Pseudogap and spin fluctuations in the cuprates

P. Prelovšek and A. Ramšak

Faculty of Mathematics and Physics, University of Ljubljana
J. Stefan Institute, Ljubljana, Slovenia

Trieste 2002

”Jožef Stefan” Institute

Outline

- pseudogap scales in cuprates
- evidence for pseudogap in the planar t-J model: numerical
- spectral functions: equation-of-motion approach: effective spin – fermion coupling, self energy, quasiparticles etc.
- underdoped regime: pseudogap and truncated Fermi surface
- spin dynamics: experiments
- spin fluctuations: EQM approach, memory functions, spin damping, resonant peak

References:

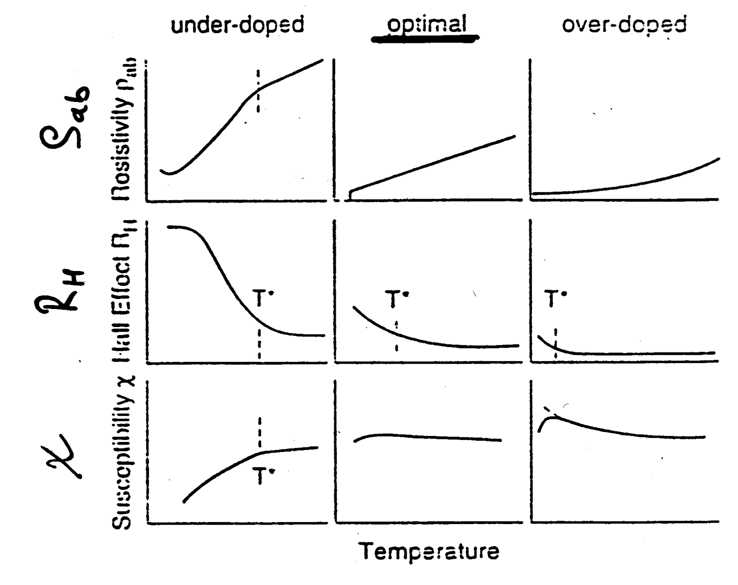
J. Jaklič and P. Prelovšek, Adv. Phys. 49, 1 (2000).

P. Prelovšek and A. Ramšak, PRB 63, 180506 (2001)

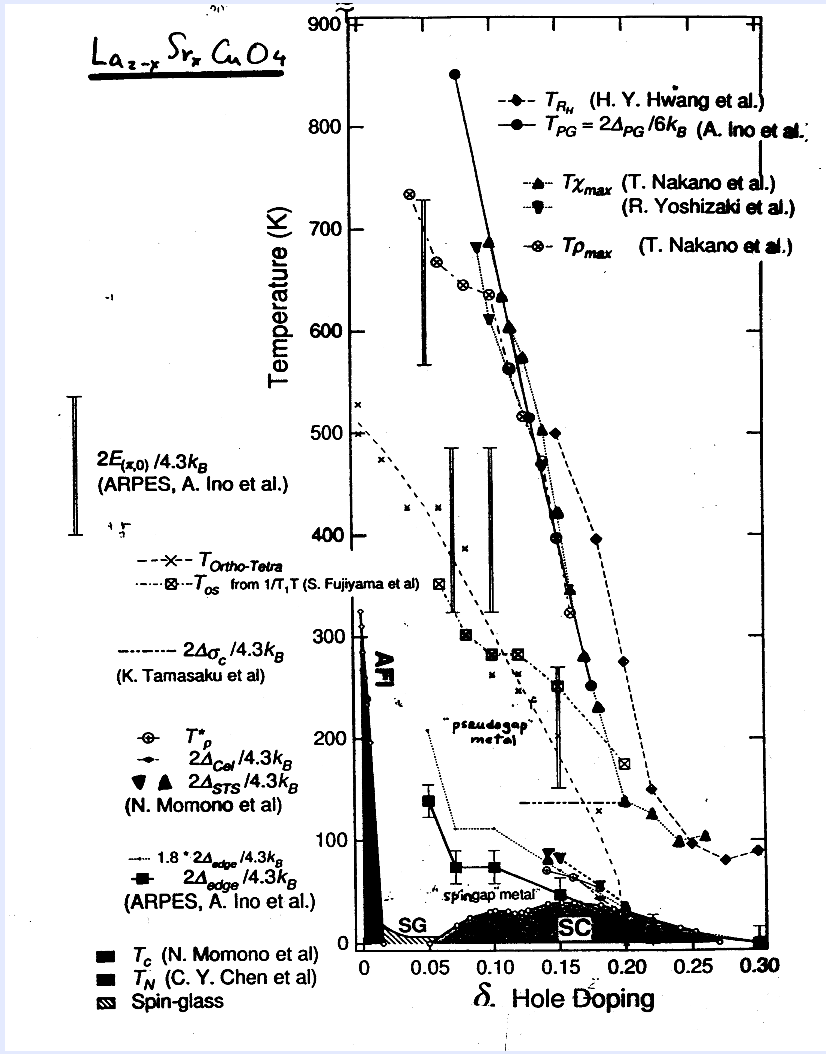
P. Prelovšek and A. Ramšak, PRB 65, 174529 (2002)

I. Sega, P. Prelovšek and J. Bonča, in preparation

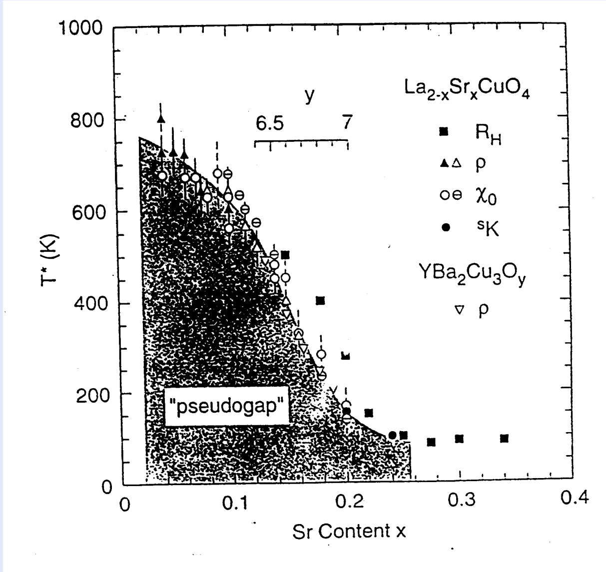
Pseudogap scales in underdoped cuprates



A.Fujimori 99



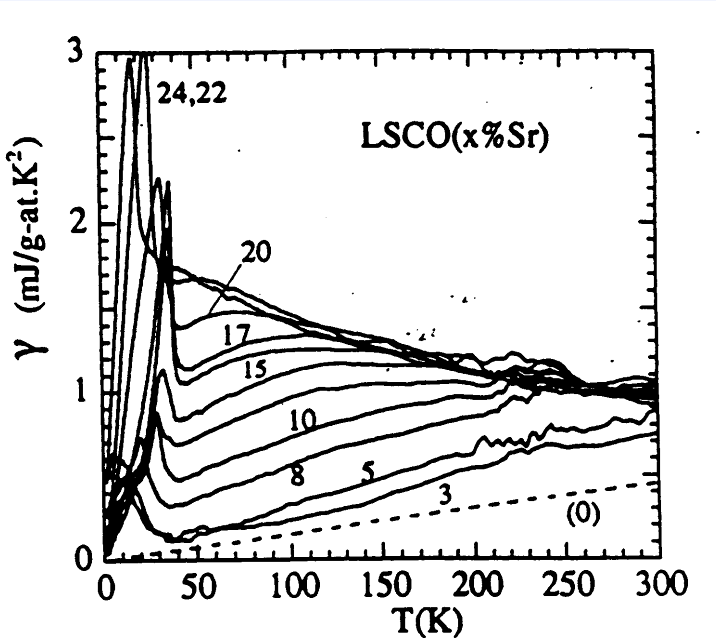
B.Batlogg 94

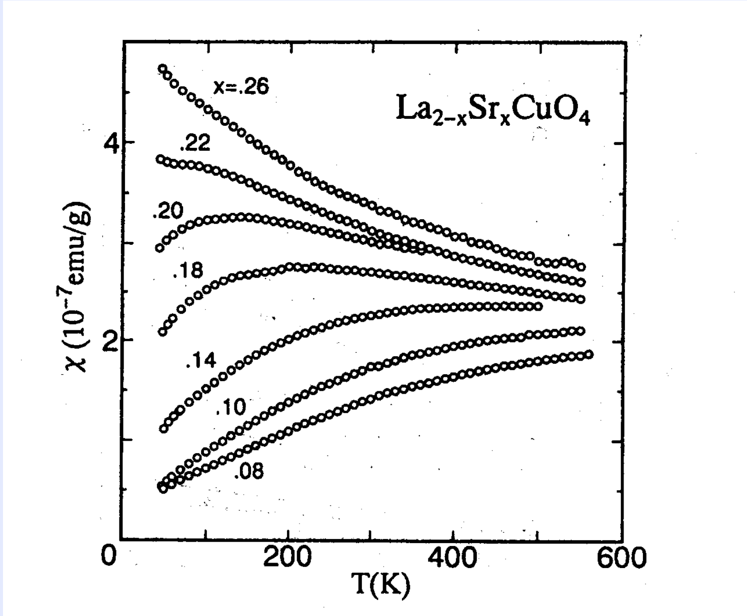


Large pseudogap

specific heat coefficient: $\gamma = C_V / T$

uniform spin susceptibility



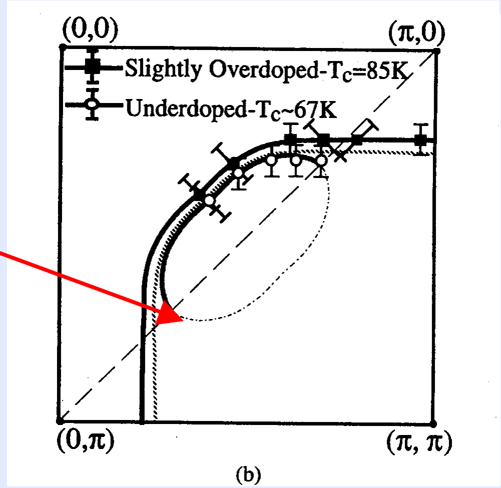


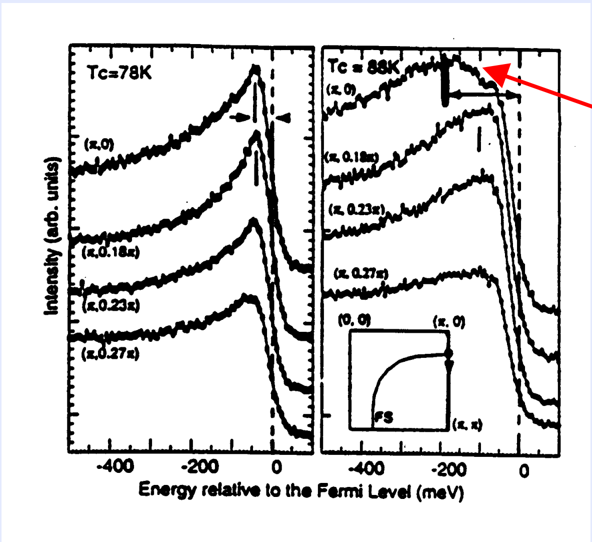
J. Loram 93, 96

Johnston, Torrance et al. 89

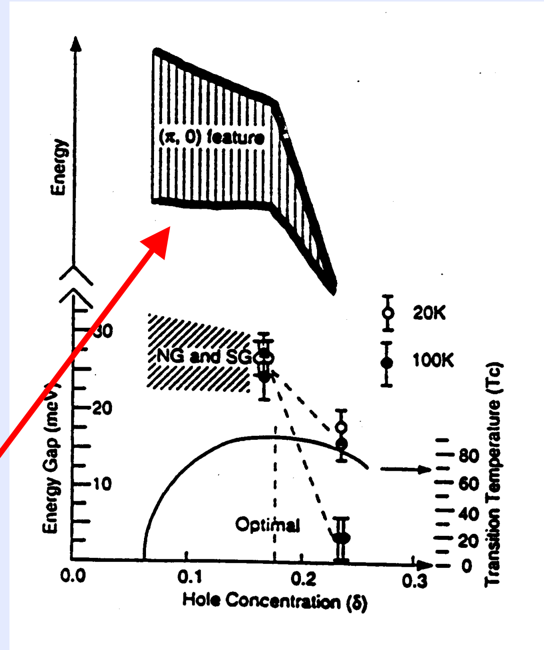
ARPES: BSCCO Fermi surface and pseudogap

truncated
FS in UD
cuprates :





hump:
large pseudogap
feature



t – J model: strong correlations

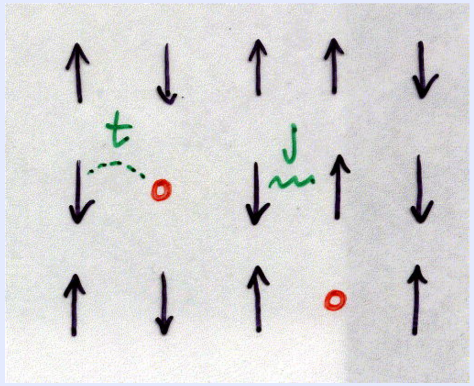
single band model

interplay : electron hopping (n.n. + n.n.n.) + spin exchange

$$H = -t \sum_{\langle ij \rangle s} \tilde{c}^{\dagger}_{js} \tilde{c}_{is} + J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j) \quad + H_{n.n.n.}(?) + \cdots$$

no double occupation of sites

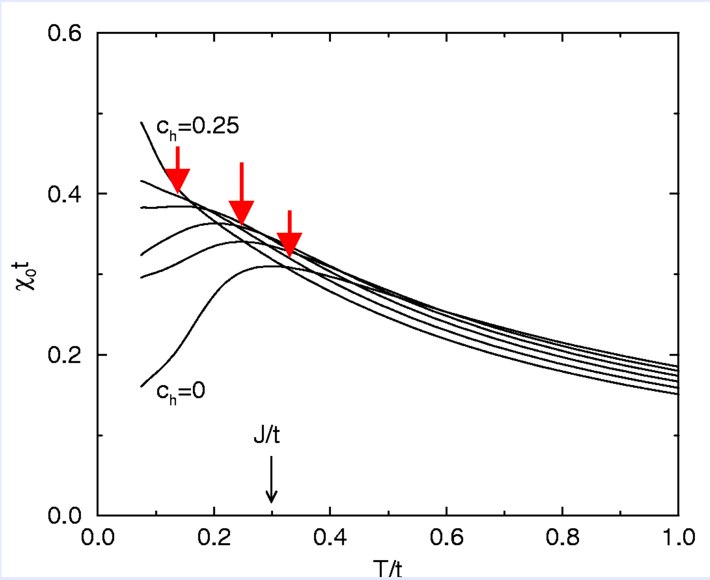
$$\tilde{c}^{\dagger}_{is} = (1 - n_{i,-s}) c^{\dagger}_{is}$$



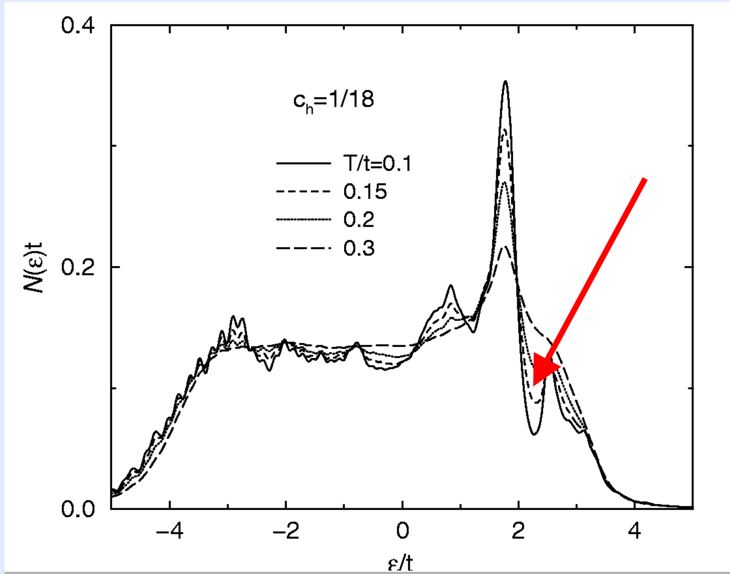
strong correlations: J = 0.3 t

Small system analysis: evidence for pseudogap

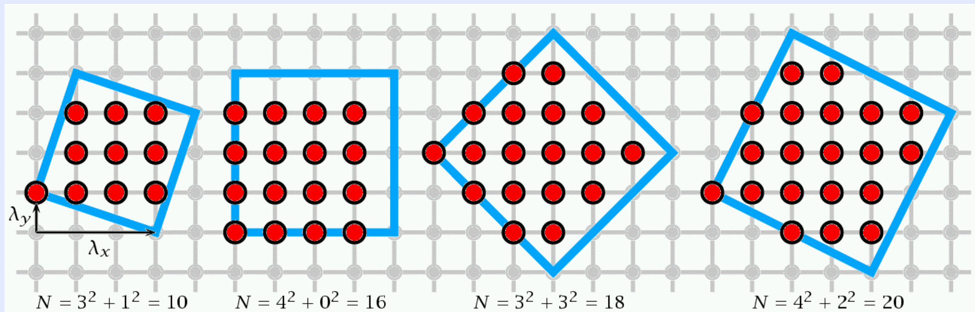
uniform spin susceptibility



density of states



finite-T Lanczos method (FTLM): J.Jaklič + PP



Pseudogap in electron density of states

$$\mathcal{N}(\omega) = 2/N \sum_{\mathbf{k}} A(\mathbf{k}, \omega - \mu)$$

ED

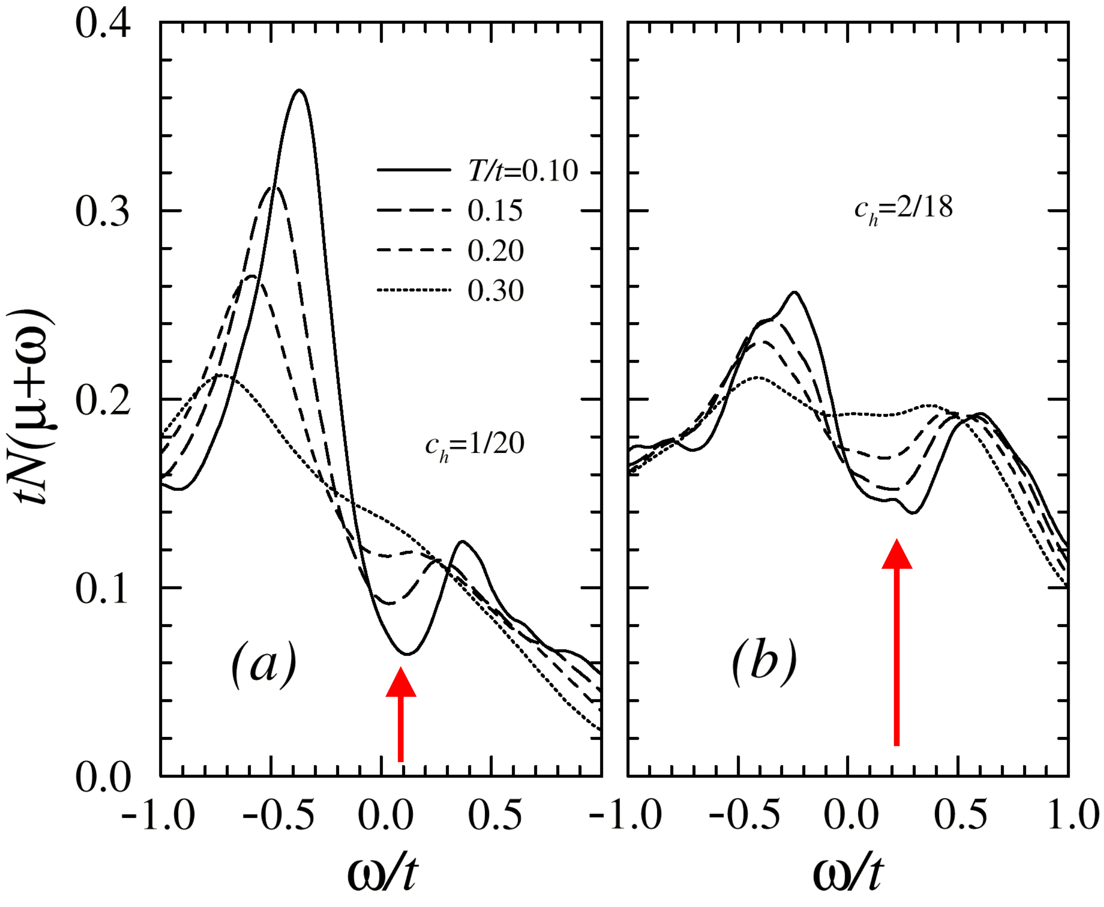


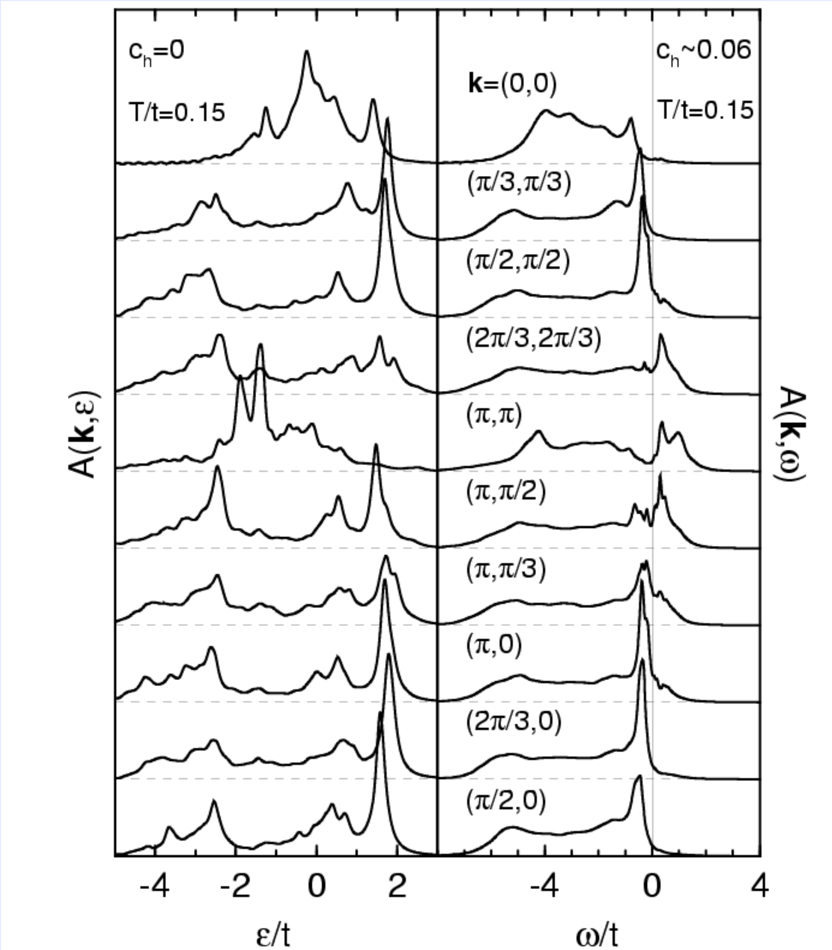
FIG. 1. The DOS $\mathcal{N}(\mu + \omega)$ at various $T \leq J$ for hole concentrations: (a) $c_h = 1/20$ and (b) $c_h = 2/18$.

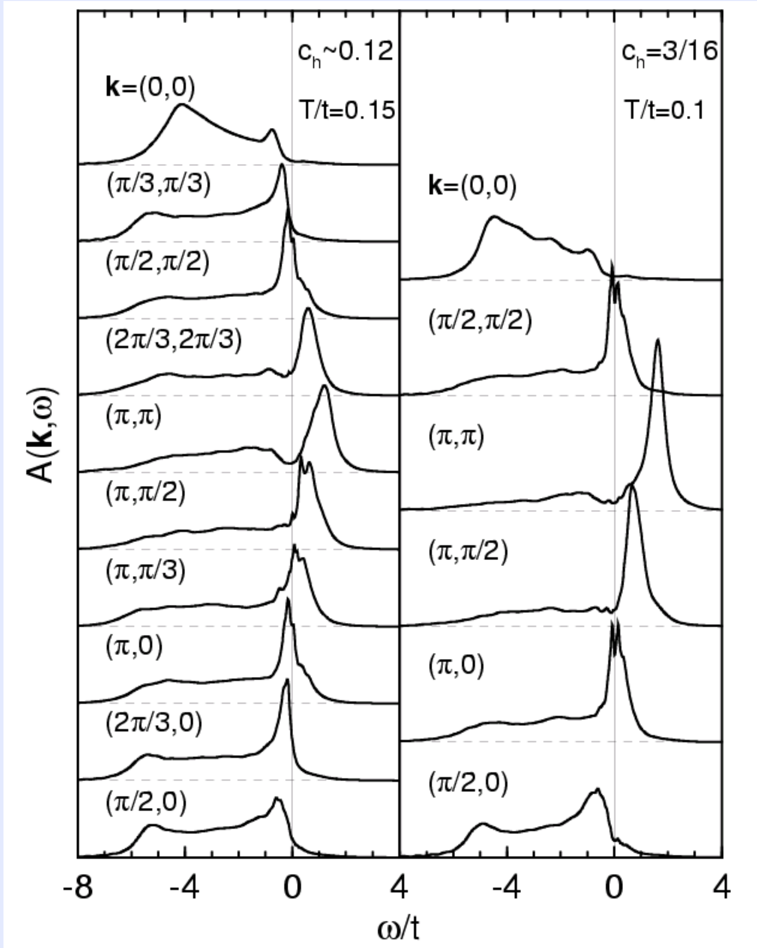
pseudogap closes with doping and T~J

P. Prelovšek, A. Ramšak, and I. Sega, Phys. Rev. Lett. **81**, 3745 (1998).

Spectral functions

undoped AFM - - underdoped - - optimal doping - - overdoped





Spectral function in t-J model: equation-of-motion approach

$$H = -\sum_{i,j,s} t_{ij}\tilde{c}^\dagger_{js}\tilde{c}_{is} + J\sum_{\langle ij\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j - \frac{1}{4}n_i n_j)$$

Green's function: projected operators $\tilde{c}^\dagger_{is} = (1-n_{i,-s})c^\dagger_{is}$

$$G(\mathbf{k},\omega) = \langle\langle \tilde{c}_{\mathbf{k}s};\tilde{c}^\dagger_{\mathbf{k}s}\rangle\rangle_\omega = -i\int_0^\infty \mathrm{e}^{i(\omega+\mu)t}\langle\{\tilde{c}_{\mathbf{k}s}(t),\tilde{c}^\dagger_{\mathbf{k}s}\}_+\rangle dt$$

$$A(\mathrm{k},\omega) = -\frac{1}{\pi}\mathrm{Im}\,G(\mathrm{k},\omega)$$

spectral function

Equations of motions for GF

$$G(\omega) = \langle\langle A; A^\dagger \rangle\rangle_\omega$$

$$\omega \langle\langle A; B \rangle\rangle_\omega = \langle \{A, B\}_+ \rangle + \langle\langle [A, H]; B \rangle\rangle_\omega = \\ = \langle \{A, B\}_+ \rangle - \langle\langle A; [B, H] \rangle\rangle_\omega .$$

$$[\tilde{c}_{is}, H] = -\sum_j t_{ij} [(1 - n_{i,-s}) \tilde{c}_{js} + S_i^{\mp} \tilde{c}_{j,-s}] + \frac{1}{4} J \sum_{j\ n.n.i} (2s S_j^z \tilde{c}_{is} \ldots$$

doping-dependent hopping

$$[\tilde{c}_{\mathbf{k}s}, H] = [(1 - \frac{c_e}{2}) \epsilon^0_{\mathbf{k}} - J c_e] \tilde{c}_{\mathbf{k}s} + \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} m_{\mathbf{kq}} \\ [s S^z_{\mathbf{q}} \tilde{c}_{\mathbf{k-q},s} + S^{\mp}_{\mathbf{q}} \tilde{c}_{\mathbf{k-q},-s} - \frac{1}{2} \tilde{n}_{\mathbf{q}} \tilde{c}_{\mathbf{k-q},s}]$$

effective spin-fermion coupling

$$\tilde{m}_{\mathbf{kq}} = 2J\gamma_{\mathbf{q}} + \frac{1}{2} (\epsilon^0_{\mathbf{k-q}} + \epsilon^0_{\mathbf{k}})$$

symmetrized coupling
involves J, t, t’-
at q=Q only J, t’ !

‘Free’ term, self energy,…

$$G(\mathbf{k},\omega) = \frac{\alpha}{\omega + \mu - \zeta_{\mathbf{k}} - \Sigma(\mathbf{k},\omega)}$$

spectral weight renormalization <1 : no upper Hubbard band

$$\alpha = \frac{1}{N}\sum_i \langle\{\tilde{c}_{is}, \tilde{c}^\dagger_{is}\}_+\rangle = 1 - \frac{c_e}{2} = \frac{1}{2}(1 + c_h).$$

$$\zeta_{\mathbf{k}} = \frac{1}{\alpha}\langle\{[\tilde{c}_{\mathbf{k}s}, H], \tilde{c}^\dagger_{\mathbf{k}s}\}_+\rangle$$
$$= \bar{\zeta} - 4\eta_1 t\gamma_{\mathbf{k}} - 4\eta_2 t'\gamma'_{\mathbf{k}},$$
$$\eta_j = \alpha + \frac{1}{\alpha}\langle \mathbf{S}_0 \cdot \mathbf{S}_j\rangle,$$

renormalized effective ‘free’ band: dependent on spin correlations

$$\Sigma(\omega) \sim \frac{1}{\alpha}\langle\langle C; C^+\rangle\rangle^{irr}_\omega$$

$$-iC_{\mathbf{k}s} = [\tilde{c}_{\mathbf{k}s}, H] - \zeta_{\mathbf{k}}\tilde{c}_{\mathbf{k}s}$$

Coupling to short-range spin fluctuations: paramagnons

$$i\frac{d}{dt}\tilde{c}_{is} \sim -t \sum_{j\ n.n.i} (S_i^{\mp} + S_j^{\mp})\tilde{c}_{j,-s}. \;= t \sum_{j\ n.n.i} h_j^{\dagger}(a_i^{\dagger} + a_j).$$

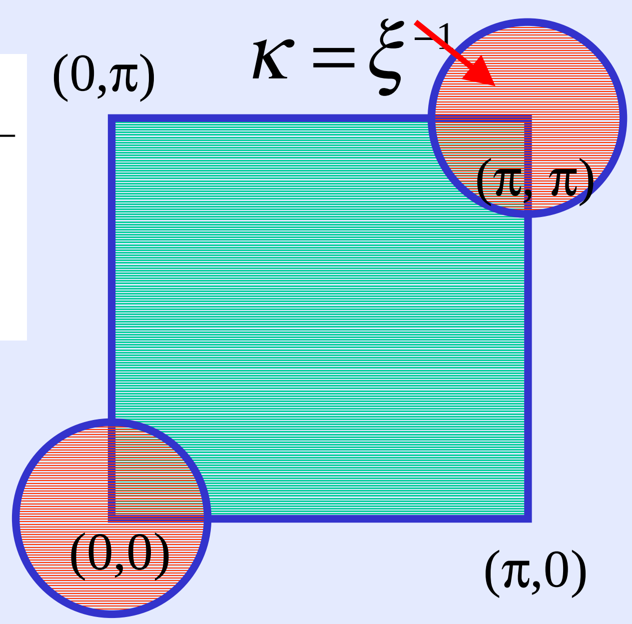
EQM in undoped system reproduce self-consistent Born approx.

extention to finite doping: finite AFM correlation length
+ electron spectral part: coupling to short range fluctuations strong !

$$\Sigma_{\rm pm}(\mathbf{k},\omega) = \frac{1}{N}\sum_{q,\tilde{q}>\kappa} [M^2_{\mathbf{kq}} G^{-}(\mathbf{k}-\mathbf{q},\omega+\omega_{\mathbf{q}}) + M^2_{\mathbf{k+q,q}} G^{+}(\mathbf{k}+\mathbf{q},\omega-\omega_{\mathbf{q}})],$$

$$M_{\mathbf{kq}} = 4t(u_{\mathbf{q}}\gamma_{\mathbf{k-q}} + v_{\mathbf{q}}\gamma_{\mathbf{k}})$$

~SCBA



Coupling to longer-range spin fluctuations

LR (longitudinal) fluctuations restore paramagnetic symmetry

coupling to LR fluctuations moderate: decoupling

$$\langle S^z_{\mathbf{q}}(t)\tilde{c}_{\mathbf{k}-\mathbf{q},s}(t)S^z_{-\mathbf{q}'}\tilde{c}^\dagger_{\mathbf{k}-\mathbf{q}',s}\rangle \sim \delta_{\mathbf{q}\mathbf{q}'}\langle S^z_{\mathbf{q}}(t)S^z_{-\mathbf{q}}\rangle\langle\tilde{c}_{\mathbf{k}-\mathbf{q},s}(t)\tilde{c}^\dagger_{\mathbf{k}-\mathbf{q},s}\rangle$$

$$\Sigma_{\mathrm{lf}}(\mathbf{k},\omega) = \frac{r_s}{\alpha}\sum_{\mathbf{q}}\tilde{m}^2_{\mathbf{kq}}\int\int\frac{d\omega_1 d\omega_2}{\pi}g(\omega_1,\omega_2)\frac{\tilde{A}(\mathbf{k}-\mathbf{q},\omega_1)\chi''(\mathbf{q},\omega_2)}{\omega-\omega_1-\omega_2},$$

← spin susceptibility: input

$$\Sigma = \Sigma_{\mathrm{pm}} + \Sigma_{\mathrm{lf}}$$

overdamped spin fluctuations

$$\chi''(\mathbf{q},\omega) \propto \frac{\omega}{(\tilde{q}^2+\kappa^2)(\omega^2+\omega_\kappa^2)}$$

$\omega_\kappa \lesssim 2J\kappa$

$\kappa = 1/\xi_{AFM}$ inv. AFM correlation length

Pseudogap (approximate) analysis

SR fluctuations modify effective band – higher frequencies

$$A^0_{\rm ef}(\mathbf{k},\omega) = \alpha Z^{\rm ef}_{\mathbf{k}}\delta(\omega+\mu-\epsilon^{\rm ef}_{\mathbf{k}})$$

$$\epsilon^{\rm ef}_{\mathbf{k}} = Z^{\rm ef}_{\mathbf{k}}[\zeta_{\mathbf{k}} + \Sigma_{\rm pm}(\mathbf{k},0) - \mu] \qquad Z^{\rm ef}_{\mathbf{k}} = \left[1 - \frac{\partial \Sigma_{\rm pm}(\mathbf{k},\omega)}{\partial\omega}\Big|_{\omega=0}\right]^{-1}$$

$\nu \to 0$

LR (slow) fluctuation origin of pseudogap

quasistatic –single mode approximation: T=0

$$\frac{1}{\pi}\chi''(\mathbf{q},\omega) \sim \frac{1}{4}\delta(\mathbf{q}-\mathbf{Q})[\delta(\omega-\nu)-\delta(\omega+\nu)]$$

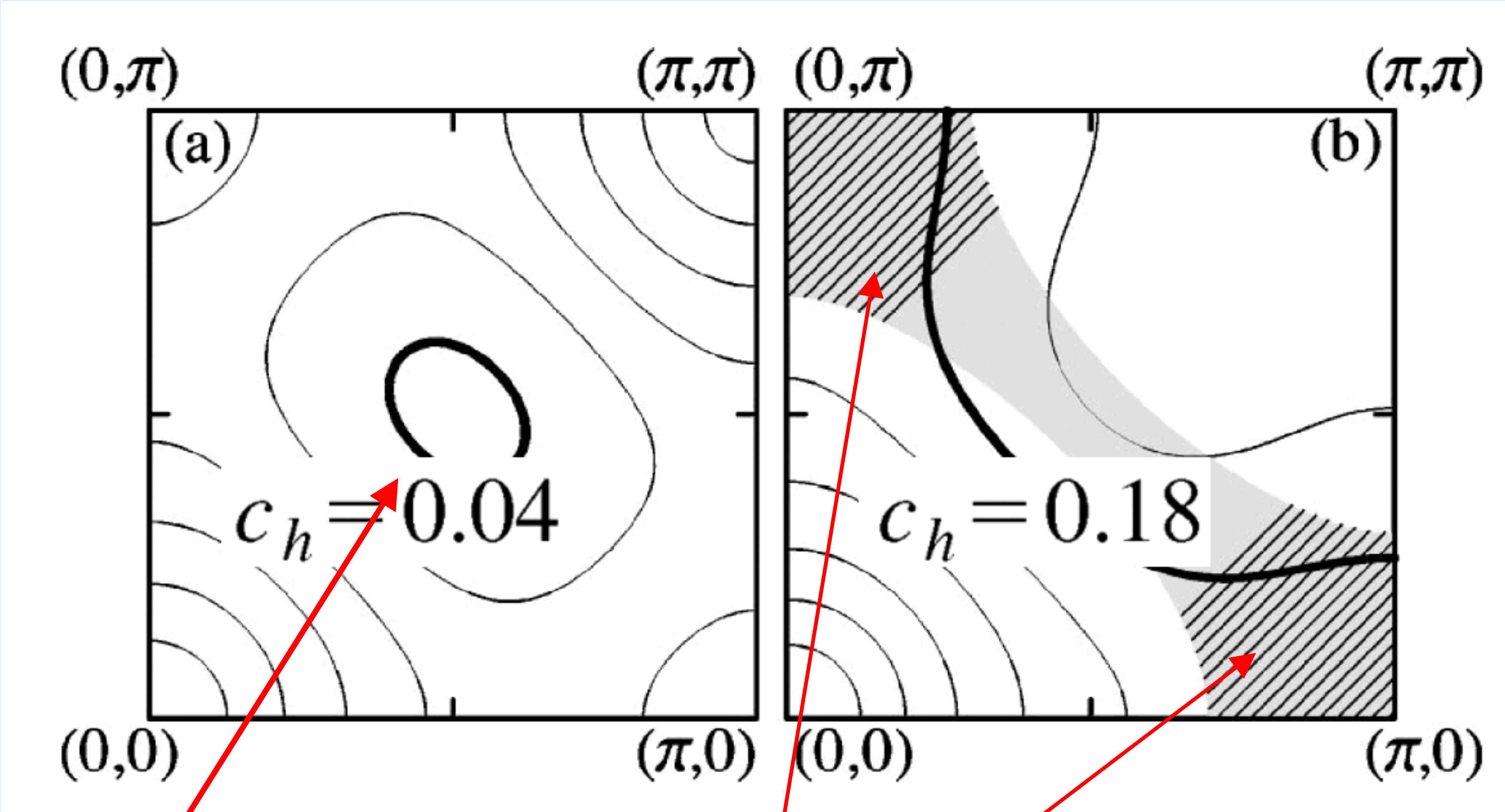
$\nu \to 0$

$$G^{QSA}(\mathbf{k},\omega) = \frac{\alpha Z_{\mathbf{k}}(\omega - \epsilon^{ef}_{\mathbf{k}-\mathbf{Q}})}{(\omega-\epsilon^{\rm ef}_{\mathbf{k}-\mathbf{Q}})(\omega-\epsilon^{\rm ef}_{\mathbf{k}}) - \Delta^2_{\mathbf{k}}}$$

$$\Delta^{PG}_{\mathbf{k}} = |\Delta_{\mathbf{k}_{AFM}}| = \frac{Z^{\rm ef}_{\mathbf{k}}}{2}\sqrt{r_s}|2J - 4t'\cos^2 k_x|$$

gap depends on J, t’ – not on t !

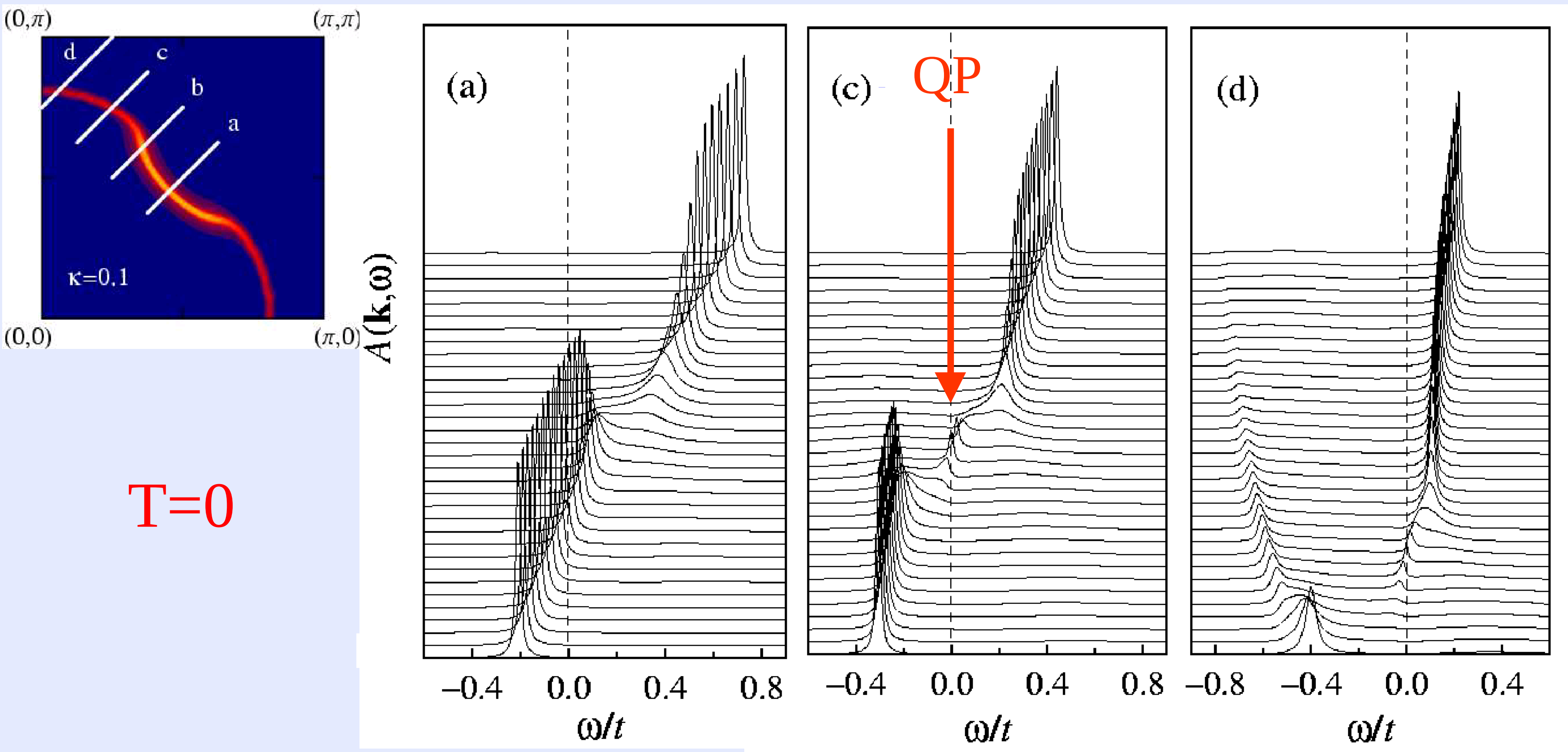
Evolution of Fermi surface



hole pockets

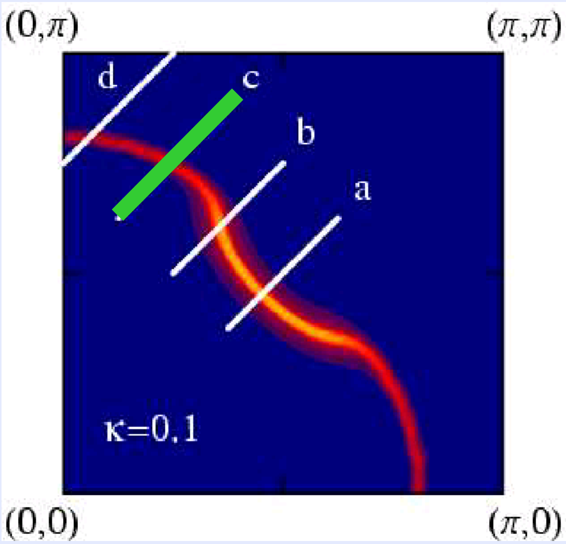
Pseudogap regions – truncated FS

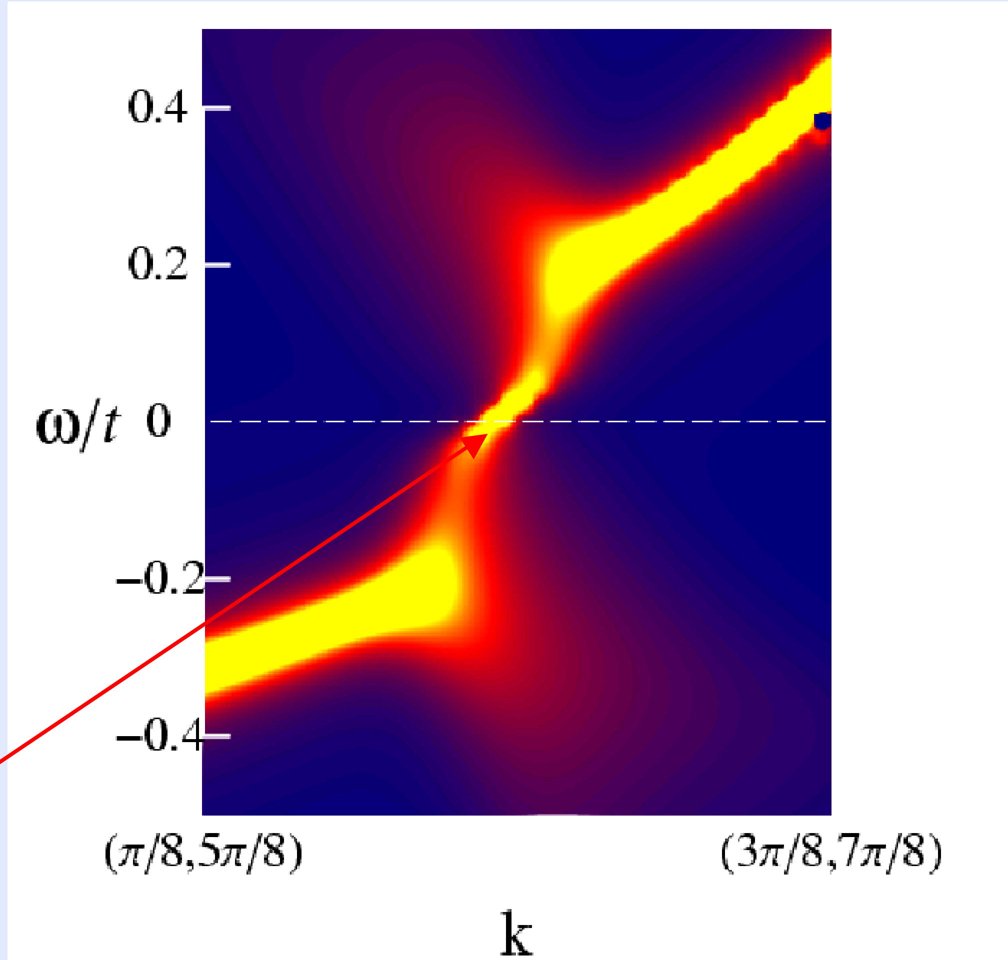
Quasiparticle in pseudogap



T=0

QP exists in pseudogap: with small weight Z and large velocity
Fermi liquid even at strong correlations ?





Large velocity of QP: smaller QP density of states !

QP in pseudogap: simplified analysis

$$\chi''(\mathbf{Q}+\tilde{\mathbf{q}},\omega) = \begin{cases} C[\delta(\omega-\omega_\kappa)-\delta(\omega+\omega_\kappa)], & \tilde{q}_\perp < \kappa, \\ 0, & \tilde{q}_\perp > \kappa, \end{cases}$$

$$\Sigma(\epsilon,\omega) = -\frac{\Delta^2}{2w}\log\frac{(w+\omega_\kappa+\bar{\epsilon}-\omega)(\omega_\kappa+\omega)}{(w+\omega_\kappa-\bar{\epsilon}+\omega)(\omega_\kappa-\omega)}$$

$\epsilon_{\mathbf{k}}^{\text{ef}} - \mu$

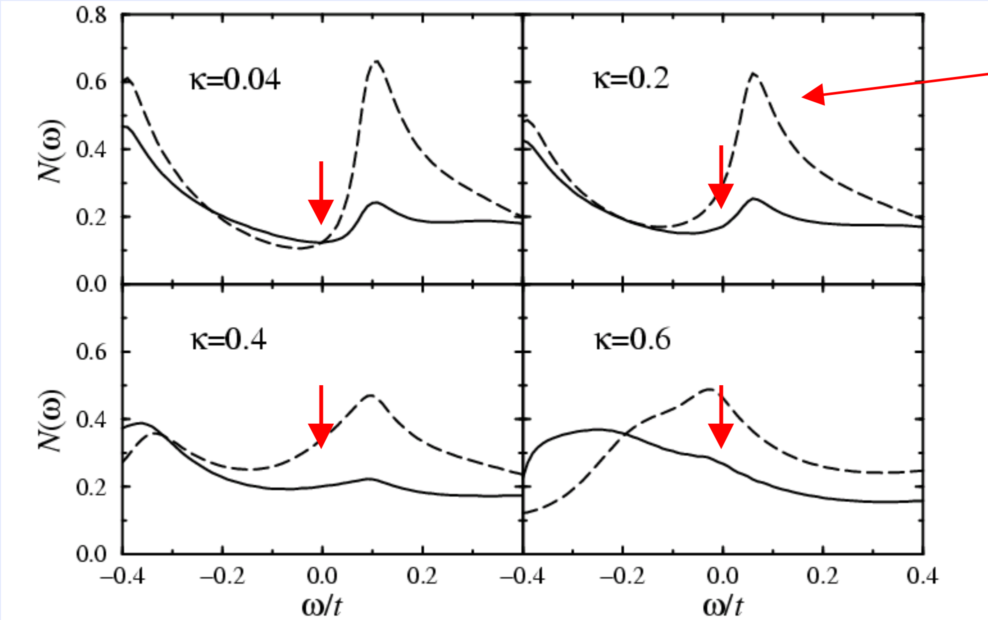
$$\frac{Z_F}{Z^{\text{ef}}} = \left[1-\frac{\partial\Sigma'}{\partial\omega}\Big|_{\omega=0,\bar{\epsilon}=0}\right]^{-1} = \left[1+\frac{\Delta^2}{\omega_\kappa(\omega_\kappa+w)}\right]^{-1}$$

$$w = v_{\mathbf{k}}^{\text{ef}}\kappa$$

$$\frac{v_F}{v_{\mathbf{k}}^{\text{ef}}} = \left(1+\frac{\partial\Sigma'}{\partial\epsilon}\right)\frac{Z_F}{Z^{\text{ef}}} \sim \frac{\omega_\kappa}{w} \sim \frac{2J}{v_{\mathbf{k}}}$$

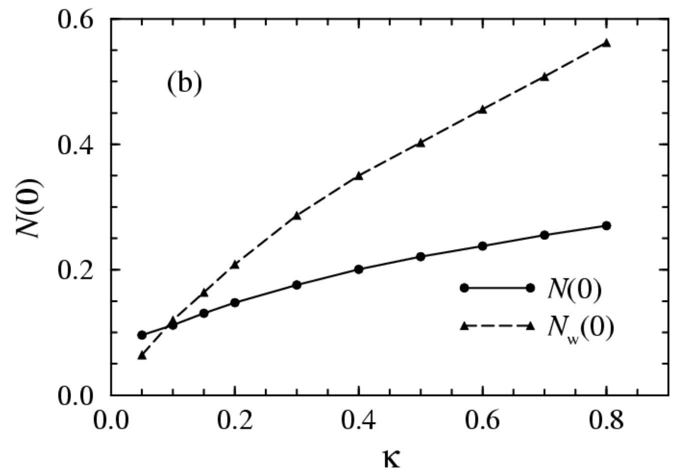
QP weight Z reduced, but QP velocity can even increase !

Single particle and QP density of states

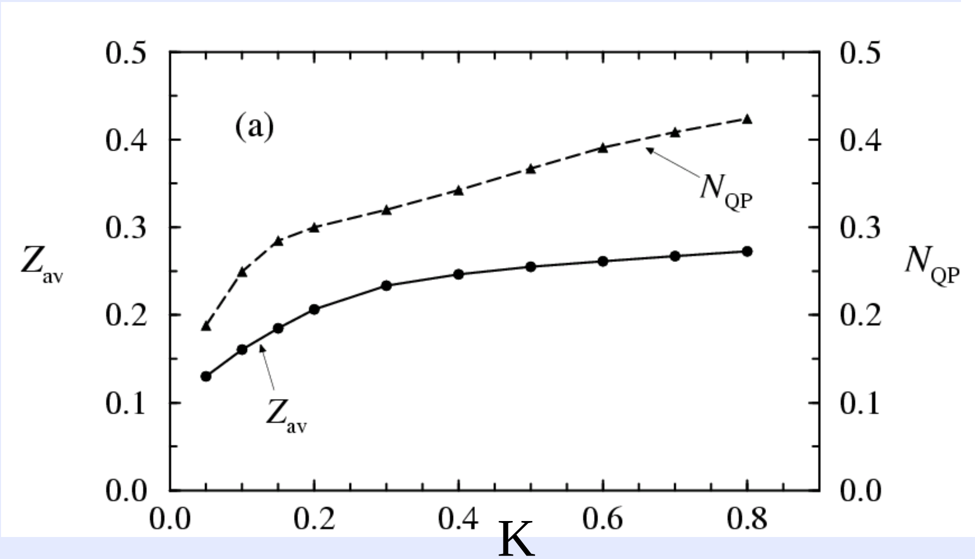


weighted DOS

$$w(\mathbf{k}) = (\cos k_x - \cos k_y)^2$$

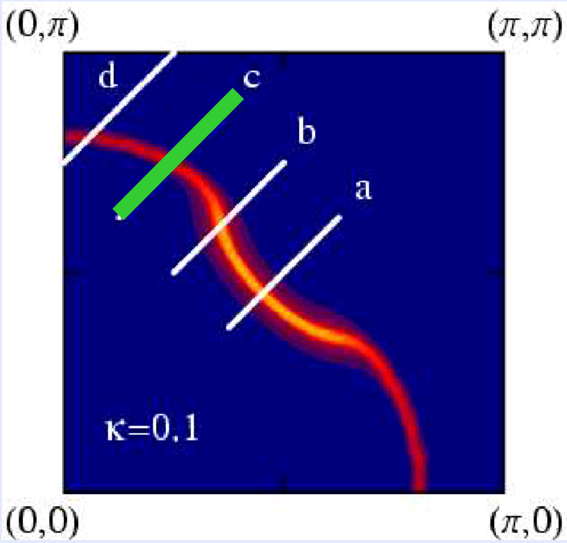


$$N_{QP} = \frac{\alpha Z^{et}}{2\pi^2} \oint \frac{dS_F}{v(\mathbf{k})}$$

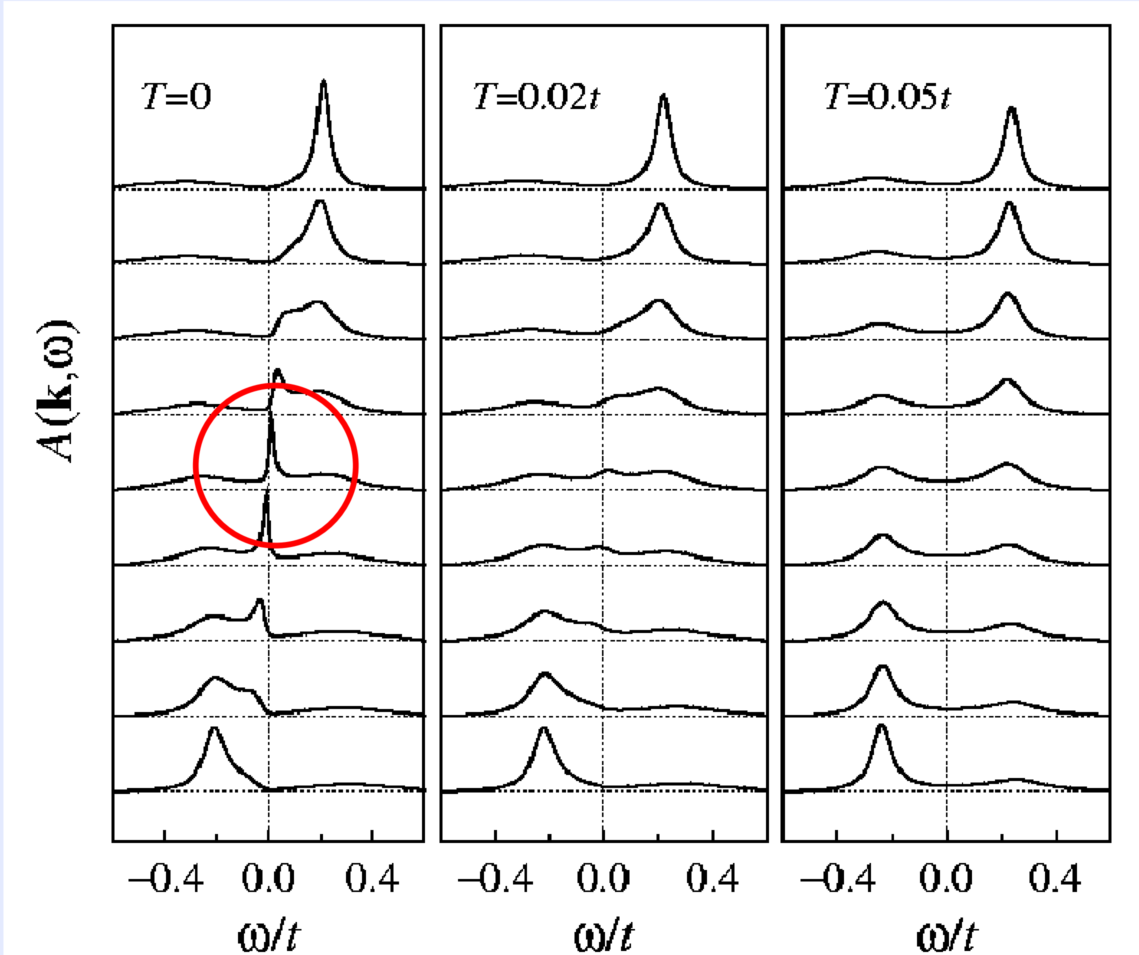


QP DOS and average Z decrease with decreasing doping

Temperature dependence



even very small T
smears out the QP
peak in pseudogap

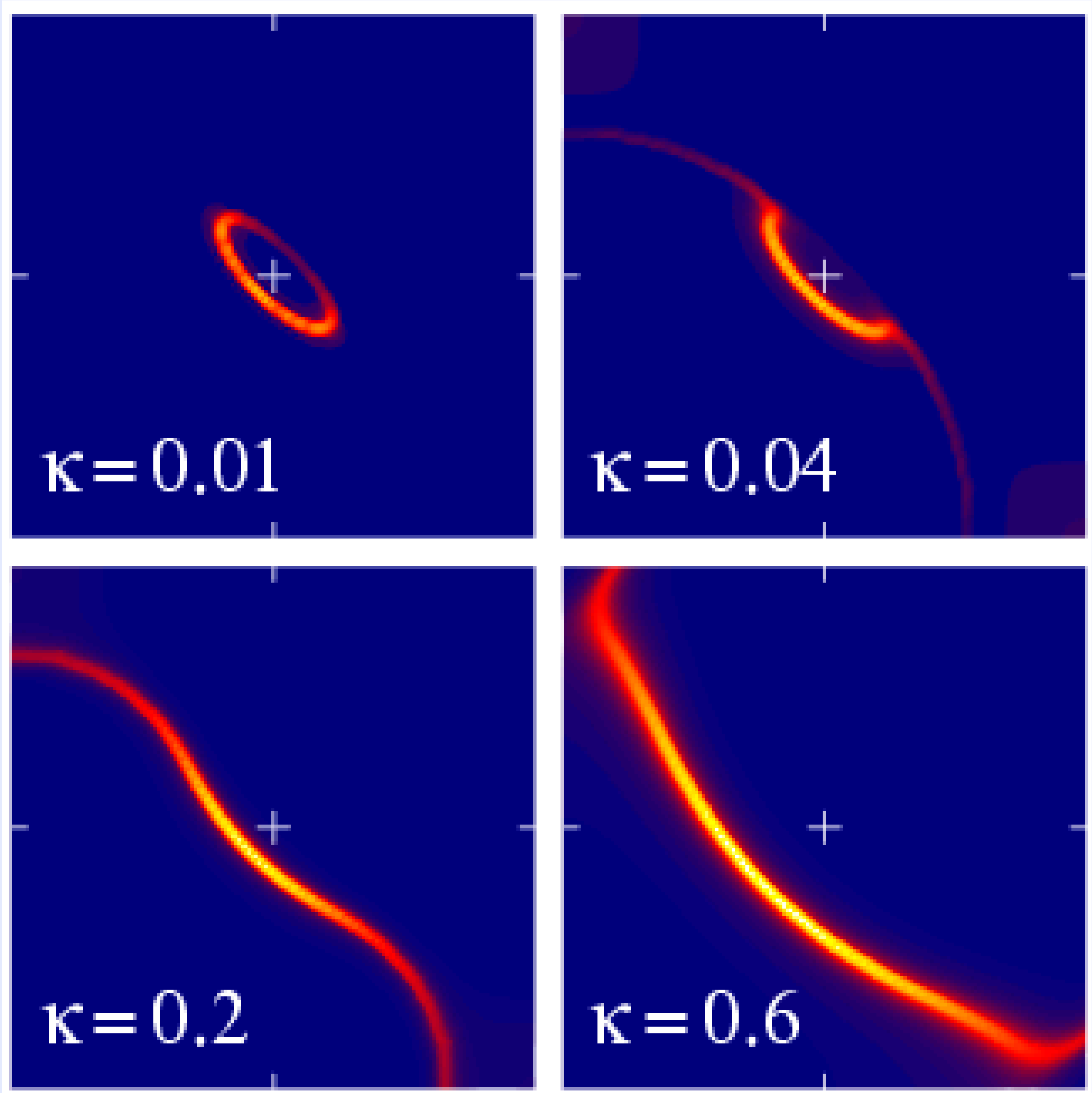


Fermi surface evolution

$$A(\mathrm{k}, \omega = 0)$$

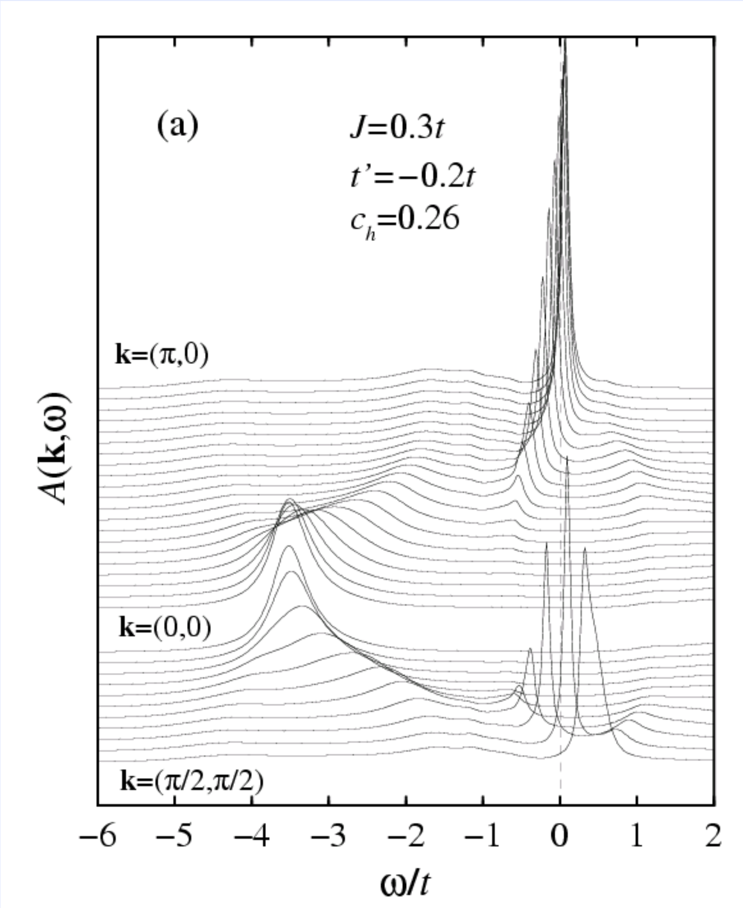
$$\xi^{-1} = \kappa = \sqrt{c_h}$$

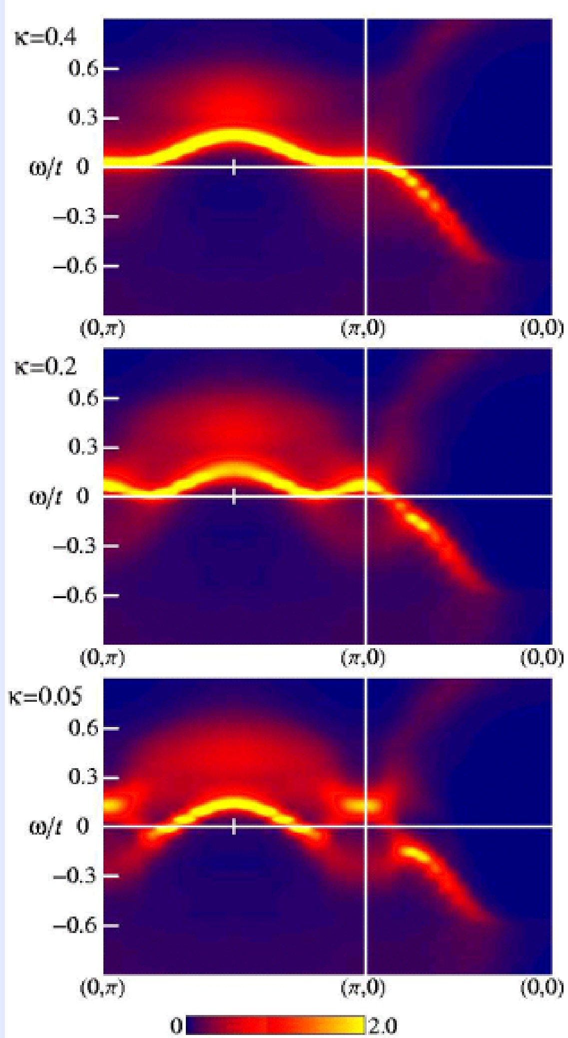
AFM correlation length

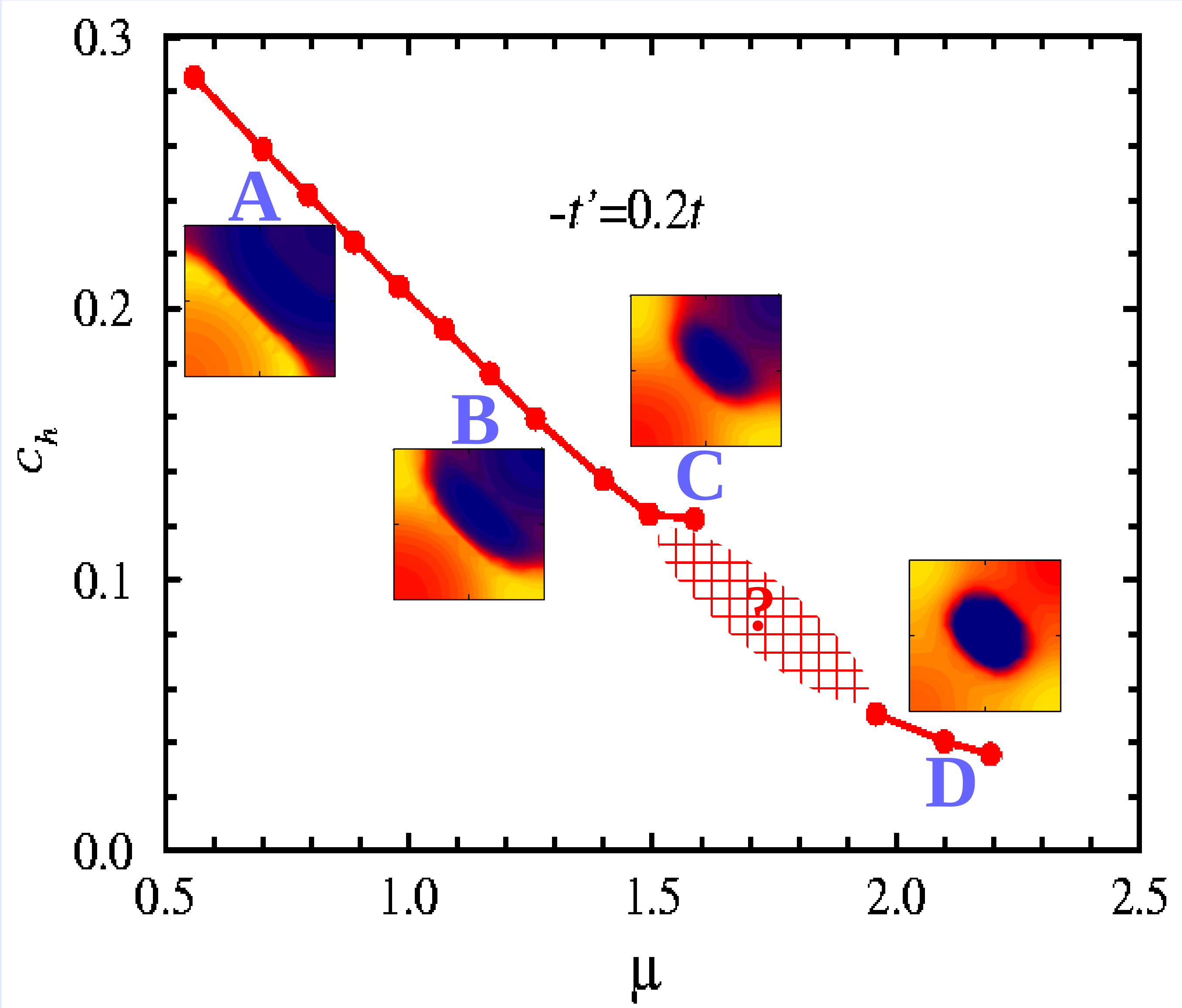


Full (selfconsistent) calculation

$$c_h = 1 - \int_{-\infty}^{\infty} f(\omega)\mathcal{N}(\omega)\,d\omega \;\Rightarrow \mu$$







$$n_{\mathbf{k}} = \langle \Psi_{\mathbf{k}_0} | \sum_\sigma c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} | \Psi_{\mathbf{k}_0} \rangle$$

FS: largest gradient n(k)

Self-consistent calculation

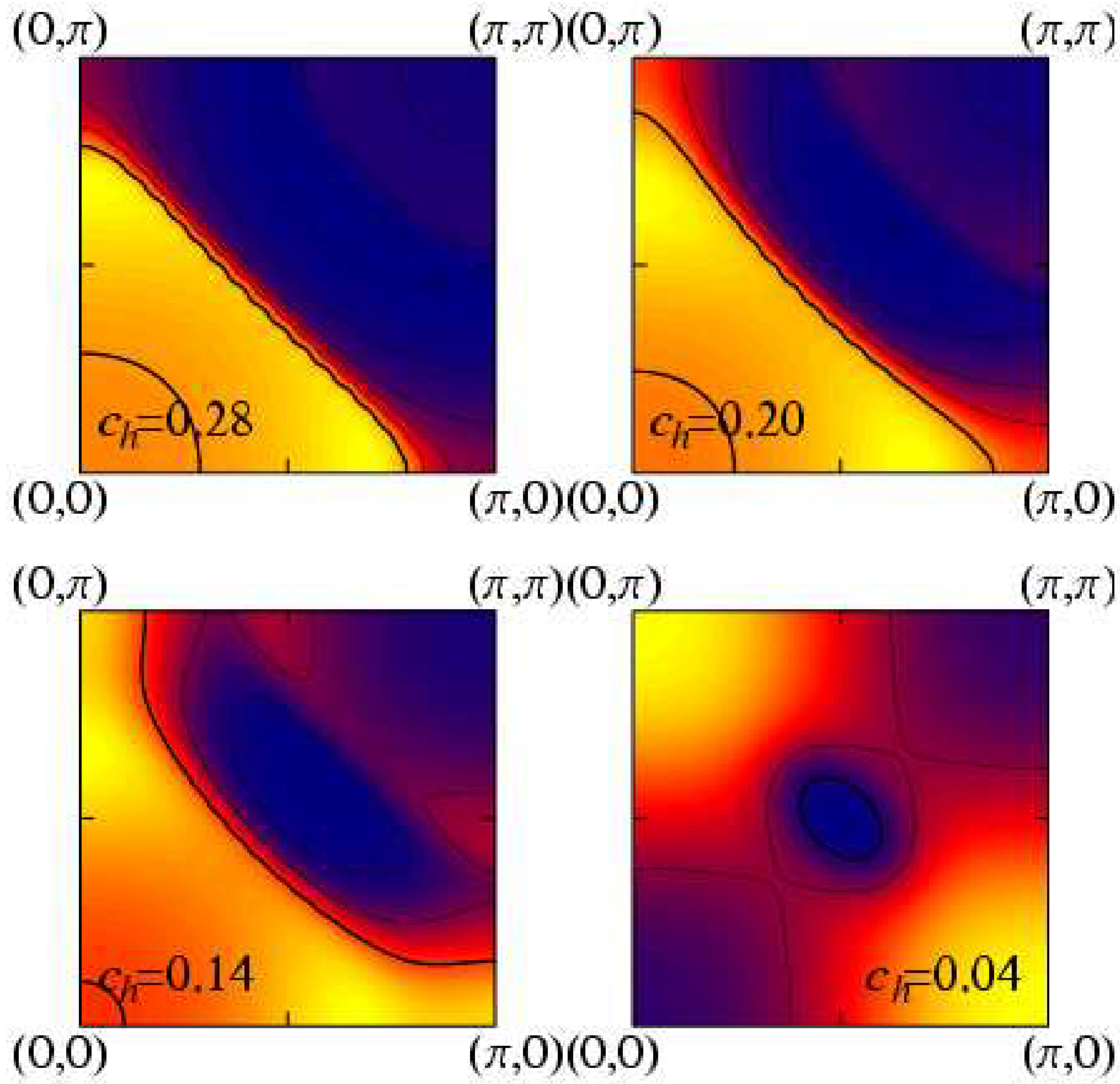


FIG. 9. (color) Electron momentum distribution $\tilde{n}(\mathbf{k})$ for various c_h. Thin contour lines represent $\tilde{n}(\mathbf{k})$ in increments 0.1 while heavy line is corresponding to $\tilde{n}(\mathbf{k}) = 0.8$ for $c_h = 0.26, 0.20, 0.14$ and $\tilde{n}(\mathbf{k}) = 0.85$ for $c_h = 0.04$.

Spin fluctuations - doped AFM - EQM approach

goal: overdamped spin fluctuations in normal state + resonance (collective) mode in SC state

Spin susceptibility: memory function representation

$$\chi_{\mathbf{q}}(\omega) = \frac{-\eta_{\mathbf{q}}}{\omega^2 + \omega \tilde{M}_{\mathbf{q}}(\omega) - \omega_{\mathbf{q}}^2}$$

$$\omega_{\mathbf{q}}^2 = \frac{\eta_{\mathbf{q}}}{\chi_{\mathbf{q}}^0}$$ coll.mode

$$\eta_{\mathbf{q}} = (\mathcal{L}S_{\mathbf{q}}^z|\mathcal{L}S_{\mathbf{q}}^z) = \langle[S_{\mathbf{q}}^{z\dagger}, \mathcal{L}S_{\mathbf{q}}^z)]\rangle$$

$$M_{\mathbf{q}}(\omega) = (\tilde{Q}\mathcal{L}^2 S_{\mathbf{q}}^z|\frac{1}{\mathcal{L}_{\tilde{Q}} - \omega}|\tilde{Q}\mathcal{L}^2 S_{\mathbf{q}}^z))$$ mode damping

$$\mathcal{L}_t^2 \mathbf{S}_j = -\sum_k t_{j,k}^2 (\mathbf{S}_j - \mathbf{S}_k)\mathcal{P}_{jk} + 2\sum_{k,l\neq j} t_{jk} t_{kl} \mathbf{S}_j (1 - n_k + \mathcal{P}_{jk}) S_{jl}^0 - 2\sum_{k\neq l} t_{jk} t_{jl} (1 - n_j + \mathcal{P}_{jl}) S_{lk}^0 \mathbf{S}_k + \mathrm{H.}c.$$

$$\mathcal{P}_{ij} = \frac{1}{2} n_i n_j + 2\mathbf{S}_i \cdot \mathbf{S}_j \qquad S_{ij}^0 = \frac{1}{2}\sum_s \tilde{c}_{is}^\dagger \tilde{c}_{js}$$

$$\mathcal{P}_{jk} \to \langle \mathcal{P}_{jk} \rangle \approx (1 - c_h)^2 (\frac{1}{2} + 2\langle \mathbf{S}_j \cdot \mathbf{S}_k \rangle)$$

$$\tilde{Q}\mathcal{L}_t^2 S_{\mathbf{q}}^z \sim \frac{1}{2\sqrt{N}} \sum_{\mathbf{k}s} w_{\mathbf{kq}} s \tilde{c}_{\mathbf{k}s}^\dagger \tilde{c}_{\mathbf{k+q},s}$$

decay of collective spin mode into fermions – effective coupling

Effective damping of collective mode

$$M''_{\mathbf{q}}(\omega) = \frac{1}{2\omega} \int d\omega_1 [f(\omega - \omega_1) - f(\omega_1)] R_{\mathbf{q}}(\omega, \omega_1)$$

$$R_{\mathbf{q}}(\omega, \omega_1) = \frac{\pi}{N} \sum_{\mathbf{k}} w_{\mathbf{kq}}^2 A_{\mathbf{k}}(\omega_1) A_{\mathbf{k+q}}(\omega - \omega_1)$$ coherent

$$\tilde{R}_{\mathbf{q}}(\omega, \omega_1) \approx 22\pi t^4 \mathcal{P}_1^2 \mathcal{N}(\omega_1) \mathcal{N}(\omega - \omega_1)$$ incoherent

$$M''_{\mathbf{q}}(\omega) \propto \sigma_c(\omega)$$

$$\gamma_{\mathbf{Q}} \sim x \bar{Z}^2 \mathcal{P}_1^2 t^4 / \tilde{W}^2 \eta$$

coupling strongly reduced due to AFM fluctuations and low doping (Z)

Conclusions

- pseudogap scales in cuprates
- evidence for pseudogap in the planar t-J model
- spectral functions: equation-of-motion approach
- effective spin – fermion coupling
- in underdoped regime pseudogap and truncated Fermi surface: coexistence of Fermi liquid and pseudogap ?
- onset of pseudogap

$$\kappa(c_h, T) < \kappa^* \sim 0.5 \quad \Rightarrow \quad T^* \sim T_0^*(1 - c_h/c_h^*)$$

- spin dynamics: EQM approach, memory functions
- collective mode: frequency and damping