Physics of Doped Mott-Hubbard Insulators and the High-Temperature Superconductors

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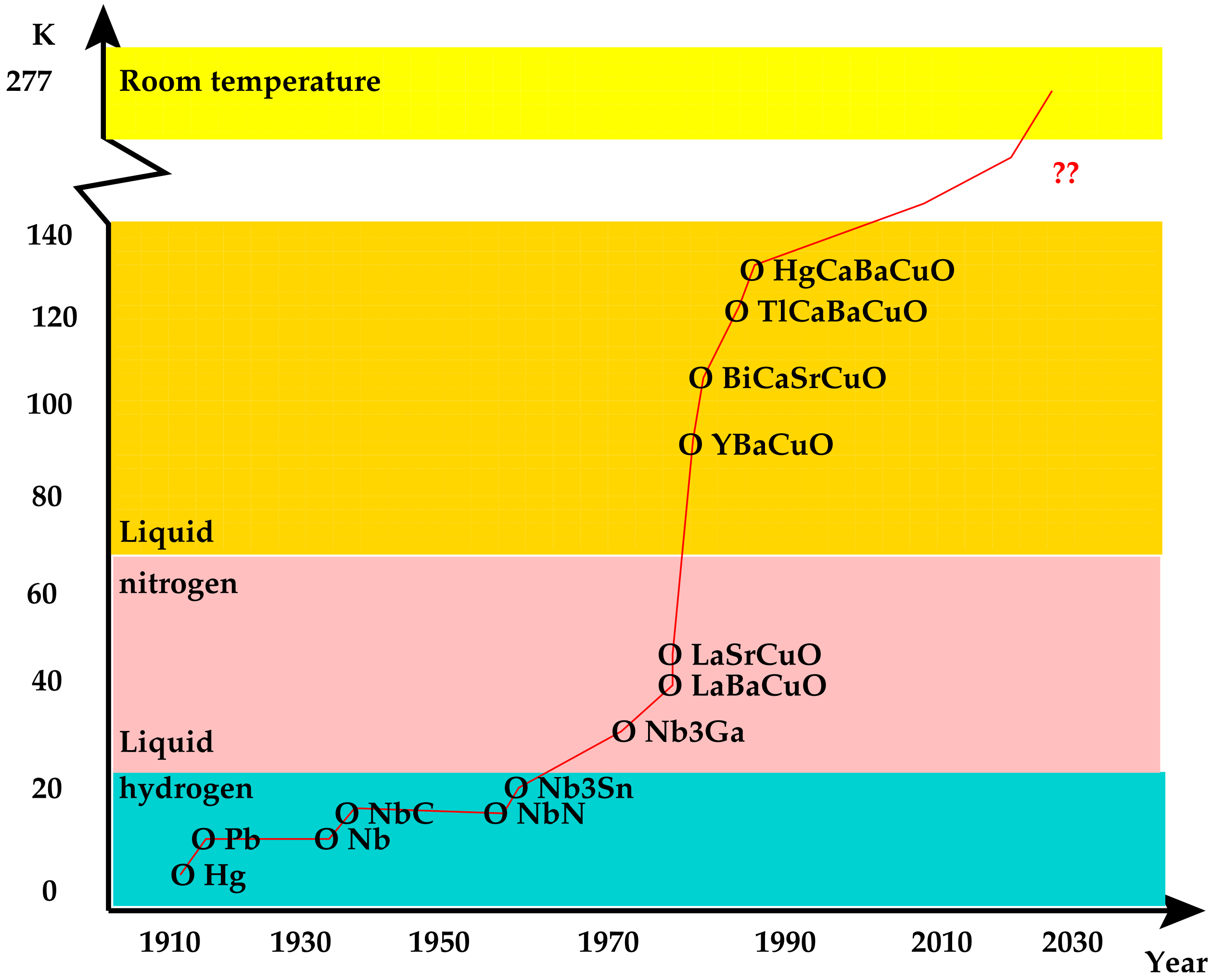
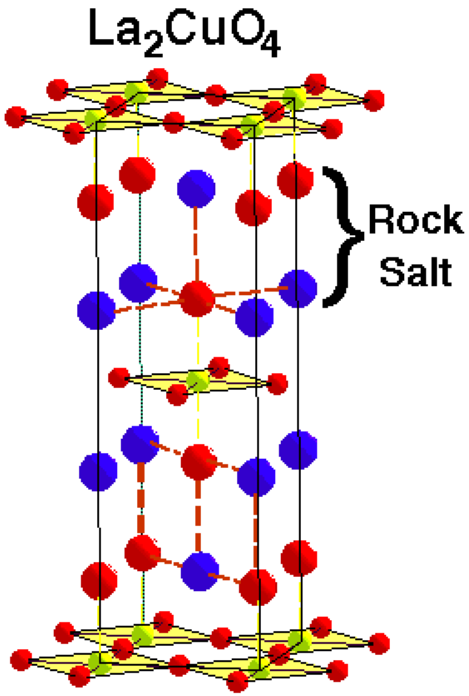
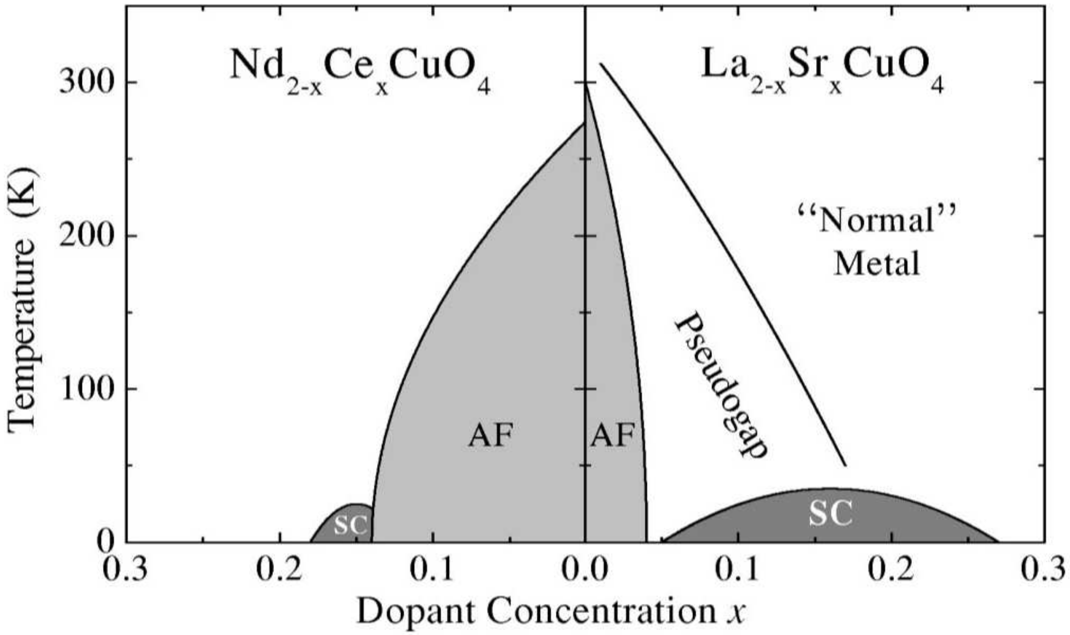
transition temperatures



1986: Discovery by of high-temperature superconductivity by Bednorz & Müller

high-temperature superconductors





novelty

superconductivity in a doped oxide (bad metal)

doped Mott-Hubbard insulator

do AF and SC compete or cooperate?

BCS superconductivity

Bardeen-Cooper-Schrieffer

▷ standard theory for ‘conventional’ superconductors.

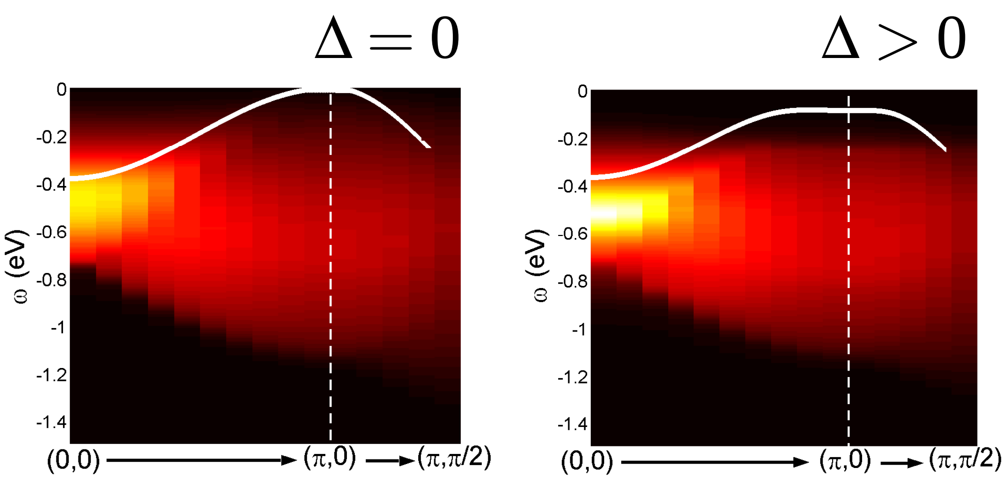
▷ superconductivity $\hat{=}$ pair condensation

$$|\Psi_{BCS}\rangle = \prod_k \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)|0\rangle \qquad u_k^2/v_k^2 = \frac{1}{2}\left(1 \pm \frac{\xi_k}{\sqrt{\xi_k^2+\Delta_k^2}}\right)$$

▷ one-particle dispersion $\xi_k = \frac{\hbar^2 k^2}{2m} - \mu$

Bogoliubov quasiparticles

- dispersion $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$
- gap $\Delta_k \equiv \Delta$ (s-wave)

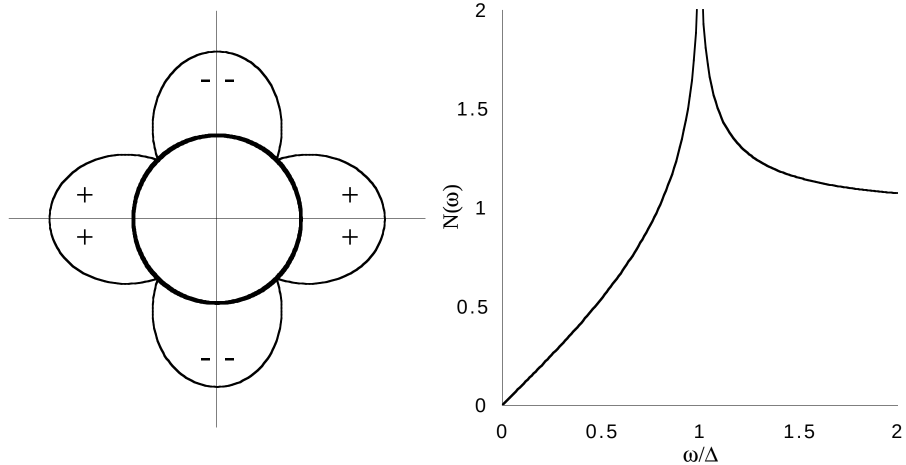


[Edegger, Muthukumar, Gros ‘06]

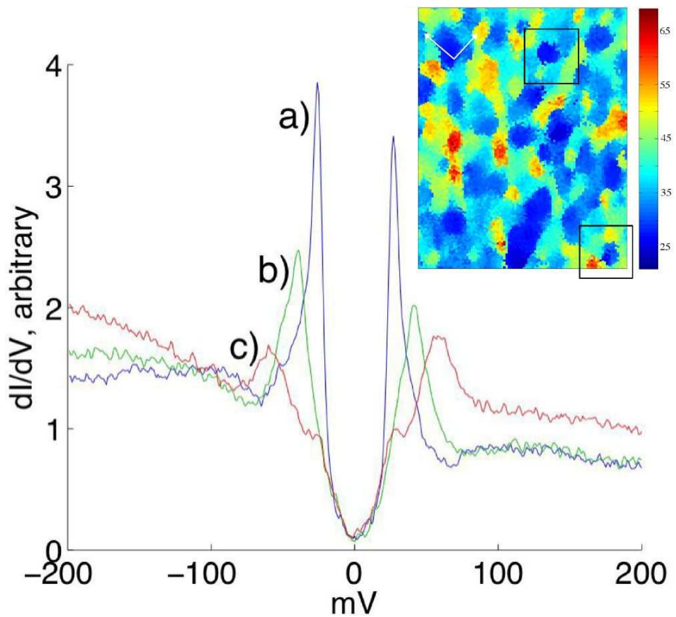
gap-function

$$\Delta_k = \Delta(\cos k_x - \cos k_y)$$

▷ nodes along $(1,1)$ direction



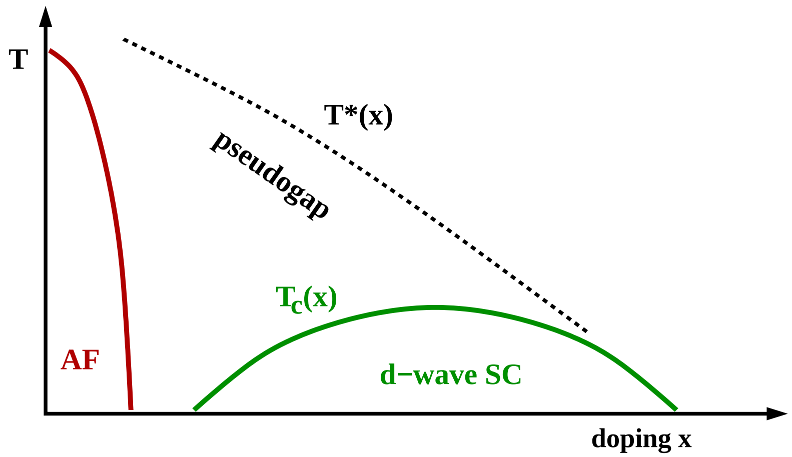
[Fang. et. al. (2005)]

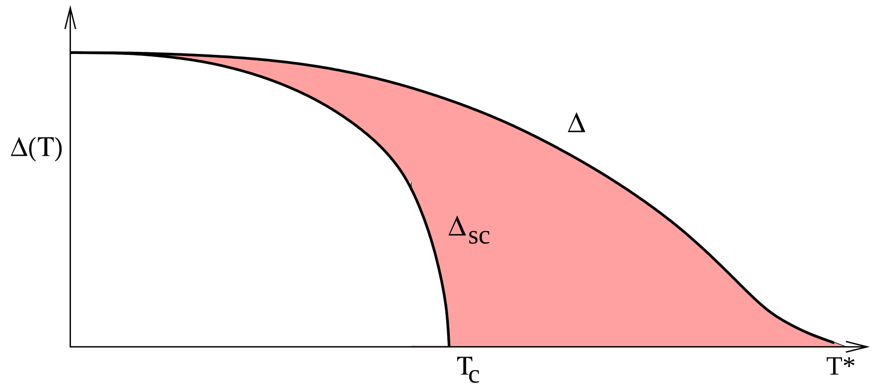


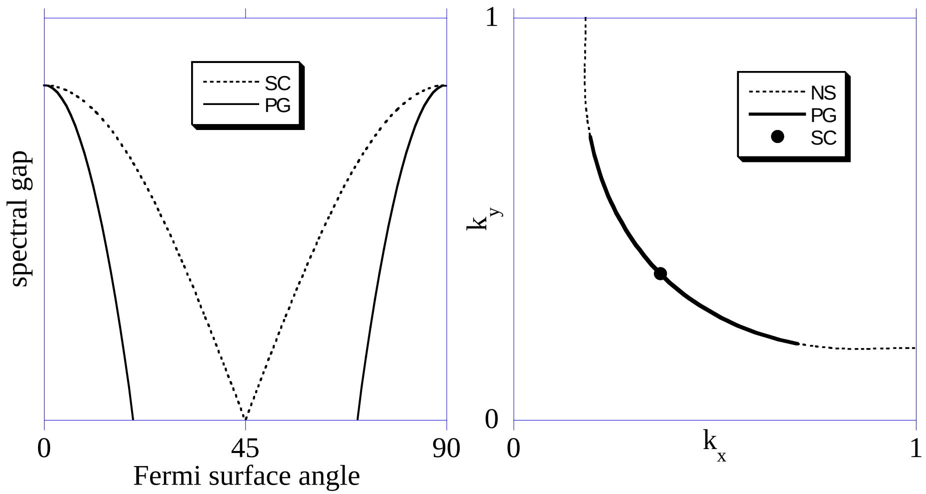
- predicted by theory
  - ▷ correlation-induced superconductivity
- experimental verification
  - ▷ phase-sensitive interference
  - ▷ tunneling, ARPES

key issue: the pseudogap

what happens for $T > T_c$?





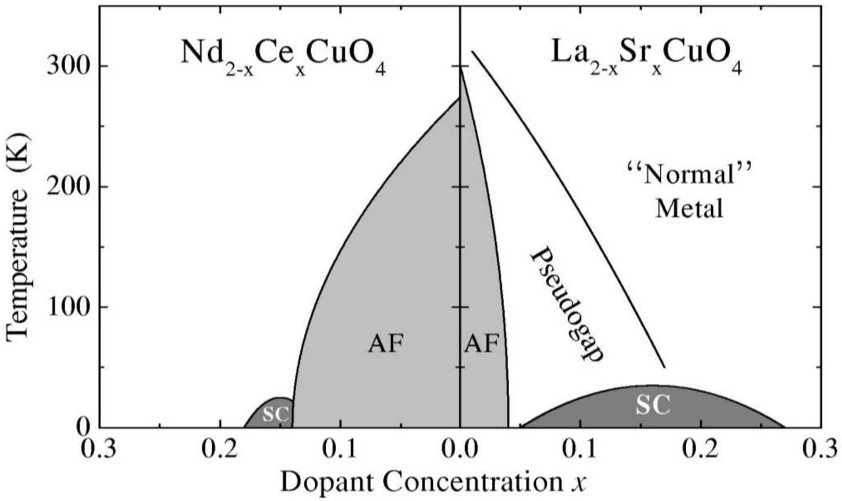


- one-particle excitations
  - ▷ transport, ARPES
  - ▷ pseudo $\Delta_k \approx \Delta(\cos k_x - \cos k_y)$
- Fermi arc

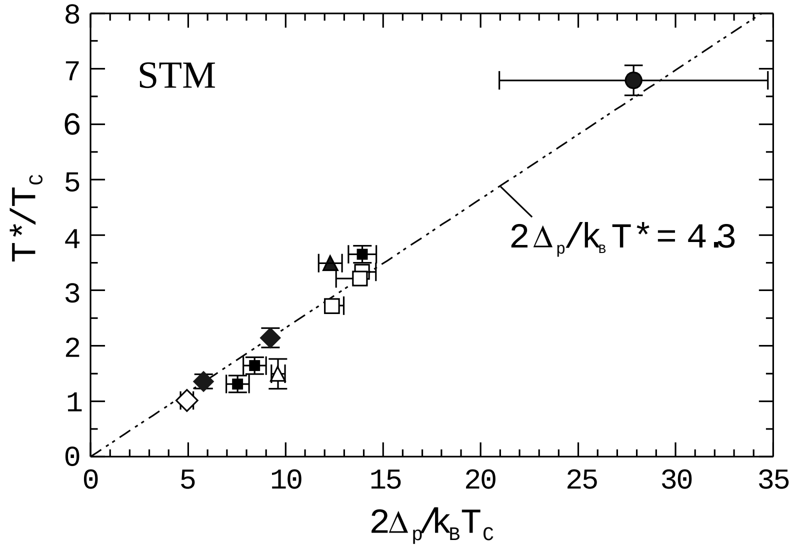
BCS-ratio

- universal for weak-coupling

$$\frac{2\Delta}{k_B T_c} = \begin{cases} 3.52 & \text{s-wave} \\ 4.3 & \text{d-wave} \end{cases}$$



[Kugler, Fischer, Renner, Ono, Ando '01]



- high-temperature superconductors

$$\frac{2\Delta}{k_B T^*} = 4.3$$

doped Mott-Hubbard insulators

$$H = -t \sum_{<i,j>,\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

strong correlation

$U \gg t$: reduced double occupancy

$c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} |0\rangle$ has energy U

low-energy states

$c^\dagger_{i\sigma}|0\rangle$ singly-occupied

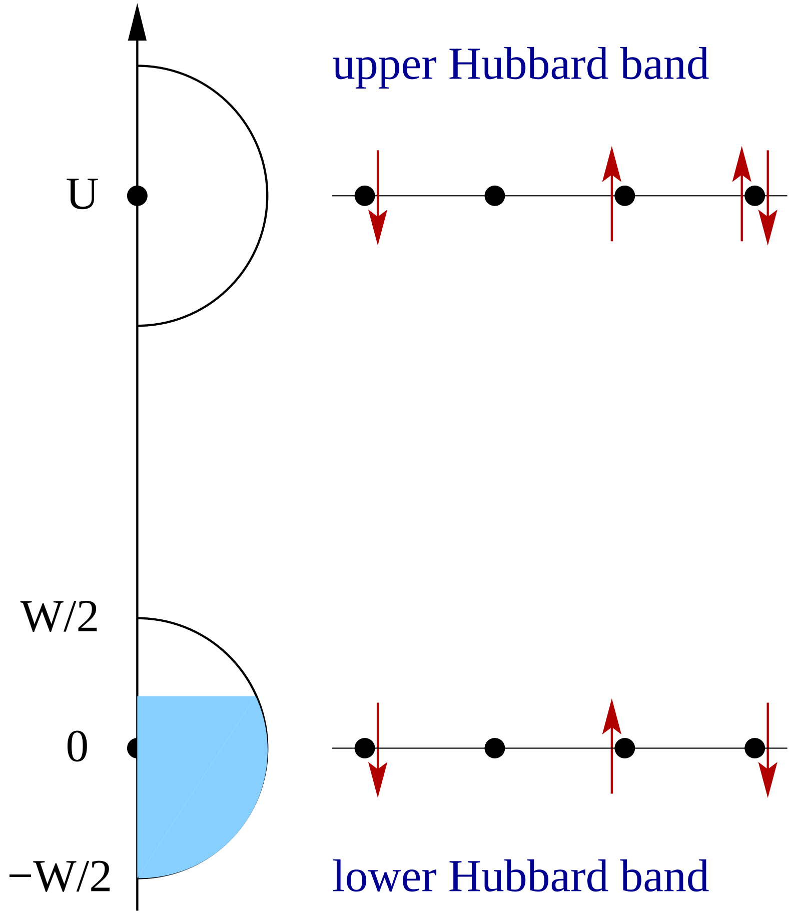
$|0\rangle$ empty sites

low-energy Hamiltonian

canonical transformation

$$H_{t-J} \approx H_{eff} = e^{iS} H e^{-iS}$$

H_{eff} block-diagonal in double-occupancy



canonical transformation

kinetic energy terms

$$T = T_e + T_d + T_+ + T_-$$

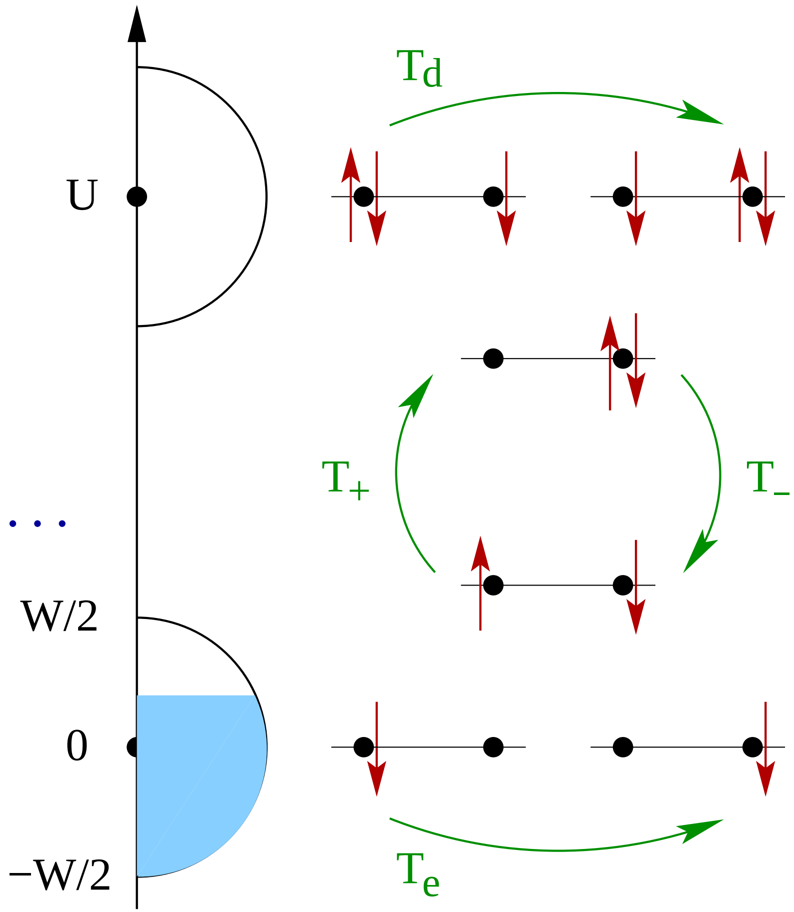
$$H = \left(T_e + T_d + U \textstyle\sum_i n_{i,\uparrow} n_{i,\downarrow}\right) + \left(T_+ + T_-\right)$$

perturbation expansion

$$H_{eff} = \mathrm{e}^{iS} H \mathrm{e}^{-iS} \approx H + i[S,H] + \frac{i^2}{2}[S,[S,H]] + \ldots$$

diagonal in double occupancy $\Rightarrow$

$$S = \frac{i}{U}\left(T_+ - T_-\right) + O(t^2/U^2)$$



projected Hilbert-space

$$H_{t-J} = H_{eff} + O(t^3/U^2) = T_e + T_d + U \textstyle\sum_i n_{i,\uparrow} n_{i,\downarrow} + J \textstyle\sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j$$

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

Gutzwiller approximation

projected wavefunctions

$$|\Psi\rangle = P\,|\Psi_0\rangle = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})\,|\Psi_0\rangle$$

projected Hilbert space : $|\Psi\rangle$

pre-projected Hilbert space : $|\Psi_0\rangle$

renormalization scheme

$$\frac{\langle\Psi|\hat{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \approx g\,\frac{\langle\Psi_0|\hat{O}|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

renormalization factors

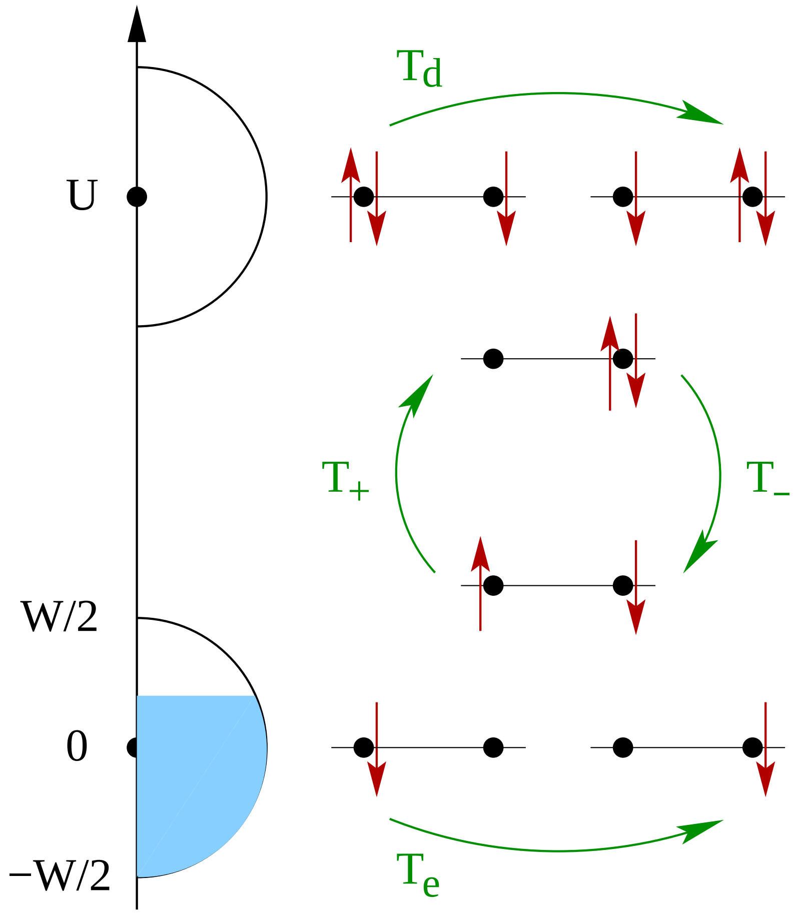
Hilbert-space arguments

Gutzwiller renormalization factors

kinetic energy

$$\frac{\langle\Psi|T_e|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle\Psi|T|\Psi\rangle}{\langle\Psi|\Psi\rangle} \quad \propto \quad n_\sigma(1-n)$$

$$\frac{\langle\Psi_0|T|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} \quad \propto \quad n_\sigma(1-n_\sigma)$$



$$\frac{\langle\Psi|T|\Psi\rangle}{\langle\Psi|\Psi\rangle} \approx g_t \frac{\langle\Psi_0|T|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

$$g_t = \frac{1-n}{1-n_\sigma} = \frac{1-n}{1-n/2}$$

renormalized Hamiltonian

in pre-projected Hilbert space

renormalization scheme

un-projected Hilbert space	Hubbard Hamiltonian

$\Downarrow$ canonical transformation $e^{iS} H e^{-iS}$ $\Downarrow$

projected Hilbert space	t-J Hamiltonian

$\Downarrow$ Gutzwiller renormalization g $\Downarrow$

pre-projected Hilbert space	renormalized Hamiltonian

$$\frac{\langle \Psi | H_{t-J} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \approx \frac{\langle \Psi_0 | H_{t-J}^{(renor)} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

$$H_{t-J}^{(renor)} = g_t T_e + g_s J \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$g_t = \frac{1-n}{1-n/2}, \qquad g_s = \frac{1}{(1-n/2)^2}$$

renormalized molecular-field theory

pre-projected Hilbert-space

$$|0\rangle,\ |\uparrow\rangle,\ |\downarrow\rangle,\ |\uparrow\downarrow\rangle$$

decoupling

$$S_i^+ S_j^- \ = \ c_{i\uparrow}^\dagger c_{i\downarrow} c_{j\downarrow}^\dagger c_{j\uparrow} \ \approx < c_{i\uparrow}^\dagger c_{j\uparrow} > c_{i\downarrow} c_{j\downarrow}^\dagger - < c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger > c_{i\downarrow} c_{j\uparrow} + \ldots$$

molecular fields

hopping-amplitude: $\xi_{i-j} \ = < c_{i\uparrow}^\dagger c_{j\uparrow} >$

pair-amplitude: $\Delta_{i-j} \ = < c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger >$

ground-state wavefunction

BCS-wavefunction

$$|\Psi_0\rangle \ = \ \prod_k \left(u_k + v_k c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger \right) |0\rangle$$

d-wave superconductivity (RMFT)

$$|\Psi_0\rangle = \prod_k \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{k\downarrow}\right)|0\rangle \qquad u_k^2/v_k^2 = \frac{1}{2}\left(1 \pm \frac{\tilde{\varepsilon}_k}{\sqrt{\tilde{\varepsilon}_k^2 + \Delta_k^2}}\right)$$

parameterization

$$\tilde{\varepsilon}_k = \left(-2g_t t + \tfrac{3}{4} g_s J \xi\right)\left(\cos k_x + \cos k_y\right)$$

$$\Delta_k = \tfrac{3}{4} g_s J \Delta \left(\cos k_x - \cos k_y\right)$$

$x \leftrightarrow y$ d-wave symmetry

results

- predicted d-wave superconductivity

[Gros '88]

- contains pseudogap

[Zhang, Gros, Rice, Shiba '88]

strong-coupling approach via RMFT

Hubbard Hamiltonian

canonical transformation $e^{iS} H e^{-iS}$ $\Updownarrow$

t-J Hamiltonian

Gutzwiller renormalization g $\Downarrow$

renormalized Hamiltonian

mean-field decoupling ξ, Δ $\Downarrow$

renormalized mean-field Hamiltonian

ground state $|\Psi_0\rangle$ $\Downarrow$

trial projected wavefunction $|\Psi\rangle = P|\Psi_0\rangle$

Variational Monte Carlo

numerical evaluation

$$\frac{\langle\Psi|H_{t-J}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle\Psi_0|PH_{t-J}P|\Psi_0\rangle}{\langle\Psi_0|PP|\Psi_0\rangle}$$

[Zhang, Gros, Rice, Shiba '88]

variational Monte Carlo (VMC)

fixed particle number

$$|\Psi_0^N\rangle = P_N \prod_k \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{k\downarrow} \right) |0\rangle = \text{const.} \times \Big(\underbrace{\sum_{r,r'} a(r-r') c^\dagger_{r\uparrow} c^\dagger_{r'\downarrow}}_{\text{pair wavefunction}} \Big)^{N/2} |0\rangle$$

$$a(\delta r) = \sum_k \frac{v_k}{u_k} e^{ik\delta r}$$

matrix elements

$$\frac{\langle\Psi|\hat{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_{\alpha,\beta} \langle\alpha|\hat{O}|\beta\rangle \frac{\langle\Psi|\alpha\rangle\langle\beta|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \sum_\alpha \left(\sum_\beta \frac{\langle\alpha|\hat{O}|\beta\rangle\langle\beta|\psi\rangle}{\langle\alpha|\psi\rangle} \right) \frac{|\langle\alpha|\Psi\rangle|^2}{\langle\Psi|\Psi\rangle} \equiv \sum_\alpha f(\alpha)\,\rho(\alpha)$$

Monte Carlo walk

weight: $\rho(\alpha)$
method: update of inverse determinants $\langle\alpha|\Psi\rangle$

order-parameter renormalization

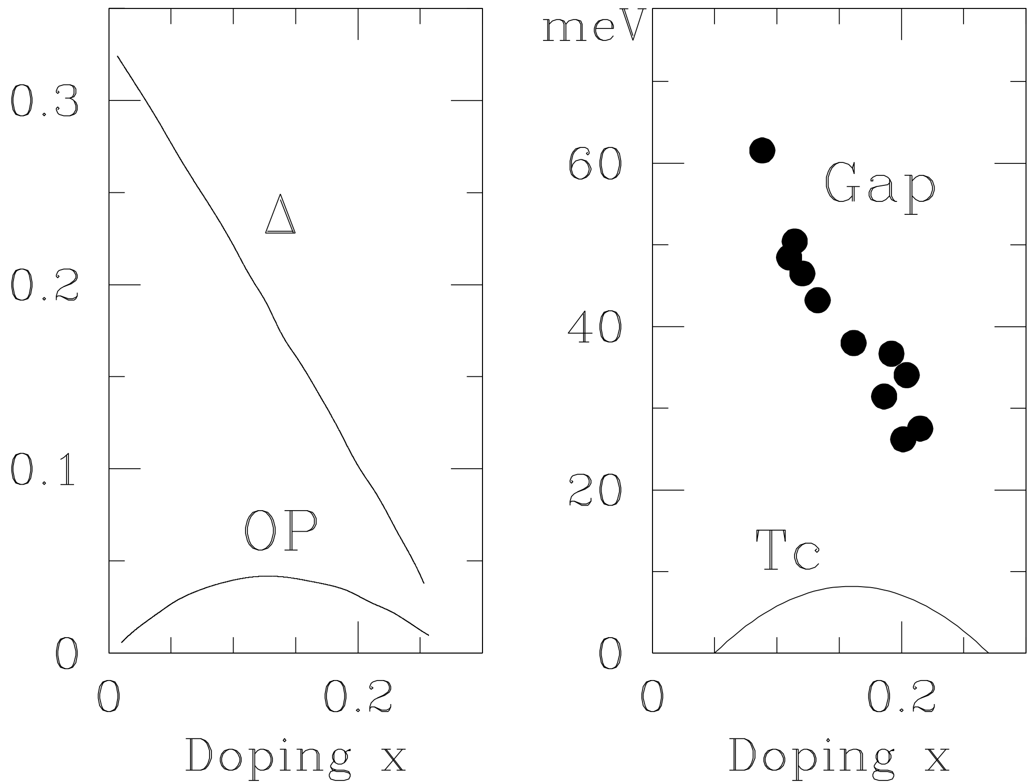
$$< c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} >_\psi = g_t < c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} >_{\psi_0}$$

$$< \Delta >_\psi = g_t < \Delta >_{\psi_0}$$

- Hubbard-U suppresses particle-number fluctuations

$$g_t = \frac{1-n}{1-n/2}$$

[Anderson *et al.* '04]

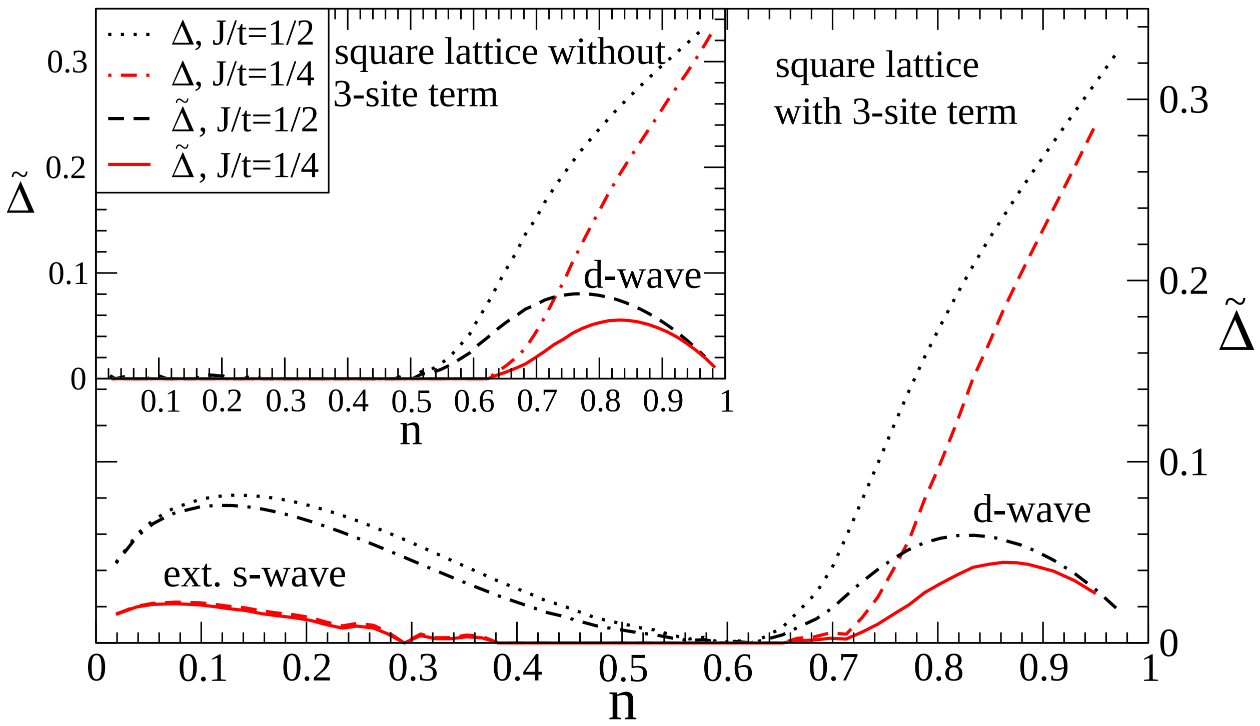


phase diagram

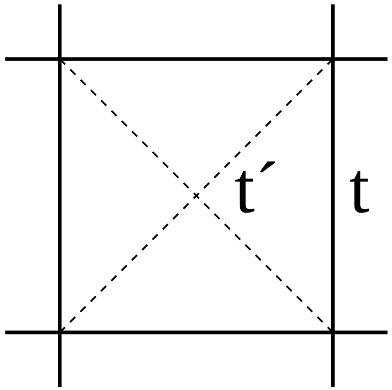
2D t-J model

$$H_{t-J} = \sum_{<i,j>,\sigma} t_{(i,j)} \left(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + \sum_{<i,j>} \frac{4t_{(i,j)}^2}{U} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right)$$
$$- \sum_{\sigma,\sigma'} \sum_{<i,j>,<j,l>} \frac{t_{(i,j)} t_{(j,l)}}{U} \left(c_{i\sigma}^\dagger c_{j\sigma} c_{j\sigma'}^\dagger c_{l\sigma'} + k.k. \right)$$

[Edegger, Gros, Muthukumar '05]

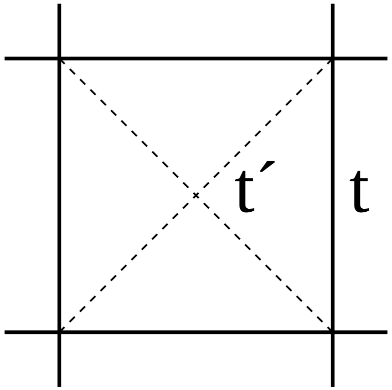


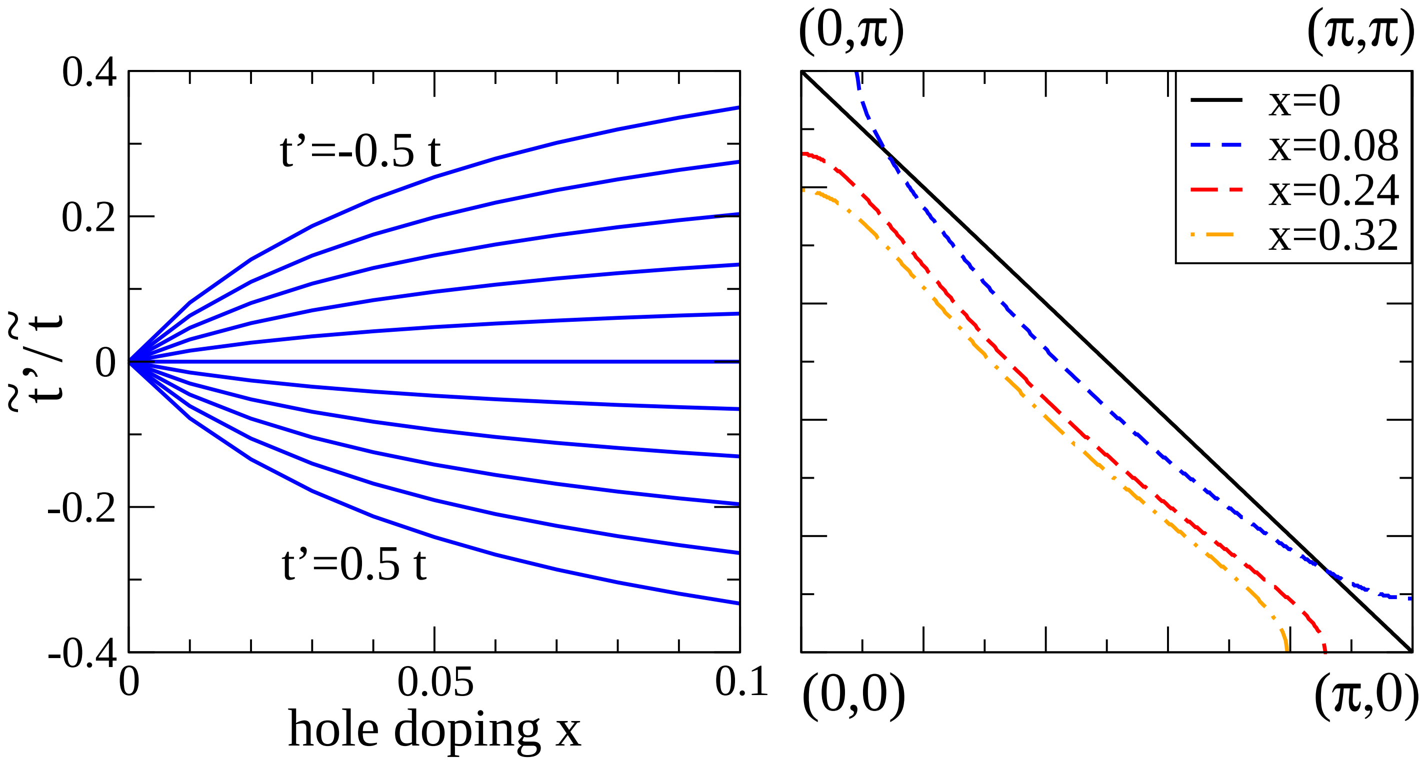
HTSC: $t_2/t_1 \approx 1/3$



renormalization towards perfect nesting

RMFT $\lim_{n\to 1} \begin{cases} \tilde{t} = (t)_{\text{renorm}} & \to & J \\ \tilde{t}' = (t')_{\text{renorm}} & \to & 0 \end{cases}$





$t' = -t/4, \; U = 12t$

[Gros, Edegger, Muthukumar & Anderson, PNAS ‘06]

Luttinger vs. Fermi surface

gap / pseudogap

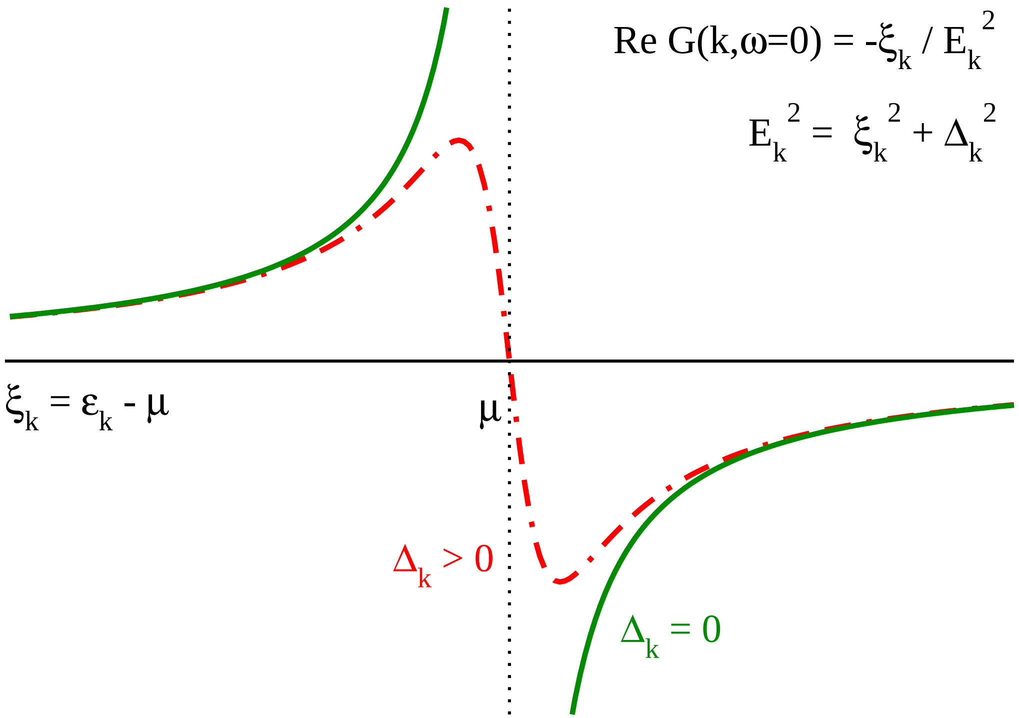
- Fermi surface (FS) not defined
- underlying Fermi surface = ?

Luttinger surface

- $ReG(k,\omega=0)$ changes sign
- underlying Fermi surface
  ≙ Luttinger surface

BCS superconductor

$$\mathrm{Re}\,G(k,\omega=0) \;=\; -\frac{\xi_k}{E_k^2}$$

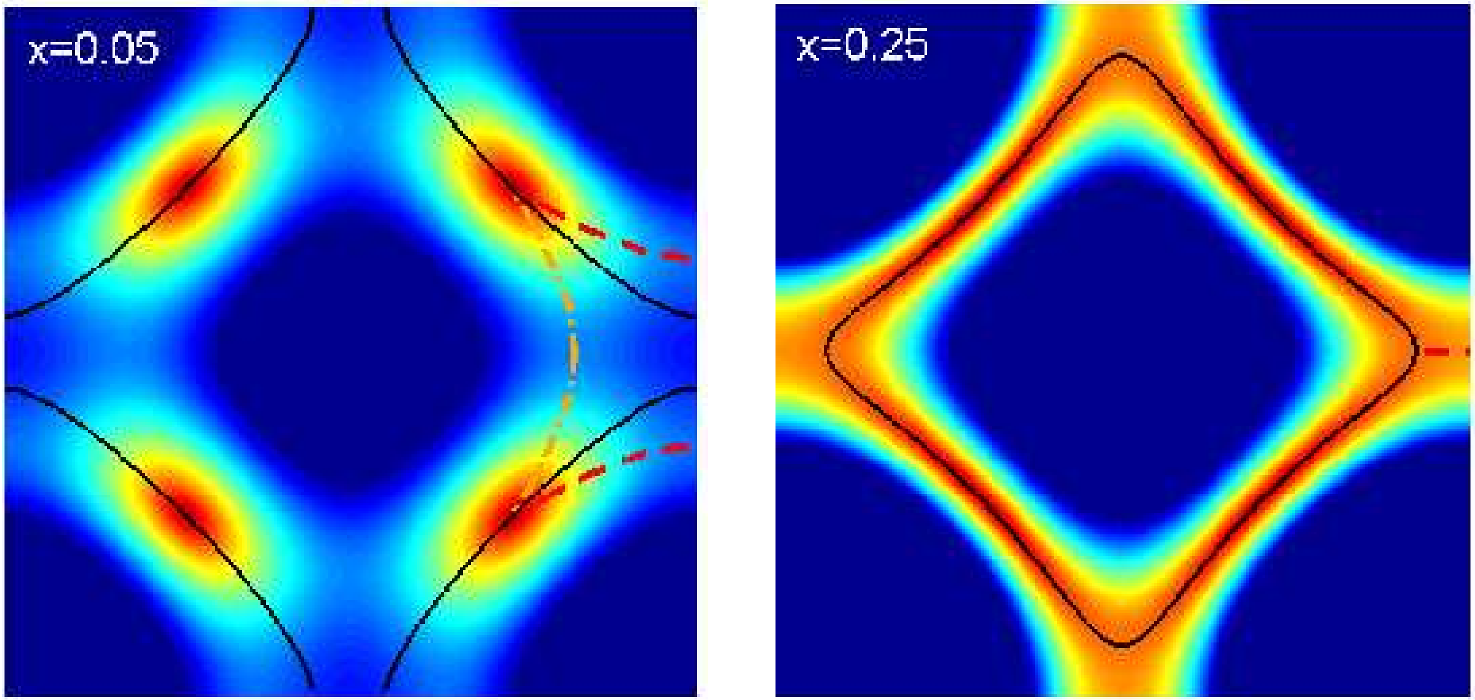


Fermi surface determination

large, momentum dependent gap Δ_k

'underlying Fermi surface' $\hat{=}$ Luttinger surface

- $ReG(k,\omega)$ changes sign



intensity plots

$$\sim \frac{\Gamma}{E_k^2 + \Gamma^2}$$

$$E_k = \sqrt{\xi_k^2 + \Delta_k^2}$$

line $\equiv$ Luttinger surf.

[Gros, Edegger, Muthukumar & Anderson, PNAS '06]

nodal Fermi velocity

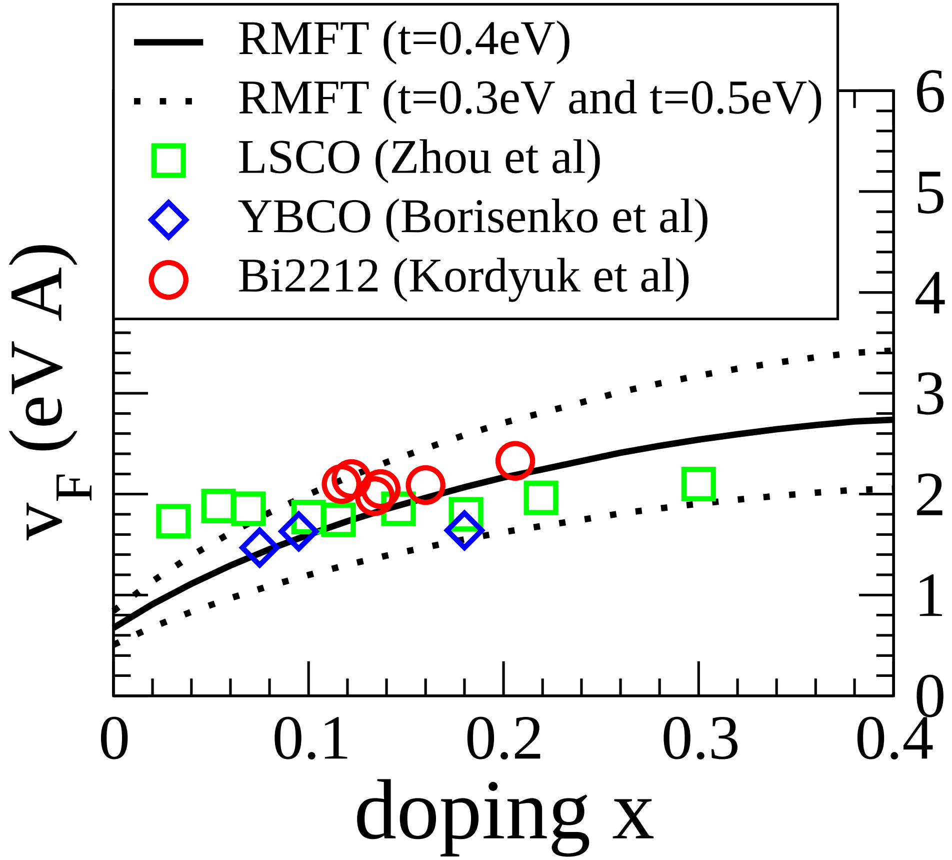
- nodes along $(1,1)$ direction

$$v_F = \frac{d\varepsilon(k)}{dk} \approx \frac{m}{m^*}$$

- RVB-Gutzwiller

$$\lim_{U/t\to\infty}\lim_{n\to1} v_F \propto J = 4\frac{t^2}{U}$$

[Edegger, Muthukumar, Gros, Anderson '06]



experiment & theory

$$\lim_{U/t\to\infty}\lim_{n\to1} v_F \longrightarrow \text{const}$$

nodal quasiparticle weight renormalization

one particle Greens function

$$G(k,\omega) = \frac{1}{\omega - \xi_k - \Sigma(k,\omega)} \approx \frac{Z}{\omega - v_F(k-k_F) + i\delta_k} + G_{inc}(k,\omega)$$

- quasiparticle weight

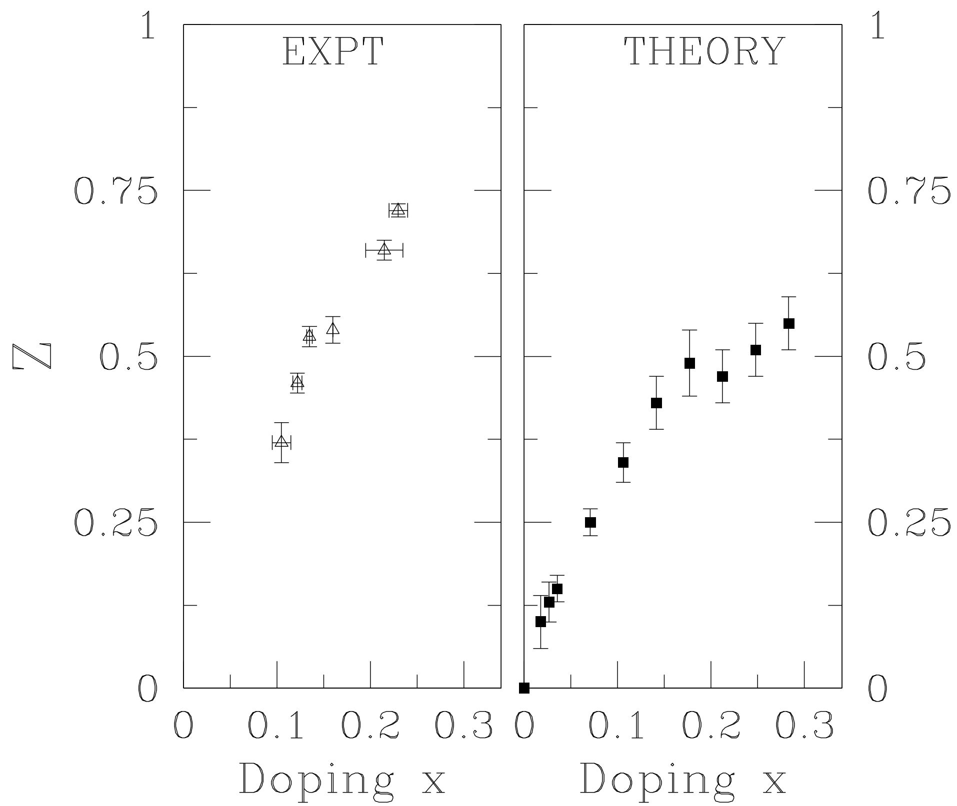
$$Z = \frac{1}{1 - \partial Re\Sigma/\partial\omega}$$

- Fermi velocity

$$v_F = Z\left(v_F^0 + \frac{\partial Re\Sigma}{\partial k}\right)$$

[Johnson *et al.* ‘01]

[Randeria, Paramekanti, Trivedi ‘04]



theory & experiment(?)

$$\lim_{U/t\to\infty} \lim_{n\to 1} Z \to 0$$

diverging momentum dependence of self energy

theory & experiment

$$\lim_{U/t\to\infty}\lim_{n\to 1} v_F \longrightarrow \text{const}$$

$$\lim_{U/t\to\infty}\lim_{n\to 1} Z \longrightarrow 0$$

- Fermi velocity

$$v_F = Z\left(v_F^0 + \frac{\partial Re\Sigma}{\partial k}\right)$$

singular momentum dependence (nodal)

$$\lim_{U/t\to\infty}\lim_{n\to 1} \frac{\partial Re\Sigma}{\partial k} \propto \frac{1}{x} \longrightarrow \infty$$

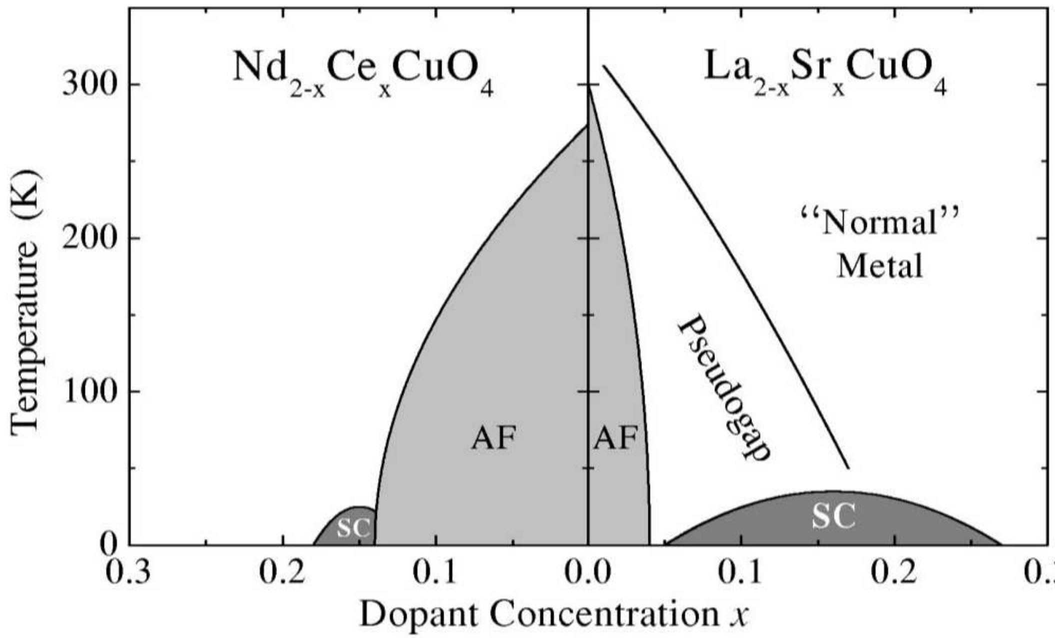
- doping $x = 1 - n$

physics of HTSC within RVB/RMFT

correlations

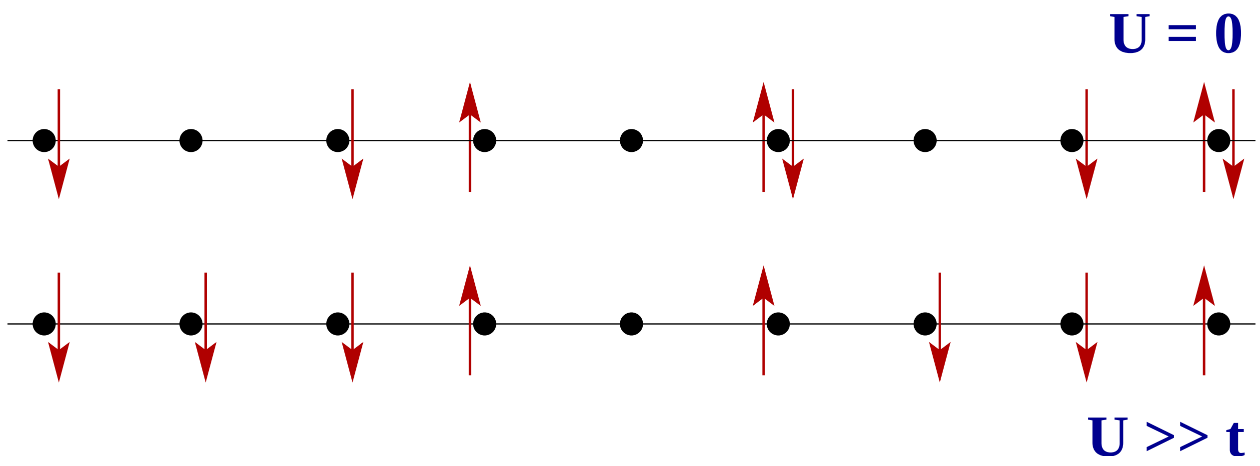
- induce antiferromagnetism — at half-filling
- induce superconductivity — at finite doping
- suppress particle-number fluctuations — close to half-filling
  - ▷ suppress long-range superconductivity — close to half-filling
  - ▷ lead to the pseudogap phase — close to half-filling

$$T_c \propto (1-n)J$$



Mottness and enhanced phase fluctuations

reduction of particle-number fluctuations by strong correlations

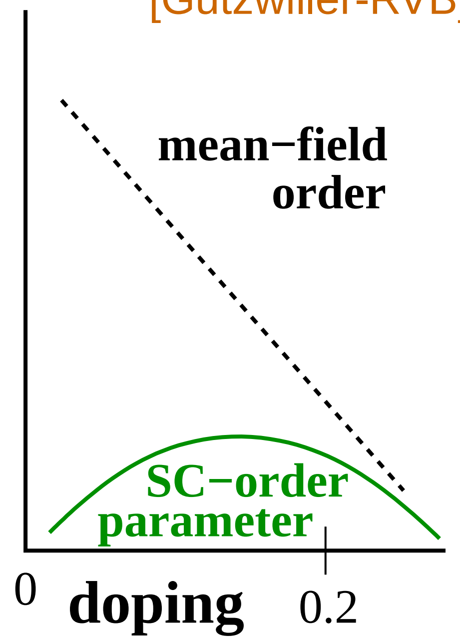


canonical conjugate variables $\langle \Delta N \rangle \langle \Delta \varphi \rangle \approx 1$

phase φ

particle number N

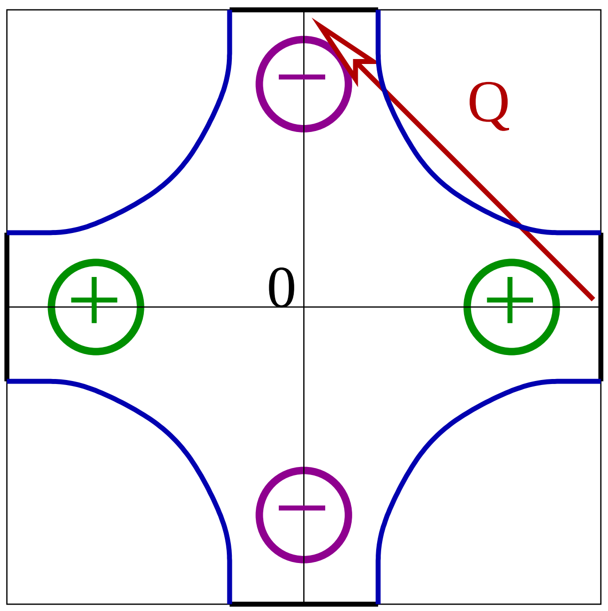
[Gutzwiller-RVB]



$$\left(\lim_{U/t \to \infty} \lim_{n \to 1} \langle \Delta N \rangle \to 0 \right) \Longleftrightarrow \left(\lim_{U/t \to \infty} \lim_{n \to 1} \langle T_c \rangle \to 0 \right)$$

- Mottness results in diverging phase fluctuations

why two dimensions?



antiferromagnetic nesting vector

- 3 dimensions $\mathbf{Q} = (\pi, \pi, \pi)$
- 2 dimensions $\mathbf{Q} = (\pi, \pi)$

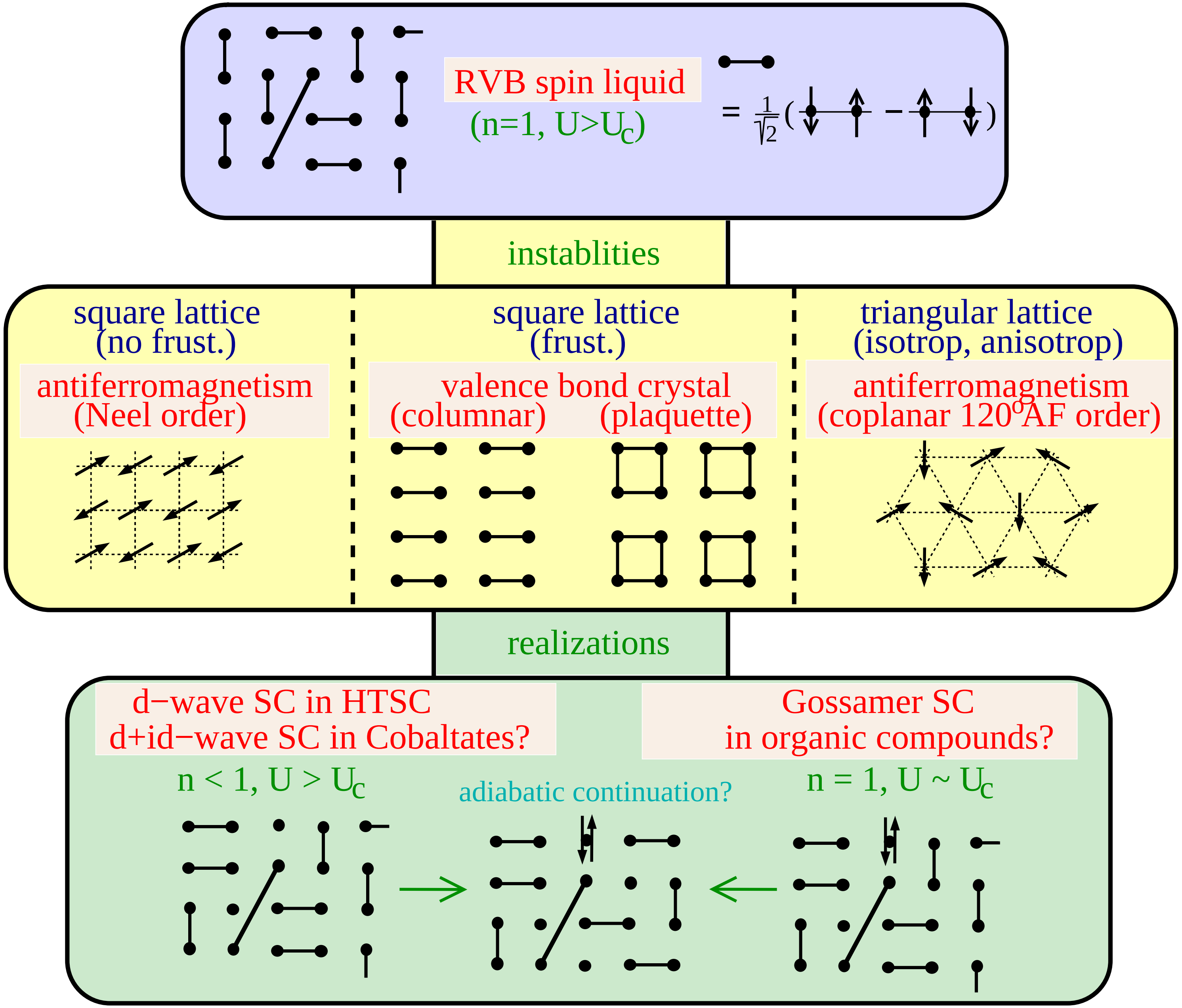
BCS gap-equation

$$\Delta_{\mathbf{k}} \;=\; -\int \frac{d^2 p}{(2\pi)^2} V_{\mathbf{k}-\mathbf{p}} \frac{\Delta_{\mathbf{p}}}{\sqrt{\xi_{\mathbf{p}}^2 + \Delta_{\mathbf{p}}^2}}$$

repulsive interaction

- $\boxed{V_{\mathbf{k}-\mathbf{p}} \;\propto\; J \;>\; 0}$
- scattering between hot-spots $(\pi, 0)$ and $(0, \pi)$ via $\mathbf{Q} = (\pi, \pi)$
  - ▷ d-wave: $\boxed{\Delta_{(\pi,0)} = -\Delta_{(0,\pi)}}$

RVB as a unstable fixpoint



RVB: applications and generalizations

high-temperature superconductors

- phase-diagram, quasi-particles, ARPES, ...
  [Randeria, Trivedi, Dagotto, Sorella, Lee, Ivanov, ...]
- stripes and dynamics
  [Seibold, Lorenzana, ...]
- ‘Gossamer superconductivity’
  [Laughlin, ...]

other correlated systems

- cobaltates and organic superconductors
  [McKenzie, Zhang, Baskaran, Trivedi, Ogata, Schmalian ...]
- frustrated magnets
  [Mila, Giamarchi, ...]
- multi-orbitals and magnetism in Fe, Ni
  [Weber, Gebhard, Bünemann, ...]

theories for HTSC

microscopic approaches

- strong coupling: RMFT and projected wavefunctions
  [Anderson, Lee, Zhang, Trivedi, Gros, ...]
- weak coupling: spin fluctuations
  [Pines, ...]
- phonons: favor s-wave
  [Müller, Shen, ...]

phenomenological approaches

- SU(5): between SC and AF order parameter
  [Zhang, Hanke, ...]
- stripes: charge vs. spin ordering, 1/8-doping
  [Kivelson, Zaanen, ...]
- marginal Fermi liquid: scattering rate in normal state $\propto |\omega|$
  [Varma, ...]

after 20 years of HTSC

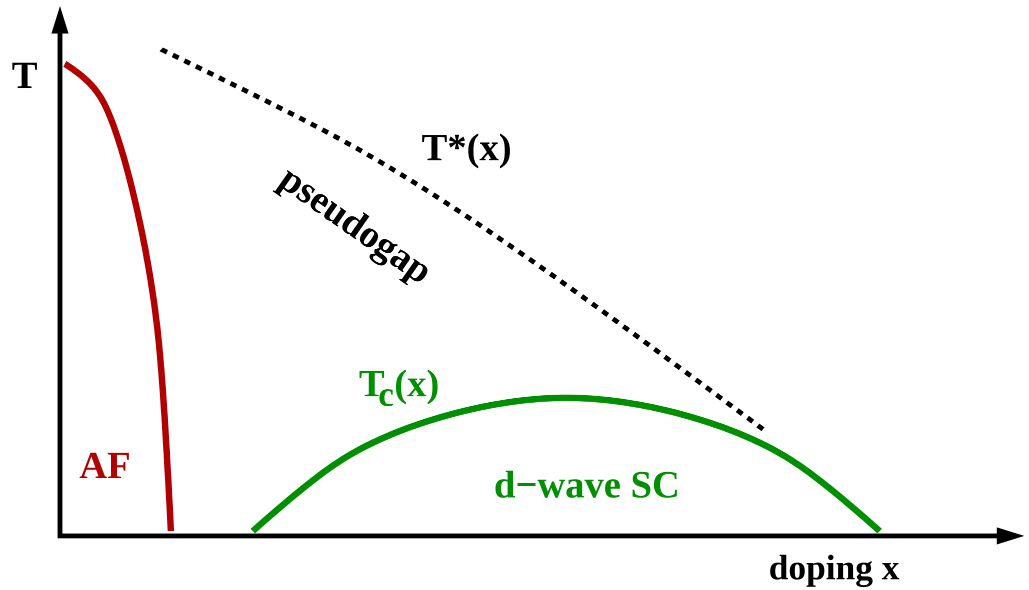
some established facts

- condensed state: correlated d-wave, e.g. $P_G|BCS\rangle$
- antiferromagnetism drives SC: $T_c \sim J \approx 1400\text{K}$
- absence of exchange bosons: ($\nexists$ weak coupling) $\Rightarrow$ preformed pairs

RVB-Gutzwiller

key open question

- theory for pseudogap state
  - spin-gap
  - phase-fluctuations
  - Fermi-arc

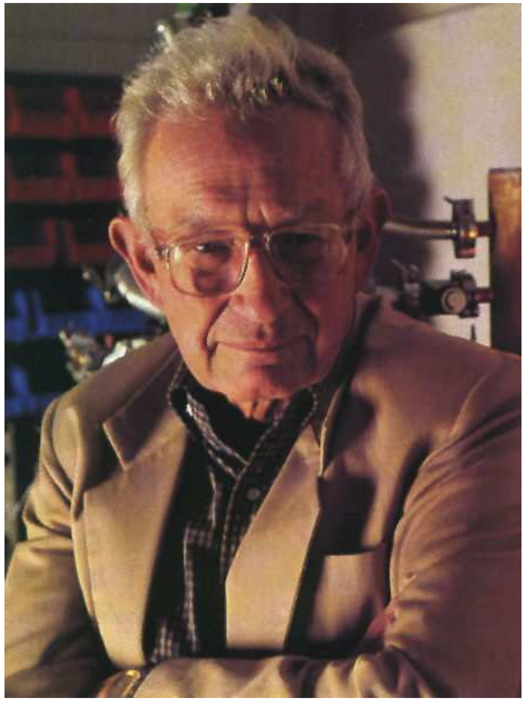


thanks

It's all fun together with ...

Bernhard Edegger

V.N. Muthukumar



P.W. Anderson