Understanding correlated electron systems by a classification of Mott insulators

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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: \( \vec{\phi} = (-1)^{i_x + i_y} \vec{S}_i \)

\[ \langle \vec{\phi} \rangle \neq 0 \; ; \; \langle \vec{S}_i \rangle \neq 0 \]
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 $T_c$

Superconductivity in a doped Mott insulator
BCS superconductor obtained by the Cooper instability of a *metallic Fermi liquid*

**Pair wavefunction**

\[ \Psi = \left( k_x^2 - k_y^2 \right) \left( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) \]

\[ \langle \vec{S} \rangle = 0 \]

(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.
Hypothesis: cuprate superconductors are characterized by additional order parameters (possibly fluctuating), associated with the proximate Mott insulator, along with the familiar order associated with the condensation of Cooper pairs in BCS theory. These orders lead to new low energy excitations, and are revealed in the presence of perturbations which locally destroy the BCS order (vortices, impurities, magnetic fields etc.)

The theory of quantum phase transitions, using expansions away from quantum critical points, allows a systematic description of states in which the order of Mott insulator is “fluctuating”
Outline

I. Order in Mott insulators
   \textbf{Magnetic order}
   \textbf{A. Collinear spins}
   \textbf{B. Non-collinear spins}

   \textbf{Paramagnetic states}
   \textbf{A. Compact U(1) gauge theory: bond order and confined spinons in $d=2$}
   \textbf{B. $Z_2$ gauge theory: visons, topological order, and deconfined spinons}

II. Class A in $d=2$
    The cuprates

III. Conclusions
I. Order in Mott insulators

Magnetic order \[
\langle S_j \rangle = N_1 \cos(\mathbf{K} \cdot \mathbf{r}_j) + N_2 \sin(\mathbf{K} \cdot \mathbf{r}_j)
\]

Class A. Collinear spins

\(\mathbf{K} = (\pi, \pi) ; N_2 = 0\)

\(\mathbf{K} = (3\pi/4, \pi) ; N_2 = 0\)

\(\mathbf{K} = (3\pi/4, \pi) \quad ; \quad N_2 = (\sqrt{2} - 1)N_1\)
I. Order in Mott insulators

*Magnetic order* \( \langle S_j \rangle = N_1 \cos(\vec{K} \cdot \vec{r}_j) + N_2 \sin(\vec{K} \cdot \vec{r}_j) \)

**Class A. Collinear spins**

**Key property**

Order specified by a single vector \( \vec{N} \).

Quantum fluctuations leading to loss of magnetic order should produce a paramagnetic state with a vector \((S=1)\) quasiparticle excitation.
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**Magnetic order** \( \langle S_j \rangle = N_1 \cos(\vec{K} \cdot \vec{r}_j) + N_2 \sin(\vec{K} \cdot \vec{r}_j) \)


\( \vec{K} = (3\pi/4, \pi) \); \n\( N_2^2 = N_1^2 \), \( N_1 \cdot N_2 = 0 \)

Solve constraints by expressing \( N_{1,2} \) in terms of two complex numbers \( z_\uparrow, z_\downarrow \)

\[
N_1 + iN_2 = \begin{pmatrix}
2z_\uparrow z_\downarrow \\
z_\downarrow - z_\uparrow^2 \\
i (z_\downarrow^2 + z_\uparrow^2)
\end{pmatrix}
\]

Order in ground state specified by a spinor \( (z_\uparrow, z_\downarrow) \) (modulo an overall sign).

This spinor can become a \( S=1/2 \) spinon in paramagnetic state.

Theory of spinons must obey the \( Z_2 \) gauge symmetry \( z_a \to -z_a \)
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Coupled ladder antiferromagnet


\[ S = \frac{1}{2} \text{ spins on coupled 2-leg ladders} \]

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

\[ 0 \leq \lambda \leq 1 \]

\[ J \quad \lambda J \]
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

\[ \langle \tilde{S}_i \rangle = 0 \]

Real space Cooper pairs with their charge localized.

Upon doping, motion and condensation of Cooper pairs leads to superconductivity
Excitations

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 La$_2$CuO$_4$

Spin gap \( \Delta \)

Neel order \( N_0 \)

\( T=0 \)

\( \delta \) in cuprates?
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.

A precise description of this physics is obtained by a compact U(1) gauge theory of the paramagnetic Mott insulator

Class A: Collinear spins and compact U(1) gauge theory

Write down path integral for quantum spin fluctuations

**Key ingredient: Spin Berry Phases**

\[ e^{iSA} \]
Class A: Collinear spins and compact U(1) gauge theory

Write down path integral for quantum spin fluctuations

Key ingredient: Spin Berry Phases

$e^{iSA}$
Class A: Collinear spins and compact U(1) gauge theory

\( S=1/2 \) square lattice antiferromagnet with non-nearest neighbor exchange

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

Include Berry phases after discretizing coherent state path integral on a cubic lattice in spacetime

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

\( \eta_a \to \pm 1 \) on two square sublattices;

\( \mathbf{n}_a \sim \eta_a \vec{S}_a \to \) Neel order parameter;

\( A_{a\mu} \to \) oriented area of spherical triangle

formed by \( \mathbf{n}_a, \mathbf{n}_{a+\mu} \), and an arbitrary reference point \( \mathbf{n}_0 \)
\[ n_0 \]

\[ n_a \]

\[ n_{a+\mu} \]

\[ A_{a\mu} \]
Change in choice of $n_0$ is like a “gauge transformation”

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

($\gamma_a$ 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

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

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 \( A_{a\mu} \)

\[
Z = \prod_{a,\mu} \int dA_{a\mu} \exp \left( -\frac{1}{2e^2} \sum_{\Box} \cos \left( \frac{1}{2} (\Delta_\mu A_{av} - \Delta_\nu A_{a\mu}) \right) - \frac{i}{2} \sum_a \eta_a A_{a\tau} \right)
\]

with \( e^2 \sim g^2 \)

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 \textit{always} in a \textit{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

$$H = 2J \sum_{\langle ij \rangle} \left( S_i^x S_j^x + S_i^y S_j^y \right) - K \sum_{\langle ijkl \rangle} \left( S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+ \right)$$
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**Paramagnetic states** \( \langle S_j \rangle = 0 \)

Class B. Topological order and deconfined spinons

Number of valence bonds cutting line is conserved modulo 2 – this is described by the same \( \mathbb{Z}_2 \) gauge theory as non-collinear spins


RVB state with free spinons

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1. **Pairing order of BCS theory (SC)**

   Bose-Einstein condensation of \(d\)-wave Cooper pairs

**Orders associated with proximate Mott insulator in class A**

2. **Collinear magnetic order (CM)**

3. **Bond order (B)**

Evidence cuprates are in class A
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- Neutron scattering shows collinear magnetic order co-existing with superconductivity
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• Proximity of $Z_2$ Mott insulators requires stable $hc/e$ vortices, vison gap, and Senthil flux memory effect

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• Proximity of $Z_2$ Mott insulators requires stable $hc/e$ vortices, vison gap, and Senthil flux memory effect

• Non-magnetic impurities in underdoped cuprates acquire a $S=1/2$ moment
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 $\chi_{\text{impurity}}(T \to 0) = \frac{S(S+1)}{3k_BT}$ with $S = 1/2$ in underdoped sample.

This behavior does not emerge out of BCS theory.

Evidence cuprates are in class A

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- Tests of phase diagram in a magnetic field
Superflow kinetic energy $\langle v_s^2 \rangle \propto \frac{H}{H_{c2}} \ln \frac{3H_{c2}}{H} \Rightarrow \delta_{\text{eff}} (H) = \delta - C \frac{H}{H_{c2}} \ln \left( \frac{3H_{c2}}{H} \right)$

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Neutron scattering observation of SDW order enhanced by superflow.

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


Solid line - fit to: $I(H) = a \frac{H}{H_{c2}} \ln \left( \frac{H_{c2}}{H} \right)$

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"Normal" (Bond order)

$H \sim \frac{(\delta - \delta_c)}{\ln \left( 1/(\delta - \delta_c) \right)}$

Prediction: SDW fluctuations enhanced by superflow and bond order pinned by vortex cores (no spins in vortices). Should be observable in STM


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:

Spectral properties of the STM signal are sensitive to the microstructure of the charge order.

Measured energy dependence of the Fourier component of the density of states which modulates with a period of 4 lattice spacings.

Theoretical modeling shows that this spectrum is best obtained by a modulation of bond variables, such as the exchange, kinetic or pairing energies.


Conclusions

I. Two classes of Mott insulators:
   (A) Collinear spins, compact U(1) gauge theory;
   bond order and confinements of spinons in $d=2$
   (B) Non-collinear spins, $Z_2$ gauge theory

II. Doping Class A in $d=2$
    Magnetic/bond order co-exist with superconductivity at low doping
    Cuprates most likely in this class.
    Theory of quantum phase transitions provides a description of “fluctuating order” in the superconductor.