Microscopic Approach to High-Temperature Superconductors

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Outline:

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2. *Projector-based renormalization method*

3. *Application to the t-J model*

4. *Results and discussion: Pseudogap phase*

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1. Introduction

One of the most important unsolved problems in solid-state physics is the understanding of copper-oxide superconductors:

- superconducting pairing mechanism not known
- pseudogap phase not understood:

  -- key features: pseudogap opens on a part of the Fermi surface (FS) around the anti-nodal point

  -- nongapped FS segment known as Fermi arc around the nodal point

  -- close connection between T* and the Fermi arc length

t-J model: generally accepted model for the copper-oxide superconductors

$$\mathcal{H} = -\sum_{ij,\sigma} t_{ij}\, \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} - \mu \sum_{i\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{i\sigma} + \sum_{ij} J_{ij} \mathbf{S}_i \mathbf{S}_j =: \mathcal{H}_t + \mathcal{H}_J$$

Hubbard operators: $\hat{c}^{\dagger}_{i\sigma} = c^{\dagger}_{i\sigma}(1 - n_{i,-\sigma})$

exclusion of doubly occupied sites

2. Projector-based Renormalization Method (PRM) :

Starting point: $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$

$\mathcal{H}_1$ leads to transitions between eigenstates of $\mathcal{H}_0$

First step: Construction of an effective Hamiltonian

$$\mathcal{H}_\lambda = \mathcal{H}_{0,\lambda} + \mathcal{H}_{1,\lambda}$$

in which all transitions $|E_n^\lambda - E_m^\lambda|$ due to $\mathcal{H}_1$ larger than a given cutoff λ are eliminated

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review article: cond-mat 0809.3360

- **Next step:** $\mathcal{H}_\lambda$ is transformed to a renormalized Hamiltonian $\mathcal{H}_{(\lambda-\Delta\lambda)}$ by eliminating all transitions between λ and a reduced cutoff $(\lambda - \Delta\lambda)$

$$\mathcal{H}_{(\lambda-\Delta\lambda)} = e^{X_{\lambda,\Delta\lambda}} \mathcal{H}_\lambda e^{-X_{\lambda,\Delta\lambda}}.$$

$X_{\lambda,\Delta\lambda}$ generator of the unitary transformation :

$$X^{(1)}_{\lambda,\Delta\lambda} = \frac{1}{\mathsf{L}_{0,\lambda}} \left[\mathsf{Q}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda}\right].$$

decomposition of $\mathcal{H}_{1,\lambda}$ into eigenmodes of $\mathcal{H}_{0,\lambda}$ is needed

- **Explicit evaluation leads to difference (or renormalization) equations which connect the parameters of $\mathcal{H}_\lambda$ with those of $\mathcal{H}_{(\lambda-\Delta\lambda)}$**

- Stepwise renormalization till $\lambda \to 0$ gives a „free“ Hamiltonian

$$\tilde{\mathcal{H}} = \mathcal{H}_{\lambda\to 0} = \mathcal{H}_{0,\lambda\to 0}$$

Note: interaction $\mathcal{H}_1$ is completely used up to renormalize the parameter of $\mathcal{H}_0$

Evaluation of expectation values for operators $\mathcal{A}$:

$$\langle \mathcal{A} \rangle = \frac{\mathrm{Tr}\,(\mathcal{A}\, e^{-\beta \mathcal{H}})}{\mathrm{Tr}\, e^{-\beta \mathcal{H}}} = \langle \mathcal{A}(\lambda) \rangle_{\mathcal{H}_\lambda} = \langle \tilde{\mathcal{A}} \rangle_{\tilde{\mathcal{H}}}$$

Note: unitary transformation has to be applied on $\mathcal{A}$ as well

$$\mathcal{A}(\lambda) = e^{X_\lambda}\, \mathcal{A} e^{-X_\lambda} \text{ and } \tilde{\mathcal{A}} = \mathcal{A}(\lambda \to 0).$$

==> renormalization equations for $\mathcal{A}(\lambda)$ are also required

3. Application to the t-J model

Decomposition: $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$

$$\mathcal{H}_0 = \mathcal{H}_t + \mathcal{H}_{0,J} =: \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \, \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} J_{\mathbf{q}} \, \mathcal{A}_0(\mathbf{q})$$

$$\mathcal{H}_1 = \sum_{\mathbf{q}} J_{\mathbf{q}} \left(\mathcal{A}_1(\mathbf{q}) + \mathcal{A}_1^\dagger(\mathbf{q}) \right)$$

$\mathcal{A}_0(\mathbf{q})$ -part of the exchange $\mathcal{H}_J$ which commutes with the hopping $\mathcal{H}_t$

$\mathcal{A}_1(\mathbf{q})$ and $\mathcal{A}_1^\dagger(\mathbf{q})$ lead to transitions between eigenstates of $\mathcal{H}_0$

$\mathcal{A}_{1,\lambda}(\mathbf{q})$ and $\mathcal{A}^{\dagger}_{1,\lambda}(\mathbf{q})$ have to be eliminated in the renormalization procedure

==> Renormalized Hamiltonians:

$$\tilde{\mathcal{H}} = \sum_{\mathbf{k}\sigma} \tilde{\varepsilon}_{\mathbf{k}}\, \hat{c}^{\dagger}_{\mathbf{k}\sigma}\, \hat{c}_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \left(\tilde{\Delta}_{\mathbf{k}}\, \hat{c}^{\dagger}_{\mathbf{k},\uparrow} \hat{c}^{\dagger}_{-\mathbf{k},\downarrow} + \tilde{\Delta}^{*}_{\mathbf{k}}\, \hat{c}_{-\mathbf{k},\downarrow} \hat{c}_{\mathbf{k},\uparrow} \right) + \tilde{E} \qquad \text{(sc)}$$

$$\tilde{\mathcal{H}} = \sum_{\mathbf{k}\sigma} \tilde{\varepsilon}_{\mathbf{k}}\, \hat{c}^{\dagger}_{\mathbf{k}\sigma}\, \hat{c}_{\mathbf{k}\sigma} + \tilde{E} \qquad \text{(nl)}$$

$\tilde{\varepsilon}_{\mathbf{k}}$, $\tilde{\Delta}_{\mathbf{k}}$, $\tilde{E}$: solutions of the renormalization equations for $\varepsilon_{\mathbf{k},\lambda}$, $\Delta_{\mathbf{k},\lambda}$

and E_{λ} in the limit $\lambda \to 0$

Note:

- Due to construction, the effective Hamiltonians are valid for moderate hole doping outside the antiferromagnetic regime and not yet in the Fermi-liquid phase
- Hamiltonains $\tilde{\mathcal{H}}$ are still strongly correlated models

4. Results and Discussion: Pseudogap phase

- Fully renormalized Hamiltonian: Model of independent strongly correlated electrons

$$\tilde{\mathcal{H}} = .\sum_{\mathbf{k}\sigma} \tilde{\varepsilon}_{\mathbf{k}}\, \hat{c}^{\dagger}_{\mathbf{k}\sigma}\, \hat{c}_{\mathbf{k}\sigma} + \tilde{E}$$

ARPES spectral function:

$$A(\mathbf{k},\omega) = \frac{1}{1+e^{\beta\omega}} G(\mathbf{k},\omega)$$

Anticommutator Green function:

$$G(\mathbf{k},\omega) \;=\; \frac{1}{2\pi}\int_{-\infty}^{\infty} \langle [\hat{c}^{\dagger}_{\mathbf{k}\sigma}(\lambda,-t)\,,\; \hat{c}_{\mathbf{k}\sigma}(\lambda)]_{+}\rangle_{\mathcal{H}_{\lambda}}\; e^{i\omega t} dt$$

Ansatz for $\hat{c}_{\mathbf{k}\sigma}(\lambda) = e^{X_\lambda}\,\hat{c}_{\mathbf{k}\sigma}\,e^{-X_\lambda}$ from lowest order perturbation theory

$$\hat{c}_{\mathbf{k}\sigma}(\lambda) = u_{\mathbf{k},\lambda}\hat{c}_{\mathbf{k}\sigma} + \frac{1}{2N}\sum_{\mathbf{q}} v_{\mathbf{k},\mathbf{q},\lambda}\,\frac{J_{\mathbf{q}}}{4\hat{\omega}^2_{\mathbf{q}}}\sum_{\alpha\beta\gamma}(\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\sigma\gamma})\sum_{\mathbf{k}'}(\varepsilon_{\mathbf{k}'}-\varepsilon_{\mathbf{k}'+\mathbf{q}})\;\hat{c}^{\dagger}_{\mathbf{k}'+\mathbf{q}\alpha}\;\hat{c}_{\mathbf{k}'\beta}\;\hat{c}_{\mathbf{k}+\mathbf{q}\gamma}$$

Parameters $u_{\mathbf{k},\lambda}$ and $v_{\mathbf{kq},\lambda}$ account for the λ- dependence of $\hat{c}_{\mathbf{k}\sigma}(\lambda)$

Result for $G(\mathbf{k},\omega)$ **from renormalization till** $\lambda \to 0$

$$G(\mathbf{k},\omega) = \tilde{u}_{\mathbf{k}}^2 D\,\delta(\omega - q\tilde{\varepsilon}_{\mathbf{k}}) +$$

(coherent excitation)

$$+\frac{3D}{2N^2}\sum_{\mathbf{q}\mathbf{q}'}\Big[\Big(\frac{J_{\mathbf{q}}}{4\hat{\omega}_{\mathbf{q}}^2}\tilde{v}_{\mathbf{k},\mathbf{q}}\Big)^2\big(\varepsilon_{\mathbf{k}+\mathbf{q}'} - \varepsilon_{\mathbf{k}+\mathbf{q}+\mathbf{q}'}\big)^2\big(\tilde{n}_{\mathbf{k}+\mathbf{q}+\mathbf{q}'}\tilde{m}_{\mathbf{k}+\mathbf{q}'} + \tilde{n}_{\mathbf{k}+\mathbf{q}}(D + \tilde{n}_{\mathbf{k}+\mathbf{q}'} - \tilde{n}_{\mathbf{k}+\mathbf{q}+\mathbf{q}'})\big)$$

$$+\cdots\Big] \times \delta\big(\omega + q(\tilde{\varepsilon}_{\mathbf{k}+\mathbf{q}+\mathbf{q}'} - \tilde{\varepsilon}_{\mathbf{k}+\mathbf{q}'} - \tilde{\varepsilon}_{\mathbf{k}+\mathbf{q}})\big)$$

(incoherent excitations)

where $\hat{\omega}_{\mathbf{q}}^2 = 2\delta\,(t_{\mathbf{q}=0}^2 - t_{\mathbf{q}}^2) \geq 0,$,

$\delta = 1 - n,$ hole filling

$D = 1 - n/2$

Gutzwiller approximation:

$$\tilde{n}_{\mathbf{k}} = \langle \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} \rangle_{\tilde{\mathcal{H}}} = (D - q) + q\, f(\tilde{\varepsilon}_{\mathbf{k}})$$

$$\tilde{m}_{\mathbf{k}} = \langle \hat{c}_{\mathbf{k}\sigma} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \rangle_{\tilde{\mathcal{H}}} = q\,(1 - f(\tilde{\varepsilon}_{\mathbf{k}}))$$

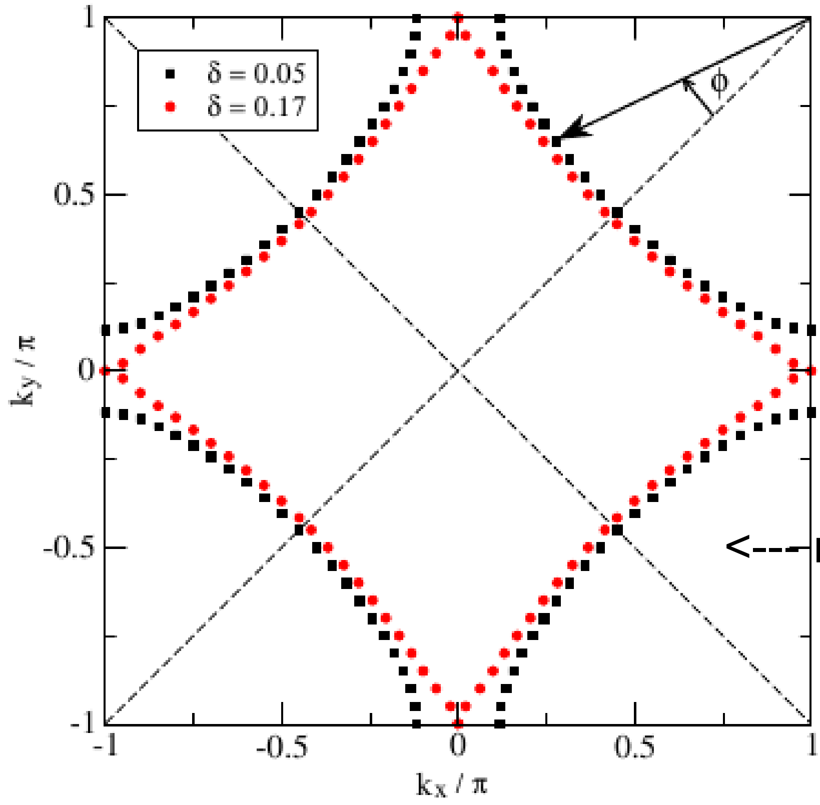
where $q = \dfrac{1-n}{1-n/2}$ attenuation factor for hopping matrix element

Note: $\tilde{u}^2_{\mathbf{k}}$ and $\tilde{v}^2_{\mathbf{k},\mathbf{q}}$ are related to each other by the **sum rule:**

$$\int_{-\infty}^{\infty} d\omega\, G(\mathbf{k},\omega) = \langle [\hat{c}^{\dagger}_{\mathbf{k}\sigma}, \hat{c}_{\mathbf{k}\sigma}]_{+} \rangle = 1 - \frac{n}{2}$$

Fermi surface similar to Fermi surface of uncorrelated electrons

(J = t' = 0.2 t ,   40 x 40 sites)



<---- antinodal region

<--- nodal region

PRM result:

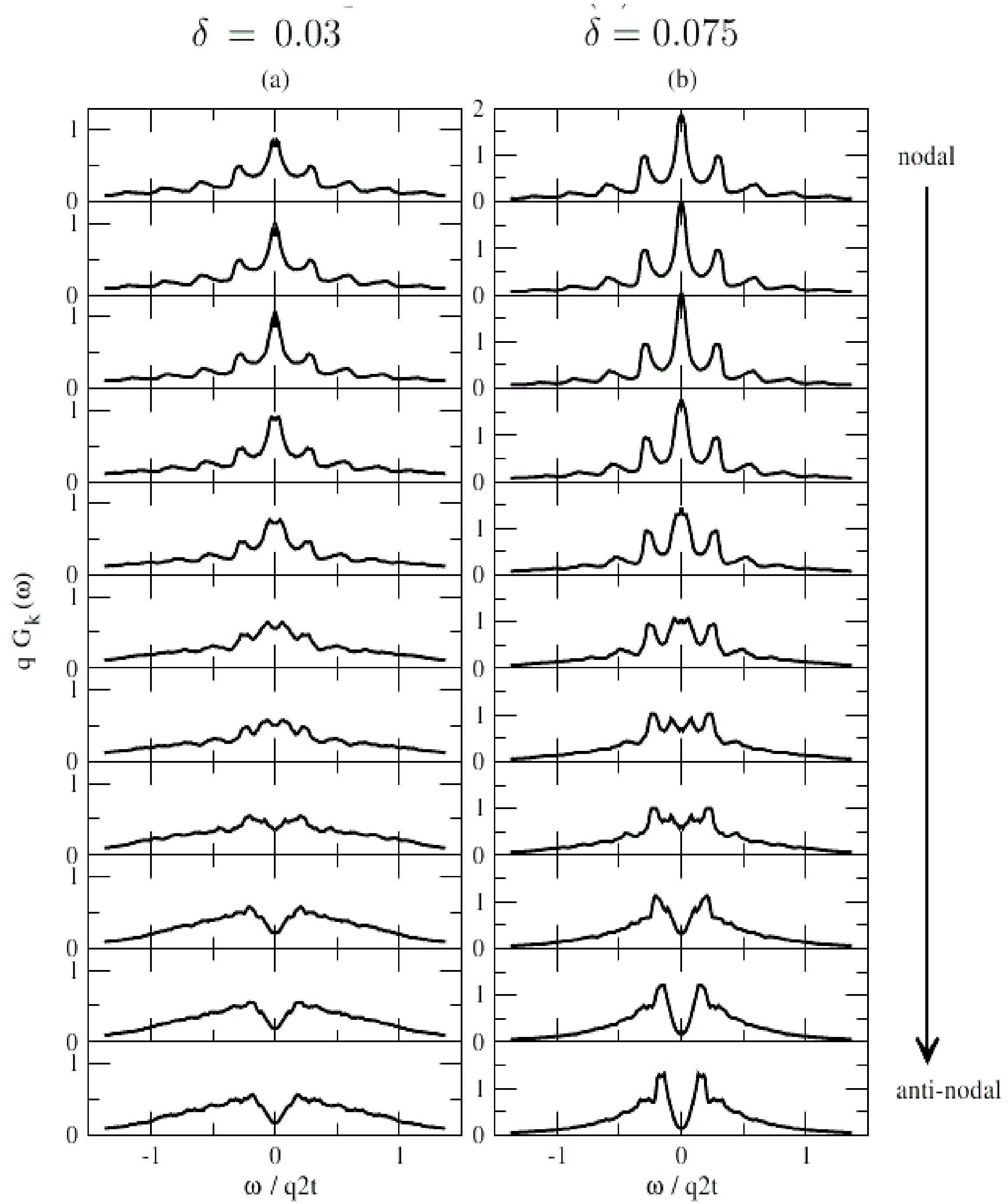
Symmetrized spectral function

$G(\mathbf{k}, \omega)$ **along Fermi surface:**

-- opening of a **pseudogap** around the anti-nodal point

-- Fermi arc of **gapless excitations** around the nodal point

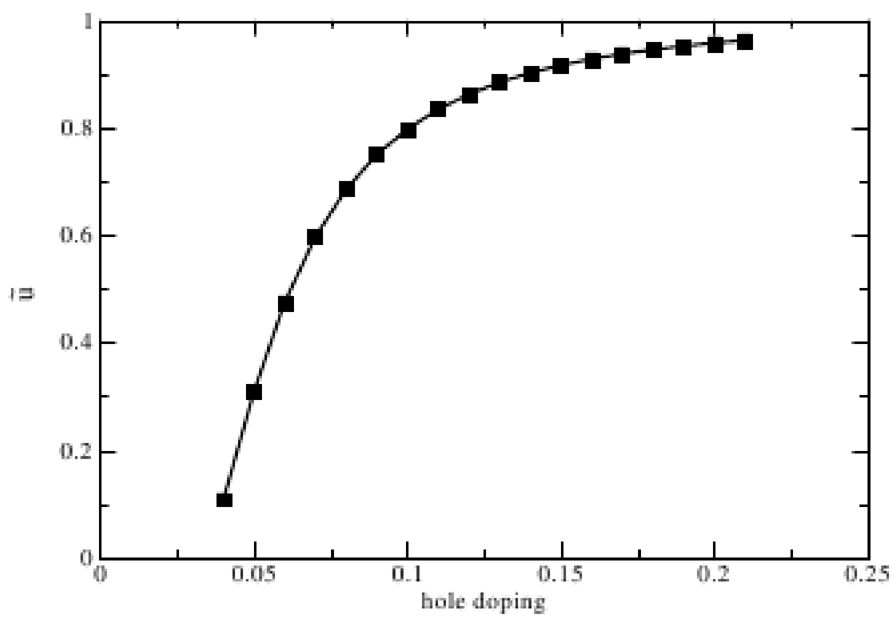
-- additional peaks in the nodal region at lower binding energies



-- Origin of pseudogap can be understood as suppression of incoherent weight in a small energy range in the anti-nodal region

-- Spectrum completely dominated by incoherent excitations of $G(\mathbf{k}, \omega)$

weight $\tilde{u}_{\mathbf{k}}^2$ of the coherent excitation small



Experiment:

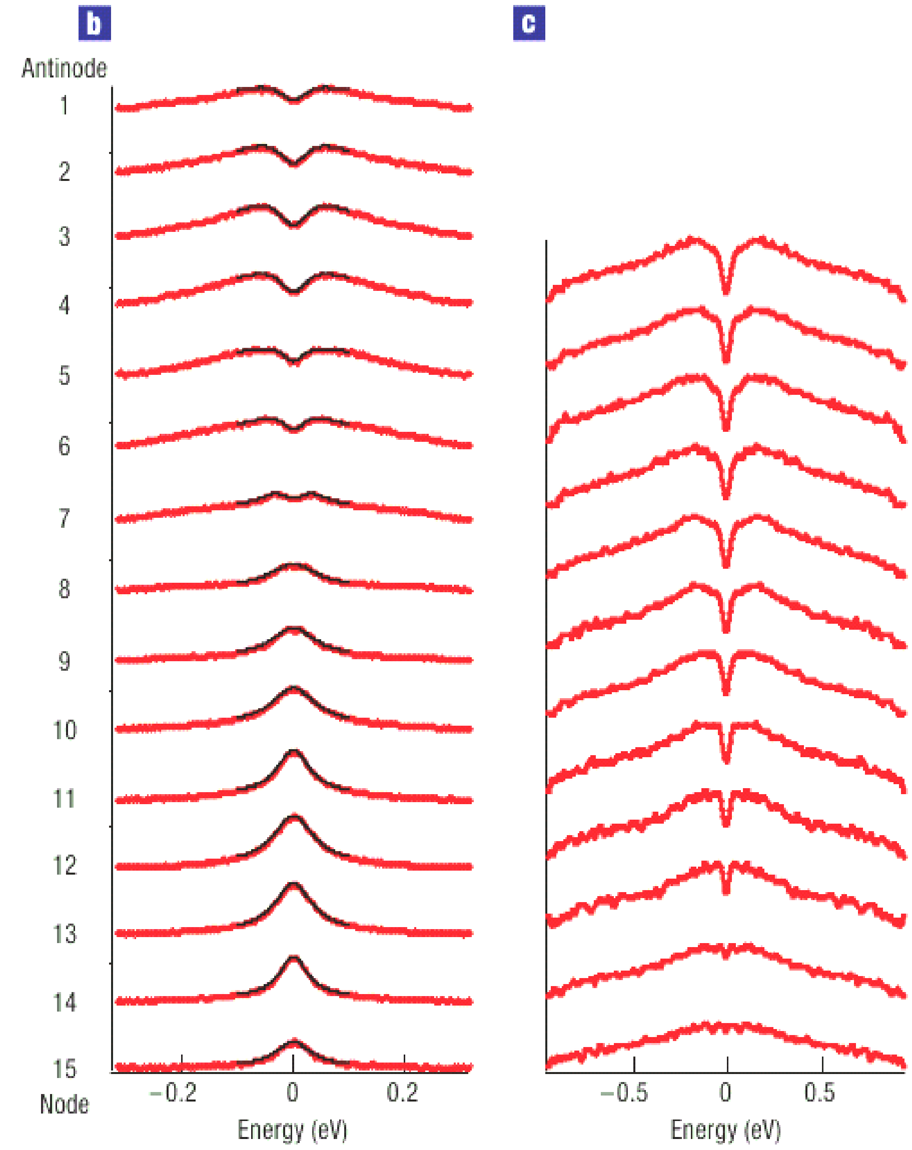
Symmetrized spectral function of Bi2212 in the pseudogap phase

b: T_c =90 K sample in the pseudogap phase at T=140 K

c: Spectral function for a very underdoped, T_c =25 K, sample measured at 55 K

Note:

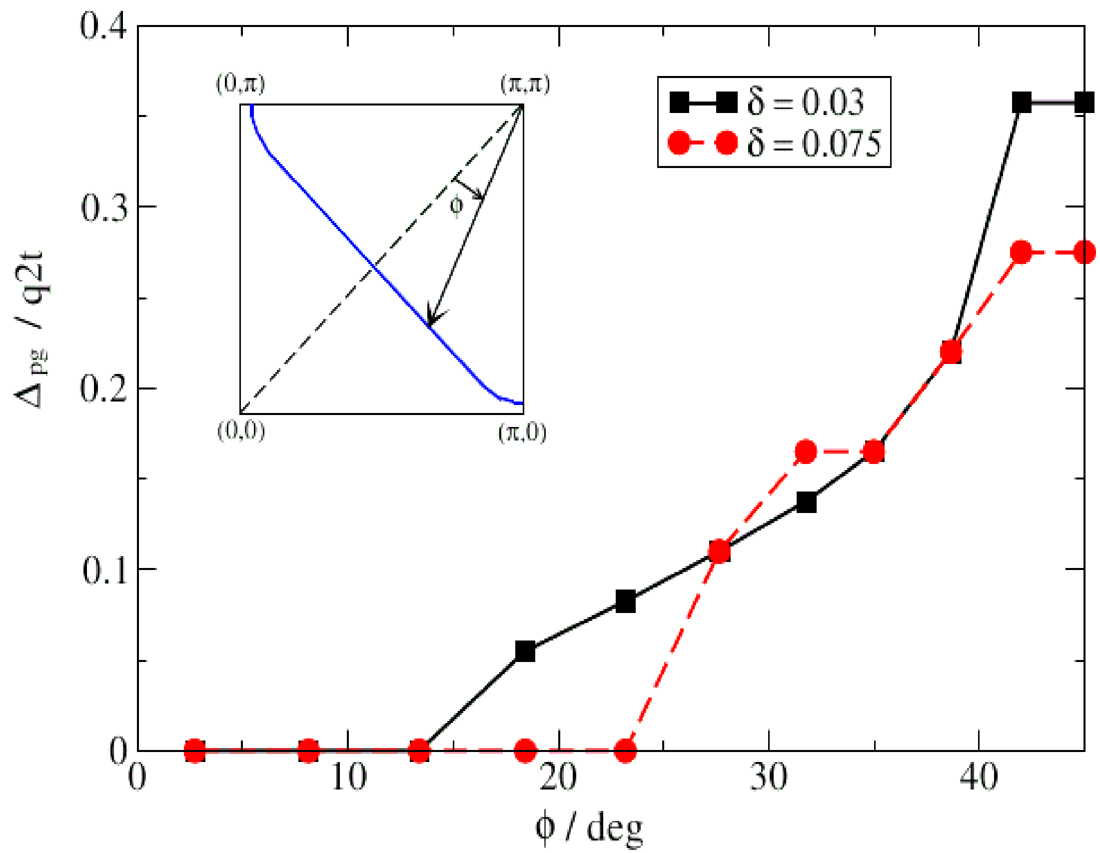
At low doping the spectral weight is reduced relative to higher doping values in agreement with theory



Kanigel et al., Nature Physics **2**. 447 (2006)

PRM: Pseudogap on the Fermi surface

- for lower hole doping δ pseudogap somewhat larger
- arc length of gapless excitat-ions somewhat smaller
- corresponds to an increase of pseudogap temperature T*



nodal

anti-nodal

direction

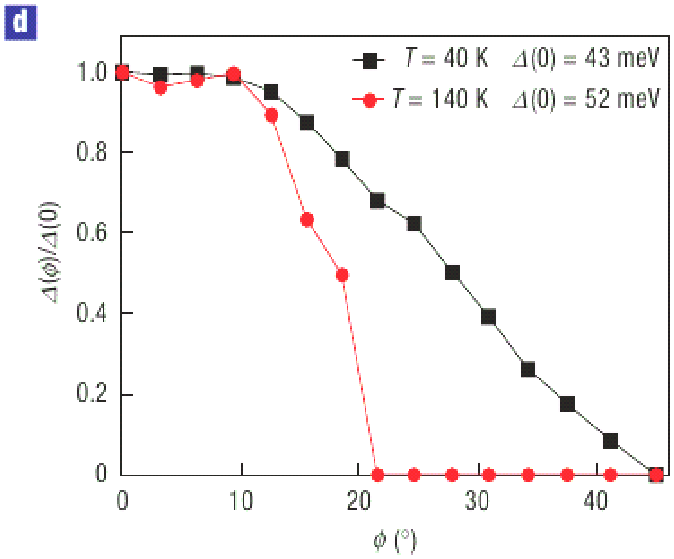
Experiment:

d: red curve: **pseudogap**

- Variation of the pseudogap along the Fermi surface extracted from figure b above

- black curve:

  superconducting phase (see below)



anti-nodal   nodal

region

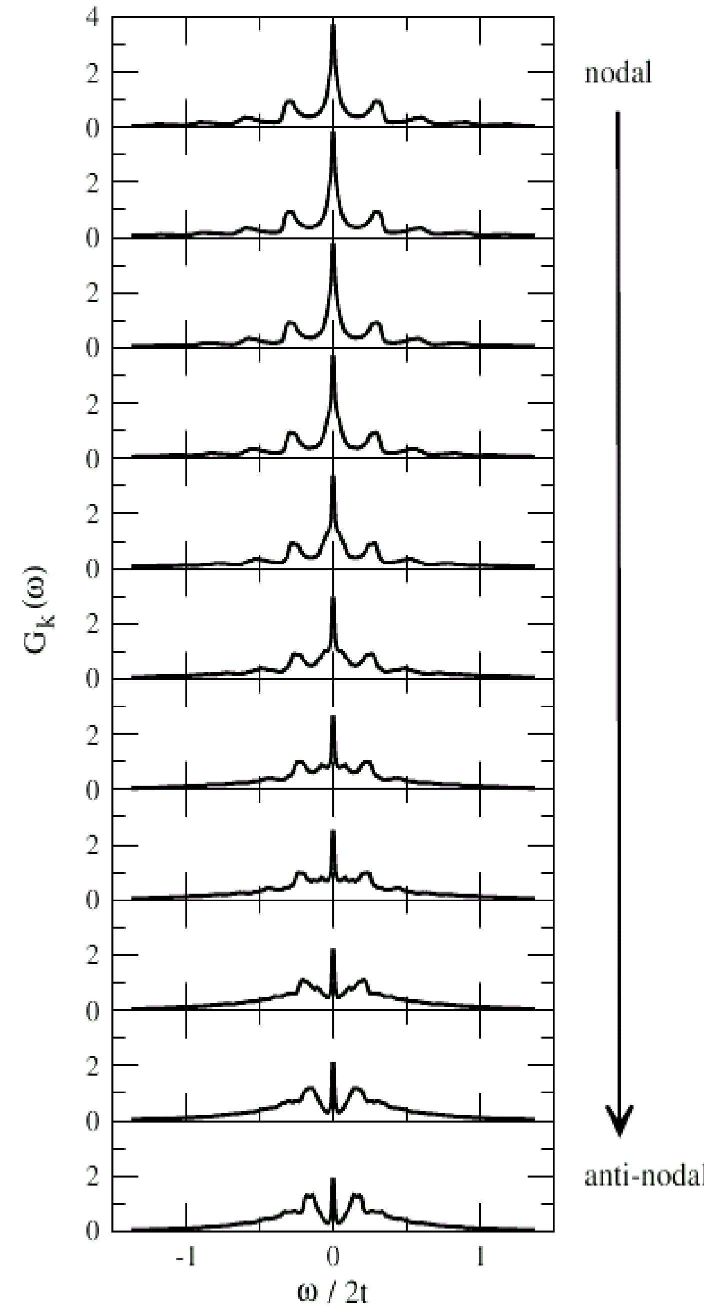
Larger hole doping: $\bar{\delta} = 0.0\dot{9}$

-- additional (narrow) coherent excitation at $\omega = 0$ evolves at the anti-nodal point

-- for larger hole filling coherent excitation becomes dominant and signals the breakdown of the pseudogap phase

-- broadening due to coupling to other degrees of freedom is expected

$\bar{\delta} = 0.0\dot{9}$

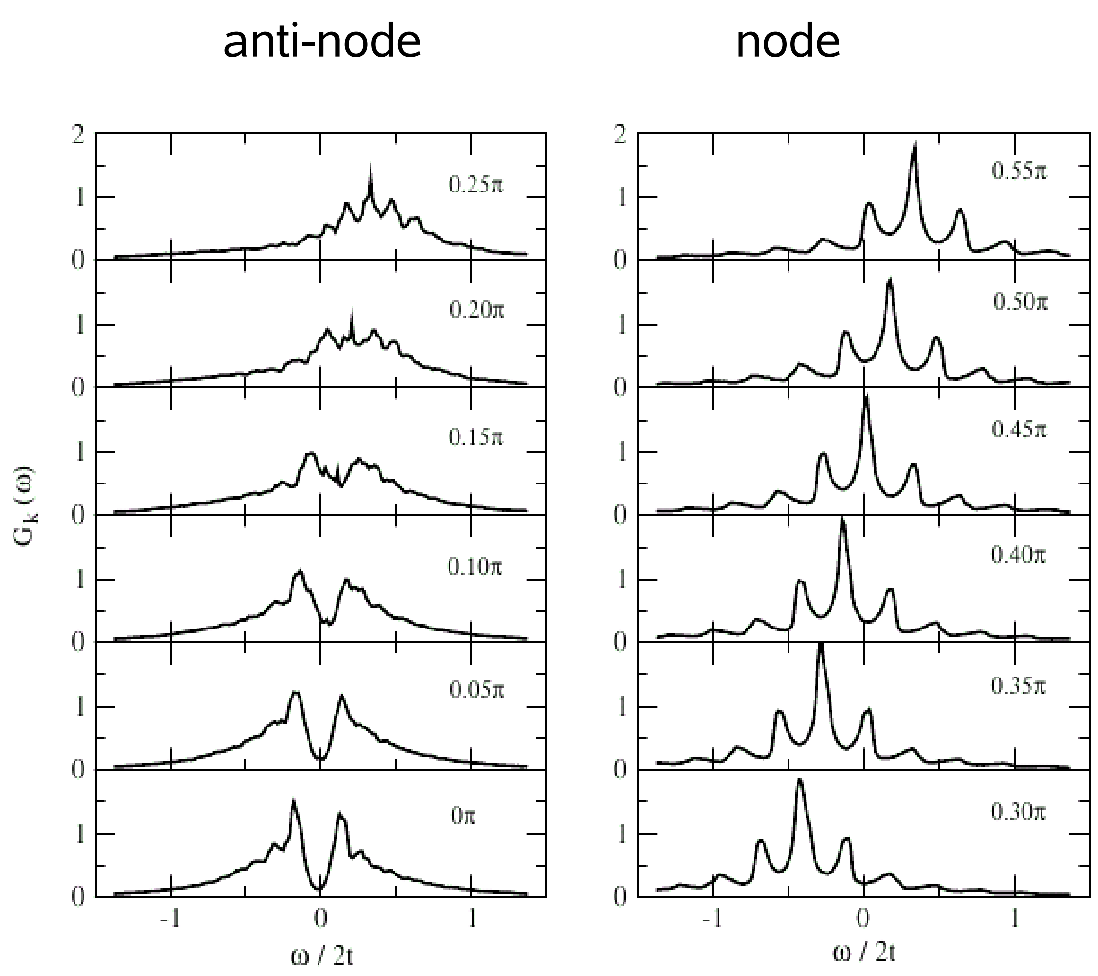


PRM result: Spectral function for different cuts crossing the Fermi surface

-- in the nodal region the whole peak structure moves through the Fermi surface

-- in the anti-nodal direction a gap is only found for $\mathbf{k}$ close to the FS

==> agreement with experiment



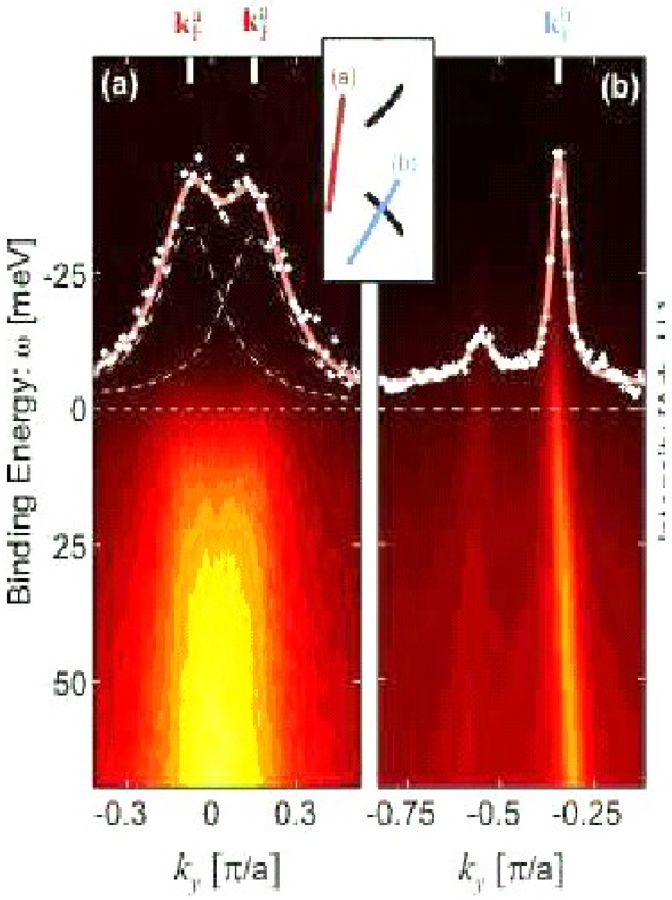
$k_x = \pi$ $\quad$ $k_x = \pi/2$

(k_x fixed, k_y varied)

Experiment:

Angle resolved photoemission spectra

recorded on La1.48 Nd0.4 Sr0.12 CuO4



Chang et al., cond-mat 0805.0302

Summary (pseudogap phase) :

-- results of the PRM approach show excellent agreement with ARPES data

-- spectrum in pseudogap phase is dominated by incoherent excitations

-- pseudogap caused by suppression of incoherent spectral weight in the anti-nodal region

-- pseudogap is an intrinsic property of the normal phase and not due to a competing order

-- by changing the hole filling (or temperature) a transition to a superconducting phase can also be found in the PRM approach

5) Superconducting phase: order parameter

Fully renormalized Hamiltonian:

$$\tilde{\mathcal{H}} = \sum_{\mathbf{k}\sigma} \tilde{\varepsilon}_{\mathbf{k}} \, \hat{c}^{\dagger}_{\mathbf{k}\sigma} \, \hat{c}_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \left(\tilde{\Delta}_{\mathbf{k}} \, \hat{c}^{\dagger}_{\mathbf{k},\uparrow} \hat{c}^{\dagger}_{-\mathbf{k},\downarrow} + \tilde{\Delta}^{*}_{\mathbf{k}} \, \hat{c}_{-\mathbf{k},\downarrow} \hat{c}_{\mathbf{k},\uparrow} \right) + \tilde{E}$$

Renomalization equation for $\Delta_{\mathbf{k},\lambda}$ leads to the sc gap function $\tilde{\Delta}_{\mathbf{k}}$

Approximate gap equation:

$$\tilde{\Delta}_{\mathbf{k}} \approx -\frac{1}{N} \sum_{\mathbf{q}, |\varepsilon_{\mathbf{k+q}}| \leq |\tilde{\Delta}_{\mathbf{k+q}}|} \frac{3 J_{\mathbf{q}}}{4 \omega_{\mathbf{q}}^2} (\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k+q}})^2 \, |\tilde{u}_{\mathbf{k+q}}|^2 \frac{1 - 2 f(\tilde{E}_{\mathbf{k+q}})}{2\sqrt{\varepsilon_{\mathbf{k+q}}^2 + |\tilde{\Delta}_{\mathbf{k+q}}|^2}} \tilde{\Delta}_{\mathbf{k+q}}$$

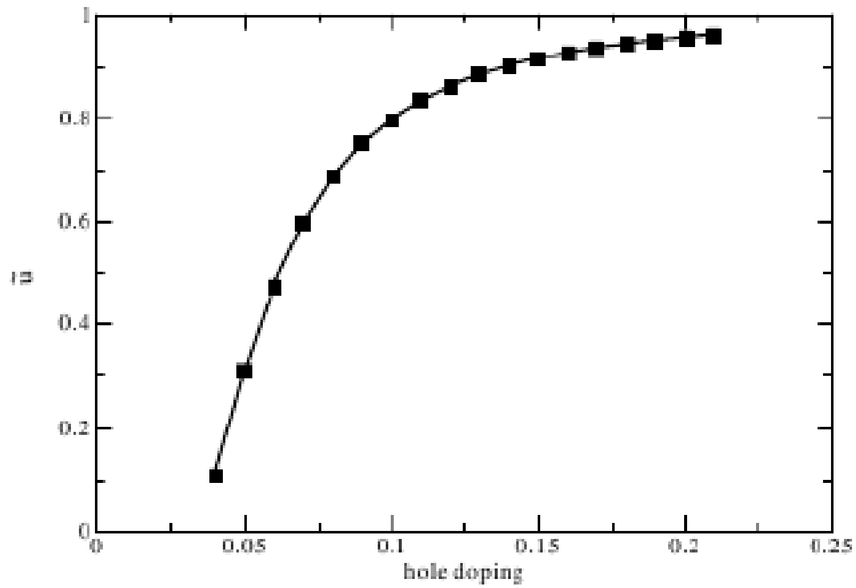
where $\tilde{E}_{\mathbf{k}} = D\sqrt{\varepsilon_{\mathbf{k}}^2 + |\tilde{\Delta}_{\mathbf{k}}|^2}$

Note: Pairing interaction proportional to J

mainly caused by the $\mathcal{A}_0$ part of $\mathcal{H}_J$ which commutes with $\mathcal{H}_t$

$\tilde{u}_{\mathbf{k}}^2$ weight of the coherent excitation

Weight of the coherent excitation $\tilde{u}_{\mathbf{k}}^2$ as function of hole doping



Superconducting gap: d-wave symmetry (T=0)

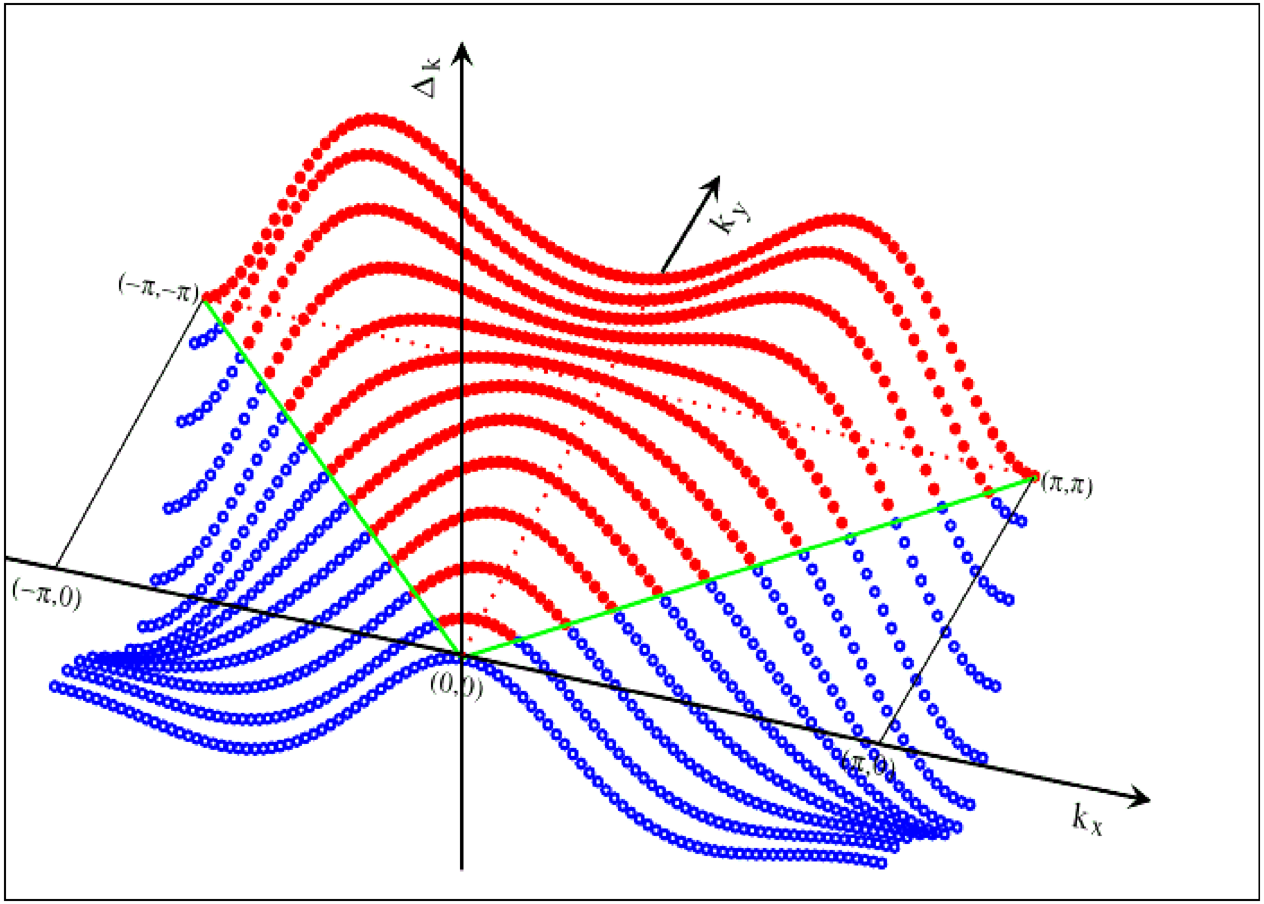
strong **k**-dependence

of $\bar{\Delta}_{\mathbf{k}}$ due to the strong

k-dependence of the

pairing interaction in the

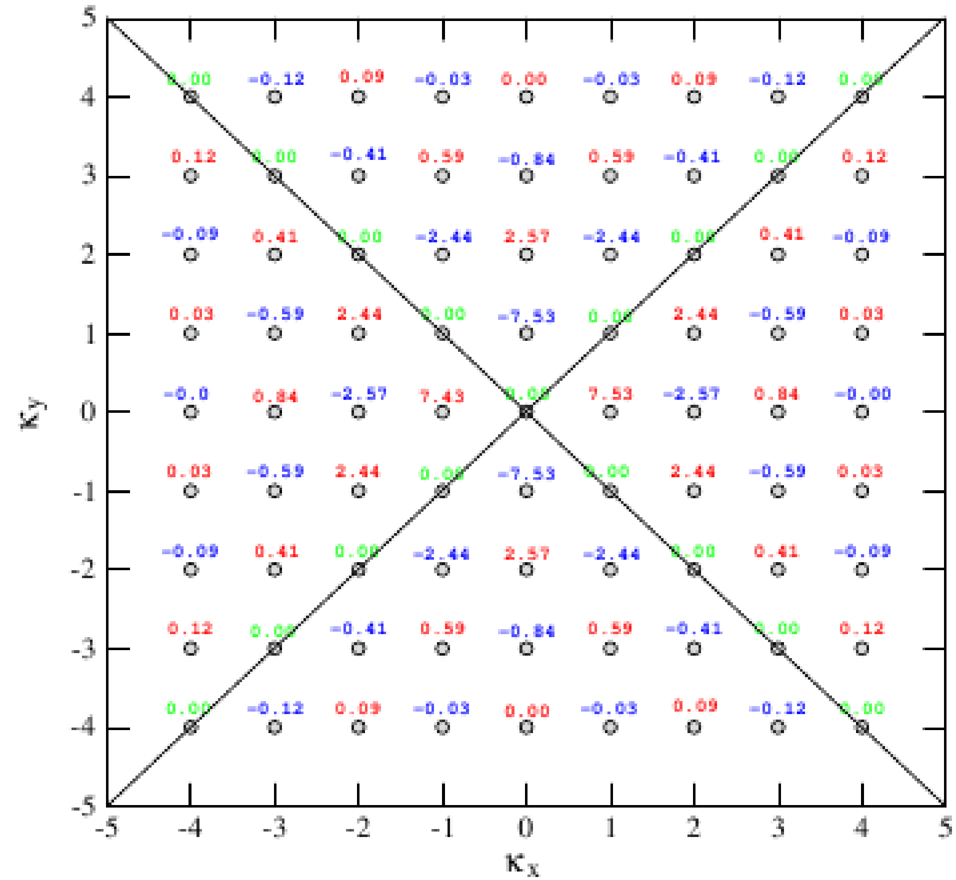
gap equation



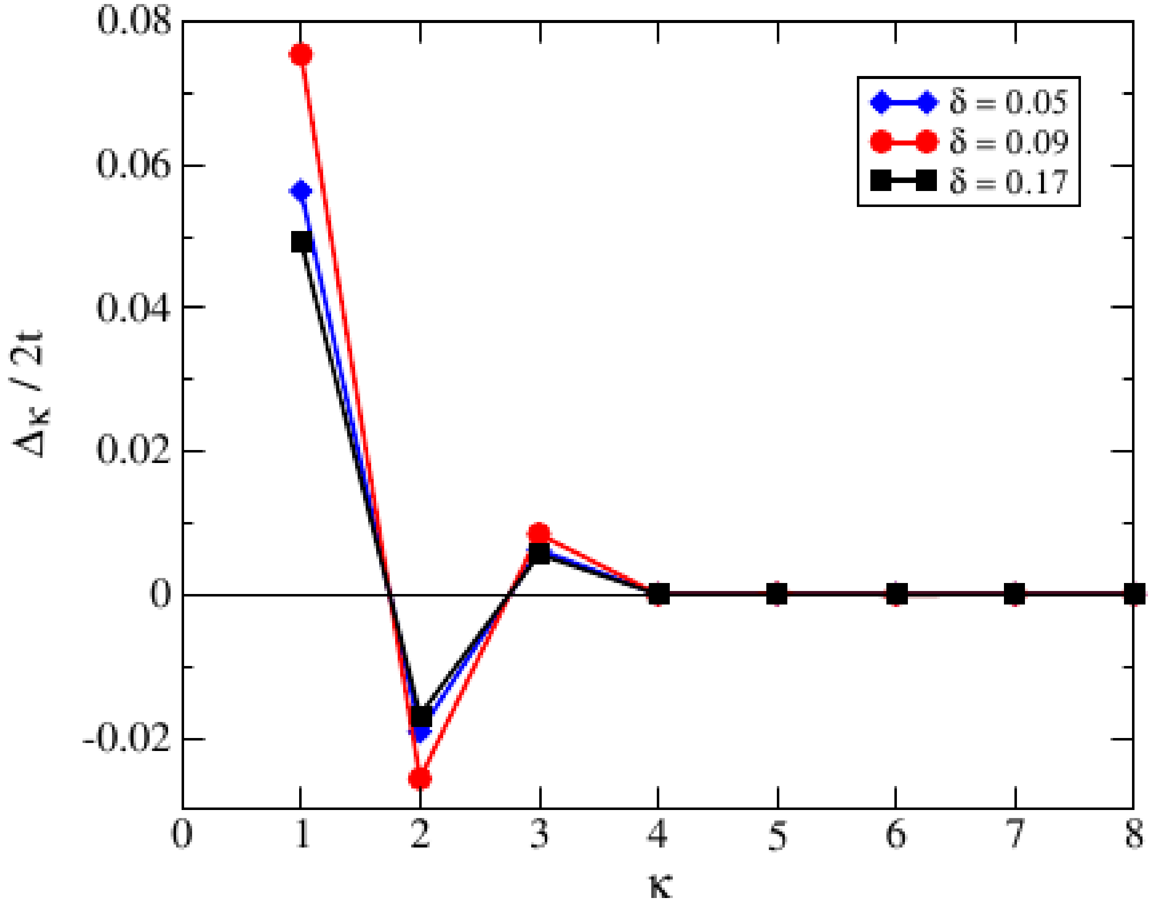
Superconducting order parameter Δ_{ij} in local space

Coherence length is of the order

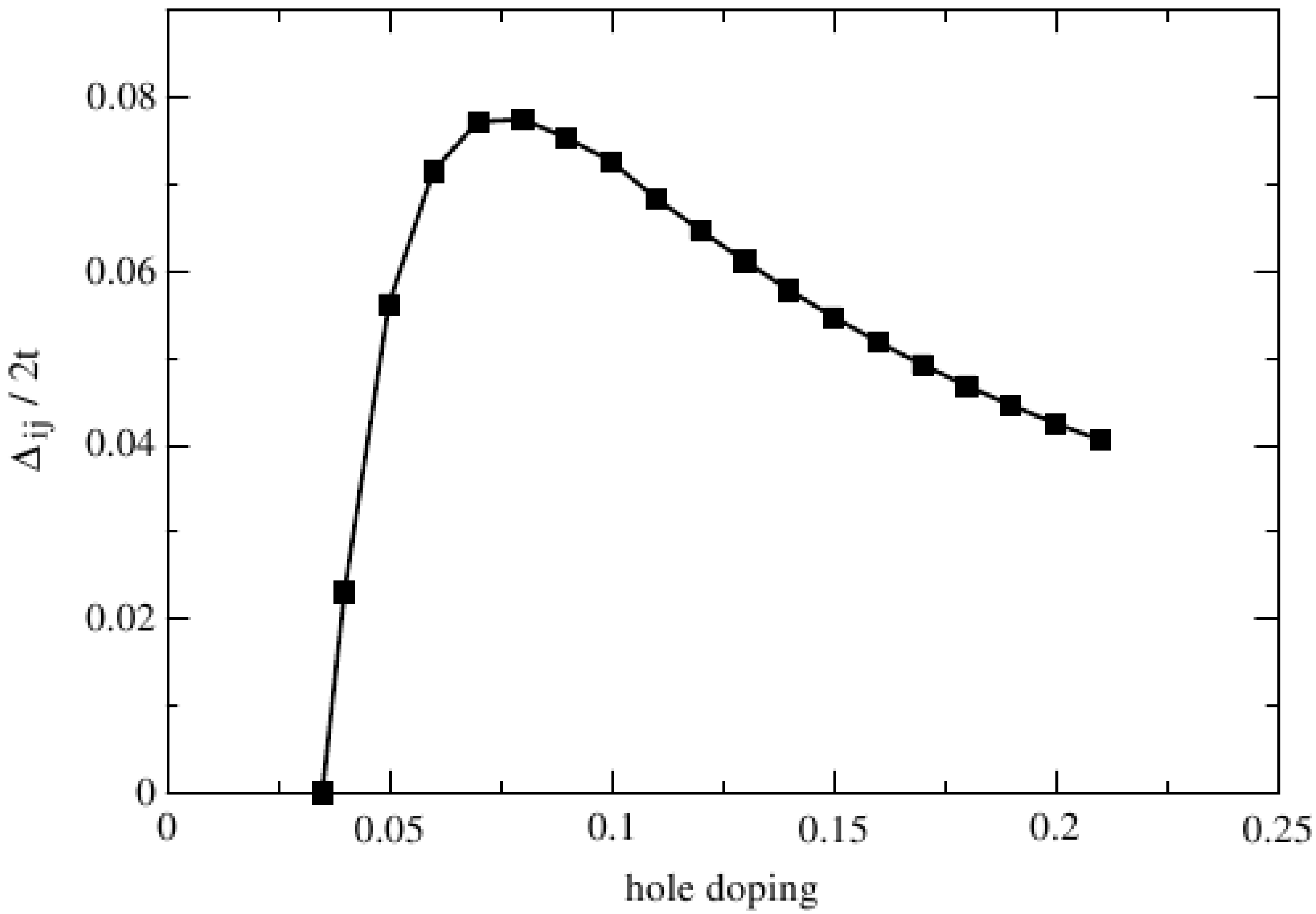
of a few lattice constants



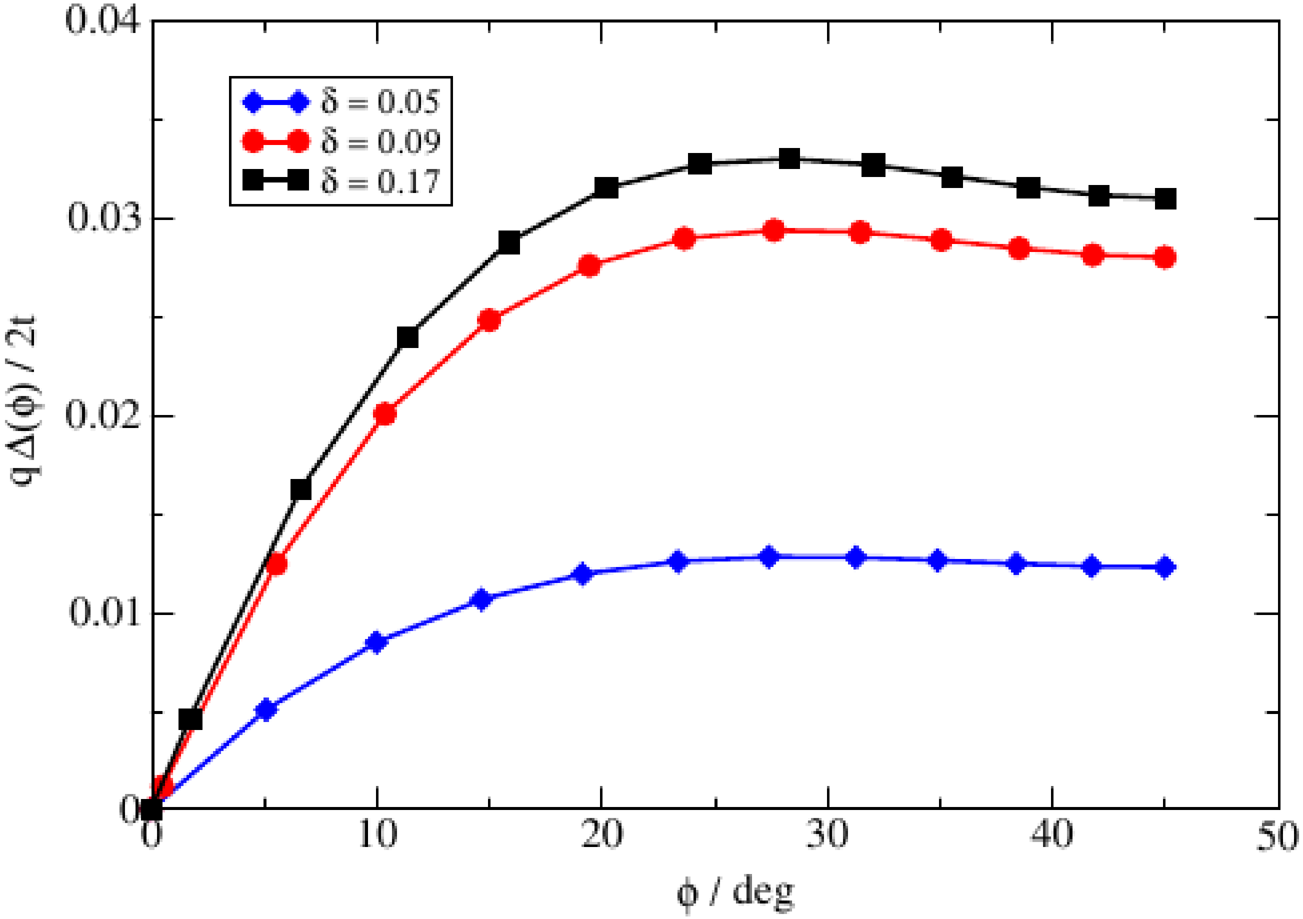
Order parameter Δ_{ij} in local space along the x direction:



Order parameter between nearest neighbor sites as function of hole doping



Superconducting order parameter Δ_k in k-space along the Fermi surface

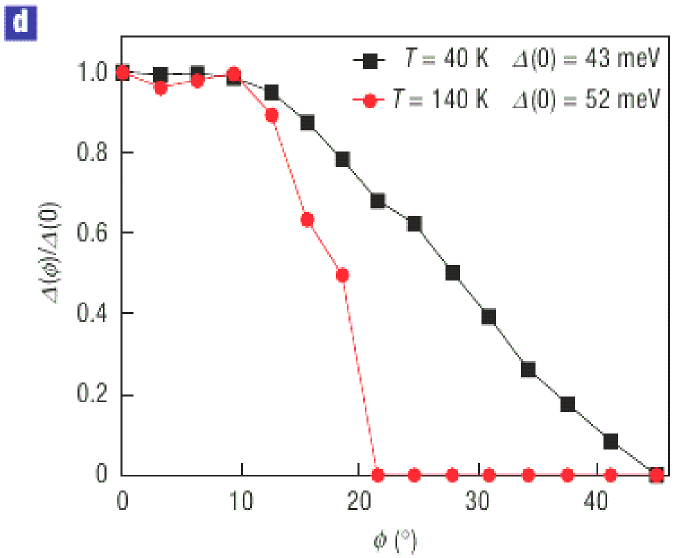


Experiment:

superconducting gap

along Fermi surface

(black curve)



anti-nodal

region

nodal

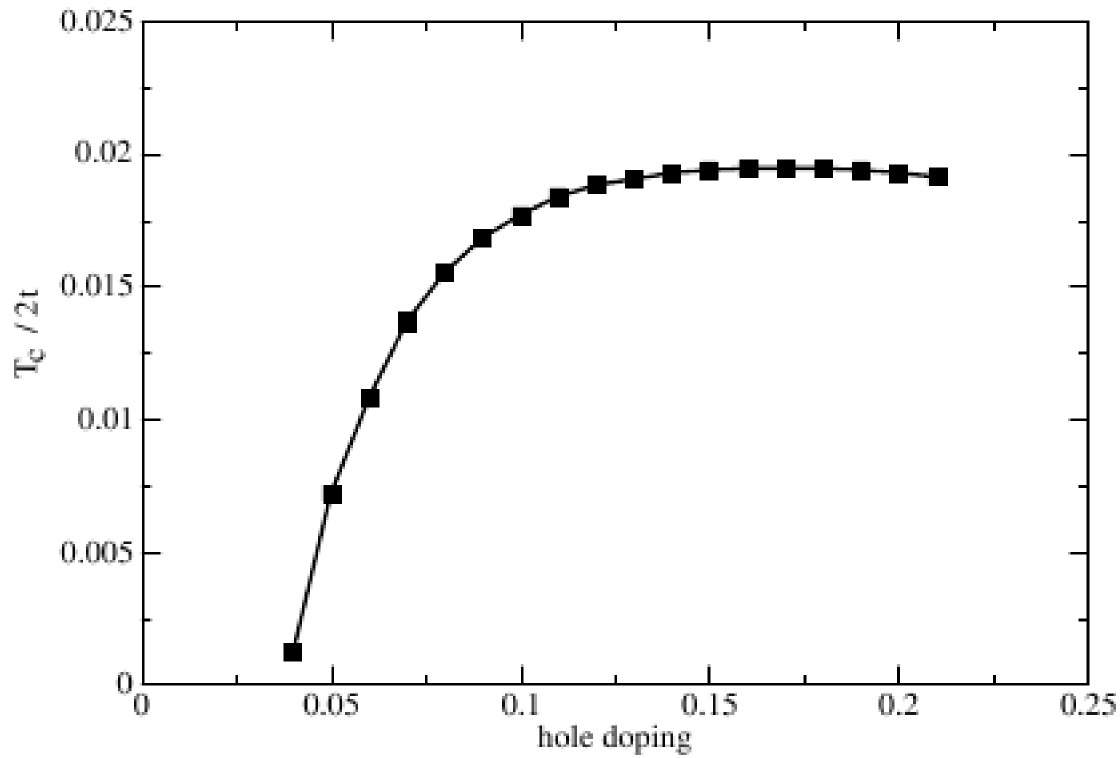
(Kanigel et al.)

Critical temperature T_c in the underdoped and optimally doped regime

-- decrease at underdoping

due the vanishing of $\tilde{u}_{\mathbf{k}}^2$

with decreasing hole doping



Summary (superconducting phase):

-- superconducting pairing interaction proportional to J

-- in contrast to the pseudogap phase the coherent weight $|\tilde{u}_{\mathbf{k}+\mathbf{q}}|^2$

is important in the sc phase

-- breakdown of the sc phase at low δ follows from vanishing of $u^2_{\mathbf{k},\lambda}$

due to renormalization behavior $u^2_{\mathbf{k},\lambda-\Delta\lambda} - u^2_{\mathbf{k},\lambda} = -\alpha_\lambda/\delta^2$

-- breakdown for large δ follows from the gap equation where in the

denominator $\hat{\omega}^2_{\mathbf{q}} \sim \delta$

-- agreement of ARPES spectra with experiments expected as well