Quantum phase transitions in Mott insulators and *d*-wave superconductors

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Outline of Lectures

I. <u>Magnetic quantum phase</u> <u>transitions in Mott insulators</u>:

paramagnetic states with confinement and deconfinement of spinons, and charge stripe order.

II. <u>Non-magnetic impurities in two-</u> <u>dimensional antiferromagnets and</u> <u>superconductors:</u>

NMR and neutron scattering experiments with and without Zn/Li impurities

III. <u>Quantum phase transitions in *d*-</u> <u>wave superconductors:</u>

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 bondcentered 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.





Square lattice antiferromagnet

Experimental realization: La_2CuO_4



Ground state has long-range magnetic (Neel) order

$$\left\langle \vec{S}_{i} \right\rangle = (-1)^{i_{x}+i_{y}} N_{0} \neq 0$$

Excitations: 2 spin waves Quasiclassical wave dynamics at low T (Chakravarty et al, 1989; Tyc et al, 1989)







 λ is close to λ_{c}



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 – rstrength is measured by the spin gap Δ

 Δ_{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.



Quantum dimer model – D. Rokhsar and S. Kivelson Phys. Rev. Lett. **61**, 2376 (1988)



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 <u>collinear</u> spin polarization)

N. Read and S. Sachdev Phys. Rev. B 42, 4568 (1990).



S=1/2 spinons are linearly confined by the line of "defect" singlet pairs between them

I.3 <u>Paramagnets on the triangular and frustrated square</u> <u>lattices – spinon deconfinement</u>



Spinons are deconfined

Translationally invariant "spin liquid" state obtained by a quantum transition from a magnetically ordered state with <u>co-planar</u> spin polarization. Transition to confined states is described by a Z_2 gauge theory

N. Read and S. Sachdev, Phys. Rev. Lett. 66, 1773 (1991).
R. Jalabert and S. Sachdev, Phys. Rev. B 44, 686 (1991).
X.G. Wen, Phys. Rev. B 44, 2664 (1991).
T. Senthil and M.P.A. Fisher, Phys. Rev. B 62, 7850 (2000).

P. Fazekas and P.W. Anderson, Phil Mag 30, 23 (1974).

S. Sachdev, Phys. Rev. B 45, 12377 (1992).

G. Misguich and C. Lhuillier, cond-mat/0002170.

R. Moessner and S.L. Sondhi, cond-mat/0007378.



Lecture II

Non-magnetic impurities in twodimensional 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 *d*-wave superconductors.

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

4. Experiments on *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 <u>Impurities in the coupled-ladder</u> <u>antiferromagnet</u>

Make any localized deformation e.g. remove a spin



Orientation of "impurity" spin -- $n_{\alpha}(\tau)$ (unit vector) <u>Action of "impurity" spin</u>

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

 $A_{\alpha}(n)$ → Dirac monopole function

Boundary quantum field theory: $S_b + S_{imp}$

Recall -

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

Coupling γ approaches *also* approaches a fixed-point value under the renormalization group flow

Beta function:

e.g.

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

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

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

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

 Δ and *c* completely determine spin dynamics near an impurity – No new parameters are necessary ! Universal properties at the critical point $\lambda = \lambda_c$

$$\left\langle \vec{S}_{Y}(\tau) \cdot \vec{S}_{Y}(0) \right\rangle = \frac{1}{\tau^{\eta'}}$$
(and $m = \left| \lambda - \lambda_{c} \right|^{\eta' \nu}$

 η ' is a new boundary scaling dimension Operator product expansion:

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

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

However

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



Finite density of impurities n_{imp}

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

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







II.2a. <u>Impurities in square lattice</u> <u>paramagnets with confinement</u>

Zn or Li impurities substitute for Cu ions



Spinon confinement implies that free S=1/2moments <u>must</u> form near each impurity

II.2b. <u>Impurities in paramagnets with spinon</u> <u>deconfinement</u>







Collective magnetic excitations, ϕ_{α} , are not damped by fermionic Bogoliubov quasiparticles

As $\Delta \rightarrow 0$ there is a quantum phase transition to a magnetically ordered state

(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 Ψ_h fermions remain gapped at quantum-critical point. II.3. Quantum paramagnets to d-wave

superconductors: evolution with density of mobile carriers of density δ

A. Doping a paramagnet with confinement



Condensate of hole pairs

E. Fradkin and S. Kivelson, Mod. Phys. Lett B 4, 225 (1990).S. Sachdev and N. Read, Int. J. Mod. Phys. B 5, 219 (1991).

B. Doping a deconfined paramagnet

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

Flux trapping (T. Senthil and M.P.A. Fisher, Phys. Rev. Lett. 86, 292 (2001))

hc/(2e) flux quantum (S. Kivelson, D.S. Rokhsar and J.P. Sethna, Europhys. Lett. 6, 353 (1988))

Stable *hc/e* vortices (S. Sachdev, Phys. Rev. B 45, 389 (1992); N. Nagaosa and P.A. Lee, Phys. Rev. B 45, 966 (1992))

Phase diagram for case A



Superconductivity coexists with charge stripe order in region without magnetic order

S. Sachdev and N. Read, Int. J. Mod. Phys. B 5, 219 (1991).
M. Vojta and S. Sachdev, Phys. Rev. Lett. 83, 3916 (1999).
M. Vojta, Y. Zhang, and S. Sachdev, Phys. Rev. B 62, 6721 (2000)
See also J. Zaanen, Physica C 217, 317 (1999),
S. Kivelson, E. Fradkin and V. Emery, Nature 393, 550 (1998),
S. White and D. Scalapino, Phys. Rev. Lett. 80, 1272 (1998); 81, 3227 (1998).







FIG. 8. Unpolarized beam, constant-Q data [Q=(3/2,1/2,-1.7)]of the 40 meV magnetic resonance obtained by subtracting the signal below T_c from the T=100 K background. The lines are fits to Gaussians, as described in the text. For clarity successive scans are offset by 100.

Spin-1 collective mode $inYBa_2Cu_3O_7$ - little observable damping at low T. Coupling to superconducting quasiparticles unimportant.

Continuously connected to S=1 particle in confined Mott insulator



II.4. <u>Recent experiments on d-wave</u> <u>superconductors</u>

NMR on Zn/Li impurities

J. Bobroff, H. Alloul, W.A. MacFarlane, P. Mendels, N. Blanchard, G. Collin, and J.-F. Marucco, cond-mat/0010234.

⁷Li NMR below T_c



Inverse local susceptibility of isolated Li impurities in YBCO

Zn impurity in YBa₂Cu₃O_{6.7}

Moments measured by analysis of Knight shifts

M.-H. Julien, T. Feher,
M. Horvatic, C. Berthier,
O. N. Bakharev, P. Segransan,
G. Collin, and J.-F. Marucco,
Phys. Rev. Lett. 84, 3422
(2000); also earlier work of
the group of H. Alloul and the
original experiment of
A.M Finkelstein, V.E. Kataev,
E.F. Kukovitskii, and
G.B. Teitel'baum, Physica C
168, 370 (1990).



Berry phases of precessing spins do not cancel between the sublattices in the vicinity of the impurity: net uncancelled phase of S=1/2





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



Goal: Classify theories in which, with <u>minimal</u> fine tuning, a *d*-wave superconductor has a fermionic quasiparticle momentum distribution curve (MDC), at the nodal points, with a width proportional to k_BT

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

In a BCS d-wave superconductor, MDC width $\sim T^3$



Necessary conditions

- 1. Quantum-critical point should be below its uppercritical 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.





<u>A spin-singlet, fermion bilinear,</u> zero momentum order parameter for X <u>is preferred.</u>

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.



Quantum field theory for critical point

Ising order parameter ϕ (except for case (G))

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

Coupling to nodal fermions

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

(A)
$$M_1 = \tau^y$$
; $M_2 = \tau^y$
(B) $M_1 = \tau^y$; $M_2 = -\tau^y$
(C) λ =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 ϕ 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 bondcentered 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 $d_{x^2-y^2} + id_{xy}$ superconductor. Such a state is expected at larger second neighbor exchange.