

# **Renormalization of the band structure and of the underlying Fermi surface in strongly correlated superconductors**

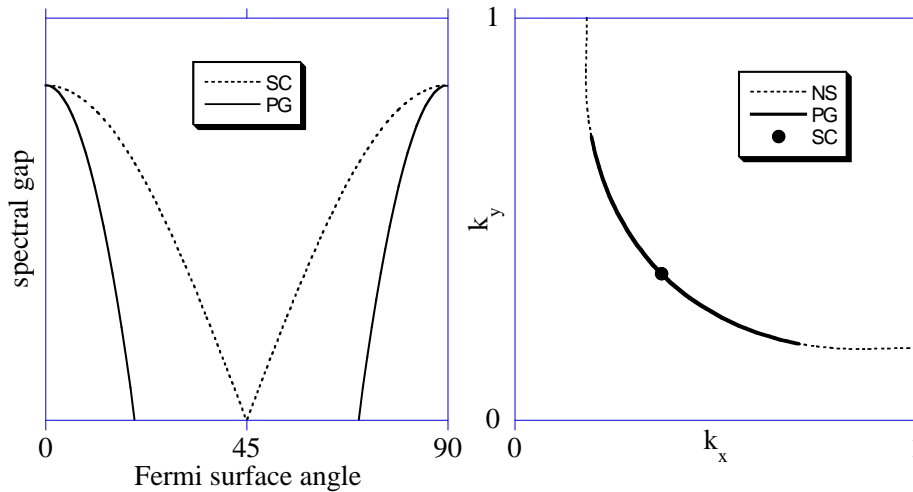
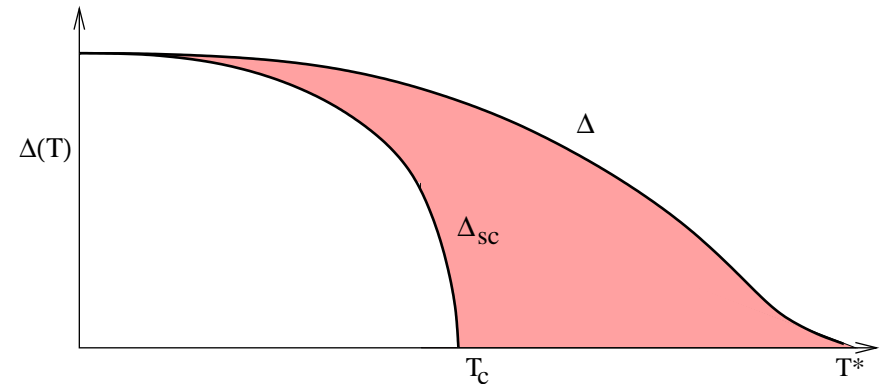
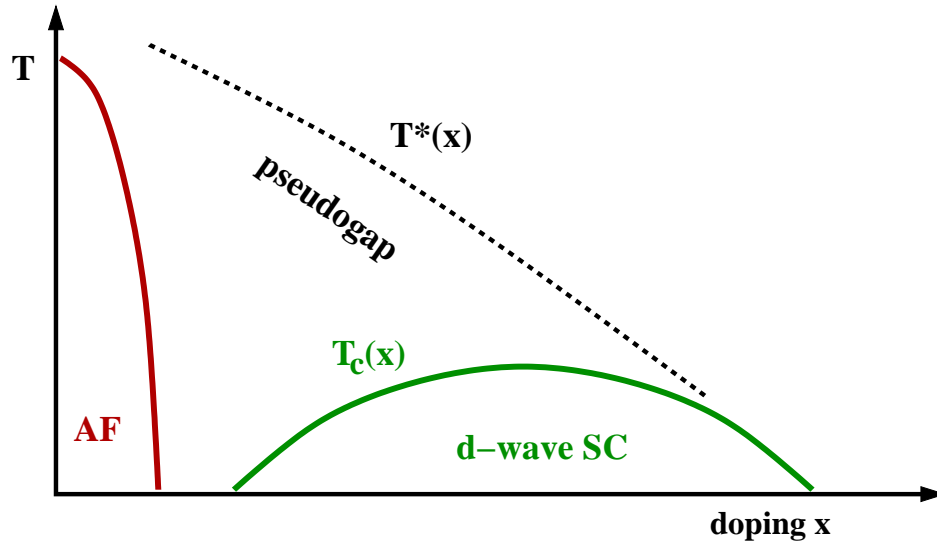
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**Claudius Gros**

J.-W. Goethe University Frankfurt

# the pseudogap phase

What happens for  $T > T_c$ ?

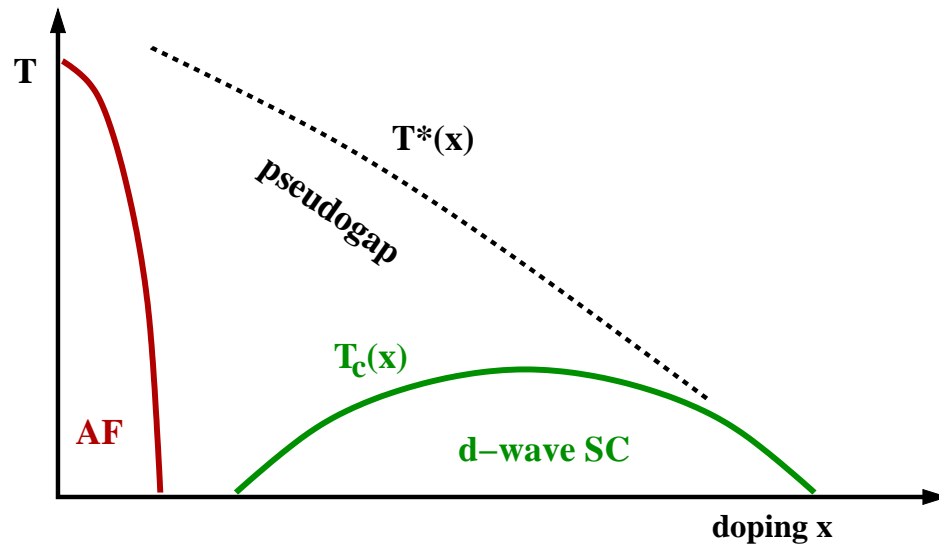


- one-particle excitations
- ▷ transport, ARPES
- ▷ pseudo  $\Delta_k \approx \Delta(\cos k_x - \cos k_y)$

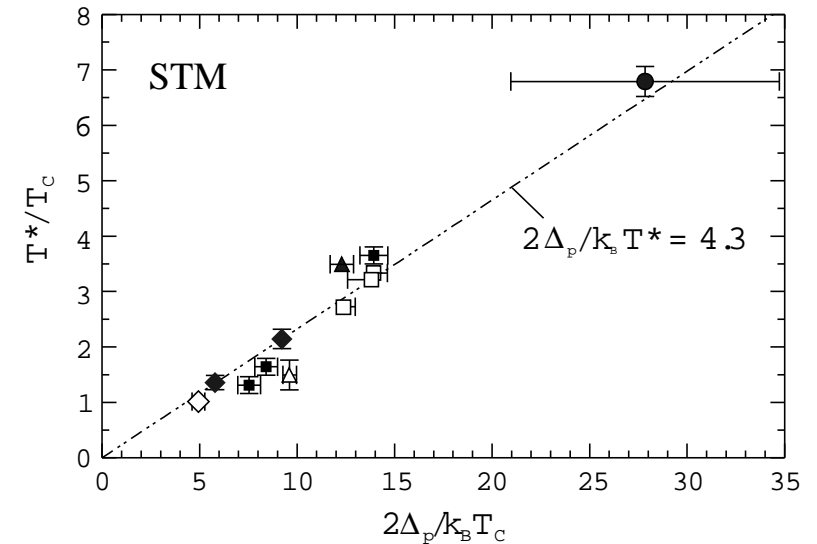
# BCS ratio and preformed pairs

- 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

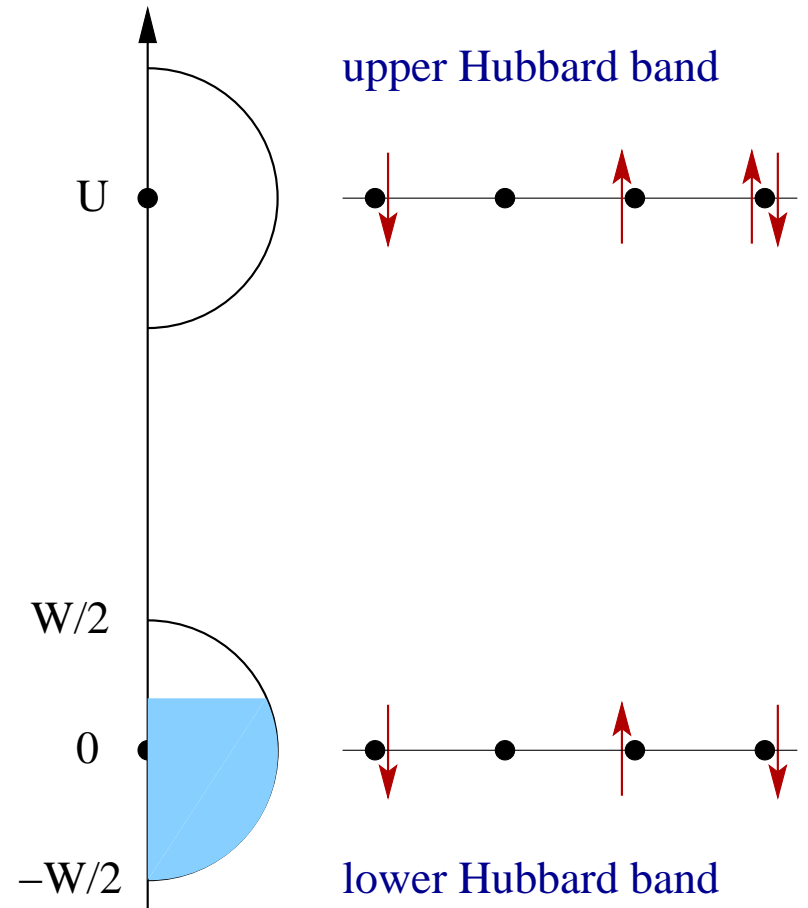
$$H = -t \sum_{\langle i,j \rangle, \sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

## strong correlation

$U \gg t$  : reduced double occupancy  
 $c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger |0\rangle$  has energy  $U$

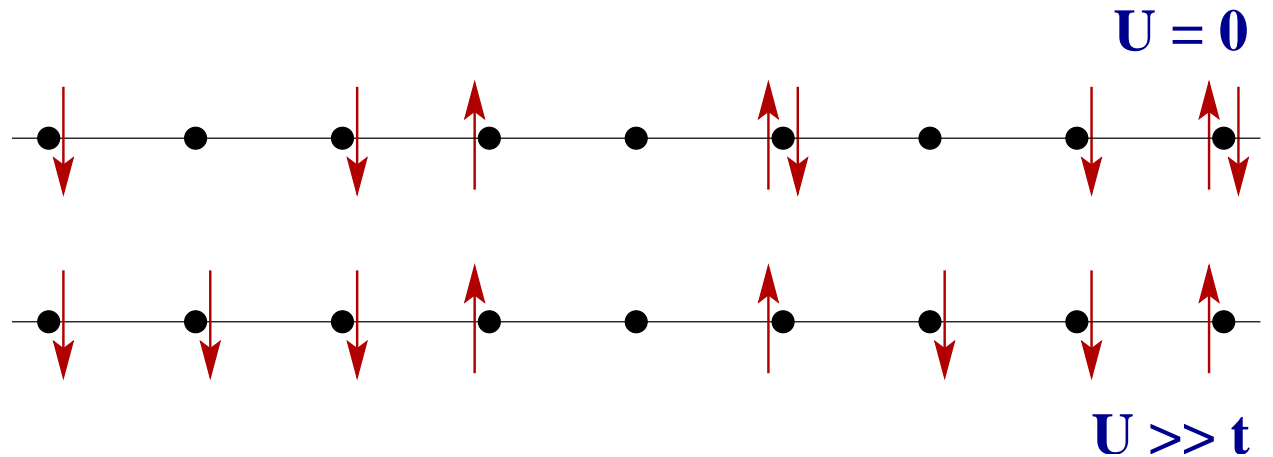
## low-energy states

$c_{i\sigma}^\dagger |0\rangle$  singly-occupied  
 $|0\rangle$  empty sites



# Mottness and enhanced phase fluctuations

reduction of particle number fluctuations  
by strong correlations

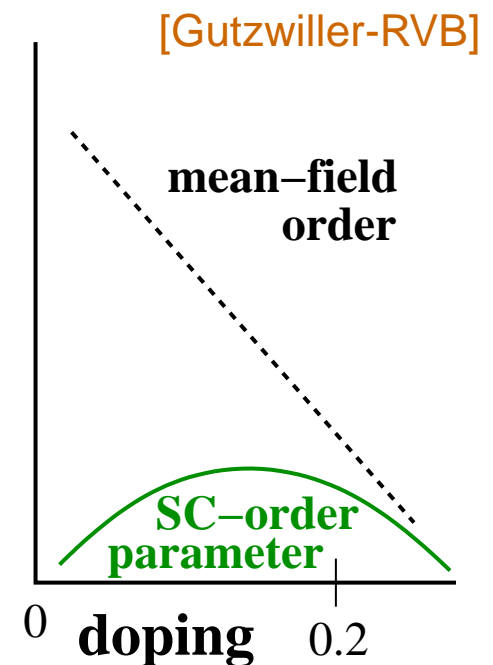


canonical conjugate variables  $\langle \Delta N \rangle \langle \Delta \phi \rangle \approx 1$

phase  $\phi$   
particle number  $N$

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

- Mottness results in diverging phase fluctuations



# nodal Fermi velocity

- nodes along (1, 1) direction

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

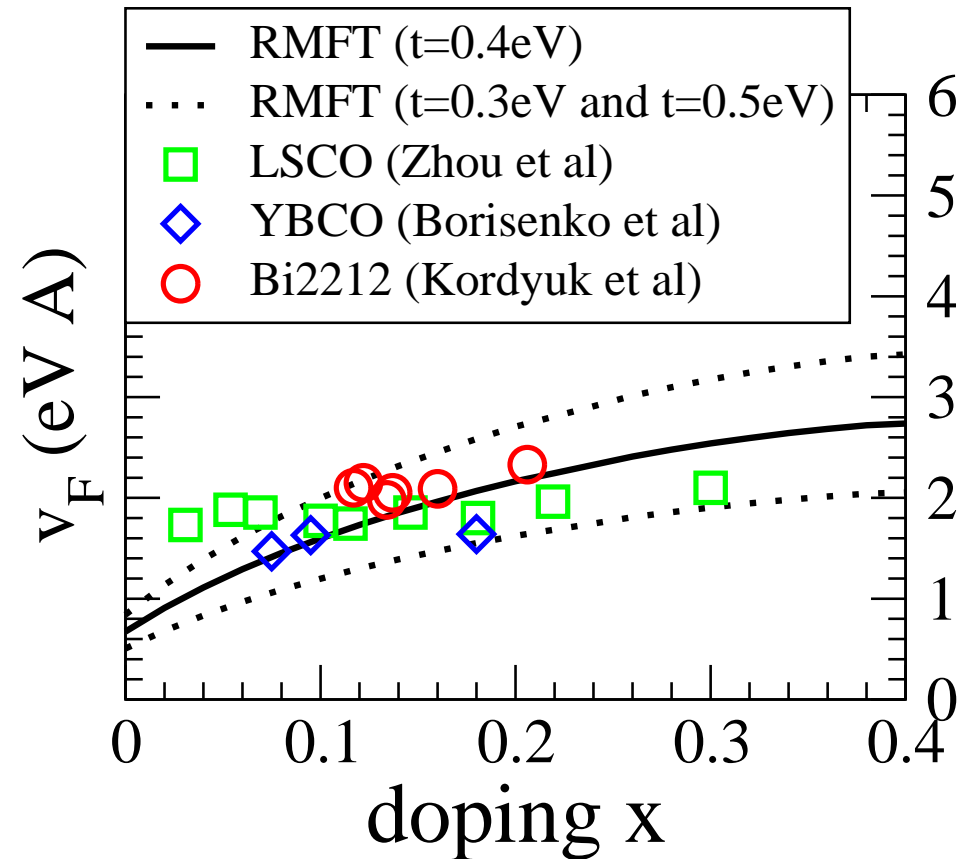
- RVB-Gutzwiller

$$\lim_{U/t \rightarrow \infty} \lim_{n \rightarrow 1} v_F \propto J = 4 \frac{t^2}{U}$$

experiment & theory

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

[Edegger, Muthukumar, Gros, Anderson '06]



# 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

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

- Fermi velocity

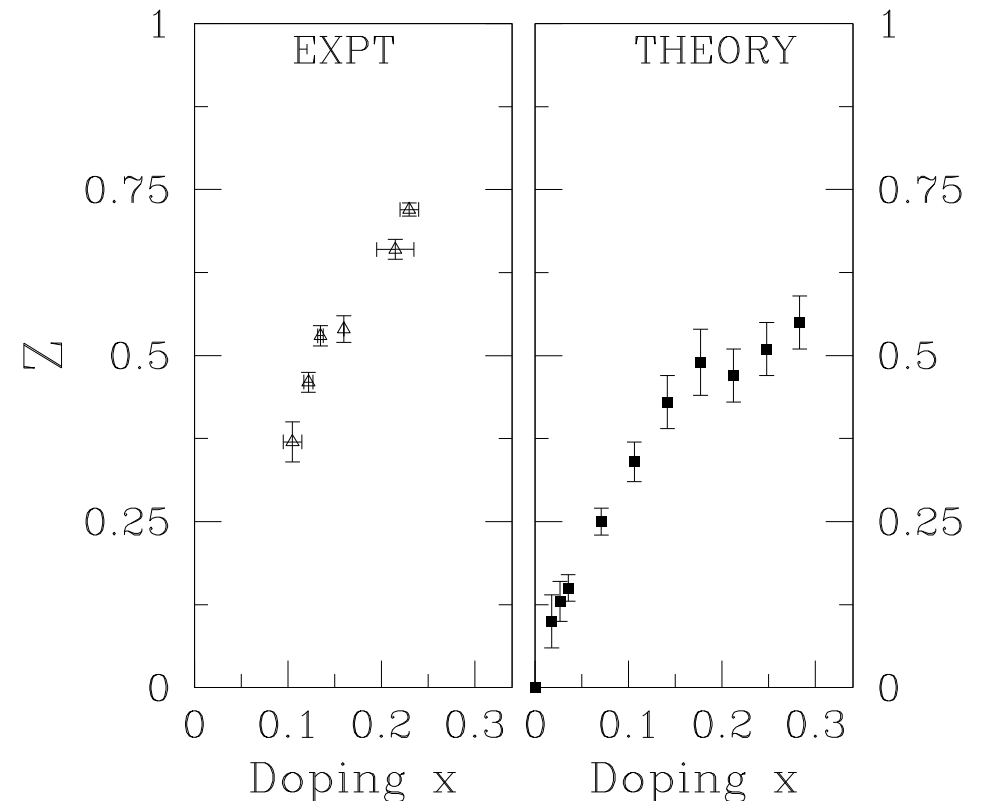
$$v_F = Z \left( v_F^0 + \frac{\partial \text{Re}\Sigma}{\partial k} \right)$$

## theory & experiment(?)

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

[Johnson *et al.* '01]

[Randeria, Paramakanti, Trivedi '04]



# diverging momentum dependence of self energy —

## theory & experiment

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

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

- Fermi velocity

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

## singular momentum dependence (nodal)

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

- doping  $x = 1 - n$



# d-wave superconductivity in the Hubbard model ---

.. as predicted by strong coupling theories in the late eighties

[Gros; Kotliar & Liu; Ogata & Shiba; Zhang, Gros, Rice & Shiba, ..]

**induced by antiferromagnetic exchange**  $\sim J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$

.. not explicitly present in the original Hubbard model  $J = 4t^2/U$

## approaches

- numerical simulations

[Maier, Jarrell & Scalapino; Kotliar, ..]

- small- $U$  RG

[Honerkamp, Salmhofer, Furukawa & Rice; Halboth & Metzner, ..]

- large- $U$  canonical transformation

$$H_{t-J} = e^{iS} H e^{-iS} \approx -t \sum_{\langle i,j \rangle, \sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \dots$$

# 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

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

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

## renormalization factors

Hilbert space counting arguments

# renormalization scheme

un-projected Hilbert space

Hubbard Hamiltonian



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



projected Hilbert space

t-J Hamiltonian



Gutzwiller renormalization  $g$



pre-projected Hilbert space

renormalized Hamiltonian

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

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

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

# renormalized molecular-field theory

## pre-projected Hilbert-space

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

## decoupling

$$S_i^+ S_j^- = c_{i\uparrow}^\dagger c_{i\downarrow} c_{j\downarrow}^\dagger c_{j\uparrow} \approx \langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle c_{i\downarrow} c_{j\downarrow}^\dagger - \langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \rangle c_{i\downarrow} c_{j\uparrow} + \dots$$

## molecular fields

hopping-amplitude:

$$\xi_{i-j} = \langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle$$

pair-amplitude:

$$\Delta_{i-j} = \langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \rangle$$

## ground-state wavefunction

BCS-wavefunction

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

# 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  $\xi, \Delta$   $\Downarrow$

renormalized mean-field Hamiltonian

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

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

**Variational Monte Carlo**

numerical evaluation

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

[Zhang, Gros, Rice & Shiba '88]

# order-parameter renormalization

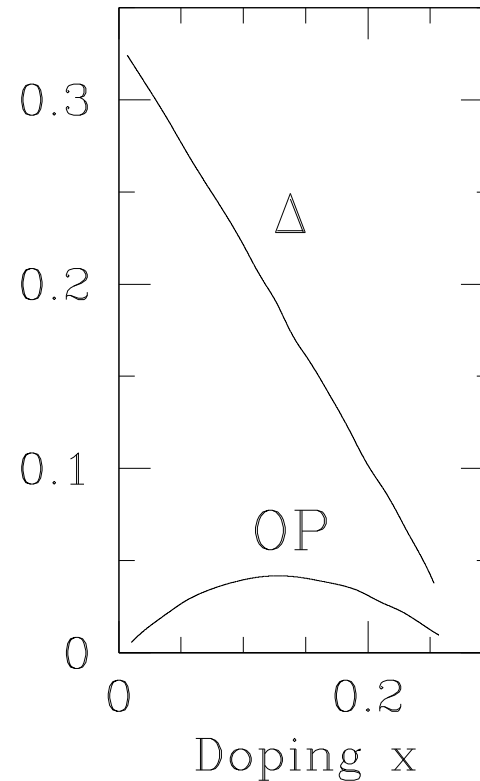
## order-parameter renormalization

$$\langle c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \rangle_\psi = g_t \langle c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \rangle_{\psi_0}$$

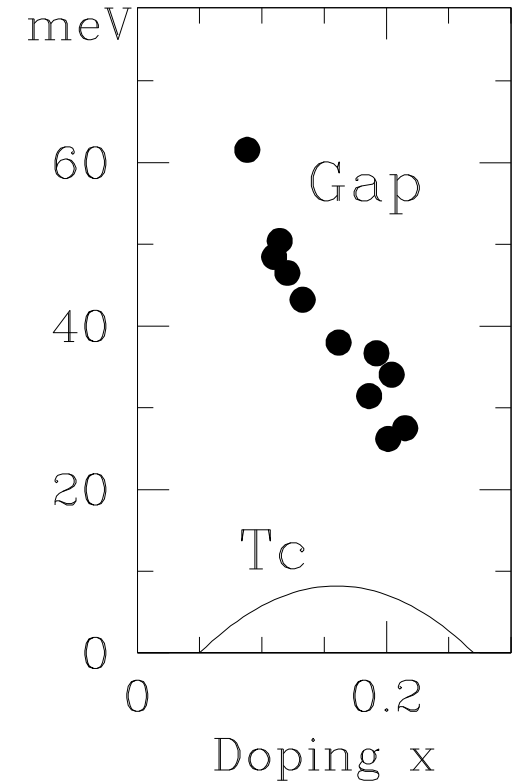
$$\langle \Delta \rangle_\psi = g_t \langle \Delta \rangle_{\psi_0}$$

- Hubbard- $U$  suppresses particle-number fluctuations

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

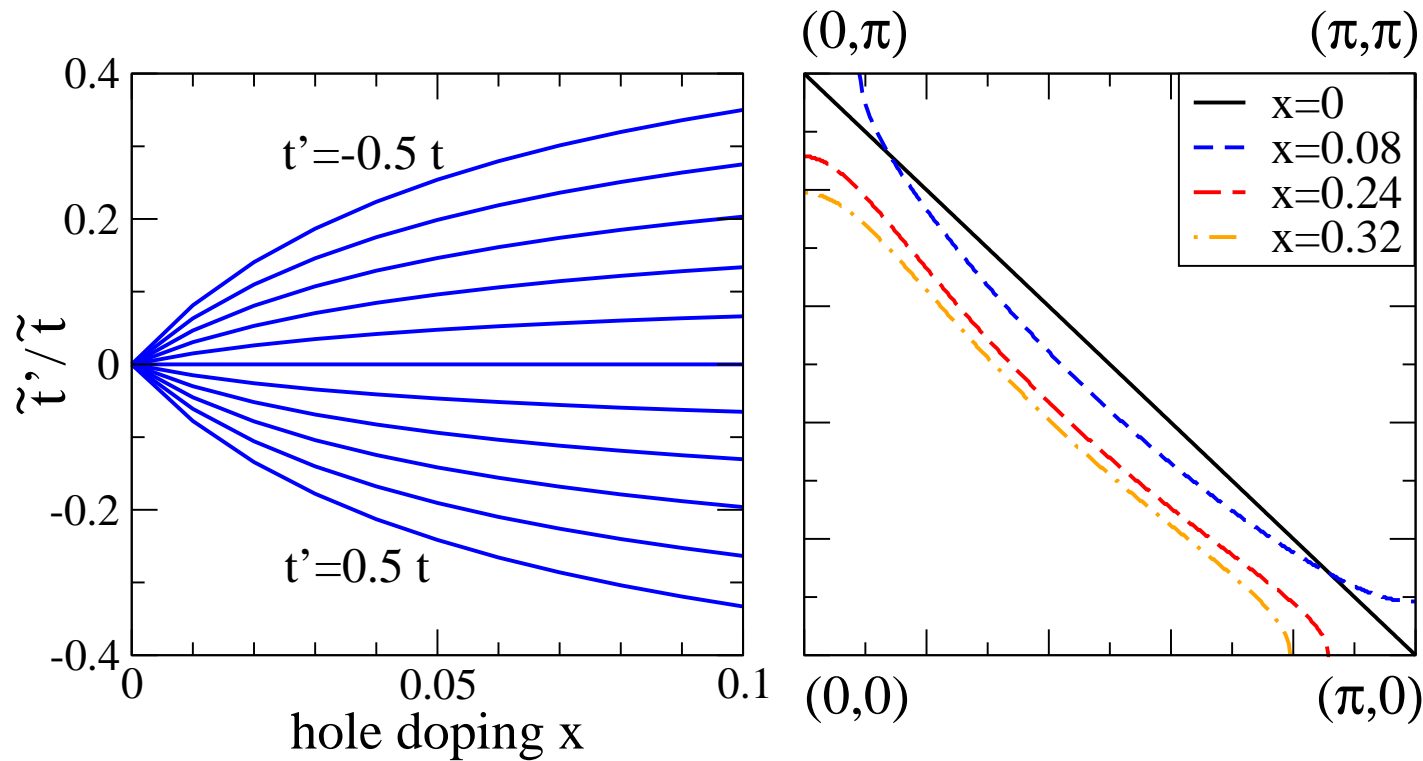
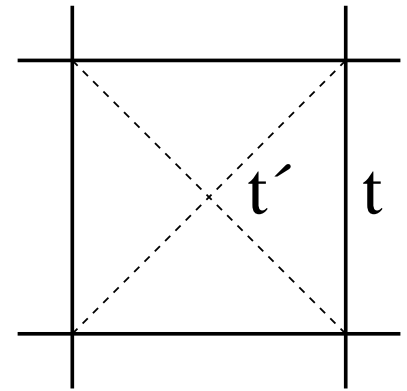


[Anderson *et al.* '04]



# renormalization towards perfect nesting

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



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

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

# Luttinger vs. Fermi surface

## gap / pseudogap

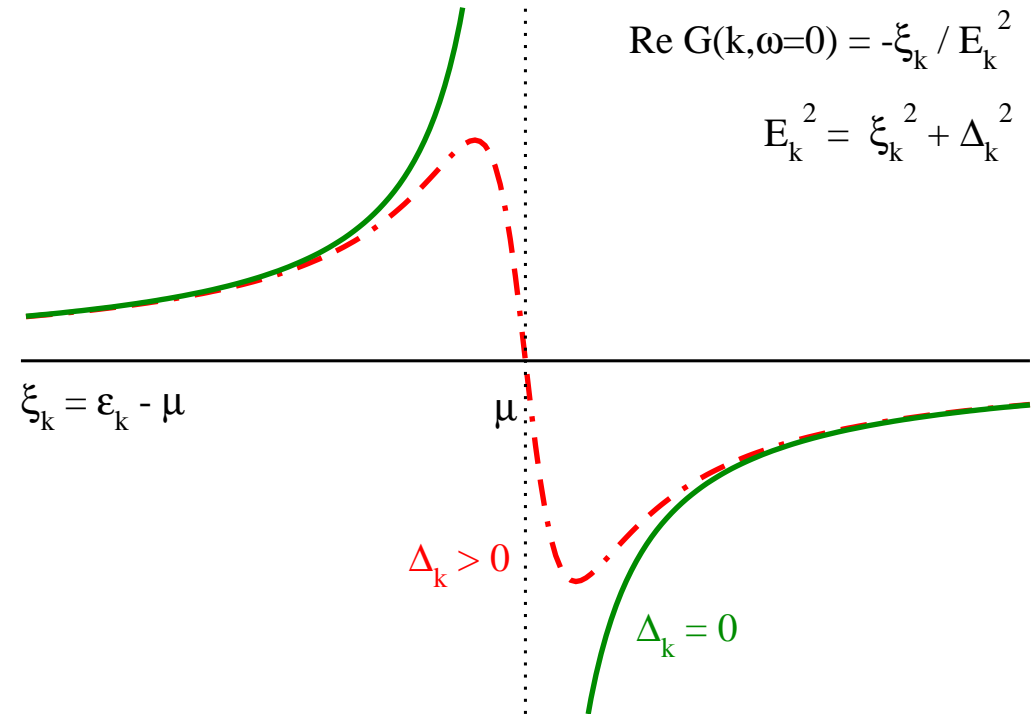
- Fermi surface (FS) not defined
- underlying Fermi surface = ?

## Luttinger surface

- $\text{Re}G(k, \omega = 0)$  changes sign
- underlying Fermi surface  $\hat{=}$  Luttinger surface

## BCS superconductor

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



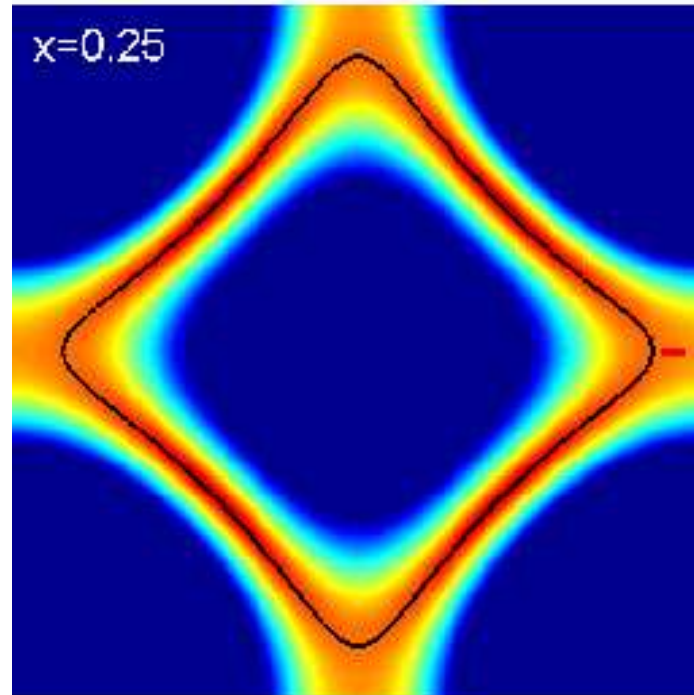
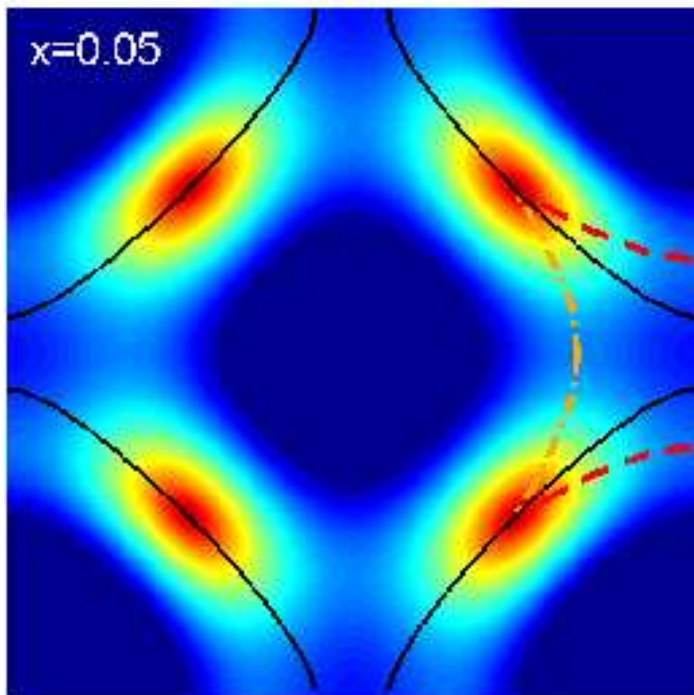


# Underlying Fermi surface determination

## Luttinger surface vs. maximal spectral intensity

maximal intensity surface  $\neq$  Luttinger surface

- large, momentum dependent gap  $\Delta_k$



intensity plots

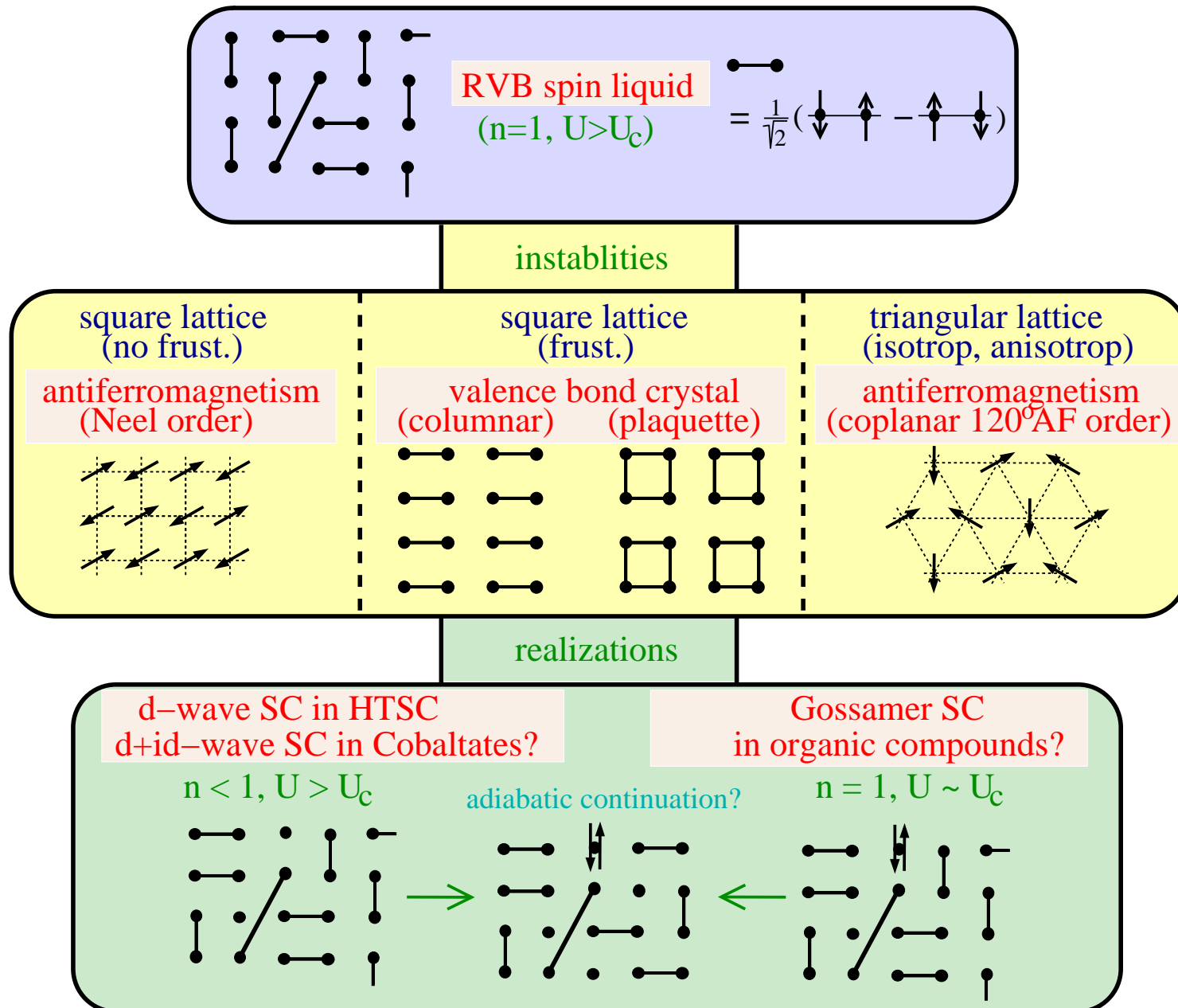
$$\sim \frac{\Gamma}{E_k^2 + \Gamma^2}$$

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

line  $\equiv$  Luttinger surf.

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

# RVB as an unstable fixpoint



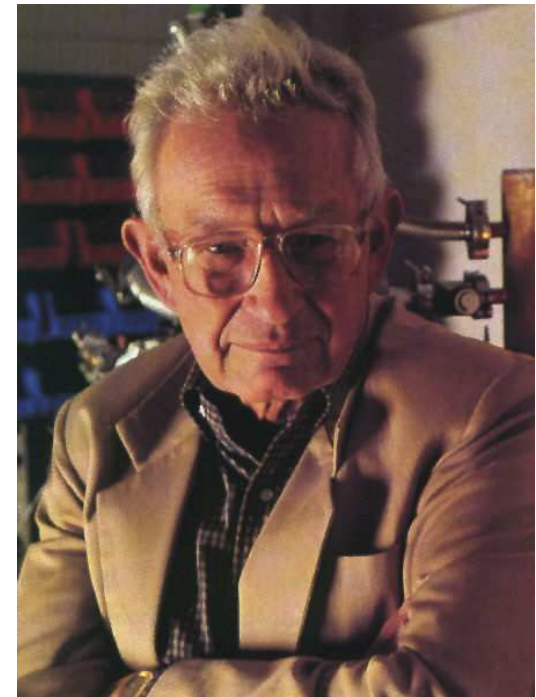
It's all fun together with ...



Bernhard Edegger



V.N. Muthukumar



P.W. Anderson

[PRL '06, PNAS '06, review on RVB-Gutzwiller '07]