Competing orders, spectral functions, and the superconducting gap in the Hubbard model

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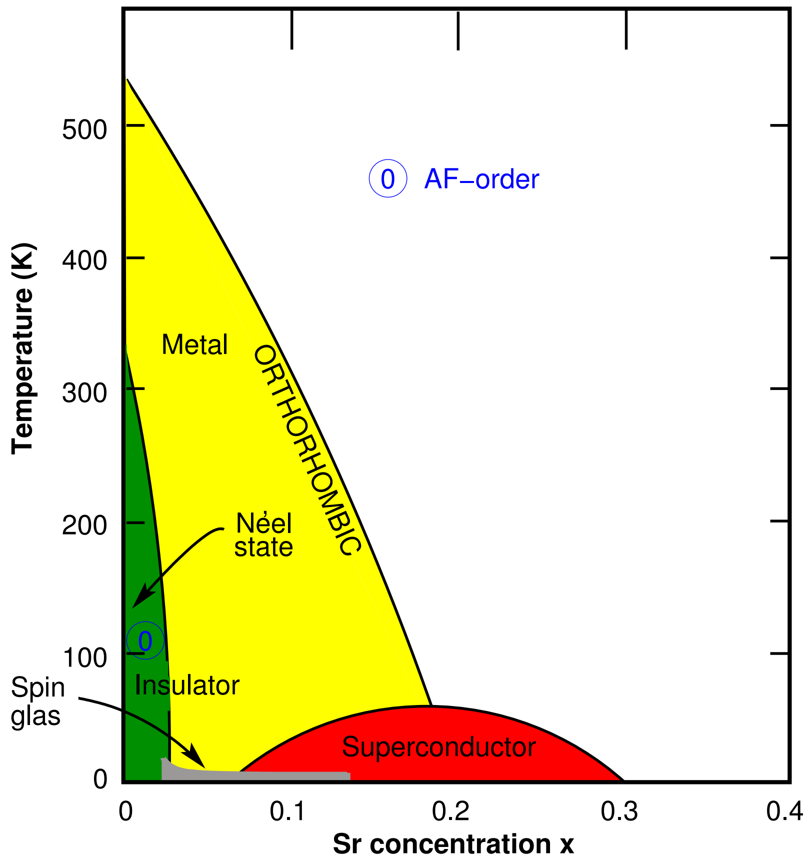
M. Potthoff, W. Hanke, Würzburg

E. Arrigoni, Graz

Z.B. Huang, Wuhan

High-temperature Superconductors



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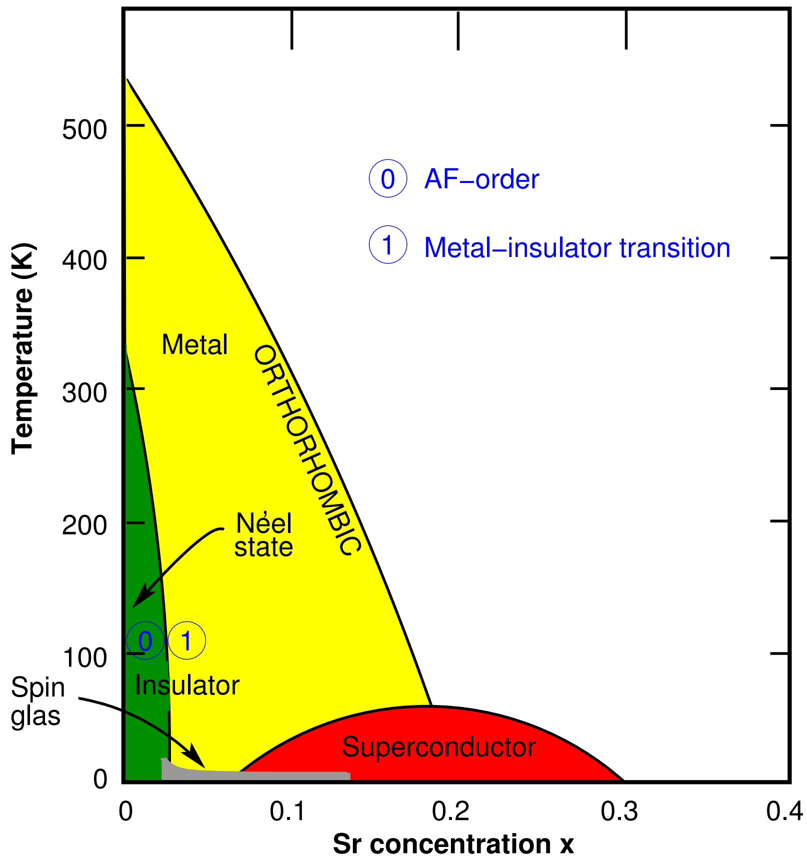

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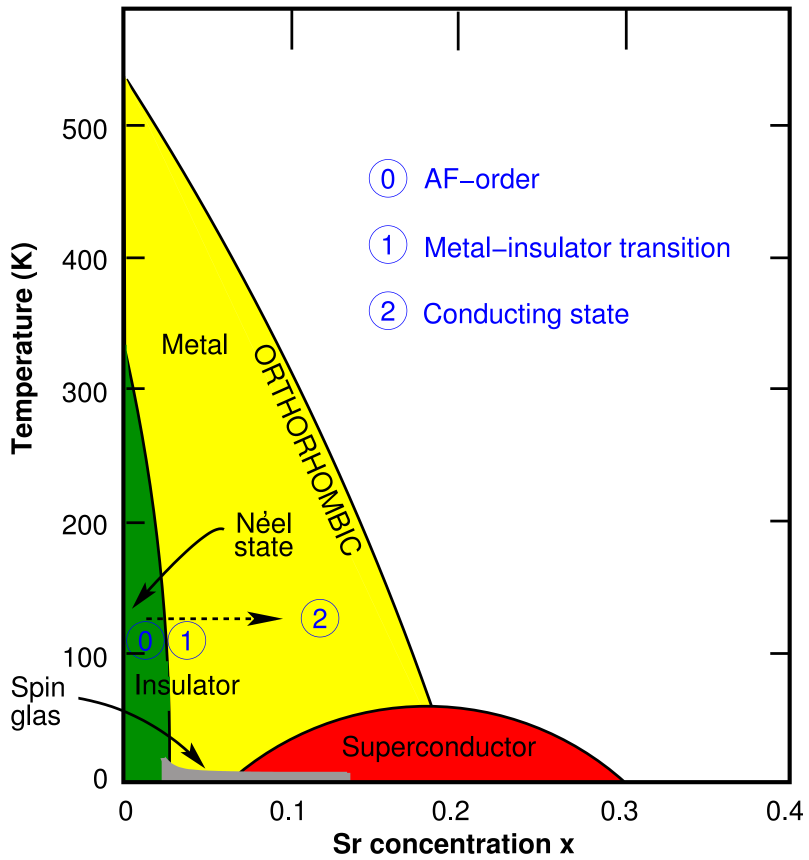

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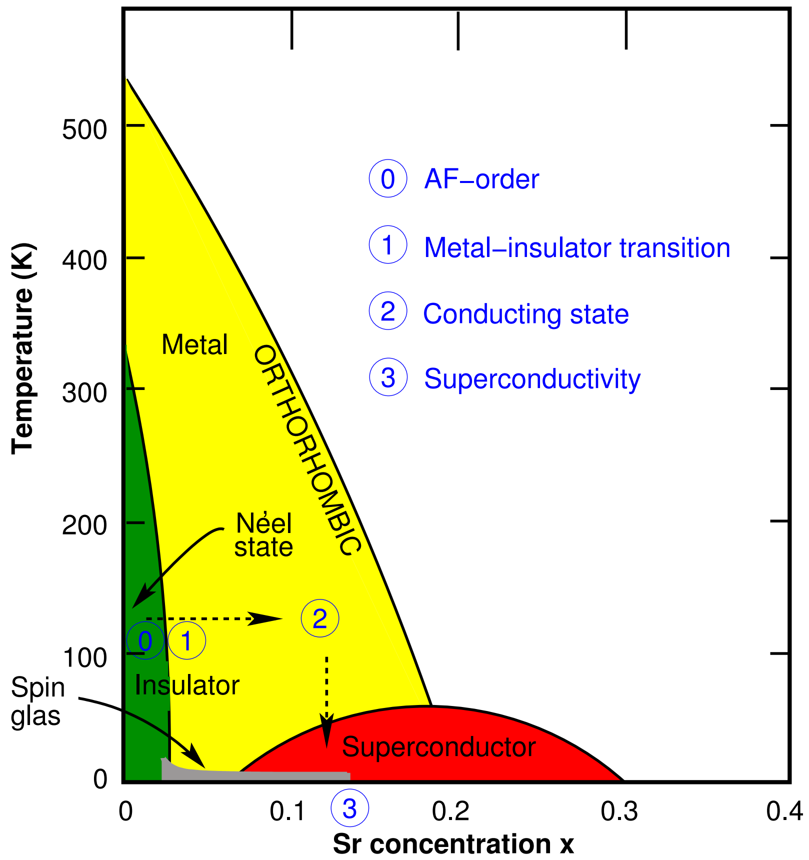

Outline

- Brief introduction to the Variational Cluster Approach

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- Antiferromagnetism and Superconductivity in the Hubbard model
  - Spectral functions
  - Order parameters

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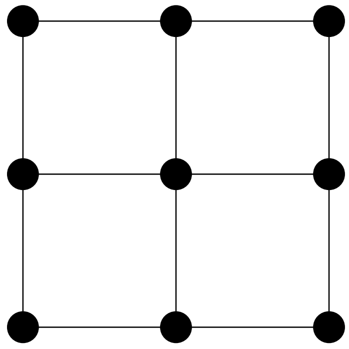
- Conclusions

Variational Cluster Approach

Main idea:

Dynamical information on clusters to approximate thermodynamic limit

$$\Sigma \approx \Sigma_{\text{cluster}}$$



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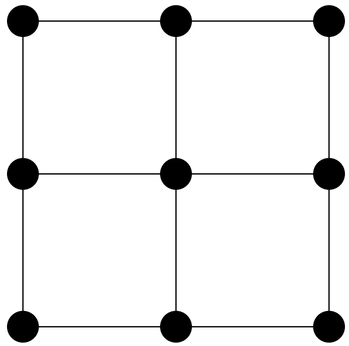

Allows to study symmetry broken phases at $T = 0$

Cluster with symmetry-breaking fields

$\Rightarrow$ Variational Parameters $\tilde{t}$

M. Potthoff *et al.*, PRL **91**, 206402 (2003); EPJB **32**, 429 (2003).

Variational Cluster Approach

$$\Omega(\tilde{t}) = \underbrace{\tilde{\Omega}(\tilde{t})}_{\text{Cluster}} + \mathrm{Tr}\ln \frac{1}{G_0^{-1} - \underbrace{\Sigma(\tilde{t})}_{\text{Cluster}}} - \mathrm{Tr}\ln \underbrace{G(\tilde{t})}_{\text{Cluster}}$$

- Reference system (Cluster) must be solvable exactly!

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- Approach includes CPT, DMFT, C-DMFT

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Competing AF and dSC order

- Model: Hubbard Model, 2D square lattice

$$H = -t \sum_{\langle ij \rangle, \sigma} c^\dagger_{i\sigma} c_{j\sigma} - t' \sum_{\langle\langle ij \rangle\rangle, \sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

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- Variational parameters:
  - AF field: $h \sum_i \mathrm{e}^{i\mathbf{Q}\mathbf{r}_i}(n_{i\uparrow} - n_{i\downarrow})$
  - dSC field: $\Delta \sum_{ij} \eta_{ij}(c_{i\downarrow} c_{j\uparrow} + \text{h.c.})$
  - Onsite Potential: Thermodynamic consistency

Spectral function - Theory

M. Aichhorn *et al.*, EPL **72**, 117 (2005); PRB **74**, 024508 (2006)

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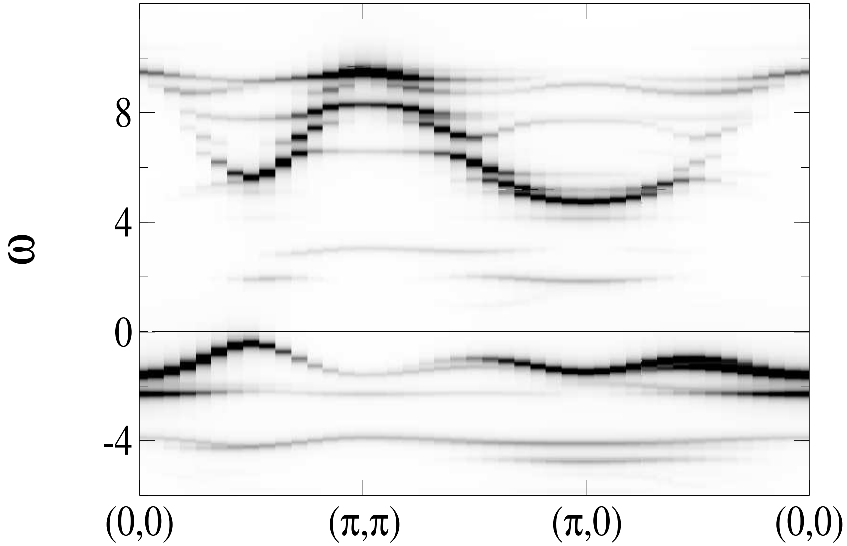

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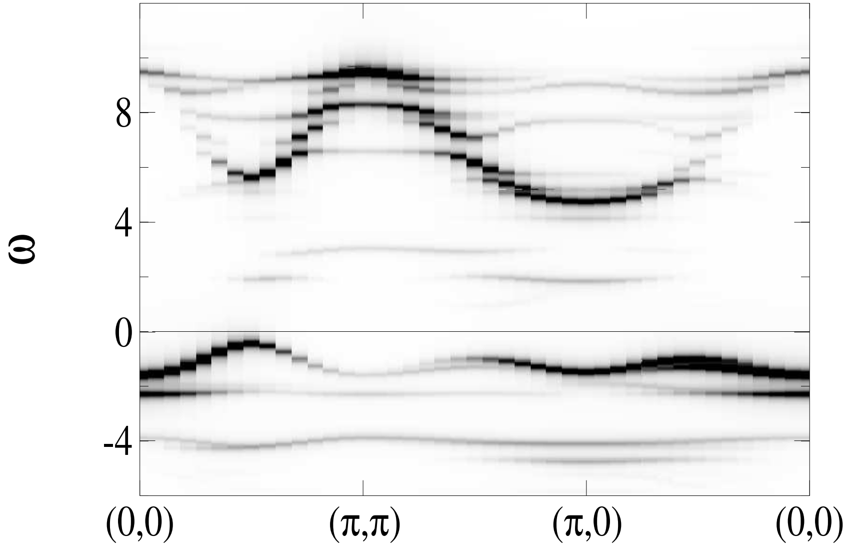

Holes first enter at $(\frac{\pi}{2}, \frac{\pi}{2})$

Consistent with experiment!

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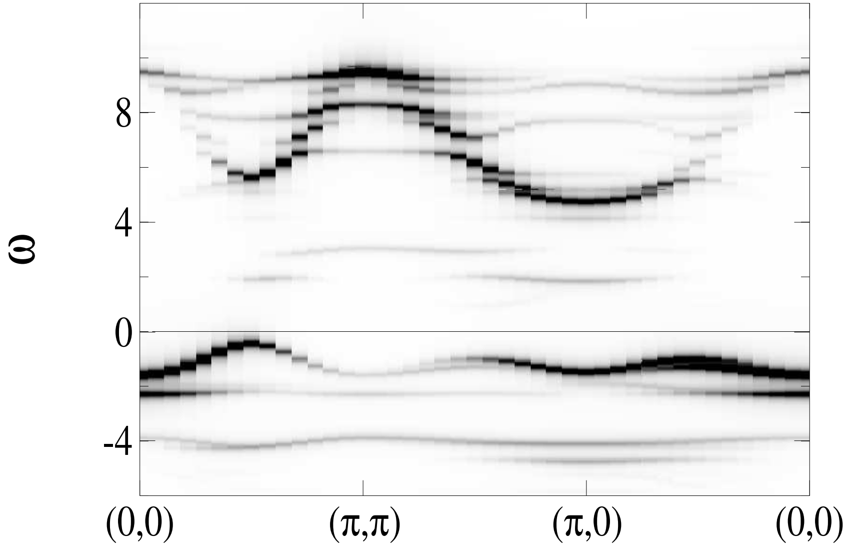
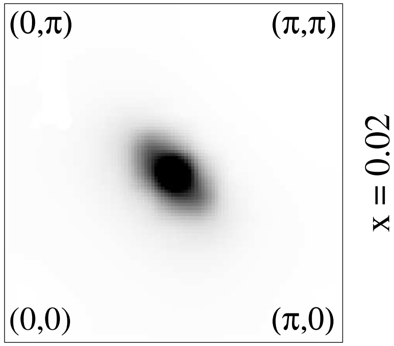


Calculated Fermisurfaces:



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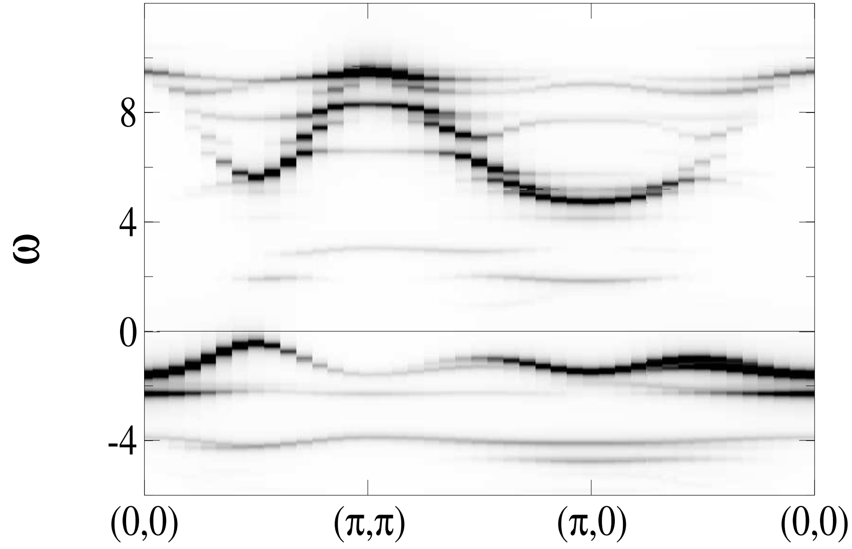

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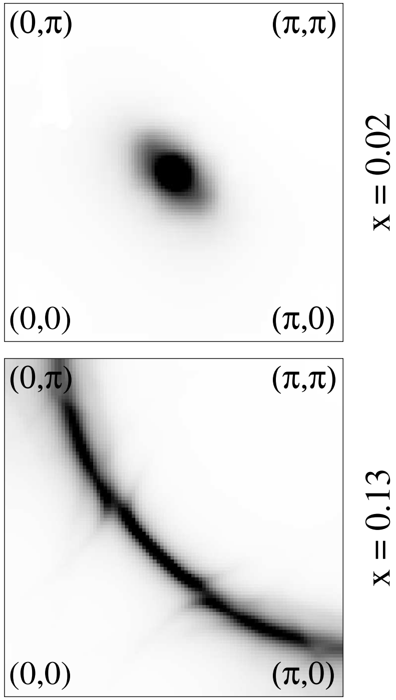

Spectral function - Theory

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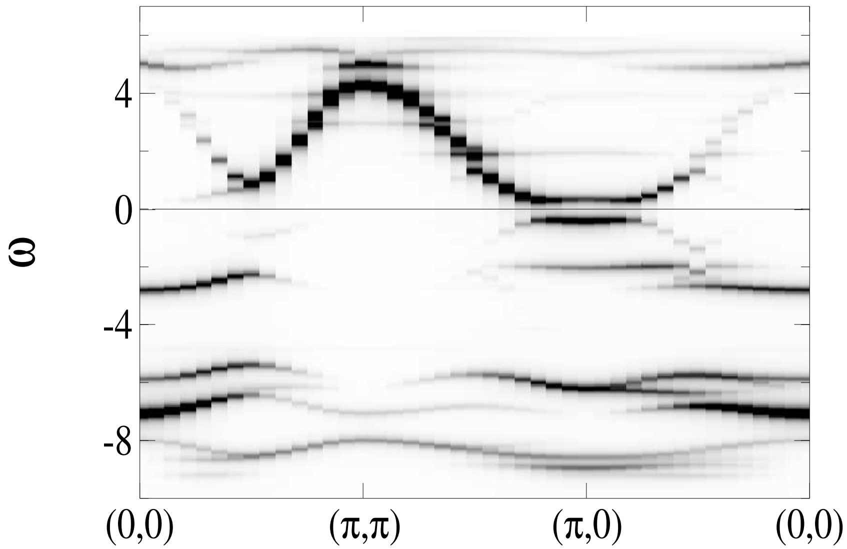
$x = 0.08$, electron doped:



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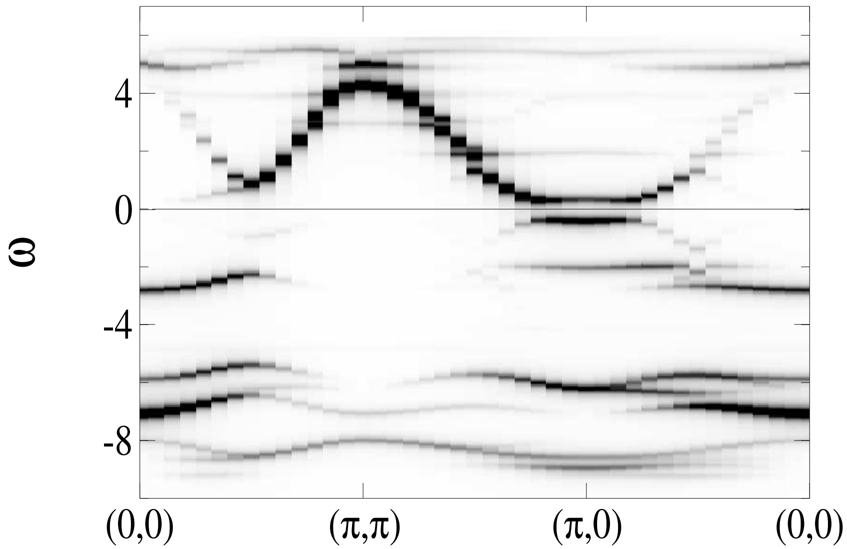

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see ARPES: Armitage *et al.*, 2001,2002

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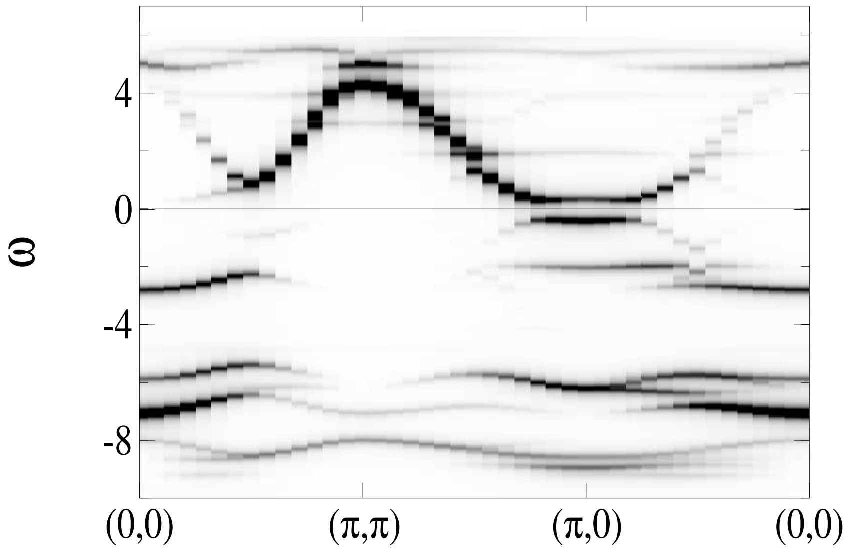

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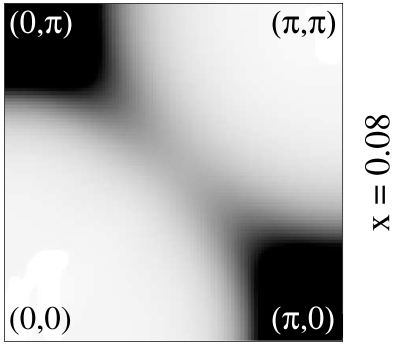

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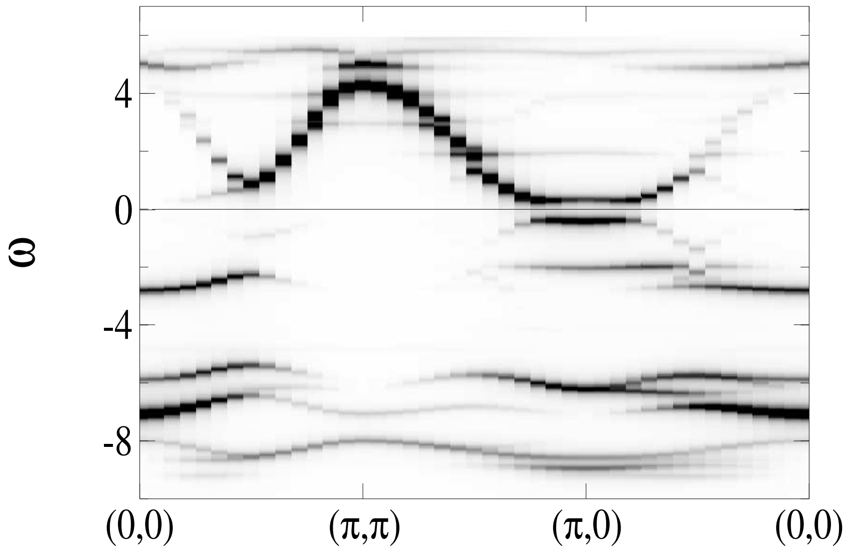

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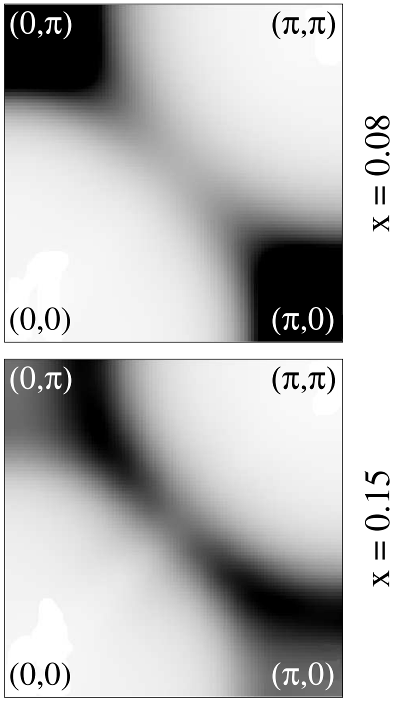

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Order parameters

- Variational Parameters / Symmetry-breaking fields:
  - AF field: $h \sum_i \mathrm{e}^{i\mathbf{Q}\mathbf{r}_i}(n_{i\uparrow} - n_{i\downarrow})$
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- Corresponding Order Parameters:

$$M_{\mathrm{AF}} = \frac{2i}{(2\pi)^3}\int \mathrm{d}^3k \int \mathrm{d}\omega \sum_\sigma (-1)^\sigma G(\mathbf{k}, \mathbf{k}+\mathbf{Q}; \omega)$$

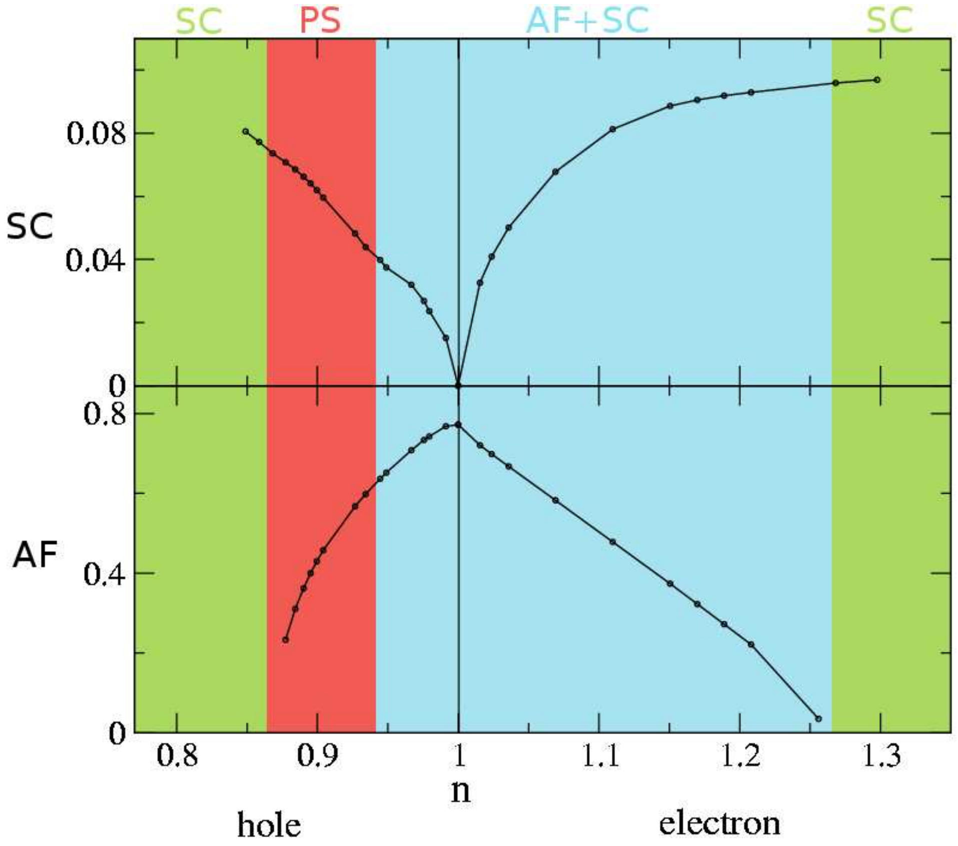
$$D_{\mathrm{SC}} = \frac{2i}{(2\pi)^3}\int \mathrm{d}^3k \int \mathrm{d}\omega\, g(\mathbf{k}) F(\mathbf{k}, \mathbf{k}; \omega)$$

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

Can be calculated from VCA single-particle Green's function.

AF to dSC Phase Transition

M. Aichhorn *et al.*, PRB **74**, 235117 (2006)



Order Parameters at $T = 0$
Hubbard model
$U = 8t$, $t' = -0.3t$

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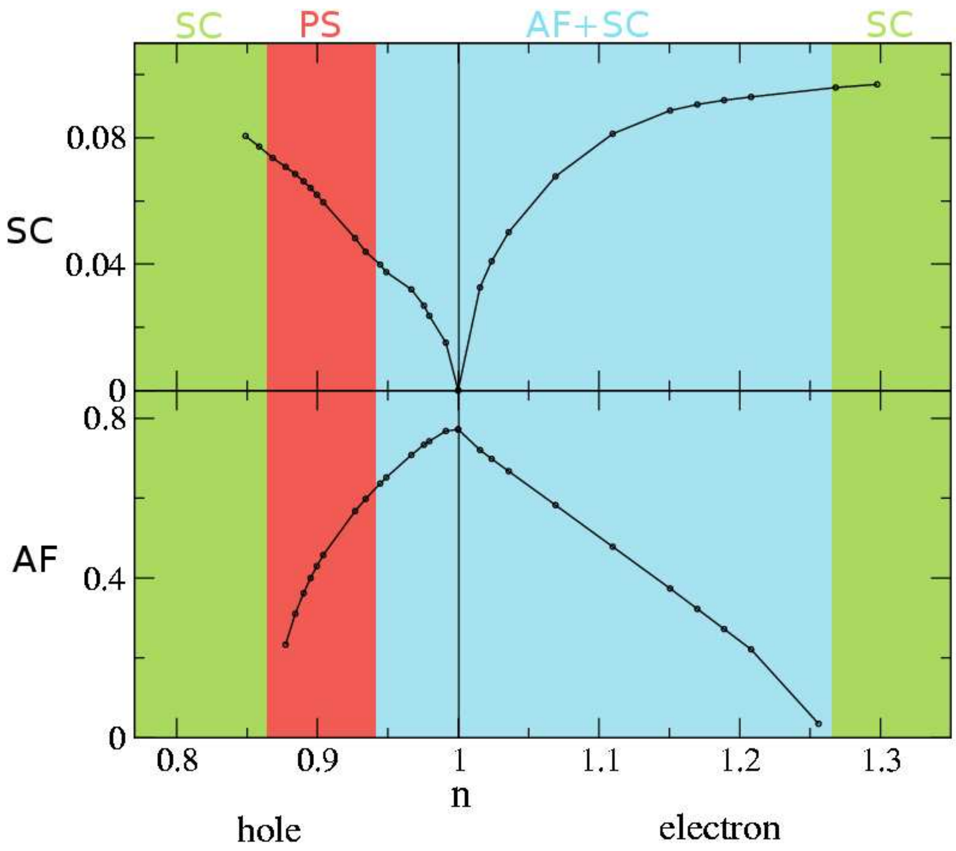

Order Parameters at $T = 0$
Hubbard model
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Salient features of the ground-state phase diagram are re-produced

The SC gap: two-gap scenario?

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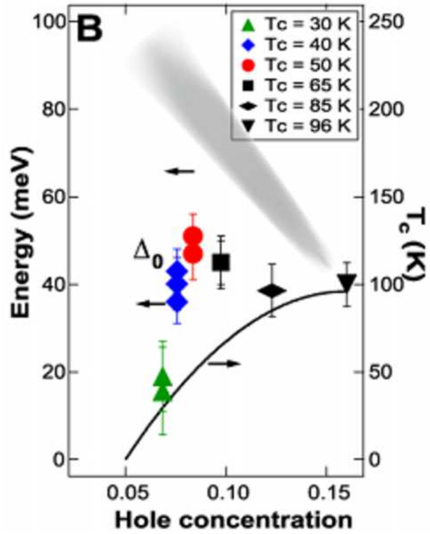
The SC gap: two-gap scenario?



K. Tanaka *et al.*, Bi2212
Science **314**, 1910 (2006)

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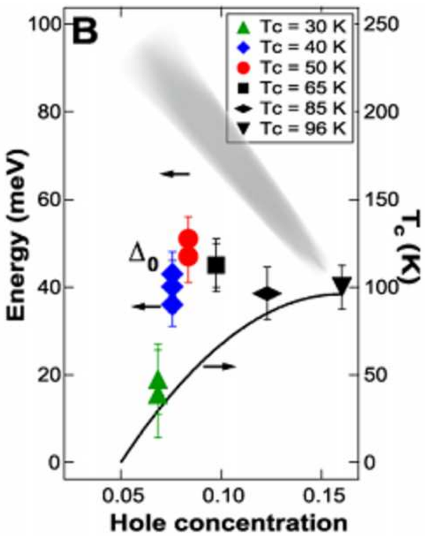

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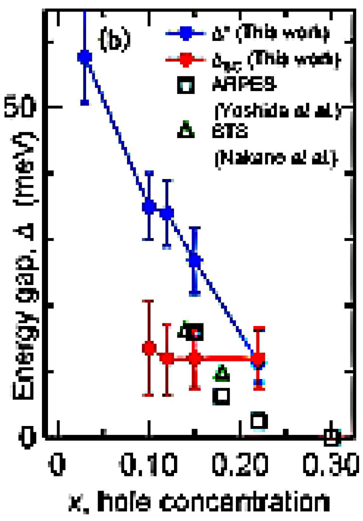

M. Hashimoto *et al.*, LSCO
cond-mat/0610758

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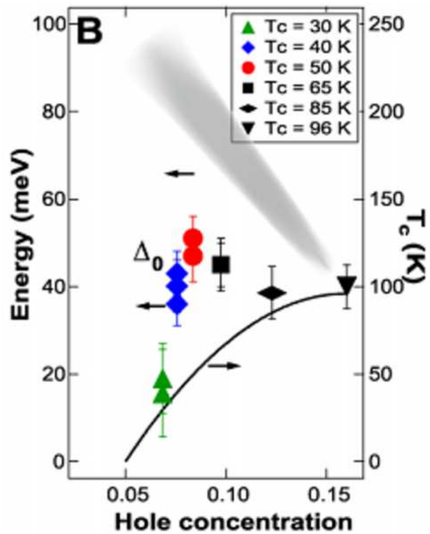

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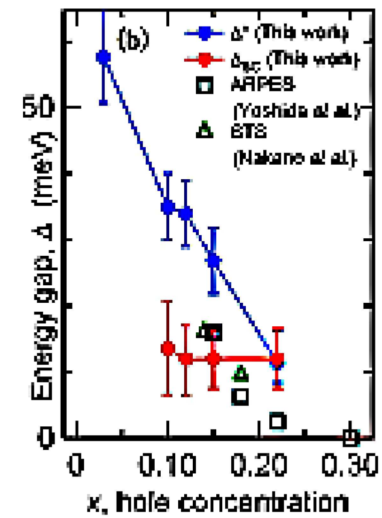

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Also evidence from Raman spectroscopy
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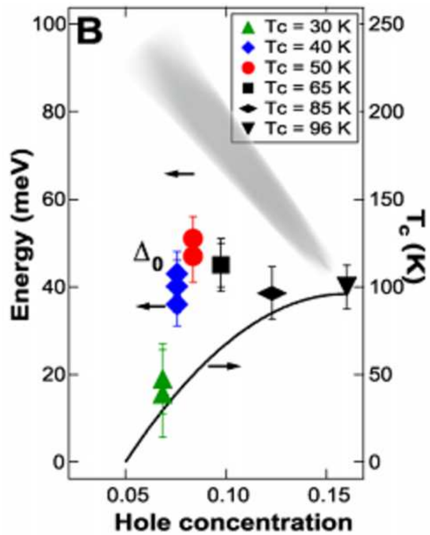

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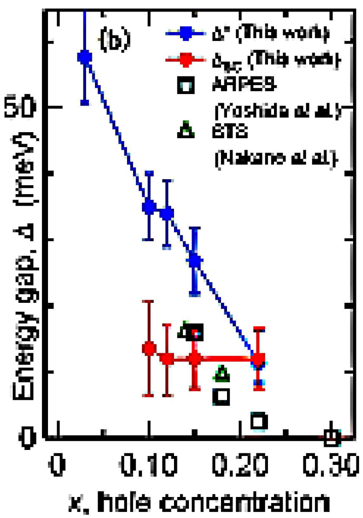

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No simple $(\cos k_x - \cos k_y)$ gap structure!

The SC gap in the Hubbard model

M. Aichhorn *et al.*, cond-mat/0702391

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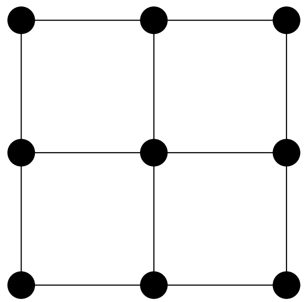

3×3 reference system

Variational parameter:
$\Delta \sum_{ij} \eta_{ij} (c_{i\downarrow} c_{j\uparrow} + \text{h.c.})$

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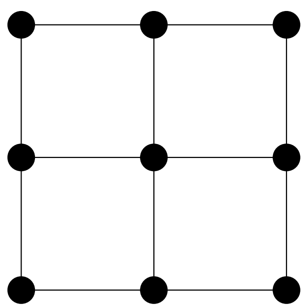

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Self-consistent solution
for finite Δ!

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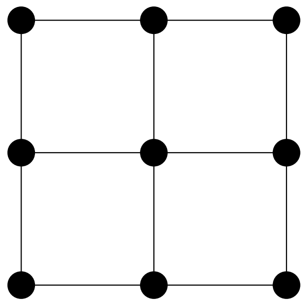

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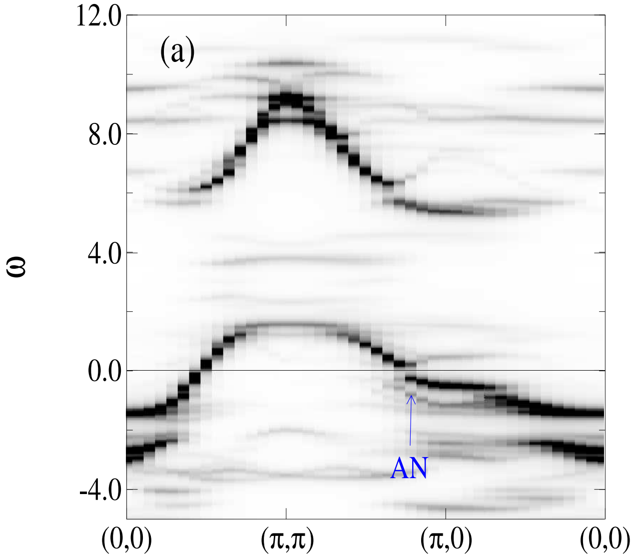

$x = 0.07$ hole doping

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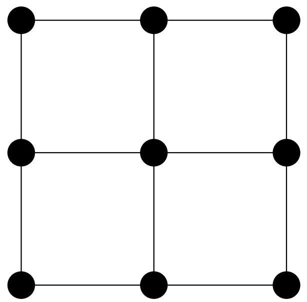

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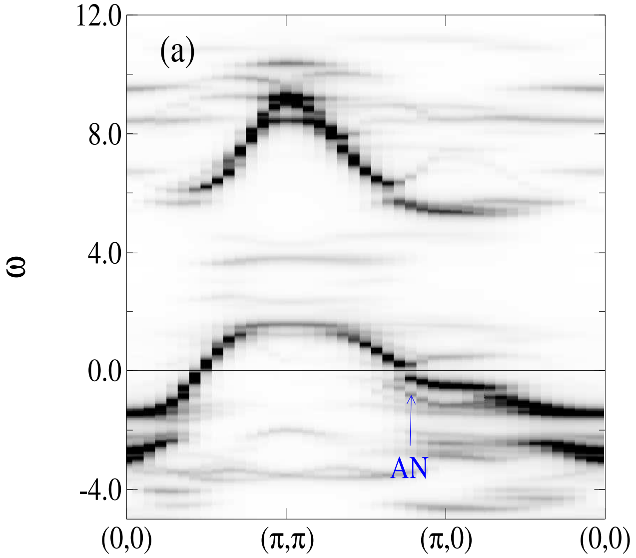

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Nodal direction: crossing

Antinodal direction: gap

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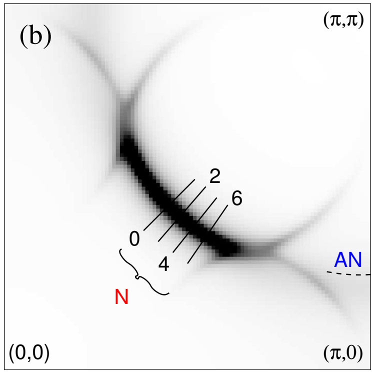
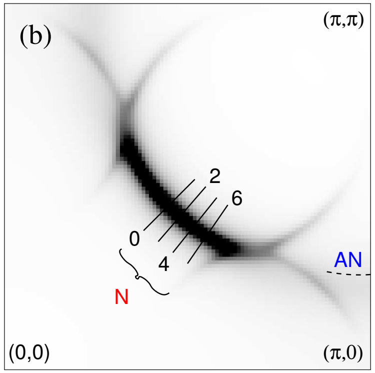
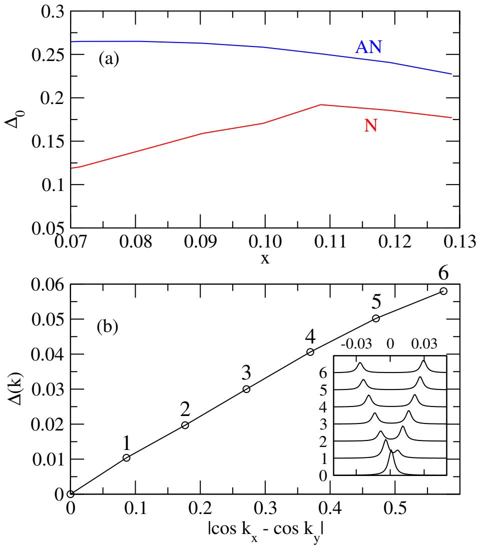


Fermi surface,
$x = 0.07$

Fermi arc

The SC gap in the Hubbard model





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Fermi arc

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

Different doping behavior
AN ↔ N

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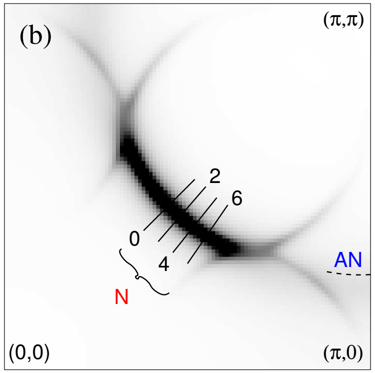

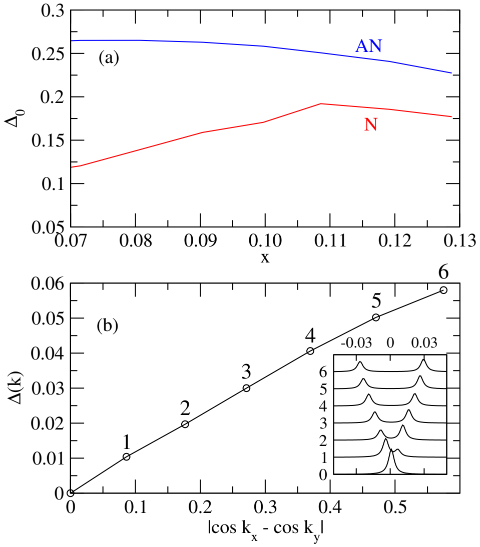

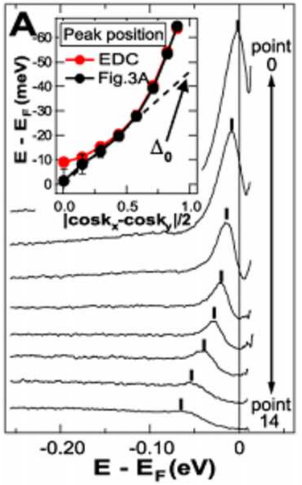

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Different doping behavior
AN $\leftrightarrow$ N

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Qualitative difference

NODAL versus ANTINODAL

Qualitative difference

NODAL versus ANTINODAL

Physical explanation?

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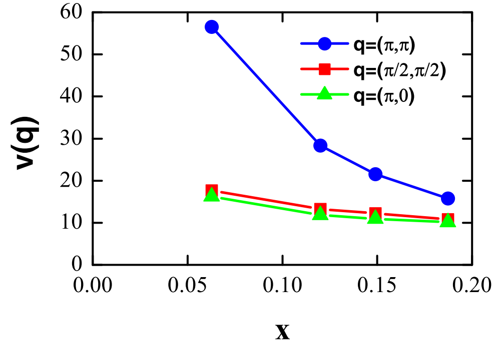
Explanation?

Explanation?

Assumption: Spin-fluctuation mediated pairing

Well known:
Doping affects strongest $q = (\pi, \pi)$



Explanation?

Assumption: Spin-fluctuation mediated pairing

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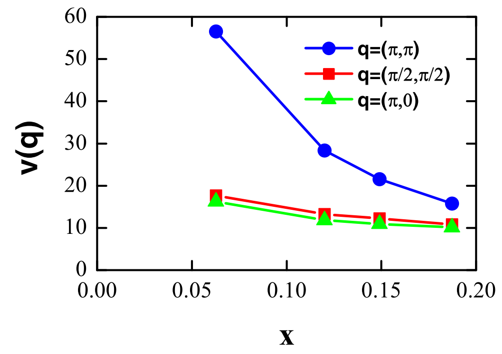

BCS model:

$$\Delta(\mathbf{k}_F) = -\frac{1}{2} \int \frac{d^2k'}{(2\pi)^2} v(\mathbf{k}' - \mathbf{k}_F) \frac{\Delta(\mathbf{k}')}{\sqrt{\varepsilon^2(\mathbf{k}') + \Delta(\mathbf{k}')^2}}$$

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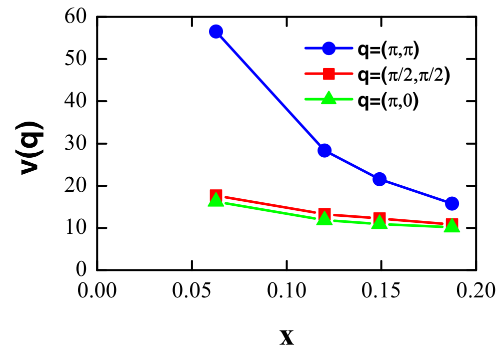

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Analyse kernel contributions for different $\mathbf{k}_F$

Natural explanation by spin fluctuations

ANTINODAL NODAL

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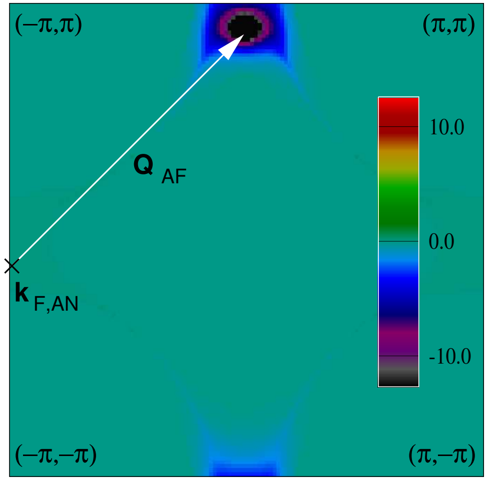

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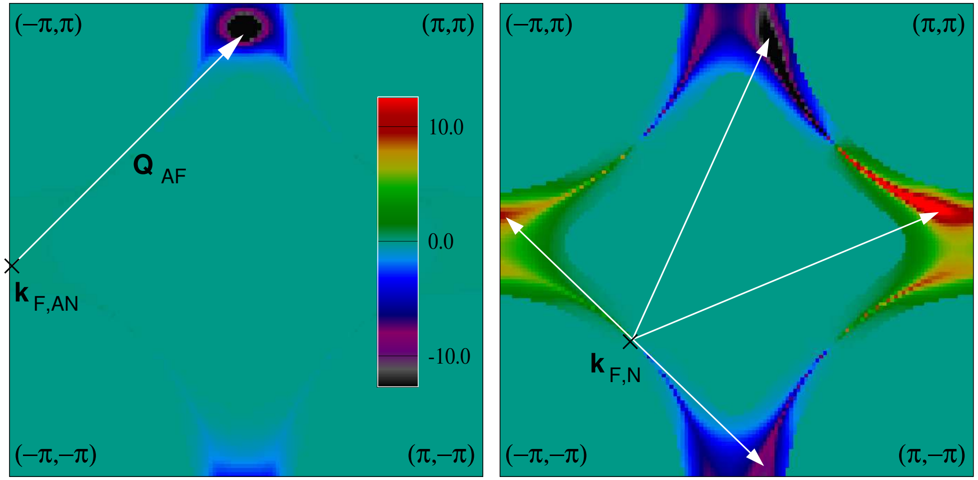
ANTINODAL NODAL



Totally different contributions!

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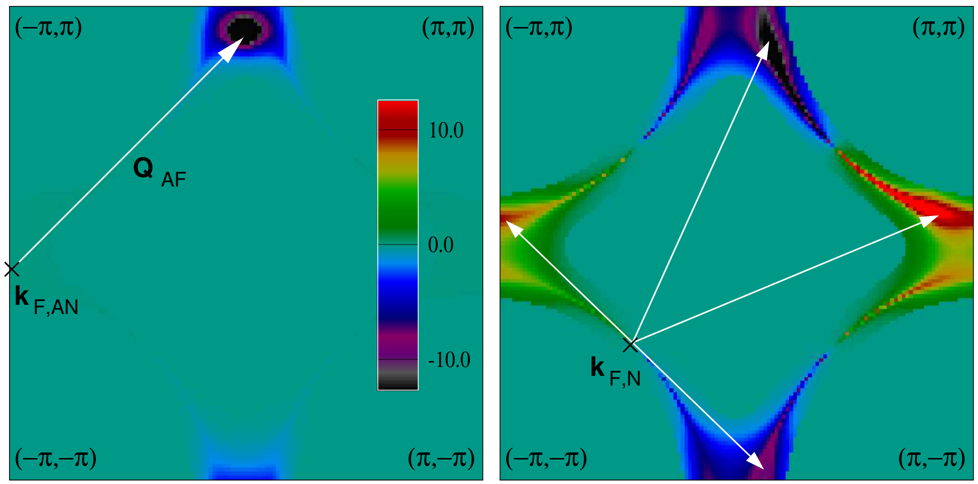

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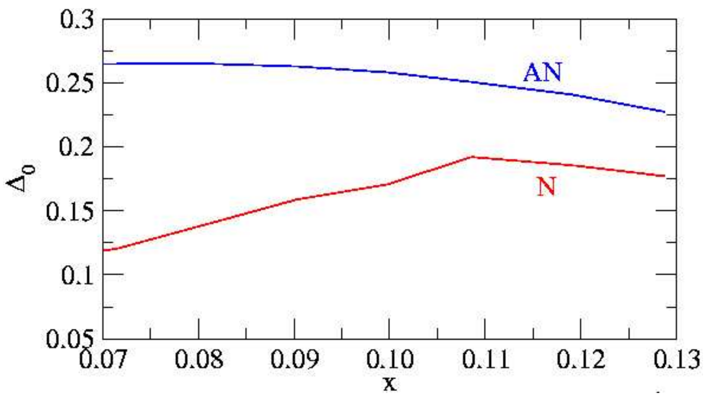

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Natural explanation by spin fluctuations

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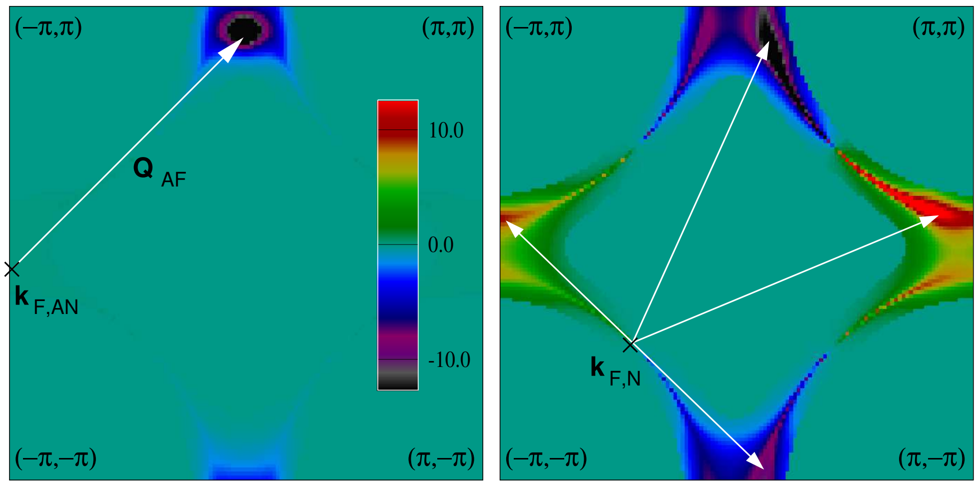

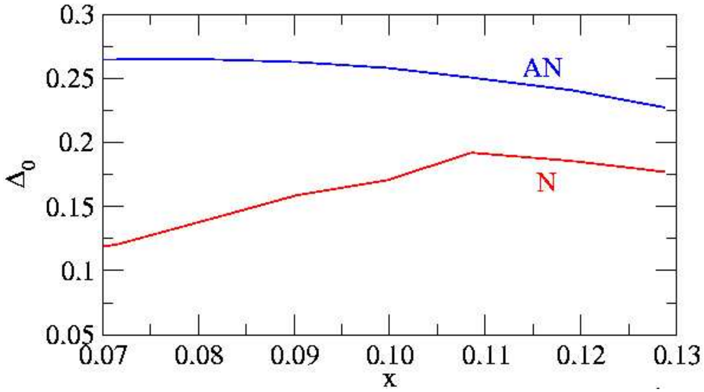

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Doping dependence of pairing interaction
$\Rightarrow$ Different response at Antinode and Node

Conclusions

Salient features are reproduced by the Hubbard model

Competition between AF and SC

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xxx.arXiv.org/cond-mat/0702391

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