Quantum phase transitions:
from Mott insulators
to the cuprate superconductors

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Talk online: 
Google Sachdev
Outline

A. “Dimerized” Mott insulators
   Landau-Ginzburg-Wilson (LGW) theory

B. Mott insulators with spin $S=1/2$ per unit cell
   Berry phases, bond order, and the breakdown of the LGW paradigm

C. Cuprate Superconductors
   Competing orders and recent experiments
“Dimerized” Mott insulators:

Landau-Ginzburg-Wilson (LGW) theory:

Second-order phase transitions described by fluctuations of an order parameter associated with a broken symmetry.
M. Matsumoto, B. Normand, T.M. Rice, and M. Sigrist, cond-mat/0309440.
TlCuCl$_3$

M. Matsumoto, B. Normand, T.M. Rice, and M. Sigrist, cond-mat/0309440.
Coupled Dimer Antiferromagnet


$S=1/2$ spins on coupled dimers

\[ H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j \]

$0 \leq \lambda \leq 1$
$\lambda$ close to 0

Weakly coupled dimers

Paramagnetic ground state

$$\langle \vec{S}_i \rangle = 0$$
$\lambda$ close to $0$  
Weakly coupled dimers

Excitation: $S=1$ *triplon*

$$\left| \begin{array}{c} \uparrow \downarrow \\ \downarrow \uparrow \end{array} \right> - \frac{1}{\sqrt{2}} \left| \begin{array}{c} \downarrow \uparrow \\ \uparrow \downarrow \end{array} \right>$$
$\lambda$ close to 0 \hspace{1cm} \text{Weakly coupled dimers}

Excitation: $S=1 \text{ triplon}$

$\frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$
\( \lambda \) close to 0

Weakly coupled dimers

Excitation: \( S=1 \) triplon (exciton, spin collective mode)

Energy dispersion away from antiferromagnetic wavevector

\[
\varepsilon_p = \Delta + \frac{c_x^2 p_x^2 + c_y^2 p_y^2}{2\Delta}
\]

\( \Delta \rightarrow \) spin gap

FIG. 1. Measured neutron profiles in the $a^*c^*$ plane of TlCuCl$_3$ for $i=(1.35,0,0)$, $ii=(0,0,3.15)$ [r.l.u]. The spectrum at $T=1.5$ K.
Coupled Dimer Antiferromagnet


$S=1/2$ spins on coupled dimers

\[
H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j
\]

\[0 \leq \lambda \leq 1\]
Square lattice antiferromagnet

Experimental realization: $La_2CuO_4$

Ground state has long-range magnetic (Neel or spin density wave) order

$$\langle \vec{S}_i \rangle = (-1)^{i_x+i_y} \vec{\phi} \neq 0$$

Excitations: 2 spin waves (**magnons**) $\varepsilon_p = \sqrt{c_x^2p_x^2 + c_y^2p_y^2}$
**TlCuCl₃**

**Neutron Diffraction Study of the Pressure-Induced Magnetic Ordering in the Spin Gap System TlCuCl₃**

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**Fig. 3.** Temperature dependence of the magnetic Bragg peak intensity for \( Q = (1,0,-3) \) reflection measured at \( P = 1.48 \) GPa in TlCuCl₃.
Neel state
\[ \langle \vec{S} \rangle = \pm \phi \]
\[ \phi \neq 0 \]

Quantum paramagnet
\[ \langle \vec{S} \rangle = 0 \]
\[ \phi = 0 \]

\[ \lambda_c = 0.52337(3) \]
M. Matsumoto, C. Yasuda, S. Todo, and H. Takayama,

LGW theory for quantum criticality

Landau-Ginzburg-Wilson theory: write down an effective action for the antiferromagnetic order parameter \( \tilde{\phi} \) by expanding in powers of \( \tilde{\phi} \) and its spatial and temporal derivatives, while preserving all symmetries of the microscopic Hamiltonian.

\[
S_\phi = \int d^2x d\tau \left[ \frac{1}{2} \left( (\nabla_x \tilde{\phi})^2 + c^2 (\partial_\tau \tilde{\phi})^2 + (\lambda - \lambda_c) \tilde{\phi}^2 \right) + \frac{u}{4!} (\tilde{\phi}^2)^2 \right]
\]


For \( \lambda < \lambda_c \) oscillations of \( \tilde{\phi} \) about \( \tilde{\phi} = 0 \) lead to the following structure in the dynamic structure factor \( S(p, \omega) \)

\[
\varepsilon(p) = \Delta + \frac{c^2 p^2}{2\Delta}; \quad \Delta = \sqrt{\lambda_c - \lambda}/c
\]

Mott insulators with spin $S=1/2$ per unit cell:

*Berry phases, bond order, and the breakdown of the LGW paradigm*
Mott insulator with two $S=1/2$ spins per unit cell
Mott insulator with one $S=1/2$ spin per unit cell
Mott insulator with one $S=1/2$ spin per unit cell

Ground state has Neel order with $\tilde{\phi} \neq 0$
Mott insulator with one $S=1/2$ spin per unit cell

Destroy Neel order by perturbations which preserve full square lattice symmetry

*e.g.* second-neighbor or ring exchange
Mott insulator with one $S=1/2$ spin per unit cell

Destroy Neel order by perturbations which preserve full square lattice symmetry

e.g. second-neighbor or ring exchange
Mott insulator with one $S=1/2$ spin per unit cell

Possible paramagnetic ground state with $\bar{\phi} = 0$
Mott insulator with one $S=1/2$ spin per unit cell

Possible paramagnetic ground state with $\tilde{\phi} = 0$

Such a state breaks the symmetry of rotations by $n\pi/2$ about lattice sites, and has $\Psi \neq 0$, where $\Psi$ is the bond order parameter

$(\Psi \to \Psi e^{in\pi/2}$ under the lattice rotation).
Mott insulator with one $S=1/2$ spin per unit cell

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($\Psi \rightarrow \Psi e^{in\pi/2}$ under the lattice rotation).
Mott insulator with one $S=1/2$ spin per unit cell

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Mott insulator with one $S=1/2$ spin per unit cell

Possible paramagnetic ground state with $\bar{\varphi} = 0$

Such a state breaks the symmetry of rotations by $n\pi/2$ about lattice sites, and has $\Psi \neq 0$, where $\Psi$ is the \textit{bond order parameter} ($\Psi \rightarrow \Psi e^{i n \pi/2}$ under the lattice rotation).
Mott insulator with one $S=1/2$ spin per unit cell

Possible paramagnetic ground state with $\phi = 0$

Another state that breaks the symmetry of rotations by $n\pi/2$ about lattice sites, and has $\Psi \neq 0$, where $\Psi$ is the \textit{bond order parameter}

$(\Psi \rightarrow \Psi e^{in\pi/2}$ under the lattice rotation).
Mott insulator with one $S=1/2$ spin per unit cell

Possible paramagnetic ground state with $\bar{\phi} = 0$

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$(\Psi \rightarrow \Psi e^{in\pi/2}$ under the lattice rotation).
Resonating valence bonds

Resonance in benzene leads to a symmetric configuration of valence bonds
\( (F. Kekulé, L. Pauling) \)

The paramagnet on the square lattice should also allow other valence bond pairings, and this implies a “resonating valence bond liquid” with \( \Psi=0 \)
\( (P.W. Anderson, 1987) \)
Quantum theory for destruction of Neel order

Ingredient missing from LGW theory:
Spin Berry Phases

$A$

$e^{iSA}$
Quantum theory for destruction of Neel order

**Ingredient missing from LGW theory:**

**Spin Berry Phases**
Quantum theory for destruction of Neel order

Discretize imaginary time: path integral is over fields on the sites of a cubic lattice of points $a$

$n_a \sim \eta_a \vec{S}_a \rightarrow$ Neel order parameter;
$\eta_a \rightarrow \pm 1$ on two square sublattices ;
$A_{a\mu} \rightarrow \text{half} \text{ oriented area of spherical triangle}$
formed by $n_a$, $n_{a+\mu}$, and an arbitrary reference point $n_0$
Quantum theory for destruction of Neel order

Partition function on cubic lattice

\[ Z = \prod_a \int d n_a \delta \left( n_a^2 - 1 \right) \exp \left( \frac{1}{g} \sum_{a, \mu} n_a \cdot n_{a+\mu} - i \sum_a \eta_a A_{a\tau} \right) \]

Modulus of weights in partition function: those of a classical ferromagnet at “temperature” \( g \)

Small \( g \) \( \Rightarrow \) ground state has Neel order with \( \left\langle n_a \right\rangle = \bar{\phi} \neq 0 \)

Large \( g \) \( \Rightarrow \) paramagnetic ground state with \( \left\langle n_a \right\rangle = 0 \)

Berry phases lead to large cancellations between different time histories \( \rightarrow \) need an effective action for \( A_{a\mu} \) at large \( g \)
Change in choice of $n_0$ is like a “gauge transformation”

$$2A_{a\mu} \rightarrow 2A_{a\mu} - \gamma_{a+\mu} + \gamma_a$$

($\gamma_a$ is the oriented area of the spherical triangle formed by $n_a$ and the two choices for $n_0$).

The area of the triangle is uncertain modulo $4\pi$, and the action is invariant under

$$A_{a\mu} \rightarrow A_{a\mu} + 2\pi$$

These principles strongly constrain the effective action for $A_{a\mu}$ which provides description of the large $g$ phase.
Simplest large $g$ effective action for the $A_{a\mu}$

$$Z = \prod \int dA_{a\mu} \exp \left( \frac{1}{2e^2} \sum \cos (\Delta_\mu A_{av} - \Delta_v A_{a\mu}) - i \sum \eta_a A_{a\tau} \right)$$

with $e^2 \sim g^2$

This is compact QED in 3 spacetime dimensions with static charges ±1 on two sublattices.

Exact duality transform on a periodic Gaussian ("Villain") action for compact QED + Berry phases leads to a representation in terms of a "height" model

\[ Z_{\text{dual}} = \sum_{\{h_j\}} \exp \left( -\frac{e^2}{2} \sum_j (\Delta_\mu h_j - \Delta_\mu \chi_j)^2 \right) \]

with the \( h_j \) integer heights.
The Berry phases lead to height ‘offsets’ \( \chi_j = 0, 1/4, 1/2, 3/4 \) on the four dual sublattices.

For large $e^2$, low energy height configurations are in exact one-to-one correspondence with nearest-neighbor valence bond pairings of the sites square lattice.

There is no roughening transition for three dimensional interfaces, which are smooth for all couplings.

⇒ There is a definite average height of the interface

⇒ **Ground state has bond order.**

Smooth interface with average height $3/8$

Smooth interface with average height $5/8$

Smooth interface with average height $7/8$

Smooth interface with average height $1/8$

“Disordered-flat” interface with average height $1/2$

“Disordered-flat” interface with average height $3/4$

“Disordered-flat” interface with average height 0

“Disordered-flat” interface with average height $1/4$

\[ Z = \prod_a \int d\mathbf{n}_a \delta(\mathbf{n}_a^2 - 1) \exp \left( \frac{1}{g} \sum_{a,\mu} \mathbf{n}_a \cdot \mathbf{n}_{a+\mu} - i \sum_a \eta_a A_{a\tau} \right) \]

Neel order
\[ \tilde{\phi} \neq 0 \]

Bond order
\[ \Psi \neq 0 \]
Not present in LGW theory of \( \tilde{\phi} \) order
Bond order in a frustrated $S=1/2$ XY magnet


First *large scale* numerical study of the destruction of Neel order in a $S=1/2$ antiferromagnet with full square lattice symmetry

\[
H = 2J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y) - K \sum_{\langle ijkl \rangle} (S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+) \]

\[
g = \frac{K}{J} \]
\[ Z = \prod_a \int d\mathbf{n}_a \delta(\mathbf{n}_a^2 - 1) \exp \left( \frac{1}{g} \sum_{a,\mu} \mathbf{n}_a \cdot \mathbf{n}_{a+\mu} - i \sum_a \eta_a A_{a\tau} \right) \]

Neel order
\[ \tilde{\varphi} \neq 0 \]
Bond order
\[ \Psi \neq 0 \]
Not present in LGW theory of \( \tilde{\varphi} \) order
Naïve approach: add bond order parameter to LGW theory “by hand”

- Neel order: $\tilde{\phi} \neq 0$
- Bond order: $\Psi \neq 0$
  - First order transition

- Neel order: $\tilde{\phi} \neq 0$
  - Coexistence: $\tilde{\phi} \neq 0, \Psi \neq 0$
- Bond order: $\Psi \neq 0$

- Neel order: $\tilde{\phi} \neq 0$
  - "disordered": $\tilde{\phi} = 0, \Psi = 0$
- Bond order: $\Psi \neq 0$

$g$
Alternative formulation to describe transition:
Express theory in terms of a complex spinor $z_{a\alpha}$, $\alpha = \uparrow, \downarrow$, with

$$n_a = z_{a\alpha}^* \sigma_{\alpha\beta} z_{a\beta}$$

$$Z = \prod_a \int dz_{a\alpha} dA_{a\mu} \delta (|z_{a\alpha}|^2 - 1) \exp \left( \frac{1}{g} \sum_{a,\mu} z_{a\alpha}^* e^{iA_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} + i \sum_a \eta_a A_{a\tau} \right)$$

Theory of a second-order quantum phase transition between Neel and bond-ordered phases

At the quantum critical point:

- Dual interface becomes *rough*.
- $A_\mu$ gauge field is effectively non-compact (monopoles are *dangerously irrelevant*)
- $\Rightarrow$ Total gauge flux is conserved.
- Fractionalized $S=1/2$ $z_\alpha$ are globally propagating degrees of freedom.

Second-order critical point described by emergent fractionalized degrees of freedom ($A_\mu$ and $z_\alpha$); Order parameters ($\varphi$ and $\Psi$) are “composites” and of secondary importance

Phase diagram of S=1/2 square lattice antiferromagnet

Neel order
\[ \bar{\phi} \sim z^*_\alpha \bar{\sigma}_{\alpha\beta} z_\beta \neq 0 \]

Bond order \( \Psi \neq 0 \),
\( S = 1/2 \) spinons \( z_\alpha \) confined,
\( S = 1 \) triplon excitations

Second-order critical point described by
\[
S_{\text{critical}} = \int d^2x d\tau \left[ \left| (\partial_\mu - i A_\mu) z_\alpha \right|^2 + r |z_\alpha|^2 + \frac{u}{2} \left( |z_\alpha|^2 \right)^2 + \frac{1}{4e^2} (\partial_\mu A_\nu - \partial_\nu A_\mu)^2 \right]
\]

where \( \mathbf{n} = z^*_\alpha \bar{\sigma}_{\alpha\beta} z_\beta \), \( z_\alpha \) are bosonic spinors, and \( A_\mu \) is non-compact

Cuprate superconductors: 
*Competing orders and recent experiments*
Main idea: *one* of the effects of doping mobile carriers is to increase the value of $g$
Neutron scattering measurements of $\text{La}_{1.875}\text{Ba}_{0.125}\text{CuO}_4$ (Zurich oxide)


Spin density wave of 8 lattice spacings along the principal square lattice axes

Possible microscopic picture

Bragg diffraction off static spin order
Neutron scattering measurements of \( \text{La}_{1.875}\text{Ba}_{0.125}\text{CuO}_4 \) (Zurich oxide)


Possible microscopic picture

Spin density wave of 8 lattice spacings along the principal square lattice axes

Bragg diffraction off static spin order with multiple domains
Neutron scattering measurements of $\text{La}_{1.875}\text{Ba}_{0.125}\text{CuO}_4$ (Zurich oxide)


Spin density wave of 8 lattice spacings along the principal square lattice axes

Bragg diffraction off static spin order with multiple domains (after rotation by 45°)
At higher energies, expect "spin-wave cones".

Only seen at relatively low energies.
High energy spectrum is the triplon excitation of two-leg spin ladders
  \[ \Rightarrow \textit{presence of bond order} \]
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Superposition and rotation by 45 degrees
Computation from isolated 2 leg ladders.

J. M. Tranquada et al., cond-mat/0401621
La$_{1.875}$Ba$_{0.125}$CuO$_4$

YBa$_2$Cu$_3$O$_{6.85}$

J. M. Tranquada et al., cond-mat/0401621
Understanding spectrum at all energies requires coupling between ladders, just past the quantum critical point to the onset of long-range magnetic order.


M. Vojta and T. Ulbricht, cond-mat/0402377
Possible evidence for spontaneous bond order in a doped cuprate

J. M. Tranquada et al., cond-mat/0401621 M. Vojta and T. Ulbricht, cond-mat/0402377
Our interpretation: STM evidence for fluctuating spin density/bond order pinned by vortices/impurities

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STM image of LDOS modulations (after filtering in Fourier space) in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ in zero magnetic field
Our interpretation: STM evidence for fluctuating spin density/bond order pinned by vortices/impurities


LDOS of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ at 100 K.
Energy integrated LDOS (between 65 and 150 meV) of strongly underdoped \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \) at low temperatures, showing only regions without superconducting “coherence peaks”


Our interpretation: STM evidence for fluctuating spin density/bond order pinned by vortices/impurities
Conclusions

I. Theory of quantum phase transitions between magnetically ordered and paramagnetic states of Mott insulators:


B. $S=1/2$ square lattice: Berry phases induce bond order, and LGW theory breaks down. Critical theory is expressed in terms of emergent fractionalized modes, and the order parameters are secondary.

II. Preliminary evidence for spin density/bond orders in superconducting cuprates