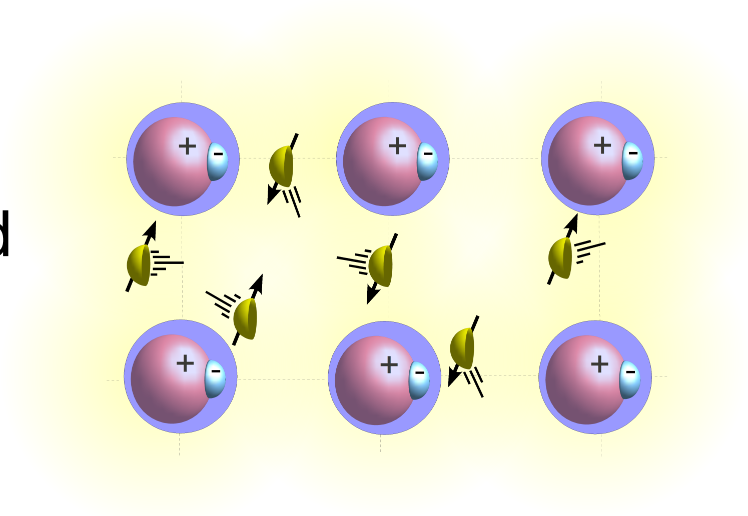
Picture of Mott transition

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?

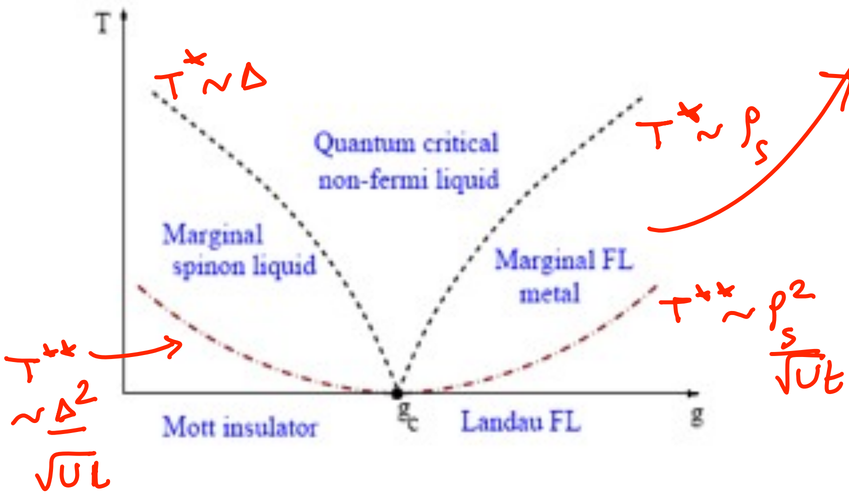
Analyse fluctuations: Concrete tractable theory of a continuous Mott transition (TS 2008); demonstrate critical Fermi surface at Mott transition;

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



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

Structure of critical theory

Field theory for critical point

$$S = S[b, a] + S[f_\alpha, a]$$

Gauge fluctuations are Landau damped by spinon Fermi surface:

$$S_{eff}[a] = \int_{\mathbf{q},\omega} \left(K_F \frac{|\omega|}{|\mathbf{q}|} + .. \right) |\mathbf{a}(\mathbf{q}, \omega)|^2$$

=> at low energies gauge field decouples from critical b fluctuations.
Charge sector is described by $S[b]$ = critical D = 2+1 XY model

Structure of critical theory (cont'd)

Though boson criticality is not affected by the gauge fields, the gauge fields are affected by the bosonic criticality.

Effective gauge dynamics

$$S_{eff}[a] = \int_{q,\omega} \left(K_F \frac{|\omega|}{|\mathbf{q}|} + \sigma_0 \sqrt{\omega^2 + q^2} \right) |\mathbf{a}(\mathbf{q},\omega)|^2$$

Second term: response of critical boson to the gauge field.

Anticipate that for fermions $|\omega| \ll |\mathbf{q}|$, replace by

$$S_{eff}[a] = \int_{q,\omega} \left(K_F \frac{|\omega|}{|\mathbf{q}|} + \sigma_0 |\mathbf{q}| \right) |\mathbf{a}(\mathbf{q},\omega)|^2$$

Spinon Fermi surface coupled to Landau damped gauge field with $z_b = 2$ (a well understood theory).

Critical theory

Effective critical action

$$S_{eff} = S[b] + S[f, a]$$

$S[b]$: critical D = 2+1 XY model
$S[f]$: spinon Fermi surface + Landau damped gauge field with $z_b = 2$
Both individually understood.

Non-zero temperature transport/dynamics

$$S_{eff}[a] = \int_{\mathbf{q}} \frac{1}{\beta} \sum_{\omega_n} \left(K_F \frac{|\omega_n|}{|\mathbf{q}|} + .. \right) |\mathbf{a}(\mathbf{q}, \omega_n)|^2$$

Static gauge fluctuations ($\omega_n = 0$) escape Landau damping, and do not decouple from critical bosons.

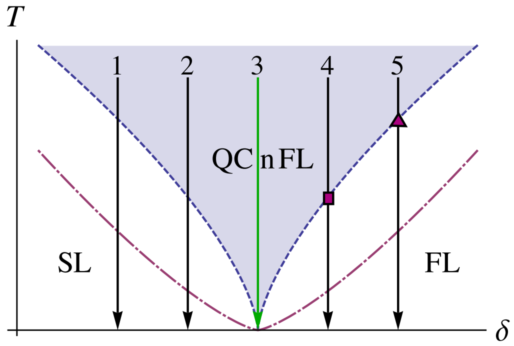
Universal transport in a large-N approximation (Witzcak-Krempa, Ghaemi, TS, Y.B. Kim, 2012):

Gauge scattering reduces universal conductivity by factor of ≈ 8 from $3D$ XY result (Damle, Sachdev '97).

Electronic Mott transition: Net resistivity $\rho = \rho_b + \rho_f$

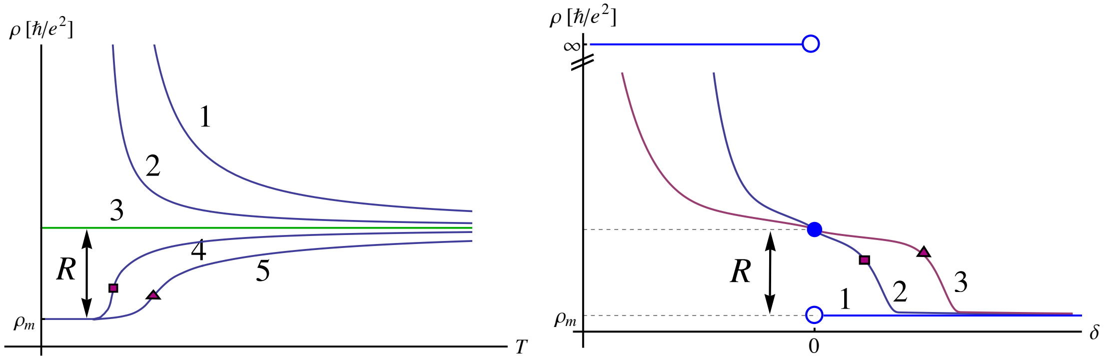
Universal resistivity jump $= \rho_b$ enhanced by factor of ≈ 8.

Non-zero temperature transport



(a)

(b)



(c)

(d)

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

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

Plan of talk

1. Theory of a continuous Mott metal-insulator transition in $d = 2$ at $x = 0$

Evolution from Fermi liquid to quantum spin liquid insulator: Predictions for transport experiments

2. Electronic Mott transition at filling 1/q : Formulation

3. Warm-up: Superfluid-insulator transitions of bosons at commensurate filling 1/q (a review)

Mott transitions at commensurate filling on square lattice

Consider filling $\nu = 1 - \frac{1}{q}$ for electrons on a square lattice.

Can drive a transition from a uniform Fermi liquid to a translation broken Mott insulator.

Address using slave bosons:

$$c_\alpha = b^\dagger f_\alpha$$

b is at filling $x = \frac{1}{q}$ and f_α at $1 - x$.

As before $\langle b \rangle \neq 0$ (and f_α form Fermi surface) yields the Fermi liquid.

To get Mott insulator put b in a boson Mott insulator.

For $q > 1$ this insulator will typically break translation symmetry.

Mott transitions at commensurate filling on square lattice

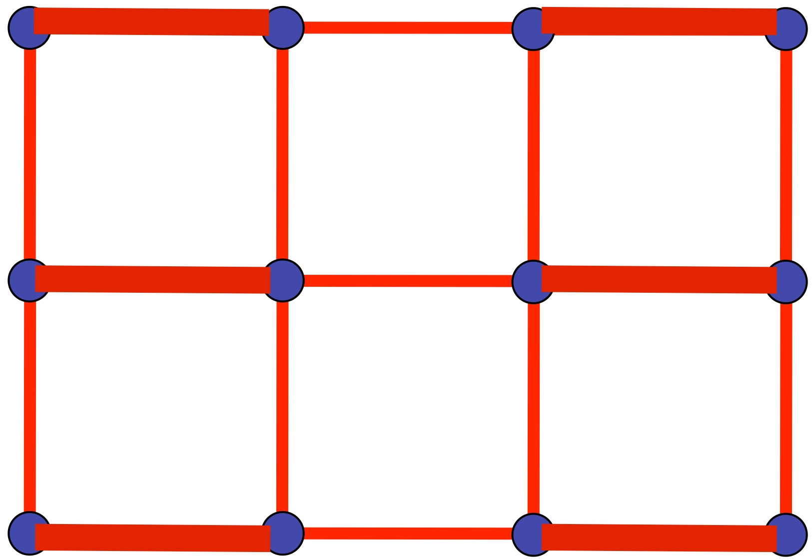
In this framework, the slave boson undergoes a transition from superfluid to a charge ordered insulator.

Such a transition could be second order, described by a deconfined quantum critical point.

Eg: q = 2

Insulator could be a period-2 stripe.

This has both stripe and `nematic' order (i.e break lattice rotation symmetry).



?? Continuous Mott transitions at commensurate filling ??

Strategy:

1. Understand theory of possible continuous superfluid - charge ordered Mott insulator transition of bosons at commensurate filling.

2. Couple this theory to spinon Fermi surface.

Many important couplings

- gauge fields of the slave boson decomposition (same as at $x = 0$)
- energy-energy coupling (same as at $x = 0$)
- charge order and nematic fluctuations

?? Continuous Mott transitions at commensurate filling ??

If the SF- charge ordered insulator transition of bosons is second order, it will be characterized by some critical exponents $\nu, z, \eta, \eta_{CO}, \eta_{Nem}$.

ν: correlation length exponent
z: dynamical critical exponent (expect $= 1$; see later)
η: anomalous dimension of b
η_{CO}: anamolous dimension of charge order.
η_{Nem}: anamolous dimension of nematic order.

Easy to derive criteria for when coupling to spinons does not change the bosonic criticality (as at x = 0).

Coupling to spinon Fermi surface

1. Gauge field coupling: Similar to x = 0 so long as boson sector is described by relativistic critical theory.

   Gauge field decouples from boson but is affected by it.

2. Energy- energy coupling

$$\int_{\omega,\mathbf{q}} \frac{|\omega|}{q} |b|^2$$

   Irrelevant if $\nu > \frac{2}{3}$.

3. Charge order fluctuations

$$\int_{\omega,\mathbf{q}} |\omega| |\rho_{CO}|^2$$

   Irrelevant if $\eta_{CO} > 1$.

4. Nematic fluctuations

$$\int_{\omega,\mathbf{q}} \frac{|\omega|}{q} |N|^2$$

   Irrelevant if $\eta_{Nem} > 2$.

Possible critical theory

Effective critical action

$$S_{eff} = S[b] + S[f, a]$$

$S[b]$: possible non-Landau critical theory for SF- CO insulator of bosons at filling $1/q$.

$S[f]$: spinon Fermi surface + Landau damped gauge field with $z_b = 2$

Need boson sector to be relativistic with $\nu > \frac{2}{3}, \eta_{CO} > 1, \eta_{Nem} > 2$.

If these are not satisfied critical theory will be more complicated.

Plan of talk

1. Theory of a continuous Mott metal-insulator transition in $d = 2$ at $x = 0$

Evolution from Fermi liquid to quantum spin liquid insulator: Predictions for transport experiments

2. Electronic Mott transition at filling 1/q : Formulation

3. Warm-up: Superfluid-insulator transitions of bosons at commensurate filling 1/q (a review)

Dual vortex theory of bosons at filling 1/q

q = 2: Lannert, Fisher, TS, 2000

General q: Balents, Bartosch, Burkov, Sachdev, Sengupta, 2005.

Dual description in terms of vortices very convenient to incorporate Berry phase effects of lattice filling.

Conventional 2d bosons: charge-vortex duality

$$\mathcal{L}_d = \mathcal{L}[\Phi, a_\mu] + \frac{1}{2\pi}\epsilon_{\mu\nu\lambda}\partial_\nu a_\lambda A_\mu$$

Dasgupta, Halperin, ’80
Peskin, Stone, ’80
Fisher, Lee, ’89

Conventional 2d bosons: charge-vortex duality

$$\mathcal{L}_d = \mathcal{L}[\Phi, a_\mu] + \frac{1}{2\pi}\epsilon_{\mu\nu\lambda}\partial_\nu a_\lambda A_\mu$$

Bosonic vortex

Dasgupta, Halperin, '80
Peskin, Stone, '80
Fisher, Lee, '89

Conventional 2d bosons: charge-vortex duality

$$\mathcal{L}_d = \mathcal{L}[\Phi, a_\mu] + \frac{1}{2\pi}\epsilon_{\mu\nu\lambda}\partial_\nu a_\lambda A_\mu$$

Bosonic vortex

Physical boson current

Dasgupta, Halperin, '80
Peskin, Stone, '80
Fisher, Lee, '89

Conventional 2d bosons: charge-vortex duality

$$\mathcal{L}_d = \mathcal{L}[\Phi, a_\mu] + \frac{1}{2\pi}\epsilon_{\mu\nu\lambda}\partial_\nu a_\lambda A_\mu$$

Bosonic vortex

Physical boson current

external probe gauge field

Boson superfluid = vortex insulator

Mott insulator = vortex condensate

Dasgupta, Halperin, '80
Peskin, Stone, '80
Fisher, Lee, '89

Dual vortex theory of bosons at filling 1/q

Bosons at filling $1/q$ => Vortices see an average flux $\frac{2\pi}{q}$.

Non-zero flux: translations realized projectively for the vortices.

"Magnetic translations": Vortex band structure q-fold degenerate.

Natural dual Landau-Ginzburg theory: q-species of vortex fields all coupled to same non-compact $U(1)$ gauge field.

Dual (possibly critical) field theory

Balents, Bartosch, Burkov, Sachdev, Sengupta 05

$$\mathcal{S}_0 = \int d^2 r d\tau \left(\sum_{\ell=0}^{q-1} \left[\left| (\partial_\mu - i A_\mu) \varphi_\ell \right|^2 + s \left| \varphi_\ell \right|^2 \right] \right.$$

$$\left. + \frac{1}{2e^2} (\epsilon_{\mu\nu\lambda} \partial_\nu A_\lambda)^2 \right). \qquad (2.19)$$

$$\mathcal{S}_1 = \int d^2 r d\tau \left(\sum_{n=0}^{q/2} \sum_{m=0}^{n} \lambda_{nm} \left[|\rho_{nm}|^2 + |\rho_{n,-m}|^2 + |\rho_{mn}|^2 \right. \right.$$

$$\left. \left. + |\rho_{m,-n}|^2 \right] \right). \qquad (2.20)$$

$\rho_{nm} = \varphi_n^* \varphi_m$ are gauge invariant charge ordering operators.

Status

Unfortunately there seem to currently be no sensible analytic ways of deciding whether there may be such a non-Landau critical point or not (for $q > 2$).

It may be possible in the future to study these theories numerically by simulating an SU(q) spin system with suitable anisotropies
(challenge for Ribhu Kaul).

Summary

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

Half-filling (organics, hyperkagome iridate):
Continuous Mott transition possible; several predictions for experiment (eg: universal resistivity jump in d = 2, resistivity peak in d = 3)

Other commensurate filling:
Criteria for certain kind of continuous Mott transition accompanied by charge order.

Other (not discussed in this talk):
Disordered limit (doped semiconductors Si:P, Si:B).
Do electrical and thermal metal-insulator transitions occur simultaneously?