

Sawubona

Khuyadakh



to levitated trains!

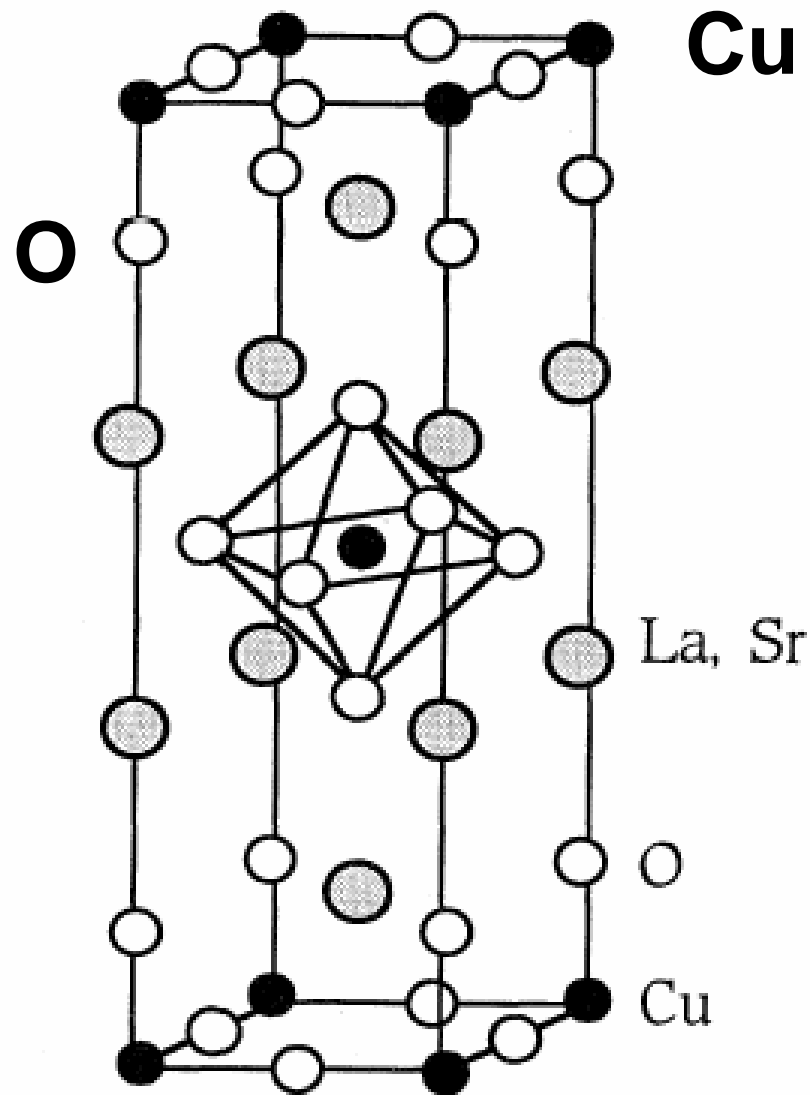
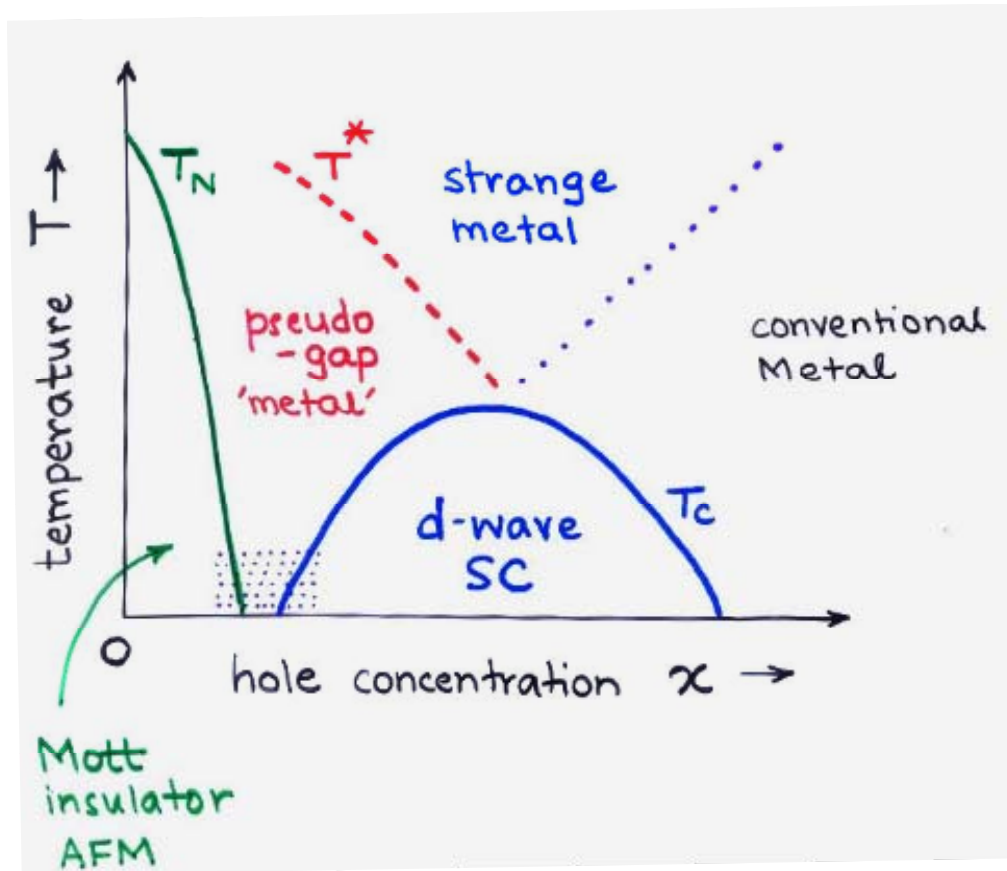


FIG. 1. Crystal structure of $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (T phase). Taken from Almasan and Maple (1991).

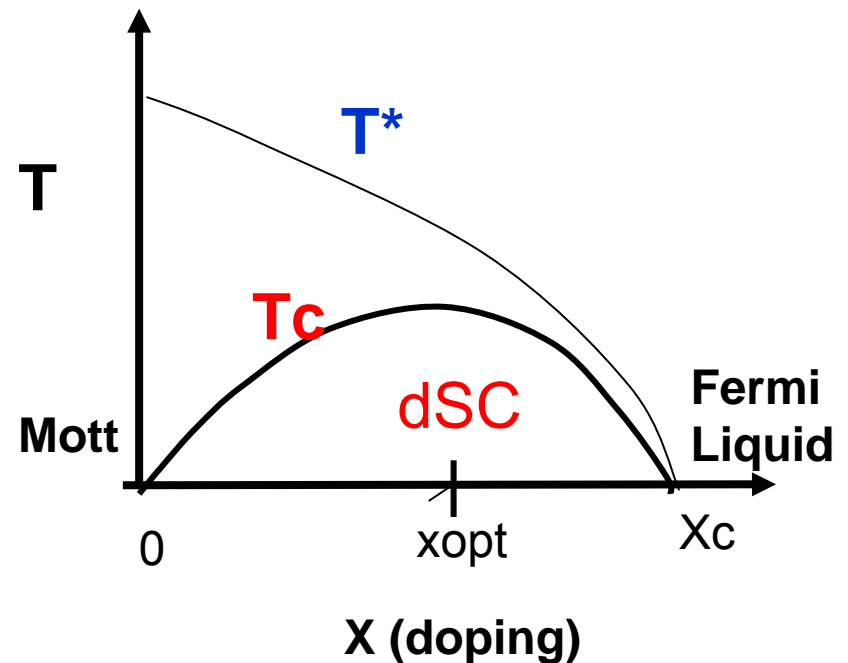
High Temperature Superconductors: schematic phase diagram



- 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

$$H = -t \sum_{\langle i,j \rangle \sigma} c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

2-site case:

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

Each site can have 4 possible states:

$$|0\rangle; |\uparrow\rangle; |\downarrow\rangle; |\uparrow\downarrow\rangle$$

Two sites can have 16 possible states:

$$|\alpha_1; \beta_2\rangle \quad e.g. |\uparrow_1; 0_2\rangle$$

Subspace with $S_{z\text{tot}}=0$ has 4 states

$$|\uparrow_1; \downarrow_2\rangle; |\downarrow_1; \uparrow_2\rangle; |\uparrow\downarrow_1; 0\rangle; |0_1; \uparrow\downarrow_2\rangle$$

2 site Hubbard Model

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

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

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

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

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

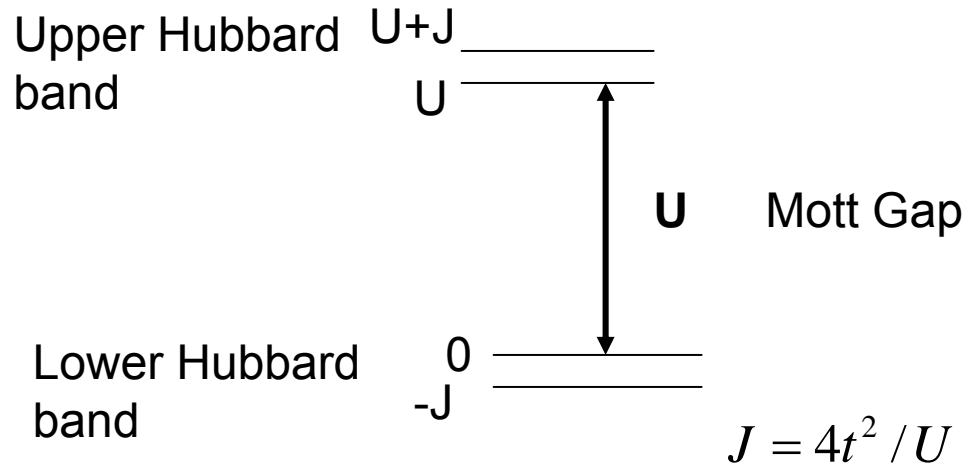
Eigenvalues: 0; U;

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

Ground state:

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

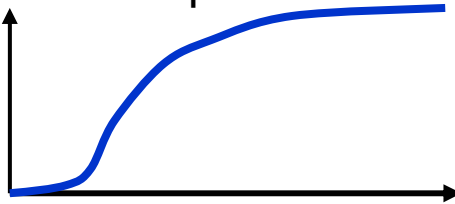
S=0 singlet



how do we construct wave functions for correlated systems?

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

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

$$|\psi_{\text{int bosons}}\rangle = \prod_{i < j} P$$


r_{ij}

Correlation physics:
Jastrow factor

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

$$|\psi_0\rangle = P |\psi_{BCS}\rangle$$

Explains the phenomenology
of correlated SC in hitc

PROPERTIES OF

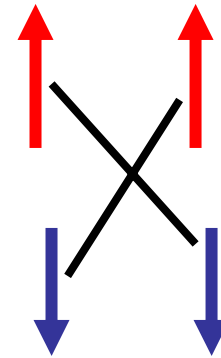
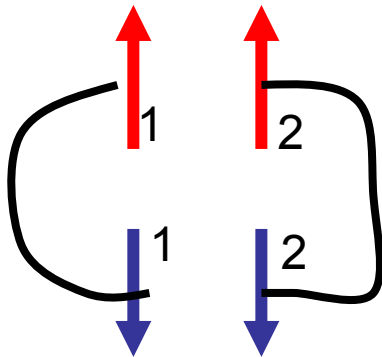
$$|\psi_0\rangle$$

and

$$|\psi_{BCS}\rangle$$

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

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

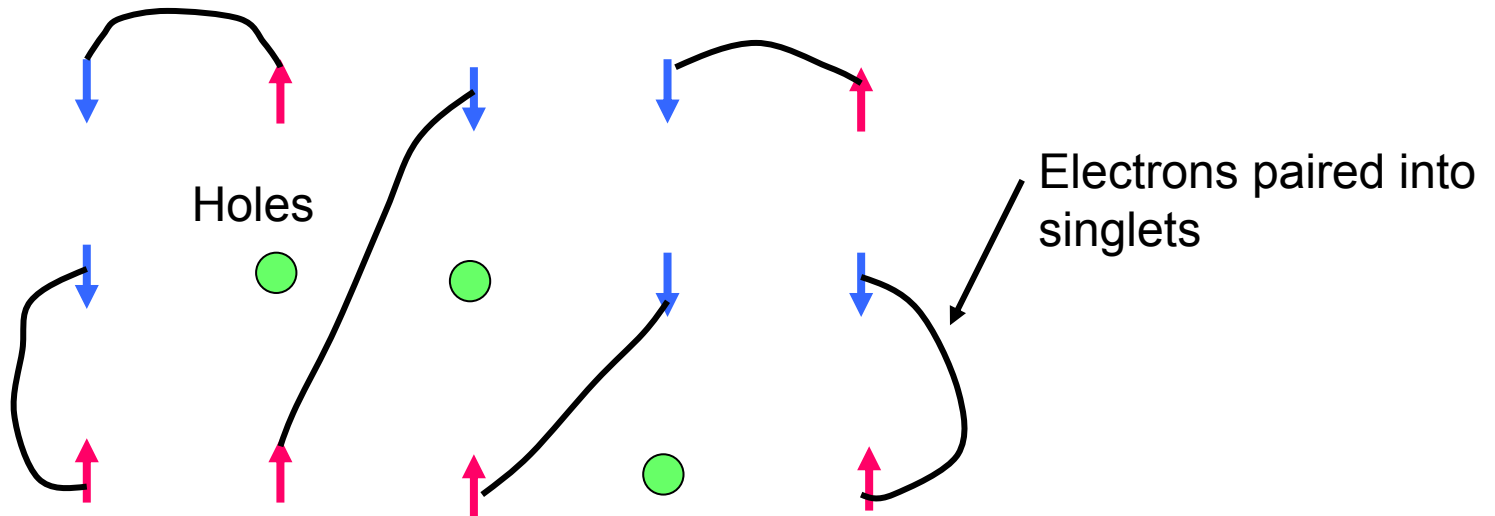
$$\mathbf{P} \langle R | \psi_{BCS} \rangle = \mathbf{P}$$

$$\phi(r_{1\uparrow} - r'_{1\downarrow}) \dots \dots \dots \phi(r_{1\uparrow} - r'_{N/2\downarrow})$$

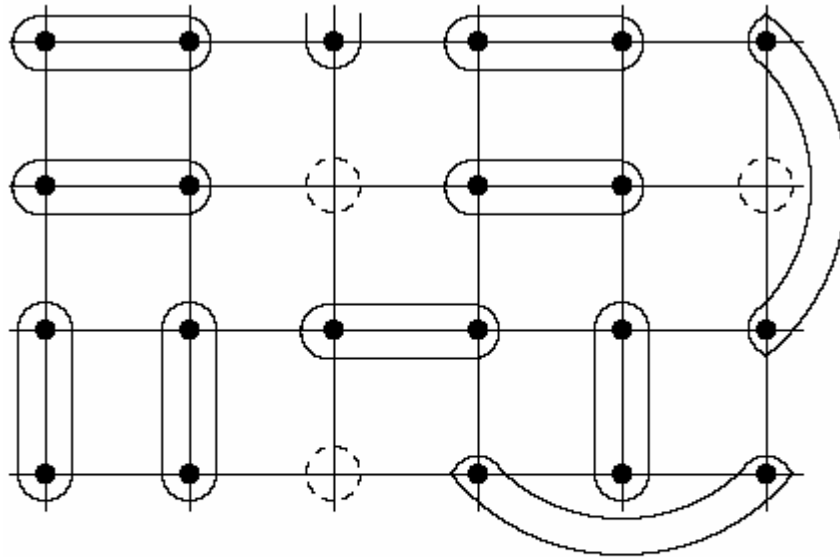
$$\phi(r_{1\uparrow} - r'_{2\downarrow}) \dots \dots \dots$$

⋮
⋮
⋮

$$\phi(r_{1\uparrow} - r'_{N/2\downarrow}) \dots \dots \dots \phi(r_{N/2\uparrow} - r'_{N/2\downarrow})$$



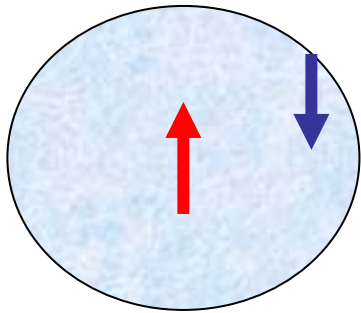
$$|\Psi_0\rangle = \mathbf{P} |d\text{BCS}\rangle$$



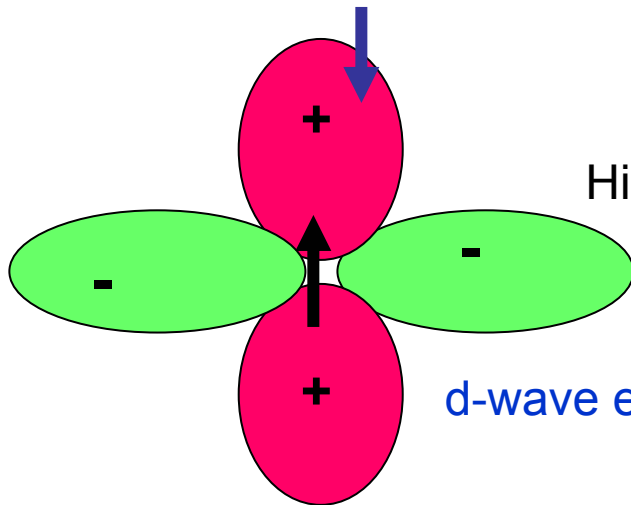
$$r \text{ --- } r' = \frac{|\uparrow_r \downarrow_{r'}\rangle - |\downarrow_r \uparrow_{r'}\rangle}{\sqrt{2}} \phi(r - r')$$

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

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

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

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

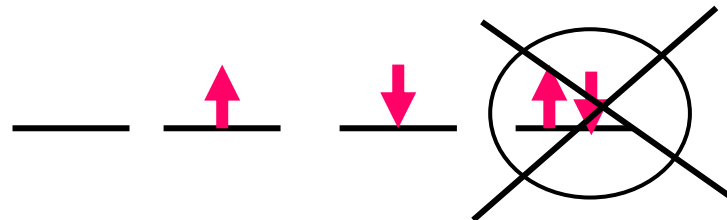
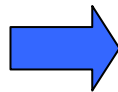
$$\varphi_k = \frac{v_k}{u_k} = \frac{\Delta_k}{\xi_k + \sqrt{\xi_k^2 + \Delta_k^2}}$$

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

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

“dwave”

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



HUBBARD MODEL

Kinetic Energy $= -t \sum_{\langle i,j \rangle \sigma} c_{i\sigma}^+ c_{j\sigma}$

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

$U \gg t$ generates AFM exchange

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

Energy Scales: $J \leq t < U$

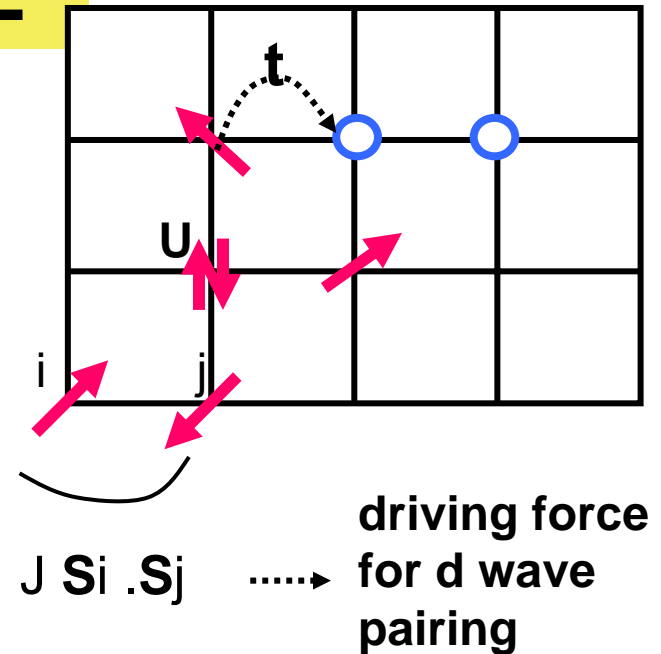
neutron scattering: $J = 4t^2 / U \sim 100$ meV

electronic structure theory
and photoemission $t \sim 300$ meV



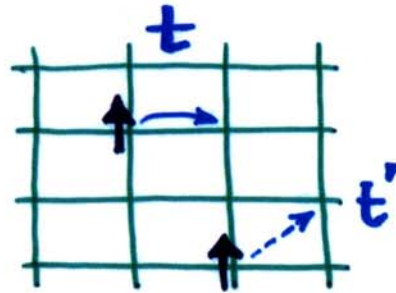
$$U \sim 12t$$

$x =$ Hole doping = fraction of vacancies

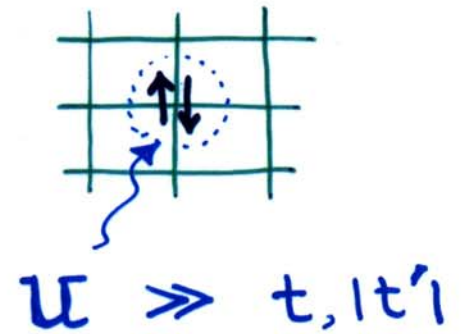


2D Hubbard Hamiltonian

kinetic energy

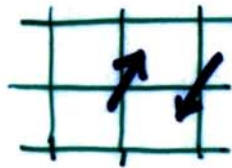


Coulomb potential



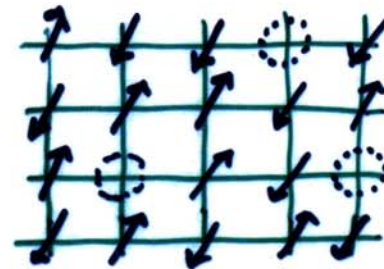
AF superexchange

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



Hole doping:

$$x \ll 1$$



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

\uparrow $\approx 100 \text{ meV}$ \uparrow $\approx 300 \text{ meV}$ \uparrow $\approx 3.6 \text{ eV}$

$t' = -t/4$

Unitary Transformation

$$H = \begin{array}{|c|c|c|} \hline D=0 & K_1 & \\ \hline K_{-1} & D=1 & K_1 \\ \hline & K_{-1} & D=2 \\ \hline \end{array}$$

D=number of doubly occupied sites

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

| Kinetic energy

Unitary transformation to diagonalize H

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

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

$$iS = \frac{1}{U} (K_{+1} - K_{-1}) + \dots$$

• Transform ALL operators

Kohn, PR 133, A171 (1964)

Gros, Joynt, Rice (1988)

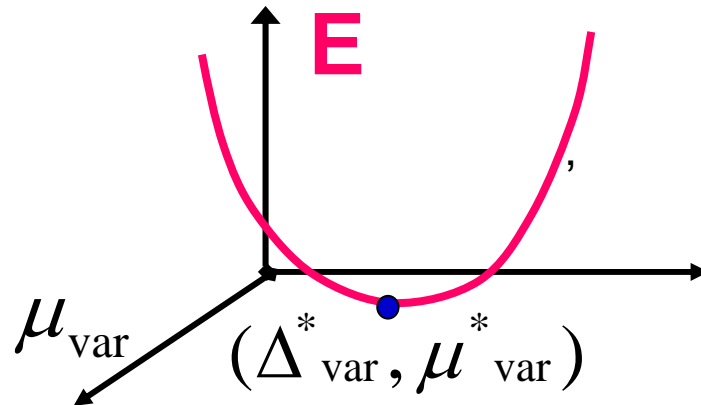
MacDonald, Girvin and Yoshioka (1988)

Variational Monte Carlo

$$\langle \psi_0 | \hat{O} | \psi_0 \rangle = \int dr_{1\uparrow}, dr_{2\uparrow}, \dots, dr_{N/2\uparrow}; dr_{1\downarrow}, dr_{2\downarrow}, \dots, dr_{N/2\downarrow} \\ |\psi(r_{1\uparrow}, \dots, r_{N/2\uparrow}; r_{1\downarrow}, \dots, r_{N/2\downarrow})|^2 \hat{O}(r_{1\uparrow}, \dots, r_{N/2\uparrow}; r_{1\downarrow}, \dots, r_{N/2\downarrow})$$

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

$$E(\Delta_{\text{var}}, \mu_{\text{var}}) = \frac{\langle \psi_0 | H | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle}$$



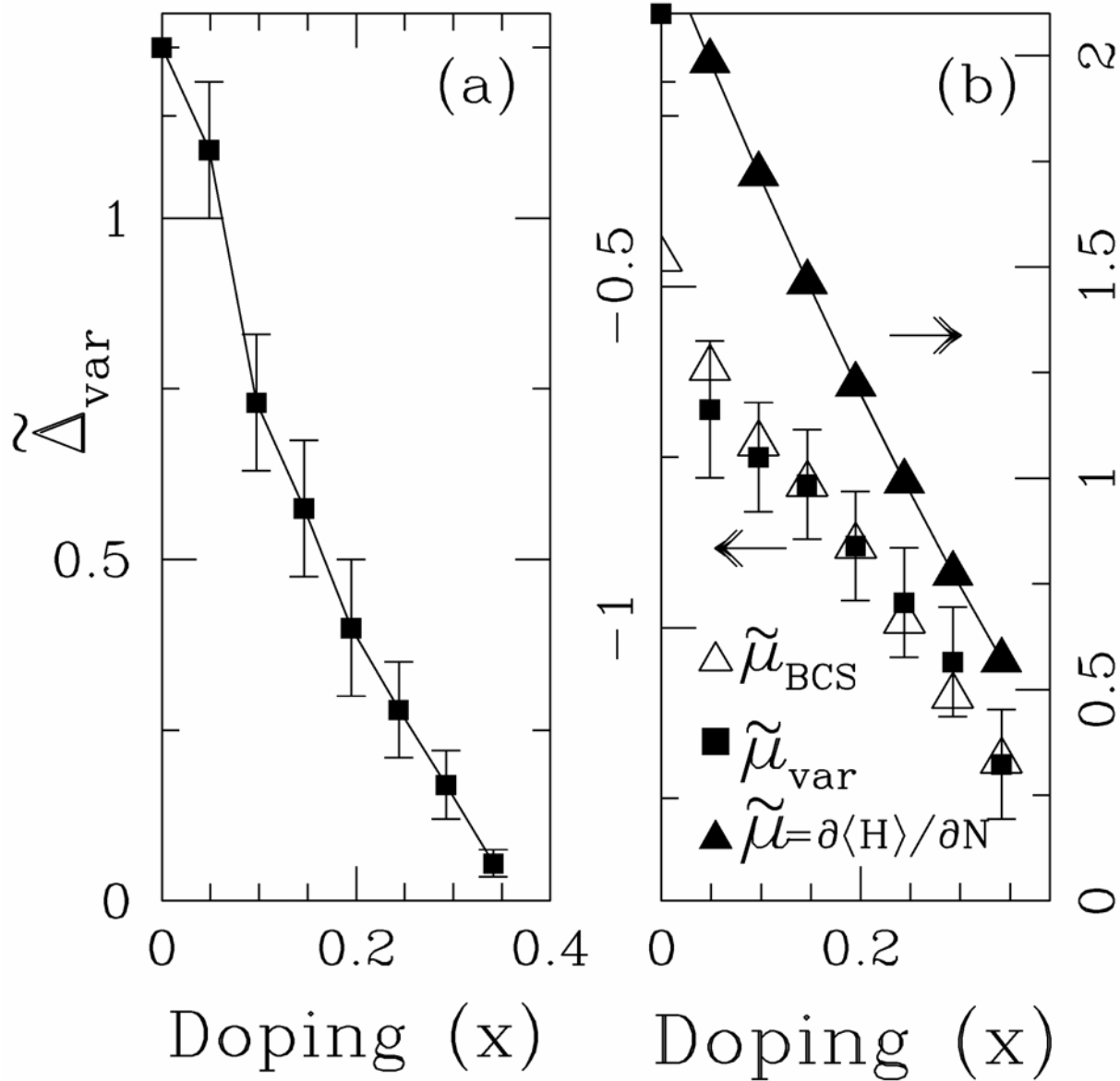
Limitation:

- 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

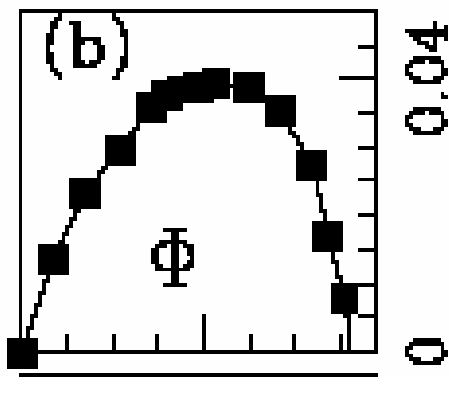
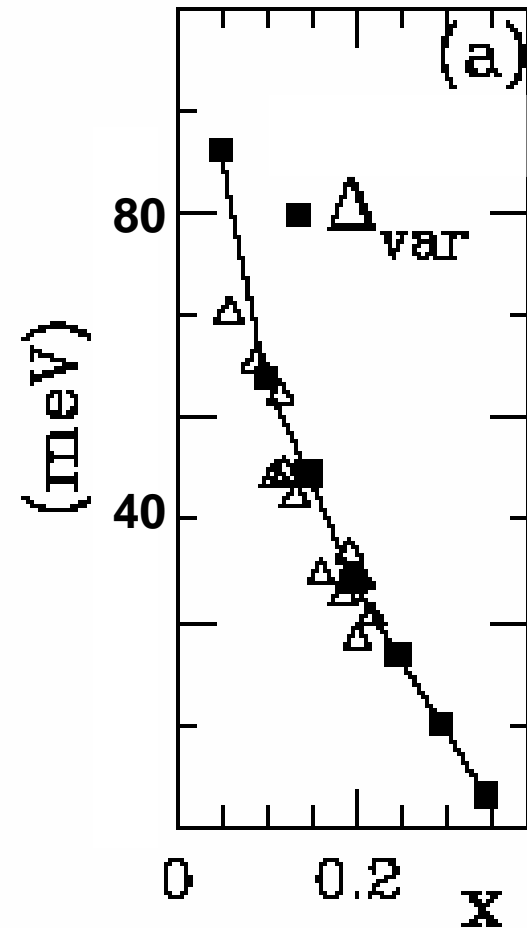
Scale $\sim J$

$\Phi(x)$ = SC order
parameter

Strong
Coulomb 'U'
leads to

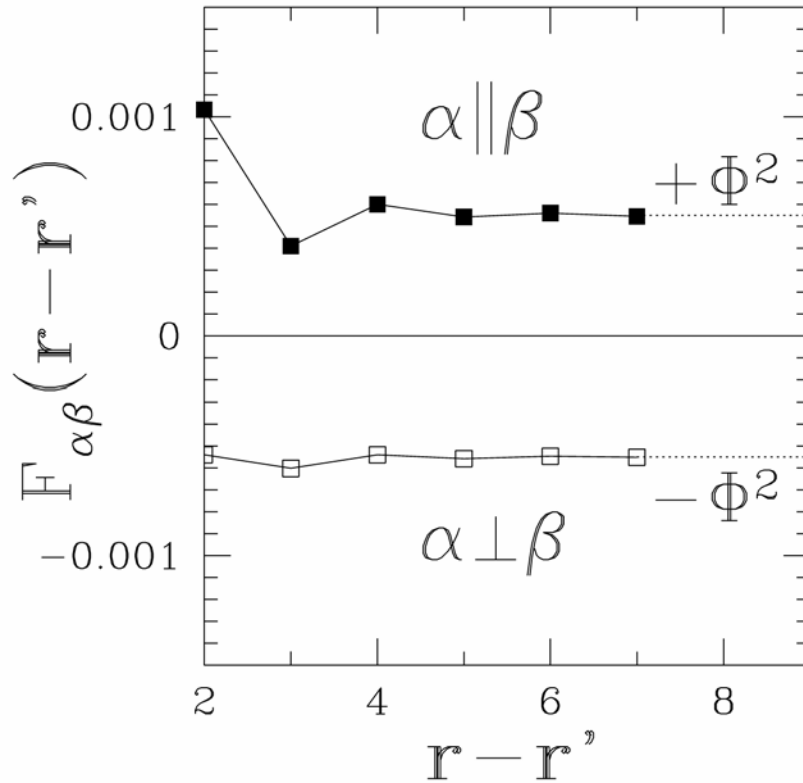
$$\Phi(x) \sim x$$

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



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

OFF DIAGONAL LONG RANGE ORDER



$$\langle C_{r_{\uparrow}}^{+} C_{r+x_{\downarrow}}^{+} C_{r'_{\downarrow}} C_{r'+x_{\uparrow}} \rangle \xrightarrow{|r-r'| \rightarrow \infty} \phi^2$$

SUPERFLUID

Off diagonal long range order

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

In a subspace with fixed number of particles

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

Condensate fraction

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

Diagonal long range order

MAGNET

Magnetization in XY plane

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

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

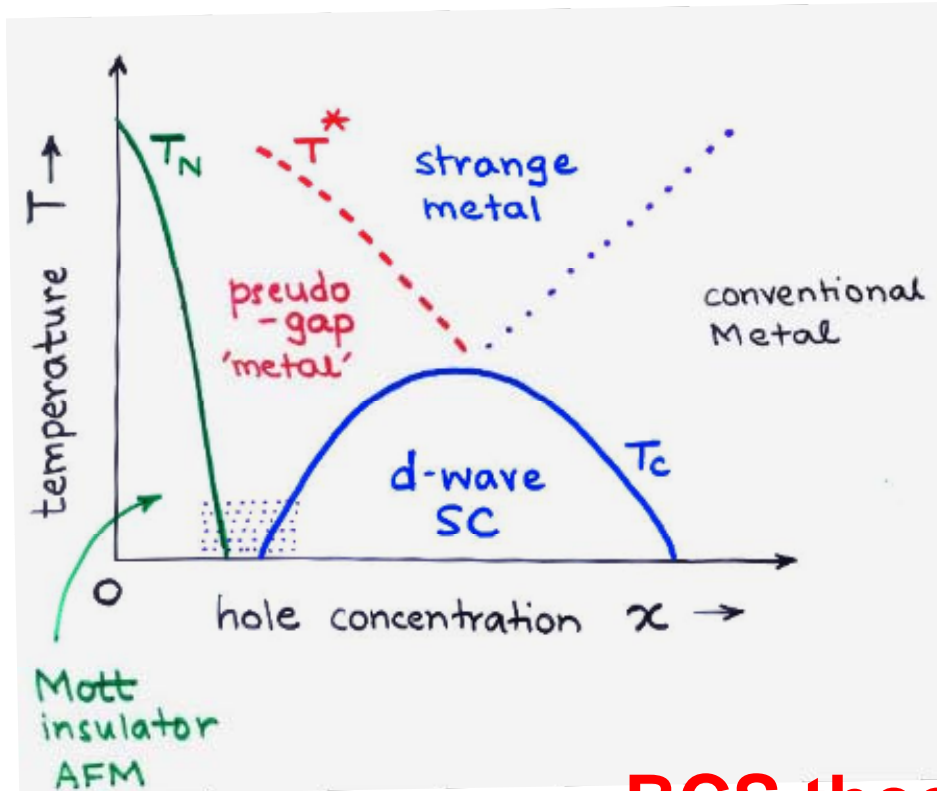
Sublattice magnetization in XY plane

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

Sublattice magnetization along z

Summary of experiments:

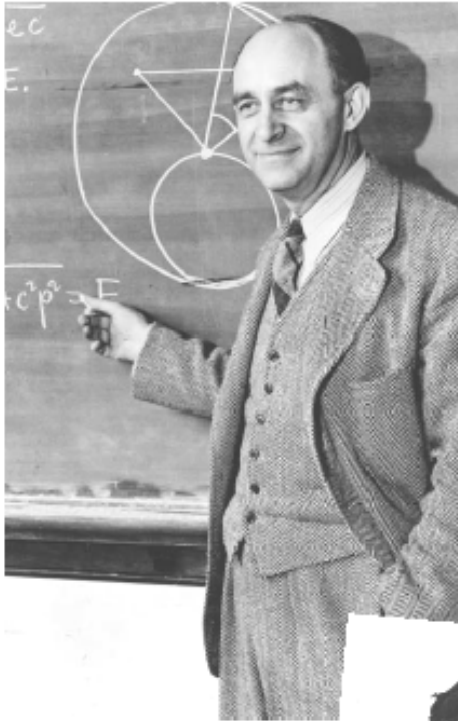
Band theory fails
for $x=0$
parent insulator



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 $x \ll 1$



physical picture, a so strong that not reach your calculation to introduce arbitrariness that are not based on solid physics or solid mathematics. In desperation I was not impressed between our calculated measured numbers many arbitrary parameters for your calculation moment about our and said, "Four." He my friend Johnny we say, with four parallel elephant, and with I wiggle his trunk." Worsation was over. I th time and trouble, an bus back to Ithaca t to the students. Becau for the students to I a published paper, v our calculations. fi

What is the role of theory?

to understand phenomena

to make predictions

Understanding is not curve fitting...

Crossed paths: A discussion with Enrico Fermi (above) made Freeman Dyson (right) change his career direction.

ions a package of our theoretical are- graphs to show to Fermi. tude When I arrived in Fermi's sing office, I handed the graphs to ,and Fermi, but he hardly glanced per- at them. He invited me to sit mics down, and asked me in a tons friendly way about the health recs. of my wife and our new- eak, born baby son, now fifty sses years old. Then he delivered ntly his verdict in a quiet, even voice. "There are were two ways of doing calculations in theoretical



little bags of quarks. B