Simulations of strongly interacting Fermions and Bosons in Optical Lattices

Nandini Trivedi
The Ohio State University
trivedi@mps.ohio-state.edu

Hubbard Models simulated using Quantum Monte Carlo methods

1) World line QMC for bosons at zero and finite T

   Y. Kato, N. Kawashima, and N. Trivedi

2) Determinantal QMC for attractive fermions with equal fermion populations at finite T

   B. Peters, M. Randeria, R. Scalettar and N. Trivedi

3) Variational MC at T=0 with RVB wave functions for repulsive fermions with equal populations

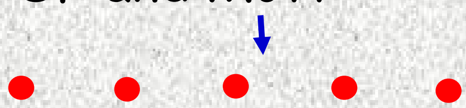
   A. Paramekanti, M. Randeria and N. Trivedi;

   S. Pathak, V. Shenoy, M. Randeria and N. Trivedi

Optical Lattices: Tune well depth
1-band Hubbard Models: tune t/|U|

BHM

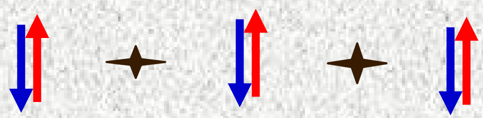
MFT gets phases
SF and Mott



QMC: quantitative insights

FHM: U<0

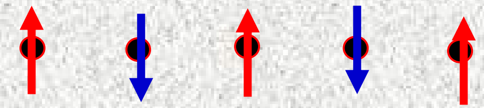
MFT:
s-SF and CDW



QMC reveals
reveals pseudo gap

FHM:U>0

AF-Mott



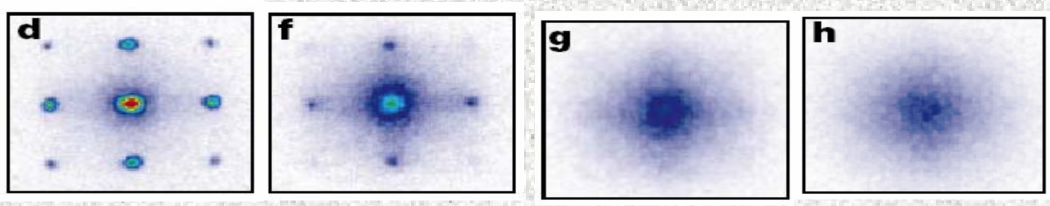
Multiple MFTs:

Dynamical MFT
Density Matrix RG on strips

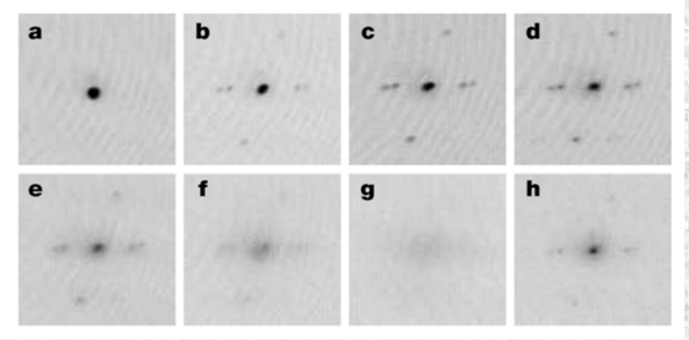
Standard QMC: limited
To high temperature

VMC (T=0): tremendous qualitative and quantitative insight

big questions



Bosons



Attractive Fermions

Understanding of quantum and thermal fluctuations

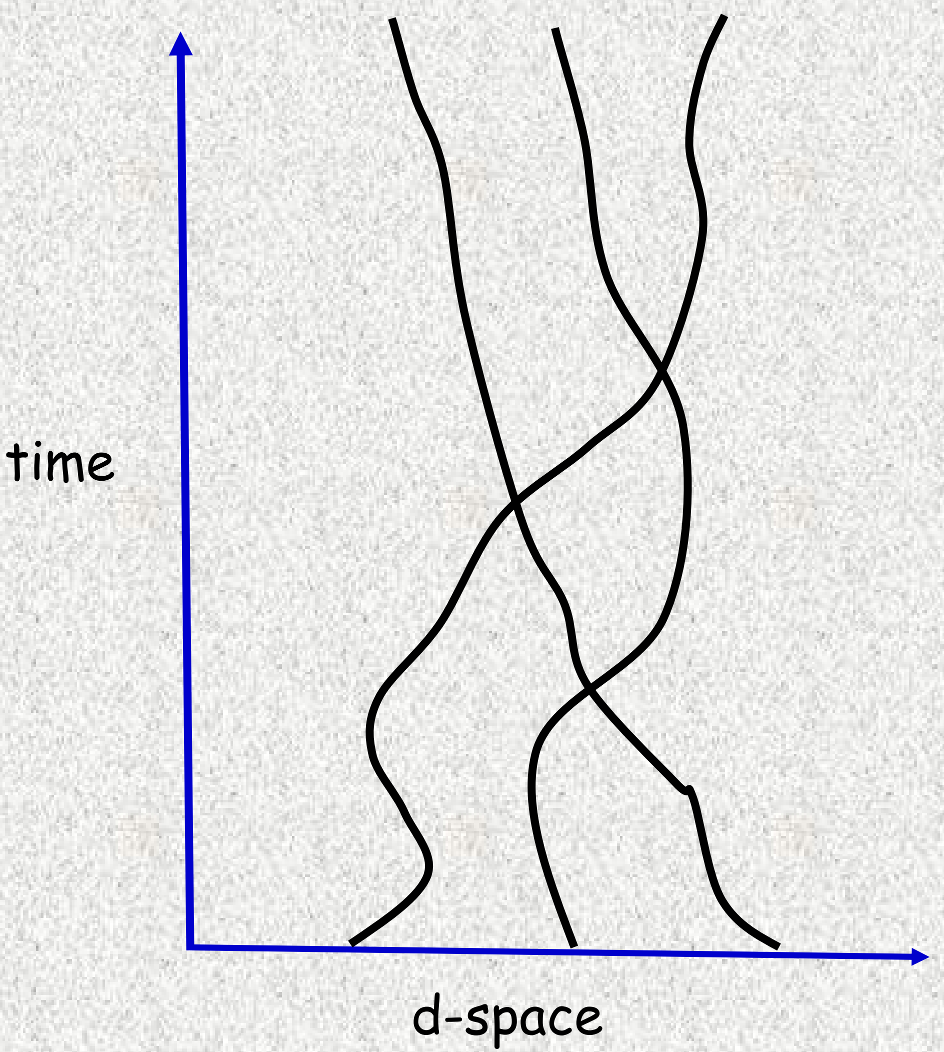
Is there a superfluid phase in the positive U Hubbard model?

Is there a pseudogap phase at T=0?

Bose Hubbard Model

World Lines

Path integrals in configuration / occupation basis



$$Z = \sum_{\substack{\text{spaghetti} \\ \text{configurations}}} e^{-\beta H}$$

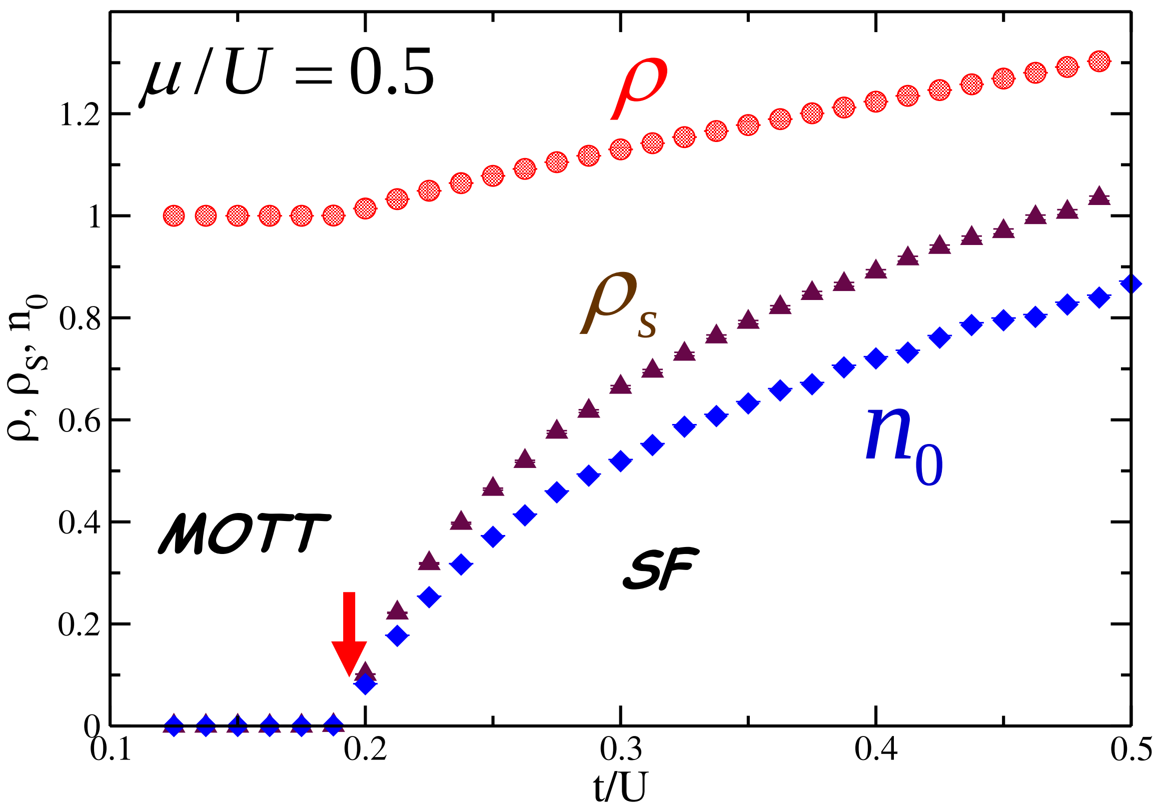
Sample the configurations using Monte Carlo

Method is "exact" with only statistical errors

Prokofeev, Troyer and collaborators
Sorensen and collaborators
Batrouni and collaborators

Superfluid-Mott Insulator Transition: Bose Hubbard Model in 3D

$$\mathcal{H} = -\frac{t}{z}\sum_{\langle i,j\rangle}\left(\phi_i^\dagger \phi_j + \phi_i \phi_j^\dagger\right) + \frac{u}{2}\sum_i n_i(n_i - 1) - \mu\sum_i n_i,$$



ge t: SF with $\rho_s \approx \rho$

all t: Mott with $\rho = 1$

$\rho_s = 0$

$N = 24 \times 24 \times 24$

$T \approx 0$

Also have results in 2D

$$\left(\frac{t}{U}\right)_c = 0.195$$

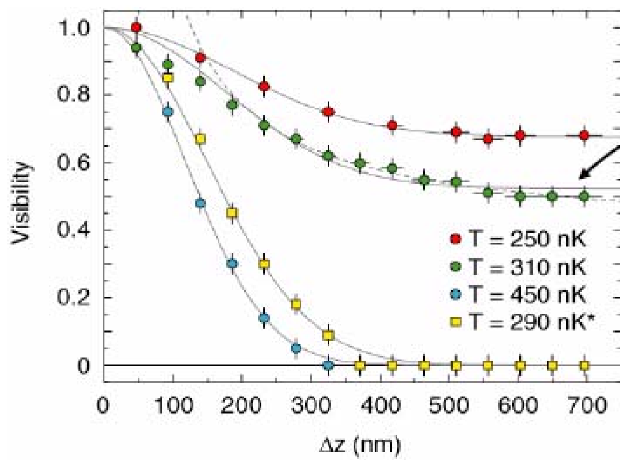
d NT, preprint

See also Prokofeev and collaborators

Measuring SF order parameter

$$\left\langle \phi^{+}(0,\tau)\phi(r,\tau)\right\rangle$$

Spatial Correlation Function of a Trapped Bose Gas



Constant correlation function indicates the presence of long-range phase coherence !

temperature	thermal de Broglie wavelength		measured width
250 nK	373±15 nm	<<	463±16 nm
310 nK	335±11 nm		428±26 nm
nK	278±6 nm	<	294 ± 6 nm
nK	346±12 nm		372±8 nm

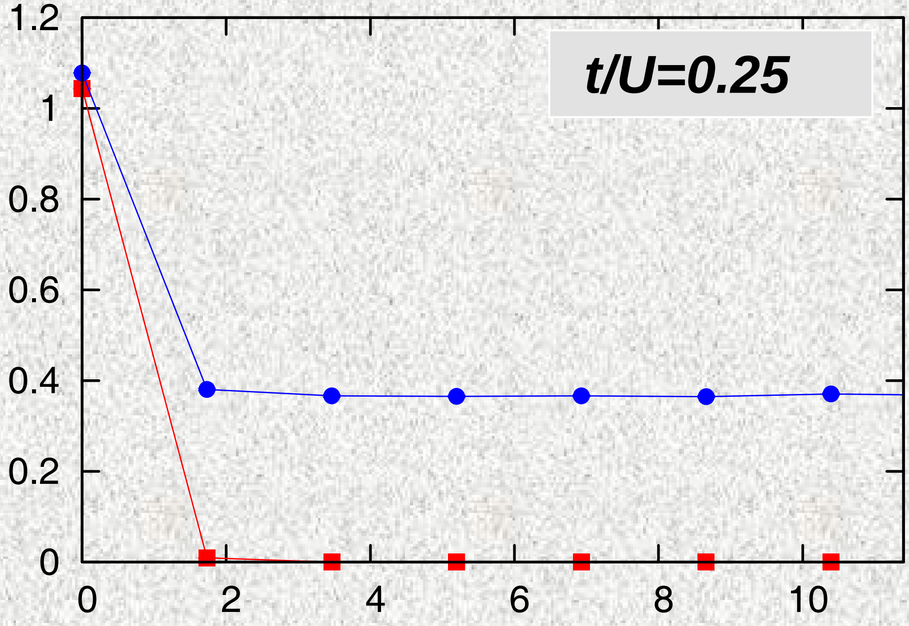
änsch, and T. Esslinger, Nature 403, 166 (2000).

$$\rho(\mathbf{r},\mathbf{r}') = \left\langle \hat{\Psi}^{+}(\mathbf{r}), \hat{\Psi}(\mathbf{r}')\right\rangle \rightarrow \frac{N_0}{V} \qquad \text{for} \qquad |\mathbf{r},\mathbf{r}'| \rightarrow \infty$$

Condensate fraction

Order parameter correlations

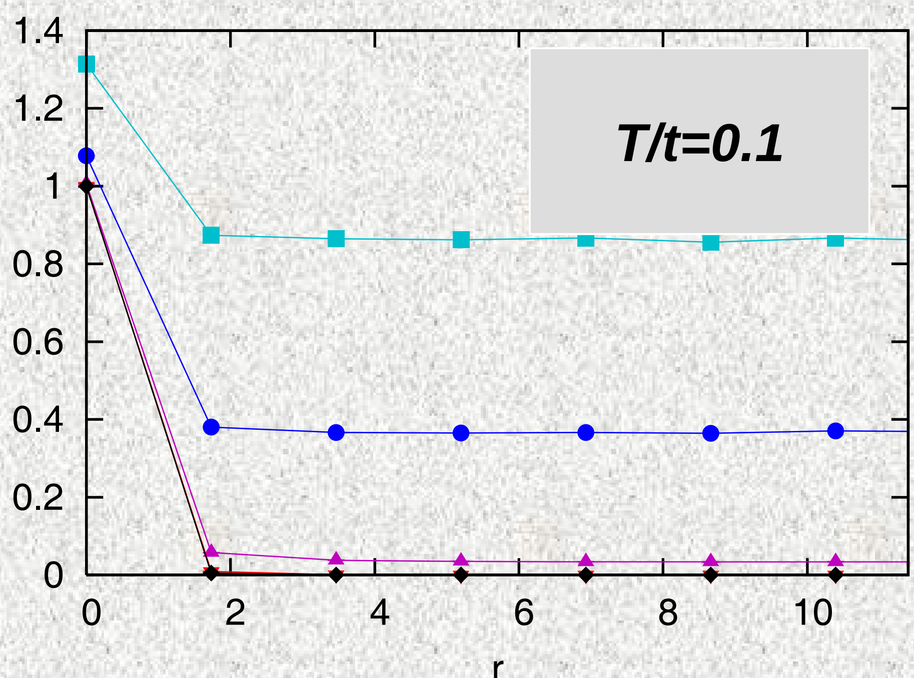
$$\left\langle \phi^{+}(0,\tau)\phi(r,\tau) \right\rangle$$



T/t=0.1

T/t=2.0

Order parameter suppressed by thermal fluctuations

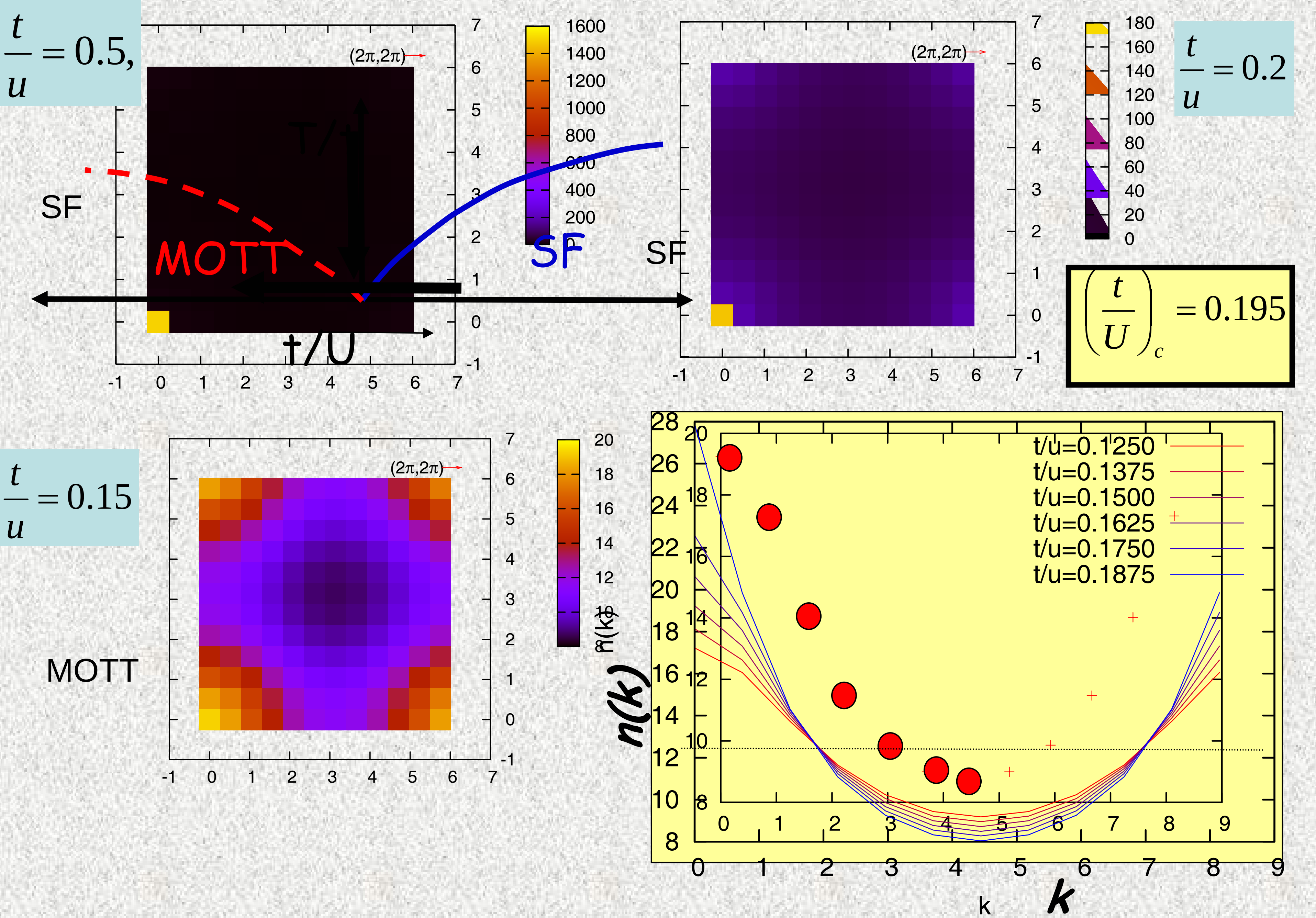


t/U=0.5

t/U=0.25

t/U=0.195

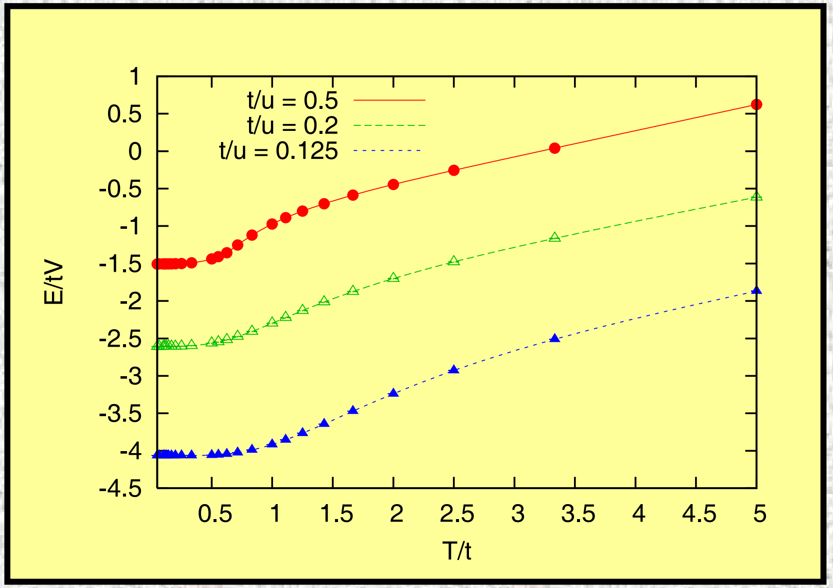
Order parameter suppressed by quantum fluctuations

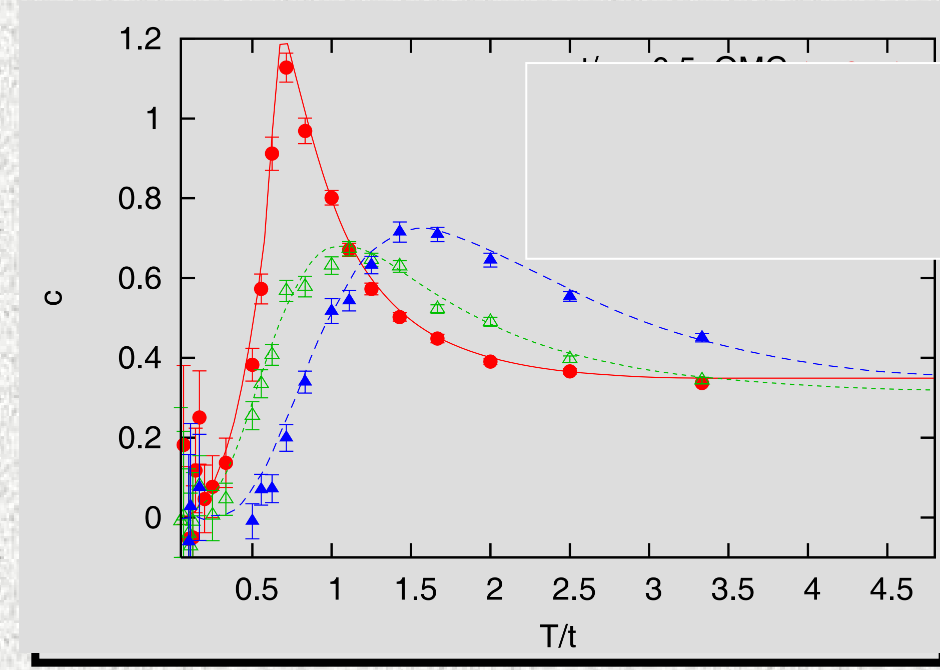


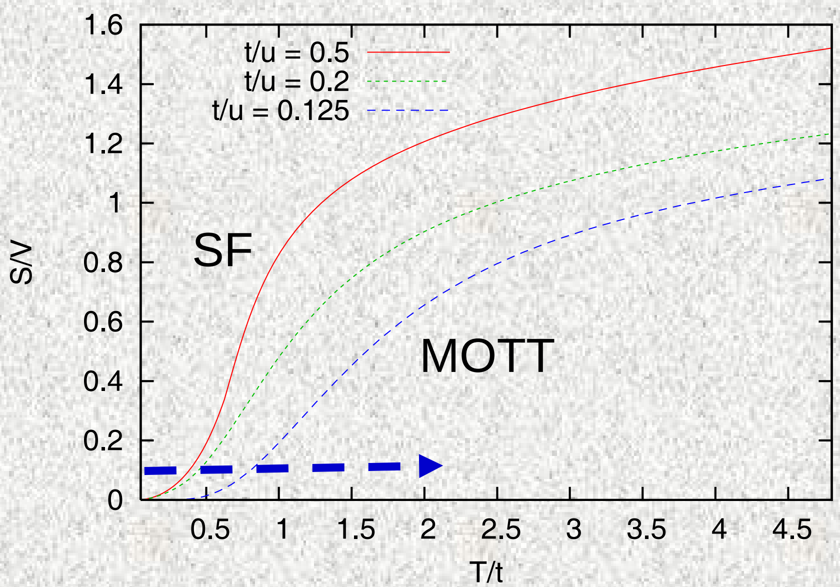
$\frac{t}{u} = 0.5,$
(2π,2π)
SF
MOTT
T/t
t/U
SF
SF
$\frac{t}{u} = 0.2$
$\left(\frac{t}{U}\right)_c = 0.195$
$\frac{t}{u} = 0.15$
(2π,2π)
MOTT
n(k)
t/u=0.1250
t/u=0.1375
t/u=0.1500
t/u=0.1625
t/u=0.1750
t/u=0.1875
k
k

How to determine Temperature in an interacting system?

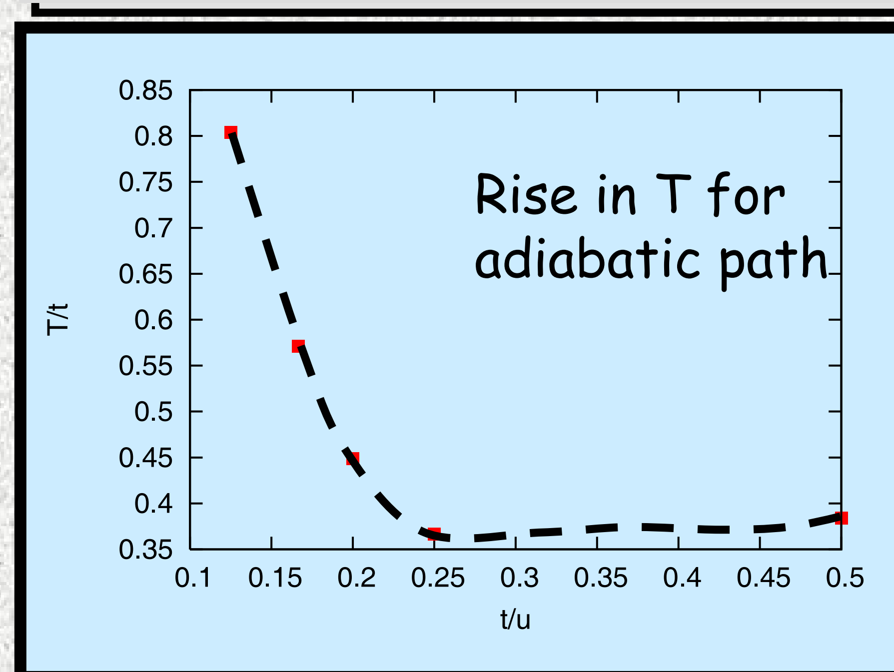
$S(T/t, t/U)$







Adiabatic path



Fermion Hubbard Model U<0

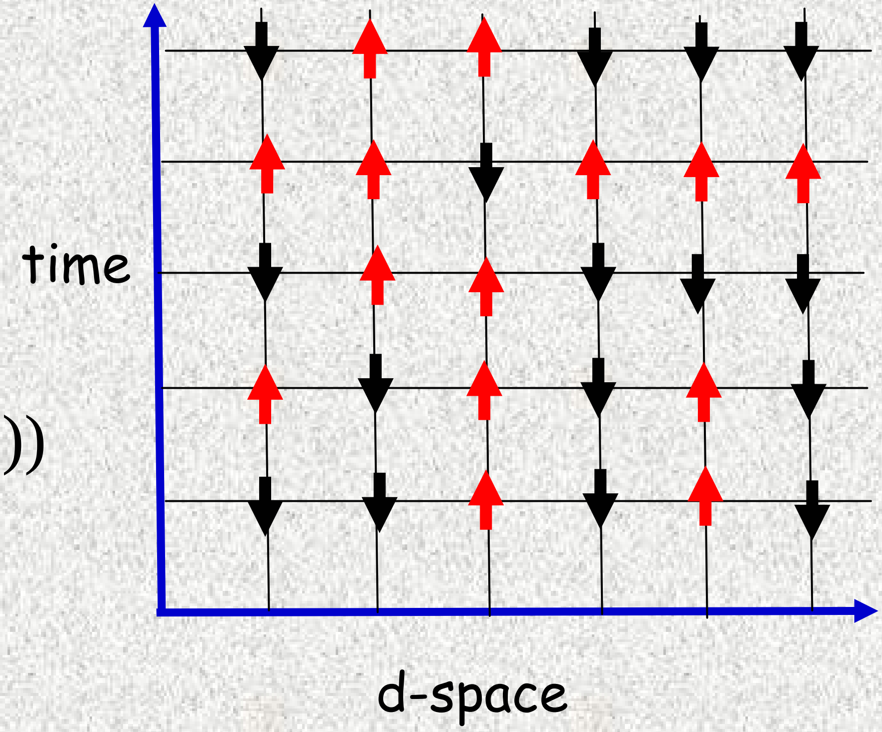
Fermion Hubbard Model U<0

Technique:Coherent State Path Integral→Determinantal QMC

- exact evaluation of density matrix with only statistical errors
- equal populations

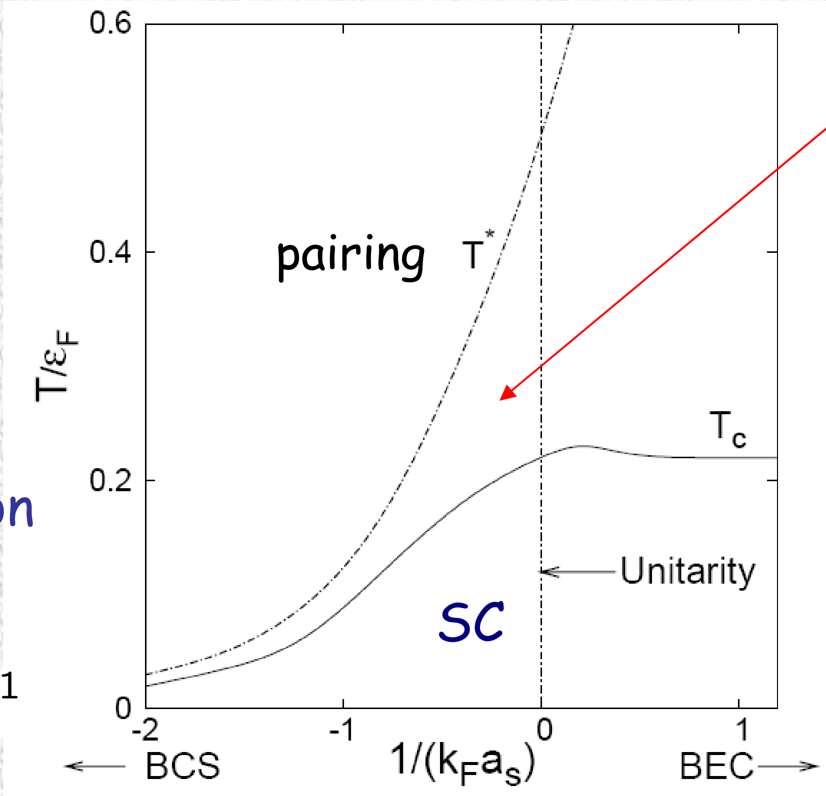
Sample configurations of $\{S_i(\tau)\}$ using Monte Carlo with probability

$$Z = \sum_{\{S_i(\tau)\}} Det(M_{\uparrow}(S))Det(M_{\downarrow}(S))$$



Scalapino and collaborators

How do the properties of a system evolve from a normal FLto a Bose Liquid : Pseudogap

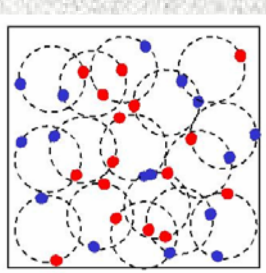


"attraction" →

pseudogap

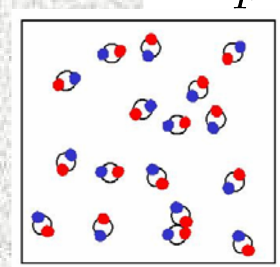
Normal
Fermi liquid

BCS regime:
- weak attraction
- cooperative Cooper pairing
- pair size $\gg k_F^{-1}$

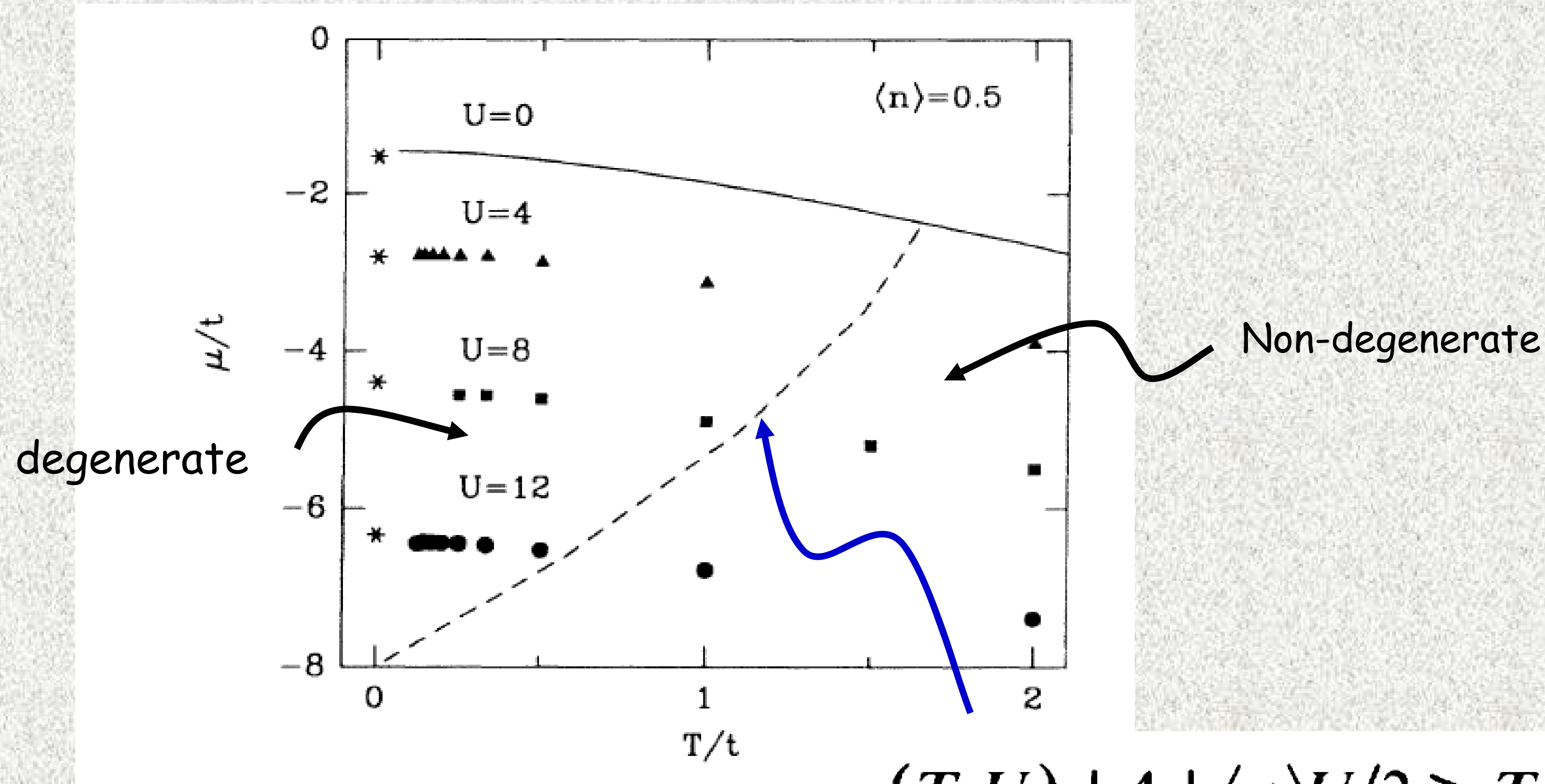


Normal
Bose liquid

BEC regime:
- strong attraction
- condensate of tightly bound molecules
- pair size $\ll k_F^{-1}$

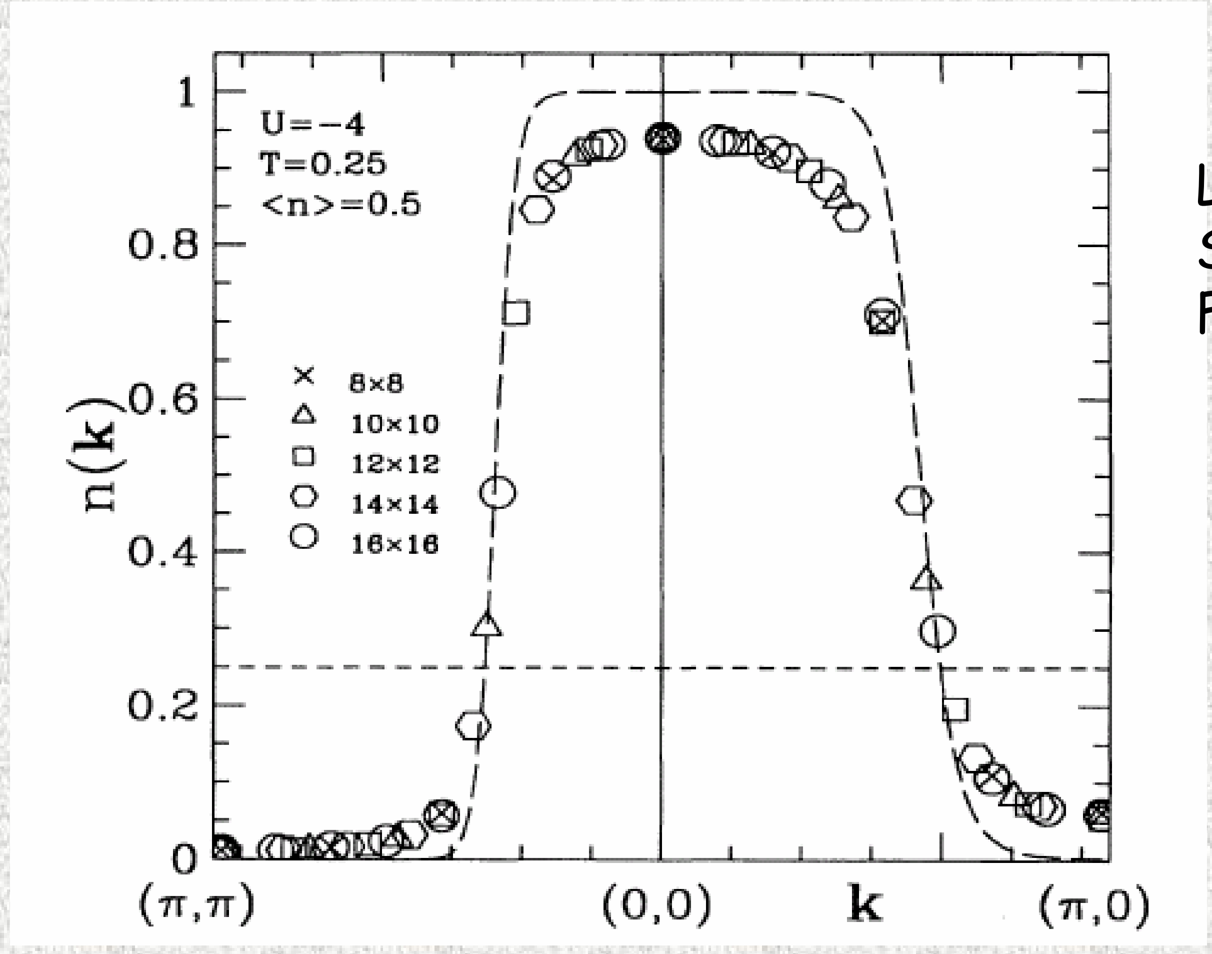


Leggett (80) Nozieres & Schmitt-Rink (85)
Randeria in "Bose-Einstein Condensation" ('95)



$$\mu(T,U)+4+\langle n\rangle U/2>T$$

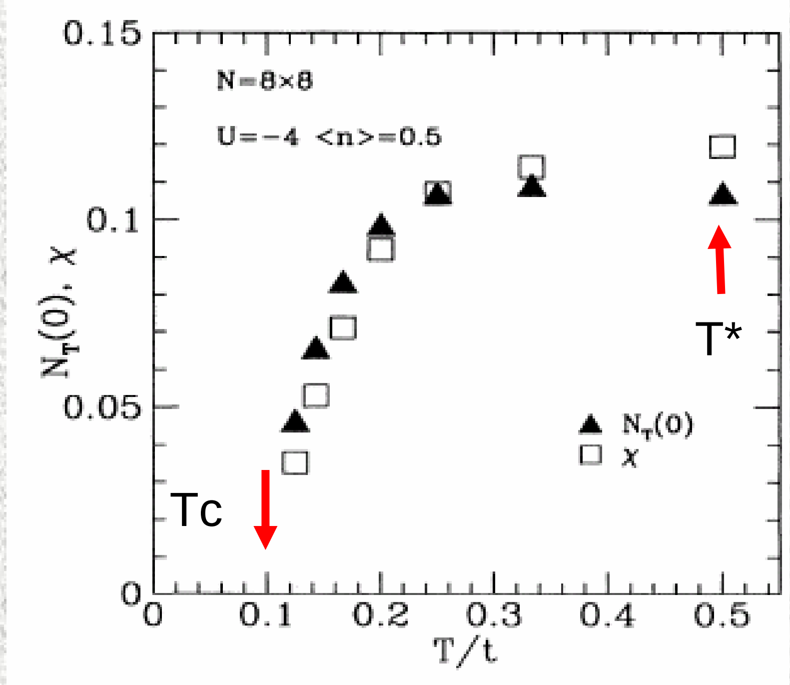
Momentum distribution function



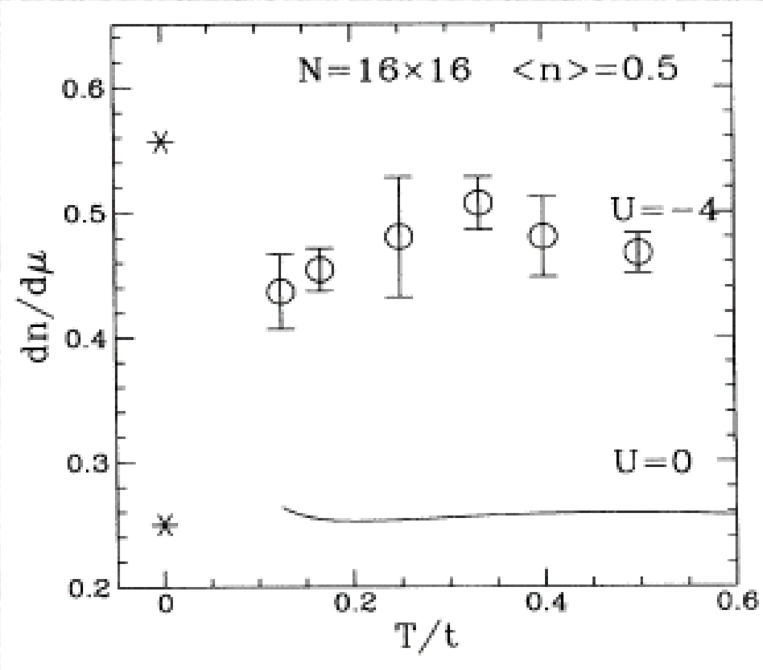
Looks rather boring:
Slightly broadened
Fermi distribution

FIRST EVIDENCE OF PSEUDOGAP

Spin susceptibility



compressibility



Randeria, Trivedi, Scalettar, Moreo;
PRL 69, 2001 (1992)

Trivedi and Randeria PRL 75, 312 (1995)

Pseudogap State: (1) Suppression of low energy density of states below T*
(2) Opening of gap in low energy spin spectrum below T*
(3) T-independent Compressibility; does not follow the spin susceptibility

c.f. Fermi Liquid $\chi \sim N(\varepsilon_F)$ $\kappa \sim N(\varepsilon_F)$ Both equal and independent of T

Probing density and spin correlations

$$C_{\uparrow\uparrow} = \frac{1}{N}\sum_{rr'}\left\langle n_{r\uparrow} n_{r'\uparrow}\right\rangle$$

$$C_{\uparrow\downarrow} = \frac{1}{N}\sum_{rr'}\left\langle n_{r\uparrow} n_{r'\downarrow}\right\rangle$$

$$\boxed{\kappa} = \frac{1}{n^2}\frac{\partial n}{\partial \mu} = \frac{2\beta}{n^2}\boxed{[C_{\uparrow\uparrow} + C_{\uparrow\downarrow}]} - \beta N$$

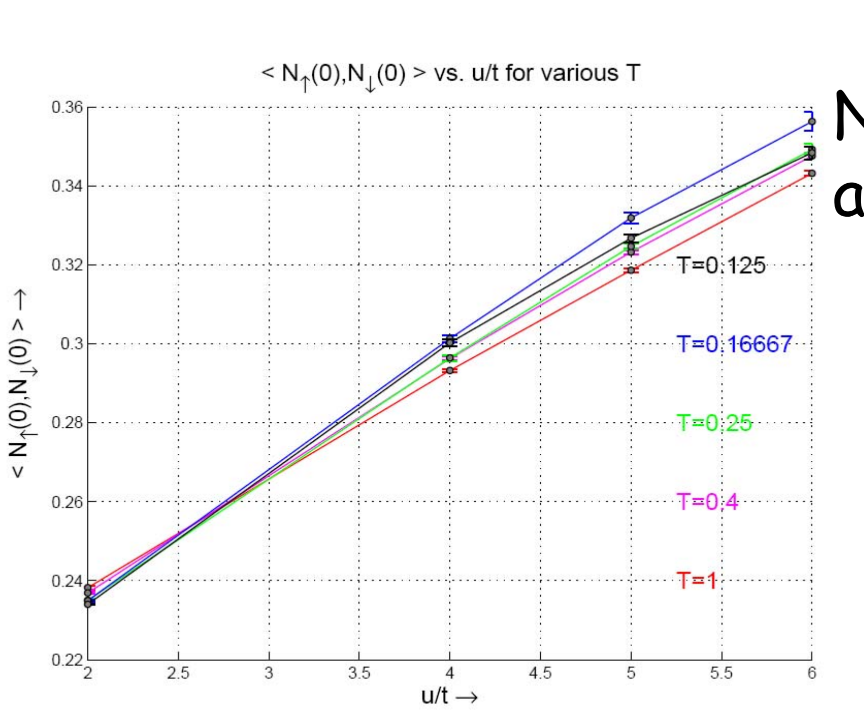
Charge channel: compressibility

$$\chi = \frac{\beta}{N}\sum_{rr'}\left\langle S_r^z S_{r'}^z\right\rangle$$

$$S_r^z = n_{r\uparrow} - n_{r\downarrow}$$

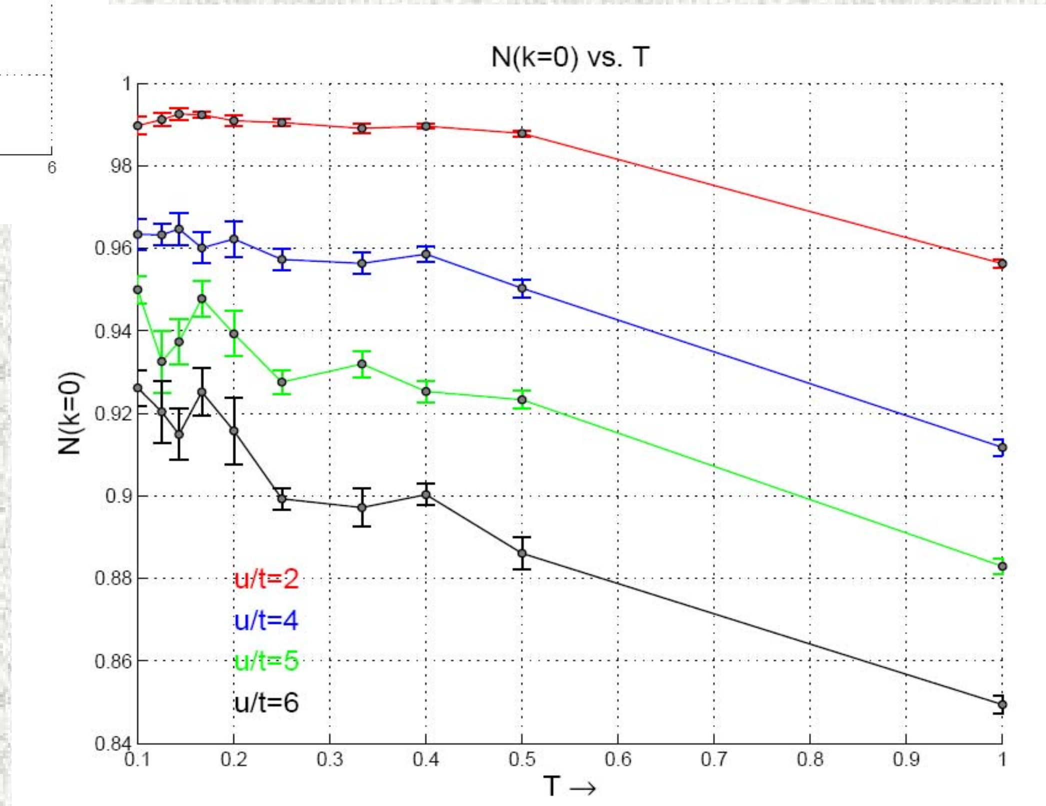
$$\boxed{\chi} = 2\beta\boxed{[C_{\uparrow\uparrow} - C_{\uparrow\downarrow}]}$$

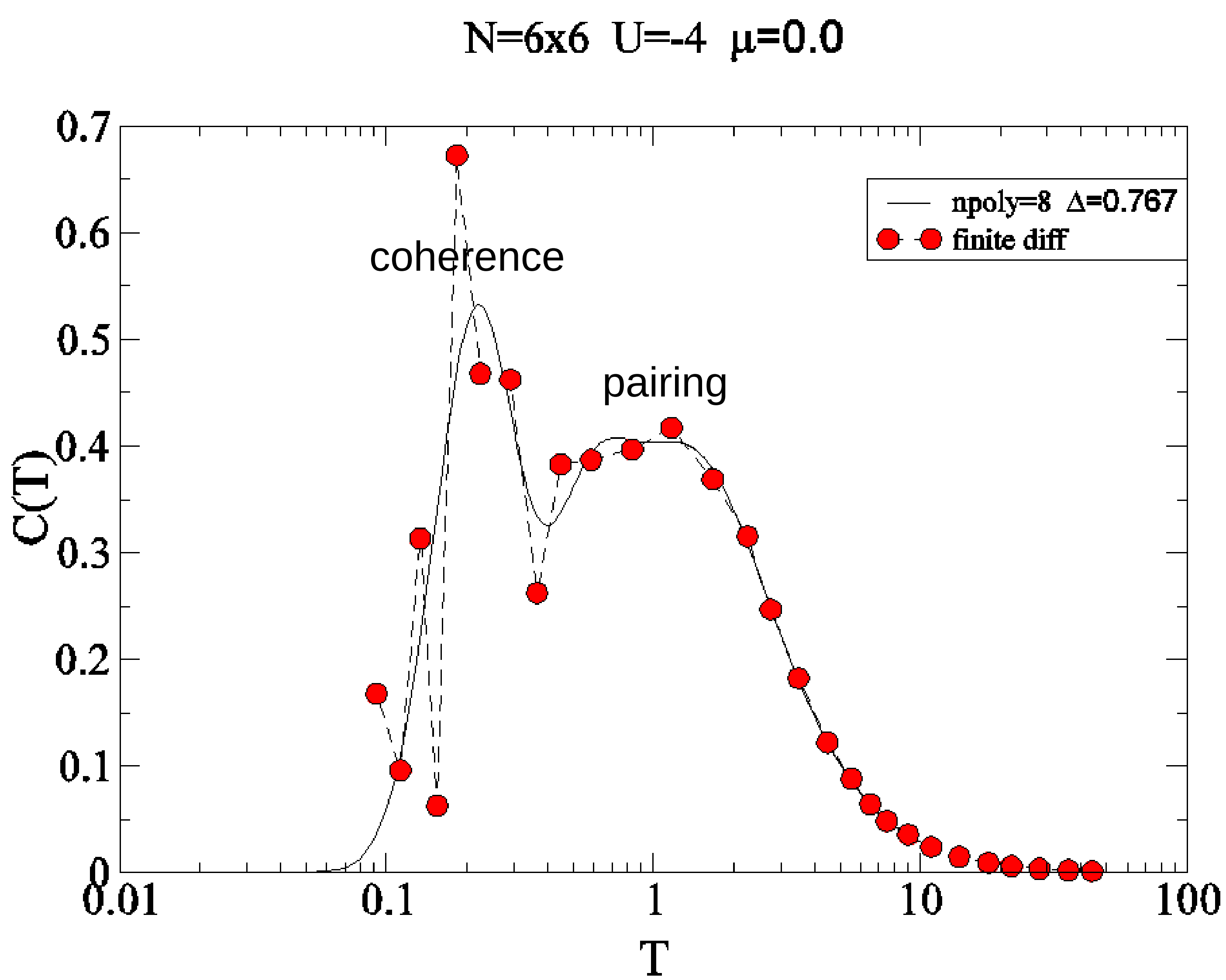
Spin channel: susceptibility



Number of doubly occupied sites as a function of U

Momentum distribution at k=0 as a function of T and U



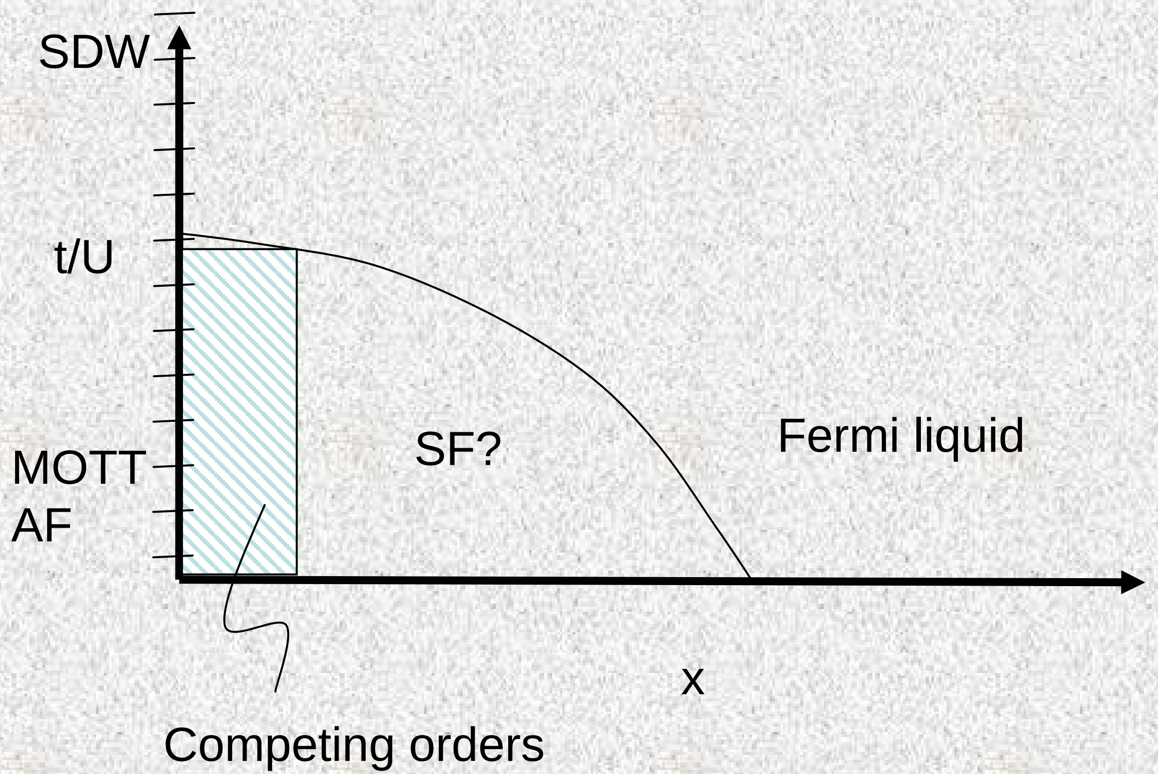


N=6x6 U=-4 μ=0.0
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
C(T)
0.01
0.1
1
10
100
T
npoly=8 Δ=0.767
finite diff
coherence
pairing

Fermion Hubbard Model U>0

Square lattice

What is the phase diagram?



Repulsive Fermion Hubbard model

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

repulsion

Large U/t : charge fluctuations are frozen and spin physics emerges

$$J \approx \frac{t^2}{U}$$

$$H_J = J \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \left(\mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}'} - \frac{1}{4} n_{\mathbf{r}} n_{\mathbf{r}'} \right)$$

$$B^{\dagger}_{\mathbf{r},\mathbf{r}'} \equiv c^{\dagger}_{\mathbf{r},\uparrow} c^{\dagger}_{\mathbf{r}',\downarrow} - c^{\dagger}_{\mathbf{r},\downarrow} c^{\dagger}_{\mathbf{r}',\uparrow}$$

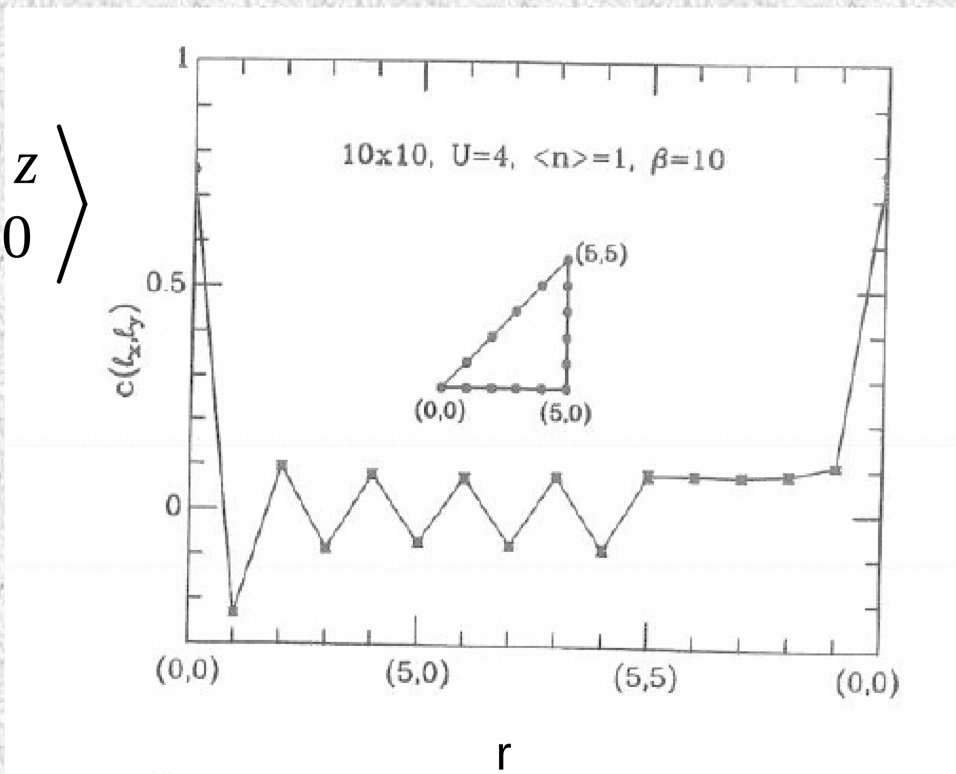
Singlet bond operator

$$H_J = -\frac{J}{2} \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} B^{\dagger}_{\mathbf{r},\mathbf{r}'} B_{\mathbf{r},\mathbf{r}'} = J \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \left(\mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}'} - \frac{1}{4} n_{\mathbf{r}} n_{\mathbf{r}'} \right)$$

Attraction
D-wave channel
Pairing scale J

Antiferromagnetism

$$\left\langle S_r^z S_0^z \right\rangle$$

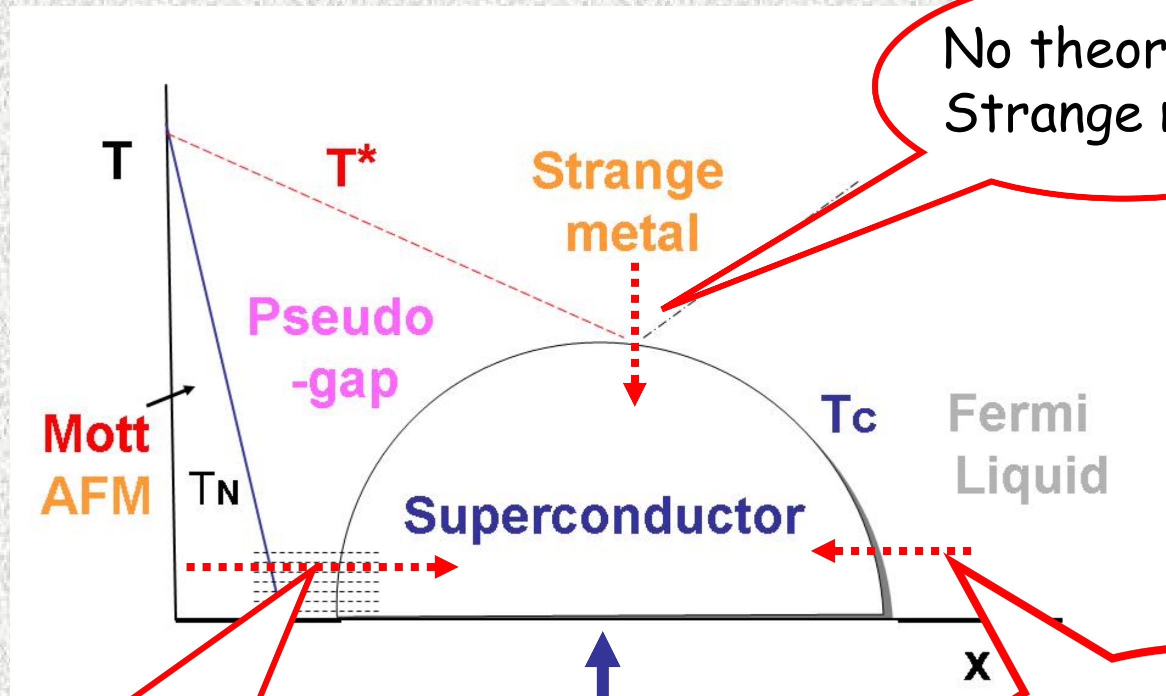


Scalapino and collaborators

T=0 :Quantum Fluctuations reduce the moment from 0.5 to 0.33

Trivedi & Ceperley, 1987

Strategy for theoretical attack on the superconducting state



No theory of Strange metal

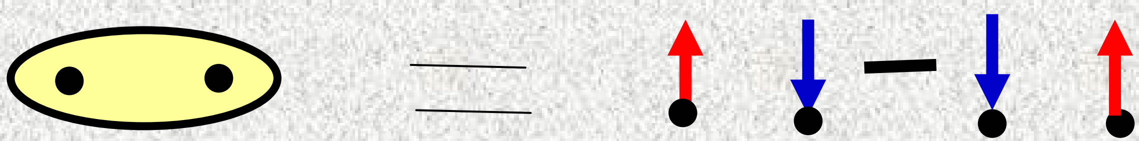
Need to cross many phases to reach the SC

Diagrammatic approaches -- Cannot reach Mott insulator

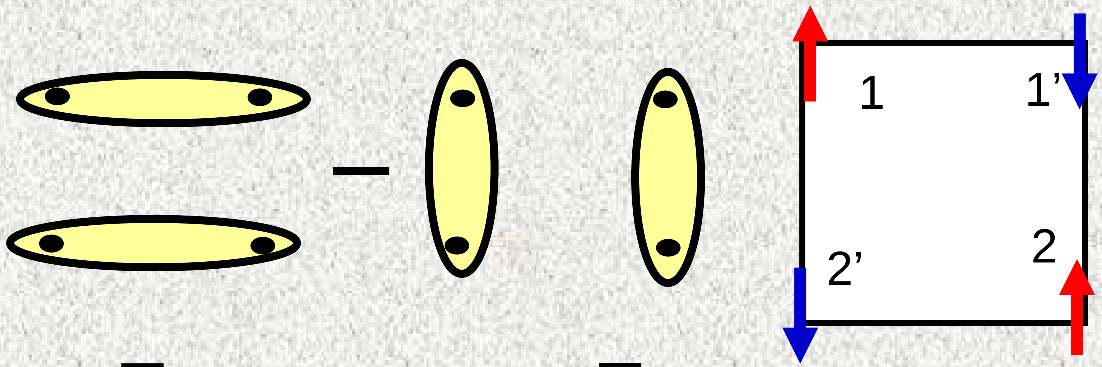
Use a variational approach to look directly at the T=0 SC state and low-lying excitations

RVB states

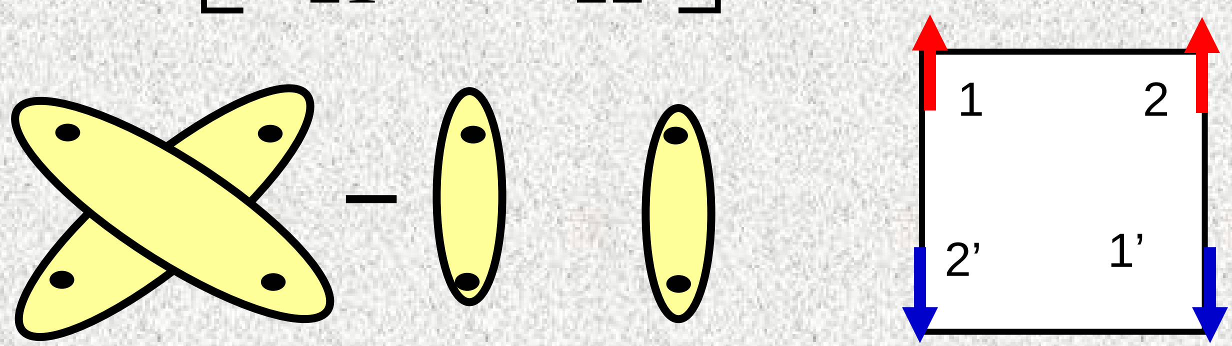
2 sites



4 sites



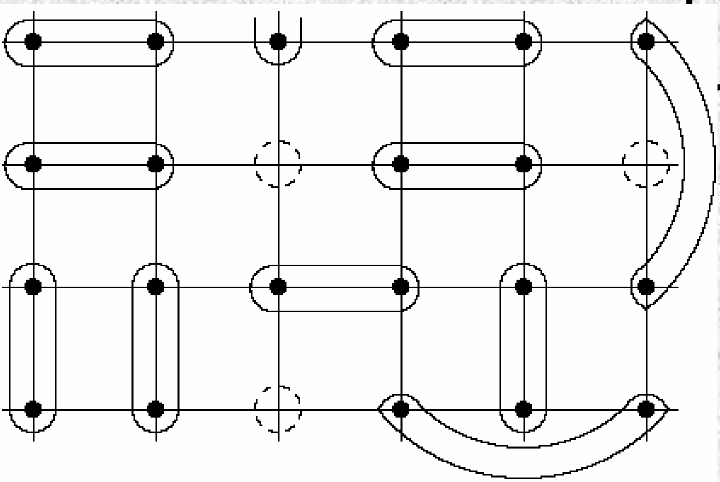
$$\Psi_{RVB} = \begin{bmatrix} \phi_{11'} & \phi_{12'} \\ \phi_{21'} & \phi_{22'} \end{bmatrix}$$

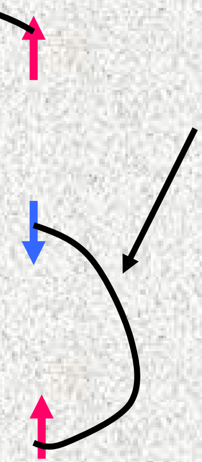


Configuration of electrons

$$R = \{ r_{1\uparrow}, r_{2\uparrow}, \cdots r_{N/2\uparrow}; r_{1\downarrow}, r_{2\downarrow}, \cdots r_{N/2\downarrow} \}$$

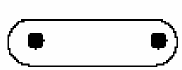
$$\mathbf{P} \langle R | \psi_{BCS} \rangle = \mathbf{P} \begin{vmatrix} \phi(r_{1\uparrow} - r'_{1\downarrow}) \cdots\cdots\cdots \phi(r_{1\uparrow} - r'_{1\downarrow}) \\ \phi(r_{1\uparrow} - r'_{2\downarrow}) \cdots\cdots \\ \vdots \\ \vdots \\ \phi(r_{1\uparrow} - r'_{N/2\downarrow}) \cdots\cdots\cdots \phi(r_{N/2\uparrow} - r'_{N/2\downarrow}) \end{vmatrix}$$





Projected SC Resonating Valence Bond (RVB) liquid

P.W. Anderson, Science 235, 1196 (1987)



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

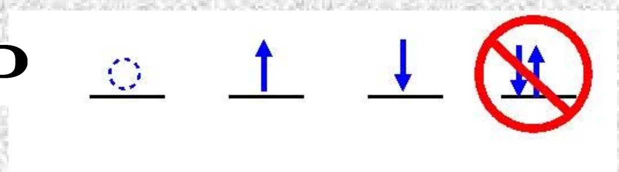
Electrons paired into singlets

$$\varphi(\mathbf{r} - \mathbf{r}') = \sum_k \exp(i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}'))\,(v_{\mathbf{k}}/u_{\mathbf{k}})$$

Signature of Strongly Correlated Superconductor

$$|\Psi_0\rangle = \mathbf{P}|dBCS\rangle$$

$\mathbf{P}$



$U \gg t$

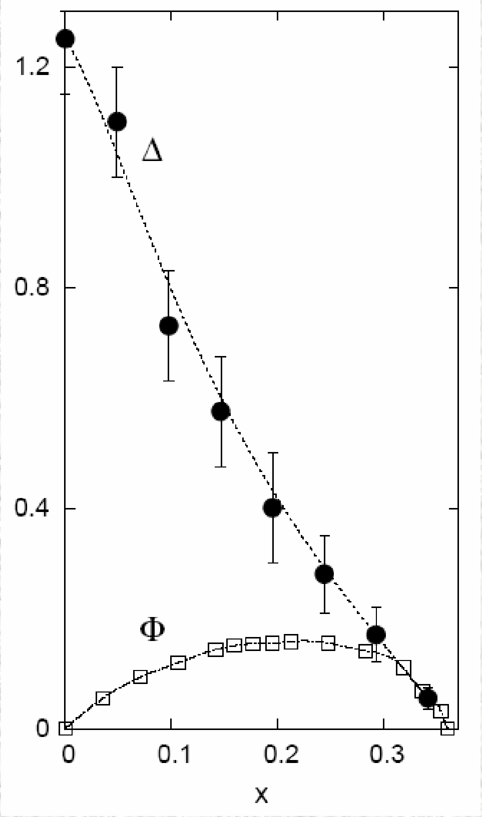
Hubbard model

RVB: Anderson ('87)
Kotliar & Liu ('88)
Zhang, Gross, Rice & Shiba ('88)

Projected Variational Wavefunctions

- SC "dome" with optimal doping

- pairing gap Δ(x) and SC order parameter have qualitatively different x-dependences.



Paramekanti, Randeria & Trivedi
PRL 87, 217002 (2001);
PRB 70, 054504 (2004)

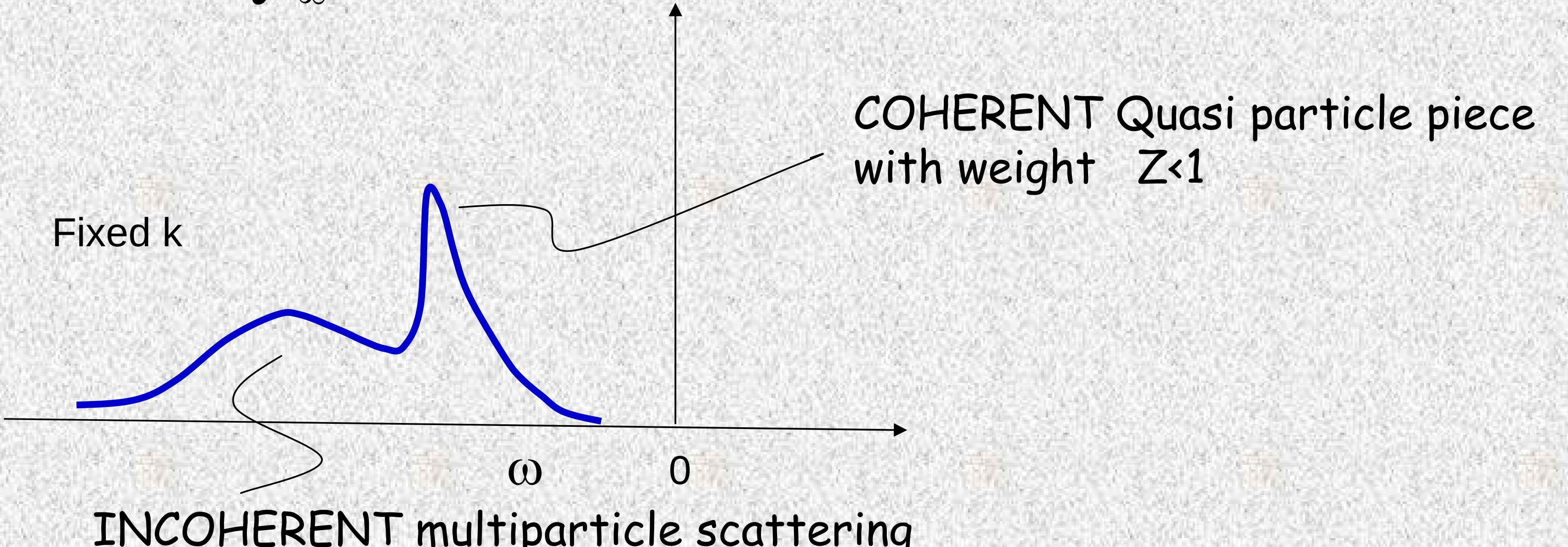
Anderson, Lee, Randeria, Rice, Trivedi & Zhang,
J. Phys. CM 16, 755 (2004)

How does the SC evolve to a Mott Insulator

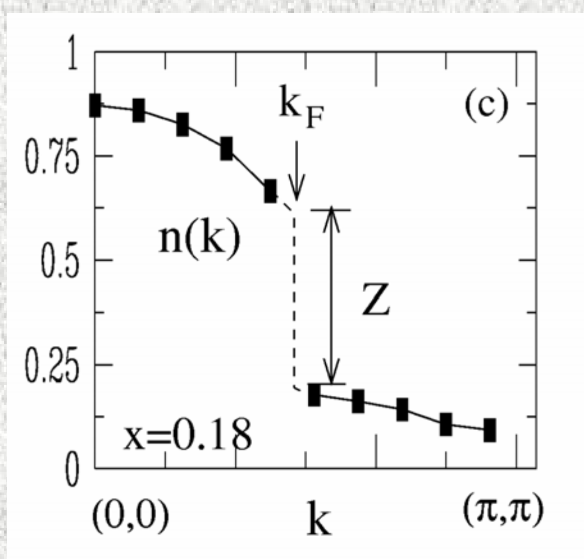
$A(k,\omega)$ SPECTRAL FUNCTION $\longrightarrow \left\langle c_{r'}^{+}(\tau) c_{r}(0) \right\rangle$

$$\sum_k A(k,\omega) = N(\omega)$$

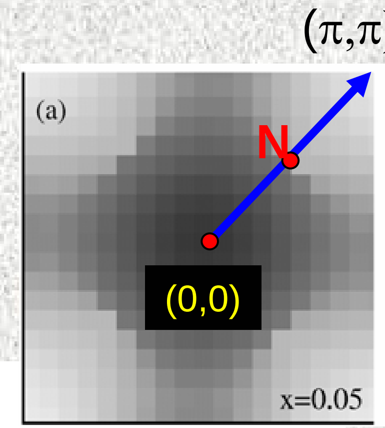
$$\int_{-\infty}^{0} d\omega A(k,\omega) = n(k)$$



COHERENT QUASIPARTICLE WEIGHT



Discontinuity in n(k)



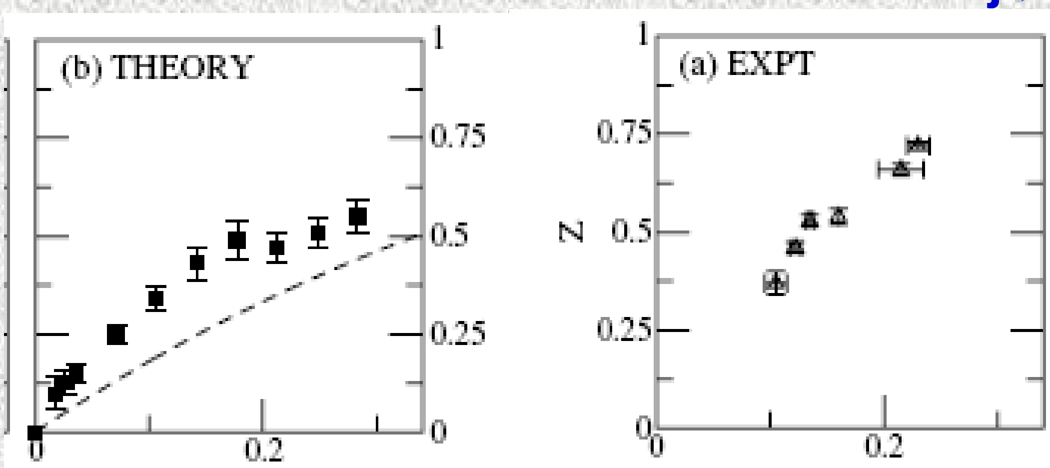
Existence of **gapless**

QUASIPARTICLES at nodal point N

Coherent weight (QP residue)

Z~x as x → 0

Projection leads to incoherence

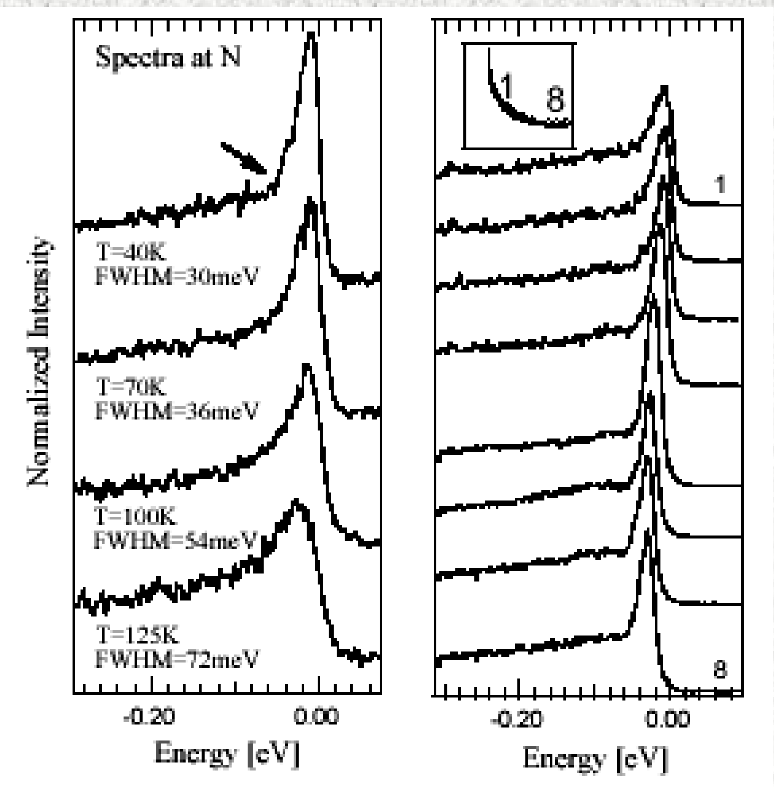


Route to Mott Insulator

Vanishing Quasiparticle wt. Z

Quasiparticles in SC state

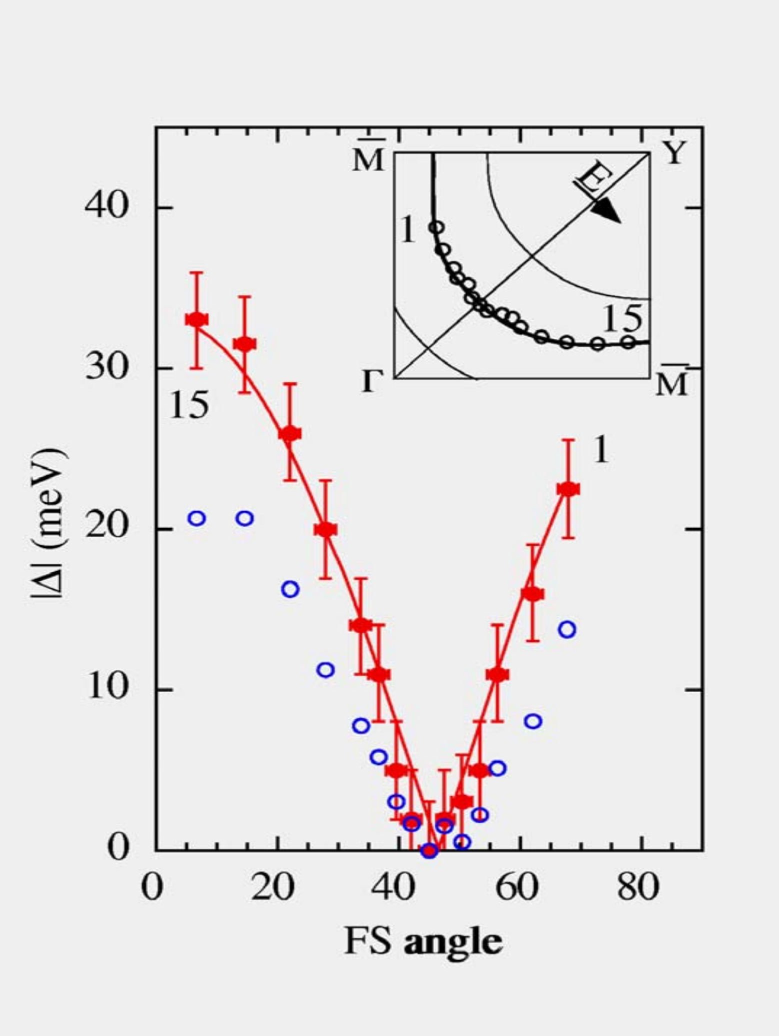
A. Kaminski et al., PRL (2000; 2001)



$$\Delta(\mathbf{k}) = \Delta_0 (\cos k_x - \cos k_y)$$

ARPES: Bi2212 SC Gap Anisotropy

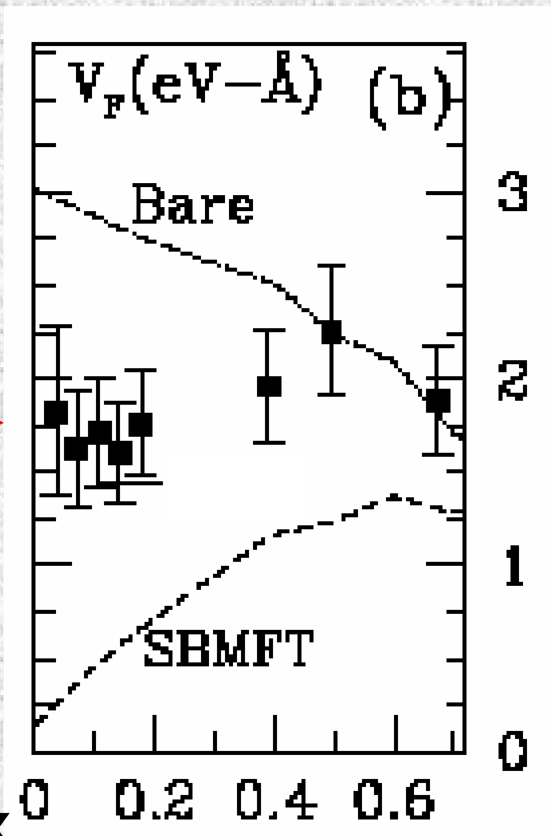
H. Ding et al., PRB (1996)



Velocity of Nodal Quasiparticles:

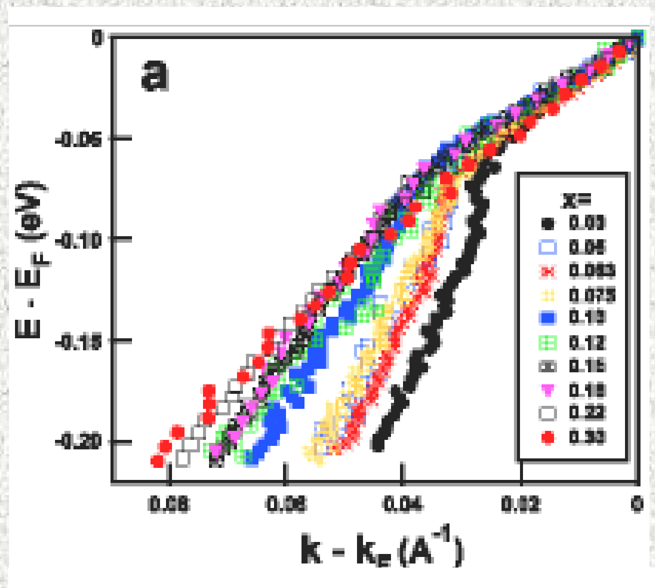
const. V_F

V_F indep. of x



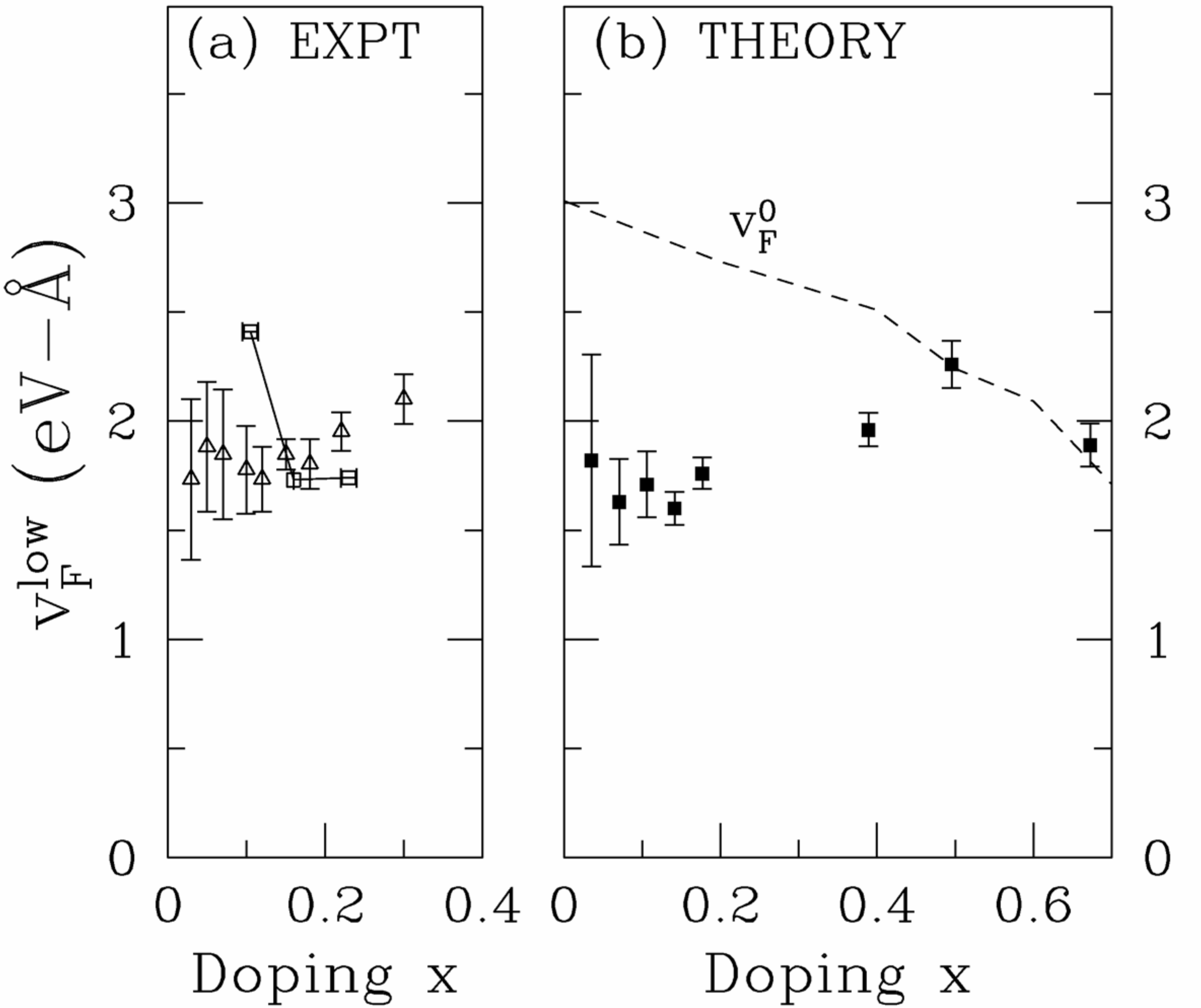
x

Theory: Paramekanti et al, PRL (2001)



Expt: Zhou et al, Nature (2003)

Z ~ x <u>and</u> V_F ~ const.
→ Σ (k,ω) singularities!



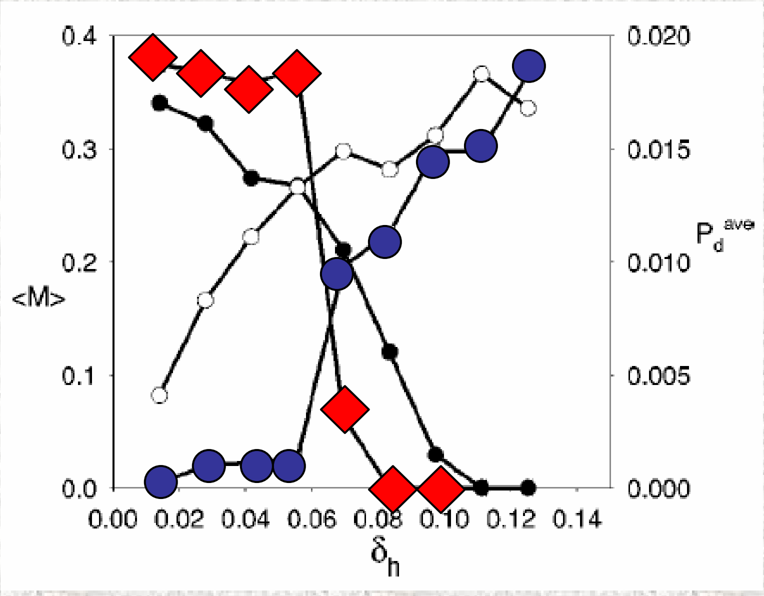
Expt: Zhou et. al
Nature **423**, 398 (2003)

Theory: Paramekanti, Randeria, NT;
PRL **87,** 217002 (2001)

Competition between SC and AFM as x → 0

Energetics: energies of different states differ by < few %

→ need to know details of H

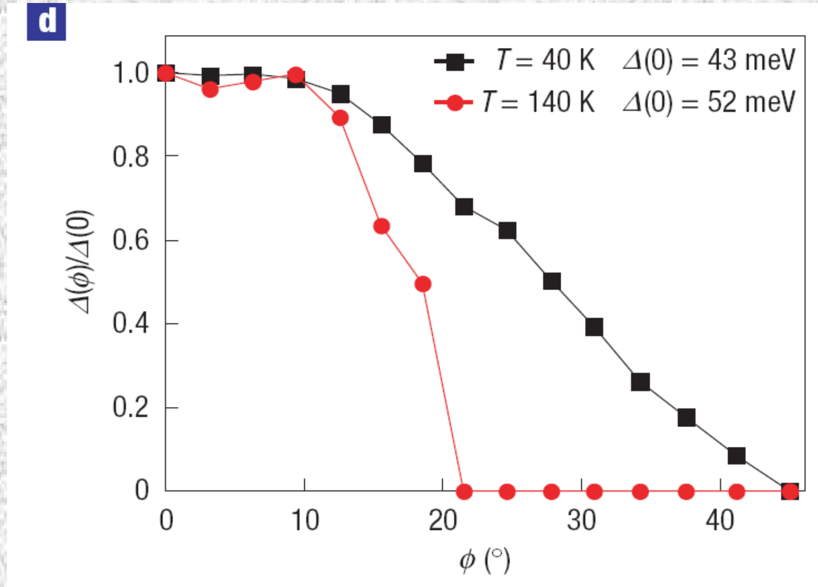


t' = 0:
Large region of coexsitence
Giamarchi & Lhuillier, PRB 1991
Himeda & Ogata, PRB 1999

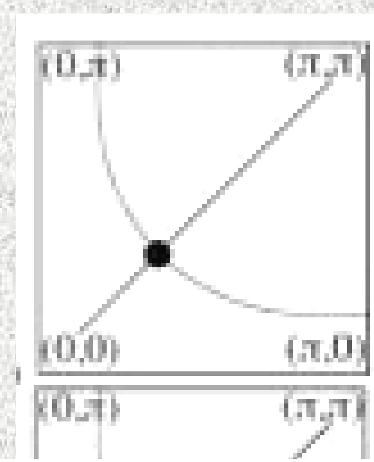
- ◆ AFM order parameter for x < 8%
- ● SC order parameter for x > 6%

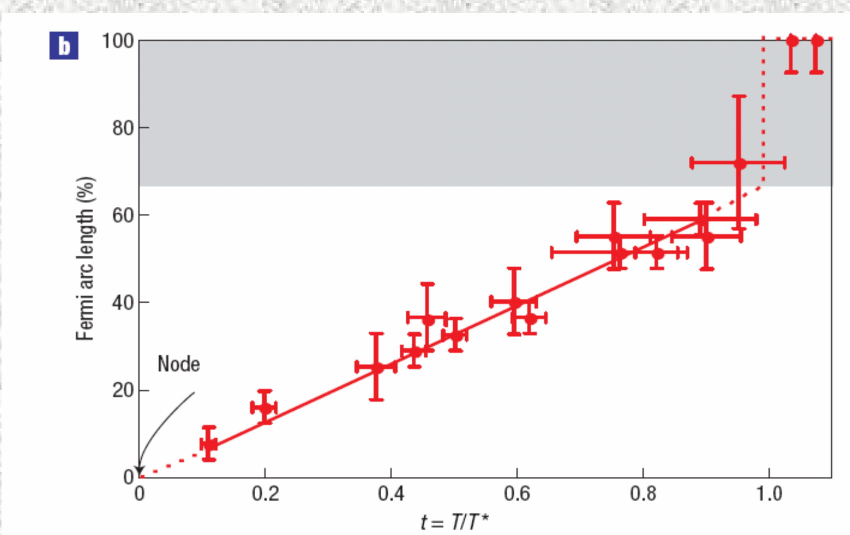
For J/ t =0.3, t ' / t= - 0.3 and t"/ t=0.2

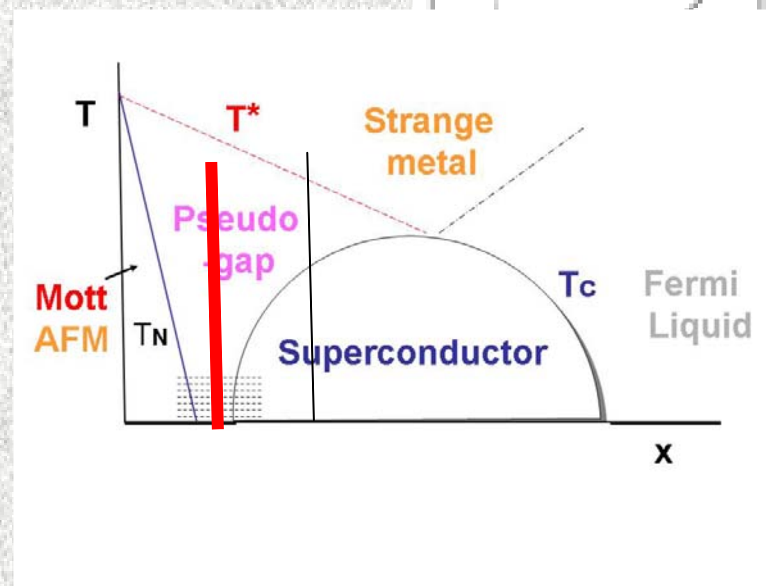
Shih, Chen, Chou, & Lee, PRB**70**, 220502 (2004)
S. Pathak, V, Shenoy, M. Randeria and N. Trivedi, preprint



SC
T <Tc







NODAL METAL?? NEW PHASE OF MATTER

Kanigel et al, Nature Physics 2, 447 (2006)

Norman et al, Nature (1998)

Next…

- Quantitative comparison with experiments

BHM: (i) Quantitative determination of phase boundaries and exponents;

(ii) quantum and thermal fluctuations; n(k); entropy and thermometry; visibility; role of trap

FHM U<0: pseudogap: charge and spin correlations; entropy

FHM U>0: (i) interplay of AF and SF;

(ii) RVB wavefunctions from stripes to 2D

(iii) Unusual normal states

end