Quantum phase transitions in Mott insulators and \textit{d}-wave superconductors

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\textit{Quantum Phase Transitions}
Cambridge University Press
Concentration of mobile carriers $\delta$ in e.g. $\text{La}_{2-\delta}\text{Sr}_\delta\text{CuO}_4$.

Change magnetic interactions to produce a quantum paramagnet or a "spin liquid".

$\langle S \rangle = 0$

Experiments

La$_2$CuO$_4$

Magnetic order
$\langle S \rangle \neq 0$

High temperature superconductivity

Zn

Theory
Outline of Lectures

I. Magnetic quantum phase transitions in Mott insulators:
   paramagnetic states with confinement and deconfinement of spinons, and charge stripe order.

II. Non-magnetic impurities in two-dimensional antiferromagnets and superconductors:
   NMR and neutron scattering experiments with and without Zn/Li impurities

III. Quantum phase transitions in $d$-wave superconductors:
   Photo-emission experiments and the case for fluctuating $d_{x^2-y^2} + id_{xy}$ pairing order.
Lecture I

**Magnetic quantum phase transitions in Mott insulators:**

1. Neel and paramagnetic states of the coupled ladder antiferromagnet.
   Coherent state path integral and field theory for the quantum phase transition

2. Paramagnets on the square lattice.
   Confinement of spinons and bond-centered charge stripe order.
   Generalization to magnetic transitions in $d$-wave superconductors

3. Magnetically ordered and paramagnetic states on strongly frustrated square lattices and the triangular lattice.
   Non-collinear spin correlations and the deconfinement of spinons.
I.1 Neel and paramagnetic states of the coupled ladder antiferromagnet

(Katoh and Imada; Tworzydlo, Osman, van Duin and Zaanen)

S=1/2 spins on coupled 2-leg ladders

\[
H = \sum_{<ij>} J_{ij} \mathbf{\hat{S}_i} \cdot \mathbf{\hat{S}_j}
\]

Follow ground state as a function of \( \lambda \)

\( 0 \leq \lambda \leq 1 \)
Square lattice antiferromagnet

Experimental realization: $La_2CuO_4$

Ground state has long-range magnetic (Neel) order

$$\langle \tilde{S}_i \rangle = (-1)^{i_x+i_y} N_0 \neq 0$$

Excitations: 2 spin waves

Quasiclassical wave dynamics at low T

(Chakravarty et al, 1989; Tyc et al, 1989)
λ close to 0

Weakly coupled ladders

\[ \begin{align*}
\hat{S}_i = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \\
\end{align*} \]

Paramagnetic ground state \[ \langle \hat{S}_i \rangle = 0 \]

Excitation: \( S=1 \), \( \phi_\alpha \) particle (collective mode)

Energy dispersion away from antiferromagnetic wavevector

\[ \epsilon = \Delta_{\text{res}} + \frac{c^2 k^2}{2 \Delta_{\text{res}}} \]

\( \Delta_{\text{res}} \rightarrow \text{Spin gap} \)
Quantum paramagnet \( \langle \vec{S} \rangle = 0 \)

Neel state \( \langle \vec{S} \rangle = N_0 \neq 0 \)

Spin gap \( \Delta_{\text{res}} \)

Neel order \( N_0 \)

\( \lambda_c \)
Nearly-critical paramagnets

\( \lambda \) is close to \( \lambda_c \)

Quantum field theory:

\[
S_b = \int d^2x d\tau \left[ \frac{1}{2} \left( (\nabla_x \phi_\alpha)^2 + c^2 (\partial_\tau \phi_\alpha)^2 + r \phi_\alpha^2 \right) + \frac{g}{4!} (\phi_\alpha^2)^2 \right]
\]

\( \phi_\alpha \rightarrow \) 3-component antiferromagnetic order parameter

\( r > 0 \rightarrow \lambda < \lambda_c \)

\( r < 0 \rightarrow \lambda > \lambda_c \)

Oscillations of \( \phi_\alpha \) about zero (for \( r > 0 \))

\( \rightarrow \) spin-1 collective mode

\( \text{T}=0 \) spectrum
Coupling $g$ approaches fixed-point value under renormalization group flow: beta function ($\varepsilon = 3-d$):

$$\beta(g) = -\varepsilon g + \frac{11g^2}{6} - \frac{23g^3}{12} + O(g^4)$$

Only relevant perturbation – $r$ strength is measured by the spin gap $\Delta$

$\Delta_{\text{res}}$ and $c$ completely determine entire spectrum of quasi-particle peak and multiparticle continua, the $S$ matrices for scattering between the excitations, and $T > 0$ modifications.
I.2 **Paramagnets on the square lattice**

Square lattice with first ($J_1$) and second ($J_2$) neighbor exchange interactions

- **Neel state**
- **Spin-Peierls state**
  - "Bond-centered charge stripe"

\[
\frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)\]

Quantum “entropic” effects prefer one-dimensional striped structures in which the largest number of singlet pairs can resonate. The state on the upper left has more flippable pairs of singlets than the one on the lower left. These effects always lead to a broken square lattice symmetry near the transition to the Neel state (more generally, this behavior is generic near magnetically ordered states with a collinear spin polarization)

Excitations
Stable S=1 particle

Energy dispersion
\[ \epsilon_k = \Delta + \frac{c_x^2 k_x^2 + c_y^2 k_y^2}{2 \Delta} \]

\[ \Delta \rightarrow \text{Spin gap} \]

S=1/2 spinons are linearly confined by the line of “defect” singlet pairs between them
I.3 Paramagnets on the triangular and frustrated square lattices – spinon deconfinement

Translationally invariant “spin liquid” state obtained by a quantum transition from a magnetically ordered state with \textit{co-planar} spin polarization. Transition to confined states is described by a $Z_2$ gauge theory


G. Misguich and C. Lhuillier, cond-mat/0002170.
R. Moessner and S.L. Sondhi, cond-mat/0007378.
Antiferromagnet on the Shastry-Sutherland lattice

Experimentally realized by $\text{SrCu}_2(\text{BO}_3)_2$

Attractive candidate for accessing states with spin-charge separation

S. Sachdev, C.-H. Chung, and J.B. Marston, to appear
Lecture II

Non-magnetic impurities in two-dimensional antiferromagnets and superconductors

1. Impurities in the coupled ladder antiferromagnet

   Berry phases and properties across the bulk quantum phase transition

2. Impurities in paramagnets with and without spinon deconfinement square.

3. From quantum paramagnets to \textit{d-wave} superconductors.

   Nature of magnetic ordering transition; fate of charge stripe order and non-magnetic impurities.

4. Experiments on \textit{d-wave} superconductors.

   NMR on Zn/Li impurities; neutron scattering measurements of phonon spectra and collective spin excitations; effective of Zn impurities on collective spin resonance
II.1 Impurities in the coupled-ladder antiferromagnet

Make *any* localized deformation e.g. remove a spin

Susceptibility

\[ \chi = A \chi_b + \chi_{imp} \]

\( (A = \text{area of system}) \)

In paramagnetic phase as \( T \to 0 \)

\[ \chi_b = \left( \frac{\Delta}{\hbar^2 c^2 \pi} \right) e^{-\Delta/k_B T} \]

\[ ; \chi_{imp} = \frac{S(S+1)}{3k_B T} \]

For a general impurity \( \chi_{imp} \) defines the value of \( S \)

\[ \lim_{\tau \to \infty} \langle \vec{S}_Y(\tau) \cdot \vec{S}_Y(0) \rangle = m^2 \neq 0 \]
Orientation of “impurity” spin -- \( n_\alpha (\tau) \) (unit vector)

Action of “impurity” spin

\[
S_{\text{imp}} = \int d\tau \left[ iSA_\alpha (n) \frac{dn_\alpha}{d\tau} - \gamma S n_\alpha (\tau) \phi_\alpha (x = 0, \tau) \right]
\]

\( A_\alpha (n) \rightarrow \) Dirac monopole function

Boundary quantum field theory: \( S_b + S_{\text{imp}} \)

Recall -

\[
S_b = \int d^2x d\tau \left[ \frac{1}{2} \left( (\nabla_x \phi_\alpha)^2 + c^2 (\partial_\tau \phi_\alpha)^2 + r\phi_\alpha^2 \right) + \frac{g}{4!} (\phi_\alpha^2)^2 \right]
\]
Coupling $\gamma$ approaches also approaches a fixed-point value under the renormalization group flow

(Sengupta, 97  
Sachdev+Ye, 93  
Smith+Si 99)

Beta function:

$$\beta(\gamma) = -\frac{\varepsilon \gamma}{2} + \gamma^3 - \gamma^5 + \frac{5g^2\gamma}{144} + \pi^2 \left(S(S + 1) - \frac{1}{3}\right) g^3 \gamma + \mathcal{O}\left((\gamma, \sqrt{g})^7\right)$$

No new relevant perturbations on the boundary; All other boundary perturbations are irrelevant –

e.g.

$$\lambda \int d\tau \phi^2_{\alpha}(x = 0, \tau)$$

$\Delta$ and $c$ completely determine spin dynamics near an impurity –

No new parameters are necessary!
Universal properties at the critical point $\lambda = \lambda_c$

$$\langle \vec{S}_Y(\tau) \cdot \vec{S}_Y(0) \rangle = \frac{1}{\tau^{\eta'}}$$

(and $m = |\lambda - \lambda_c|^{\eta'\nu}$)

$\eta'$ is a new boundary scaling dimension

Operator product expansion:

$$\lim_{x \to 0} \phi_\alpha(x, \tau) \sim \frac{n_\alpha(\tau)}{|x|^{(d-1+\eta-\eta')/2}}$$

However

$$\chi_{imp} \neq \frac{1}{T^{1-\eta'}}$$

This last relationship holds in the multi-channel Kondo problem because the magnetic response of the screening cloud is negligible due to an exact “compensation” property. There is no such property here, and naïve scaling applies. This leads to

$$\chi_{imp} = \frac{\text{Universal number}}{k_B T}$$

Curie response of an irrational spin
In the Neel phase

\[ \chi_{\text{imp}} = \frac{S(S + 1)}{3k_BT} \]

\[ \chi_{\text{imp}}^\perp = C_3/\rho_s \]

Bulk susceptibility vanishes while impurity susceptibility diverges as \( \rho_s \to 0 \)

At \( T > 0 \), thermal averaging leads to

\[ \chi_{\text{imp}} = \frac{S^2}{3k_BT} + \frac{2}{3} \chi_{\text{imp}}^\perp \]
Finite density of impurities $n_{\text{imp}}$

Relevant perturbation – strength determined by only energy scale that is linear in $n_{\text{imp}}$ and contains only bulk parameters

$$\Gamma \equiv \frac{n_{\text{imp}}(\hbar c)^2}{\Delta}$$

Two possible phase diagrams

(a) $\Gamma / \Delta = 0^+$

Magnetic long-range order

Quantum paramagnet

$b$ $\Gamma / \Delta = \text{constant}$

Magnetic long-range order

Quantum paramagnet
Fate of collective mode peak

Without impurities \( \chi(G, \omega) = \frac{A}{\Delta^2 - \omega^2} \)

With impurities \( \chi(G, \omega) = \frac{A}{\Delta^2} \Phi\left( \frac{\hbar \omega}{\Delta}, \frac{\Gamma}{\Delta} \right) \)

\( \Phi \rightarrow \text{Universal scaling function. We computed it in a "self-consistent, non-crossing" approximation} \)

Predictions: Half-width of line \( \approx \Gamma \)
Universal asymmetric lineshape
II.2a. Impurities in square lattice paramagnets with confinement

Zn or Li impurities substitute for Cu ions

Spinon confinement implies that free $S=1/2$ moments must form near each impurity
II.2b. Impurities in paramagnets with spinon deconfinement

G. Misguich and C. Lhuillier, cond-mat/0002170.
R. Moessner and S.L. Sondhi, cond-mat/0007378.
Concentration of mobile carriers $\delta$ in e.g. $\text{La}_{2-\delta}\text{Sr}_\delta\text{CuO}_4$

Change magnetic interactions to produce a quantum paramagnet or a "spin liquid"

$\langle S \rangle = 0$

$\langle \bar{S} \rangle \neq 0$

Experiments

Magnetic order

High temperature superconductivity

Theory

Zn

$\text{La}_2\text{CuO}_4$
Constraints from momentum conservation in d-wave superconductors

Collective magnetic excitations, $\phi_\alpha$, are not damped by fermionic Bogoliubov quasiparticles
As \( \Delta \to 0 \) there is a quantum phase transition to a magnetically ordered state

(A) Insulating Neel state (or collinear SDW at wavevector \( \mathbf{Q} \)) \( \iff \) insulating quantum paramagnet

(B) \( d \)-wave superconductor with collinear SDW at wavevector \( \mathbf{Q} \) \( \iff \) \( d \)-wave superconductor (paramagnet)

Transition (B) is in the same universality class as (A) provided \( \Psi_h \) fermions remain gapped at quantum-critical point.
II.3. **Quantum paramagnets to \textit{d}-wave superconductors:** evolution with density of mobile carriers of density $\delta$

A. **Doping a paramagnet with confinement**

\[ \text{Condensate of hole pairs} \]


B. **Doping a deconfined paramagnet**

If holes are bosons, single hole condensation leads to a superconductor with some exotic properties


**Stable $hc/e$ vortices** (S. Sachdev, Phys. Rev. B \textbf{45}, 389 (1992);
Superconductivity coexists with charge stripe order in region without magnetic order

See also J. Zaanen, Physica C 217, 317 (1999),
Neutron scattering measurements of phonon spectrum of superconducting $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$ by R. J. McQueeney, Y. Petrov, T. Egami, M. Yethiraj, G. Shirane, and Y. Endoh, Phys. Rev. Lett. 82, 628 (1999)

Thanks to S. Kivelson
Computation of phonon spectrum by McQueeney et al using a simple model based on lattice modulation below.

Evidence for coexistence of spin-Peierls order and "d-wave" superconductivity.

Spin-1 collective mode in YBCO - little observable damping at low T. Coupling to superconducting quasiparticles unimportant.

Continuously connected to S=1 particle in confined Mott insulator

Zn or Li impurities in doped Mott insulators

Case A

Striped insulator with spinon confinement

$d$-wave superconductor

Moments form near each Zn or Li.

This moment is quenched at a quantum phase transition at $\delta=\delta_c$.


Case B

Spin liquid with spinon deconfinement

$d$-wave superconductor

No moments form near Zn or Li ions substituted for Cu and impurity response evolves smoothly
II.4. Recent experiments on d-wave superconductors

NMR on Zn/Li impurities


$^7$Li NMR below $T_c$

Inverse local susceptibility of isolated Li impurities in YBCO
Moments measured by analysis of Knight shifts


Berry phases of precessing spins do not cancel between the sublattices in the vicinity of the impurity: net uncancelled phase of \( S=1/2 \)
$YBa_2Cu_3O_7 + 0.5\% \text{ Zn}$

YBa$_2$Cu$_3$O$_7$ + 0.5% Zn


\[ n_{\text{imp}} = 0.005 \]
\[ \Delta = 40 \text{ meV} \]
\[ \hbar c = 0.2 \text{ eV} \]
\[ \Rightarrow \Gamma = 5 \text{ meV}, \quad \Gamma/\Delta = 0.125 \]

Quoted half-width = 4.25 meV
Lecture III

Quantum phase transitions in \(d\)-wave superconductors

1. Motivation from photo-emission experiments.

2. Field theories for low energy fermionic excitations near quantum phase transitions.

   Classification of all possible spin singlet order parameters with zero total momentum

3. Renormalization group analysis.

   Selection of \(d_{x^2-y^2} + id_{xy}\) order
Photoemission on BSSCO

(Valla et al Science 285, 2110 (1999))

Quantum-critical damping of quasi-particles along (1,1)
Goal: Classify theories in which, with minimal fine tuning, a d-wave superconductor has a fermionic quasiparticle momentum distribution curve (MDC), at the nodal points, with a width proportional to $k_B T$.

In a Fermi liquid, MDC width $\sim T^2$

In a BCS d-wave superconductor, MDC width $\sim T^3$
Proximity to a quantum-critical point

\[ T_c \]

Superconducting state \( X \)

Quantum critical

Superconducting \( T \)

d-wave superconductor

\[ S \]
Necessary conditions

1. Quantum-critical point should be below its upper-critical dimension and obey hyperscaling.

2. Nodal quasi-particles should be part of the critical-field theory.

3. Critical field theory should not be free – required to obtain damping in the scaling limit.
Low energy fermionic excitations of a \textit{d}-wave superconductor

Gapless Fermi Points in a \textit{d}-wave superconductor at wavevectors $(\pm K, \pm K)$

\[ K = 0.391 \pi \]

\[
\Psi_1 = \begin{pmatrix} f_{1\uparrow} \\ f_{3\downarrow}^* \\ f_{1\downarrow} \\ -f_{3\uparrow}^* \end{pmatrix} \quad \quad \Psi_2 = \begin{pmatrix} f_{2\uparrow} \\ f_{4\downarrow}^* \\ f_{2\downarrow} \\ -f_{4\uparrow}^* \end{pmatrix}
\]

\[
S_\Psi = \int \frac{d^2k}{(2\pi)^2} T \sum_{\omega_n} \Psi_1^\dagger (-i\omega_n + v_F k_x \tau^z + v_\Delta k_y \tau^x) \Psi_1
+ \int \frac{d^2k}{(2\pi)^2} T \sum_{\omega_n} \Psi_2^\dagger (-i\omega_n + v_F k_y \tau^z + v_\Delta k_x \tau^x) \Psi_2.
\]

$\tau^x, \tau^z$ are Pauli matrices in Nambu space
2a. Charge stripe order

Charge density
\[ \delta \rho \sim \text{Re}[\Phi_x e^{iG_x} + \Phi_y e^{iG_y}] \]

If \( G \neq 2K \) fermions do not couple efficiently to the order parameter and are not part of the critical theory

Action for quantum fluctuations of order parameter
\[
S_{\Phi} = \int d^d x d\tau \left[ |\partial_\tau \Phi_x|^2 + |\partial_\tau \Phi_y|^2 + |\nabla \Phi_x|^2 + |\nabla \Phi_y|^2 \right. \\
\left. + s_0 \left( |\Phi_x|^2 + |\Phi_y|^2 \right) + \frac{u_0}{2} \left( |\Phi_x|^4 + |\Phi_y|^4 \right) \right. \\
\left. + v_0 |\Phi_x|^2 |\Phi_y|^2 \right]
\]

Coupling to fermions \( \sim \lambda \int d^d x d\tau |\Phi_a|^2 \Psi \Psi \)
and \( \lambda \) is irrelevant at the critical point

\[ \text{Im} \Sigma \sim T^{2d+1-2/\nu} \]

\[ \sim T^{(\text{between 2 and 3})} \text{ for } 2/3 < \nu < 1 \]
A spin-singlet, fermion bilinear, zero momentum order parameter for \( X \) is preferred.

If ordering wavevector does not connect two nodal points, nodal fermions are not part of the critical theory, and do not suffer critical damping.

Similar reasoning can be used to argue against magnetic order parameters and the staggered-flux order.
Order parameter for $X$ should be a component of

$$\Delta_k = \langle c_{k\uparrow} c_{-k\downarrow} \rangle \text{ (fermion pairing)}$$

or

$$A_k = \langle c_{k\alpha}^\dagger c_{k\alpha} \rangle \text{ (excitonic order)}$$

**Complete group-theoretic classification**

$X$ has $d_{x^2-y^2}$ pairing plus

- (A) $is$ pairing
- (B) $id_{xy}$ pairing
- (C) $ig$ pairing
- (D) $s$ pairing
- (E) $d_{xy}$ excitons
- (F) $d_{xy}$ pairing
- (G) $p$ excitons

**Superconducting nematics**

**Fermion spectrum fully gapped**

**Nodal points**
Quantum field theory for critical point

Ising order parameter $\phi$ (except for case (G))

$$S_\phi = \int d^2x d\tau \left[ \frac{1}{2} (\partial_\tau \phi)^2 + \frac{c^2}{2} (\nabla \phi)^2 + \frac{s}{2} \phi^2 + \frac{u}{24} \phi^4 \right]$$

Coupling to nodal fermions

$$S_{\Psi \phi} = \int d^2x d\tau \left[ \lambda \left( \bar{\Psi}_1 M_1 \Psi_1 + \bar{\Psi}_2 M_2 \Psi_2 \right) \right].$$

(A) $M_1 = \tau^y$; $M_2 = \tau^y$

(B) $M_1 = \tau^y$; $M_2 = -\tau^y$

(C) $\lambda = 0$, so fermions are not critical

(D) $M_1 = \tau^x$; $M_2 = \tau^x$

(E) $M_1 = \tau^z$; $M_2 = -\tau^z$

(F) $M_1 = \tau^x$; $M_2 = -\tau^x$

(G) $M_1 = 1$; $M_2 = 1$ but $\phi$ has

2 components
Main results

Only cases

(A) \( d_{x^2-y^2} \leftrightarrow d_{x^2-y^2} + is \) pairing and

(B) \( d_{x^2-y^2} \leftrightarrow d_{x^2-y^2} + id_{xy} \) pairing

have renormalization group fixed points with a non-zero interaction strength between the bosonic order parameter mode and the nodal fermions.

Only cases (A) and (B) satisfy conditions 1,2,3

\( d_{xy} \) pairing vanishes along the (1,0),(0,1) directions, and so only case (B) does not strongly scatter the anti-nodal quasiparticles.

Transition to \( d_{xy} \) pairing is expected with increasing \( J_2 \).
Conclusions

1. Argued that many properties of the superconductor can be understood by adiabatic continuity from a reference paramagnetic Mott insulator with confinement – such a state requires $S=1$ spin resonance, broken translational symmetry (stripe order), and moments near non-magnetic impurities.

2. Clear NMR evidence for $S=1/2$ moment near non-magnetic impurities.

3. Quantitative comparison of neutron scattering experiments on Zn impurities with theory.

4. Evidence for theoretically predicted bond-centered stripe correlations in paramagnetic phase with $d$-wave superconductivity.

5. Damping of nodal quasiparticles may be associated with proximity to a quantum critical point to a $d_{x^2-y^2} + i d_{xy}$ superconductor. Such a state is expected at larger second neighbor exchange.