

High T_c superconductivity in doped Mott insulators

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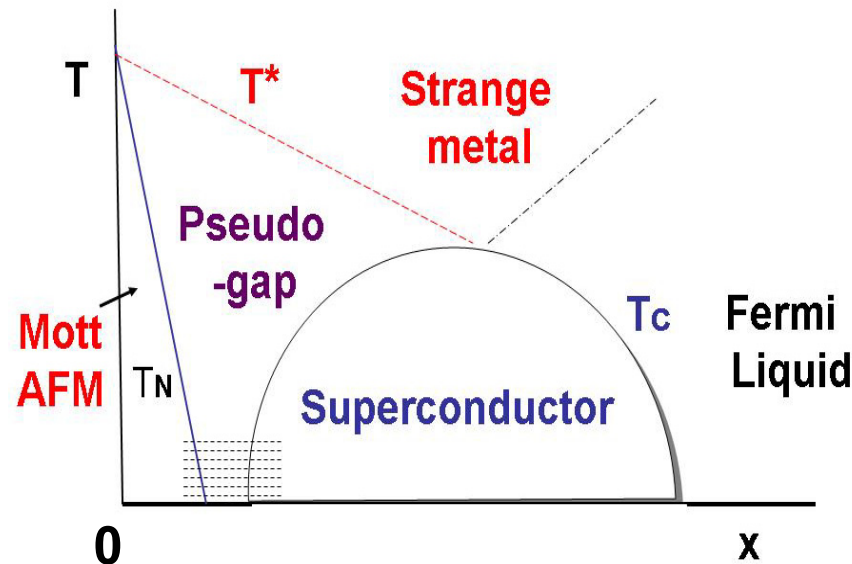
Larkin Memorial Conference
Chernogolovka
June 2007

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

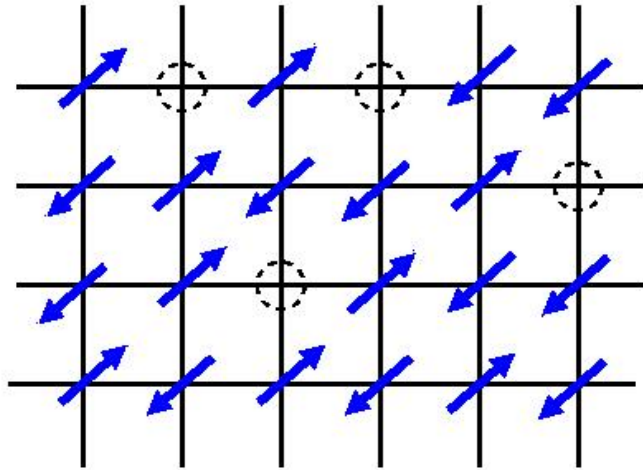
(3) BCS theory fails for Unconventional SC particularly for $x \ll 1$

Competing orders:

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

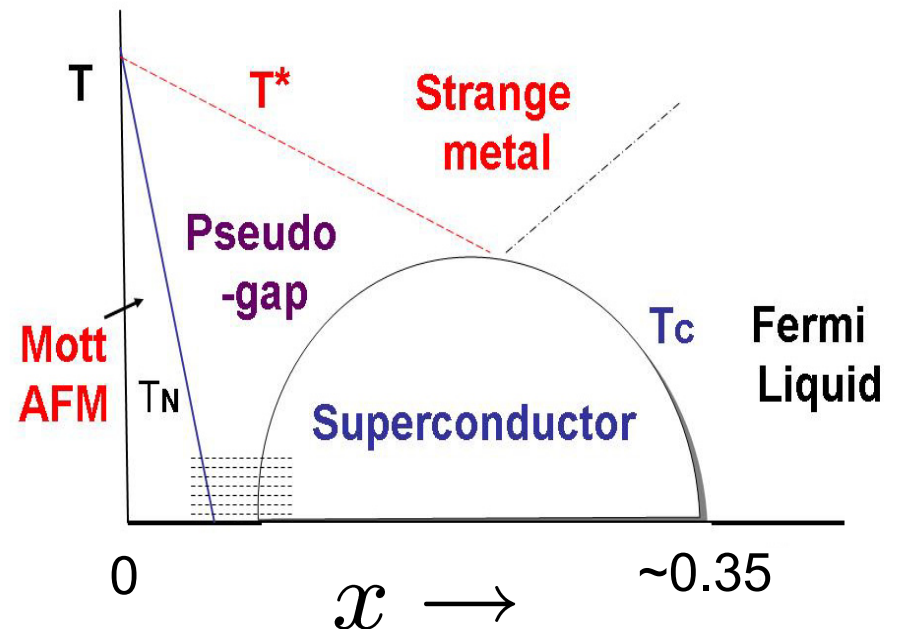
Hidden **Quantum Critical Point** under the dome(?)

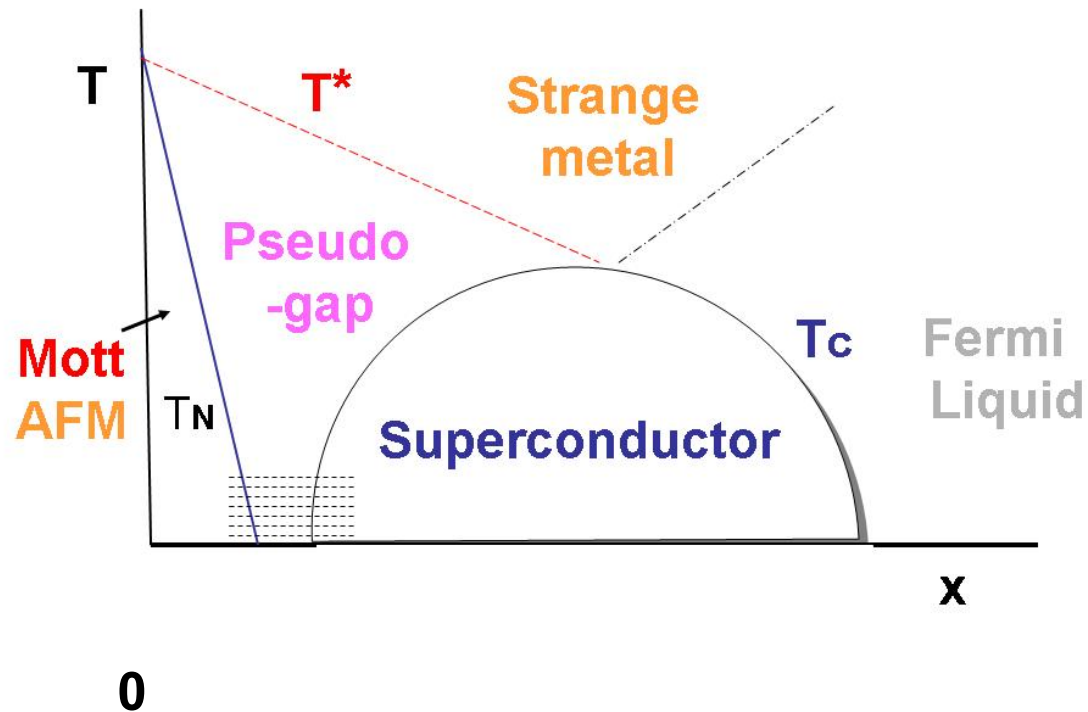
Key question:
holes in a 2-d $S=1/2$ Mott insulator



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PRL 98, 027004 (2007) and unpublished.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).

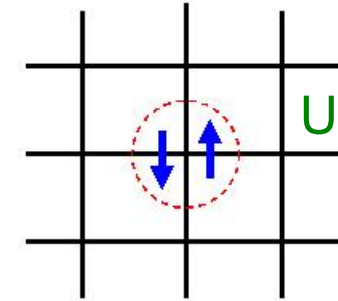
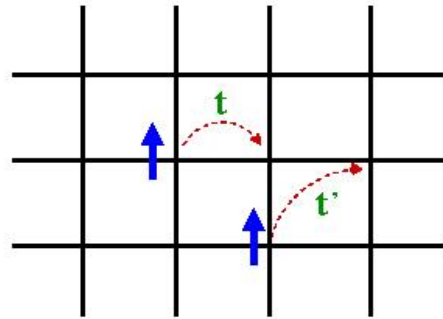
P.W. Anderson, Princeton

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

Hubbard model:

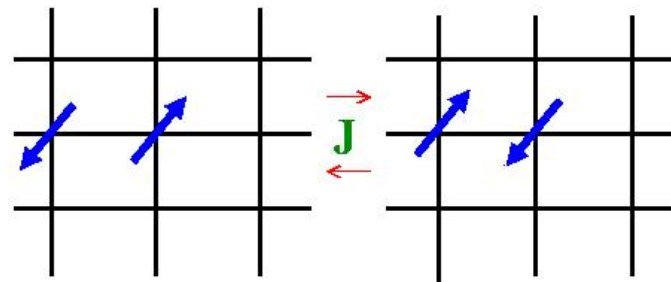
Minimal
Model for
CuO₂ planes

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



$$\epsilon(\mathbf{k}) = -2t (\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y$$

$$U \gg t, |t'|$$



$$J = 4t^2/U$$

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

- neutron
- Raman

↓
~ 100 meV

↓
300 meV
t' ~ -t/4

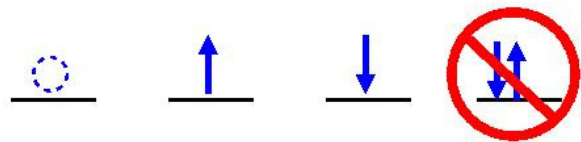
- photoemission
- band theory

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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)
- Anderson & Ong, cond-mat/0405518; J. Phys. Chem. Sol. (2006)



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

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

No assumptions about

- ground state
- broken symmetries
- translational invariance

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

Lehmann Representation
 → **Energy-integrated**
Sum Rules

P-H asymmetry: Exact sum rules for local DOS

Local Hole doping

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

Extracting electrons:

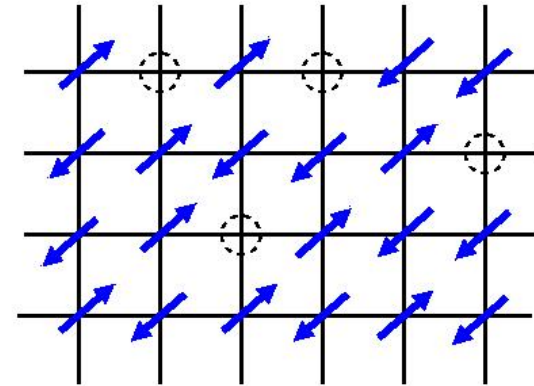
$$\int_{-\infty}^0 d\omega N(\mathbf{r}; \omega) = 1 - x(\mathbf{r}) \quad (\text{filled sites})$$

Adding electrons:

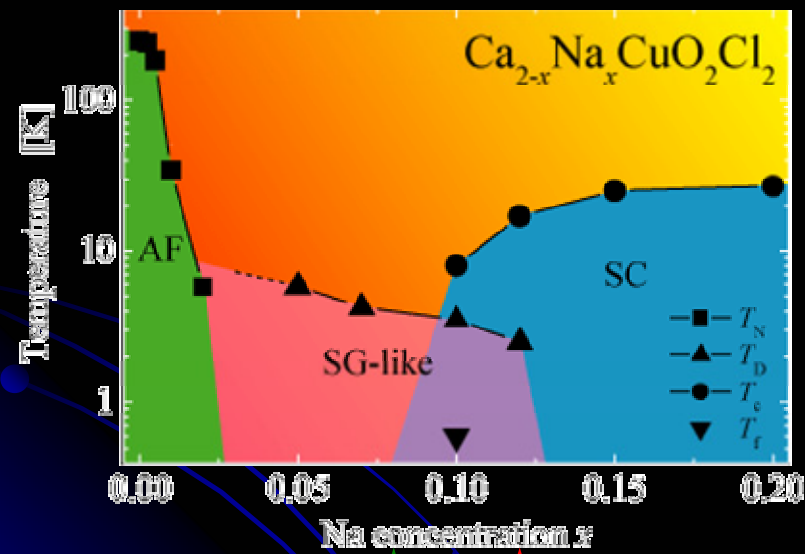
$$\int_0^{\Omega_L} d\omega N(\mathbf{r}; \omega) = 2x(\mathbf{r}) + 2 |\langle K(\mathbf{r}) \rangle| / U$$

$$J < t \ll \Omega_L \ll U \quad (\text{empty sites} + \dots)$$

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

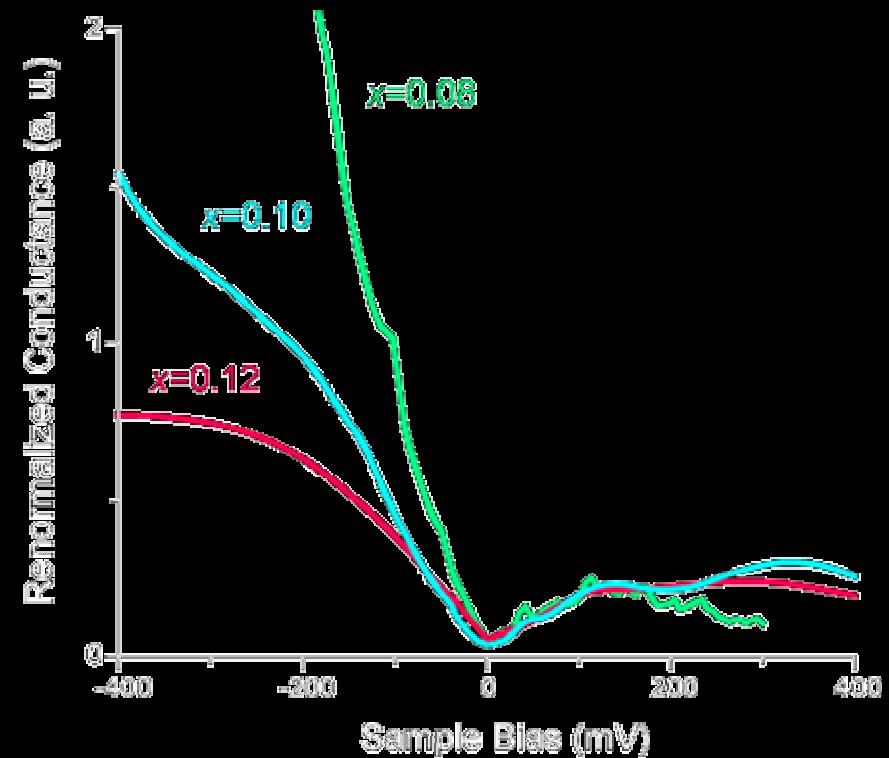


Increasing p-h Asymmetry with Underdoping



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**

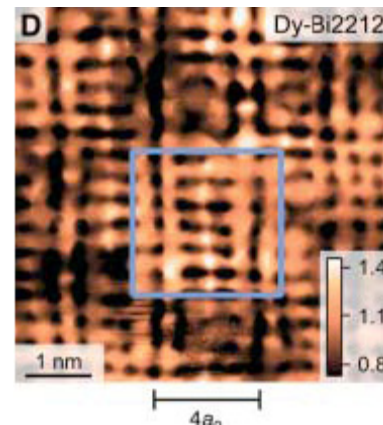
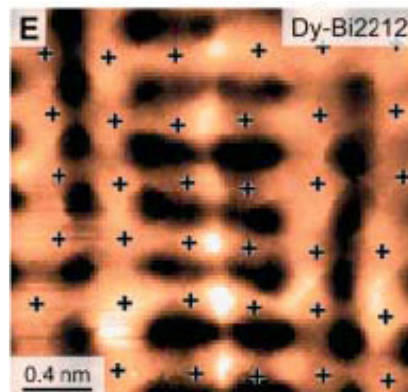
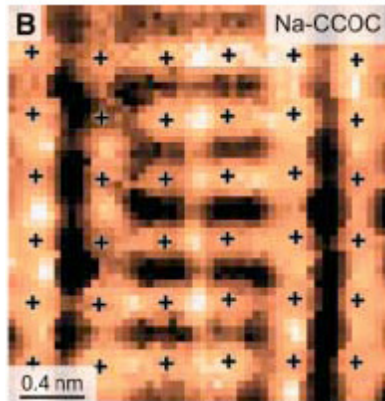
conductance $g(\mathbf{r}; eV) = M(\mathbf{r})N(\mathbf{r}; \omega = eV)$

Unknown matrix element $M(\mathbf{r})$ 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

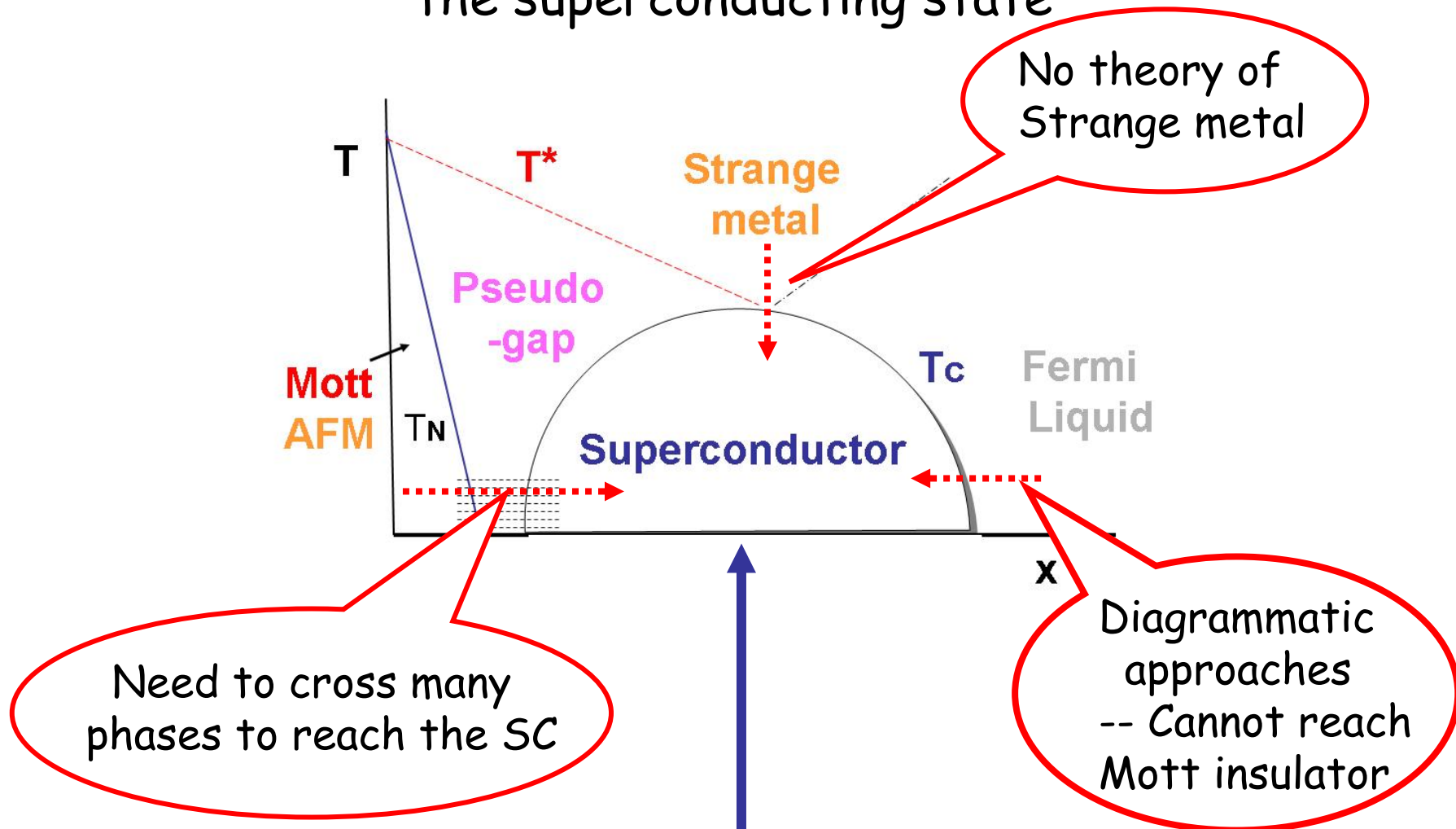
Determine $x(\mathbf{r})$



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

Y. Kohsaka et al,
Science (2007)

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

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- **Variational Theory of SC State**
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Variational Ground State Wavefunction

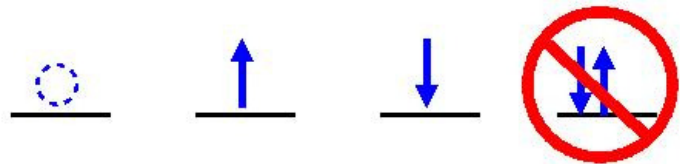
$$|\Psi_0\rangle = \exp(-iS) \mathbf{P} |dBCS\rangle$$

$|dBCS\rangle =$ d-wave BCS state

variational parameters Δ and μ

$$U = \infty$$

Gutzwiller Projection:

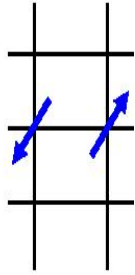


$$P = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$$

$\exp(-iS) =$ Unitary transformation:

Hubbard $\rightarrow tJ + \dots$ brings in the scale J

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



← $S=0$ pairing induced by superexchange $J = 4t^2/U$

Anderson (1987)

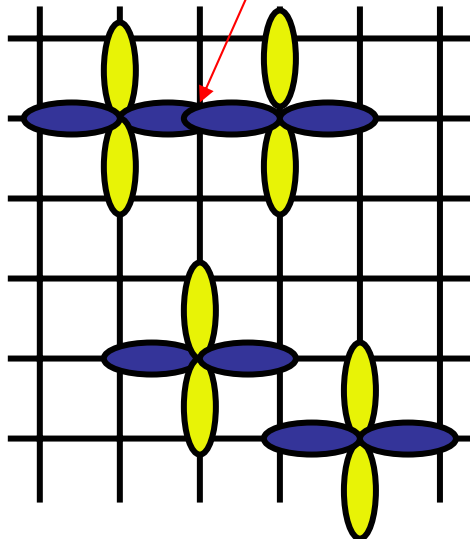
Baskaran et al (1987)

Kotliar(1988)

Zhang, Gros, Rice, and Shiba (1988)



Not allowed by P



Allowed by P

d-wave symmetry

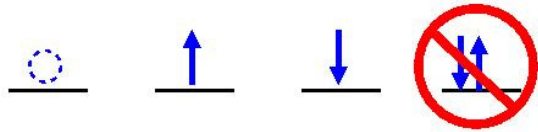
→ Partners in a pair never at the same site

Projection P

→ eliminate all double occupancy

- What are the properties of the Projected SC $P|dBCS\rangle$?
- How do these compare with those of the High T_c cuprates?

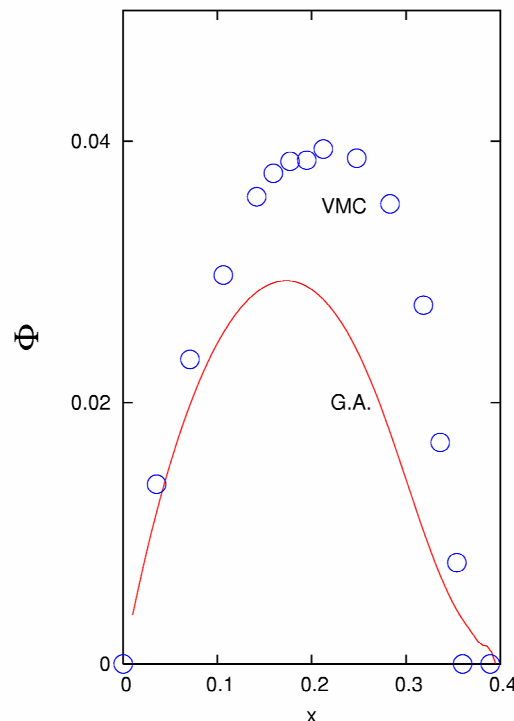
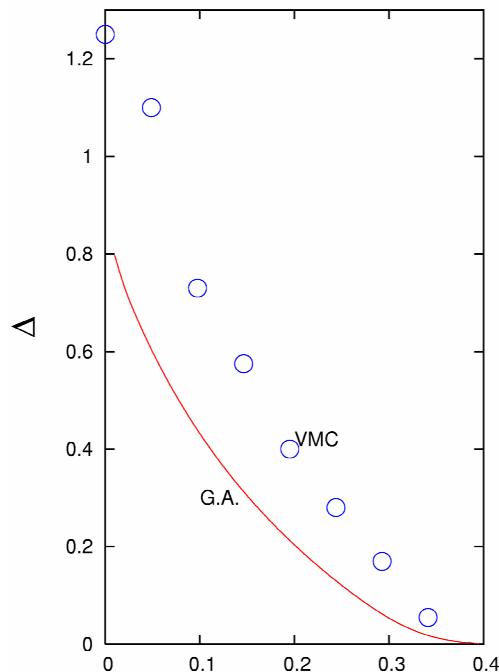
$$|\Psi_0\rangle = \mathcal{P}|BCS\rangle$$



variational Monte Carlo
method: only known way
to treat P exactly

Gutzwiller approximation:

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



GA Calculation:
"renormalized"
mean field theory

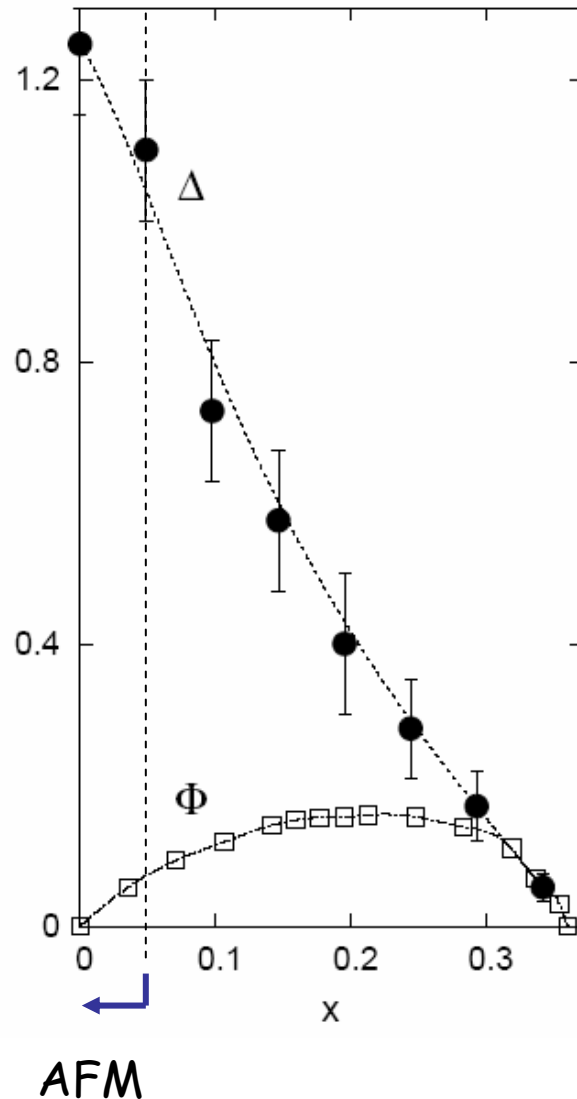
- analytical insights
- excited states
- dynamical correlations
- disorder effects

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

Pairing & Superconductivity

Pairing \rightarrow variational Δ

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



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

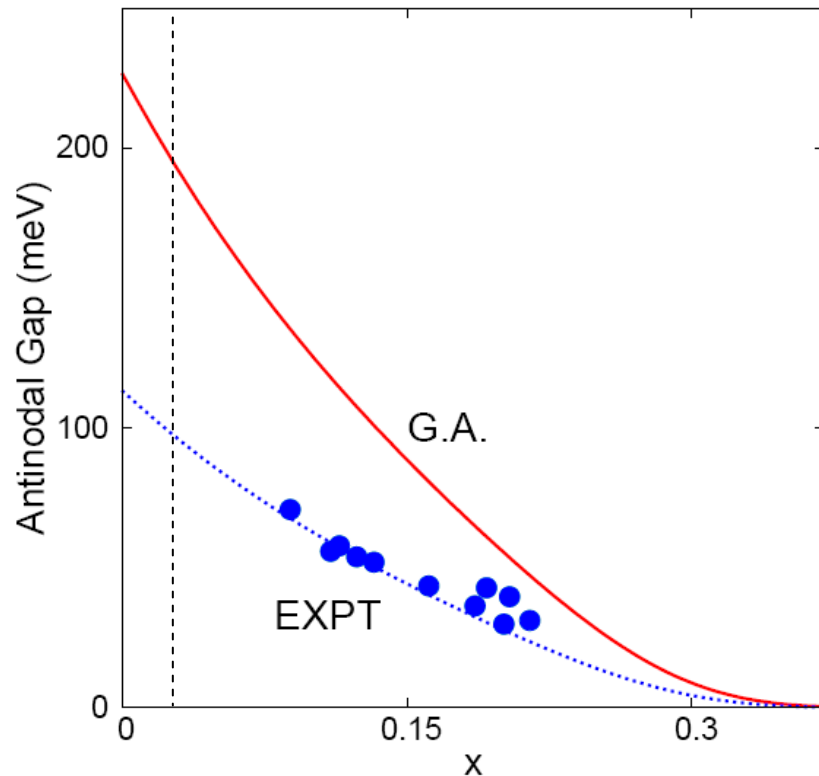
$P \rightarrow$ local, quantum
 phase fluctuations

$$\rightarrow \boxed{\Delta \neq \Phi_{SC}}$$

Variational Estimate of SC Energy Gap

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

QP excitation energy \rightarrow SC gap



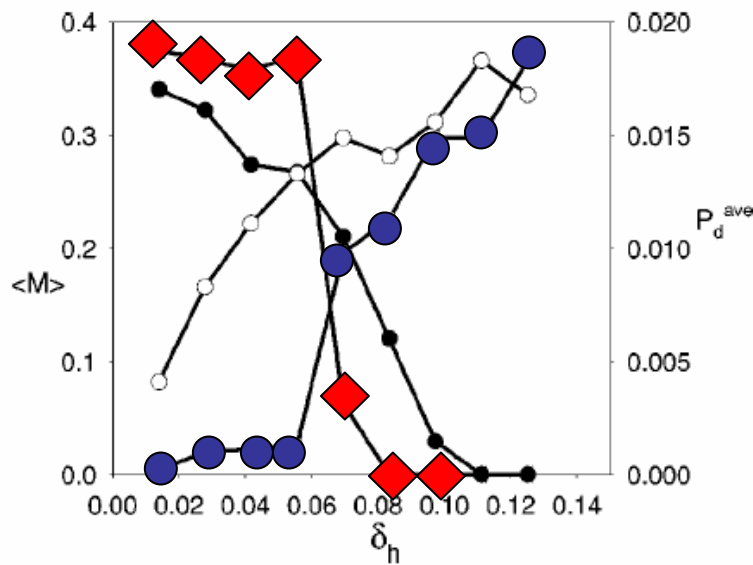
ARPES Expt:
Campuzano et al, PRL (1999)

SC Gap = Variational Δ

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

Competition between SC and AFM as $x \rightarrow 0$

Energetics: energies of different states differ by few % $J \rightarrow$ details of H are important



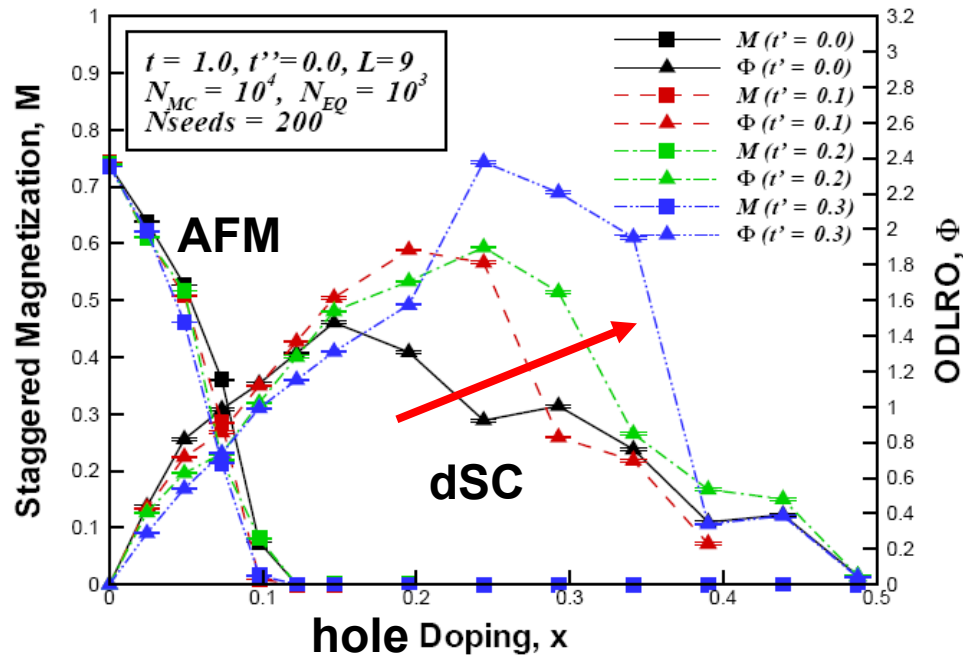
At $x=0$ AF magnetism wins;
 RVB spin-liquid insulator
 Energy/bond = $-0.3199 J$
 v/s
 AFM Long range order
 Energy/bond = $-0.3346 J$
 Trivedi & Ceperley, (1989)

- ◆ 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)

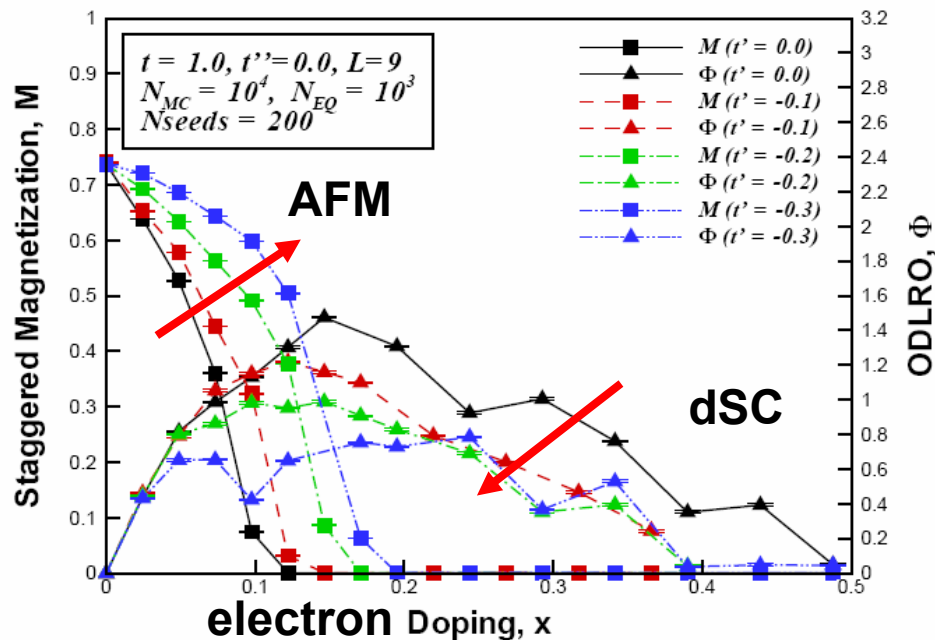
Electron-Hole Asymmetry In Phase Diagram

t, t', J model



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

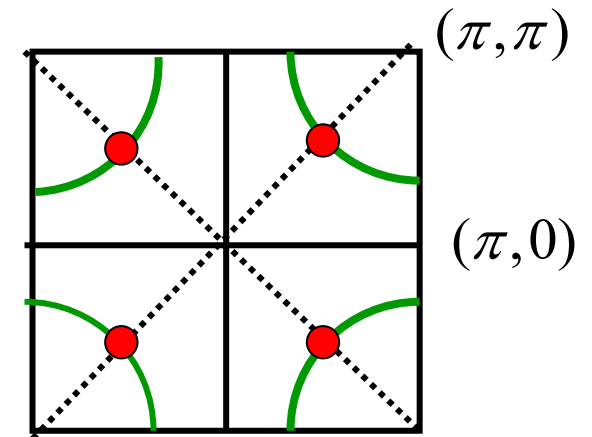
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- Variational Theory of SC State
- **Low energy excitations:**
 - * nodal quasiparticles
 - * "underlying Fermi surface"
- Superfluid density
- Disorder Effects

Low Energy Excitations in SC state

Sharp Nodal Quasiparticles

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



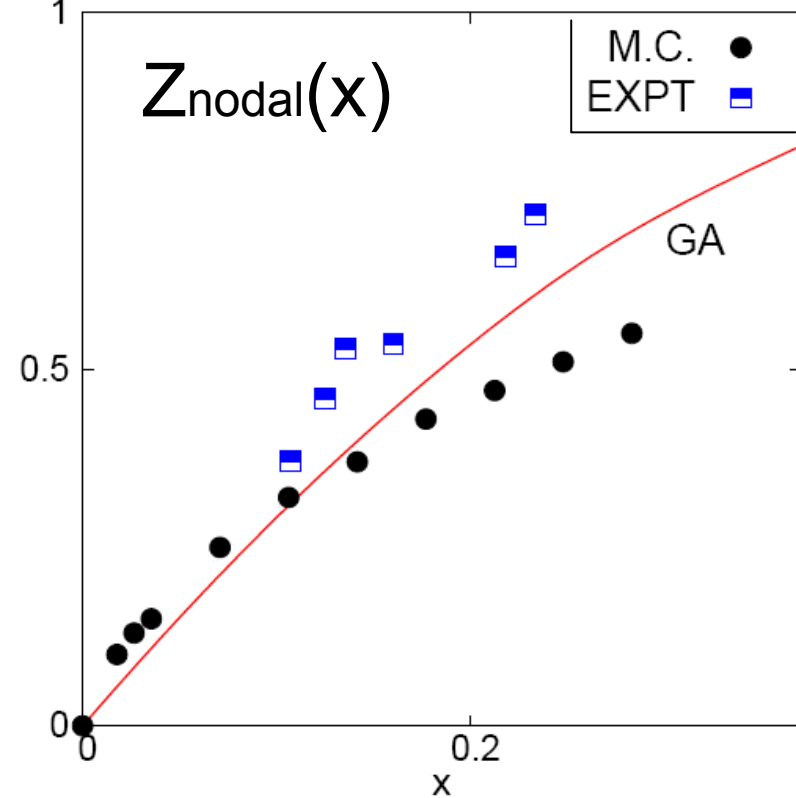
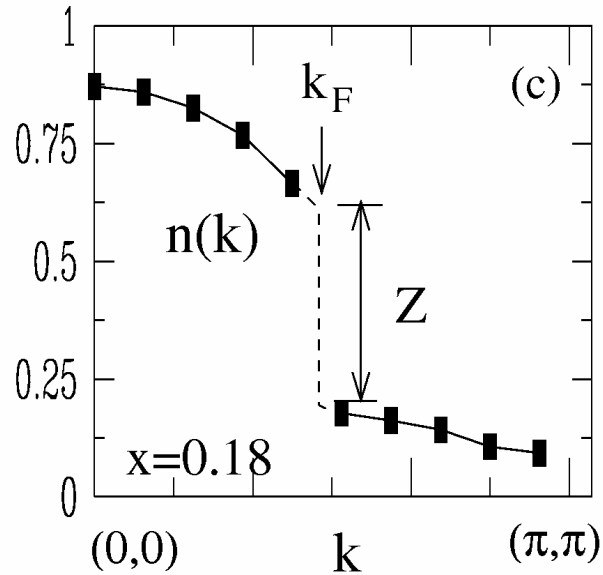
Moments of spectral function = equal-time correlators

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

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

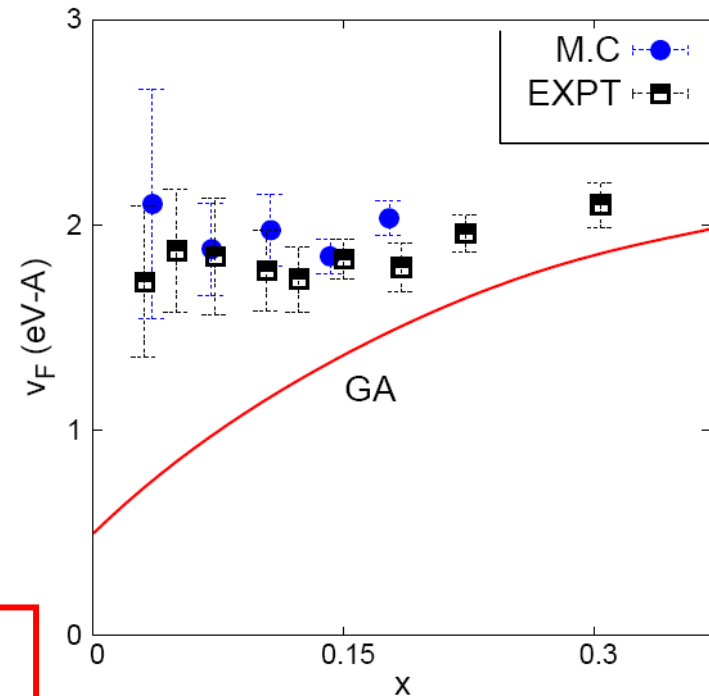
Dispersion of Nodal Quasiparticles

Nodal v_F or m^*
independent of x

as $x \rightarrow 0$

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

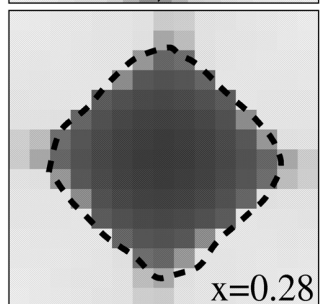
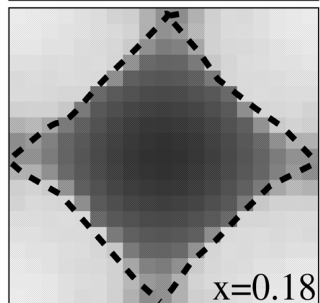
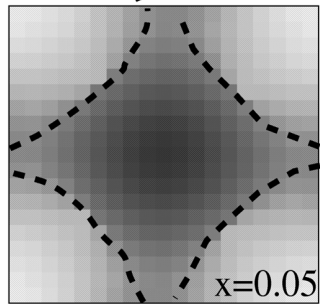
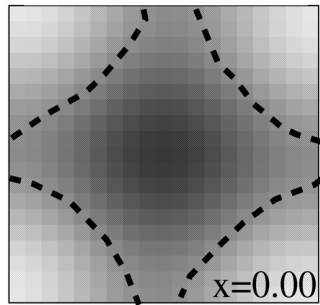
$$v_F = \text{const.} \Rightarrow |\partial \Sigma' / \partial k| \sim Ja/x$$



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)

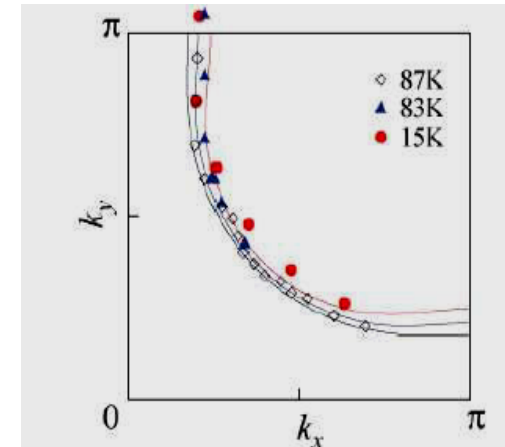
$n(k)$ from MC



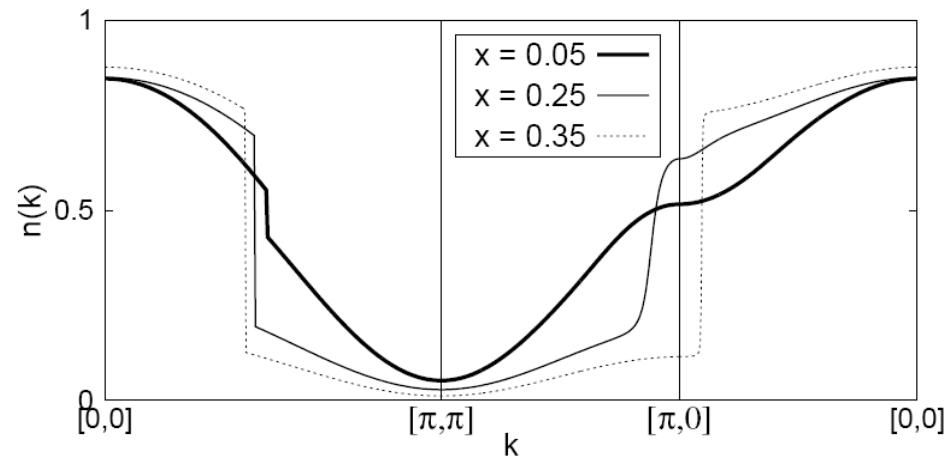
x-dependence of the Momentum distribution

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

"FS" topology change at $x \sim 0.2$; depends sensitively on t'/t



Expt: H. Ding, *et al*
PRL (1997)



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)

BCS answer: $G_{11}^{\text{BCS}}(\mathbf{k}, \omega) = \frac{\omega - \xi_{\mathbf{k}}}{\omega^2 + E_{\mathbf{k}}^2}$ $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$

$$G_{11}^{\text{BCS}}(\mathbf{k}, 0) = 0 \Rightarrow \xi_{\mathbf{k}} = 0 \quad (\text{but ... see below!})$$

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

↑
(1,1)-component of Nambu G

cf. Fermi surface in Landau's FLT $G(\mathbf{k}, 0) = \infty$

Unlike the normal Landau FL, the SC state "FS"...

$G(\mathbf{k}, 0) = 0$ does not enclose n electrons

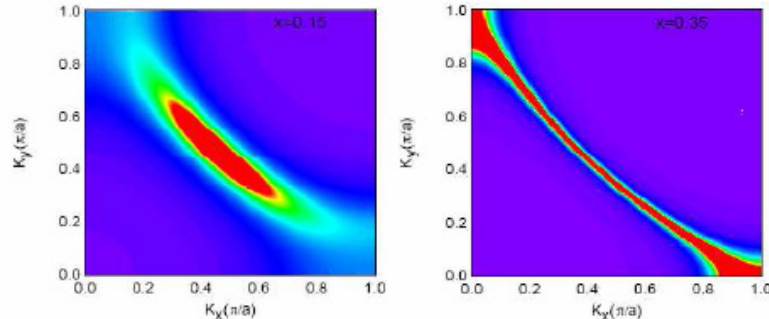
No Luttinger Sum Rule for state with ODLRO

$\Phi[\hat{G}]$ with $\delta\Phi/\delta\hat{G} = \hat{\Sigma}$

$$\int d\omega \sum_{\mathbf{k}} \text{Tr}\{\tau_3 \hat{G}\} = (n_{\uparrow} + n_{\downarrow})$$

"Number is
not conserved
in SC state"

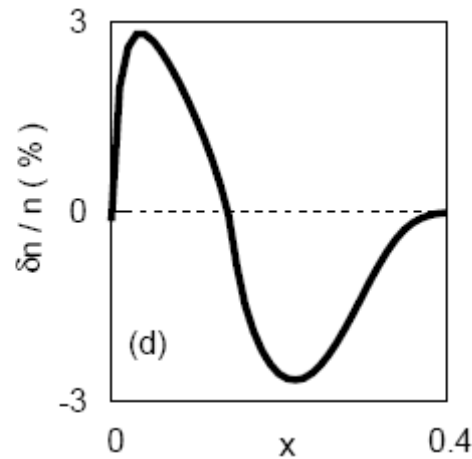
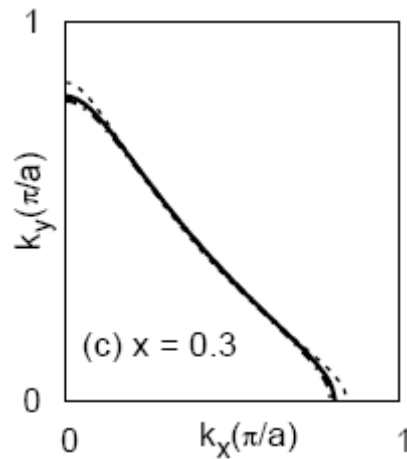
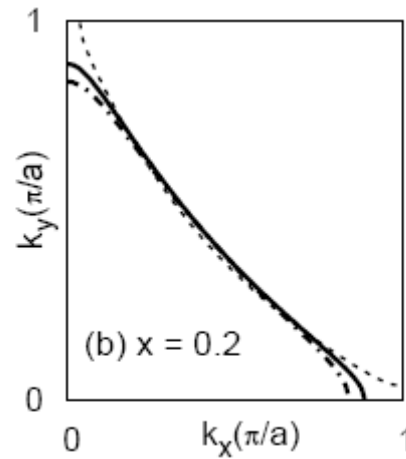
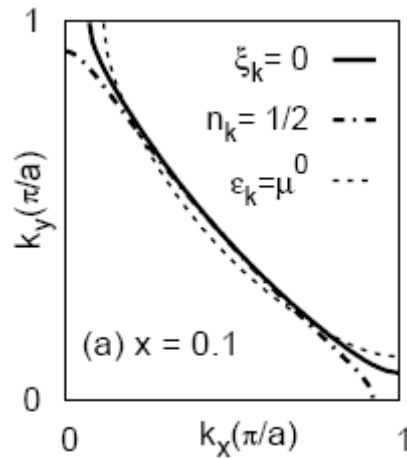
[Dzyloshinskii, PRB(2003)]



- 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

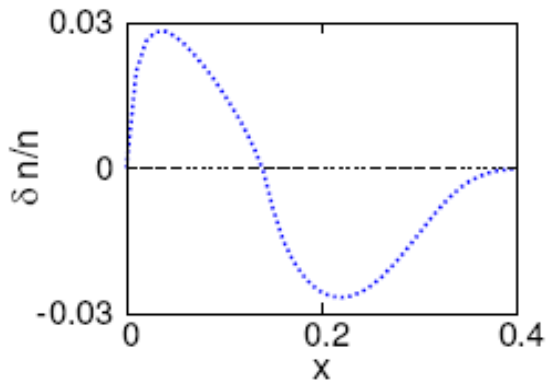
all of them violate the Luttinger count



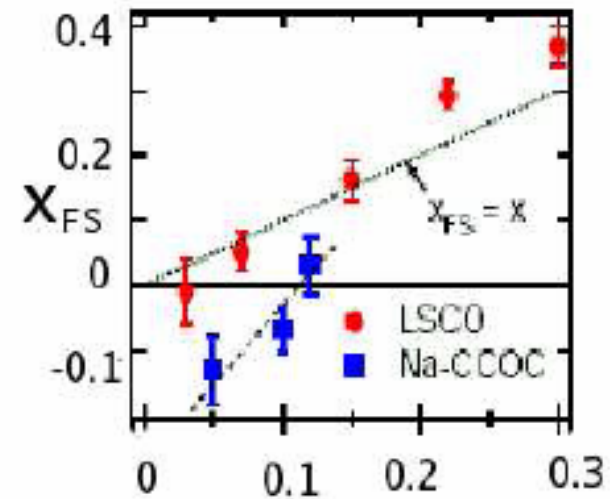
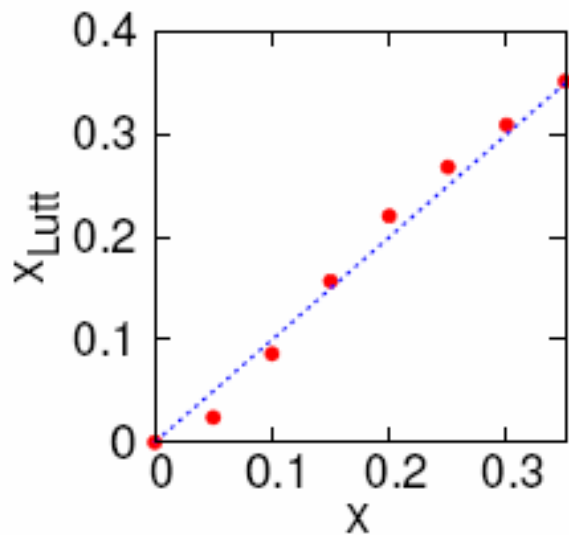
Size of violation

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

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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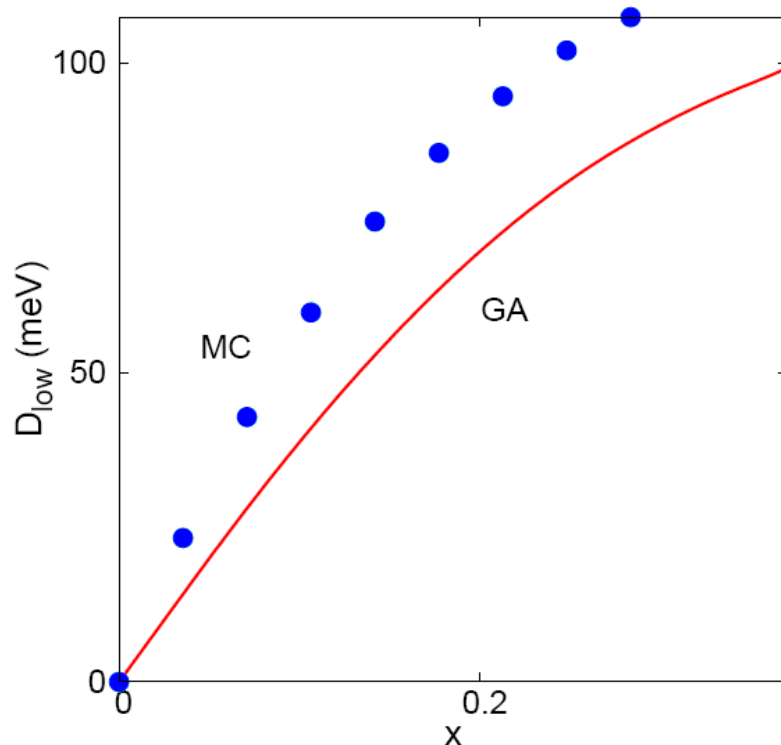
Optical Spectral Weight or Drude Weight

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

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

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

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



Upper Bound on Superfluid Density

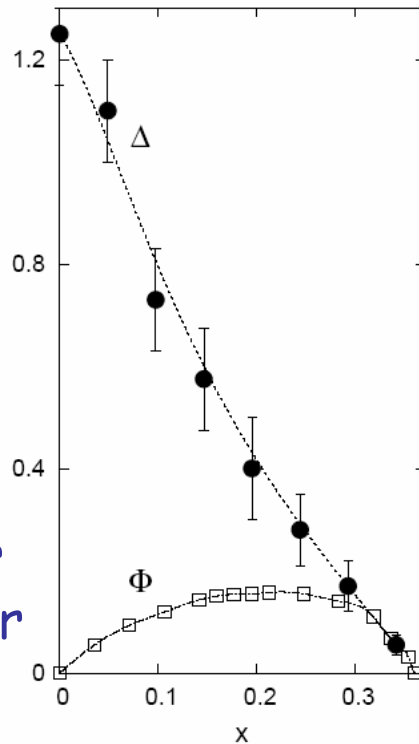
$$\rho_s \leq D_{\text{low}}$$

$$\Rightarrow \rho_s \rightarrow 0$$

$$\text{as } x \rightarrow 0$$

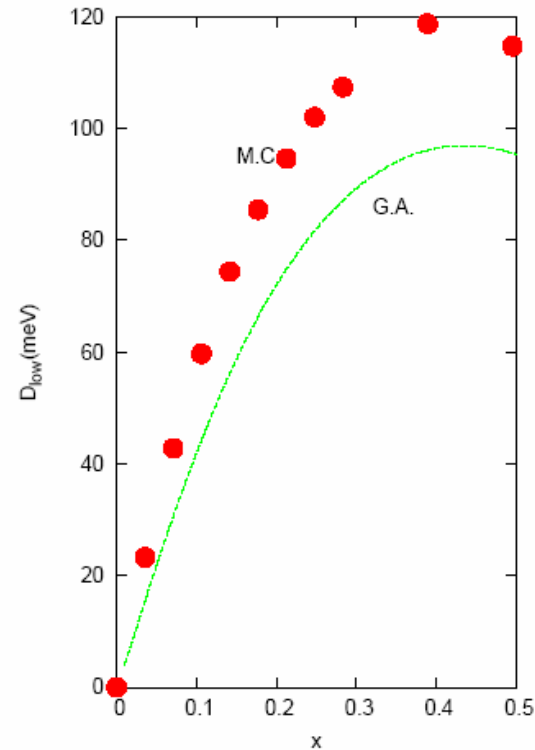
Implications of SC state results for Pseudogap: ³⁵

Energy Gap



SC Order parameter

Superfluid density:



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

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

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

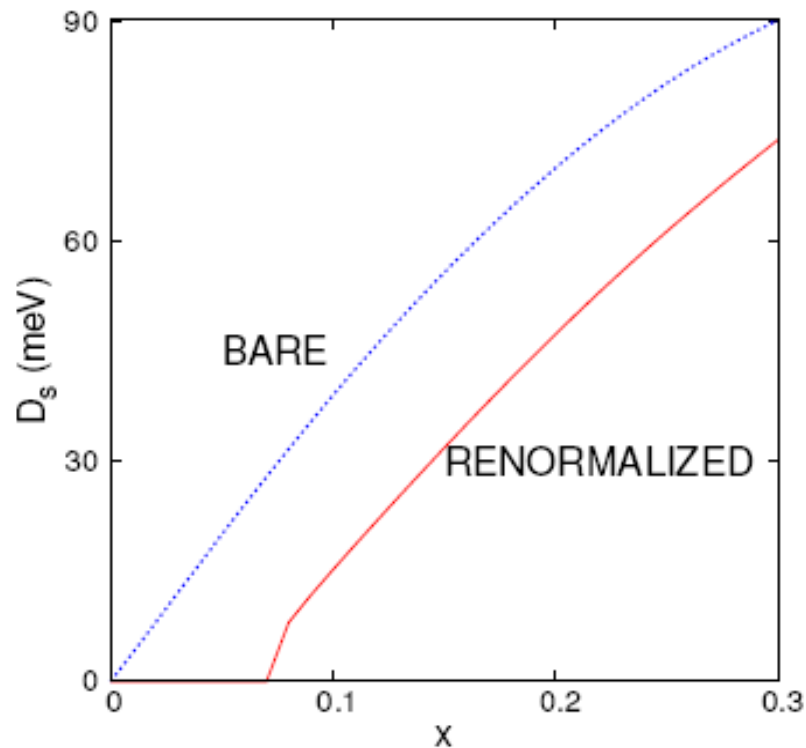
Emery & Kivelson, Nature (1995)

Pairing Pseudogap: MR *et al*, PRL (1992); Trivedi & MR, PRL (1995)

Effect of Long-Wavelength Quantum Phase Fluctuations:

T= 0 Self-Consistent
Harmonic Approximation

Paramekanti, MR,
Ramakrishnan & Mandal
PRB (2000)



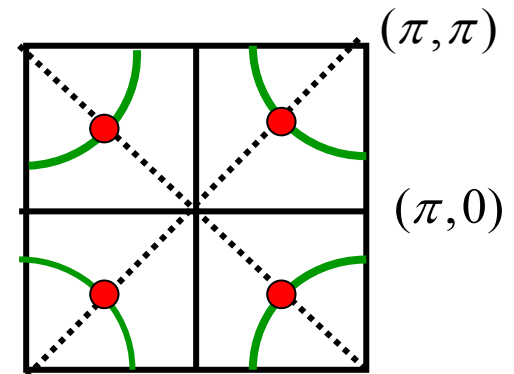
$$\rho_s = \rho_s^0 \exp \left(-\langle \delta\theta^2 \rangle / 2 \right)$$

T-dependence of Superfluid density $(T \ll T_c)$

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

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

$\rho_s(0, x)$ ← doping dependence
near Mott insulator



T-dependence from **nodal QPs**

Nodal QP dispersion

$$E_{\mathbf{k}} \approx \sqrt{(v_F \delta k_{\perp})^2 + (v_2 \delta k_{\parallel})^2}$$

$j = \alpha e v_F$ ← 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

α = "Effective charge" of QP

tJ Monte Carlo

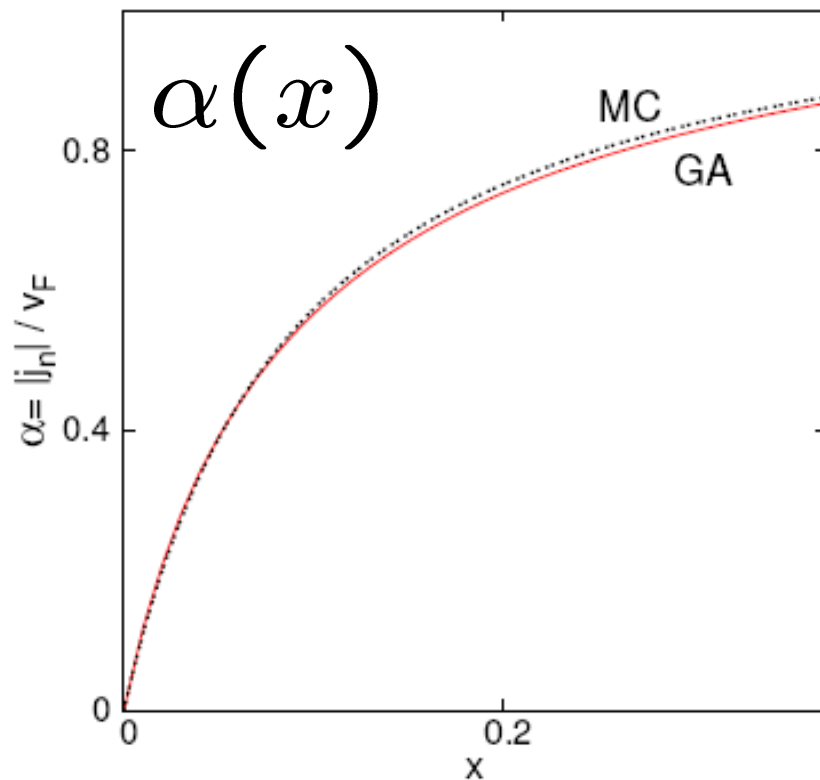
Nave, Ivanov & P.A.Lee, PRB (2005)

our Gutzwiller Approximation result for tJ model:

$$J_{nqp} = e Z v_F^0$$

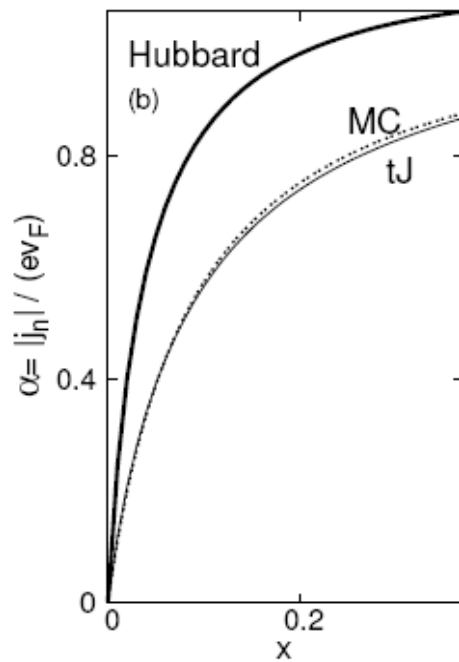
$$\alpha \approx g_t / (g_t + 1/6)$$

$$= x / (1.08x + 0.08)$$

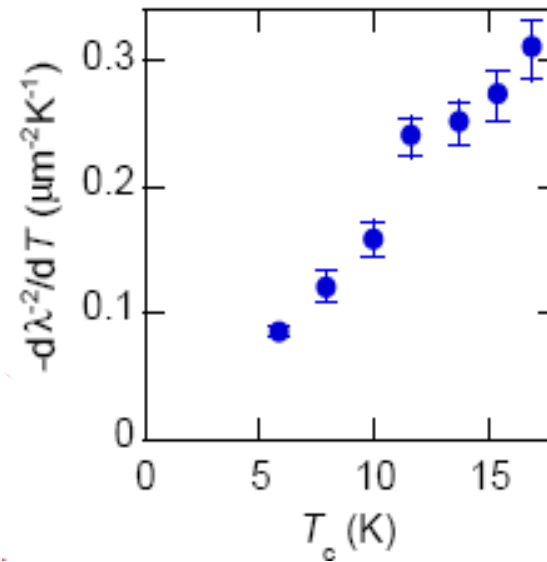
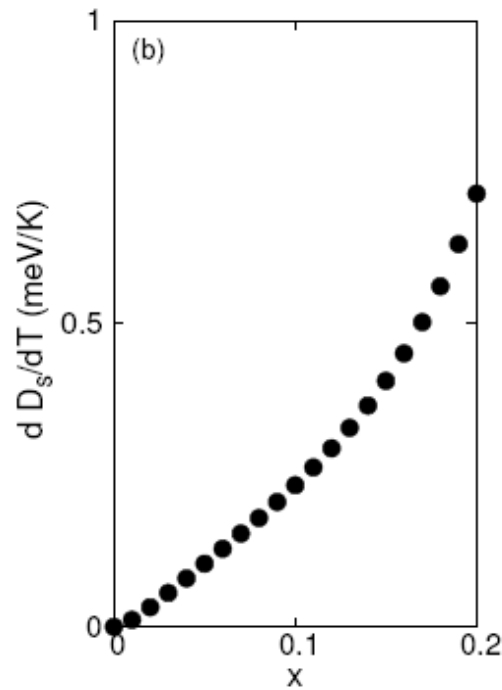


Slope of SF density:

$$\alpha(x)$$



$$d\rho_s/dT$$



UBC YBCO data
Broun et al,
cond-mat/0509223

Outline:

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

Why are HTSC's so robust against disorder?

- * (most) impurities lie off CuO_2 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

Arti Garg, N. Trivedi & MR, cond-mat/0609666

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:

- fewer low-energy excitations
- robust nodal QPs - "V" in DOS protected
 - nodes in k-space protected

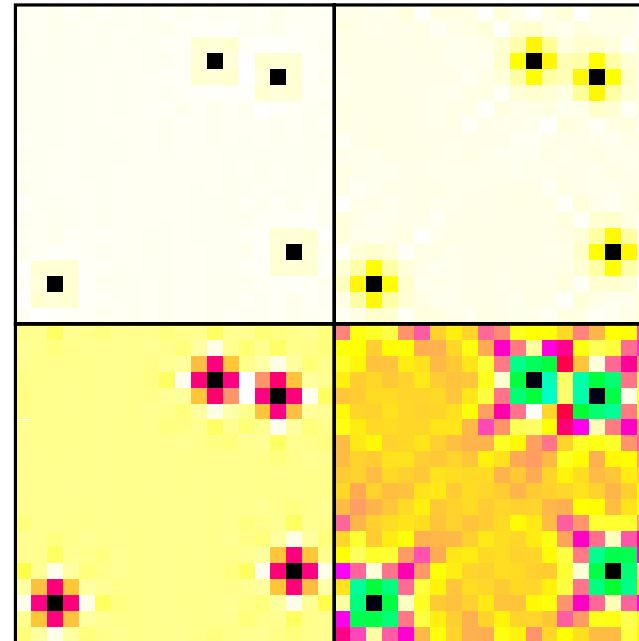
Response to weak (Born) impurities:

Local density

$n(i)$

Correlations
+ disorder

Only
disorder



$$\langle n \rangle = 0.8$$

$$n_{imp} = 0.01$$

$$V_{imp} = t$$

Local d-wave
Pairing amplitude

$\Delta(i)$

Short healing
length in
correlated system

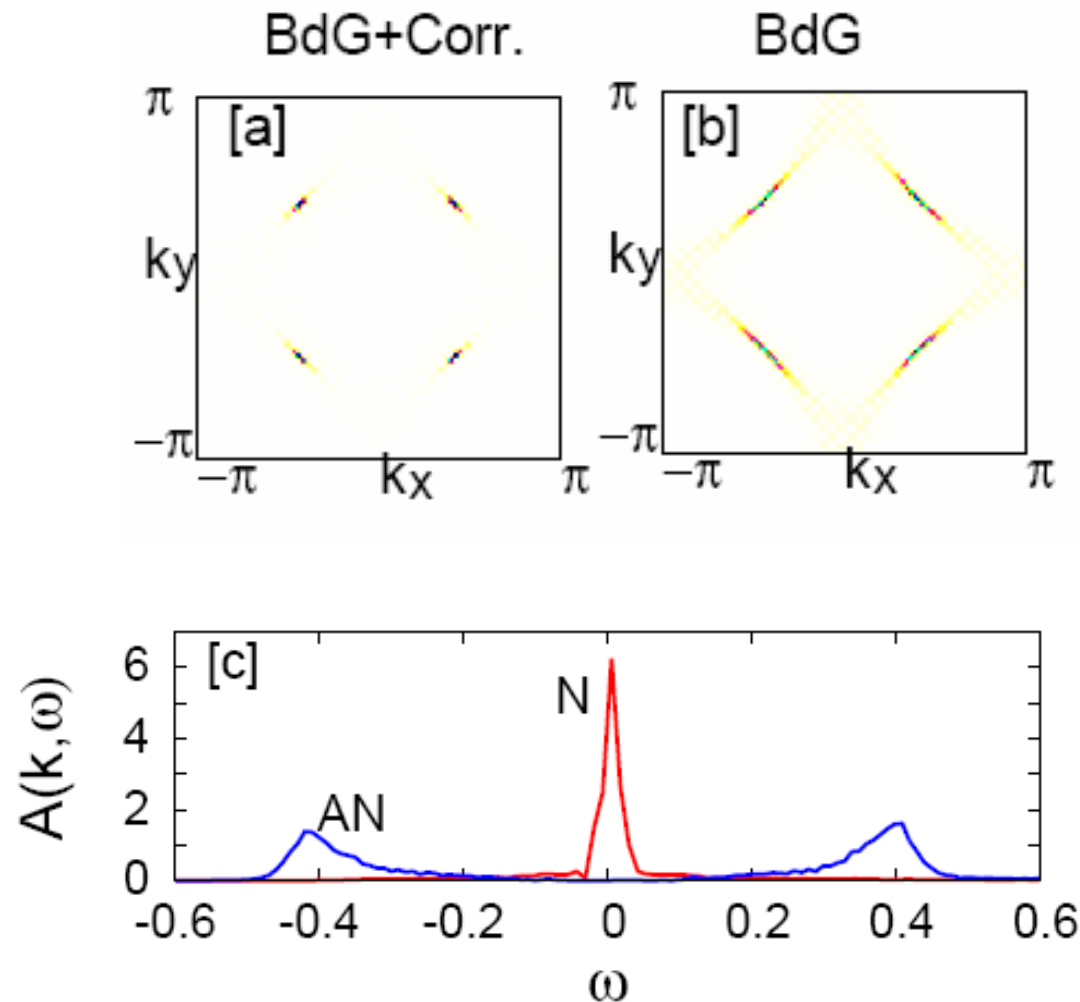
Impurity potential is
renormalized by interactions

Longer healing Length
in calculation which
ignores correlations

Where do the low energy excitations live?

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

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

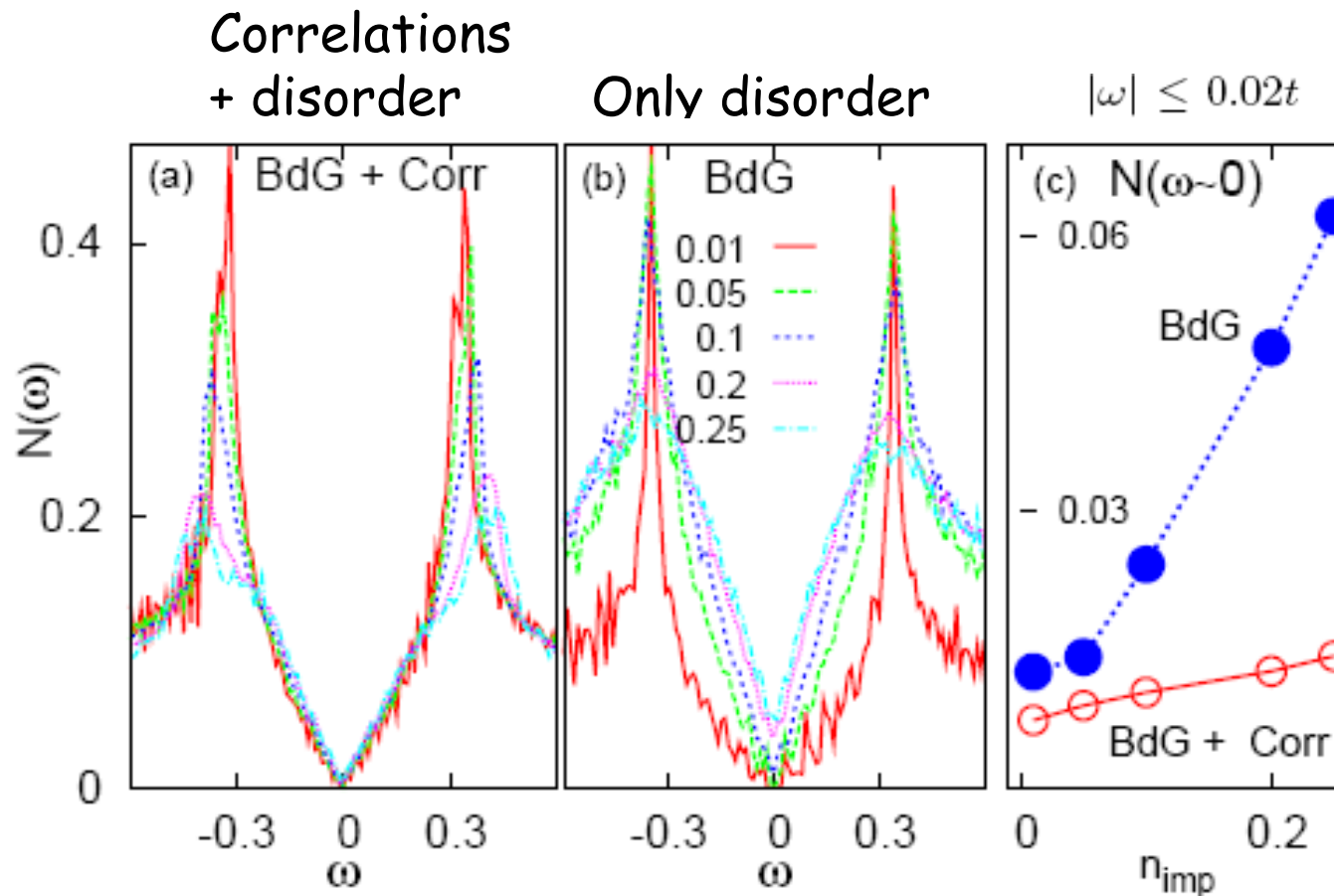


$$A(\mathbf{k}, |\omega| \leq 0.02)$$

Nodes are
protected

Nodal QPs much
less affected by
Disorder than the
Antinodal QPs

Spatially averaged DOS



In the correlated system

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

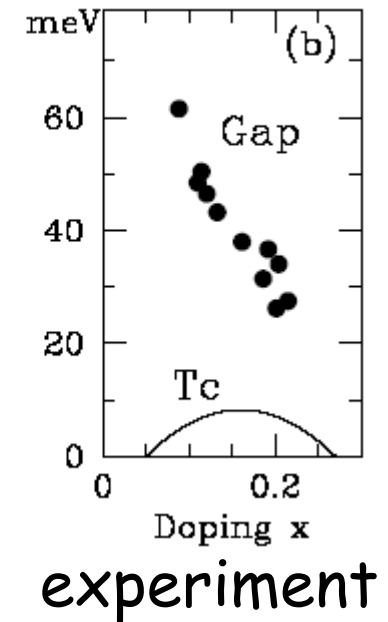
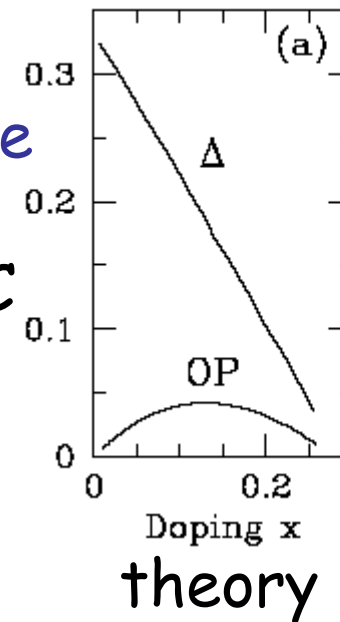
Summary: SC in doped Mott insulators

- 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)

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

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

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

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

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

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

Gutzwiller Approximation:

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

approximation scheme to analytically
evaluate matrix elements in Projected states

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

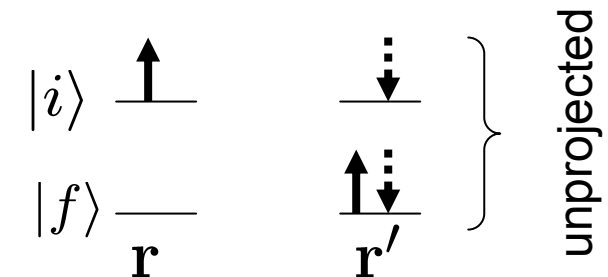
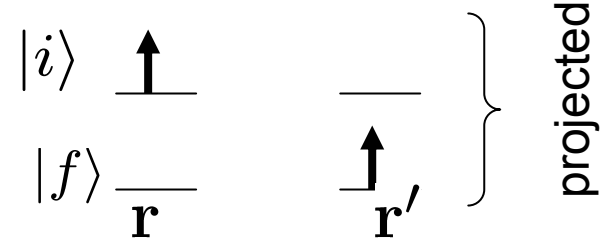
examples:

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

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

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

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



Singularities of Spectral Moments & Gapless QPs

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

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

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

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

Jump discontinuity: k_F & Z

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

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

Slope discontinuity: V_F