High Tc superconductivity in doped Mott insulators

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Outline:

• Introduction

• Sum Rules & p-h asymmetry

• Variational Theory of SC State

• Low energy excitations

• Superfluid density

• Disorder Effects
Failure of three central paradigms of Condensed Matter Physics

(1) Band theory fails for $x = 0$
parent insulator

(2) Landau's Fermi liquid theory fails for strange metal and pseudogap regimes

(3) BCS theory fails for Unconventional SC particularly for $x \ll 1$

Competing orders:
Antiferromagnetism;
Charge ordering; Spin glass
Circulating currents; DDW (?)

Hidden Quantum Critical Point under the dome(?)
Key question:
holes in a 2-d $S=1/2$ Mott insulator

hole concentration

$x \ll 1$
will focus here on: 
T=0 SC state and low-lying excitations
In collaboration with:

A. Paramekanti, Toronto
N. Trivedi, Ohio State

A. Paramekanti, MR & N. Trivedi,
PRL 87, 217002 (2001); PRB 69, 144509 (2004);
PRB 70, 054504 (2004); PRB 71, 069505 (2005).

R. Sensarma, Ohio State

R. Sensarma, MR & N. Trivedi,
PRL 98, 027004 (2007) and unpublished.

F.C. Zhang, Hong Kong

MR, R. Sensarma, N. Trivedi & F.C. Zhang,
PRL 95, 137001 (2005).

P.W. Anderson, Princeton

P.W. Anderson, P.A. Lee, MR,
T. M. Rice, N. Trivedi & F.C. Zhang,
**Hubbard model:**

**Minimal Model for CuO$_2$ planes**

\[ \mathcal{H} = \sum_{\mathbf{k}, \sigma} \epsilon(\mathbf{k}) c_{\mathbf{k} \sigma}^\dagger c_{\mathbf{k} \sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r} \uparrow} n_{\mathbf{r} \downarrow} \]

\[ \epsilon(\mathbf{k}) = -2t \left( \cos k_x + \cos k_y \right) + 4t' \cos k_x \cos k_y \]

\[ U \gg t, |t'| \]

\[ J = \frac{4t^2}{U} \]

\[ J \leq |t'| \leq t \ll U \rightarrow 3.6 \text{ eV} \]

- neutron \( \sim 100 \text{ mev} \)
- Raman \( t' \sim -t/4 \)
- photoemission
- band theory

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\(~ 300 \text{ meV} \)
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Qs: How does large $U$ affect the low-energy properties of doped materials?

- MR, SenSarma, Trivedi & Zhang, PRL 95, 137001 (2005)

Particle-hole asymmetry in Spectral function:
**Exact** sum rules for Projected electrons at $T=0$

$P = \prod_i \left( 1 - n_i^\uparrow n_i^\downarrow \right)$

No assumptions about
- ground state
- broken symmetries
- translational invariance

Im$G(r, r'; \omega)$
Lehmann Representation
$\rightarrow$ Energy-integrated
Sum Rules
P-H asymmetry: **Exact** sum rules for local DOS

Local Hole doping

\[ \langle n(r) \rangle = 1 - x(r) \]

Extracting electrons:

\[ \int_{-\infty}^{0} d\omega N(r; \omega) = 1 - x(r) \]  
(filled sites)

Adding electrons:

\[ \int_{0}^{\Omega_L} d\omega N(r; \omega) = 2x(r) + 2 |\langle K(r) \rangle| / U \]

\( J < t \ll \Omega_L \ll U \)  
(empty sites + ...)

\[ |\langle K(r) \rangle| / U \sim O(xt/U) \]
Increasing p-h Asymmetry with Underdoping

Phase diagram of \( \text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2 \)

K. Ohishi et al., cond-mat/0412313

Averaged dI/dV spectra


Davis group (Cornell)
Using **Sum Rules** to estimate local density from STM data

conductance \( g(r; eV) = M(r)N(r; \omega = eV) \)

**Unknown** matrix element \( M(r) \) cancels out in **ratio**

\[
R(r) \equiv \frac{\int_0^{\Omega_L} d\omega g(r; \omega)}{\int_{-\infty}^0 d\omega g(r; \omega)} = \frac{2x(r)}{[1-x(r)]} + \mathcal{O}\left(\frac{xt}{U}\right)
\]

Measured

Determine \( x(r) \)

\( R(r) \)-maps

Strategy for theoretical attack on the superconducting state

No theory of Strange metal

Diagrammatic approaches -- Cannot reach Mott insulator

Use a variational approach to look directly at the T=0 SC state and low-lying excitations

Need to cross many phases to reach the SC
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Variational Ground State Wavefunction

\[ | \Psi_0 > = \exp(-iS) \mathbf{P} | \text{dBCS} > \]

\[ | \text{dBCS} > = \text{d-wave BCS state} \]

variational parameters \( \Delta \) and \( \mu \)

\[ U = \infty \]

Gutzwiller Projection:

\[ P = \prod_i \left( 1 - n_{i\uparrow}n_{i\downarrow} \right) \]

\[ \exp(-iS) = \text{Unitary transformation:} \]

Hubbard \( \rightarrow tJ + \ldots \) brings in the scale \( J \)

Kohn (‘64); Gross, Joynt, Rice (‘87)
\[ |\Psi_0\rangle \equiv \mathcal{P}|BCS\rangle = \mathcal{P}
\sum_{r,r'} \varphi(r-r') c_{r\uparrow}^\dagger c_{r'\downarrow}^\dagger \frac{N^2}{2} |0\rangle \]
S=0 pairing induced by superexchange $J = \frac{4t^2}{U}$

Anderson (1987)
Baskaran et al (1987)
Kotliar (1988)
Zhang, Gros, Rice, and Shiba (1988)

\textbf{d-wave symmetry} \\
\rightarrow \text{Partners in a pair never at the same site}

\textbf{Projection P} \\
\rightarrow \text{eliminate all double occupancy}
• What are the properties of the Projected SC \( P|dBCS\) \>? 

• How do these compare with those of the High Tc cuprates?
\[ |\Psi_0\rangle = P |BCS\rangle \]

**Variational Monte Carlo method:** only known way to treat $P$ exactly

**Gutzwiller approximation:**

\[ \langle K.E. \rangle \sim \frac{2x}{(1+x)} \langle K.E. \rangle_0; \quad \langle s(i)s(j) \rangle \sim \frac{4}{(1+x)^2} \langle s(i)s(j) \rangle_0 \]

**GA Calculation:**

- “renormalized”
- mean field theory

- analytical insights
- excited states
- dynamical correlations
- disorder effects
Pairing & Superconductivity

Pairing $\rightarrow$ variational $\Delta$

d-wave SC order parameter $\Phi$
$\rightarrow$ from ODLRO $\langle c^\dagger c^\dagger cc \rangle$

Strong Coulomb $U$
$\Phi(x) \sim x \text{ as } x \rightarrow 0$

P $\rightarrow$ local, quantum phase fluctuations

$\Delta \neq \Phi_{SC}$
Variational Estimate of SC Energy Gap

Variational QP state \( |k\sigma\rangle = e^{-iS} P \gamma_{k\sigma}^\dagger |\text{dBCS}\rangle \)

QP excitation energy \( \rightarrow \) SC gap

\( \text{SC Gap} = \text{Variational} \ \Delta \)

- \( \sim \) factor of 2 larger than experiment
- same \( x \)-dependence as experiment

Competition between SC and AFM as \( x \to 0 \)

**Energetics:** energies of different states differ by few \( \% \) \( J \to \) details of \( H \) are important

At \( x = 0 \) AF magnetism wins;
RVB spin-liquid insulator
Energy/bond = \(-0.3199\) J

\( \nu/s \)
AFM Long range order
Energy/bond = \(-0.3346\) J
Trivedi & Ceperley, (1989)

- AFM for \( x < 7\% \)
- SC for \( x > 7\% \)

\( J/ t = 0.3, \)
\( t'/ t = -0.3 \)
\( t''/ t = 0.2 \)

Shih, Chen, Chou, & TK Lee,
PRB 70, 220502(R) (2004)
Hole Doping:
- AFM insensitive to \( t' \)
- SC grows with \( t' \)

Electron Doping:
- AFM grows with \( t' \)
- SC suppressed with \( t' \)

S. Pathak, V. Shenoy, N. Trivedi & MR
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- Variational Theory of SC State
- Low energy excitations:
  * nodal quasiparticles
  * “underlying Fermi surface”
- Superfluid density
- Disorder Effects
Low Energy Excitations in SC state

Sharp Nodal Quasiparticles
- existence
- $k_F(x)$
- coherent spectral weight $Z(x)$
- dispersion $v_F(x)$

Moments of spectral function = equal-time correlators

$$M_\ell(k) = \int_{-\infty}^{0} d\omega \, \omega^\ell A(k, \omega)$$

Singularities in $M_\ell(k) \iff$ gapless Quasiparticles
Nodal QP Spectral Weight $Z$

Loss of coherence with underdoping

$Z_{\text{nodal}}(x)\propto 2\frac{x}{(1+x)} + O(xt/U)$

- **GA**

- **MC**: Paramekanti, MR, Trivedi, PRL (2001)
- **MR**: Sensarma et al., PRL (2005)
- **Expt**: Johnson et al., PRL (2001)

ARPES Bi2212
Dispersion of Nodal Quasiparticles

Nodal $V_F$ or $m^*$ independent of $x$

as $x \to 0$

\[ Z \sim x \Rightarrow |\partial \Sigma'/\partial \omega| \sim 1/x \]

\[ v_F = \text{const.} \Rightarrow |\partial \Sigma'/\partial k| \sim Jax/x \]

$\Sigma'$ has singular $1/x$ dependence on both $\omega$ and $k$ along zone diagonal

- **MC**: Paramekanti. MR, Trivedi, PRL(2001)
- **GA**: Sensarma et al, PRL (2005)
x-dependence of the Momentum distribution

\[ n(k) = \frac{1}{2} \]

"FS" topology change at \( x \approx 0.2 \); depends sensitively on \( t'/t \)

Expt: H. Ding, et.al
PRL (1997)
Qs: Is there a way to determine the "underlying FS" that is gapped out in a SC state at $T = 0$?


BCS answer: $G_{11}^{bcs}(k, \omega) = \frac{\omega - \xi_k}{\omega^2 + E_k^2}$

$G_{11}^{bcs}(k, 0) = 0 \Rightarrow \xi_k = 0$

(but ... see below!)

Is SC state "FS" given by $G(k, 0) = 0$?

(1,1)-component of Nambu $G$

cf. Fermi surface in Landau's FLT $G(k, 0) = \infty$
Unlike the normal Landau FL, the SC state “FS”...

\[ G(k, 0) = 0 \] does not enclose \( n \) electrons

No Luttinger Sum Rule for state with ODLRO

\[ \Phi[\tilde{G}] \text{ with } \frac{\delta \Phi}{\delta \tilde{G}} = \sum \int d\omega \sum_k \text{Tr}\{\tau_3 \tilde{G}\} = (n_{\uparrow} + n_{\downarrow}) \]

“Number is not conserved in SC state”

[Dzyloshinskii, PRB(2003)]

• Angle-Resolved Photoemission expts.
-- measure locus of zero-energy ARPES intensity
-- “minimum gap locus”
which “looks like a Fermi surface”. What does this mean?
Various SC state “FS” definitions lead to similar contours, but all of them violate the Luttinger count.

\[
\left| \frac{\delta n}{n} \right| \sim \left( \frac{\Delta}{E_f} \right)^2
\]

**Size of violation**

**Sign of violation** related to “FS” topology.
Experiments:
Consistent with prediction, but not definitive yet
* determination of $x$
* $k$-resolution

Theory:
Sensarma, MR & Trivedi
PRL 98, 027004 (2007)

ARPES experiment:
T. Yoshida et. al,
PRB 74, 224510 (2006)
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Optical Spectral Weight or Drude Weight

\[ \omega_p^* = \frac{4\pi e^2}{d} D_{\text{low}} \]

\[ D_{\text{low}} = \frac{2}{\pi} \int_0^{\Omega_c} d\omega \, \text{Re} \sigma(\omega) \]

\[ J < t \ll \Omega_c \ll U \]

Values & trend in agreement with optics:
Orenstein, et al., PRB (1990)
Cooper, et al., PRB (1993)

Upper Bound on Superfluid Density

\[ \rho_s \leq D_{\text{low}} \]

\[ \Rightarrow \rho_s \to 0 \]

as \( x \to 0 \)
Implications of SC state results for Pseudogap:

For large $x$, BCS-like: $\Delta \ll \rho_s$  
For small $x$, non-BCS: $\rho_s \ll \Delta$

$T_C \sim \min \{\rho_s, \Delta\}$  

Effect of Long-Wavelength Quantum Phase Fluctuations:

T= 0 Self-Consistent Harmonic Approximation

Paramekanti, MR, Ramakrishnan & Mandal
PRB (2000)

\[ \rho_s = \rho_s^0 \exp \left( -\langle \delta \theta^2 \rangle / 2 \right) \]
T-dependence of Superfluid density \((T \ll T_c)\)

\[
\rho_s(T) = \rho_s(0) - \frac{2 \ln 2}{\pi} \alpha^2 \left(\frac{v_F}{v_2}\right) T + \ldots
\]

\[
\lambda^{-2}(T) = 4\pi e^2 D_s(T)/(\hbar^2 c^2 d)
\]

\[
\rho_s(0, x) \leftarrow \text{doping dependence near Mott insulator}
\]

T-dependence from nodal QPs

Nodal QP dispersion

\[
E_k \approx \sqrt{(v_F \delta k_\perp)^2 + (v_2 \delta k_\parallel)^2}
\]

\[
j = \alpha e v_F \leftarrow \text{Current carried by nodal QPs}
\]

backflow corrections
\[ J_{nqp} = \langle qp | \hat{J} | qp \rangle = \alpha e v_F \]

Current carried by a Nodal Quasiparticle
\[
\alpha = \text{"Effective charge" of QP}
\]

\[ \alpha(x) \]

tJ Monte Carlo
Nave, Ivanov & P.A.Lee, PRB (2005)

our Gutzwiller Approximation result for tJ model:

\[ J_{nqp} = e Z v_F^0 \]

\[ \alpha \approx g_t / (g_t + 1/6) \]

\[ = x/(1.08x + 0.08) \]
Slope of SF density:

\[ \alpha(x) \quad \text{and} \quad \frac{d\rho_s}{dT} \]

UBC YBCO data
Broun et al,
cond-mat/0509223
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Why are HTSC's so robust against disorder?

* (most) impurities lie off CuO$_2$ planes

* the coherence length is very short
  \( \rightarrow \) Spatially inhomogeneous response
  not captured by standard A-G theory

* Disorder effects are suppressed
  in strongly correlated SCs
Inhomogeneous response to impurities:
--- Bogoliubov-deGennes (BdG) theory

**Correlation effects**
--- inhomogeneous Gutzwiller approx. (GA)

\[ g_t(r, r') = g_t(r)g_t(r') \]
\[ g_t(r) = \left[ \frac{2x(r)}{1 + x(r)} \right]^{1/2} \]

Compare results with and without correlations:

For correlated system:
- fewer low-energy excitations
- robust nodal QPs - “V” in DOS protected
  - nodes in k-space protected
Response to weak (Born) impurities:

Local density $n(i)$

Local $d$-wave pairing amplitude $\Delta(i)$

Short healing length in correlated system

Impurity potential is renormalized by interactions

Correlations + disorder

Only disorder

$\langle n \rangle = 0.8$

$n_{imp} = 0.01$

$V_{imp} = t$

Longer healing length in calculation which ignores correlations
Where do the low energy excitations live?

\[ A(k, \omega) = \mathcal{F} \mathcal{T}_{r \rightarrow k} \langle \text{Im} \ G(r, R, \omega) \rangle_R \]

\[ r = r_1 - r_2; \quad R = (r_1 + r_2)/2 \]

Nodes are protected

Nodal QPs much less affected by Disorder than the Antinodal QPs

\[ A(k, |\omega| \leq 0.02) \]
In the correlated system

- low energy ‘V’ from nodal QPs
  - very weakly affected by disorder
- disorder induces fewer low-energy excitations

Spatially averaged DOS

Correlations + disorder

Only disorder

\[ |\omega| \leq 0.02t \]
Summary: SC in doped Mott insulators

- p-h asymmetry in STM & ARPES
- local $x(r)$ from sum rule ratio

- SC “dome” with optimal doping
- energy gap and SC order have qualitatively different $x$-dependence

- Evolution from large $x$ BCS-like SC to small $x$ SC near Mott insulator
- nodal QPs: $k_F(x), Z(x), V_F(x)$
- underlying “Fermi surface”
- optical spectral weight and superfluid density $\rho_S(x; T)$

- disorder effects suppressed in presence of strong correlations
The end
Canonical Transformation $\exp(iS)$
transforms Hubbard to $tJ$ model
(plus three-site terms)

\[
\begin{align*}
\mathcal{K}_0 &= - \sum_{\mathbf{r}, \mathbf{r}', \sigma} t_{\mathbf{r}\mathbf{r}'} \left[ n_{\mathbf{r}\bar{\sigma}} c_{\mathbf{r}\sigma}^{\dagger} c_{\mathbf{r}'\sigma} n_{\mathbf{r}'\bar{\sigma}} + h_{\mathbf{r}\bar{\sigma}} c_{\mathbf{r}\sigma}^{\dagger} c_{\mathbf{r}'\sigma} h_{\mathbf{r}'\bar{\sigma}} \right] \\
\mathcal{K}_{+1} &= - \sum_{\mathbf{r}, \mathbf{r}', \sigma} t_{\mathbf{r}\mathbf{r}'} n_{\mathbf{r}\bar{\sigma}} c_{\mathbf{r}\sigma}^{\dagger} c_{\mathbf{r}'\sigma} h_{\mathbf{r}'\bar{\sigma}} \\
\mathcal{K}_{-1} &= - \sum_{\mathbf{r}, \mathbf{r}', \sigma} t_{\mathbf{r}\mathbf{r}'} h_{\mathbf{r}\bar{\sigma}} c_{\mathbf{r}\sigma}^{\dagger} c_{\mathbf{r}'\sigma} n_{\mathbf{r}'\bar{\sigma}} \\
&= \frac{1}{U} (\mathcal{K}_{+1} - \mathcal{K}_{-1}) + \frac{1}{U^2} ([\mathcal{K}_{+1}, \mathcal{K}_0] + [\mathcal{K}_{-1}, \mathcal{K}_0])
\end{align*}
\]

Kohn (1964); Gros, Joynt, Rice (1987); MacDonald, Girvin, Yoshioka (1988)
Gutzwiller Approximation:

approximation scheme to analytically evaluate matrix elements in Projected states

\[ \langle \Phi_0 | \mathcal{P} Q \mathcal{P} | \Phi_0 \rangle \simeq g_Q(x) \langle \Phi_0 | Q | \Phi_0 \rangle \]

examples:

\[ \langle c_{i \sigma}^\dagger c_{j \sigma} \rangle \simeq \frac{2x}{(1+x)} \langle c_{i \sigma}^\dagger c_{j \sigma} \rangle_0 \]

\[ \langle s_i s_j \rangle \simeq \frac{4}{(1+x)^2} \langle s_i s_j \rangle_0 \]

\[ g_t = \frac{\langle c_{i \sigma}^\dagger c_{j \sigma} \rangle}{\langle c_{i \sigma}^\dagger c_{j \sigma} \rangle_0} \]

\[ g_t = \left[ \frac{n_{r' \uparrow} (1-n_r) n_{r \uparrow} (1-n_{r'})}{n_{r' \uparrow} (1-n_{r' \uparrow}) n_{r \uparrow} (1-n_{r \uparrow})} \right]^{1/2} = \frac{2x}{1+x} \]

\[
\begin{array}{c}
| i \rangle \uparrow & \quad \text{projected} \\
| f \rangle & \quad \text{unprojected}
\end{array}
\]

\[
\begin{array}{c}
| i \rangle \uparrow & \quad \text{projected} \\
| f \rangle & \quad \text{unprojected}
\end{array}
\]
Singularities of Spectral Moments & Gapless QPs

\[ A(k, \omega) = -\text{Im} G(k, \omega + i0^+) / \pi \]
\[ = \sum_m \left[ |\langle m | c_{k\sigma}^\dagger |0 \rangle|^2 \delta(\omega + \omega_0 - \omega_m) + |\langle m | c_{k\sigma} |0 \rangle|^2 \delta(\omega - \omega_0 + \omega_m) \right] \]

\[ M_\ell(k) \equiv \int_{-\infty}^{0} d\omega \omega^\ell A(k, \omega) \]

\[ M_0(k) = \int_{-\infty}^{0} d\omega A(k, \omega) = \sum_m |\langle m | c_{k\sigma} |0 \rangle|^2 = n(k) \]

Jump discontinuity: \( k_F \) & \( Z \)

\[ M_1(k) = \int_{-\infty}^{0} d\omega \omega A(k, \omega) = \sum_m (\omega_0 - \omega_m) |\langle m | c_{k\sigma} |0 \rangle|^2 \]
\[ = \langle c_{k\sigma}^\dagger [ c_{k\sigma}, \mathcal{H} - \mu N ] \rangle \]

Slope discontinuity: \( V_F \)