Order and quantum phase transitions in the cuprate superconductors

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Talk online: Google Sachdev
Parent compound of the high temperature superconductors: \( \text{La}_2\text{CuO}_4 \)

**Band theory**

Half-filled band of Cu 3d orbitals – ground state is predicted to be a metal.

However, \( \text{La}_2\text{CuO}_4 \) is a very good insulator
Parent compound of the high temperature superconductors: \( \text{La}_2\text{CuO}_4 \)

A Mott insulator

Ground state has long-range magnetic Néel order, or “collinear magnetic (CM) order”

Néel order parameter: \( \phi = (-1)^{i_x + i_y} \hat{S}_i \)

\[ \langle \phi \rangle \neq 0 \quad ; \quad \langle \hat{S}_i \rangle \neq 0 \]
Introduce mobile carriers of density $\delta$ by substitutional doping of out-of-plane ions e.g. $\text{La}_{2-\delta}\text{Sr}_\delta\text{CuO}_4$

Exhibits superconductivity below a high critical temperature $T_c$
BCS superconductor obtained by the Cooper instability of a metallic Fermi liquid

Pair wavefunction

$$\Psi = (k_x^2 - k_y^2)(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$\langle \vec{S} \rangle = 0$$

(Bose-Einstein) condensation of Cooper pairs

Many low temperature properties of the cuprate superconductors appear to be qualitatively similar to those predicted by BCS theory.
BCS theory of a vortex in the superconductor

Pairs are disrupted and Fermi surface is revealed.

Vortex core

Superflow of Cooper pairs
Superconductivity in a doped Mott insulator


**Hypothesis:**
Competition between orders of BCS theory (condensation of Cooper pairs) and Mott insulators

**Needed:**
Theory of zero temperature transitions between competing ground states.
Minimal phase diagram

- Paramagnetic Mott Insulator
  \[ \left< \vec{S} \right> = 0 \]
- Magnetic Mott Insulator
  \[ \left< \vec{S} \right> \neq 0 \]
- Paramagnetic BCS Superconductor
  \[ \left< \vec{S} \right> = 0 \]
- Magnetic BCS Superconductor
  \[ \left< \vec{S} \right> \neq 0 \]

La\textsubscript{2}CuO\textsubscript{4}

High temperature superconductor

Quantum phase transitions
Magnetic-paramagnetic quantum phase transition in a Mott insulator
**Coupled ladder antiferromagnet**


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

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

$0 \leq \lambda \leq 1$
Square lattice antiferromagnet

Experimental realization: $La_2CuO_4$

Ground state has long-range collinear magnetic (Neel) order

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

Excitations: 2 spin waves

$$\varepsilon_p = \sqrt{c_x^2 p_x^2 + c_y^2 p_y^2}$$
\( \lambda \) close to 0

Weakly coupled ladders

\[
\mathcal{S}_i = \frac{1}{\sqrt{2}} (|\uparrow \downarrow \rangle - |\downarrow \uparrow \rangle)
\]

Real space Cooper pairs with their charge localized. Upon doping, motion and condensation of Cooper pairs leads to superconductivity

\[
\left\langle \mathcal{S}_i \right\rangle = 0
\]

Paramagnetic ground state
Excitations

$\lambda$ close to 0

Excitation: $S=1$ exciton
(vector $N$ particle of paramagnetic state)

Energy dispersion away from antiferromagnetic wavevector

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

$S=1/2$ spinons are confined by a linear potential.
Quantum paramagnet
Electrons in charge-localized Cooper pairs

Neel state
\( \langle \vec{S} \rangle = N_0 \)
Magnetic order as in \( \text{La}_2\text{CuO}_4 \)

Neel order \( N_0 \)
Spin gap \( \Delta \)

\( \lambda \) in cuprates?

\( T=0 \)
Bond and charge order Mott insulator
Paramagnetic ground state of coupled ladder model
Can such a state with *bond order* be the ground state of a system with full square lattice symmetry?
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 leads to a “resonating valence bond liquid”
(P.W. Anderson, 1987)
Quantum “entropic” effects prefer bond-ordered configurations 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 lead to a broken square lattice symmetry near the transition to the magnetically ordered states with collinear spins.


(Slightly) Technical interlude:
*Quantum theory for bond order*

**Key ingredient: Spin Berry Phases**
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**Key ingredient: Spin Berry Phases**

\[ e^{iSA} \]
$A_{a\mu} \rightarrow$ oriented area of spherical triangle formed by $N_a$, $N_{a+\mu}$, and an arbitrary reference point $N_0$
Change in choice of $n_0$ is like a “gauge transformation”

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

($\gamma_a$ 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

$$A_{a\mu} \rightarrow A_{a\mu} + 4\pi$$

These principles strongly constrain the effective action for $A_{a\mu}$ which provides description of the paramagnetic phase.
Simplest effective action for $A_{a\mu}$ fluctuations in the paramagnet

$$Z = \prod_{a,\mu} \int dA_{a\mu} \exp \left( \frac{1}{2e^2} \sum_{\square} \cos \left( \frac{1}{2} (\Delta_{\mu} A_{av} - \Delta_{v} A_{a\mu}) \right) - i \sum_{a} \eta_{a} A_{a\tau} \right)$$

$\eta_{a} \rightarrow \pm 1$ on two square sublattices.

This is compact QED in $d+1$ dimensions with static charges $\pm 1$ on two sublattices.

This theory can be reliably analyzed by a duality mapping.

$d=2$: The gauge theory is always in a confining phase and there is bond order in the ground state.

$d=3$: A deconfined phase with a gapless “photon” is possible.

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

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

See also C. H. Chung, Hae-Young Kee, and Yong Baek Kim, cond-mat/0211299.
Experiments on the superconductor revealing order inherited from the Mott insulator
Effect of static non-magnetic impurities (Zn or Li)

Spinon confinement implies that free $S=1/2$ moments form near each impurity

$$\chi_{\text{impurity}}(T \to 0) = \frac{S(S + 1)}{3k_B T}$$
Spatially resolved NMR of Zn/Li impurities in the superconducting state

Inverse local susceptibility in YBCO

Measured $\chi_{\text{impurity}}(T \to 0) = \frac{S(S+1)}{3k_B T}$ with $S = 1/2$ in underdoped sample.

This behavior does not emerge out of BCS theory.


Tuning across the phase diagram by an applied magnetic field

Neutron scattering of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ at $x=0.1$


Talk today at 11:00 AM

STM around vortices induced by a magnetic field in the superconducting state


**Local density of states**

1Å spatial resolution image of integrated LDOS of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (1meV to 12 meV) at B=5 Tesla.

Vortex-induced LDOS of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ integrated from 1meV to 12meV

Our interpretation: LDOS modulations are signals of bond order of period 4 revealed in vortex halo

See also:

Conclusions

I. Cuprate superconductivity is associated with doping Mott insulators with charge carriers.

II. Order parameters characterizing the Mott insulator compete with the order associated with the Bose-Einstein condensation of Cooper pairs.

III. Classification of Mott insulators shows that the appropriate order parameters are collinear magnetism and bond order.

IV. Theory of quantum phase transitions provides semi-quantitative predictions for neutron scattering measurements of spin-density-wave order in superconductors; theory also proposes a connection to STM experiments.