Lecture # 3

High Tc superconductivity in doped Mott insulators

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Ohio State University

2014 Boulder School on
"Modern aspects of
Superconductivity"

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).
S. Pathak, V. Shenoy, MR & N. Trivedi, PRL 102, 027002 (2009)

R.Sensarma, Tata Institute

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

F.C.Zhang, Hong Kong

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

A.Garg, SINP, Kolkata

A. Garg, MR & N. Trivedi, Nature Physics 4, 762 (2008)

P.W.Anderson, Princeton

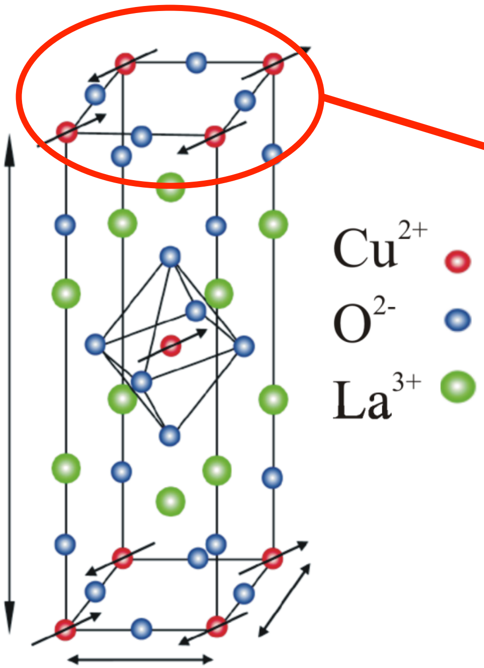
P.W. Anderson, P.A. Lee, MR, T. M. Rice, N. Trivedi & F.C. Zhang,
J. Phys. Cond. Mat. 16, R755 (2004). "The A-Z paper"

Outline:

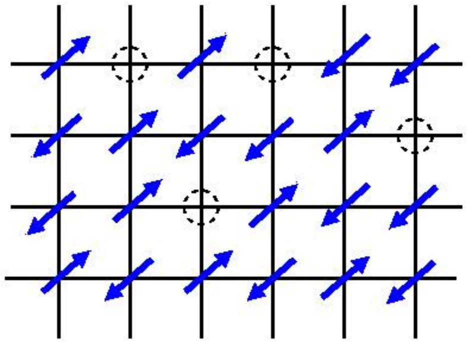
- Introduction
- Sum Rules & p-h asymmetry
- Variational Theory of SC State
- Low energy excitations
- Disorder Effects

* Effective Hamiltonian

Structure → Electronic Structure → Hubbard Model



CuO_2 plane



- Single band
- S=1/2
- 2D
- At/near half-filling
- $U \gg t$

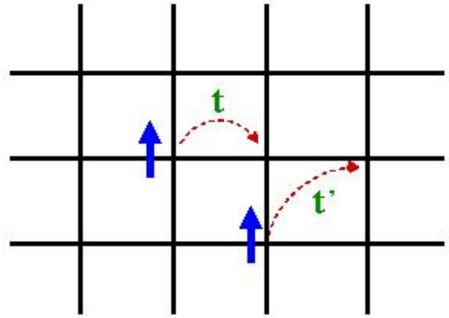
P. W. Anderson, Science **235**, 1196 (6 March 1987)

t-J model: Zhang & Rice (1988)

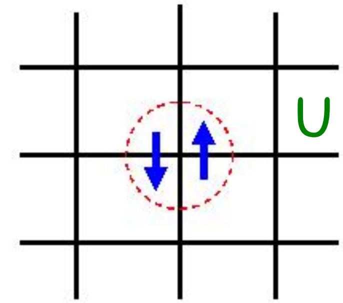
Hubbard model: <u>minimal</u> model for CuO_2 planes

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \epsilon(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}$$

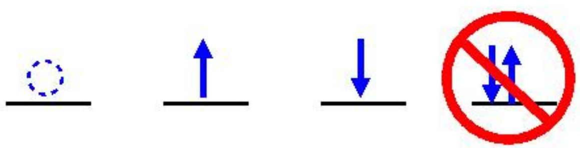
$\epsilon(\mathbf{k})$



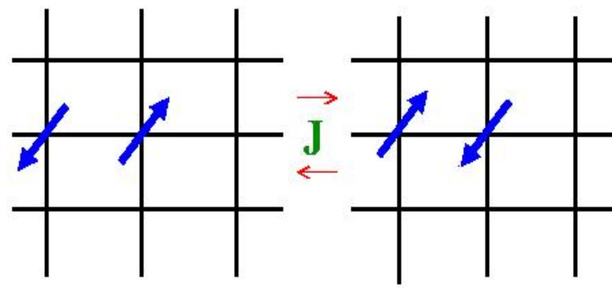
$U \gg t, |t'|$



Gutzwiller Projection



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



$J = 4t^2/U$

AF superexchange $J \sum \mathbf{S}_i \cdot \mathbf{S}_j$

$$J \le |t'| \le t \ll U$$

U → 3.6 eV

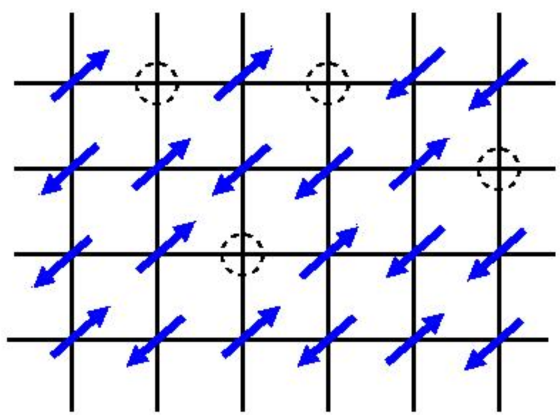
J ← ~ 100-150 mev
- neutron
- Raman

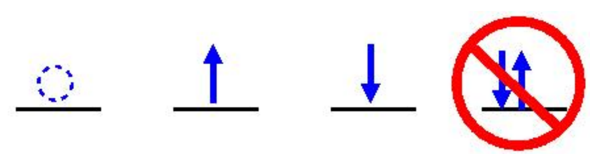
t ↓ 300 meV
t' ~ t/4

- photoemission
- electronic structure calc.

Hubbard/Heisenberg Model describes parent AFM Mott Insulator at half-filling

But is the large Hubbard U
also important in the doped materials?
Or does screening make it look like a conventional metal?





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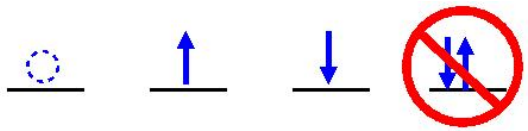


$$P = \prod_i \left(1 - n_{i\uparrow} n_{i\downarrow}\right)$$

Exact sum rules for Projected electrons
→ Particle-hole asymmetry in spectral function

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

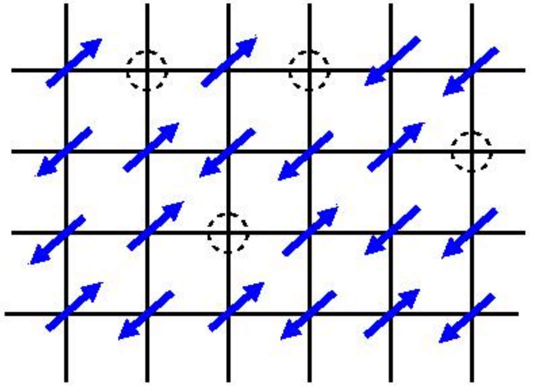
$$\mathrm{Im}G(\mathbf{r},\mathbf{r}';\omega)$$

Spectral Representation
→Energy-integrated Sum Rules

MR, SenSarma, Trivedi & Zhang, PRL **95**, 137001 (2005)
Anderson & Ong, J. Phys. Chem. Sol. (2006)

Meinders, Eskes & Sawatzky, Phys. Rev. B (1993)
Harris & Lange, Phys. Rev. (1967)

P-H asymmetry: Exact sum rules for local DOS



Local Hole doping

$$\langle n(\mathbf{r})\rangle = 1 - x(\mathbf{r})$$

Extracting electrons:

$$\int_{-\infty}^{0} d\omega N(\mathbf{r};\omega) = 1 - x(\mathbf{r})$$

(filled sites)

Adding electrons:

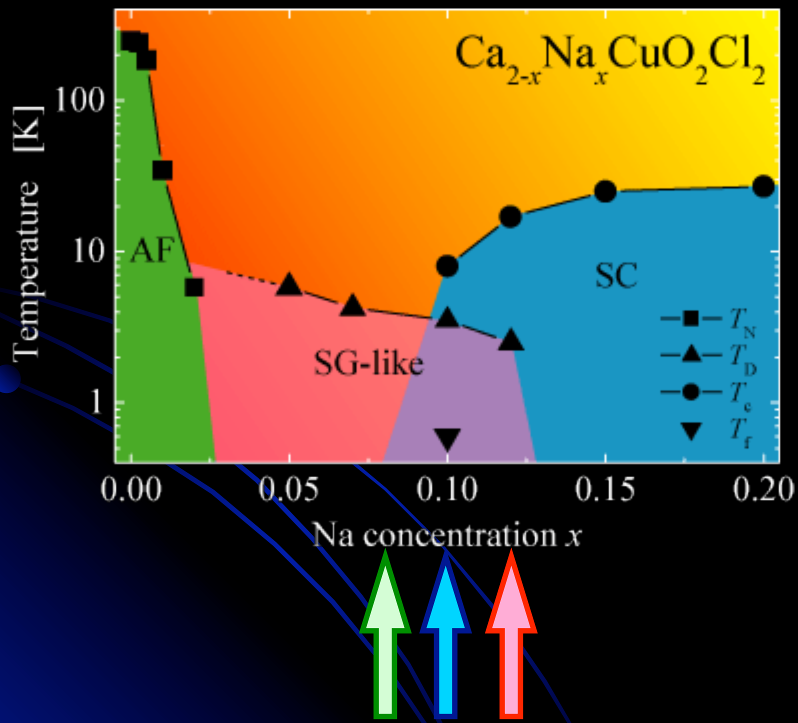
$$\int_{0}^{\Omega_L} d\omega N(\mathbf{r};\omega) = 2x(\mathbf{r}) + 2\left|\langle K(\mathbf{r})\rangle\right|/U$$

$$J < t \ll \Omega_L \ll U$$

(empty sites + ...)

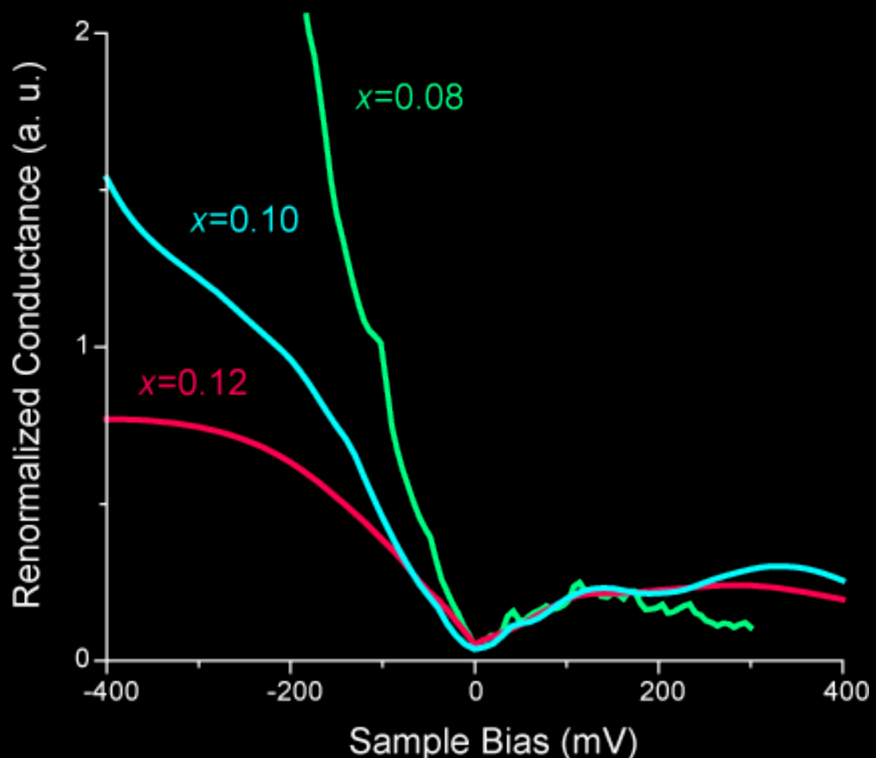
$$\left|\langle K(\mathbf{r})\rangle\right|/U \sim \mathcal{O}\left(xt/U\right)$$

Increasing p-h Asymmetry with Underdoping



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

Averaged dI/dV spectra



T. Hanaguri *et al.*, Nature **430**, 1001 (2004)

Davis group (Cornell)

Using Sum Rules to estimate local density from STM data

conductance $g(\mathbf{r}; eV) = M(\mathbf{r}) N(\mathbf{r}; \omega = eV)$

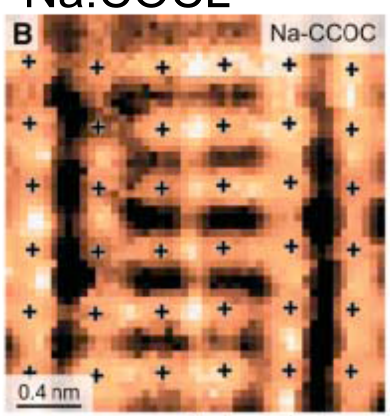
Unknown matrix element M(r) cancels out in ratio

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

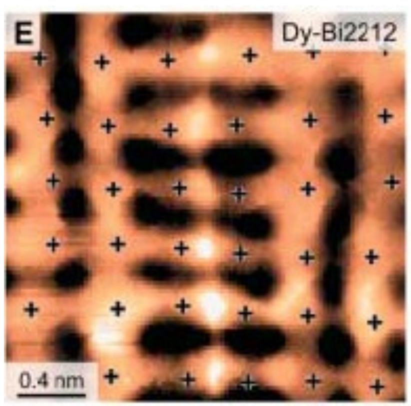
Measured

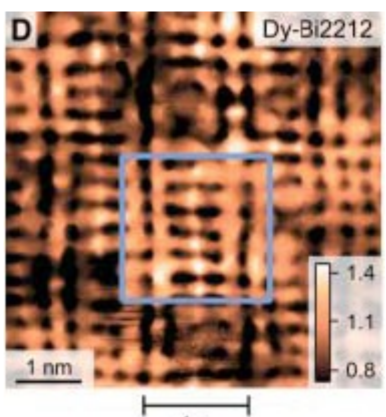
Determine x(r)

Na:COCL



Dy:Bi2212

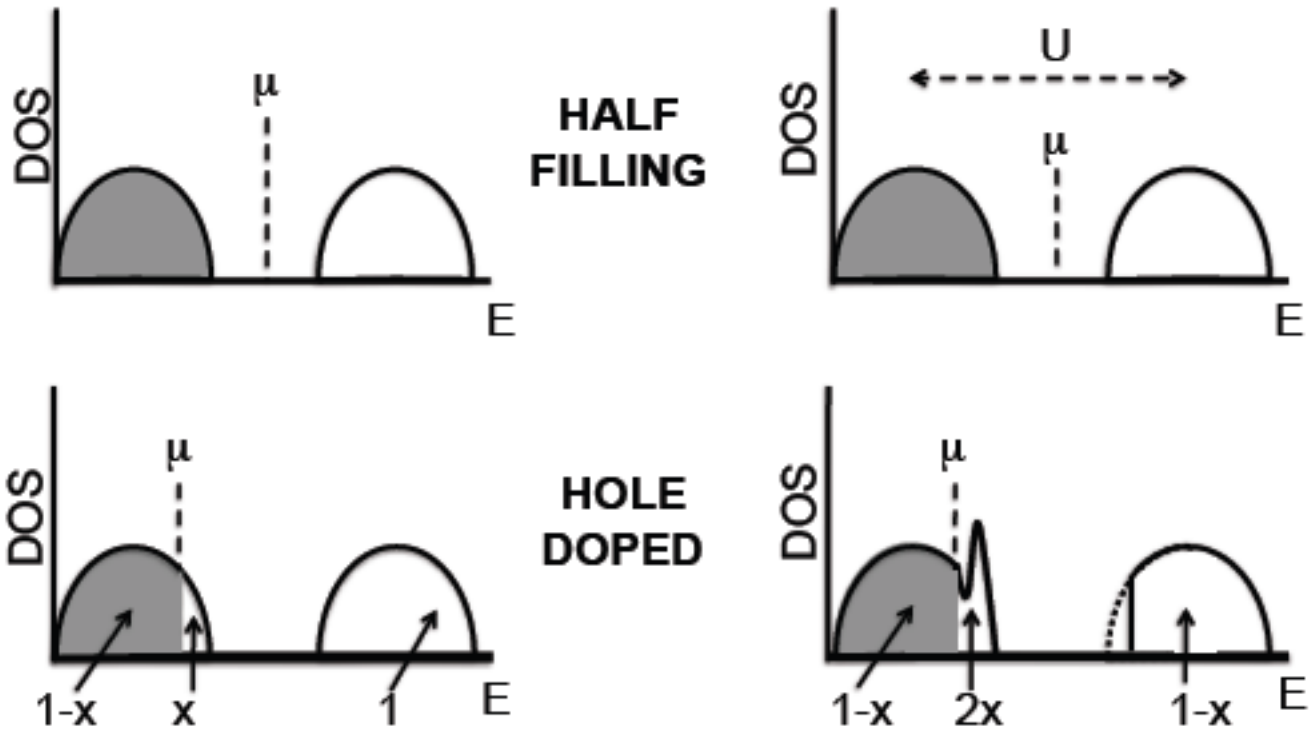




$R(\mathbf{r})$-maps

Y. Kohsaka ...
J.C. Davis
Science (2007)

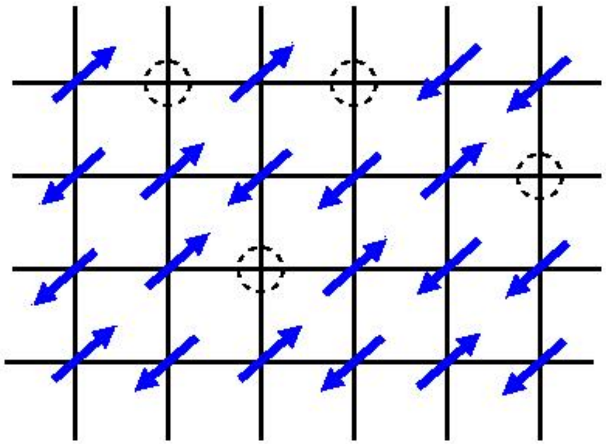
Hole Doping in
Band Insulator v/s. Mott Insulator



Rigid bands in a band insulator

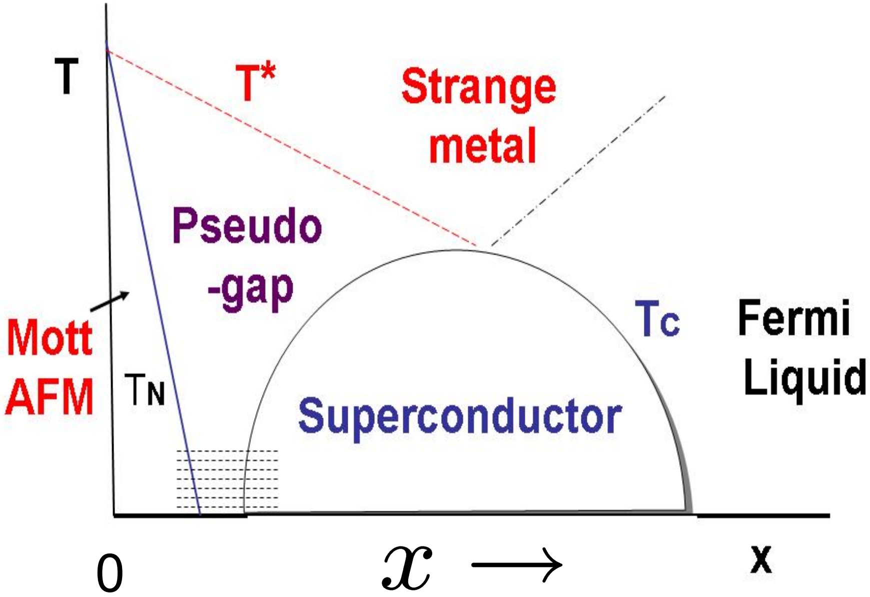
Spectral weight transfer → new low-energy states in a Mott insulator

holes in a 2-d S=1/2 Mott insulator



?

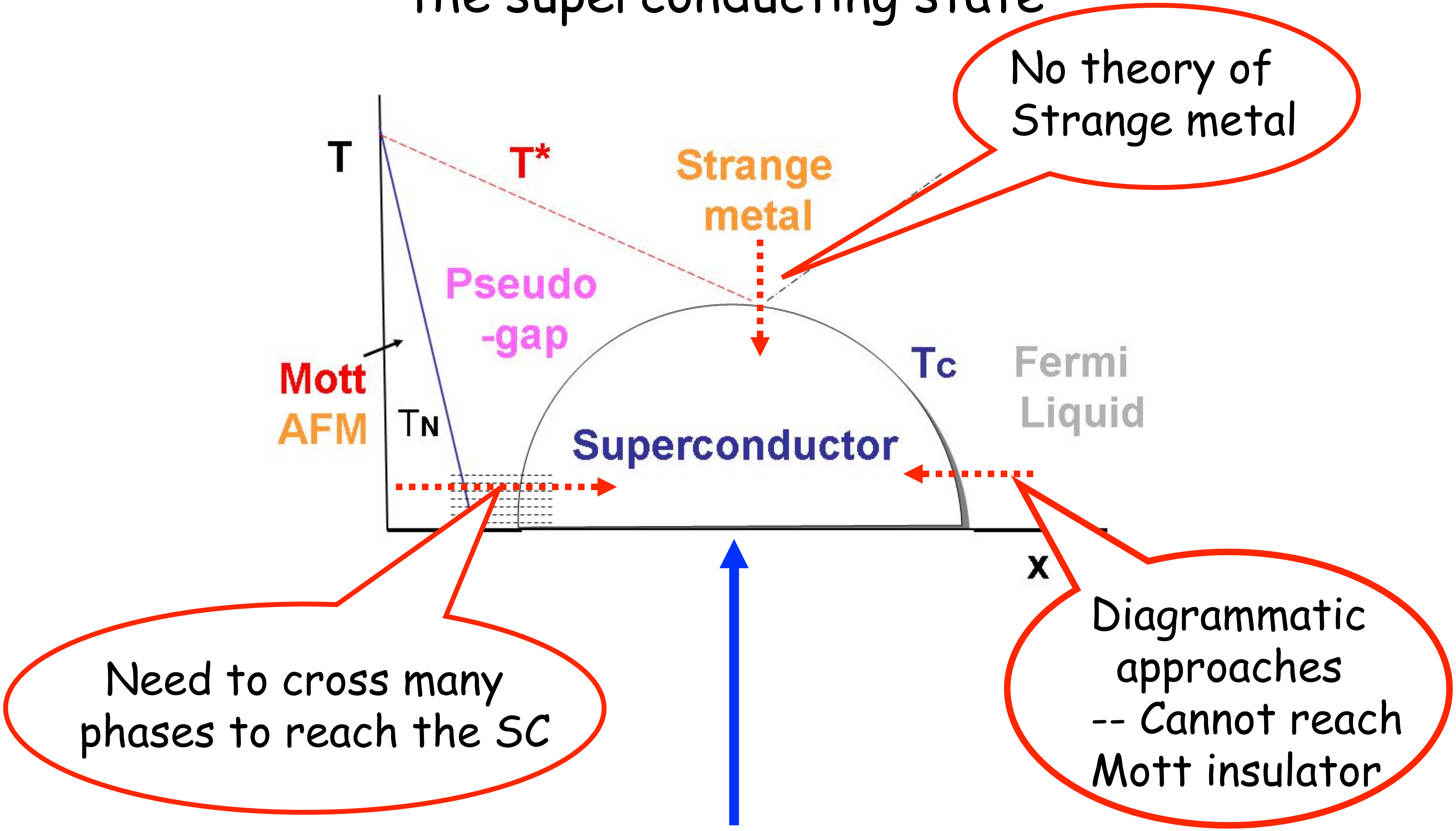
$\Rightarrow$



Focus on the

T=0, H=0 SC state and low-lying excitations

Strategy for theoretical attack on the superconducting state



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

Outline:

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* Our goal is (obviously) <u>not</u> to "prove" that the 2D Hubbard model has a SC ground state

in fact, it would be too much to expect that the simple Hubbard Hamiltonian can describe all the complexities of LSCO, YBCO, BSCO…

Goals:

* Treat the largest energy scale U as well as one can
* Understand the properties of Projected SC w.f.'s, -- the simplest description of SC + strong correlations
* How do these properties differ from SC's without strong correlations?
* How do these compare with the properties of the HTSC cuprates?
* Assess strengths & limitations

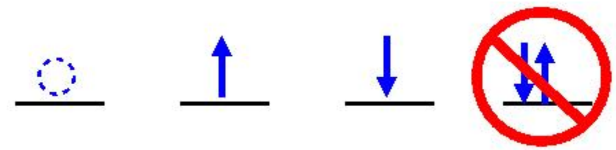
Variational Ground State Wavefunction

$$|\Psi_0\rangle = \exp(iS)\mathbf{P}|\mathrm{dBCS}\rangle$$

$|\mathrm{dBCS}\rangle$ = d-wave BCS state
variational parameters
Δ and μ that enter via u_k, v_k

Gutzwiller Projection:

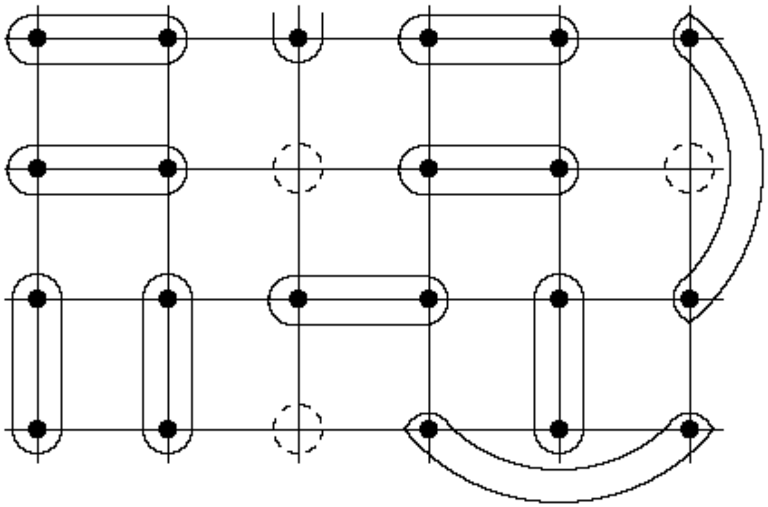
$$P = \prod_i \left(1 - n_{i\uparrow}n_{i\downarrow}\right)$$



$\exp(iS)$ = Unitary transformation
Hubbard → tJ + ... & brings in the scale J

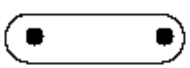
Kohn (64); Gross, Joynt, Rice *(87)*

$$|\Psi_0\rangle \equiv \mathcal{P}|BCS\rangle = \mathcal{P}[\sum_{\mathbf{r},\mathbf{r}'} \varphi(\mathbf{r}-\mathbf{r}') c^\dagger_{\mathbf{r}\uparrow} c^\dagger_{\mathbf{r}'\downarrow}]^{N/2}|0\rangle$$



Projected SC ≡ a Resonating Valence Bond (RVB) liquid

P.W. Anderson, Science (1987)

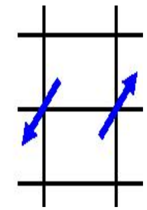
r  r′ $= \dfrac{|\uparrow_{\mathrm{r}}\downarrow_{\mathrm{r}'}\rangle - |\downarrow_{\mathrm{r}}\uparrow_{\mathrm{r}'}\rangle}{\sqrt{2}} \; \varphi(\mathbf{r}-\mathbf{r}')$

$$\varphi(\mathbf{r}-\mathbf{r}') = \sum_k e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \left(\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}}\right)$$

variational w.f. to be optimized,
not just NN singlet pairs

RVB theory of SC in doped Mott insulators

- SC from repulsion:
  super-exchange J → S=0 pairing



- Not as a "Fermi surface instability"

- Real-space description

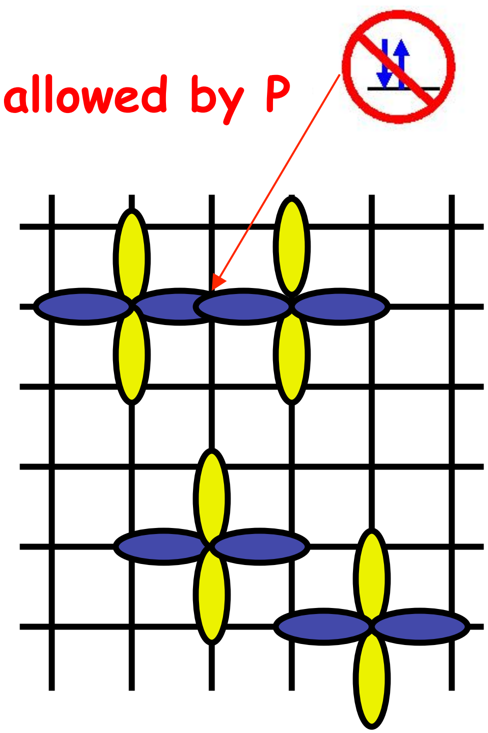
Anderson (1987); Baskaran, Zou, Anderson (1987)

→s-wave pairing

Kotliar & Liu (1988) (slave boson)
Gros (1988) (VMC)
Zhang, Gros, Rice & Shiba (1988)
Fukuyama et al (1988)

→d-wave pairing

natural for large U



Variational Monte Carlo (VMC)

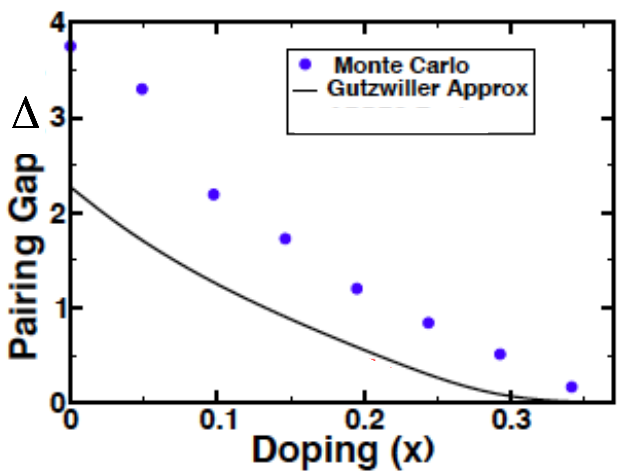
only known way to treat P *exactly*

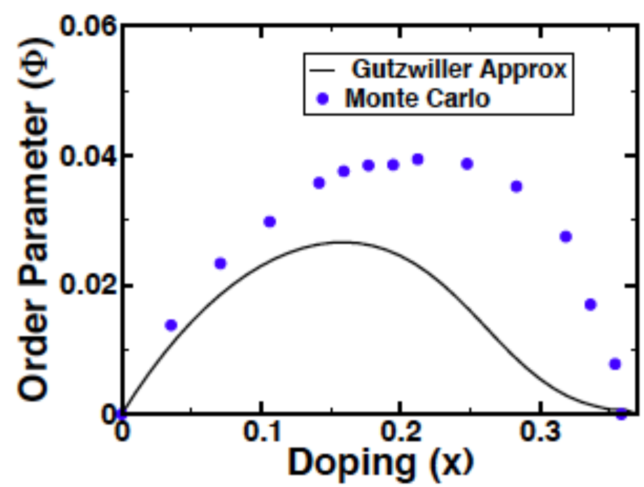
$$\frac{\langle\Psi_0|Q|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

$$|\Psi_0\rangle = \mathcal{P}|BCS\rangle$$

Gutzwiller approximation (GA):

$$\langle \text{K.E.}\rangle \simeq \frac{2x}{(1+x)}\langle \text{K.E.}\rangle_0; \ \langle s(i)s(j)\rangle \simeq \frac{4}{(1+x)^2}\ \langle s(i)s(j)\rangle_0$$





GA results in rough qualitative agreement with VMC

GA Calculation: "renormalized" mean field theory

→ analytical insights

→ excited states

→ disorder effects

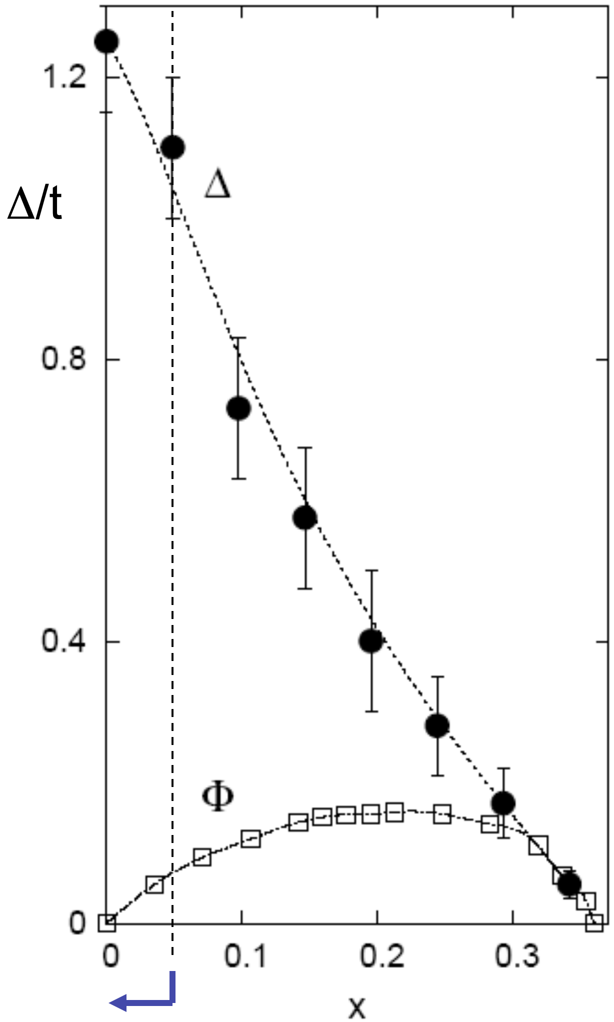
MR, Sensarma & Trivedi in "The Hubbard Model: Theoretical Methods for Strongly Correlated Systems" ed. F. Mancini & A. Avella, (Springer 2012)

$$\min \frac{\langle \Psi_0 | H | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

Pairing & Superconductivity

Pairing → variational Δ

d-wave SC order parameter $\mathbf{\Phi}$
→ from ODLRO $\langle c^\dagger c^\dagger c c \rangle$



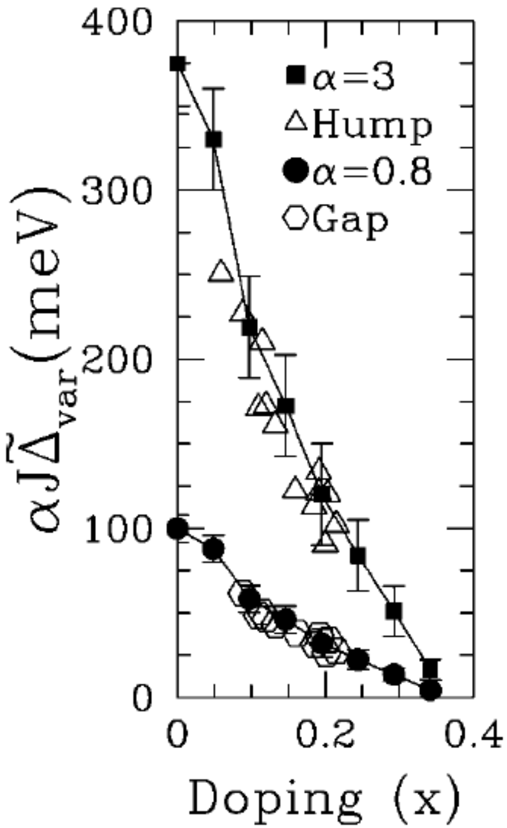
AFM (see later)

Strong Coulomb U
$\Phi(x) \sim x$ as $x \to 0$

P → enhanced (local, quantum) phase fluctuations, as number fluctns. suppressed

→ $\Delta \neq \Phi_{sc}$

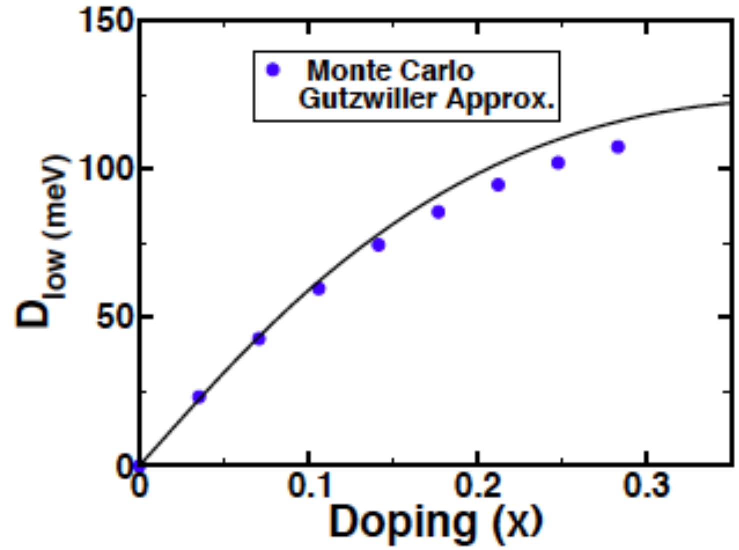
"Gap" and Superfluid Stiffness



Do not gain Insight into Change in Gap Anisotropy with underdoping

Filled symbols: VMC
Open symbols: ARPES

αJ = fudge factor to go from dim'less variational parameter to an energy



Optical spectral weight

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

$$J < t \ll \Omega_c \ll U$$

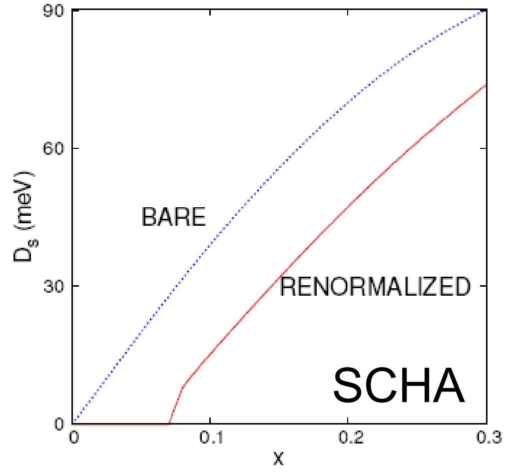
Good agreement with optics: Orenstein, et al., PRB (1990) Cooper, et al., PRB (1993)

Rigorous Bound on Superfluid stiffness

$$\rho_s \leq D_{\text{low}}$$

* Does SC persist down to $x=0^+$ in this approach?

(1) Long-wavelength quantum phase fluctuations drive superfluid stiffness to zero



(2) AFM LRO (1st order transition -- see next)

* Nature of the insulator described by P|dBCS> at x=0?

Z_2 spin liquid with algebraic AFM order [Ivanov-Senthil; Paramekanti, MR & Trivedi]

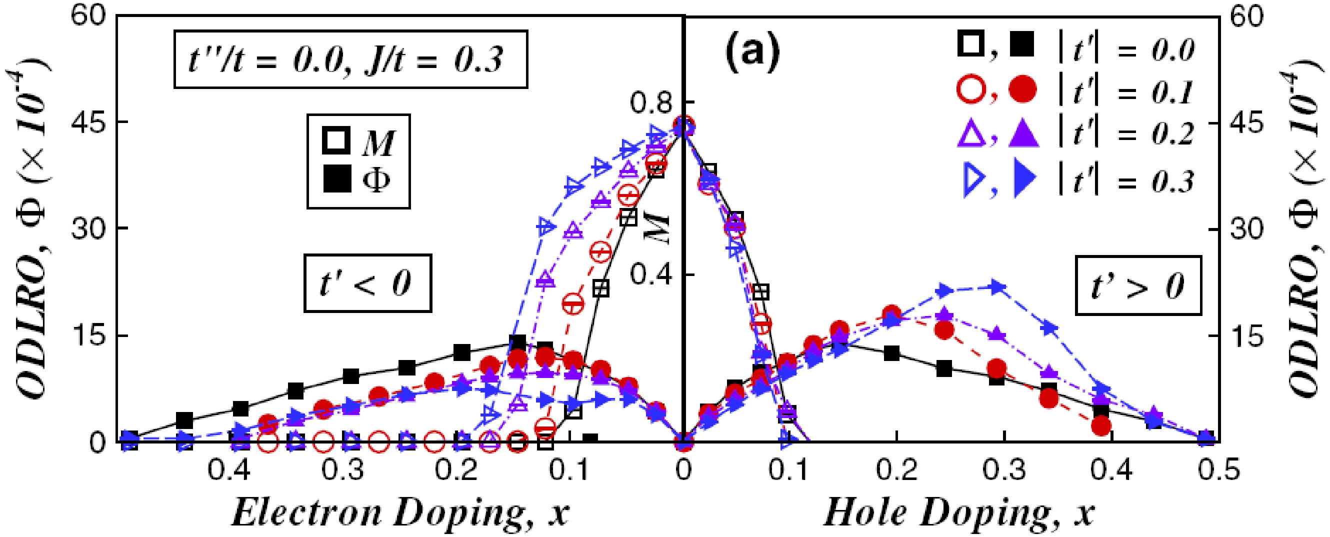
projected w.f.'s are an important tool in the study of quantum spin liquids.

* Although the x=0 state for the 2D square lattice is <u>not</u> a spin liquid, P|dBCS> is still a conceptually and computationally useful way to think about the strongly correlated SC.

SC and AFM & electron-hole Doping Asymmetry

Electron Doping:
- AFM grows with t'
- SC suppressed with t'

Hole Doping:
- AFM insensitive to t'
- SC grows with t'

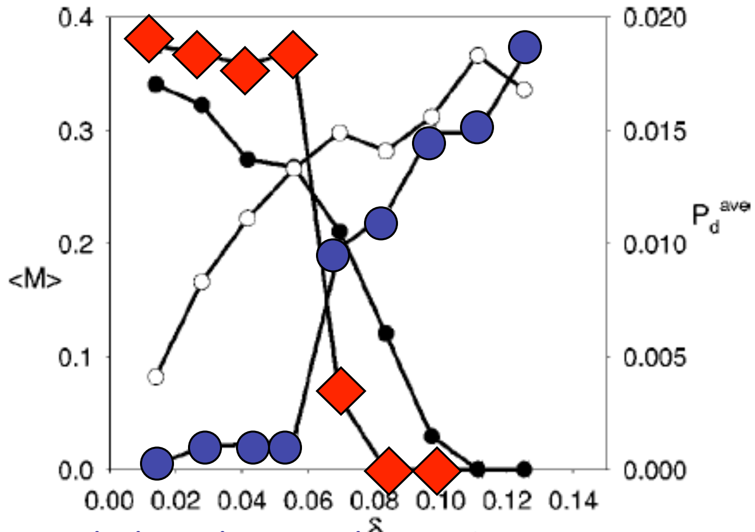


- Qualitative agreement with e v/s h doped cuprates
- Connection with Pavarini et al. "range" parameter

Pathak, Shenoy, MR & Trivedi, PRL **102**, 027002 (2009)

Competition between states at small x

Energetics: energies of different states differ by few % J → details of H are important (& not known!)



Shih, Chen, Chou, & TK Lee, PRB **70**, 220502(R) (2004)

- ◆ AFM for x < 7%
- ● SC for x > 7%

J/ t =0.3,

t ' / t= - 0.3

t"/ t=0.2

At x=0 AF magnetism wins;
RVB spin-liquid insulator
Energy/bond = - 0.3199 J
v/s
AFM Long range order
Energy/bond = - 0.3346J
Trivedi & Ceperley, (1989)

Important New Progress:
arXiv:1402.2859; Competing states in the t-J model: uniform d-wave state versus stripe state,
P. Corboz, T. M. Rice, M. Troyer

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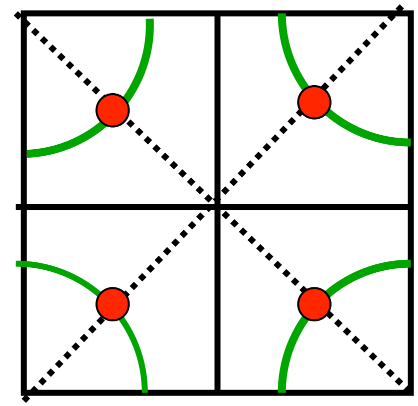
- Introduction
- Sum Rules & p-h asymmetry
- Variational Theory of SC State
- Low energy excitations:
  - * nodal quasiparticles
  - * “underlying Fermi surface”
- Disorder Effects

Low Energy Excitations in SC state



Sharp Nodal Quasiparticles

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

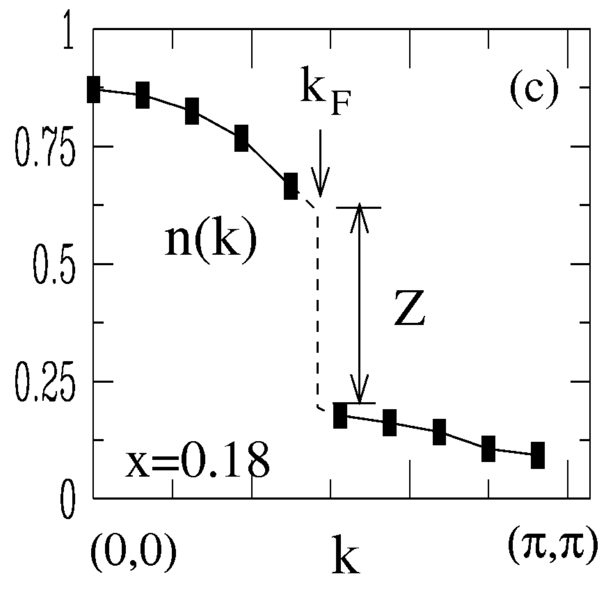
Moments of spectral function = equal-time correlators

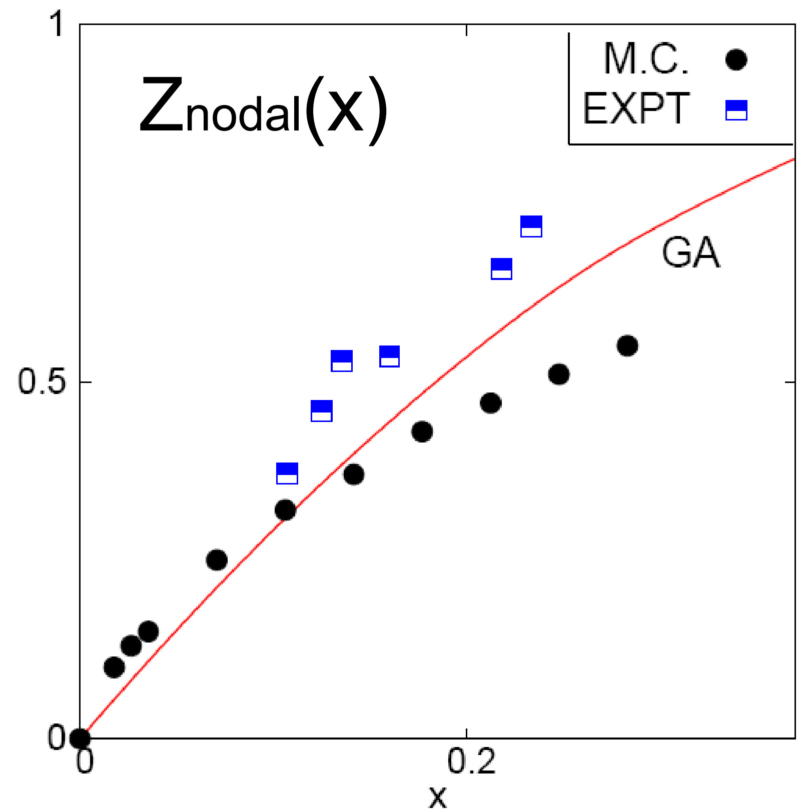
$$M_\ell(\mathbf{k}) = \int_{-\infty}^{0} d\omega\, \omega^\ell A(\mathbf{k},\omega)$$

Singularities in

$M_\ell(\mathbf{k}) \Leftrightarrow$ gapless Quasiparticles

Nodal QP Spectral Weight Z





Loss of coherence with underdoping

— GA $Z = \frac{2x}{(1+x)} + \mathcal{O}(xt/U)$

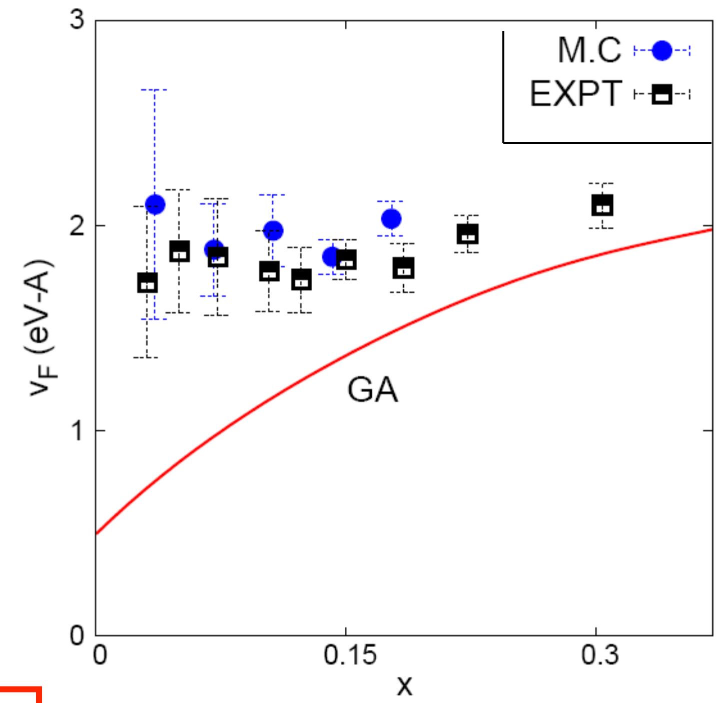
MR, Sensarma et al., PRL (2005)

● MC: Paramekanti, MR, Trivedi, PRL(2001)

Expt: Johnson *et al.*, PRL (2001)
ARPES Bi2212

Dispersion of Nodal Quasiparticles

VMC v_F independent of x
-- agrees with old ARPES data (on ~10s meV scale)
-- but not with laser ARPES data (Vishik, PNAS)



as $x \to 0$

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

$$v_F = \text{const.} \Rightarrow |\partial\Sigma'/\partial k| \sim Ja/x$$

Σ' has singular 1/x dependence on both ω and k along zone diagonal

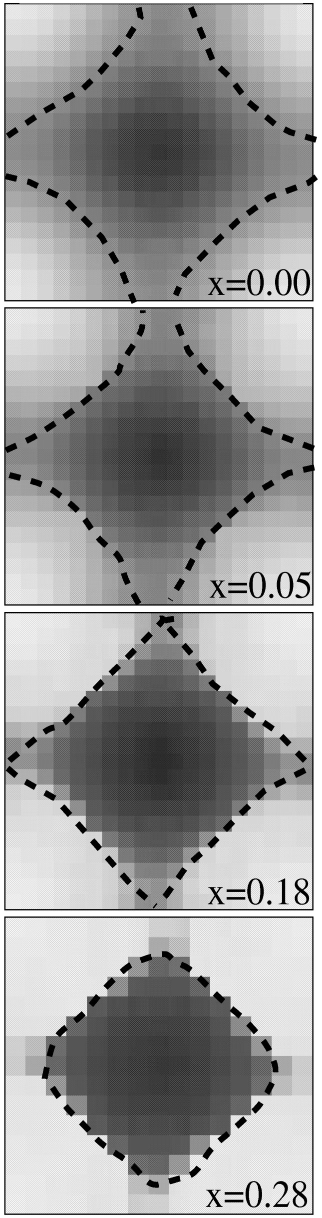
● MC: Paramekanti. MR, Trivedi, PRL(2001)

■ ARPES Expt: Zhou et al, Nature (2003)

— GA: Sensarma et al, PRL (2005)

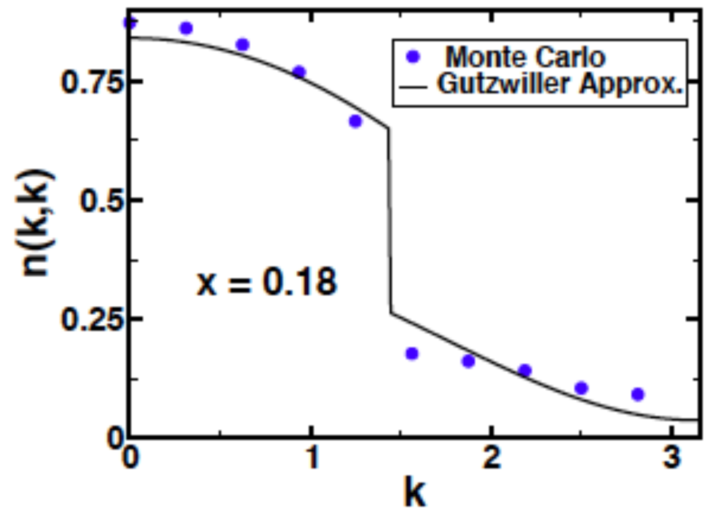
x-dependence of the Momentum distribution

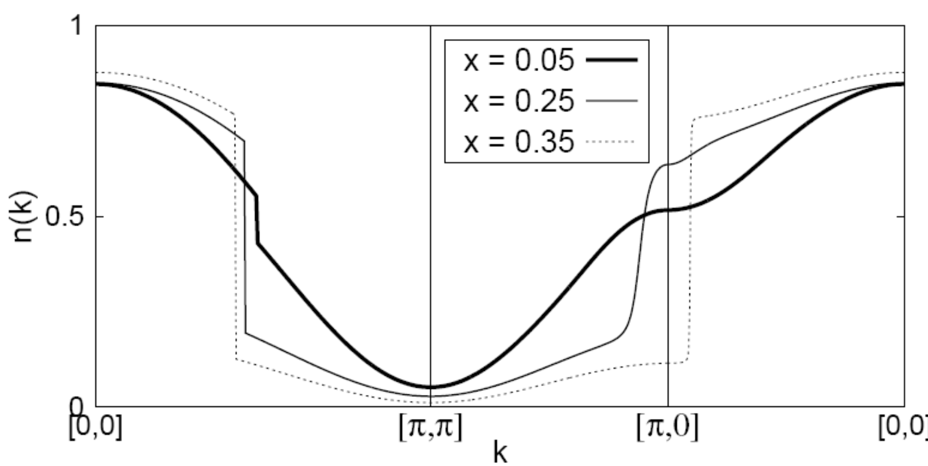
n(k) from MC



---- n(k) = 1/2

"FS" topology change at x~0.2 very sensitive to t' /t





GA n(K)

Qs: Is there a way to determine the "underlying FS" that is gapped out in a SC state at T = 0?

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

C. Gros, B. Edegger, V. Muthukumar & P.W. Anderson, PNAS (2006)

Will not discuss here…

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Disorder Effects in SCs

- Standard theory [Abrikosov-Gorkov] of "unconventional" (non s-wave) SCs → impurities are pair-breaking

e.g., rapid suppression of Tc with disorder in Sr_2RuO_4

Review on disorder effects in HTSC

H. Alloul, J. Bobroff, M. Gabay, P.J. Hirschfeld
Rev. Mod. Phys. 81, 45 (2009)

Why are HTSC's so robust against disorder?

* (most) impurities lie off CuO2 planes

* the coherence length is very short
  → spatially inhomogeneous response
  not captured by standard A-G theory

* Disorder effects are suppressed in strongly correlated SCs

* Nodal/Antinodal dichotomy

A. Garg, N. Trivedi & MR, Nature Phys. 4, 762 (2008).

Inhomogeneous response to impurities:
-- Bogoliubov-deGennes (BdG) theory

Correlation effects
-- inhomogeneous Gutzwiller approx.(GA)

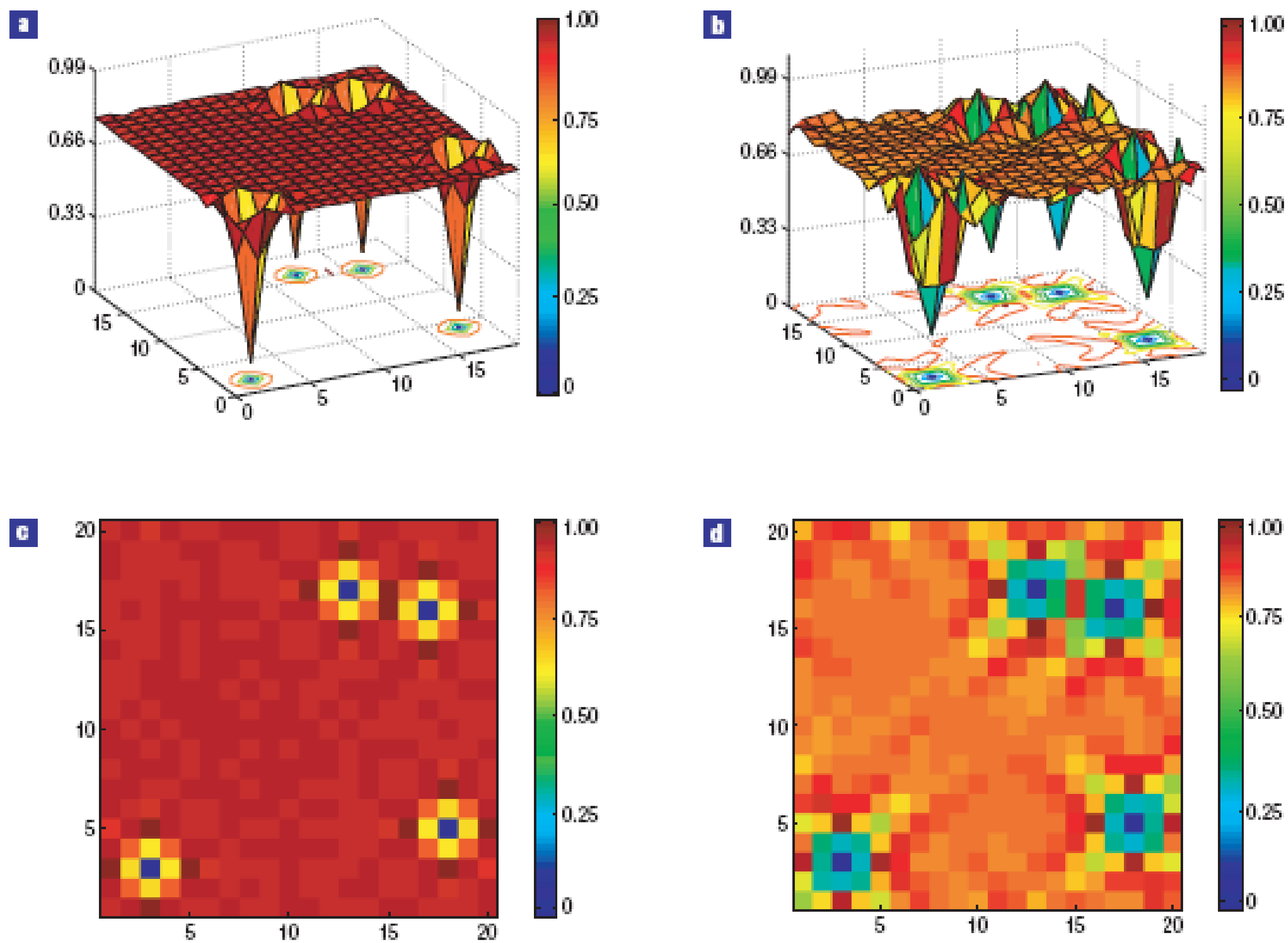
e.g., KE renormalization: $g_t(\mathbf{r},\mathbf{r}') = g_t(\mathbf{r})g_t(\mathbf{r}')$
where $g_t(\mathbf{r}) = [2x(\mathbf{r})/(1+x(\mathbf{r}))]^{1/2}$

Compare results with and without correlations:

For correlated system:
* suppression of pair-breaking
* robust nodal QPs
  - "V" in DOS protected
  - nodes in k-space protected

Response to weak (Born) impurities:
Local d-wave Pairing amplitude

Including Correlations | Ignoring Correlations



Correlations Lead to a Shorter healing length in correlated system

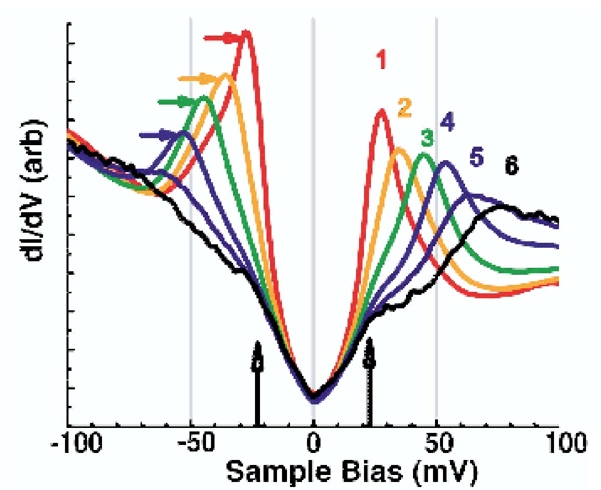
- renormalized vf (or m*)
- "screened" potential
- local changes in hopping

$V_{imp} = t$

Low-Energy Excitations Protected against Disorder

In the correlated system

- nodal QPs robust against disorder
- antinodal excitations much more affected than nodal qp's

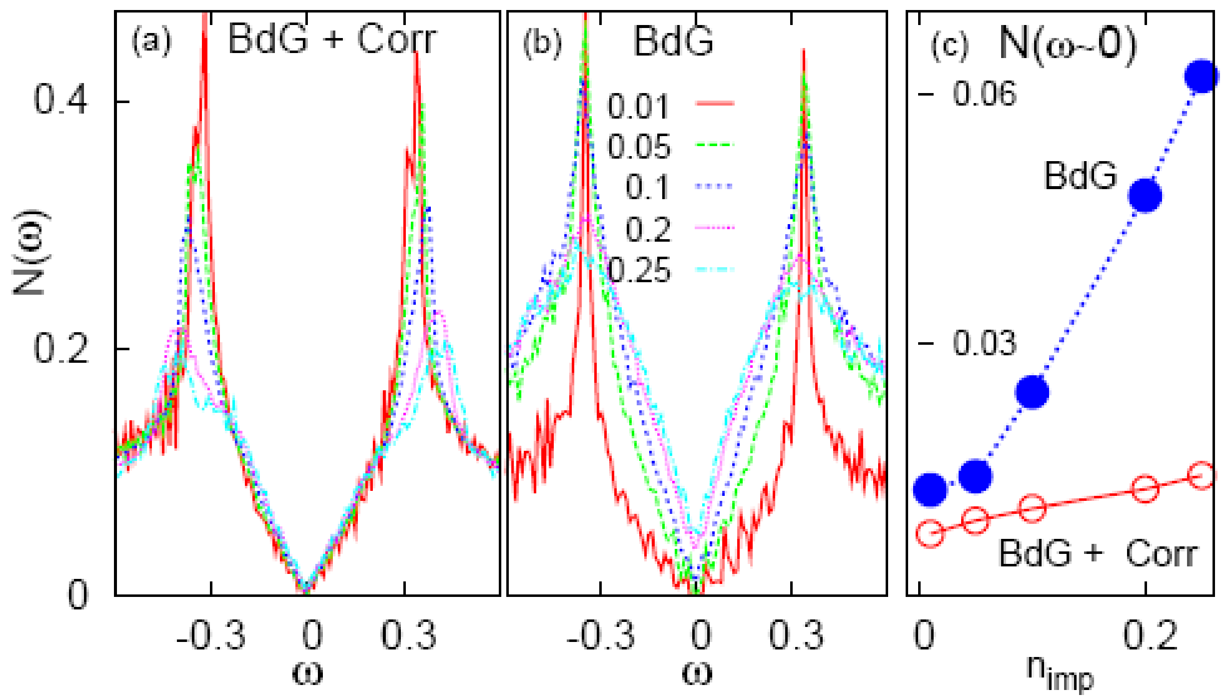


STM: McElroy et al., PRL (2005)

Spatially averaged DOS

Correlations + disorder

Only disorder; no correlations

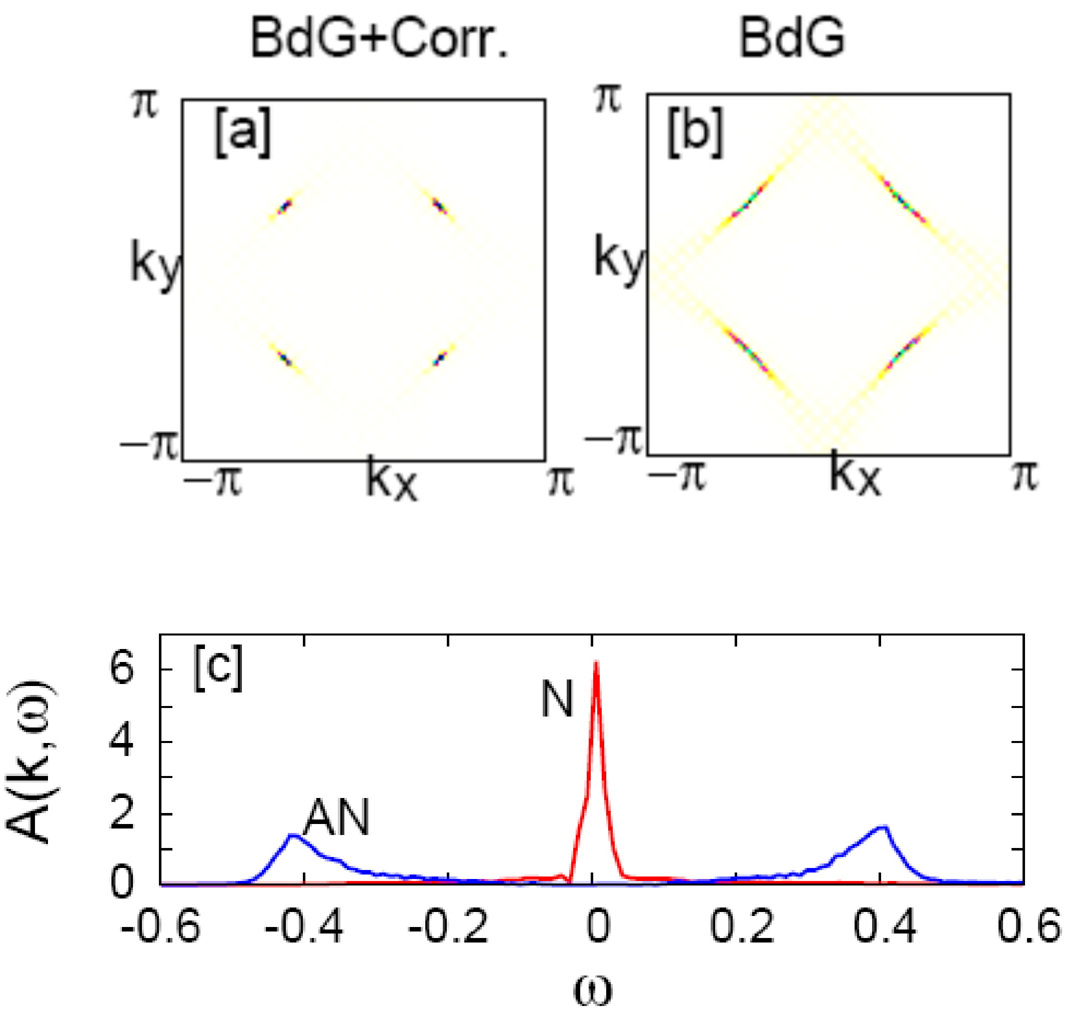


Garg, Trivedi & MR, Nature Phys. (2008)

Where do the low energy excitations live?

$$A(\mathbf{k},\omega) = \mathsf{FT}_{\mathbf{r}\to\mathbf{k}}\,\langle \mathrm{Im}\,\mathsf{G}(\mathbf{r},\mathbf{R},\omega)\rangle_{\mathbf{R}}$$

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2; \quad \mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$$



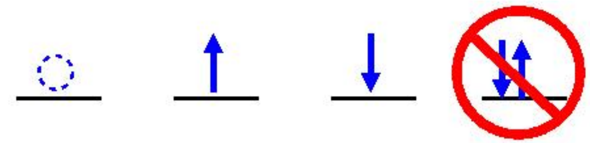
$$A(\mathbf{k},|\omega| \le 0.02)$$

Nodes are protected

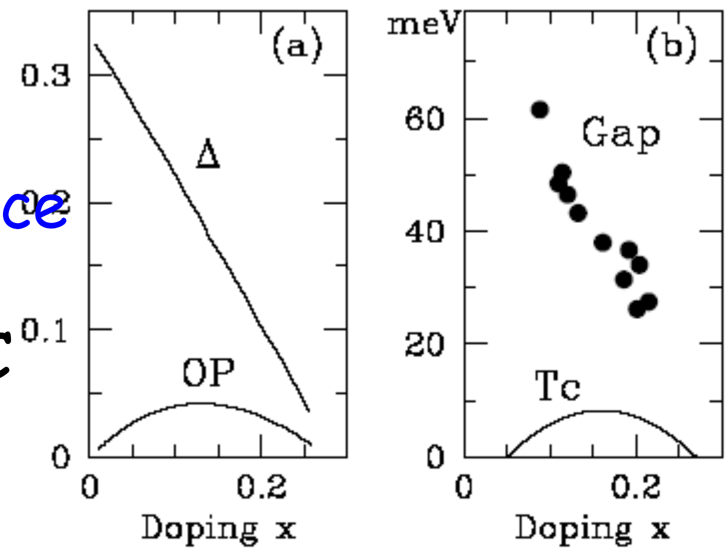
Nodal QPs much less affected by Disorder than the Antinodal QPs

Summary: d-wave SC in doped Mott insulators

- p-h asymmetry in STM
- local x(r) & sum rules



- SC "dome" with optimal doping
- energy gap and SC order have qualitatively different x-dependence



theory experiment

- 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

- disorder effects suppressed in presence of strong correlations

* T=0, H=0
* Competing Orders Not adequately described

Some technical details
Not covered in the lecture

Canonical Transformation exp(iS)

transforms Hubbard to tJ model

(plus three-site terms)

$$\mathcal{K}_0 = -\sum_{\mathbf{r},\mathbf{r}',\sigma} t_{\mathbf{r}\mathbf{r}'}[n_{\mathbf{r}\bar{\sigma}} c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} n_{\mathbf{r}'\bar{\sigma}} + h_{\mathbf{r}\bar{\sigma}} c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} h_{\mathbf{r}'\bar{\sigma}}]$$

$$\mathcal{K}_{+1} = -\sum_{\mathbf{r},\mathbf{r}',\sigma} t_{\mathbf{r}\mathbf{r}'} n_{\mathbf{r}\bar{\sigma}} c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} h_{\mathbf{r}'\bar{\sigma}}$$

$$\mathcal{K}_{-1} = -\sum_{\mathbf{r},\mathbf{r}',\sigma} t_{\mathbf{r}\mathbf{r}'} h_{\mathbf{r}\bar{\sigma}} c^\dagger_{\mathbf{r}\sigma} c_{\mathbf{r}'\sigma} n_{\mathbf{r}'\bar{\sigma}}$$

$$h_{\mathbf{r}\sigma} = (1 - n_{\mathbf{r}\sigma}) \qquad \bar{\sigma} = -\sigma$$

$$iS \equiv iS^{[1]} + iS^{[2]}$$

$$= \frac{1}{U}(\mathcal{K}_{+1} - \mathcal{K}_{-1}) + \frac{1}{U^2}([\mathcal{K}_{+1}, \mathcal{K}_0] + [\mathcal{K}_{-1}, \mathcal{K}_0])$$

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

Gutzwiller Approximation:

Gutzwiller; Brinkman-Rice
Vollhardt; Zhang *et al.*

approximation scheme to analytically
evaluate matrix elements in Projected states

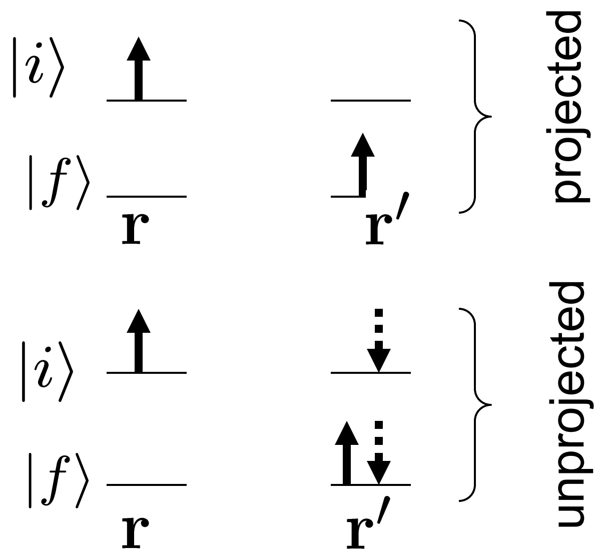
$$\langle \Phi_0 | \mathcal{P} Q \mathcal{P} | \Phi_0 \rangle \simeq g_Q(x) \langle \Phi_0 | Q | \Phi_0 \rangle$$

examples:

$$\langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle \simeq \frac{2x}{(1+x)} \langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle_0 \qquad \langle s_i s_j \rangle \simeq \frac{4}{(1+x)^2} \langle s_i s_j \rangle_0$$

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

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



Singularities of Spectral Moments & Gapless QPs

$$A(\mathbf{k},\omega) = -\mathrm{Im}G(\mathbf{k},\omega+i0^+)/\pi$$

$$= \sum_m [|\langle m|c^\dagger_{\mathbf{k}\sigma}|0\rangle|^2\delta(\omega+\omega_0-\omega_m) \quad +|\langle m|c_{\mathbf{k}\sigma}|0\rangle|^2\delta(\omega-\omega_0+\omega_m)]$$

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

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

Jump discontinuity: k_F & Z

$$M_1(\mathbf{k}) = \int_{-\infty}^{0} d\omega\omega A(\mathbf{k},\omega) = \sum_m(\omega_0-\omega_m)|\langle m|c_{\mathbf{k}\sigma}|0\rangle|^2$$

$$= \langle c^\dagger_{\mathbf{k}\sigma}[c_{\mathbf{k}\sigma},\mathcal{H}-\mu\mathcal{N}]\rangle$$

Slope discontinuity: V_F