Sawubona

Khuyadakh

to levitated trains!

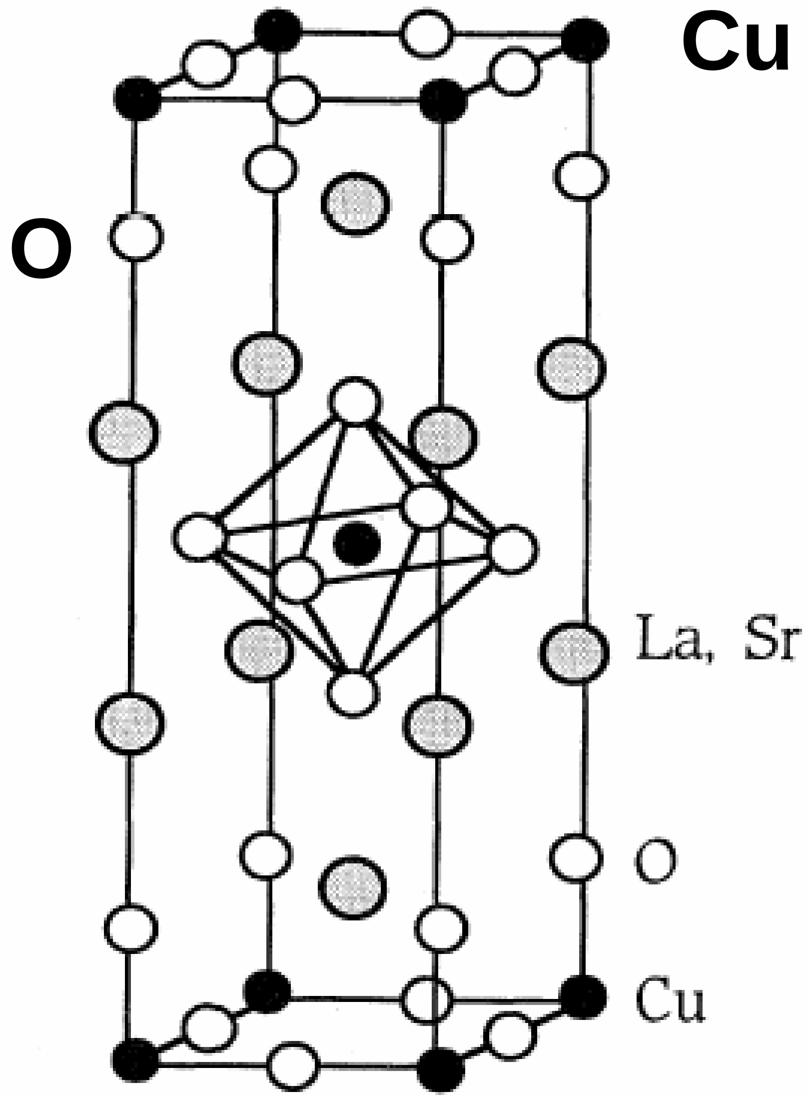
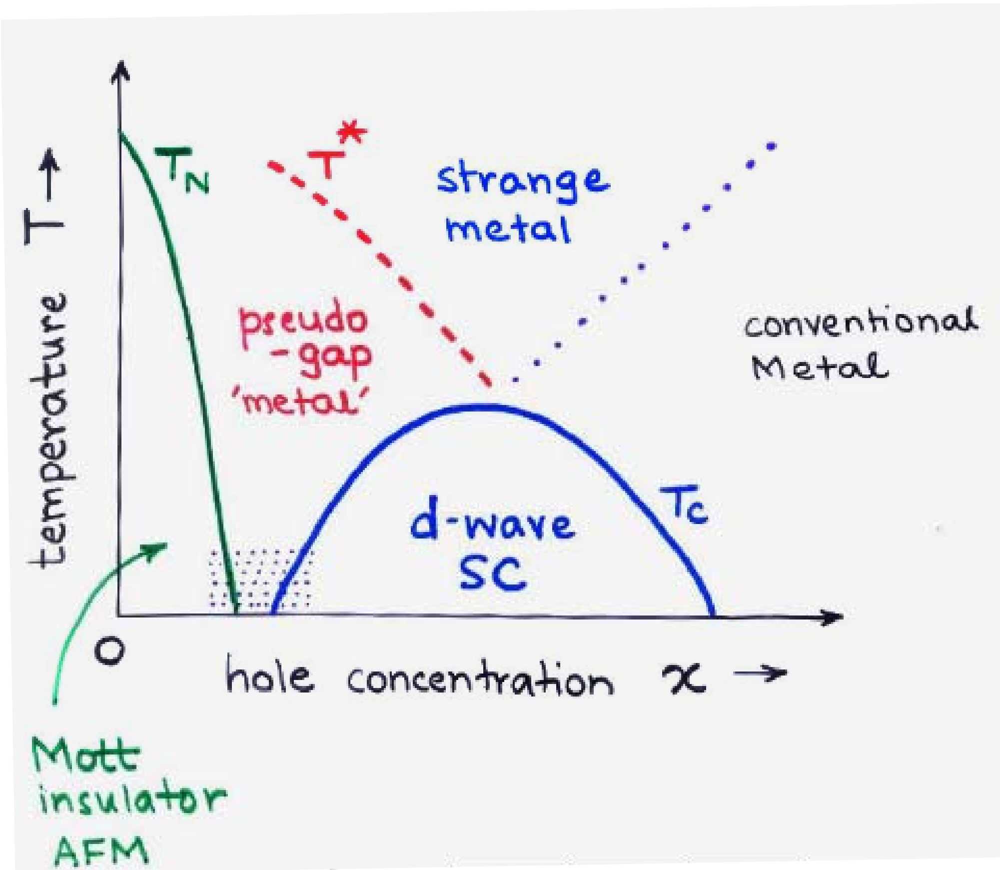


FIG. 1. Crystal structure of $La_{2-x}Sr_xCuO_4$ (T phase). Taken from Almasan and Maple (1991).

High Temperature Superconductors:

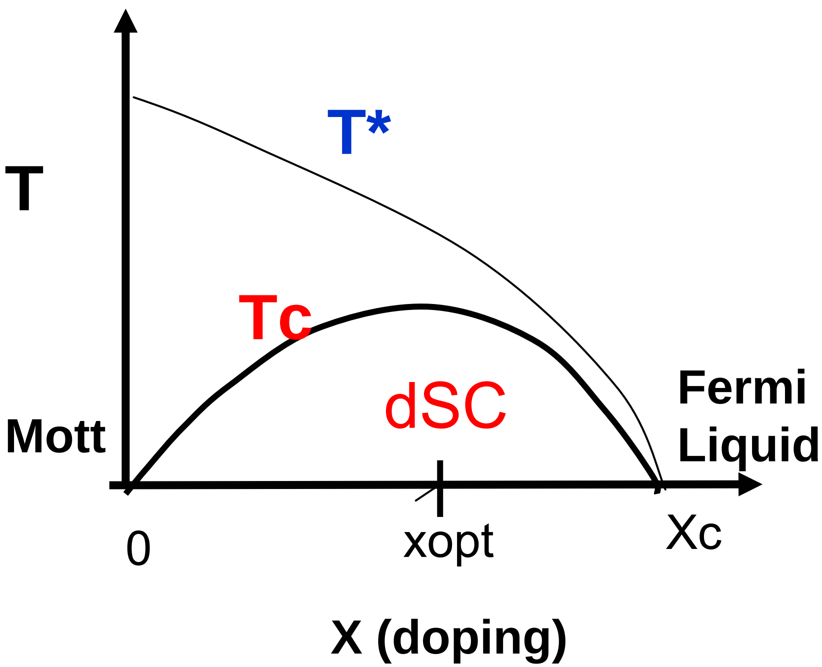
schematic phase diagram



- novel phases
- unusual phase transitions
- unusual crossovers

Our Philosophy

- Look at the strongly correlated SC state by itself; not as an instability from another state
- Look at instabilities out of the SC state
- Minimal model to understand
- Systematically build up to get entire complexity of the cuprates



Hubbard Model

$$H = -t \sum_{<i,j>\sigma} c^{+}{}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i_\uparrow} n_{i_\downarrow}$$

$$n_{i\sigma} = c^{+}_{i\sigma} c_{i\sigma}$$

2-site case:

Each site can have 4 possible states: $|0\rangle; |\uparrow\rangle; |\downarrow\rangle; |\updownarrow\rangle$

Two sites can have 16 possible states: $|\alpha_1; \beta_2\rangle$ $\quad e.g. |\uparrow_1; 0_2\rangle$

Subspace with Sztot=0 has 4 states

$$|\uparrow_1; \downarrow_2\rangle; |\downarrow_1; \uparrow_2\rangle; |\updownarrow_1; 0\rangle; |0_1; \updownarrow_2\rangle$$

2 site Hubbard Model

$$H = -t(c_{1\uparrow}^{+}c_{2\uparrow} + c_{2\uparrow}^{+}c_{1\uparrow} + c_{1\downarrow}^{+}c_{2\downarrow} + c_{2\downarrow}^{+}c_{1\downarrow}) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow})$$

$$|\chi_1\rangle = |\uparrow_1;\downarrow_2\rangle; |\chi_2\rangle = |\downarrow_1;\uparrow_2\rangle; |\chi_3\rangle = |\updownarrow_1;0\rangle; |\chi_4\rangle = |0_1;\updownarrow_2\rangle$$

$$\langle \chi_n | H | \chi_m \rangle$$

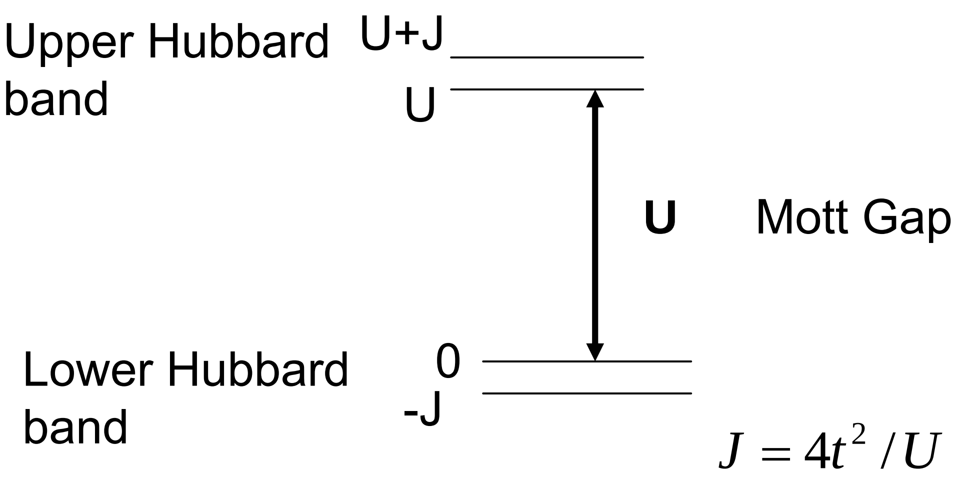
H=

$$\begin{pmatrix} 0 & 0 & -t & -t \\ 0 & 0 & -t & -t \\ -t & -t & U & 0 \\ -t & -t & 0 & U \end{pmatrix}$$

$$\mathbf{H} = \begin{pmatrix} 0 & 0 & -t & -t \\ 0 & 0 & -t & -t \\ -t & -t & U & 0 \\ -t & -t & 0 & U \end{pmatrix}$$

Eigenvalues: 0; U;

$$\frac{1}{2}\left(U \pm \sqrt{U^2 + 16t^2}\right) \approx -\frac{4t^2}{U}; U + \frac{4t^2}{U}$$



Ground state:

$$\frac{1}{\sqrt{2}}\left(\left|\uparrow_1;\downarrow_2\right\rangle - \left|\downarrow_1;\uparrow_2\right\rangle\right)$$

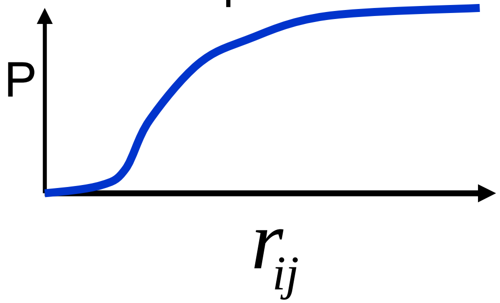
S=0 singlet

how do we construct wave functions for correlated systems?

$$\left|\phi_{bose}\right\rangle = \left(a^{+}_{k=0}\right)^{N}\left|0\right\rangle$$ = uniformly spread out in real space

What is the w.f for bosons with repulsive interactions?

$$\left|\psi_{\text{int}\,bosons}\right\rangle = \prod_{i<j}$$



Correlation physics:
Jastrow factor

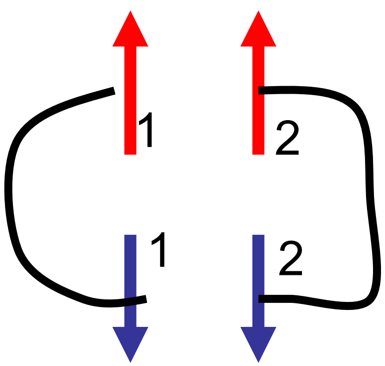
$$\left|\psi_{BCS}\right\rangle = \sum_{k}\left(\phi(k)c^{+}_{k\uparrow}c^{+}_{-k\downarrow}\right)^{N/2}\left|0\right\rangle$$

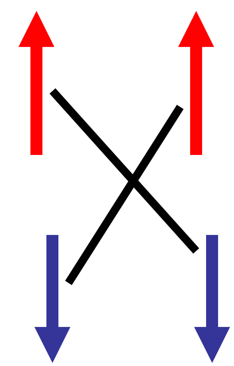
$$\left|\psi_{0}\right\rangle = P\left|\psi_{BCS}\right\rangle$$

Explains the phenomenology of correlated SC in hitc

PROPERTIES OF $\left|\psi_{0}\right\rangle$ and $\left|\psi_{BCS}\right\rangle$ completely different

$$\mathbf{P}\begin{pmatrix} \phi(r_{1\uparrow}-r'_{1\downarrow}) & \phi(r_{1\uparrow}-r'_{2\downarrow}) \\ \phi(r_{2\uparrow}-r'_{1\downarrow}) & \phi(r_{2\uparrow}-r'_{2\downarrow}) \end{pmatrix}$$



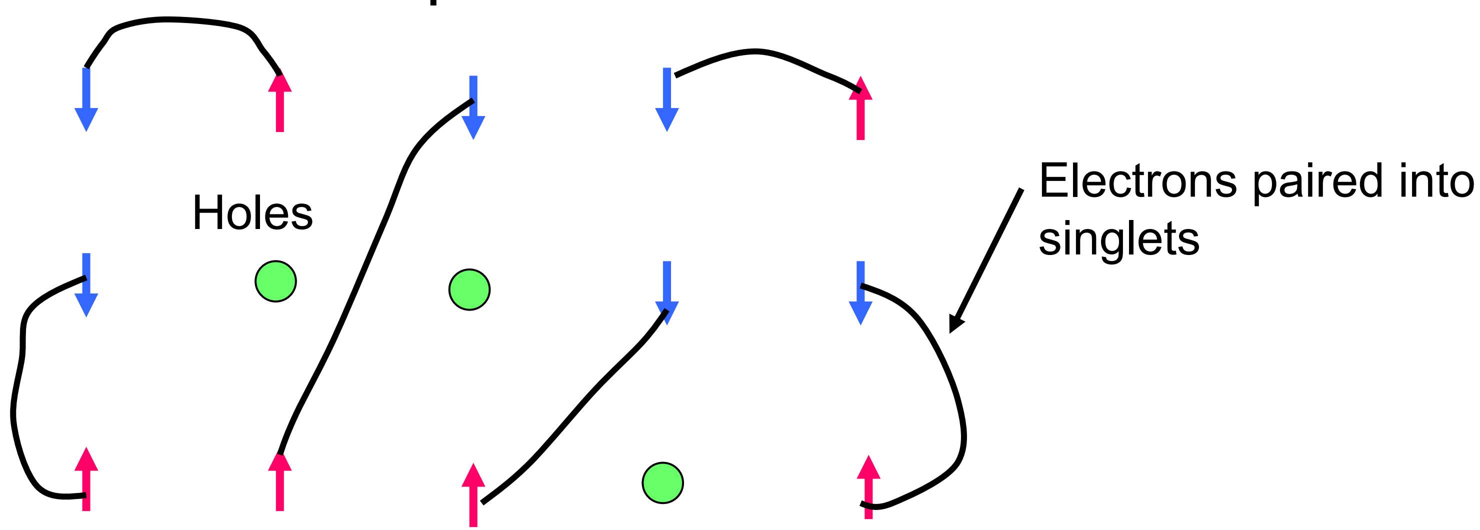


Projected wave function is a linear superposition of singlets

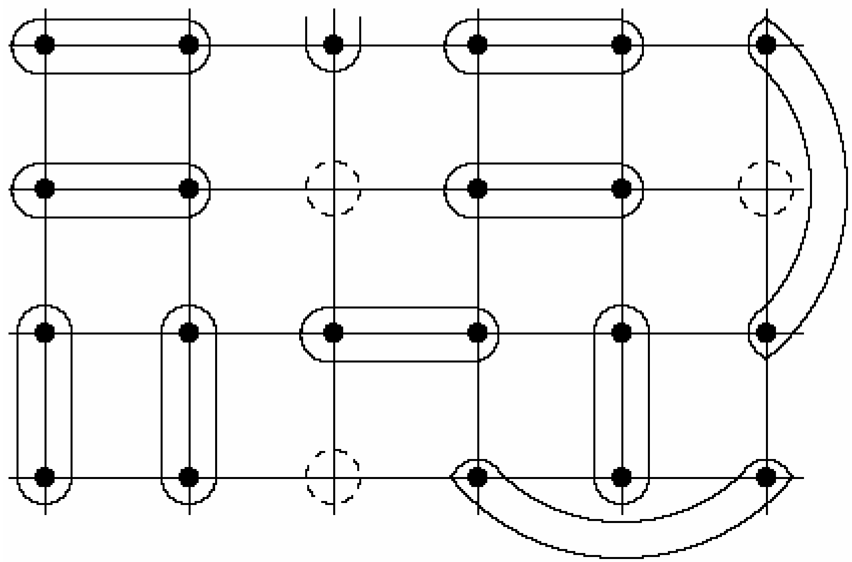
Configuration of electrons

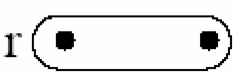
$$R = \{ r_{1\uparrow}, r_{2\uparrow}, \cdots r_{N/2\uparrow}; r_{1\downarrow}, r_{2\downarrow}, \cdots r_{N/2\downarrow} \}$$

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



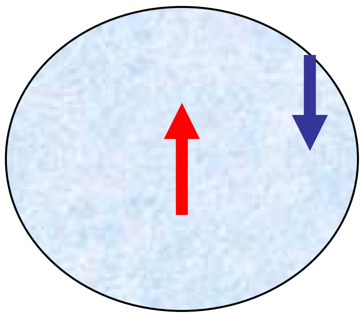
$$| \Psi_0 > = \mathbf{P} \, | \, \mathrm{dBCS} >$$



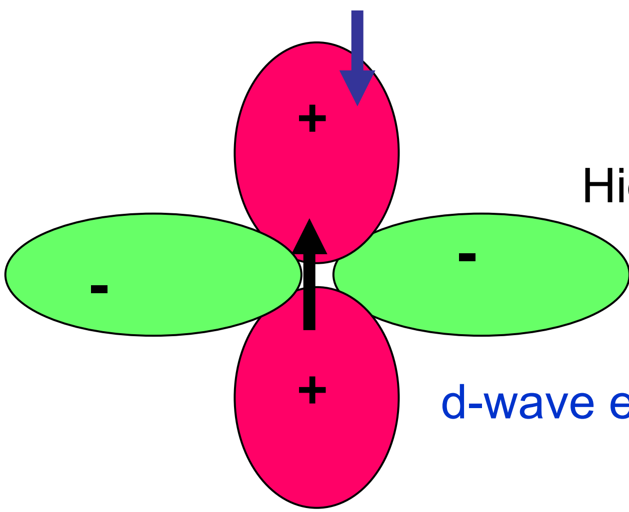
r  r′ $= \dfrac{|\uparrow_r \downarrow_{r'}\rangle - |\downarrow_r \uparrow_{r'}\rangle}{\sqrt{2}} \quad \phi\,(r - r')$

What is $\phi(r_\uparrow - r'_\downarrow)$

Relative orbital wave function of the down electron around the up electron



Usual SCs: “swave” L=0



High Tc SCs

d-wave evidence   Josephson interferometry expts

van Harlingen et al.(1994)

Tsuei and Kirtley (1994)

Lowest energy solution

C. Gros (1998); Kotliar and Liu

Variational Approach: PROJECTED WAVE FUNCTIONS

$$\left|\psi_0\right\rangle = e^{iS} P \left|\psi_{BCS}\right\rangle$$

$$\left|\psi_{BCS}\right\rangle = \left(\sum_k \phi(k) c^+_{k_\uparrow} c^+_{k_\downarrow} \right)^{N/2} \left|0\right\rangle$$

Fixed number BCS wave function: macroscopic occupation of paired state $\varphi(r_\uparrow - r'_\downarrow)$

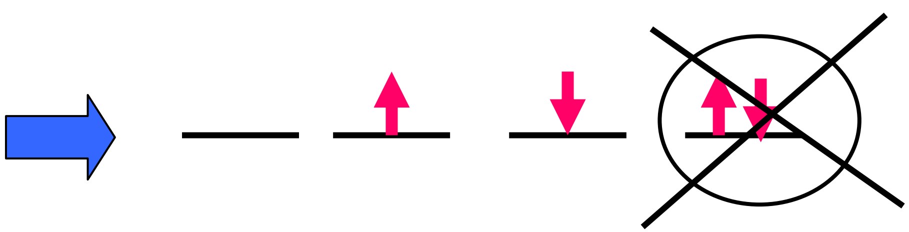
$$\varphi_k = \frac{v_k}{u_k} = \frac{\Delta_k}{\xi_k + \sqrt{\xi_k^2 + \Delta_k^2}}$$

$$\xi_k = \varepsilon_k - \boxed{\mu_{\text{var}}}$$

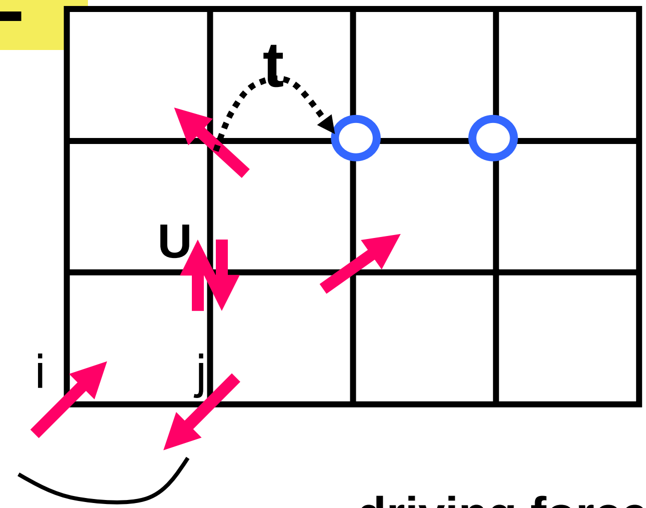
$$\Delta_k = \Delta_{\text{var}} (\cos k_x - \cos k_y)$$

"dwave"

$$P = \prod_r (1 - n_{r\uparrow} n_{r\downarrow})$$



HUBBARD MODEL



Kinetic Energy $= -t \sum_{<i,j>\sigma} c^{+}{}_{i\sigma} c_{j\sigma}$

Potential Energy $= U \sum_{i} n_{i_\uparrow} n_{i_\downarrow}$

U >> t generates AFM exchange

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

J Si .Sj → driving force for d wave pairing

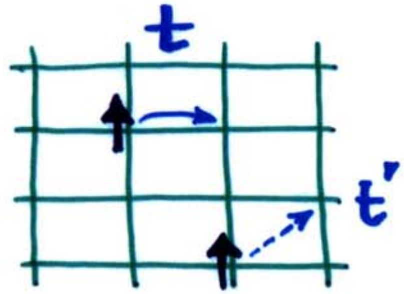
Energy Scales: $J \leq t < U$

neutron scattering: $J = 4t^2 / U$ **~100 mev**

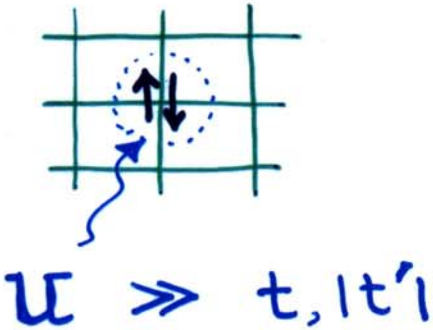
electronic structure theory
and photoemission **t~300 meV** → **U~12t**

x= Hole doping =fraction of vacancies

kinetic energy



Coulomb potential



2D Hubbard Hamiltonian

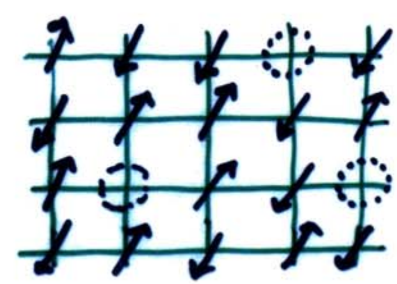
AF superexchange

$J = 4t^2 / U$

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

$J \simeq 100$ meV, $t \simeq 300$ meV, $U \simeq 3.6$ eV, $t' = -t/4$

Hole doping:
$x << 1$



Unitary Transformation

$$H=\left|\begin{array}{c:c:c} D=0 & K_1 & \\ \hdashline K_{-1} & D=1 & K_1 \\ \hdashline & K_{-1} & D=2 \end{array}\right|$$

D=number of doubly occupied sites

$$K = K_0 + K_{+1} + K_{-1}$$

Kinetic energy

Unitary transformation to diagonalize H

$$H_{eff} = e^{iS} H e^{-iS} = H - [iS, H] + \frac{1}{2!}[iS,[iS,H]] + \ldots$$

$$= K_0 + \sum_{r,r',R,\sigma,\sigma'} \frac{t_{rR} t_{Rr'}}{U} \text{ (3 site terms)}$$

$$iS = \frac{1}{U}\left(K_{+1} - K_{-1}\right) + \ldots$$

•Transform ALL operators

Kohn, PR 133, A171 (1964)
Gros, Joynt, Rice (1988)
MacDonald, Girvin and Yoshioka (1988)

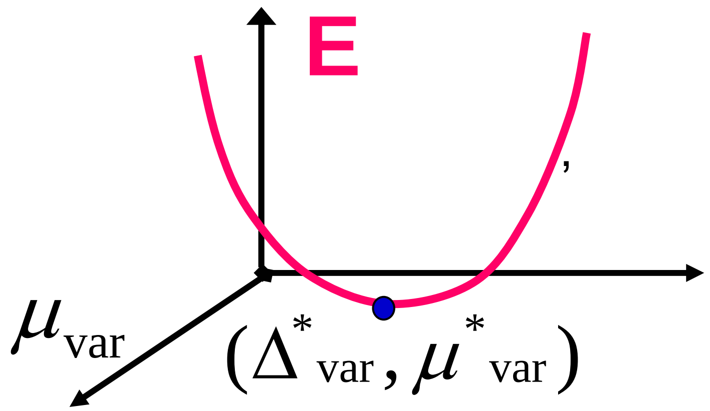
Variational Monte Carlo

$$\langle \psi_0 | \hat{O} | \psi_0 \rangle = \int dr_{1\uparrow}, dr_{2\uparrow}, \cdots dr_{N/2\uparrow}; dr_{1\downarrow}, dr_{2\downarrow}, \cdots dr_{N/2\downarrow}$$

$$| \psi(r_{1\uparrow}, \cdots r_{N/2\uparrow}; r_{1\downarrow}, \cdots r_{N/2\downarrow}) |^2 \hat{O}(r_{1\uparrow}, \cdots r_{N/2\uparrow}; r_{1\downarrow}, \cdots r_{N/2\downarrow}) \}$$

Monte Carlo: only known method to implement P exactly for evaluate 2N - dim integrals for ~1000 particle system

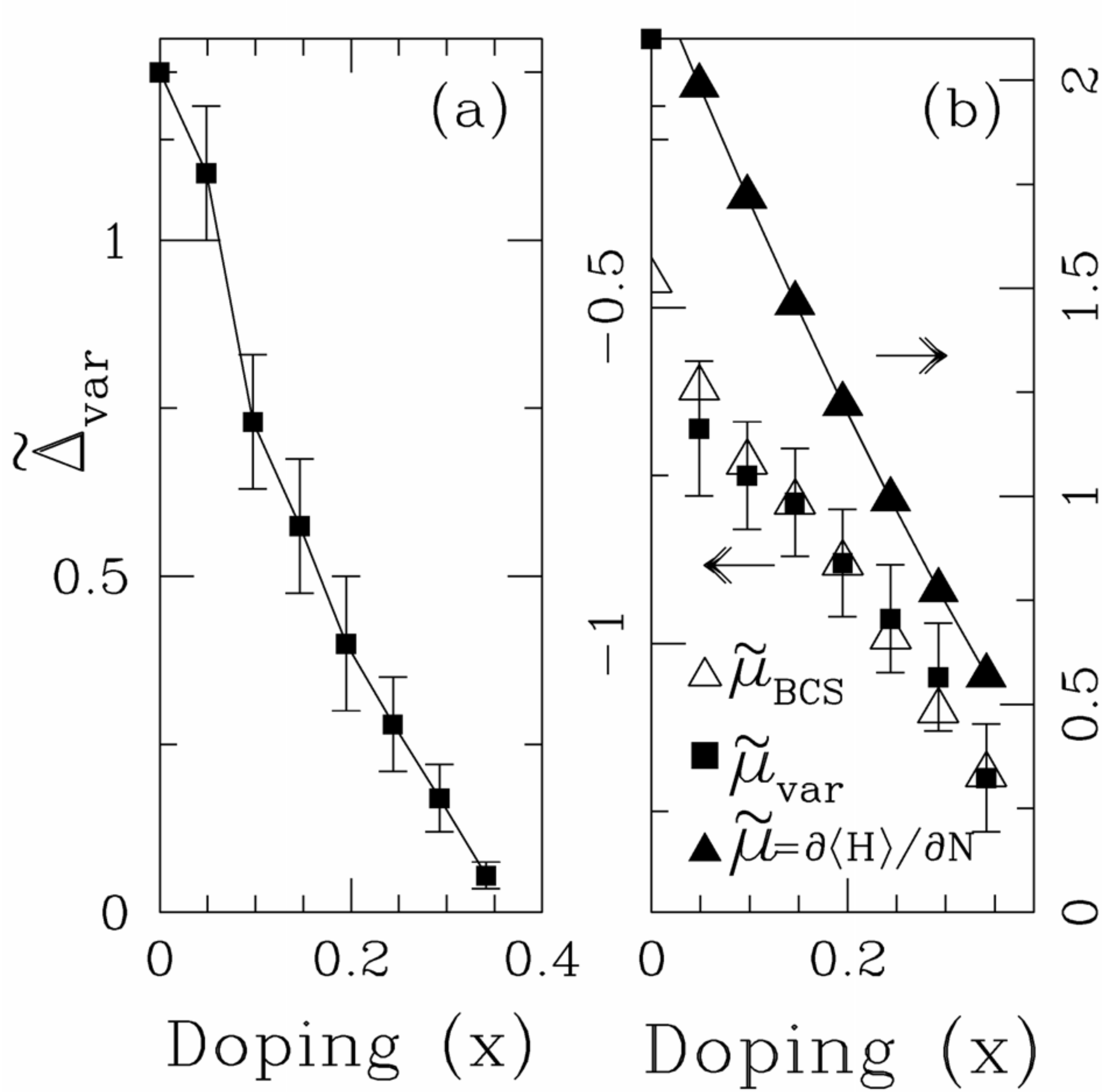
$$E(\Delta_{\text{var}}, \mu_{\text{var}}) = \frac{\langle \psi_o | H | \psi_o \rangle}{\langle \psi_o | \psi_o \rangle}$$



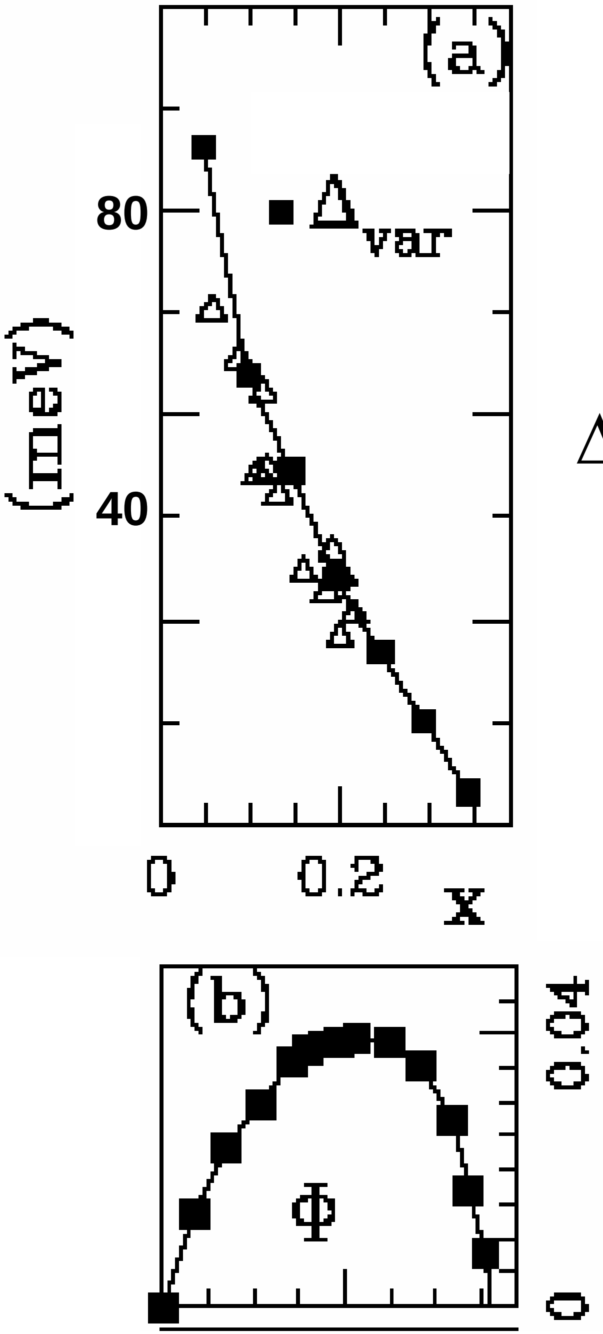
Limitation:
- T=0
- equal time correlations

Advantages:
Projection P implemented exactly
c.f. approximate analytical methods

Optimized variational parameters



Pairing & Superconductivity



Fluct
Com. op

Δ = Pairing scale
= energy gap

Scale ~ J

Φ(x) = SC order parameter

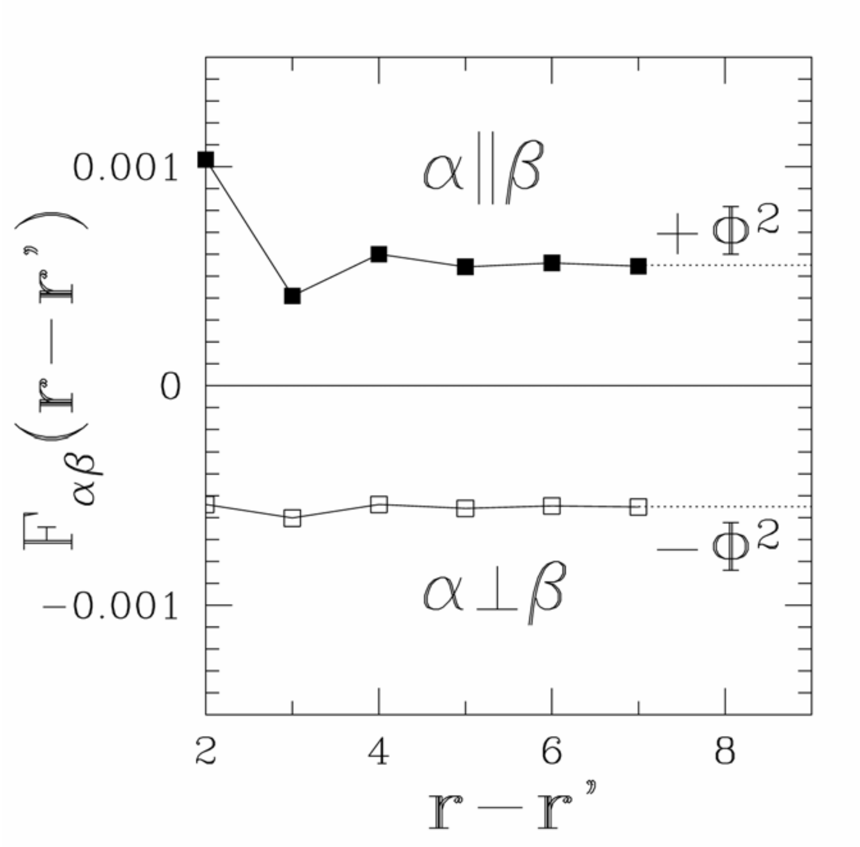
Strong Coulomb 'U' leads to

Φ(x) ~ x

as x → 0

Paramekanti, Randeria, NT
PRL 87, 217002 (2001)
PRB 69, 144509 (2004)
cond-mat/ 0303360

OFF DIAGONAL LONG RANGE ORDER



$$\langle C^{+}{}_{r\uparrow} C^{+}{}_{r+x\downarrow} C_{r'\downarrow} C_{r'+x\uparrow} \rangle \xrightarrow[|r-r'|\to\infty]{} \phi^2$$

SUPERFLUID

MAGNET

Off diagonal long range order

$$\langle a_i^+ \rangle \neq 0$$

Magnetization in XY plane

$$\langle S_i^+ \rangle \neq 0$$

In a subspace with fixed number of particles

$$h(l) = \langle a_i^+ a_{i+l} \rangle \xrightarrow[l \to \infty]{} condensate \neq 0$$

Condensate fraction

$$\langle S_i^+ S_{i+l}^- \rangle_{l \to \infty} = (m_x^+)^2 + (m_y^+)^2$$

Sublattice magnetization in XY plane

$$g(l) = \langle n_i n_{i+l} \rangle \xrightarrow[l \to \infty]{} n^2$$

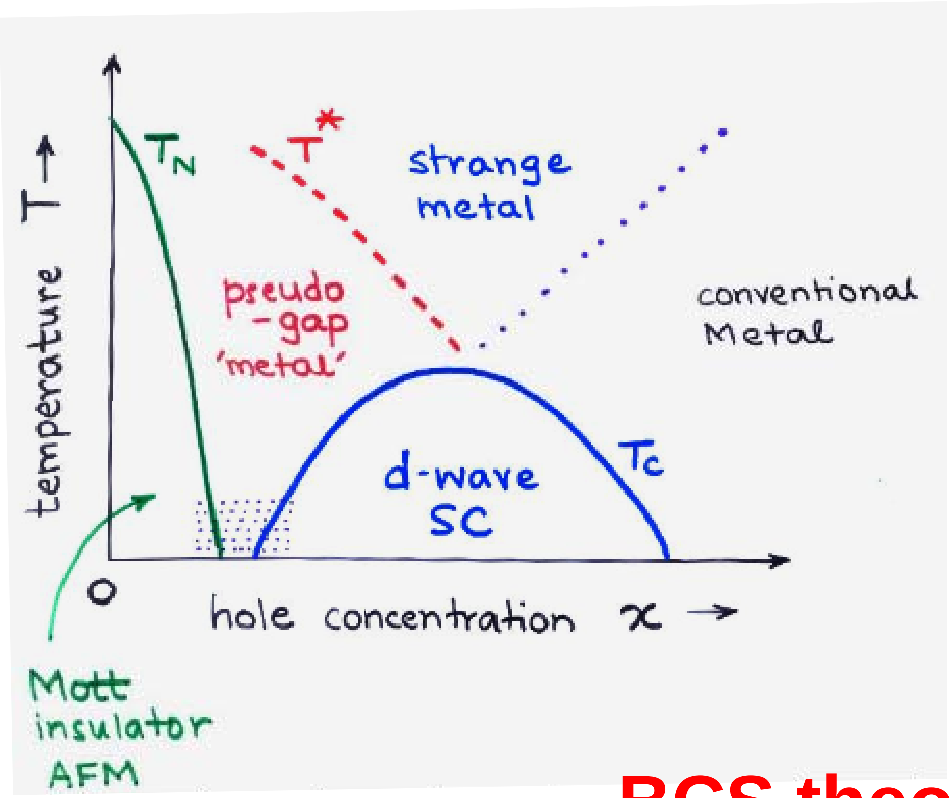
Diagonal long range order

$$\langle S_i^z S_{i+l}^z \rangle \xrightarrow[l \to \infty]{} (m_z)^2$$

Sublattice magnetization along z

Summary of experiments:

Band theory fails for x=0 **parent insulator**



Landau's Fermi liquid theory fails for **strange metal** and **pseudogap regimes**

Competing orders:
Antiferromagnetism;
Charge-density waves;
Superconductivity

BCS theory fails for **Unconventional SC** particularly for x << 1

What is the role of theory?

to **understand** phenomena

to make **predictions**

Understanding is not curve fitting…

Nature 427, 297 (2004)