FLEX and beyond: how to calculate kink and resonance peak within the spin-fluctuation scenario

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work done together with: I. Eremin (MPI Dresden)
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*thanks to:
Alexander von Humboldt-Foundation

Content

- Motivation: what are fingerprints of Cooper-pairing?
- Theory: generalized Eliashberg theory, simple FLEX approach
- Results: kink, resonance peak, anisotropy(!)
- Extensions of FLEX: bilayer case, underdoped regime, …

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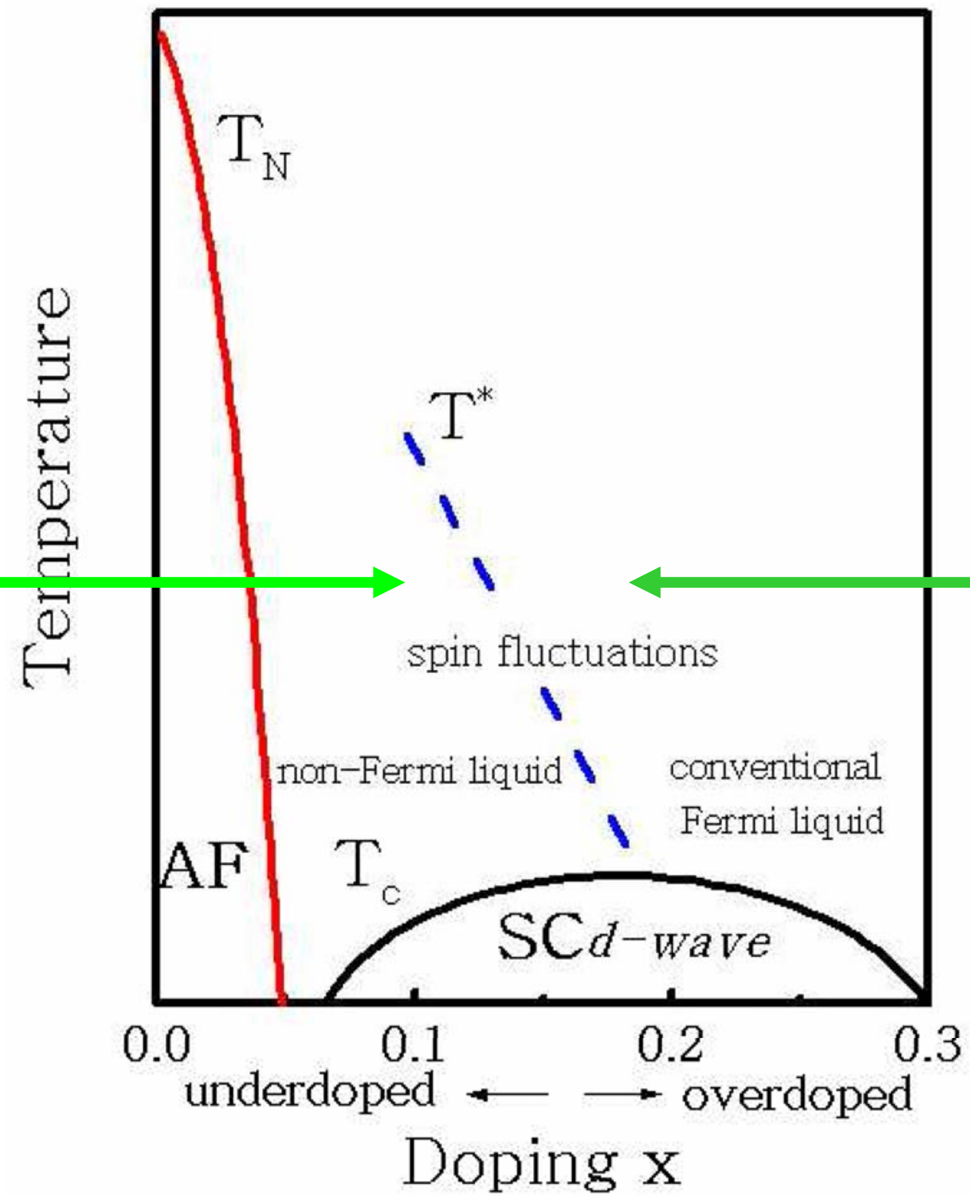
Phase diagram (hole-doped)

Theory I



Theory II

Important questions

- how to identify the pairing mechanism?
- what are key experiments?
- why *d*-wave pairing?

Symmetry of the order parameter in cuprates (unconventional superconductivity)

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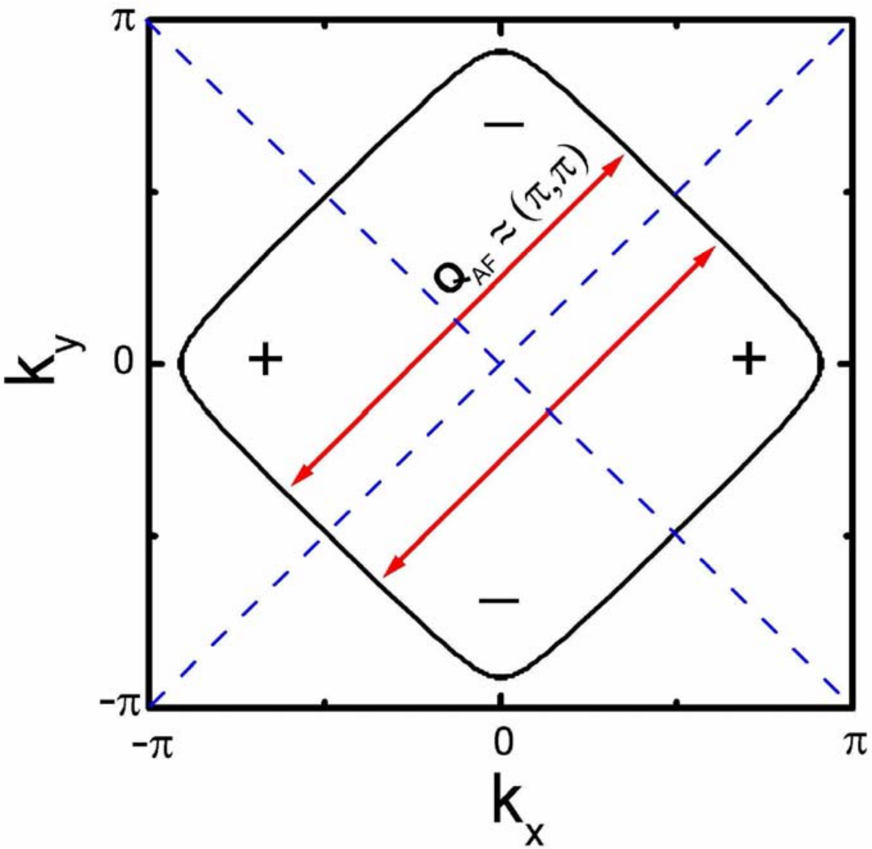
gap equation: $$\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'} \frac{V_{eff}(\mathbf{k}-\mathbf{k}')}{2E_{\mathbf{k}'}}\Delta(\mathbf{k}')$$ **with**

$$E^2_{\mathbf{k}} = \epsilon^2_{\mathbf{k}} + \Delta^2_{\mathbf{k}}$$ **(qp dispersion)**

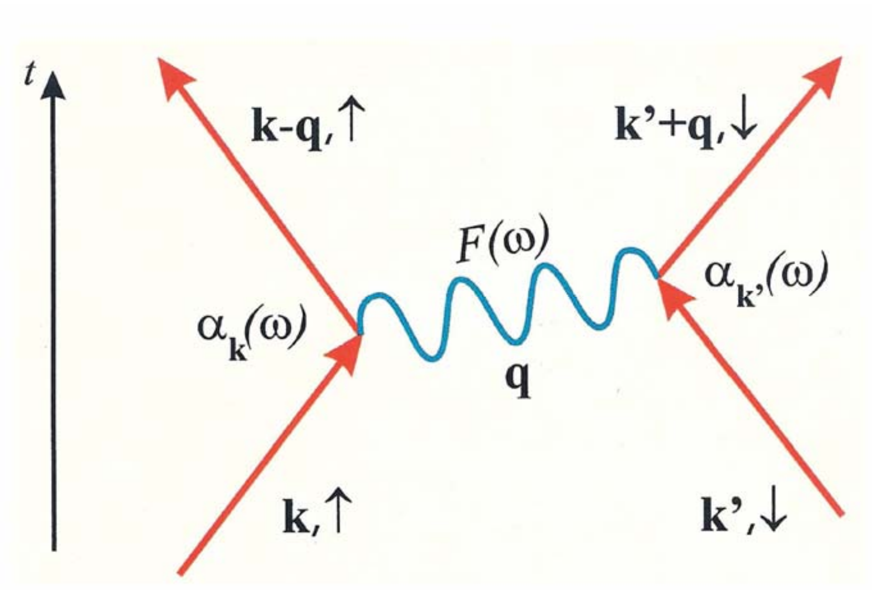
V_{eff} is calculated from χ.

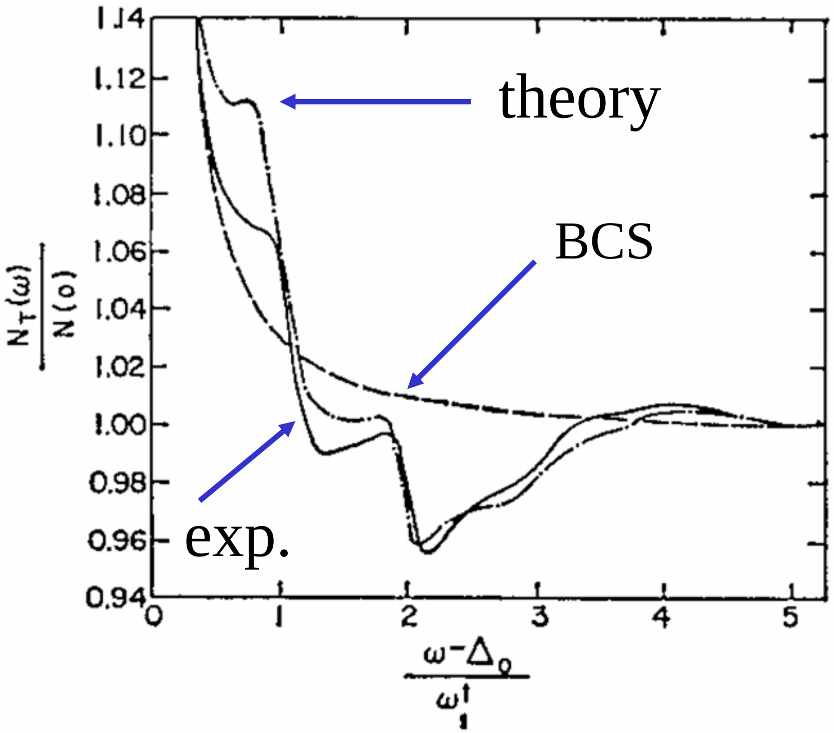


d_{x2-y2}-wave order parameter

$$\Delta(\mathbf{k}) = \frac{\Delta_0}{2}\left[\cos(k_x) - \cos(k_y)\right]$$

Cooper-pairing mechanism for phonons





pairing interaction is determined by $V_{eff} = \alpha^2_{k,k'} F(\omega)$
Eliashberg equations yield $\Delta(\omega)$ and tunneling density of states

$$\frac{N_T(\omega)}{N(0)} = \mathrm{Re}\left[\frac{\omega}{\sqrt{\omega^2 - \Delta^2(\omega)}}\right]$$

D.J. Scalapino, J.R. Schrieffer, J.W. Wilkins PR **148**, 148 (1966)

Coupling of holes to spin excitations

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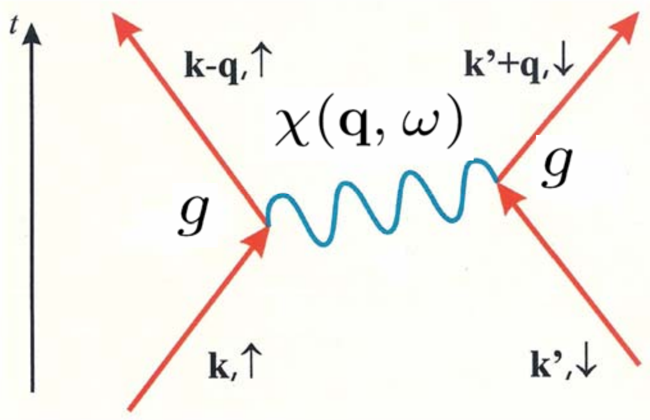

□ Cooper-pairing is controlled by spin excitations:

Ornstein-Zernicke form for the spin susceptibility ($\mathbf{Q} = (\pi, \pi)$), parameters from NMR (Millis, Monien, Pines (PRB 1989))

$$\chi(\mathbf{q},\omega) = \frac{\chi_{\mathbf{Q}}}{1 + \xi^2(\mathbf{q} - \mathbf{Q})^2 - i\frac{\omega}{\omega_{sf}}}$$

leads with $g = U_{eff} = U$

$$V_{eff}(\mathbf{q},\omega) = g^2\,\chi(\mathbf{q},\omega)$$

$\Longrightarrow$ high-T_c and d-wave is possible

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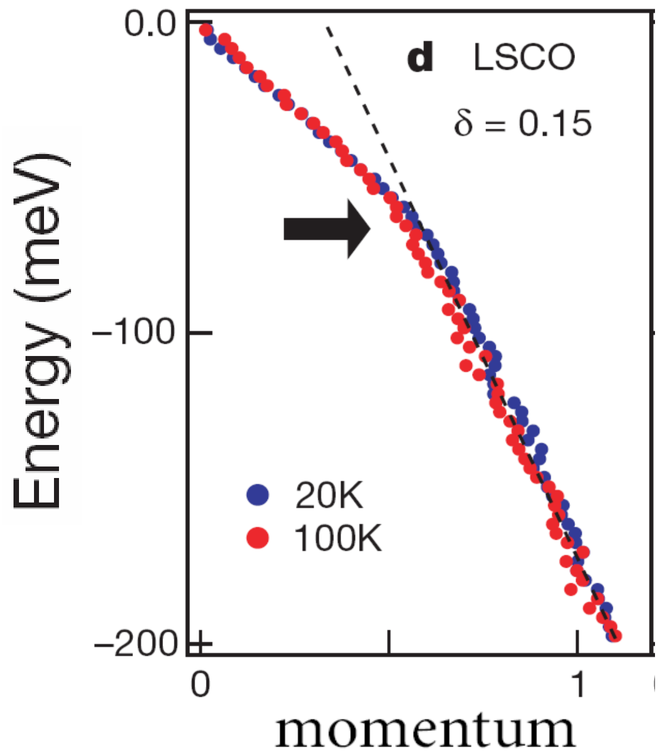
Motivation (1): kink in ARPES



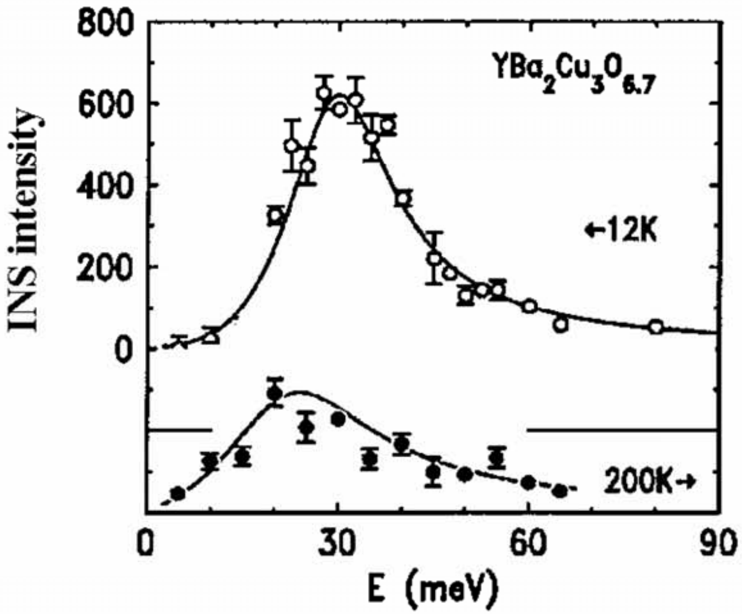
A. Lanzara et al., Nature 412, 510 (2001)

see also, e.g.
T. Valla et al., Science 285, 2110 (1999)
P.V. Bogdanov et al., PRL 85, 2581 (2000)
A. Kaminski et al., PRL 86, 1070 (2001)

A.A. Kordyuk et al., PRL 2004, PRB 2004, PRB 2005, …
S.V. Borisenko et al., PRL 2006, PRB 2004

- **are the various kinks fingerprints of spin fluctuations or phonons?**
- **how to understand the anisotropy in k-space and *d*-wave pairing?**

Motivation (2): resonance peak



H.F. Fong *et al.*, PRB **61**, 14773 (2000)

pairing mechanism:
strong feedback on $\chi(q, \omega)$

$$\frac{\omega_{res}}{T_c}(x) = \textbf{?} = \mathbf{5.4}$$

He et al., PRL 86, 1610 (2001)

- ❑ why mainly observed in **hole-doped cuprates**?
- ❑ what is the **dispersion** of the resonance peak?

Is a Scalapino-Schrieffer-Wilkins-like analysis for high-T_c cuprates possible?

Motivation (3): anisotropic spin excitations

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Fermi-liquid theory? **stripe scenario?**

new experiments on fully untwinned YBCO

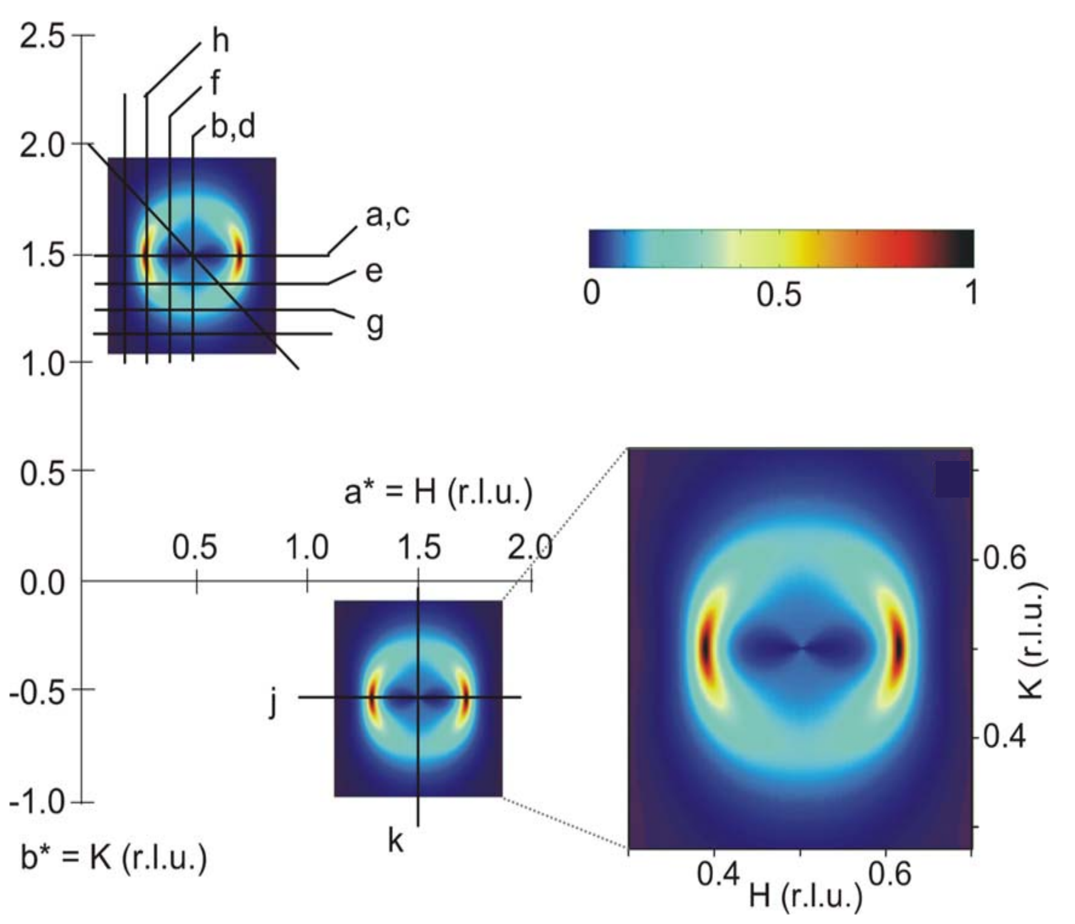
earlier data on partially untwinned YBCO by *Mook et al. (Nature, 2000)* reveal 1D excitations

***Keimer's* recent results *(V. Hinkov et al., Nature, 2004)*:**

- **INS data show 2D magnetic fluctuations**
- **but strong anisotropy → one-dimensional width and amplitude ansiotropy (dependent on the excitation energy)**

B. Keimer's recent results:

$\chi''(q,\omega=35meV)$ for opt. doped untwinned YBCO



V. Hinkov et al., *Nature* **430**, 650 (2004).

Theory: Aim

Generalized Eliashberg equations for spin fluctuation-mediated Cooper-pairing (FLEX approximation)

- ❑ **understanding of the kink, high-T_c values, and *d*-wave**
- ❑ **understanding of the resonance peak, its dispersion, and the strong anisotropy**

What is the FLEX approximation?

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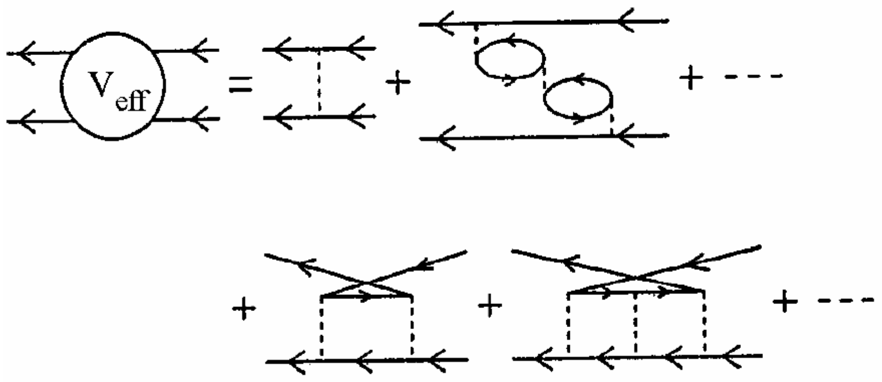
FLEX (FLuctuation EXchange) is a numerical technique for strongly correlated systems which
(a) satisfies macroscopic conservation laws
(b) treats strong frequency and momentum dependences
(Bickers, Scalapino, White, PRL 1989)

our case:
finite-*T* Bethe-Salpeter equation employing the 2D Hubbard model



$$H = -\sum_{\langle ij\rangle\sigma} t_{ij}(c^{+}_{i\sigma}c_{j\sigma} + c^{+}_{j\sigma}c_{i\sigma}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

input parameters: **(a) ab-initio, LDA+FLEX**
or **(b) model parameters**

→ $\boxed{\textbf{generalized Eliashberg equations}}$

Generalized Eliashberg equations

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The dressed one-particle propagator

mass renormalization

energy renormalization

$$G(\mathbf{k}, i\omega_n) = \frac{i\omega_n Z(\mathbf{k}, i\omega_n) + \epsilon_\mathbf{k} + \xi(\mathbf{k}, i\omega_n)}{\left(i\omega_n Z(\mathbf{k}, i\omega_n)\right)^2 - \left(\epsilon_\mathbf{k} + \xi(\mathbf{k}, i\omega_n)\right)^2 - \phi^2(\mathbf{k}, i\omega_n)}$$

sc gap function

and

$$F(\mathbf{k}, i\omega_n) = \frac{\phi(\mathbf{k}, i\omega_n)}{\left(i\omega_n Z(\mathbf{k}, i\omega_n)\right)^2 - \left(\epsilon_\mathbf{k} + \xi(\mathbf{k}, i\omega_n)\right)^2 - \phi^2(\mathbf{k}, i\omega_n)}$$

with a tight-binding dispersion relation

$$\epsilon_\mathbf{k} = -2t\left[\cos(k_x) + \cos(k_y) - 2t' \cos(k_x)\cos(k_y) + \mu/2\right]$$

is used for calculating the spin and charge susceptibilities

$$\chi_{s0,c0} = \sum_\mathbf{k} \int_{-\infty}^{\infty} d\omega \; GG \pm FF$$

→ **from this we calculate the self-energy $\Sigma(\mathbf{k}, \omega)$ of the quasiparticles**

FLEX: method and applications ...

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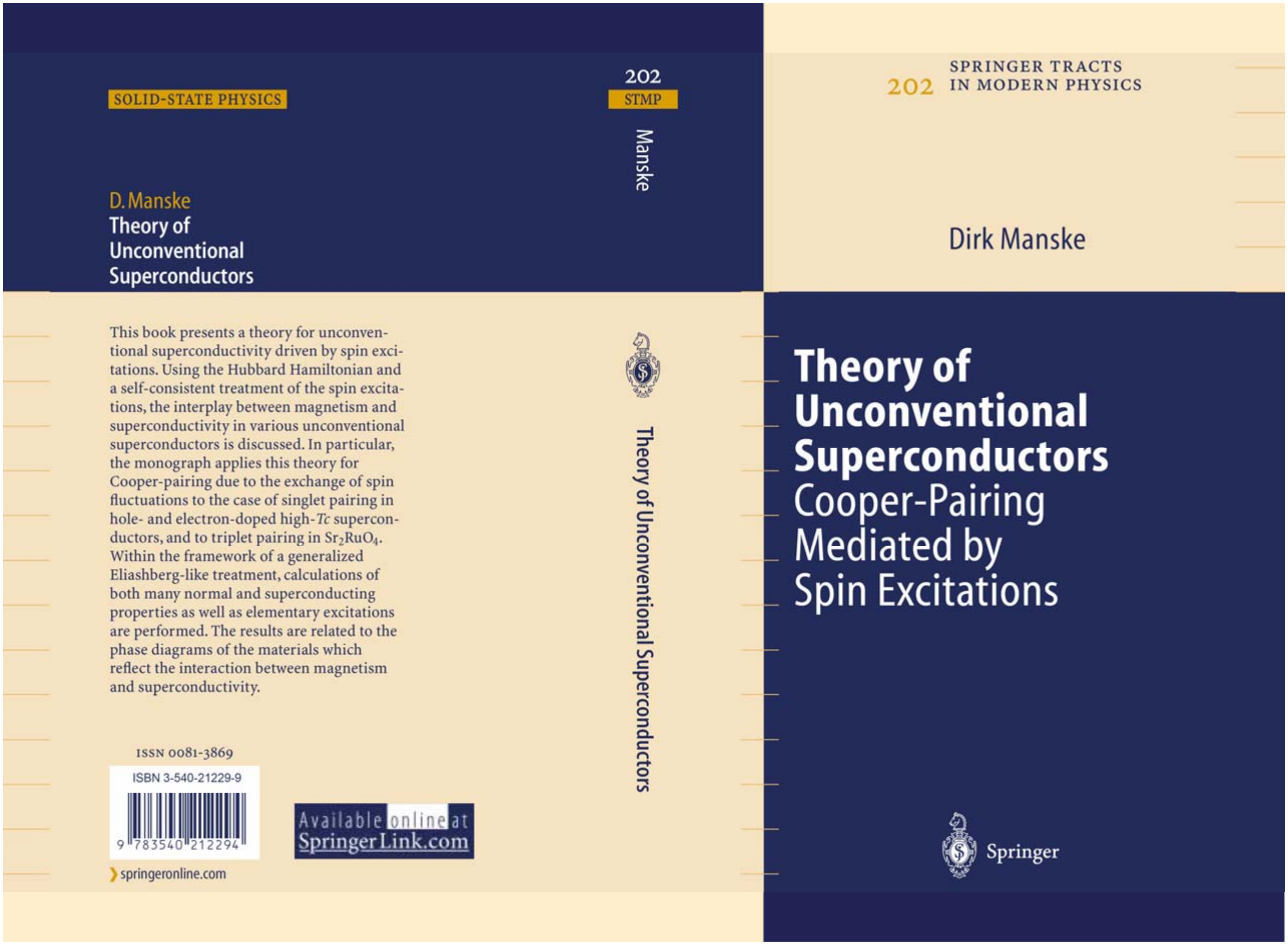
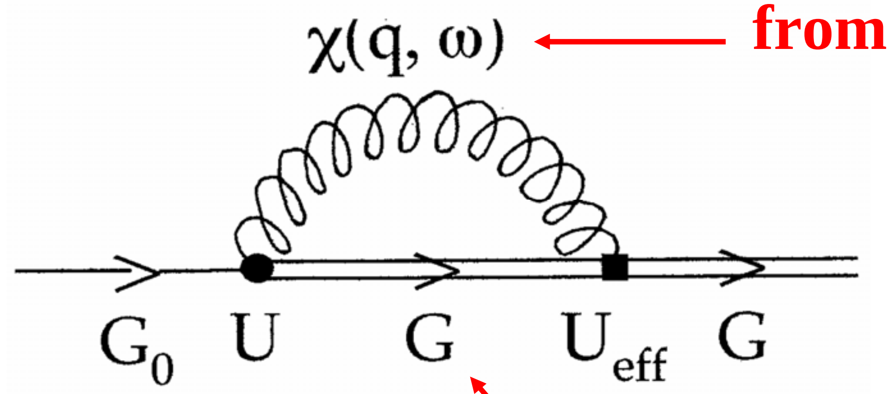


Results: elementary excitations

$$\omega(\mathbf{k}) = \epsilon_{\mathbf{k}} + \mathrm{Re}\ \Sigma(\mathbf{k},\omega)$$

$$\Sigma(\mathbf{k},\omega) =$$



from INS

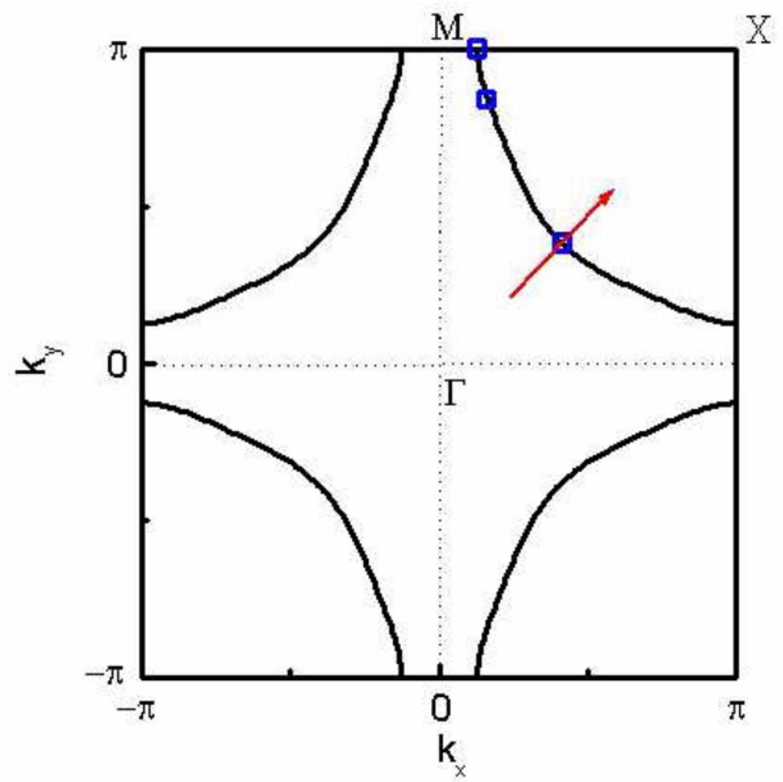
from ARPES

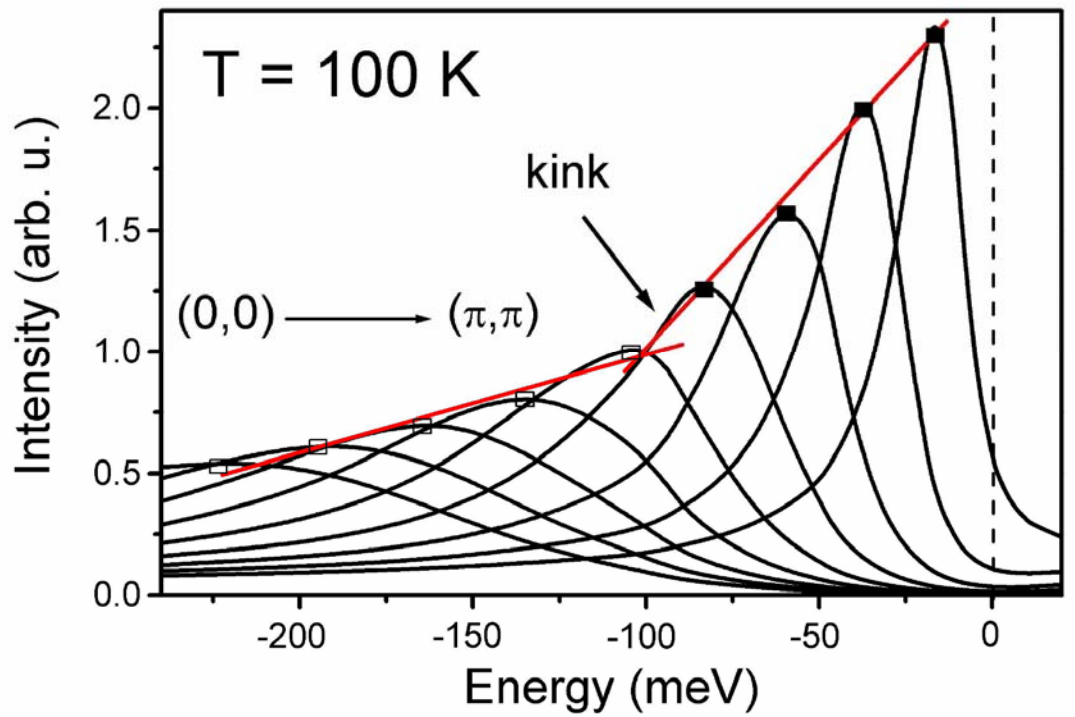
structure in Re $\Sigma(\mathbf{k},\omega)$?

- ☐ characteristic for interaction of quasiparticles $\longleftrightarrow$ spin fluctuations?
- ☐ anisotropy in momentum space?
- ☐ feedback on $\chi(\mathbf{q},\omega)$?
- ☐ doping dependence?

Results: kink (nodal direction)

$(0,0) \rightarrow (\pi,\pi)$**-direction**





- fingerprints of spin fluctuations

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Results (1): kink (nodal direction)

VOLUME 87, NUMBER 17 PHYSICAL REVIEW LETTERS 22 OCTOBER 2001

Analysis of the Elementary Excitations in High-T_c Cuprates: Explanation of the New Energy Scale Observed by Angle-Resolved Photoemission Spectroscopy

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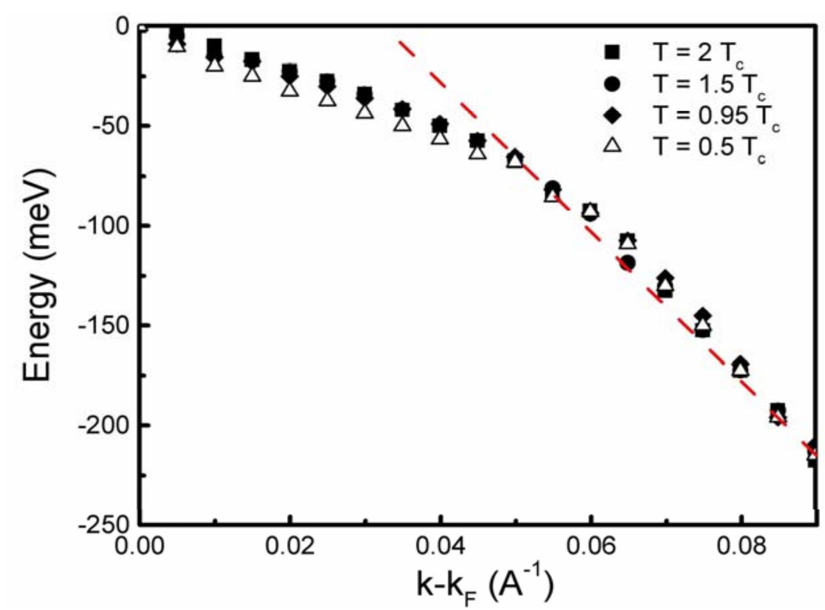
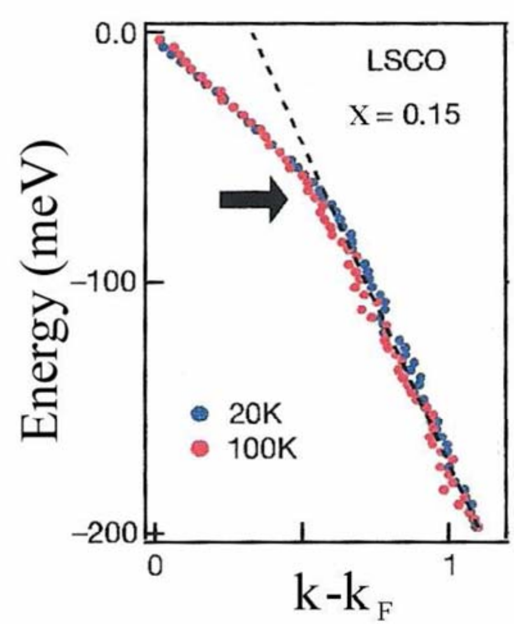
(Received 9 April 2001; published 8 October 2001)





- fingerprints of spin fluctuations

A. Lanzara *et al.*, Nature **412**, 510 (2001)

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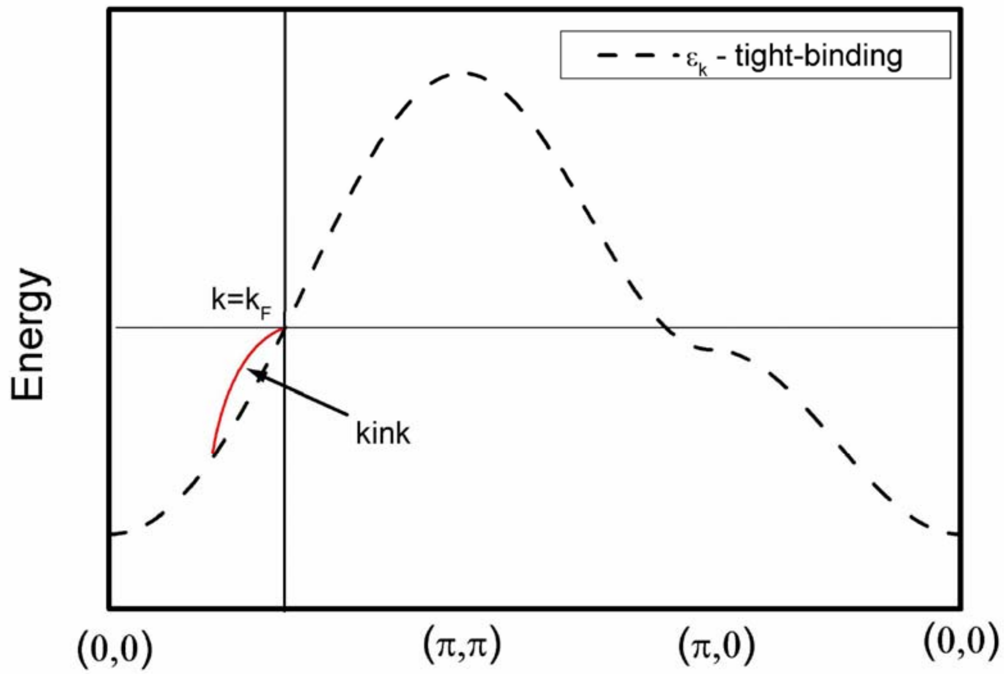
On the origin of the kink



see also discussion by:

M. Eschrig and M.R. Norman, PRL 2000
R. Zeyher and A. Greco, PRB 2001
E. Schachinger, J.P. Carbotte et al, PRB 2003
A.V. Chubukov and M.R. Norman, PRB 2004

Renormalized Dispersion: $\omega(\mathbf{k}) = \epsilon_{\mathbf{k}} + \text{Re}\ \Sigma(\mathbf{k},\omega)$

D. Manske et al., PRL 2001
D. Manske et al., PRB 2003

Results (1): kink (self-energy, antinodal)

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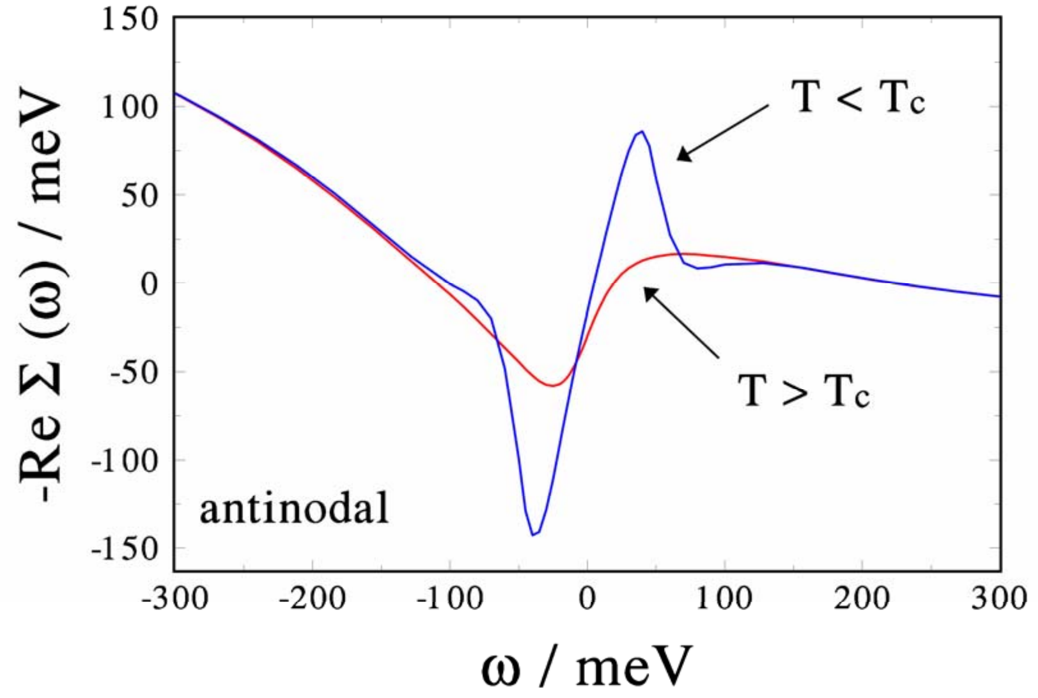
- ❑ **below T_c the ω-dependence of the superconducting gap Δ(k,ω) becomes important, i.e.**

$$\omega_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \mathrm{Re}\,\Sigma(\mathbf{k},\omega)$$



Discussion

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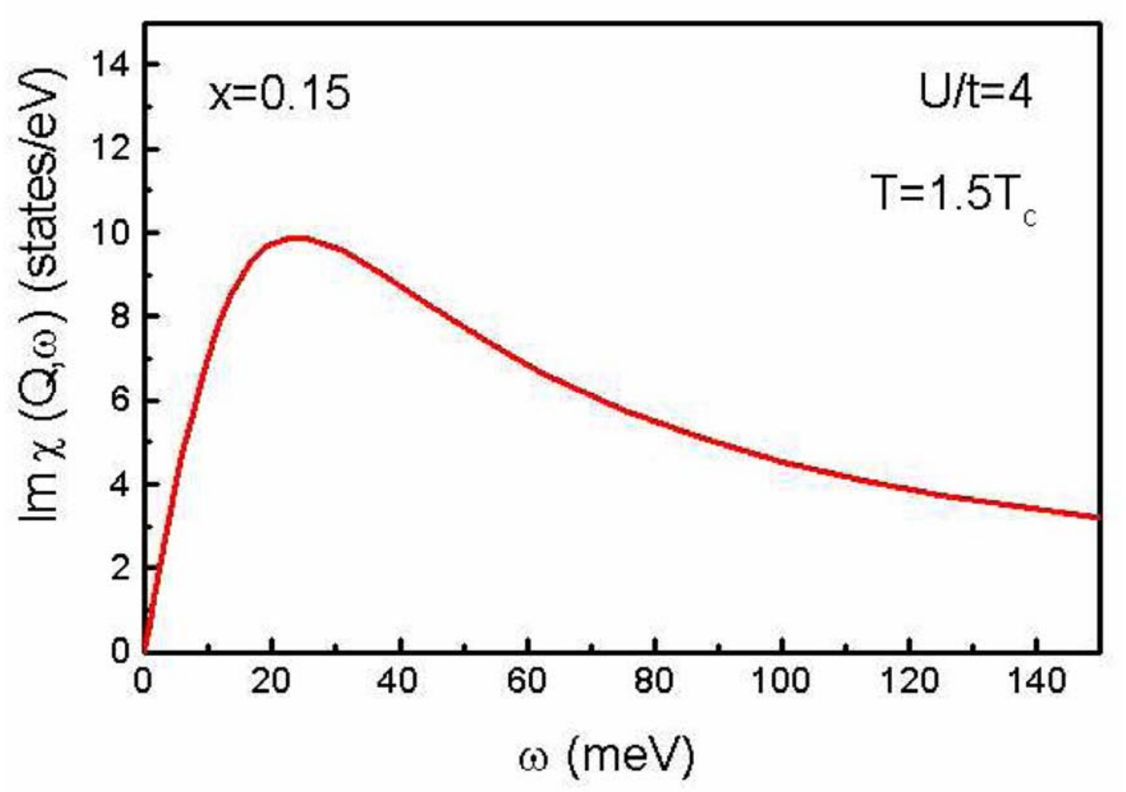
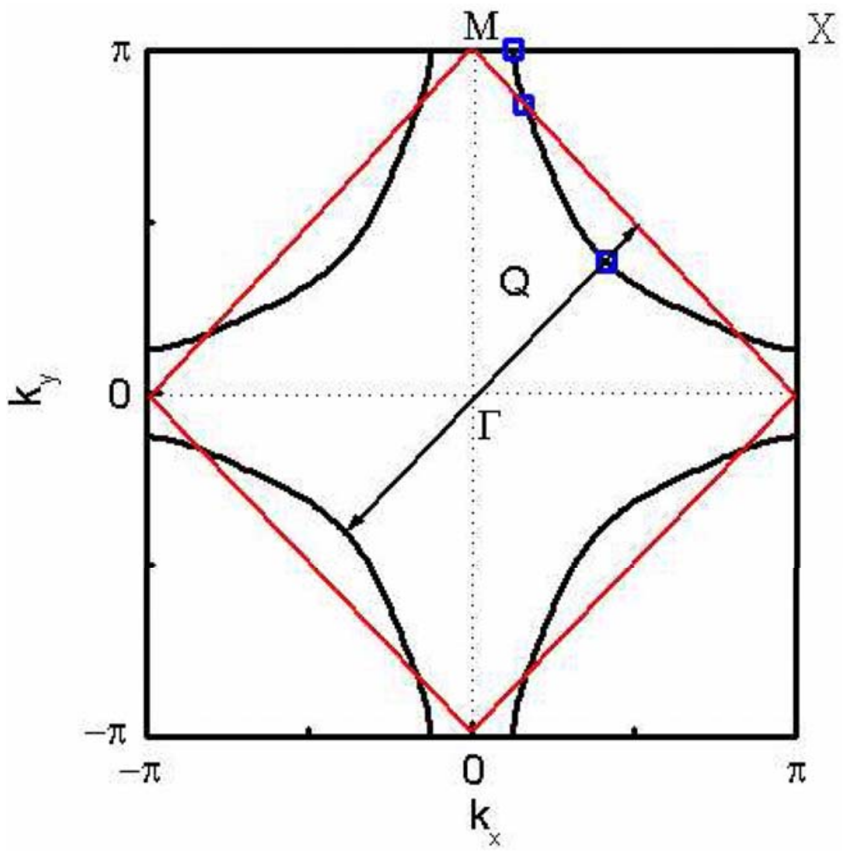
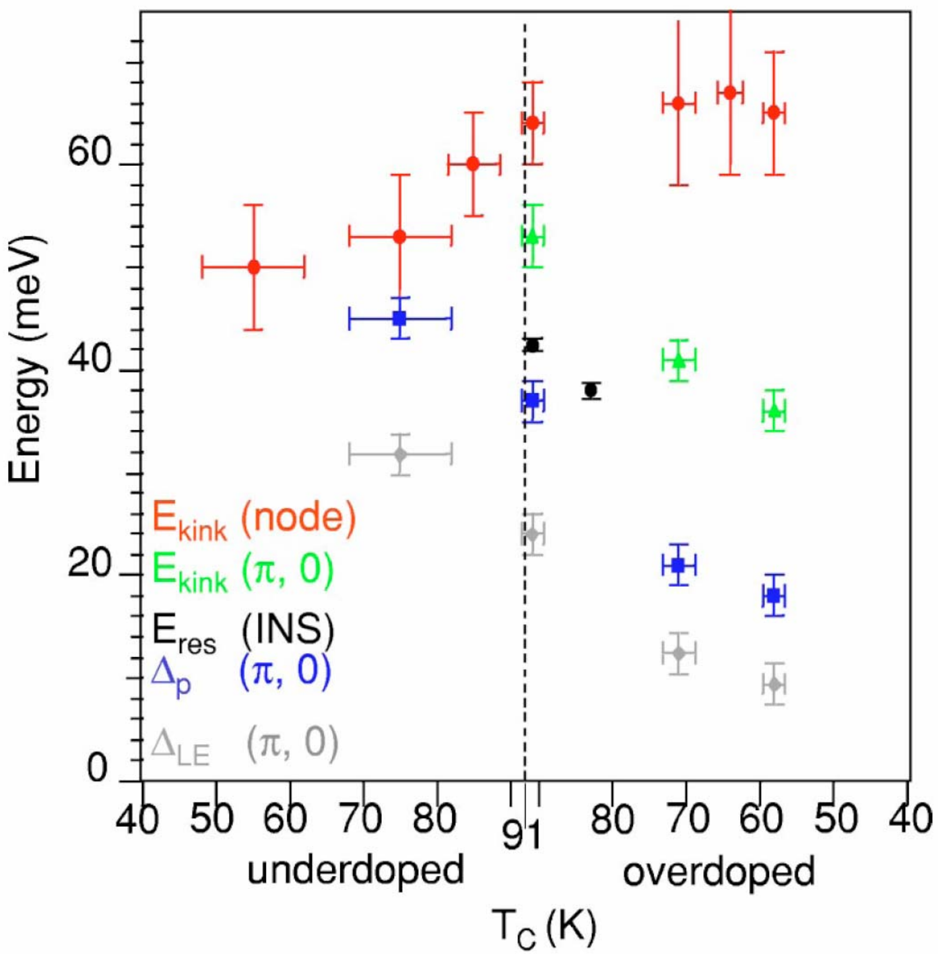
kink structure due to coupling of holes to spin fluctuations

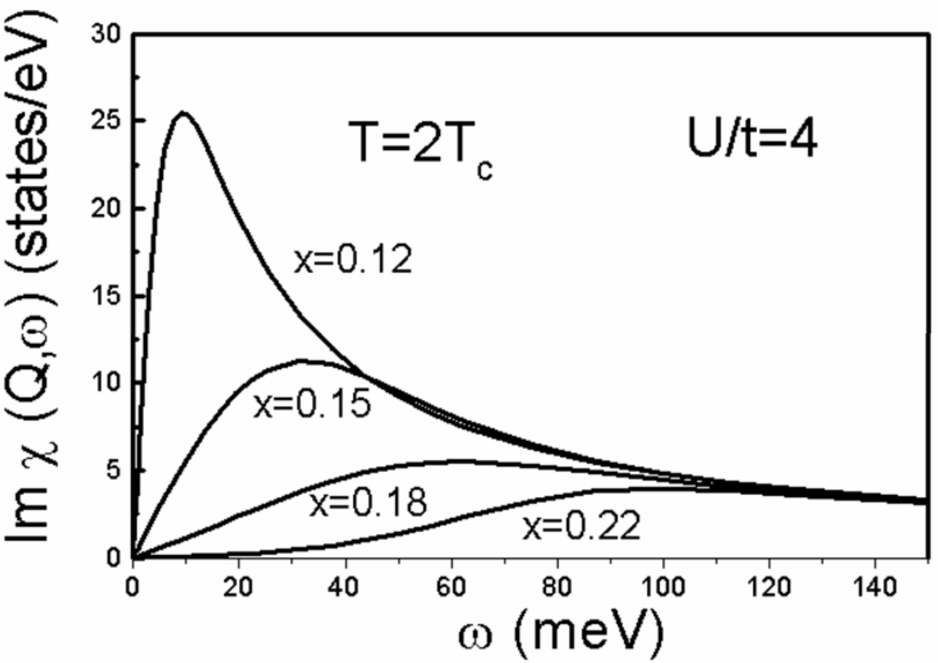




doping dependence?

Exp: A.D. Gromko *et al.*, PRB **68**, 174520 (2003) **(Bi2212)**





D. Manske et al., PRB 2003

☐ kink energy in the $(0,\pi) \rightarrow (\pi,\pi)$-direction decreases with overdoping because the superconducting gap decreases

Results (2): resonance peak

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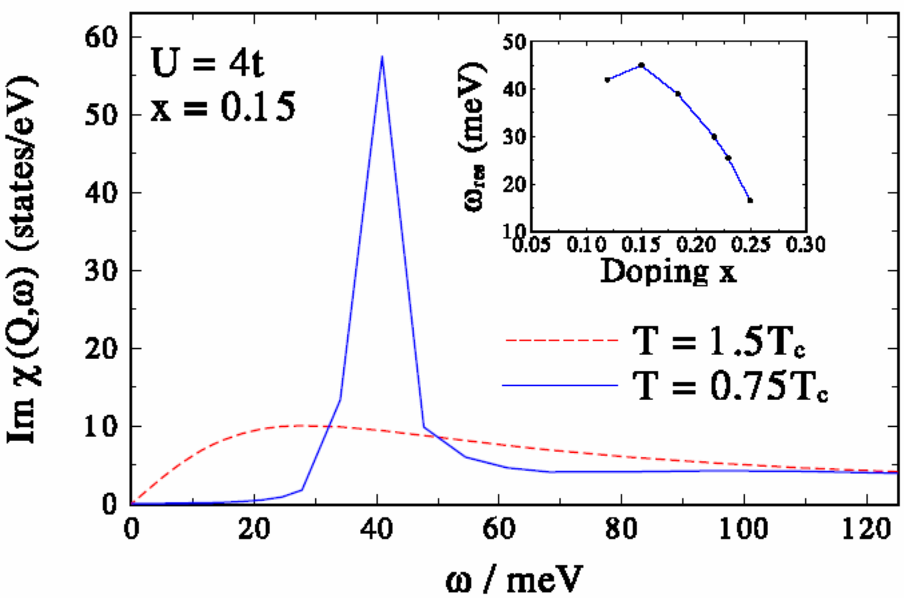

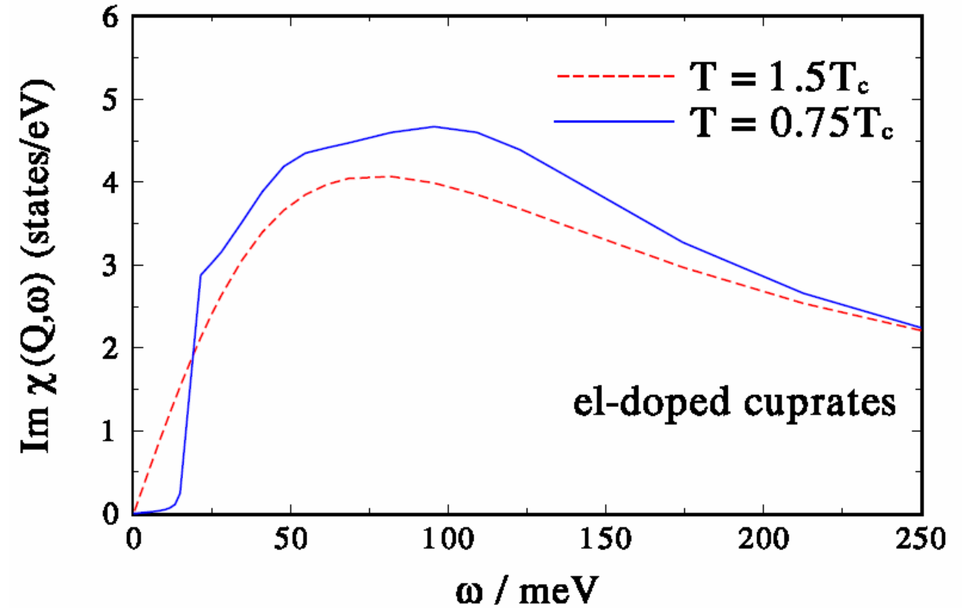

spin excitations (calculated self-consistently)

$$\mathrm{Im}\,\chi(Q,\omega) = \frac{\mathrm{Im}\,\chi_0(Q,\omega)}{(1 - U\,\mathrm{Re}\,\chi_0(Q,\omega))^2 + U^2\,(\mathrm{Im}\,\chi_0(Q,\omega))^2}$$

may become resonant, if $\quad \dfrac{1}{U_{cr}} = \mathrm{Re}\chi_0(q = Q, \omega = \omega_{res})$

(D. Manske et al., PRB 2000, PRB 2001, PRB 2003)

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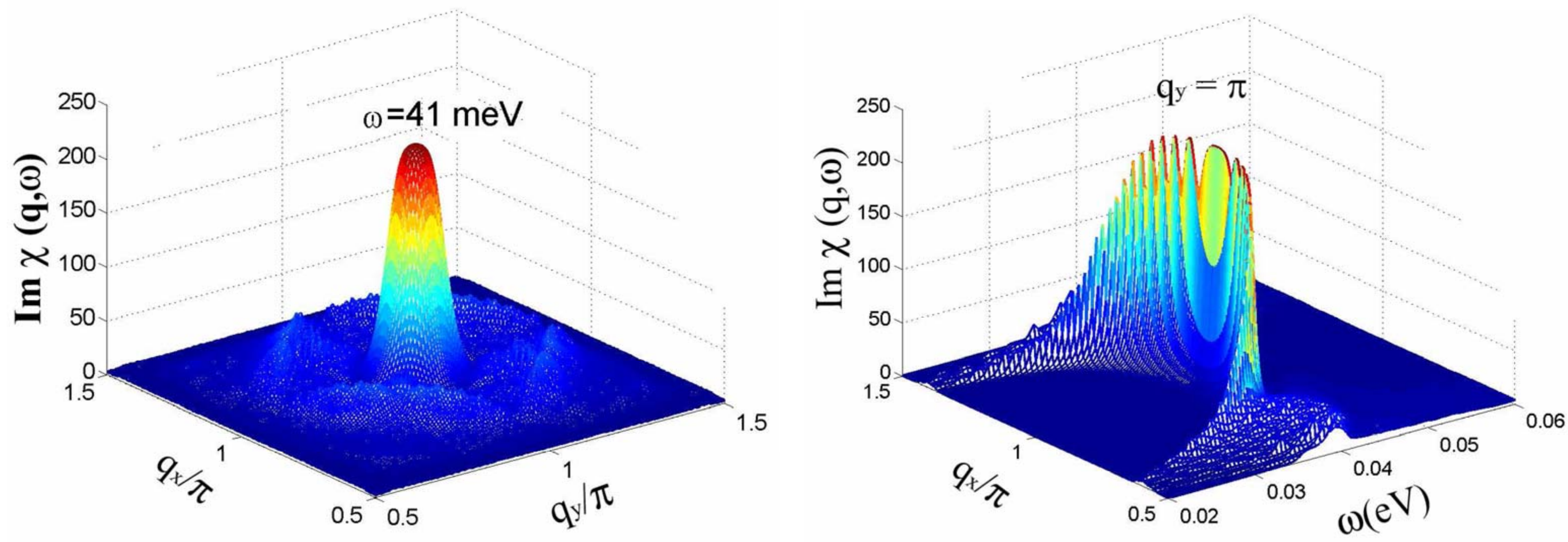
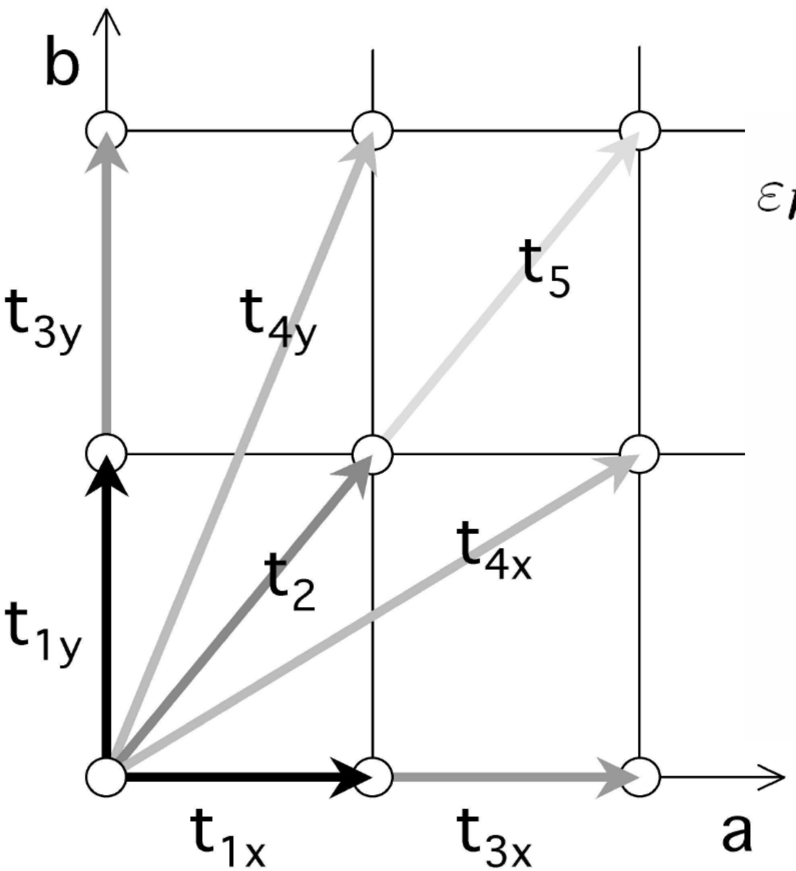
Results (2): resonance peak



- ❑ **resonance condition is fulfilled around (π,π)**
- ❑ **parabolic-like shape of the dispersion**

orthorhombic YBCO: Fermiology

orthorhombic case ($t_x \neq t_y$): new parameter δ_0

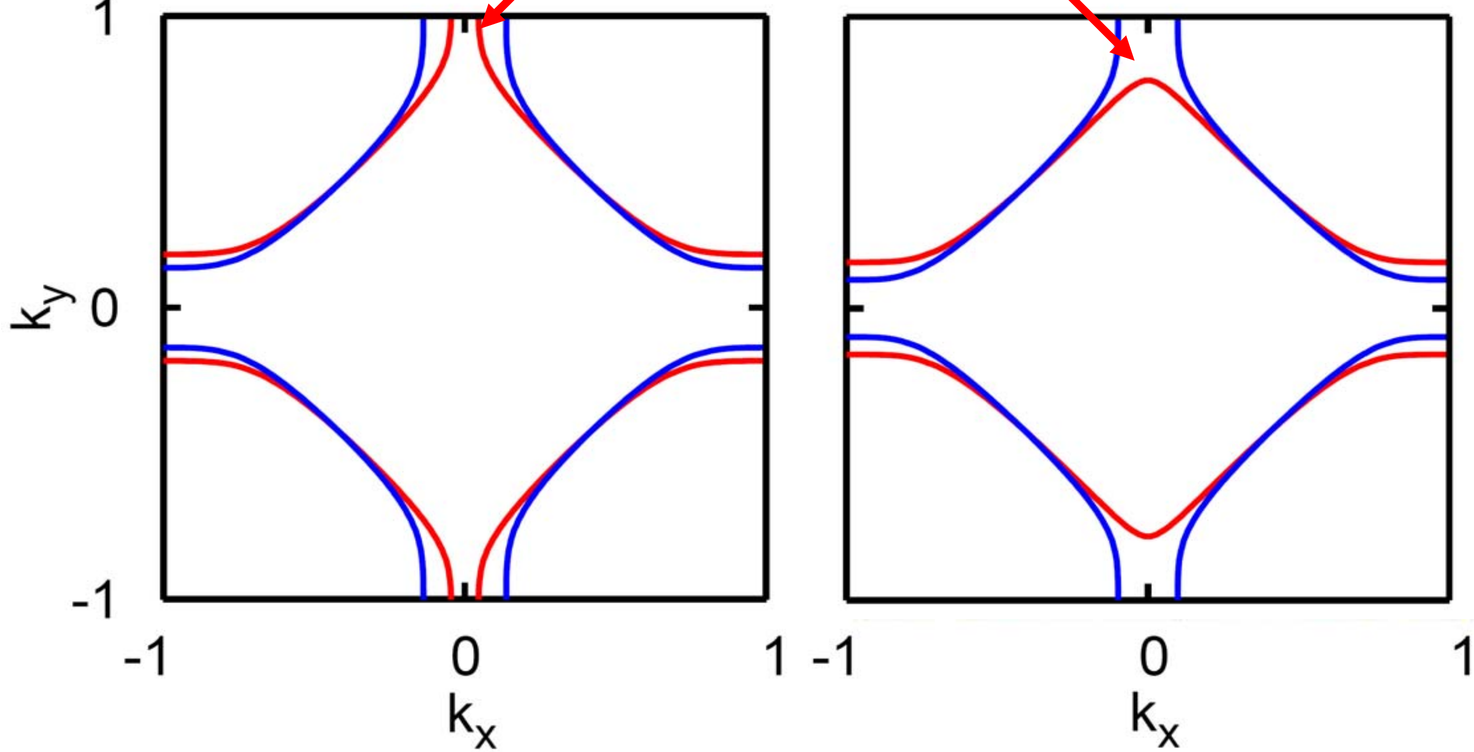


$$\begin{aligned}\varepsilon_{\boldsymbol{k}} &= \frac{t_1}{2}(1+\delta_0)\cos k_x + \frac{t_1}{2}(1-\delta_0)\cos k_y \\ &+t_2 \cos k_x \cos k_y \\ &+\frac{t_3}{2}(1+\delta_0)\cos 2k_x + \frac{t_3}{2}(1-\delta_0)\cos 2k_y \\ &+\frac{t_4}{2}\cos 2k_x \cos k_y + \frac{t_4}{2}\cos k_x \cos 2k_y \\ &+t_5 \cos 2k_x \cos 2k_y + \mu\end{aligned}$$

$$\delta_0 = -0.03$$

change of the Fermi surface topology

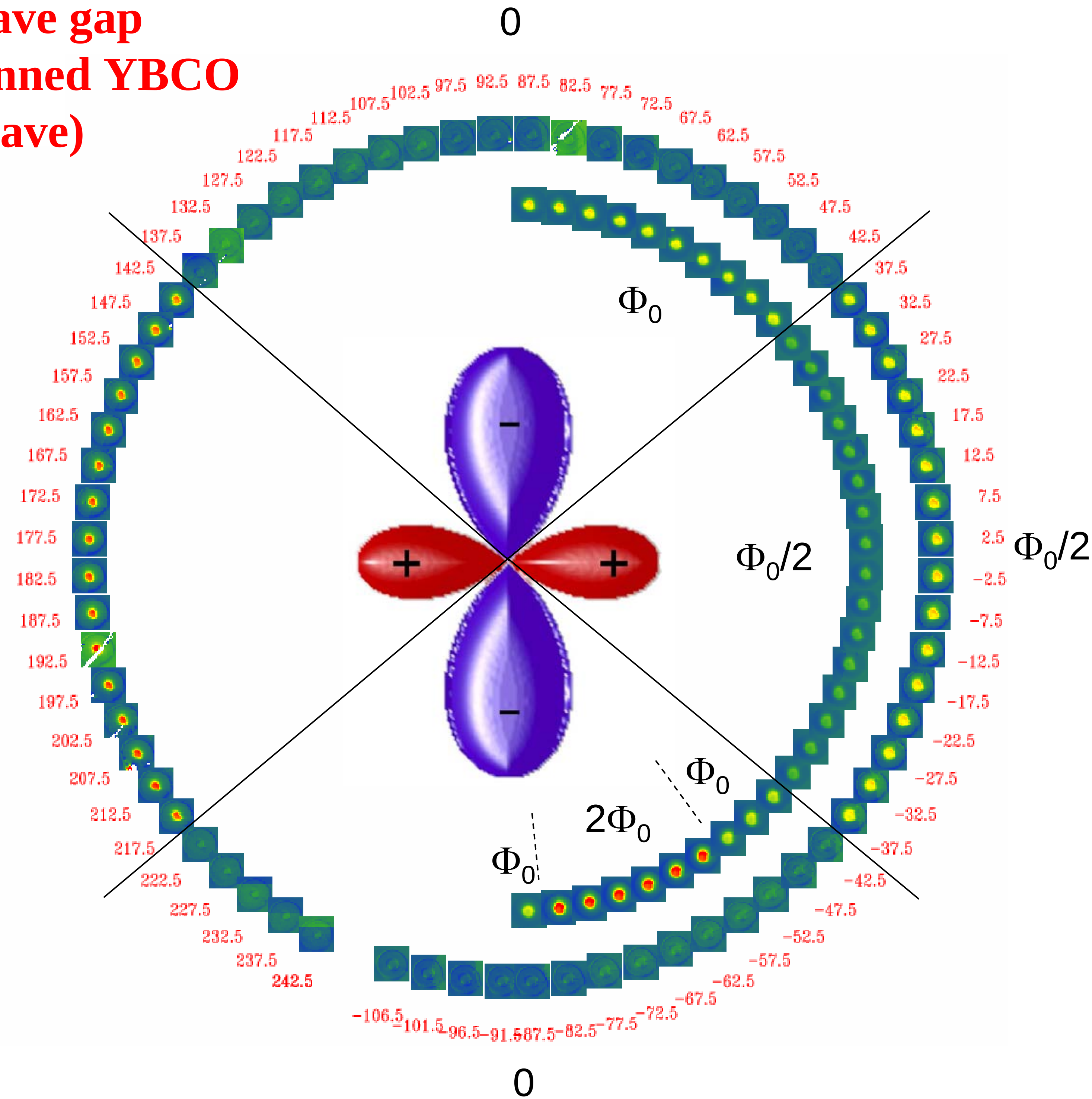
δ_0 = -0.03



- ❑ the chemical potential μ is important
- ❑ how large is the s-wave component?

Admixtures to d-wave gap symmetry in untwinned YBCO (15 % isotropic s-wave)

angle-resolved electron tunneling



H. Hilgenkamp and co-workers

PRL 2005, Nature Phys, 2006

Results (3): spin anisotropy

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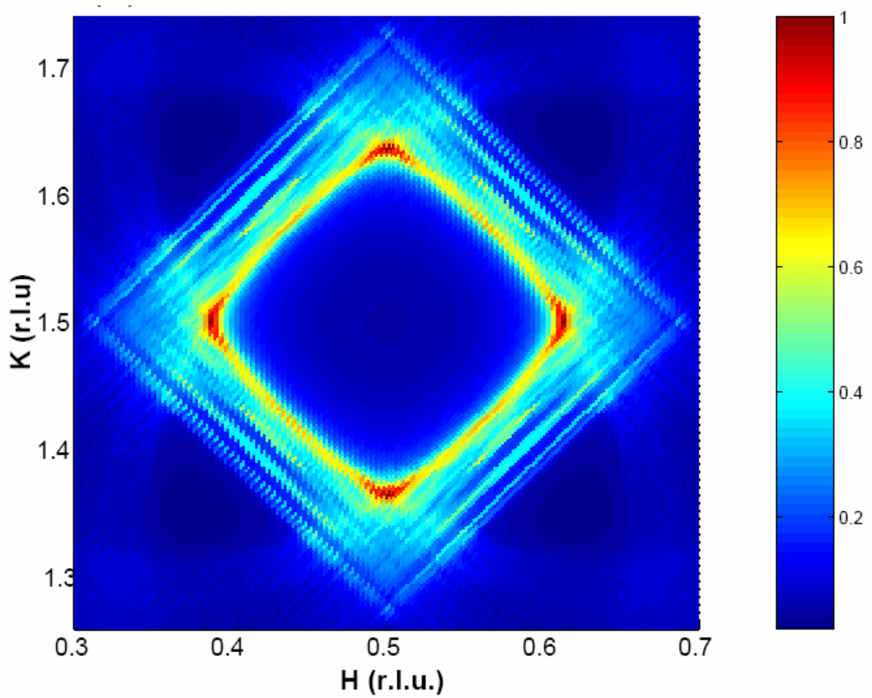
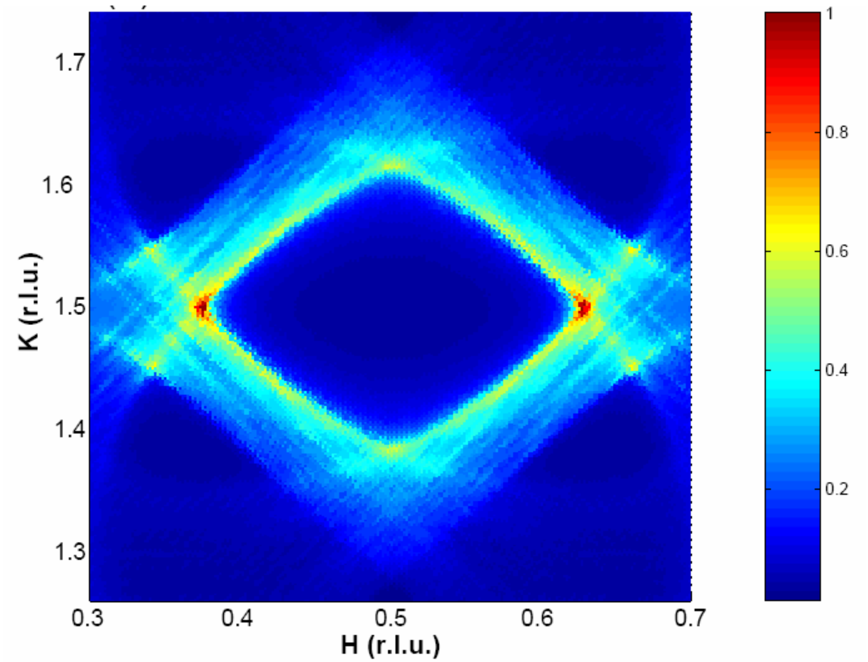




- **tetragonal case: ring-like excitations**
  four incommensurate peaks for ω = 35meV < ω_{res}

- **orthorhombic case ($t_x \neq t_y$, δ_0 = -0.03): two peaks are suppressed**

→ **alternative explanation to the stripe scenario**

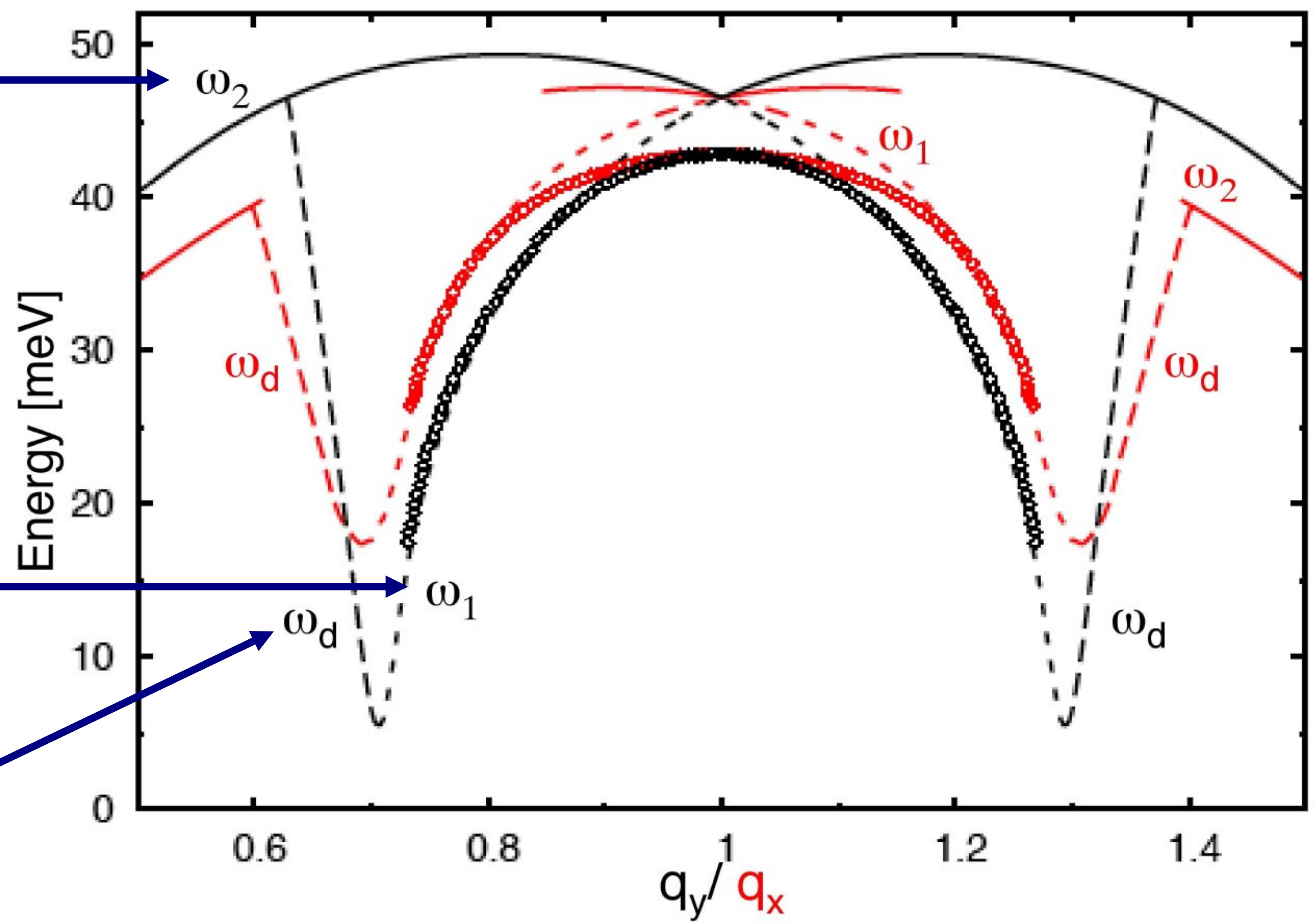
(I. Eremin and D. Manske, PRL 94, 067006 (2005); PRL 98, 139702 (2007))

prediction: two parabolic dispersions

2nd jump in χ_0

1st jump in χ_0

direct gap in χ_0



q_x-direction: downward parabola has a larger opening angle

A. Schnyder et al., PRB 73, 224523 (2006)

Summary (1)

- we obtain a kink due to coupling to spin fluctuations; it occurs, since the ω-dependence of the self-energy becomes important $\omega(\mathbf{k}) = \epsilon_k + \mathrm{Re}\ \Sigma_k(\omega)$
- the resonance peak occurs due to a feedback effect of the elementary excitations via the gap $\Delta(k,\omega)$ on the spin excitation spectrum
- theory ($t_x \neq t_y$) is able to describe anisotropic 2D spin excitations; two parabolic dispersions expected

D. Manske et al., PRL 87, 177005 ('01); PRB 63, 054517 ('03), PRB 70, 172507 (2004)

I. Eremin and D. Manske, PRL 2005, PRL 2007, A. Schnyder et al., PRB 2006

D. Manske, Theory for Unconventional Superconductors, Springer, Heidelberg (2004)

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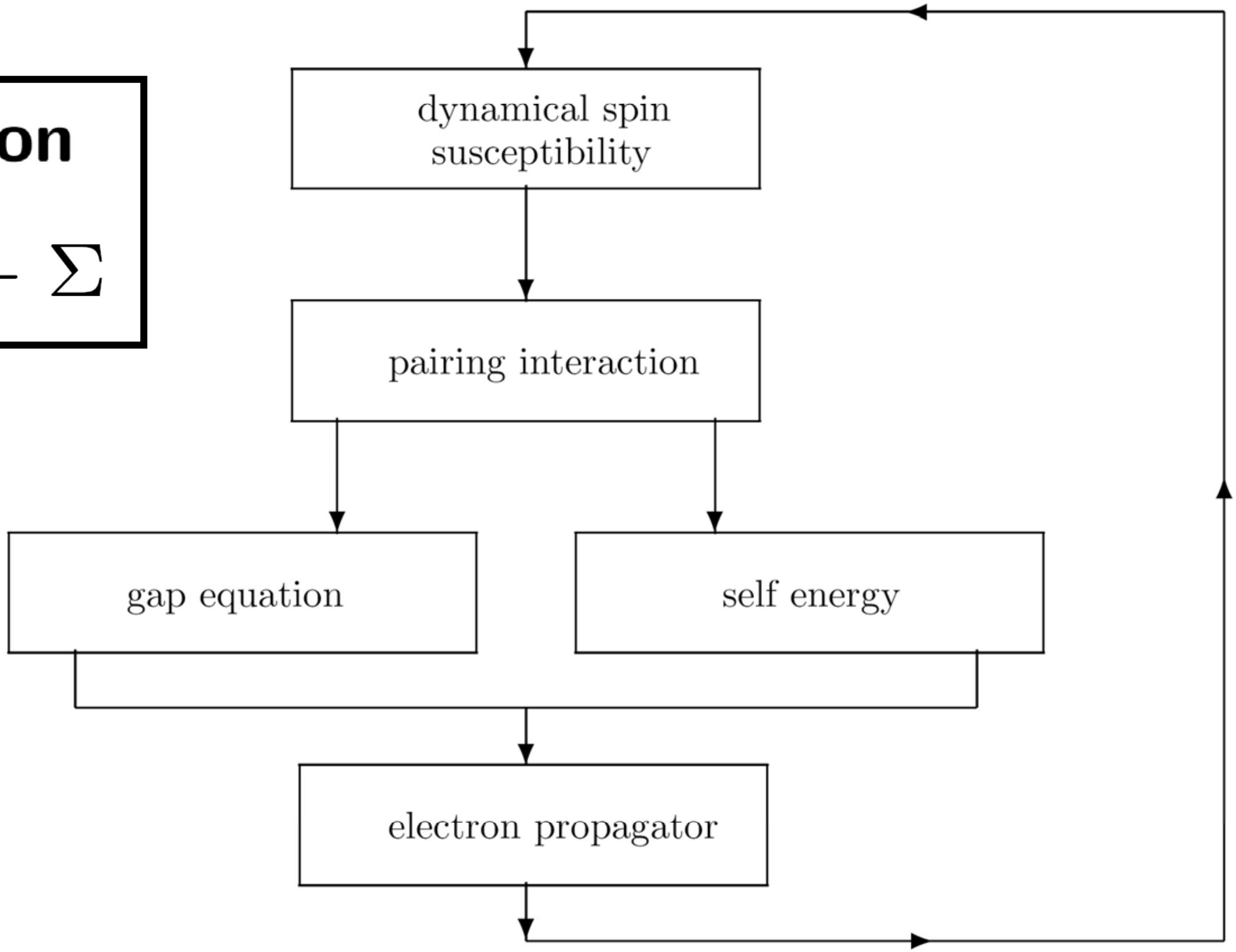
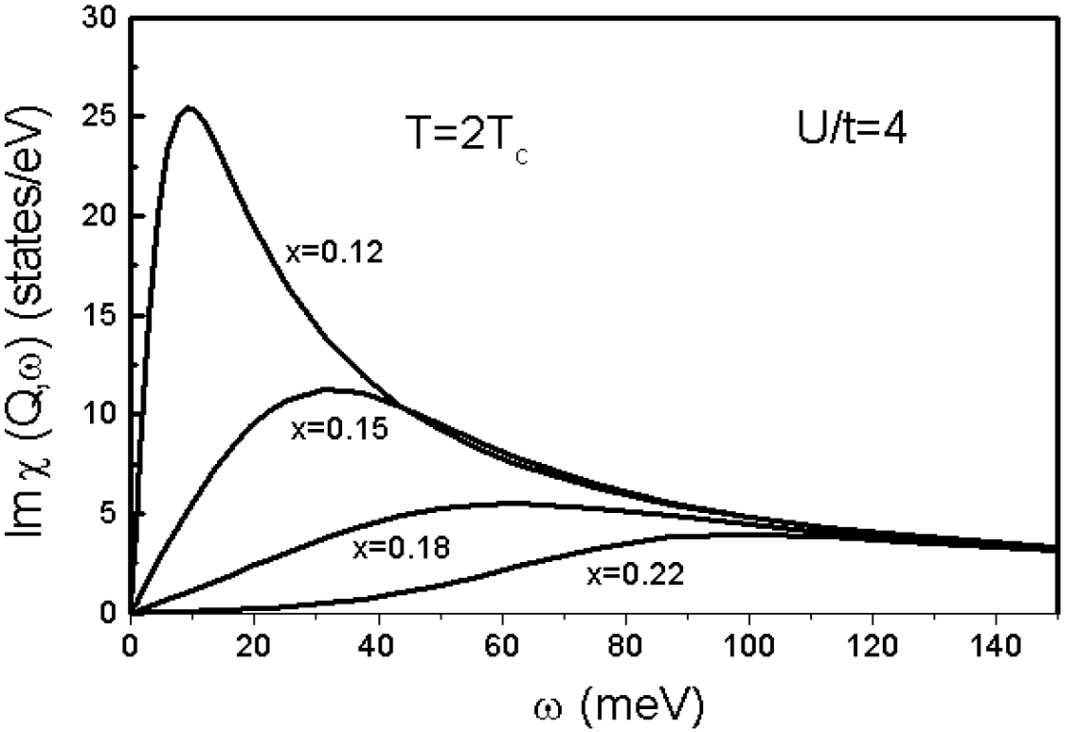
Self-consistent solution

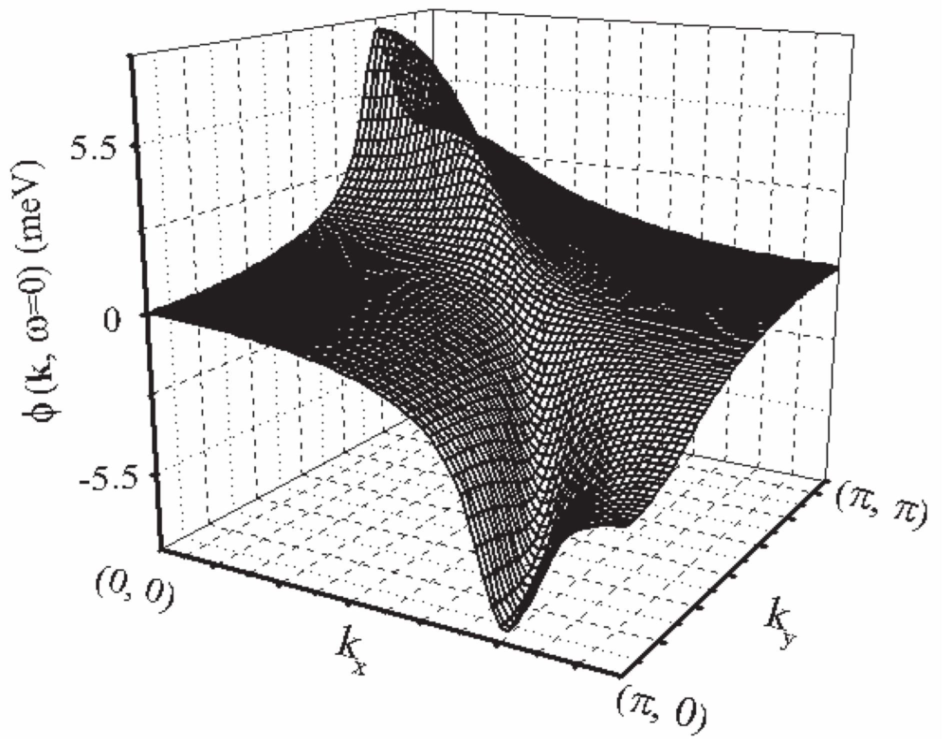
Dyson equation

$$G^{-1} = G_0^{-1} - \Sigma$$



Results (basic FLEX approach), 1





dynamical spin susceptibility, Ornstein-Zernicke-like

d_{x2-y2}-wave order parameter, 'higher harmonics'

Results (basic FLEX approach), 2

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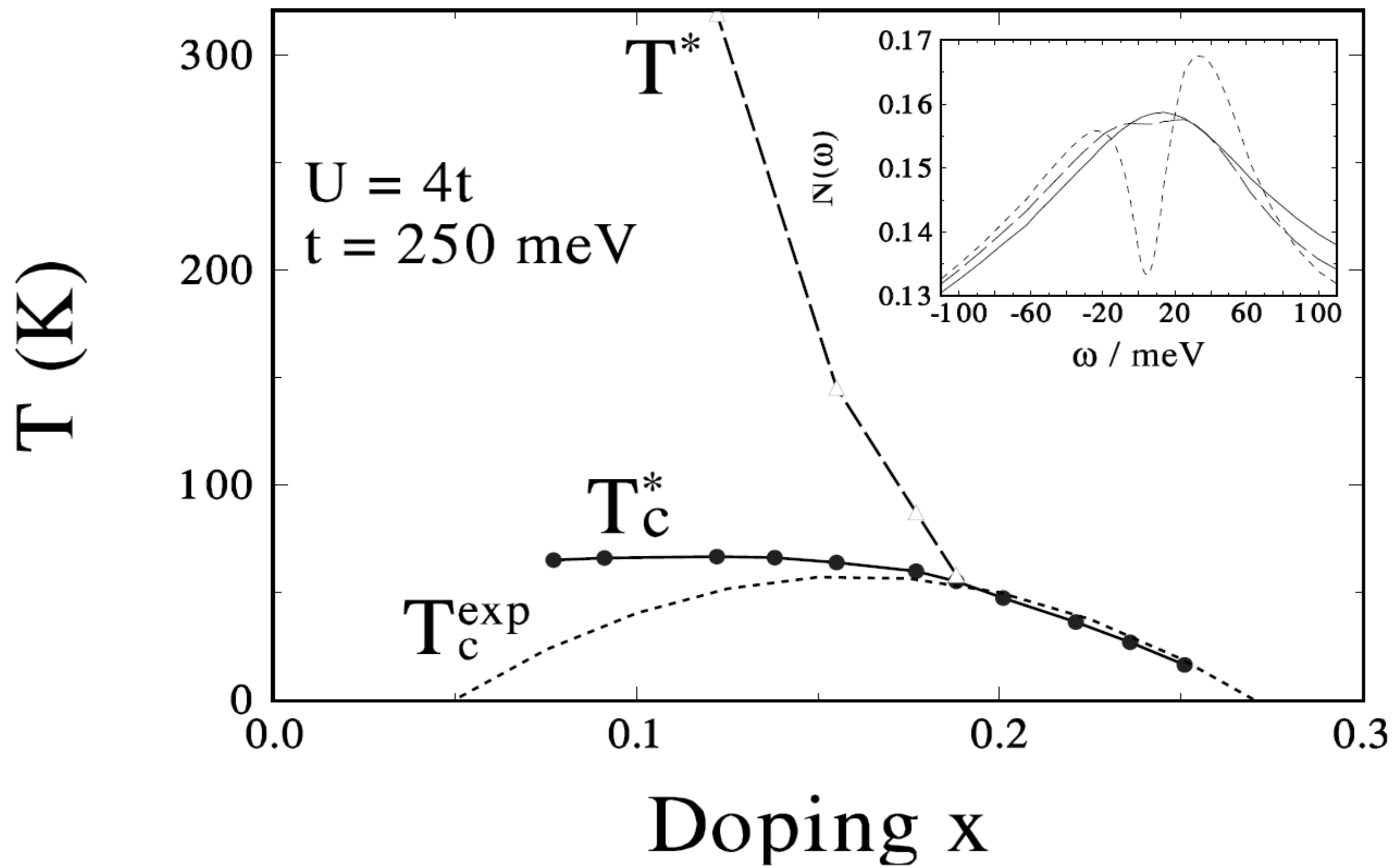
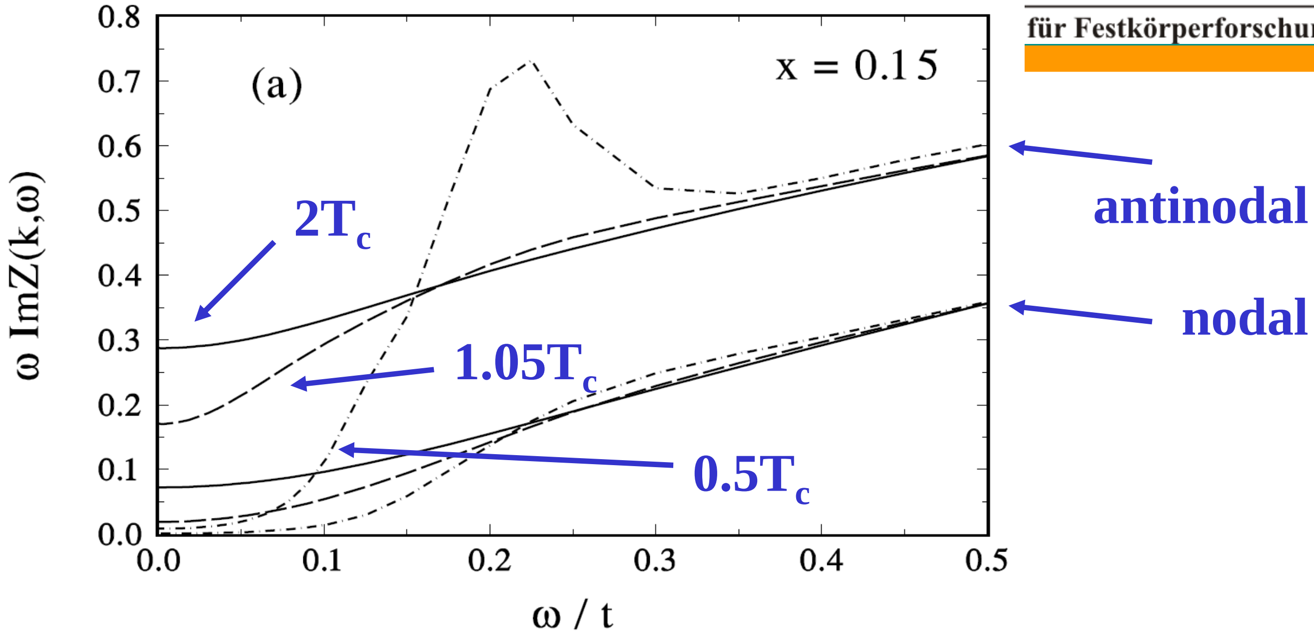
simple phase diagram (hole-doped cuprates)

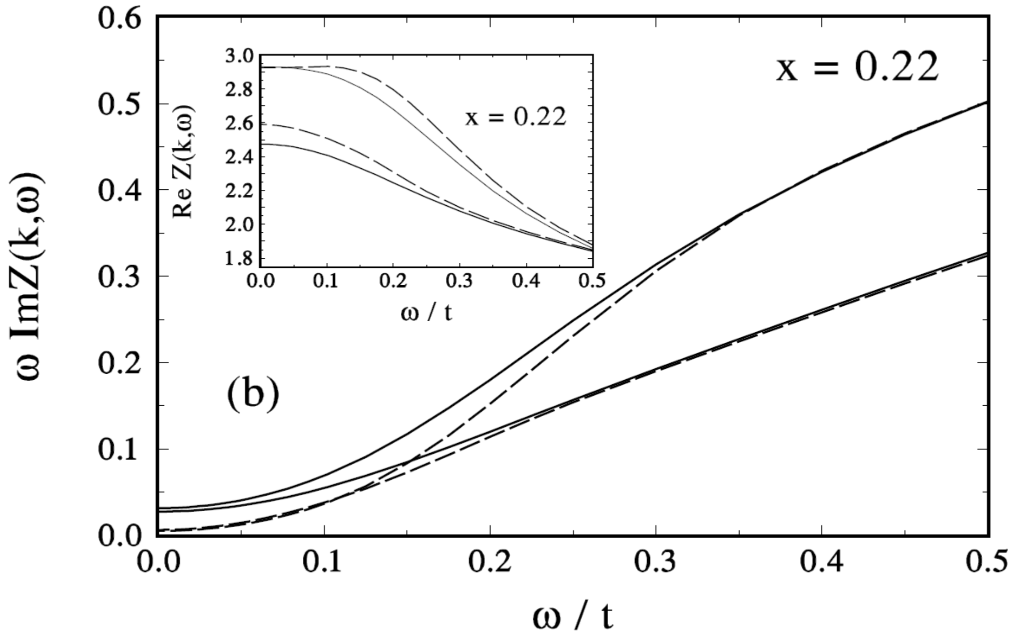


Results (basic FLEX approach), 3

calculated quasiparticle damping



anisotropy decreases in the OD regime



Contrasting FLEX with similar approaches

- Spin Bag Mechanism
- Nearly Antiferromagnetic Fermi Liquid (NAFL)
- BCS-like model calculations
- Extended Eliashberg equations for *d*-wave
- Spin-Fermion model

Contrasting FLEX with similar approaches

(1) The Spin Bag Mechanism (*Schrieffer et al.*)

Idea: a hole injected into a SDW system depresses the staggered magnetization; this region provides a bag inside of which the hole is trapped self-consistently (bag + hole = new quasiparticle)
→ 2 holes attract eachother by sharing a common bag

$$\rightarrow \quad V_{APM} = U + \frac{U^3 \chi_0^2(\mathbf{k}' - \mathbf{k})}{1 - U^2 \chi_0^2(\mathbf{k}' - \mathbf{k})} + \frac{U^2 \chi_0(\mathbf{k}' - \mathbf{k})}{1 - U \chi_0(\mathbf{k}' - \mathbf{k})}$$

+ taking explicitly into account the local AF order on the self-energy
- only simple model susceptibilities were used (parametrization)

→ extensions to describe 'shadow states'

❑ non-local character not included in FLEX, but paramagnon exchange described self-consistently, shadow states included ('hot spots')

Contrasting FLEX with similar approaches

(2) The Theory of a Nearly AF Fermi liquid (*Pines et al.*)

Idea: construct effective interaction between quasiparticles and spin fluctuations, use NMR data as an input: $H = H_0 + H_{int}$

$$H_{int} = \sum_{\mathbf{q}} g(\mathbf{q})\, \mathbf{s}(\mathbf{q}) \cdot \mathbf{S}(-\mathbf{q}) \qquad \mathbf{s}(\mathbf{q}) = \frac{1}{2} \sum_{\alpha,\beta,\mathbf{k}} \psi^{\dagger}_{\mathbf{k}+\mathbf{q},\alpha}\, \sigma_{\alpha\beta}\, \psi_{\mathbf{k},\beta}$$

$$\rightarrow \quad \chi(\mathbf{q},\omega) = \chi_{MMP}(\mathbf{q},\omega) = \frac{\chi_Q}{1 + \xi^2(\mathbf{q} - \mathbf{Q}) - i\omega/\omega_{sf}}$$

+- parametrization of the dynamical spin susceptibility
- only n-state description, no self-consistency

- ❑ **FLEX contains NAFL properties, takes all momenta into account**

Contrasting FLEX with similar approaches

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(3) BCS-like model calculations (*Levin, Norman et al.*)

Idea: construct effective interaction between quasiparticles and spin fluctuations, use INS or ARPES data as an input, employ RPA

$$\begin{aligned}\chi(\mathbf{q},\omega) &= \chi_{RUNL}(\mathbf{q},\omega)\\ &= C\left[\frac{1}{1+J_0\left[\cos(q_x a)+\cos(q_y a)\right]}\right]^2\\ &\times \frac{3(T+5)\omega}{1.05\omega^2-60|\omega|+900+3(T+5)^2}\,\Theta(\Omega_c-|\omega|)\end{aligned}$$

$$\chi(\mathbf{q},\omega)=\frac{\chi_0(\mathbf{q},\omega)}{1-J(\mathbf{q})\chi_0(\mathbf{q},\omega)}$$

$$J(\mathbf{q})=-J_0\left[\cos(q_x a)+\cos(q_y a)\right]$$

$$\mathrm{Im}\,\Sigma=\frac{\mathrm{Im}\,G}{(\mathrm{Re}\,G)^2+(\mathrm{Im}\,G)^2}\qquad \mathrm{Re}\,\Sigma=\omega-\epsilon_{\mathbf{k}}-\frac{\mathrm{Re}\,G}{(\mathrm{Re}\,G)^2+(\mathrm{Im}\,G)^2}$$

- **FLEX contains RPA properties**

Contrasting FLEX with similar approaches

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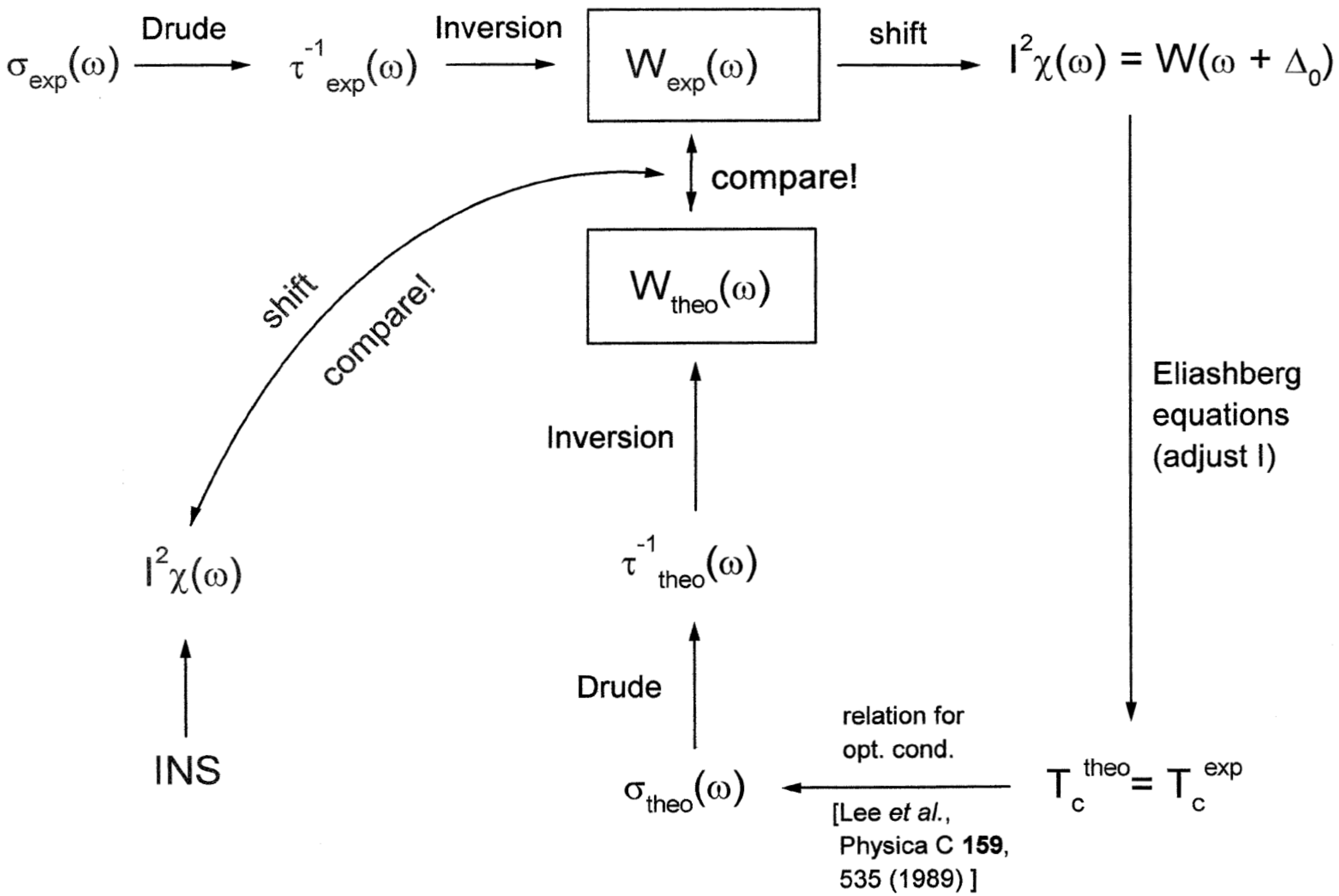
(3) Extended Eliashberg equations for *d*-wave (*Carbotte et al.*)

recent idea (*Marsiglio*): extract the pairing potential from conductivity data



Schachinger, Carbotte, Basov, Nature **401**, 354 (1999)

❑ **Fermi surface restricted, no microscopic explanation**

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Contrasting FLEX with similar approaches

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(4) Spin-Fermion model (*Chubukov et al.*)

Idea: **find a microscopic basis for the NAFL picture:**
start from a Hubbard-type Hamiltonian with a 4-fermion interaction, then generate an effective model by integrating out higher modes

$$H = \sum_{\mathbf{k},\alpha} \varepsilon_{\mathbf{k}} \psi^\dagger_{\mathbf{k},\alpha}\psi_{\mathbf{k},\alpha} + \sum_{\mathbf{q}} U(\mathbf{q})\mathbf{S}_{\mathbf{q}}\cdot\mathbf{S}_{-\mathbf{q}} + \sum_{\mathbf{k},\mathbf{q},\alpha,\beta} U(\mathbf{q})\psi^\dagger_{\mathbf{k}+\mathbf{q},\alpha}\sigma_{\alpha\beta}\psi_{\mathbf{k},\beta}\cdot\mathbf{S}_{-\mathbf{q}}$$

$$\rightarrow \qquad \mathcal{S} = -\int_k^\Lambda G_0^{-1}(k)\psi^\dagger_{k,\alpha}\psi_{k,\alpha} + \frac{1}{2}\int_q^\Lambda \chi_0^{-1}(q)\,\mathbf{S}_{\mathbf{q}}\cdot\mathbf{S}_{-\mathbf{q}} + g\int_{k,q}^\Lambda \psi^\dagger_{k+q,\alpha}\sigma_{\alpha\beta}\psi_{k,\beta}\cdot\mathbf{S}_{-\mathbf{q}} \quad .$$

with $$G_0(k) = \frac{z_0}{i\omega_m - \epsilon_{\mathbf{k}}} \qquad \chi_0(q) = \frac{\alpha}{\xi_0^{-2} + (\mathbf{q}-\mathbf{Q})^2 + \omega_m^2/c^2}$$

Contrasting FLEX with similar approaches

Gor'kov expressions:

$$G_{\mathbf{k}}(i\omega) = \frac{i\omega + \Sigma_{\mathbf{k}}(i\omega) + \varepsilon_{\mathbf{k}}}{\left[i\omega + \Sigma_{\mathbf{k}}(i\omega)\right]^2 - \Phi^2_{\mathbf{k}}(i\omega) - \varepsilon^2_{\mathbf{k}}}$$

$$F_{\mathbf{k}}(i\omega) = -\frac{\Phi_{\mathbf{k}}(i\omega)}{\left[i\omega + \Sigma_{\mathbf{k}}(i\omega)\right]^2 - \Phi^2_{\mathbf{k}}(i\omega) - \varepsilon^2_{\mathbf{k}}}$$

$$\chi_{\mathbf{q}}(i\omega) = \frac{\alpha\xi^2}{1 + \xi^2 \left(\mathbf{q} - \mathbf{Q}\right)^2 - \Pi_{\mathbf{Q}}(i\omega)}$$

leads to $$V_{\text{eff}}(q) = g^2\chi(q) = \frac{g^2\alpha\xi^2}{1 + \xi^2(\mathbf{q} - \mathbf{Q})^2 - \Pi_{\mathbf{Q}}(\omega)}$$

- **More parameters than FLEX: g, Λ, $v_F\xi^{-1}$, only 'one-loop' approximation**
- **BUT: easy to reach T=0**
- **Spin-Fermion model yields similar results than the FLEX approach**

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Extending the FLEX approach

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- ❑ **Bilayer effects (‘96-‘99)**
- ❑ **Inclusion of a *d*-wave pseudogap (’97-‘02)**
- ❑ **Combination with response theory (’96-now)**
- ❑ **Amplitude fluctuations (FLEX + T-matrix) of the sc order parameter (’97-‘03)**
- ❑ **Phase fluctuations of the sc order parameter, combination with the xy model and BKT theory (’98-‘03)**
- ❑ **Inclusion of electron-phonon interaction, Hubbard-Holstein model, current results and future prospects (’96, ’03-now)**

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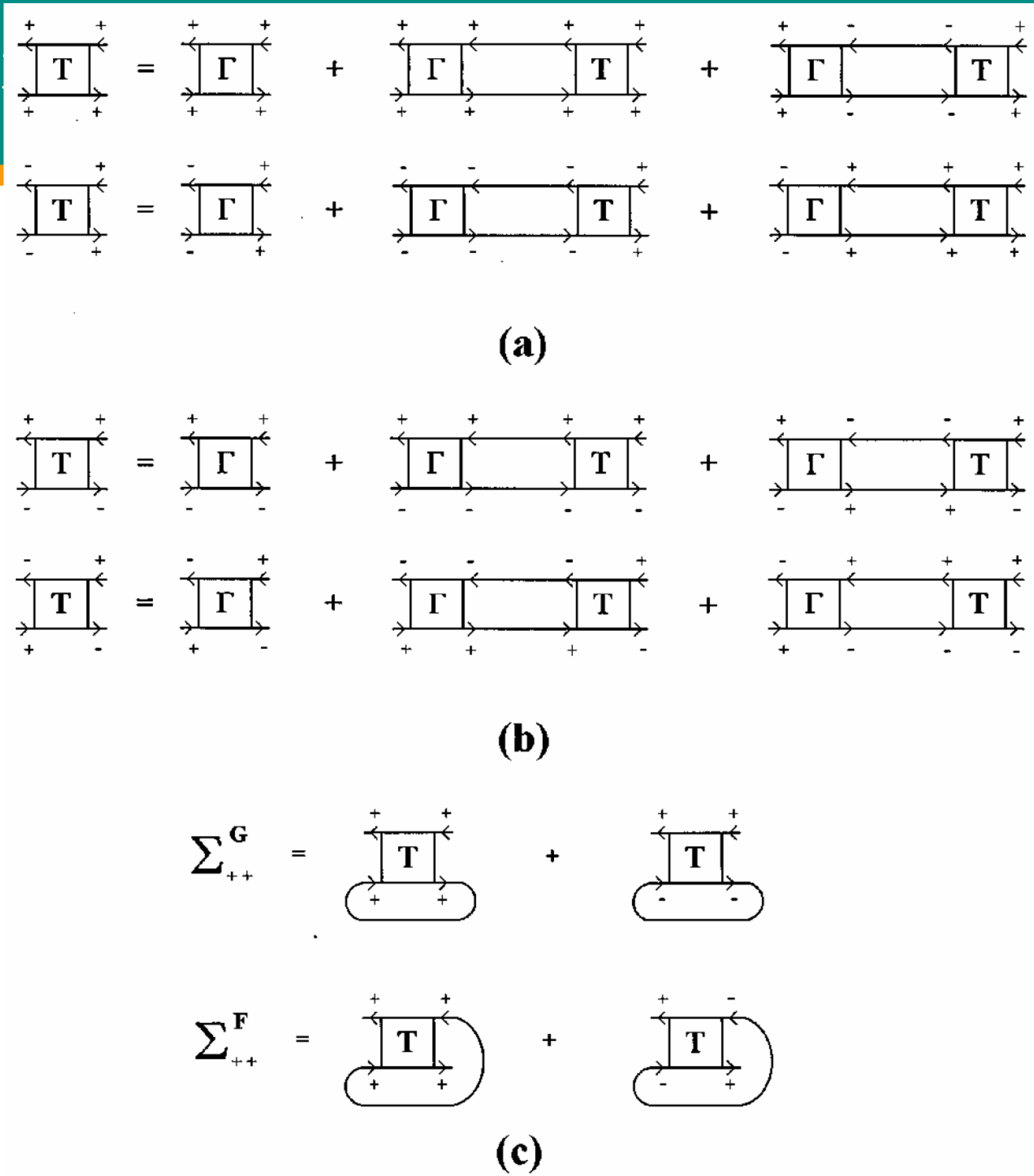
Extension 1: Bilayer effects

$$X_{i\nu}(\vec{k},\omega) = N^{-1}\sum_{k'}\sum_{\mu=+,-}\int_0^{\infty} d\Omega\,\frac{1}{2}\,P_s^{\nu\mu}(\vec{k}-\vec{k}',\Omega) \times \int_{-\infty}^{+\infty} d\omega'\; I(\omega,\Omega,\omega')A_{i\mu}(\vec{k}',\omega').$$

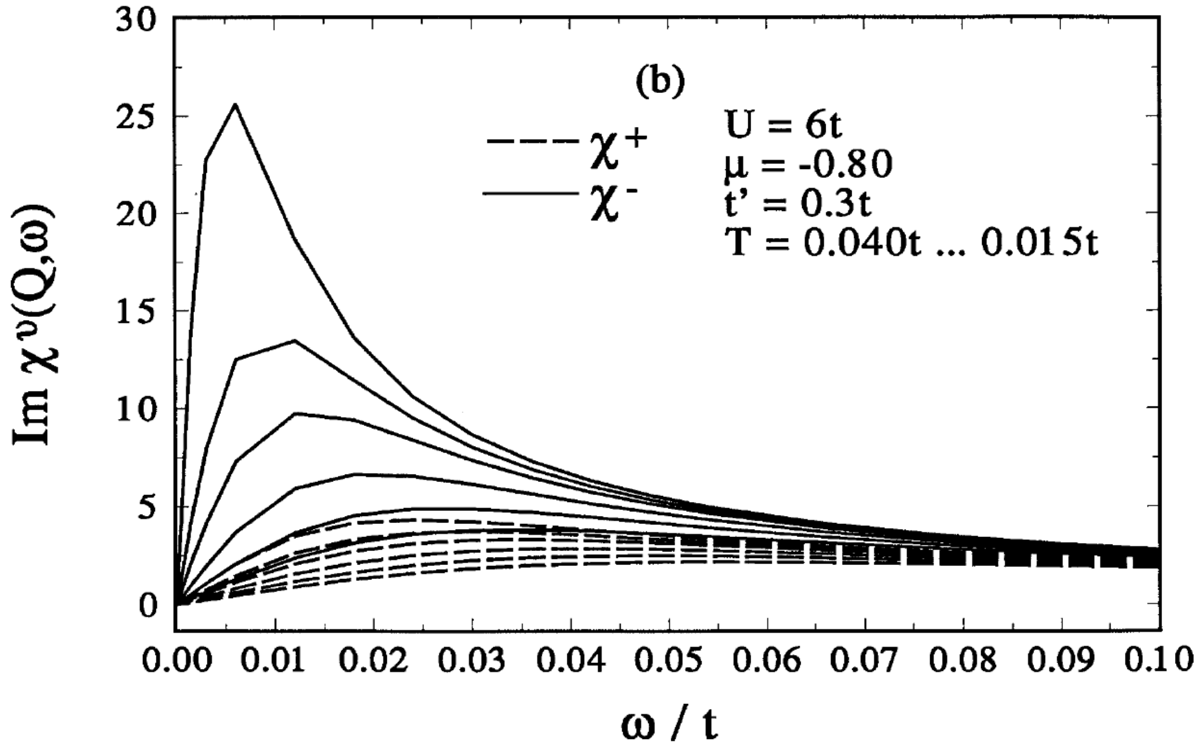
with

$$\varepsilon_{\pm}(\vec{k}) = t[-2\cos(k_x) - 2\cos(k_y) - 4(t_2/t)\cos(k_x)\cos(k_y) - \mu]\mp t'$$


(a)
(b)
(c)

Bilayer effects: even vs. odd mode

$$\chi(\vec{q},q_z,\omega)=\chi^+(\vec{q},\omega)\cos^2(q_z d/2)+\chi^-(\vec{q},\omega)\sin^2(q_z d/2)$$



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Extension 2: Inclusion of a *d*-wave PG

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start from the 4x4 matrix Green's function (e.g. CDW):

$$G(\mathbf{k},\tau) = -\langle T\alpha_{\mathbf{k}}(\tau)\alpha^\dagger_{\mathbf{k}}(0)\rangle$$ **where** $$\alpha^\dagger_{\mathbf{k}} = (c^\dagger_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}+\mathbf{Q},\sigma}, c_{-\mathbf{k},-\sigma}, c_{-\mathbf{k}-\mathbf{Q},-\sigma})$$

using $$\Sigma_{ij}(k) = \sum_{k'} P_s(k-k')G_{ij}(k')\,, \quad (k \equiv (\mathbf{k}, i\omega_n))$$

the self-energy reads

$$\Sigma_{11} = (\omega - \omega_1) + \xi_1 \quad , \quad \Sigma_{22} = (\omega - \omega_2) + \xi_2 \quad ,$$
$$\Sigma_{33} = (\omega - \omega_1) - \xi_1 \quad , \quad \Sigma_{44} = (\omega - \omega_2) - \xi_2 \quad ,$$

$$\omega \equiv i\omega_n \quad , \quad \omega_1 \equiv i\omega_n Z(\mathbf{k}, i\omega_n) \quad , \quad \omega_2 \equiv i\omega_n Z(\mathbf{k}+\mathbf{Q}, i\omega_n)$$
$$\xi_1 \equiv \xi(\mathbf{k}, i\omega_n) \quad , \quad \xi_2 \equiv \xi(\mathbf{k}+\mathbf{Q}, i\omega_n) \quad .$$

$$\Sigma_{12} = \Sigma_{21} = \phi_c(\mathbf{k}, i\omega_n) \propto \langle c^\dagger_{k+Q,\sigma} c_{k\sigma}\rangle$$
$$\Sigma_{13} = \Sigma_{31} = \phi_s(\mathbf{k}, i\omega_n) \propto \langle c_{-k-\sigma} c_{k\sigma}\rangle$$

new order parameter

Extension 2: Inclusion of a *d*-wave PG

Equation of motion for $c_{k\sigma}(\tau)$ **and Dyson equation leads to**

$$G_{11}=\left[\left(\omega_2^2-\epsilon_2^2\right)(\omega_1+\epsilon_1)-\phi_c^2(\omega_2-\epsilon_2)-\phi_s^2(\omega_1+\epsilon_1)\right]D^{-1}$$

$$G_{22}=\left[\left(\omega_1^2-\epsilon_1^2\right)(\omega_2+\epsilon_2)-\phi_c^2(\omega_1-\epsilon_1)-\phi_s^2(\omega_2+\epsilon_2)\right]D^{-1}$$

$$G_{12}=G_{21}=\phi_c\left[(\omega_1+\epsilon_1)(\omega_2+\epsilon_2)-\phi_c^2-\phi_s^2\right]D^{-1} \quad ,$$

$$G_{13}=G_{31}=\phi_s\left[\left(\omega_2^2-\epsilon_2^2\right)-\phi_c^2-\phi_s^2\right]D^{-1} \quad ,$$

with $$D=\left(\omega_1^2-\epsilon_1^2\right)\left(\omega_2^2-\epsilon_2^2\right)-\phi_c^2\left[(\omega_1-\epsilon_1)(\omega_2-\epsilon_2)+(\omega_1+\epsilon_1)(\omega_2+\epsilon_2)\right]$$

$$-\phi_s^2\left[\left(\omega_1^2-\epsilon_1^2\right)+\left(\omega_2^2-\epsilon_2^2\right)\right]+\left[\phi_c^2+\phi_s^2\right]^2 \quad ,$$

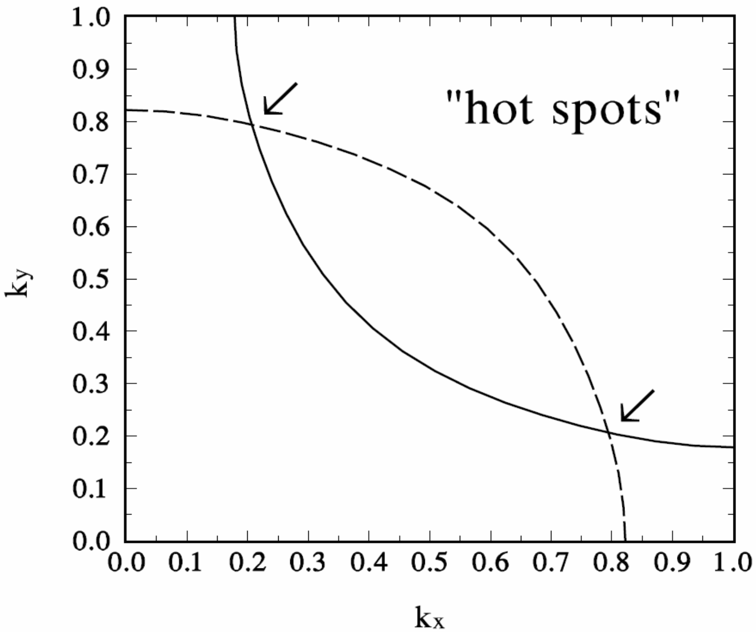
$$\epsilon_1\equiv\epsilon(\mathbf{k})+\xi_1 \quad , \quad \epsilon_2\equiv\epsilon(\mathbf{k}+\mathbf{Q})+\xi_2$$

and

$$\mathrm{Im}\chi_{s0}(\mathbf{q},\omega)=\pi\int_{-\infty}^{\infty}d\omega'\left[f(\omega')-f(\omega'+\omega)\right]\sum_{\mathbf{k}}\left[N(\mathbf{k}+\mathbf{q},\omega'+\omega)N(\mathbf{k},\omega')\right.$$

$$\left.+A_1(\mathbf{k}+\mathbf{q},\omega'+\omega)A_1(\mathbf{k},\omega')+A_g(\mathbf{k}+\mathbf{q},\omega'+\omega)A_g(\mathbf{k},\omega')\right]$$

Extension 2: Inclusion of a *d*-wave PG



$$N(\mathbf{k},\omega) = -\frac{1}{\pi}\,\mathrm{Im}\frac{\omega Z + \epsilon_k + \xi}{(\omega Z)^2 - (\epsilon_k + \xi)^2 - E_g^2 - \phi^2}$$

$$A_1(\mathbf{k},\omega) = -\frac{1}{\pi}\,\mathrm{Im}\frac{\phi}{(\omega Z)^2 - (\epsilon_k + \xi)^2 - E_g^2 - \phi^2}$$

$$A_g(\mathbf{k},\omega) = -\frac{1}{\pi}\,\mathrm{Im}\frac{E_g}{(\omega Z)^2 - (\epsilon_k + \xi)^2 - E_g^2 - \phi^2}$$

where $\phi^2 = \phi_s^2 + \phi_c^2$ **and**

$$E_g\left(\mathbf{k}, T, x\right) = E_g(T, x)\left[\cos k_x - \cos k_y\right]$$

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Extension 2: Inclusion of a *d*-wave PG

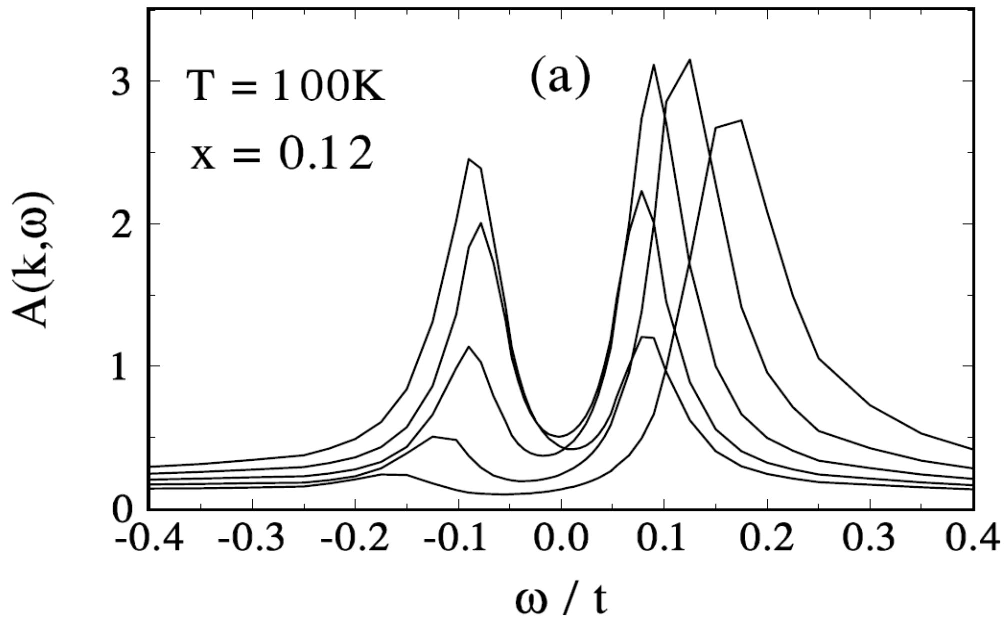
weak-coupling limit, gap equation (see also DDW, i-CDW)

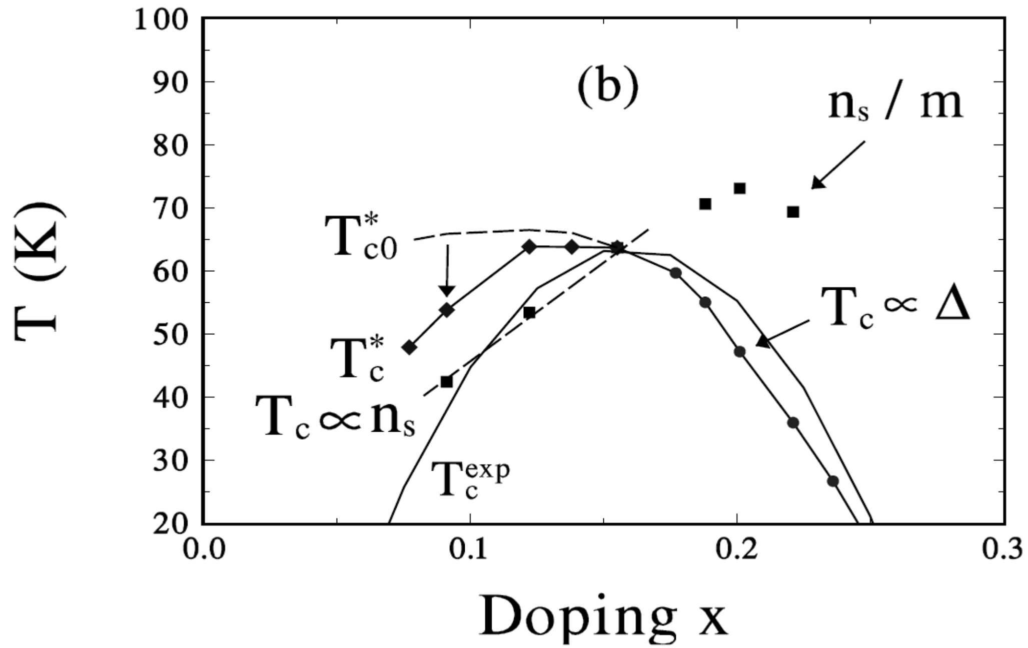
$$\Delta_s(\mathbf{k}) = -\sum_{\mathbf{k}'} P_s(\mathbf{k}-\mathbf{k}')\Delta_s(\mathbf{k}')\,\frac{1}{2}\left[\frac{1-2f(E'_+)}{2E'_+}+\frac{1-2f(E'_-)}{2E'_-}\right.$$
$$\left.+\ (\epsilon'_1-\epsilon'_2)\left[(\epsilon'_1-\epsilon'_2)^2+4\Delta_c^2\right]^{-1/2}\left(\frac{1-2f(E'_+)}{2E'_+}-\frac{1-2f(E'_-)}{2E'_-}\right)\right]$$

where $$E_\pm^2 = \left[\frac{1}{2}(\epsilon_1+\epsilon_2)\pm\frac{1}{2}\left[(\epsilon_1-\epsilon_2)^2+4\Delta_c^2\right]^{1/2}\right]^2+\Delta_s^2$$

$$\epsilon_1=\epsilon_1(\mathbf{k})\,,\qquad \epsilon_2=\epsilon_2(\mathbf{k}+\mathbf{Q})\,,\qquad \Delta_s=\Delta_s(\mathbf{k})\,,\qquad \Delta_c=\Delta_c(\mathbf{k}+\mathbf{Q})$$

Inclusion of a *d*-wave PG: Results





***d*-wave gap in the spectral density and other quantities**

reduction of T_c due to fewer DoS

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Combination with response theory

e.g., optical conductivity

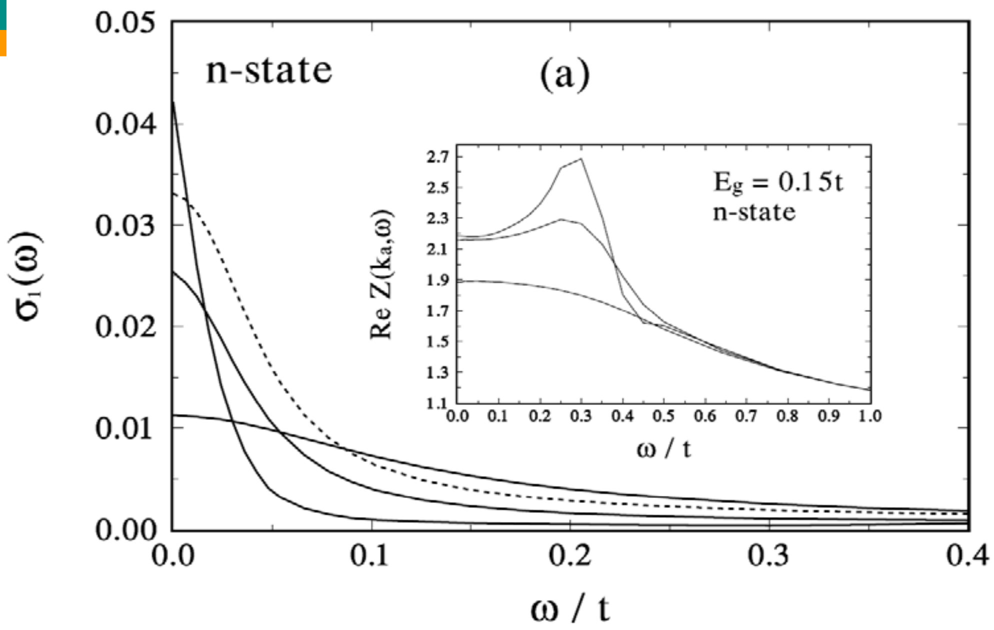
$$\sigma_{ab}(\omega) = \frac{2e^2}{\hbar c_0}\frac{\pi}{\omega}\int_{-\infty}^{\infty} \mathrm{d}\omega' \left[f(\omega') - f(\omega'+\omega)\right] \times \sum_{\mathbf{k}} \left[v_{k,x}^2 + v_{k,y}^2\right] \left[N(\mathbf{k},\omega'+\omega)N(\mathbf{k},\omega') + A_1(\mathbf{k},\omega'+\omega)A_1(\mathbf{k},\omega') + A_g(\mathbf{k},\omega'+\omega)A_g(\mathbf{k},\omega')\right]$$

$$\sigma_c(\omega) = \frac{e^2 t_\perp^2 c_0}{\hbar a_0^2}\frac{\pi}{\omega}\int_{-\infty}^{\infty} \mathrm{d}\omega' \left[f(\omega') - f(\omega'+\omega)\right] \sum \left[N(\mathbf{k},\omega'+\omega)N(\mathbf{k},\omega') + A_1(\mathbf{k},\omega'+\omega)A_1(\mathbf{k},\omega') + A_g(\mathbf{k},\omega'+\omega)A_g(\mathbf{k},\omega')\right]$$

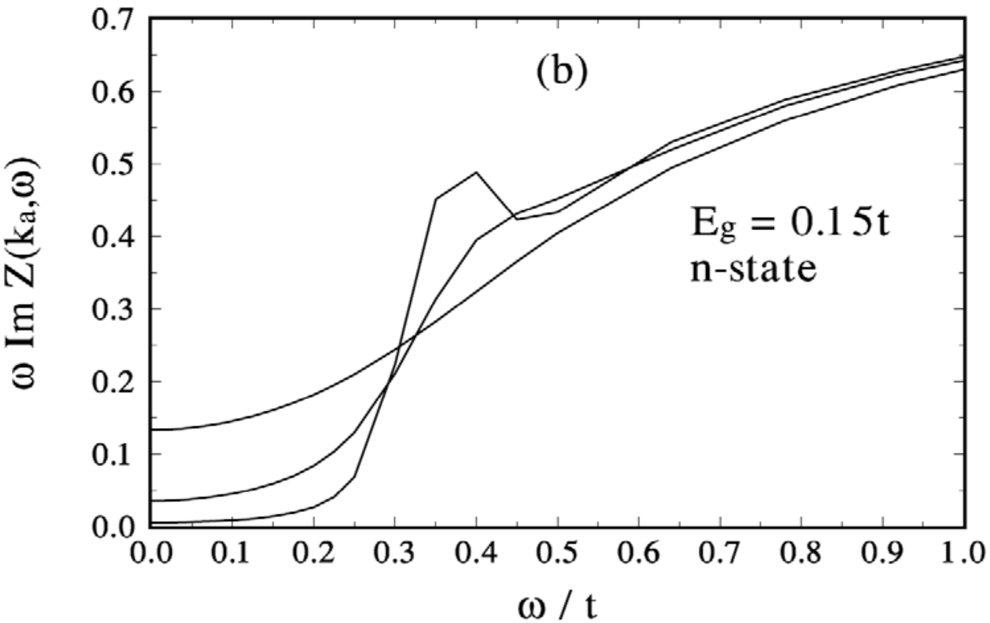
and

$$\sigma_c^{\mathrm{incoh}}(\omega) = \frac{e^2 t_\perp^2 c_0}{\hbar a_0^2}\frac{\pi}{\omega}\int_{-\infty}^{\infty} \mathrm{d}\omega' \left[f(\omega') - f(\omega'+\omega)\right] N(\omega'+\omega)N(\omega')$$

Combination with response theory: results

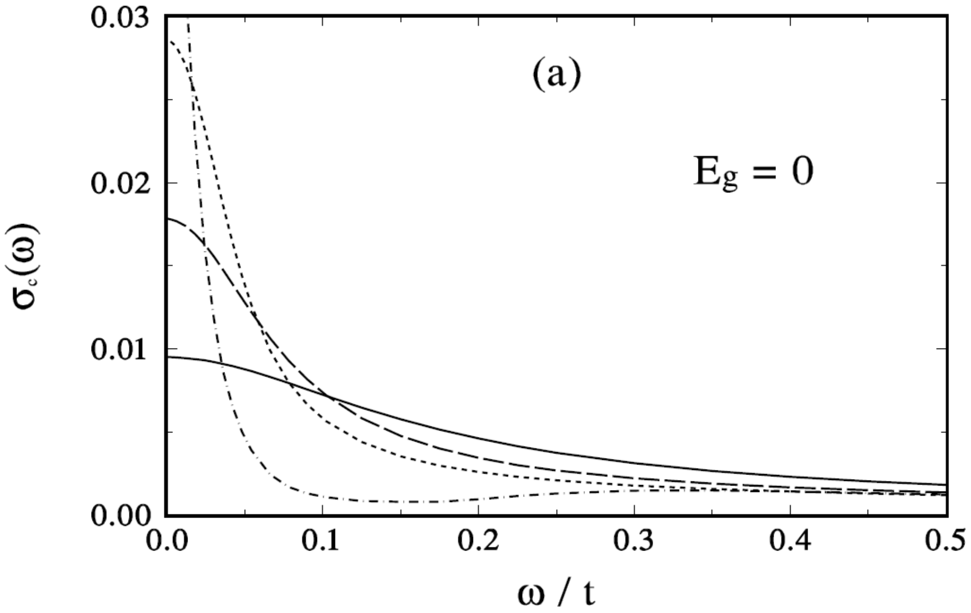


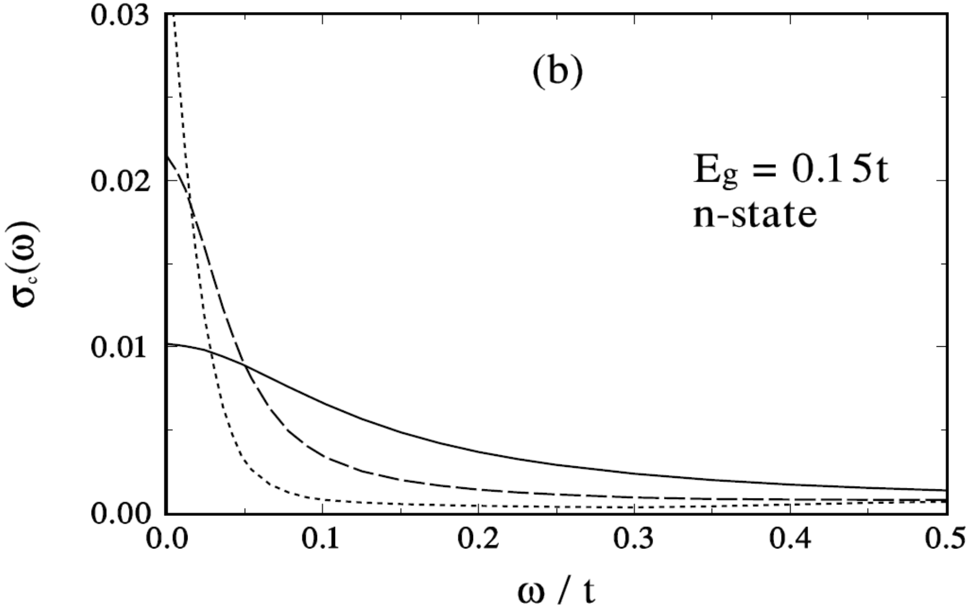
in-plane optical conductivity

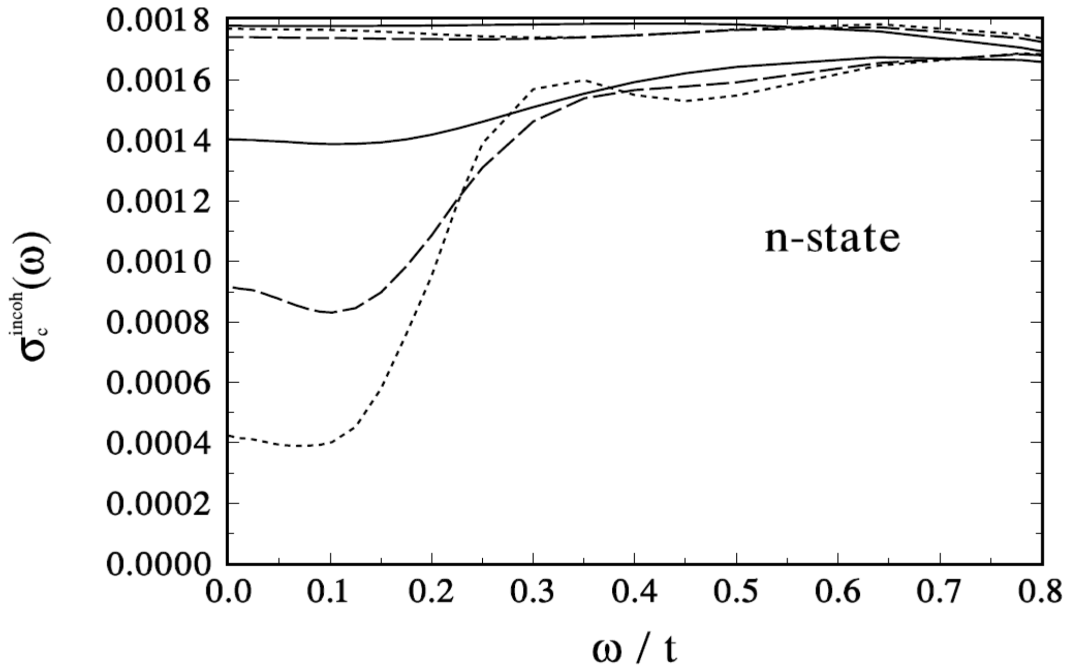


damping rate reveals a 'coherence peak'

Combination with response theory: results







coherent vs. Incoherent c-axis conductivity

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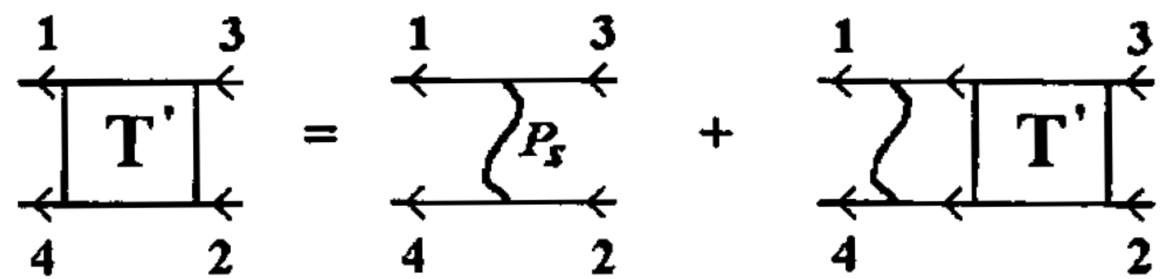
Combination with response Theory

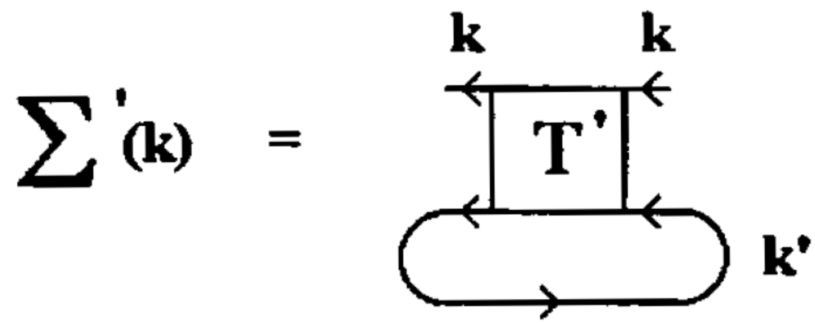
I did not talk about:

- **structure in SIN / SIS tunneling**
- **pseudogap in NMR**
- **polarization-dependent Raman scattering: ‘hot spots‘ vs. ‘cold spots‘**
- **…**

Extension 3: Amplitude fluctuations

consider FLEX + T-matrix, solve self-energy self-consistently





$$T'(k_1, k_3; q = k_1 + k_4)$$

$$= P_s(k_1 - k_3) - T \sum_{k_1'} P_s(k_1 - k_1')G(k_1')G(q - k_1')T'(k_1', k_3; q)$$

Amplitude fluctuations: FLEX + T-matrix

new self-energy

$$\Sigma'(k, i\omega_n) = T \sum_{\omega_n'} \sum_{\mathbf{k}'} T'(k, \mathbf{q} = \mathbf{k} + \mathbf{k}', i\nu_m = i\omega_n + i\omega_n') \, G(\mathbf{k}', i\omega_n')$$

leads to

$$\omega \left[1 - Z(\mathbf{k}, \omega)\right] = \sum_{\mathbf{k}'} \int_0^\infty \mathrm{d}\Omega \left[|\psi_d(\mathbf{k}, \omega)|^2 K(\mathbf{k} - \mathbf{k}', \Omega) + P_s(\mathbf{k} - \mathbf{k}', \Omega)\right] \times \int_{-\infty}^{\infty} \mathrm{d}\omega' \, I(\omega, \Omega, \omega') \, A_0(\mathbf{k}', \omega')$$

pair-fluctuation propagator

$$K(\mathbf{q}, \omega) = \frac{g}{\pi \bar{N}} \frac{\omega\tau}{\left[\ln\left(T/T_c\right) + \xi_0^2 q^2 + b\left(\omega/4T\right)^2\right]^2 + [\omega\tau]^2}$$

$$\omega\tau = (\pi/2)\tanh(\omega/4T)\,, \quad b = 7\xi(3)/\pi^2\,, \quad \xi_0^2 = (7\xi(3)/48)(v_F/\pi T)^2$$

Extension 4: Inclusion of phase fluctuations

In analogy to the FLEX equations for Cooper-pairing start with

$$\mathcal{S}_{eff}[\Phi^*, \Phi] = \int_0^\beta \mathrm{d}\tau \left\{ \sum_{i\sigma} \Phi^*_{i\sigma}(\partial_\tau - \mu)\Phi_{i\sigma} - t \sum_{\langle ij\rangle\sigma} \Phi^*_{i\sigma}\Phi_{j\sigma} \right.$$

$$\left. + V_{eff} \sum_{\langle ij\rangle} \Phi^*_{i\uparrow}\Phi^*_{j\downarrow}\Phi_{j\downarrow}\Phi_{i\uparrow} \right\} \quad ,$$

After a Hubbard-Stratonovich transformation (neglecting amplitude fluctuations) one arrives at

$$\mathcal{S}_{eff}[\varphi] = \mathcal{S}^{BCS}_{eff}(\Delta^0) + \frac{1}{\beta} \sum_{qn} \varphi(q, i\nu_n) \left[\mathcal{D}_\varphi(q, i\nu_n)\right]^{-1} \varphi(-q, -i\nu_n)$$

with $\mathcal{D}_\varphi(q, i\nu_n) = \langle\langle \varphi(q, i\nu_n)\ \varphi(-q, -i\nu_n)\rangle\rangle$ **being the phase fluctuation propagator**

Inclusion of phase fluctuations: recepy

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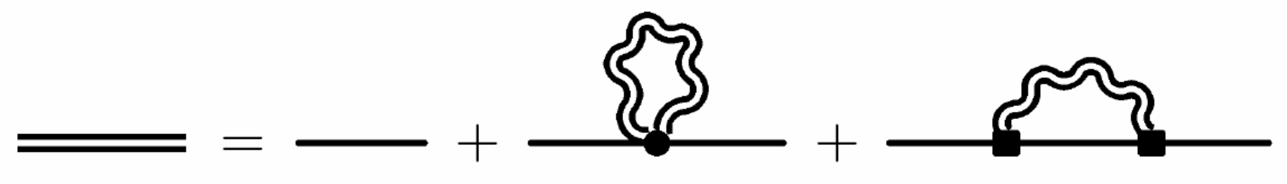
this leads finally to $\hat{\mathcal{G}}(k, i\omega_n)$

$$= \hat{\mathcal{G}}_0(k, i\omega_n) - \hat{\mathcal{G}}_0(k, i\omega_n)\ \hat{\Sigma}^{\varphi\varphi}(k, i\omega_n)\ \hat{\mathcal{G}}_0(k, i\omega_n)$$

or, diagrammatically,



and new parts of the self-energy (current–current correlation function Π **)**

$$\Sigma^{\mathcal{G}}(k, i\omega_n) = \frac{1}{4\beta N} \sum_{q,n'} [(i\nu_{n'})^2 - 2i\nu_{n'}(\epsilon_k - \epsilon_{k-q}) + (\epsilon_k - \epsilon_{k-q})^2]$$
$$\times\ \mathcal{G}_0(k-q, i\omega_n - i\nu_{n'})\ \Pi^{\varphi\varphi}(q, i\nu_n)$$
$$\Sigma^{\mathcal{F}}(k, i\omega_n) = \frac{1}{4\beta N} \sum_{q,n'} [(i\nu_{n'})^2 + (\epsilon_k - \epsilon_{k-q})^2]$$
$$\times\ \mathcal{F}_0(k-q, i\omega_n - i\nu_{n'})\ \Pi^{\varphi\varphi}(q, i\nu_n)$$

they have to be added self-consistently:
new FLEX generation

simple view: combination with BKT theory

dimensionaless stiffness $K(T) = \beta\hbar^2 \frac{n_s(T)}{m} \frac{d}{4}$ $\quad l = (r/r_0)$

recursion relations $\frac{dy}{dl} = (2 - \pi K)\, y \qquad \frac{dK}{dl} = -4\pi^3 y^2 K^2$

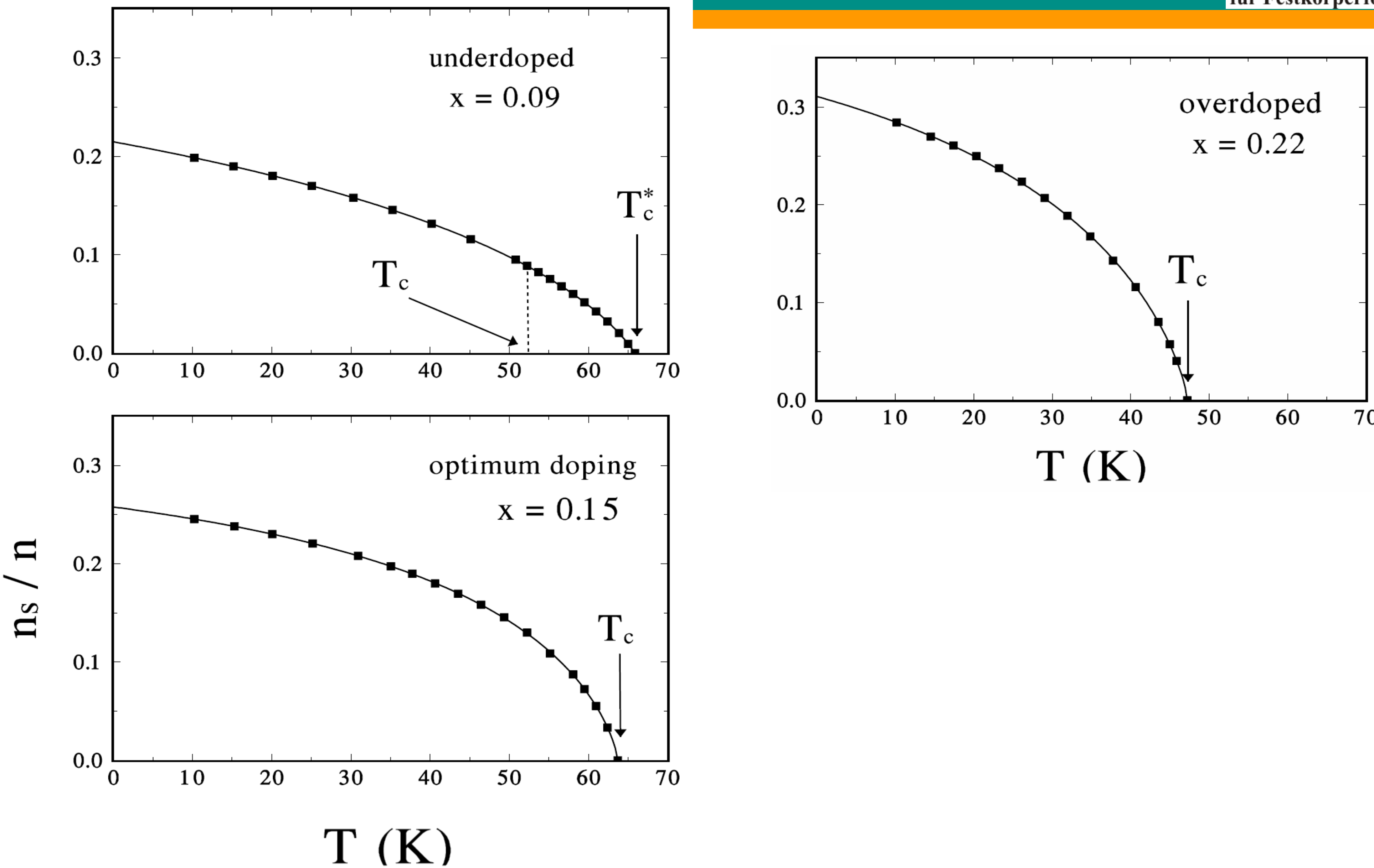
vortex fugacity $y = e^{-\beta E_c}$ **Blatter *et al.*:** $E_{core} = \pi k_B T K \ln \kappa$

obtain T$_c$ from $K(T_c) = \frac{2}{\pi}$ or $\frac{n_s(T_c, x)}{m} = \frac{2}{\pi} \frac{4 k_B T_c}{\hbar^2 d}$

and use FLEX as in input for the superfluid density $\frac{n_s}{m} = \frac{2t}{\hbar^2} (S_N - S_S)$

$$S_N = \frac{\hbar^2 c}{2\pi e^2 t} \int_{0^+}^{\infty} \sigma_1(\omega)\, \mathrm{d}\omega$$ **(f-sum rule)**

Phase fluctuations: results



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Phase fluctuations, results: phase diagram

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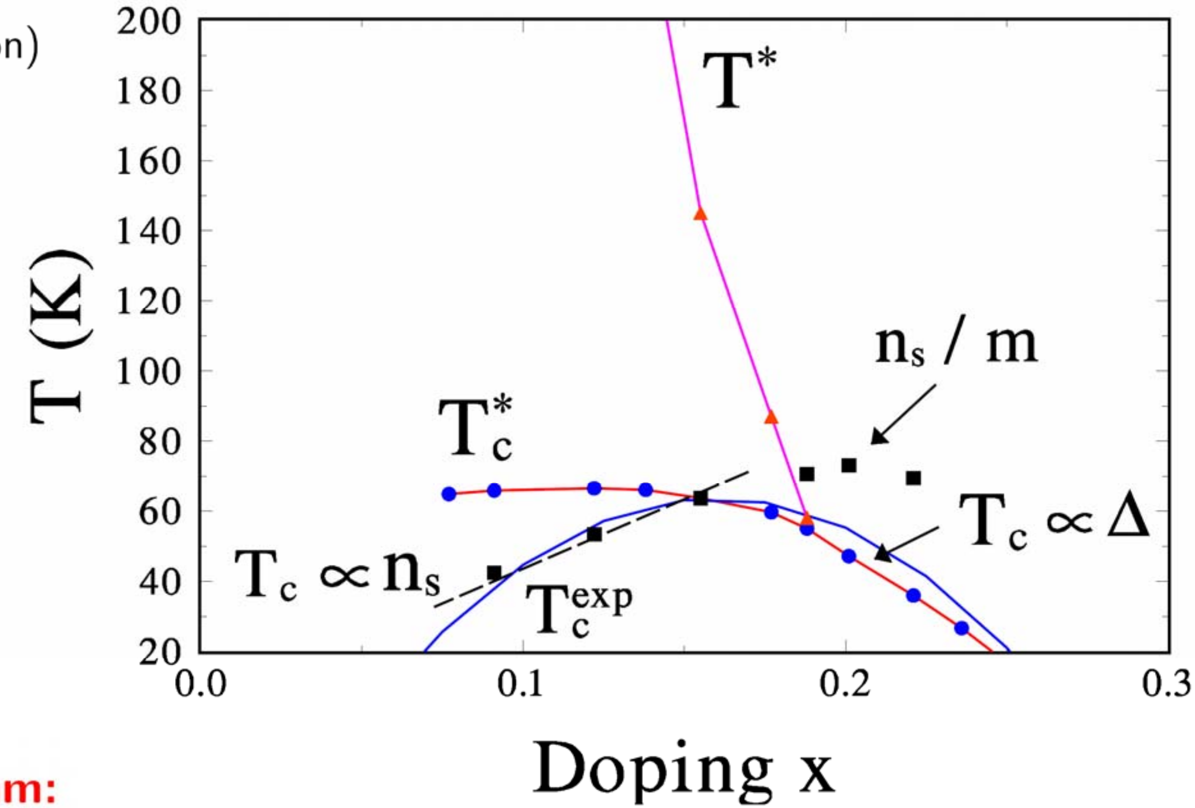
$U = 4t$, $t = 250\text{meV}$

generalized Eliashberg equations

(Berk-Schrieffer-like repulsive interaction)



- **two regions in the phase diagram:**
  $T_c \propto \Delta(T = 0)$ (overdoped)
  $T_c \propto n_s(T = 0)$ (underdoped)

Phase fluctuations: results

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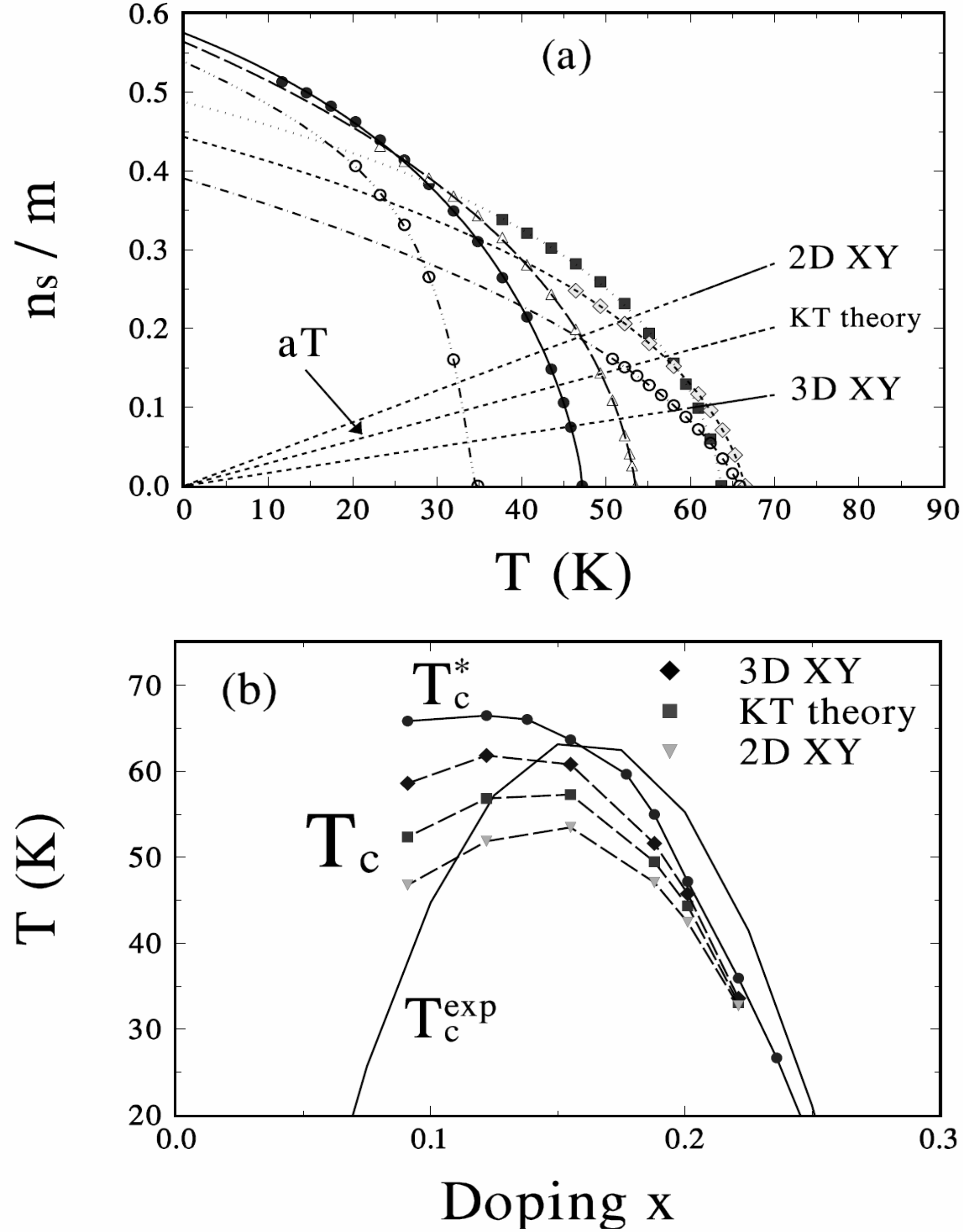
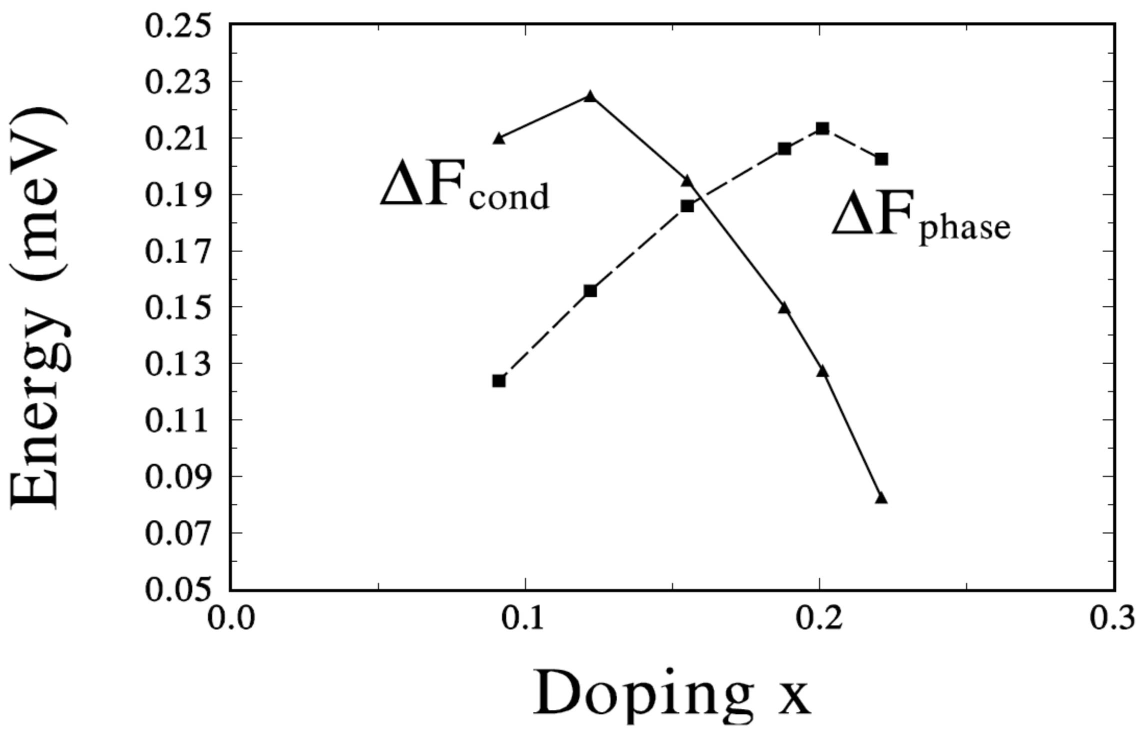
comparison of the superfluid density



Phase fluctuations: results

calculated crossover of the phase stiffness energy



Discussion: highlights and problems

- ❑ doping dependence easily obtained
- ❑ tight-binding dispersion and Hubbard U are the only input parameters
- ❑ simple calculation of the elementary excitations possible

- ❑ ‘correct‘ weak-coupling picture close to an AF phase transition

- ❑ Inclusion of vertex corrections (current research)
- ❑ Combination with RG approach

Problems:

- ❑ no Mott physics included
- ❑ only pertubation theory is used

Summary (2)

- basic FLEX approach, generalized Eliashberg equations for a repulsive interaction, comparison with similar approaches, problems/limitations
- various extensions (bilayer, pseudogap, fluctuations) and combination with response theory possible
- calculation of elementary excitations!

D. Manske, Theory for Unconventional Superconductors, Springer, Heidelberg (2004)

Outlook: isotope effect

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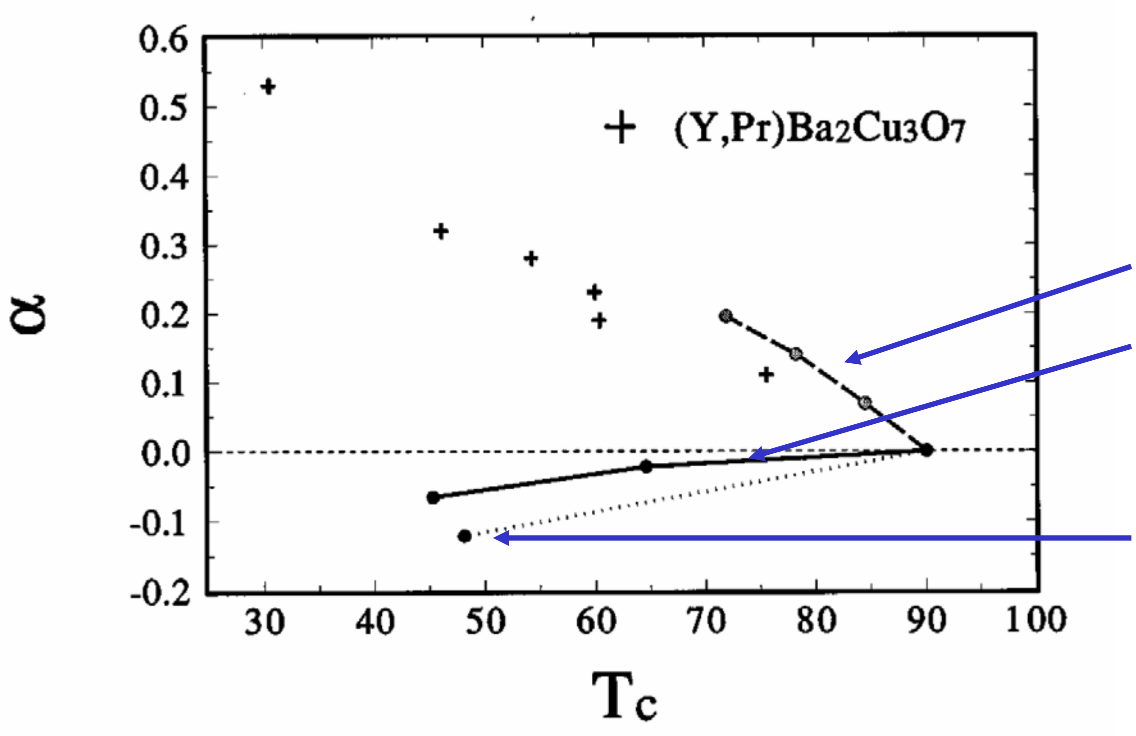
- spin fluctuations + phonons

$$\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'} \frac{[V_{\text{eff}}(\mathbf{q}) - \alpha^2 F_i(\mathbf{q})]}{2E_k} \Delta(\mathbf{k})$$

- self-consistent FLEX level (first results)

$$\alpha^2 F_i(\mathbf{q},\Omega) = g_p \frac{1}{\pi} \frac{\Omega \Gamma_0^3}{[(\Omega-\Omega_0)^2+\Gamma_0^2]^2} F_i(\mathbf{q}) \qquad (i=0,b,t)$$



d-wave with λ_p=0.25, 0.5, 0.75

$$F_t = 2 - F_b$$

$$F_0(\mathbf{q}) \equiv 1$$

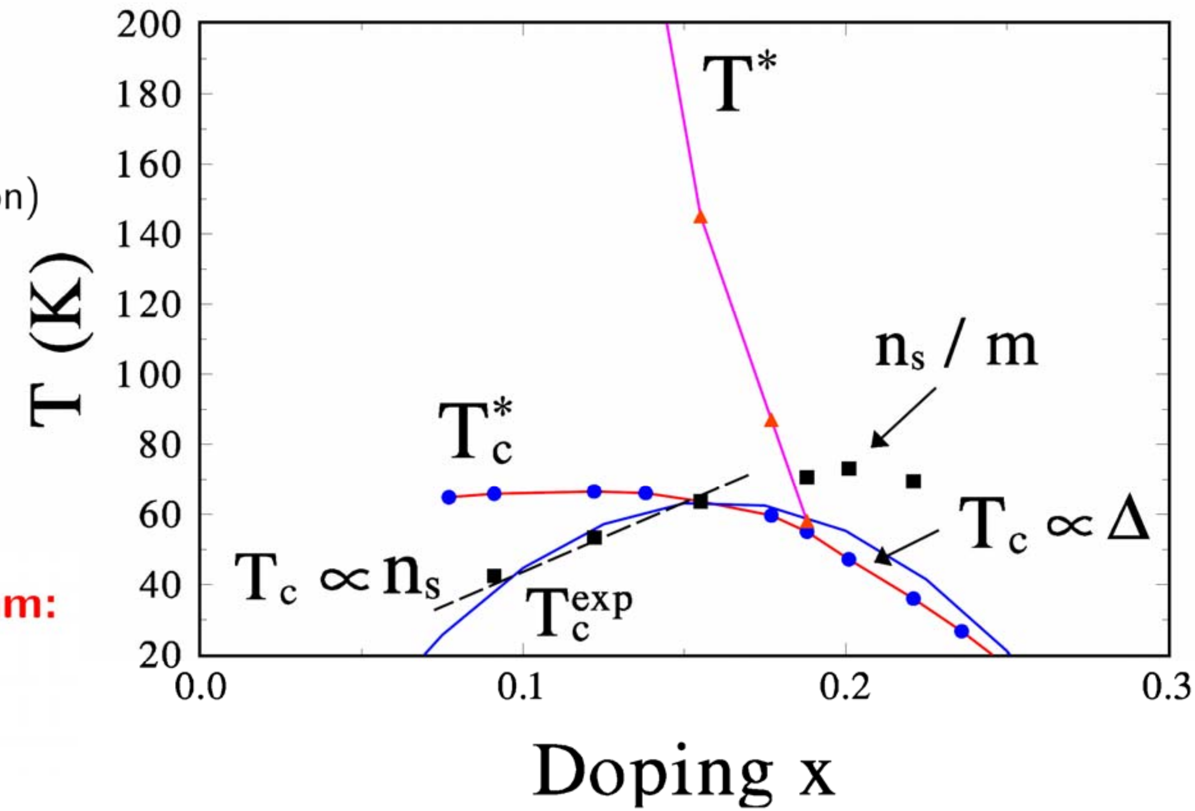
$$F_b(\mathbf{q}) = \sin^2(q_x/2) + \sin^2(q_y/2)$$

Results: phase diagram (hole-doped cuprates)

$U = 4t,\ t = 250\text{meV}$

generalized Eliashberg equations

(Berk-Schrieffer-like repulsive interaction)



- **two regions in the phase diagram:**
  $T_c \propto \Delta(T=0)$ (overdoped)
  $T_c \propto n_s(T=0)$ (underdoped)

D. Manske and K.H. Bennemann, Physica C **341-348**, 83 (2000)

D. Manske, T. Dahm, and K.H. Bennemann, PRB **64**, 144520 (2001)

C. Timm, D. Manske, K.H. Bennemann, PRB **66**, 094515 (2002)

T_c^{exp}: M.R. Presland *et al.*, Physica C **176**, 95 (1991)

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Discussion (1): new dispersion?

The BCS-Lindhard-like response function (T = 0 , ω > 0)

$$\chi_0''(\omega, \boldsymbol{q}) \; = \; \frac{\pi}{N} \sum_{\boldsymbol{k}} C^{+,-}_{\boldsymbol{q},\boldsymbol{k}} \, \delta\big(\omega - E_2(\boldsymbol{q},\boldsymbol{k})\big)$$

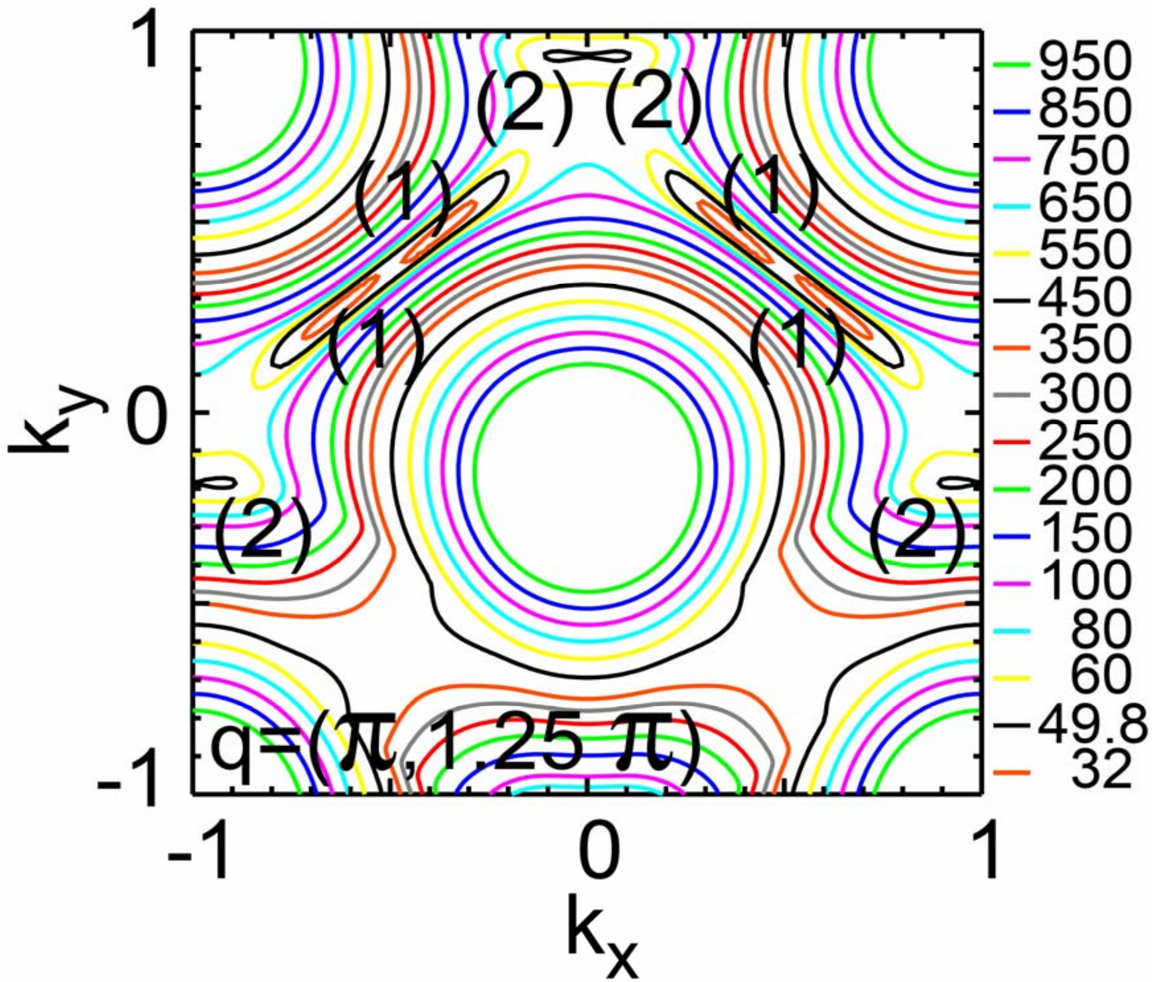
with

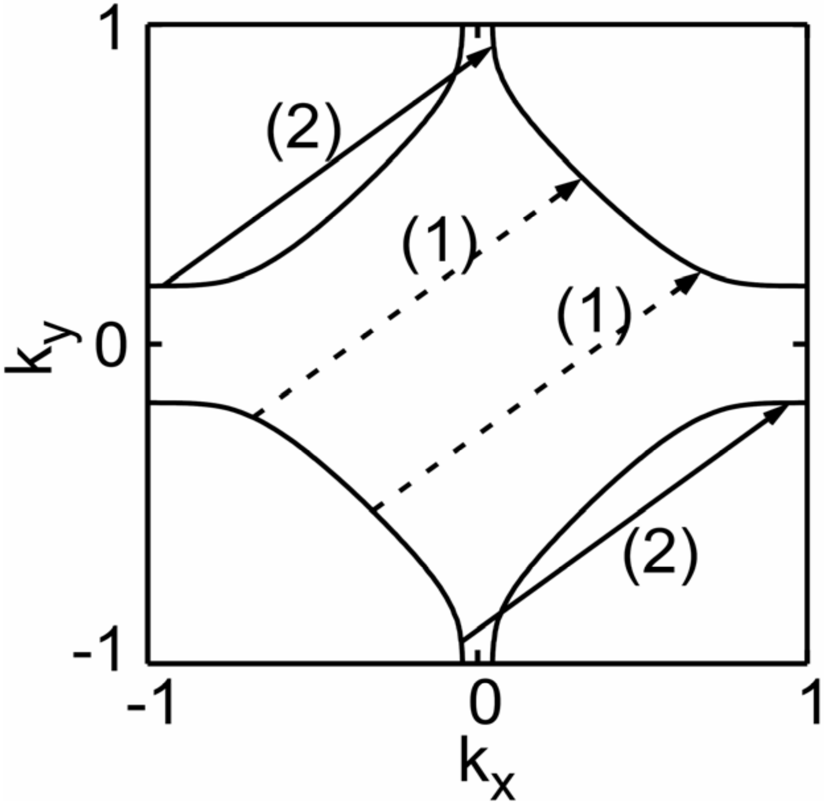
$$C^{+,-}_{\boldsymbol{q},\boldsymbol{k}} \; = \; \frac{1}{4}\left(1 - \frac{\varepsilon_{\boldsymbol{k}+\boldsymbol{q}}\varepsilon_{\boldsymbol{k}} + \Delta_{\boldsymbol{k}+\boldsymbol{q}}\Delta_{\boldsymbol{k}}}{E_{\boldsymbol{k}+\boldsymbol{q}}E_{\boldsymbol{k}}}\right)$$

and $E_2(\boldsymbol{q},\boldsymbol{k}) \; = \; E_{\boldsymbol{k}+\boldsymbol{q}} + E_{\boldsymbol{k}}$ **where** $E_{\boldsymbol{k}} \; = \; \sqrt{\varepsilon_{\boldsymbol{k}}^2 + \Delta_{\boldsymbol{k}}^2}$

vanishes below the threshold frequency $\omega_c(\boldsymbol{q}) = \min\limits_{\boldsymbol{k}\in \mathrm{BZ}} E_2(\boldsymbol{q},\boldsymbol{k})$

Discussion (2): calculated $E_2(q,k)$





PRB 2006, A. Schnyder, D. Manske, C. Mudry, and M. Sigrist

calculated inelastic scattering rates

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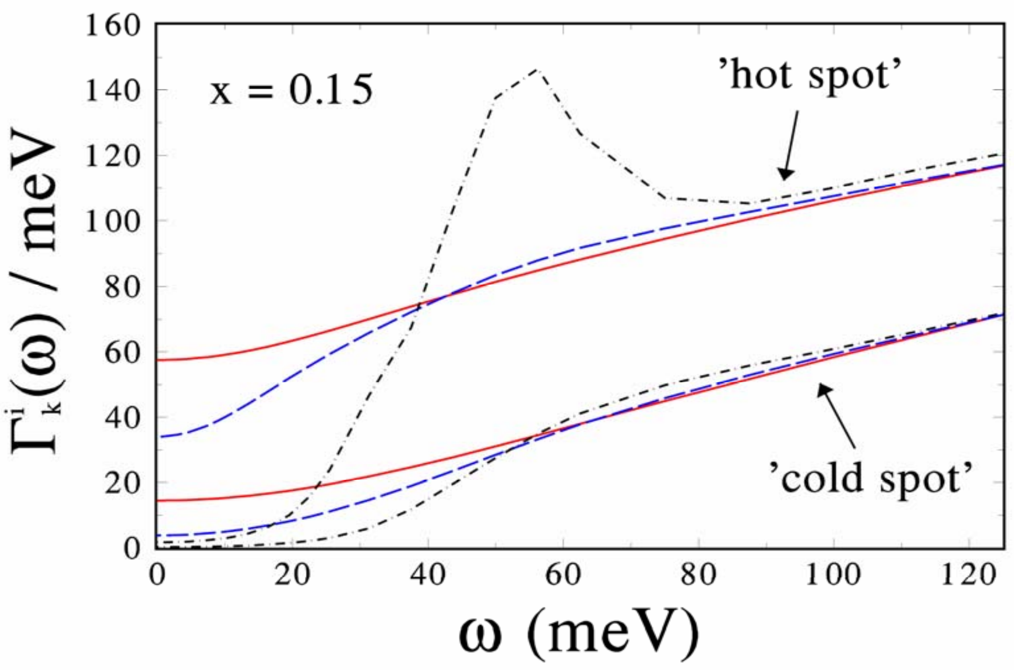

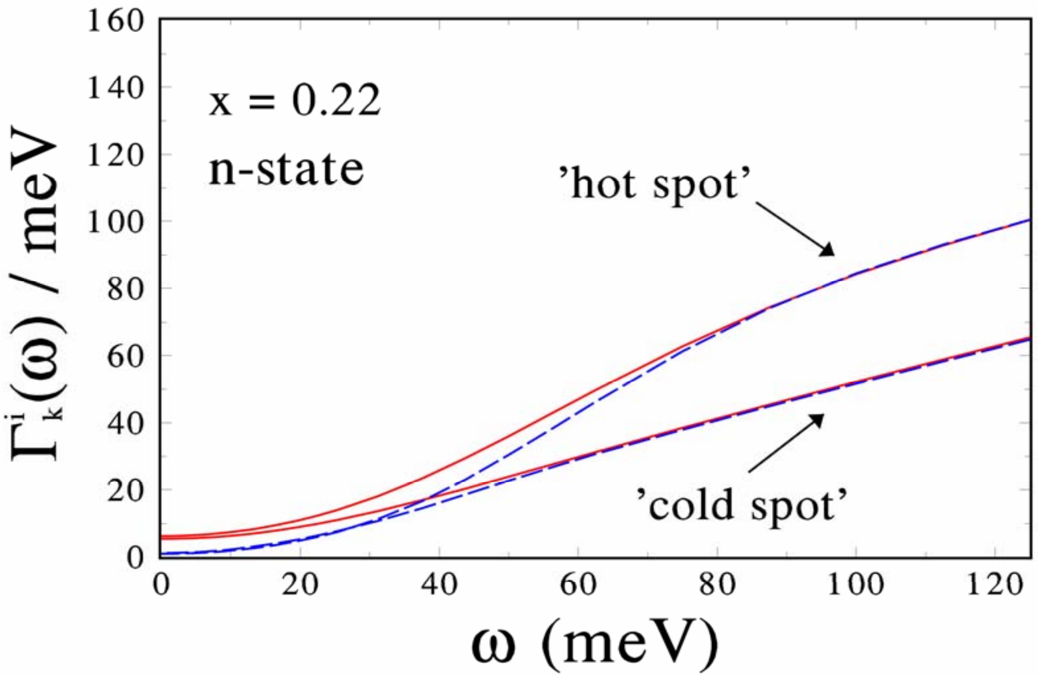

- ❑ **anisotropy for $\omega \to 0$ nearly vanishes in the overdoped regime**

(D. Manske et al., PRB 2003, PRB 2004)

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Results: kink (antinodal direction)

PHYSICAL REVIEW B **67**, 134520 (2003)

Renormalization of the elementary excitations in hole- and electron-doped cuprates due to spin fluctuations

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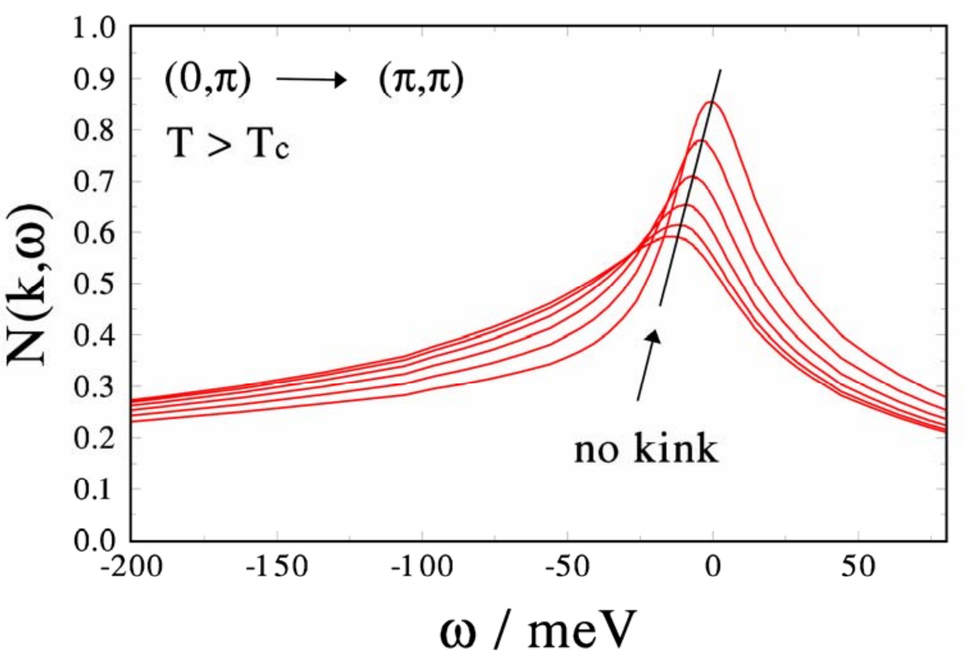
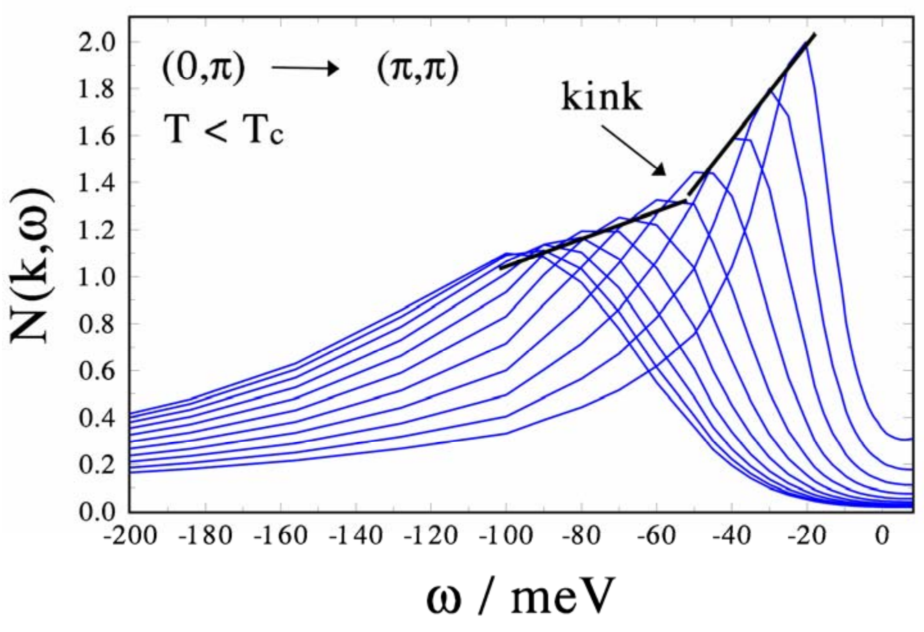
(Received 17 October 2002; revised manuscript received 10 January 2003; published 23 April 2003)





- ❑ **fingerprints of the pairing interaction via $\Delta(k,\omega)$**

rearrangement below Tc

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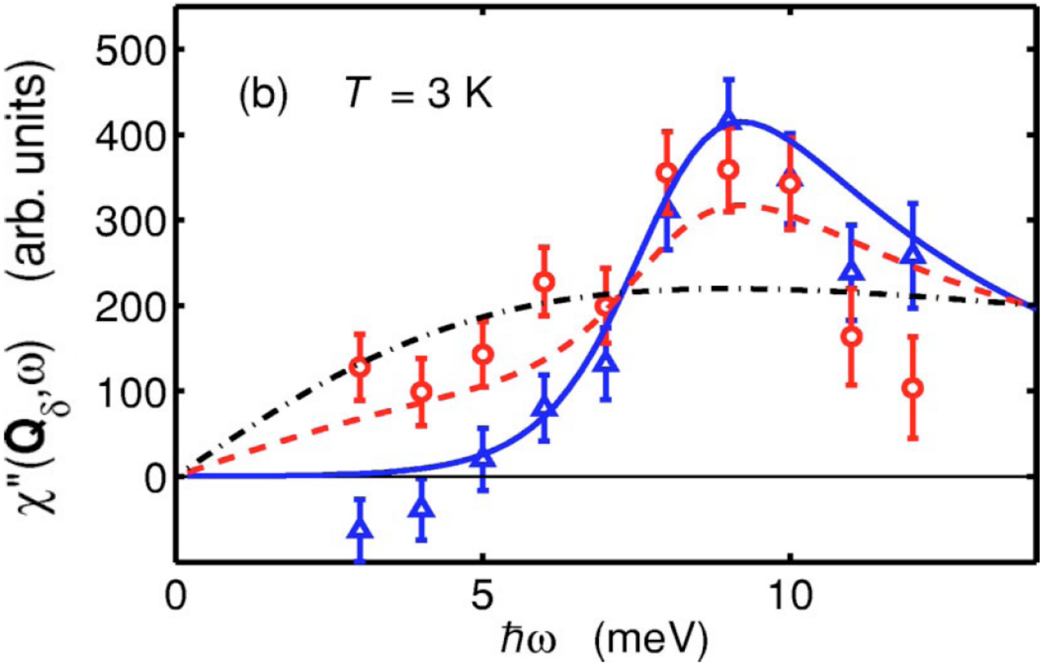

J. Tranquada et al., PRB 69, 174507 (2004)

other works

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RAPID COMMUNICATIONS

PHYSICAL REVIEW B, VOLUME 64, 140510(R)

Low-energy renormalization of the electron dispersion of high-T_c superconductors

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(Received 17 March 2001; published 19 September 2001)

High-resolution angle-resolved photoemission spectroscopy studies in cuprates have detected low-energy changes in the dispersion and absorption of quasiparticles at low temperatures, in particular, in the superconducting state. Based on a $1/N$ expansion of the t-J-Holstein model, which includes collective antiferromagnetic fluctuations already in leading order, we argue that the observed low-energy structures are mainly caused by phonons and not by spin fluctuations, at least, in the optimal and overdoped regime.

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