Theory of electronic spectrum in cuprate superconductors

N.M. Plakida

Joint Institute for Nuclear Research, Dubna, Russia

in collaboration with

V.S. Oudovenko

Rutgers University, New Jersey, USA

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- Motivation:

Is it possible to explain ARPES results *('arc' Fermi surface and pseudogap)* and high-T_c superconductivity within a microscopic theory for an effective Hubbard model for the CuO_2 plane?

- Conclusion:

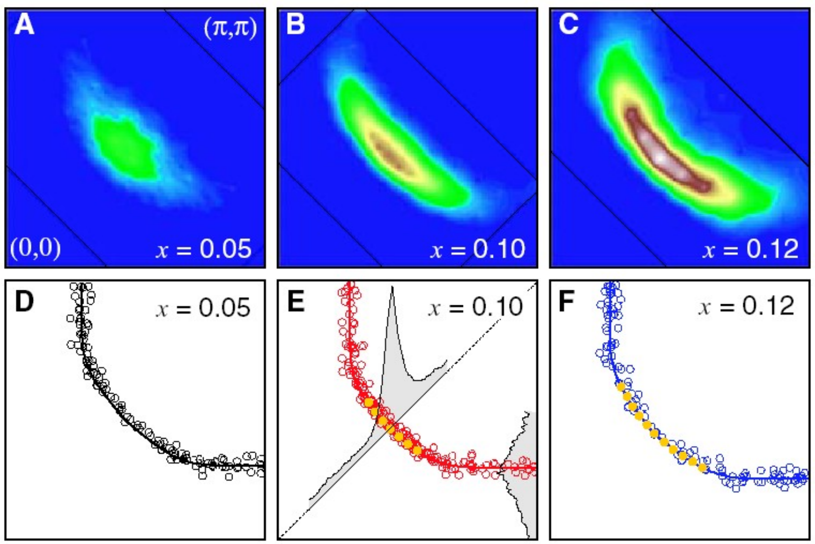
self-consistent solution of the Dyson equation for a single particle Green function in the limit of strong electron correlations for the Hubbard model provides such a possibility

Outline

- ARPES and theory of SCES
- Effective p-d Hubbard model for the CuO_2 plane
- Projection technique for Green functions:
  - Dyson equation
  - Self-energy in NCA
- Dispersion and spectral functions
- Fermi surface and arcs
- Self – energy: coupling constants and kinks
- Conclusion

ARPES

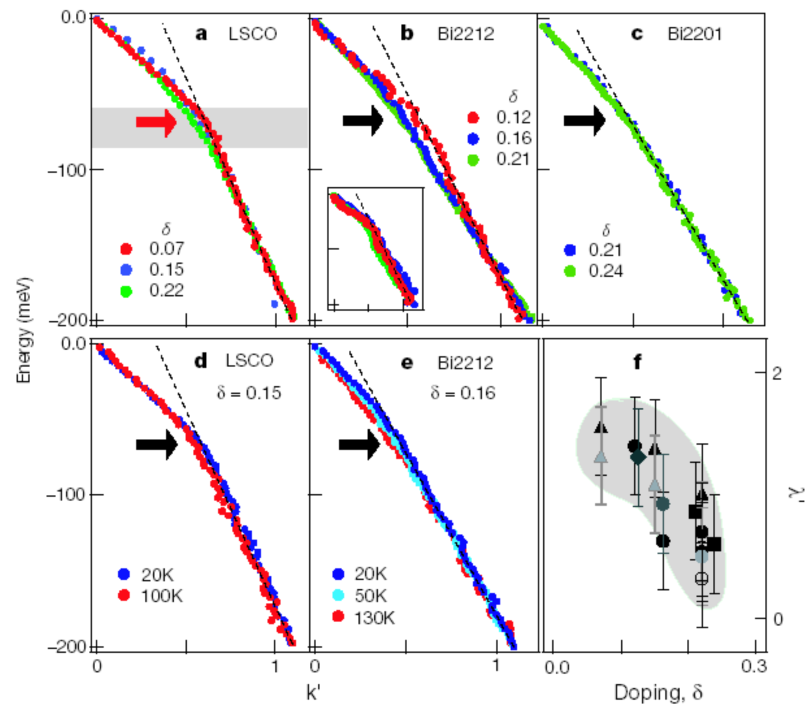
“Destruction” of FS – “arc” FS



cupric oxychloride $Ca_{2-x}Na_xCuO_2Cl_2$

*K. M. Shen, Science **307** 901 (2005).*

“Kink” phenomenon



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

Theory of SCES

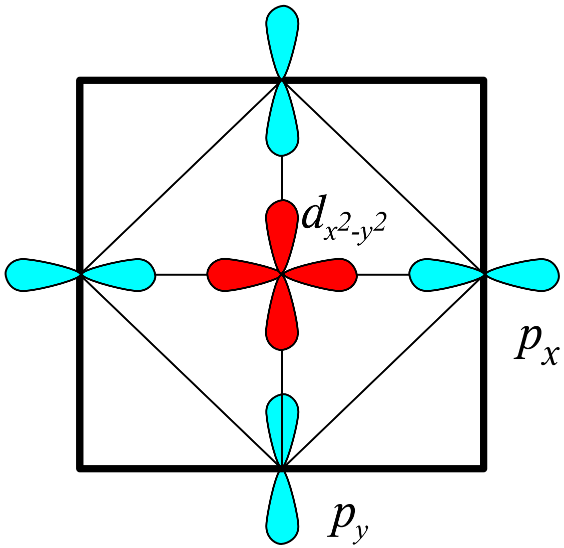
- DMFT – **q**-independent self-energy, d >> 1, *(kinks – Kollar, et al.)*,
- Momentum decomposition for GF *(K. Matho et al.)*
- Quantum cluster theories – *(review by Maier et al. RMP 2005)*

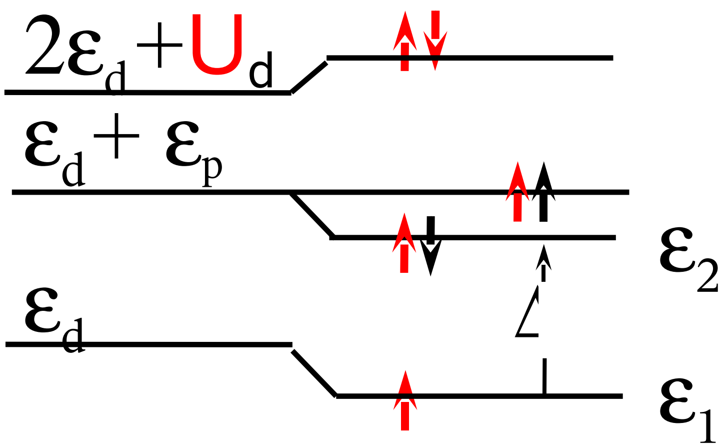
-- Quantum MC, ED *(Scalapino, Dagotto, Maekawa, Tohyama, Prelovsek)*
-- DCA – dynamical cluster approximation *(Hettler, Jarrel, et al.)*
-- CDMFT – Cellular DMFT *(Kotliar, Civelli, et al.)*
-- VCA – variational cluster approximation *(Potthoff et al.)*
-- Two-Particle Self-Consistent approach (TPSC) *(Tremblay et al.)*

- Perturbative technique

-- Phenomenological approaches (spin-fermion models)
. *(Pines, Norman, Chubukov, Eschrig, Sadovskii, et al.)*
-- FLEX (weak correlations, U < W) *(Bickers et al., Manske, Eremin)*
-- Strong correlations: Hubbard operator technique:
-- Diagram approach (involved) *(Zaitsev, Izyumov, et al.)*
-- Equation of motion method for HOs (Mori-type projection technique)
. *(Plakida, Mancini, Avella, Kakehashi – Fulde, et al.)*

Effective Hubbard p-d model for CuO_2 plane





Model for CuO_2 plane:

Cu-3d (ε_d) and O-2p (ε_p) hole states,

with $U_d > \Delta = \varepsilon_p - \varepsilon_d \approx 2\, t_{pd} \approx 3$ eV

In the strong correlation limit: $U_{eff} = \Delta > W$ it is convenient to start from the atomic basis within a two-subband Hubbard model in terms of the projected, Hubbard operators:

$$c_{i\sigma} = c_{i\sigma}\,(1 - n_{i\,-\sigma}) + c_{i\sigma}\,(n_{i\,-\sigma}) = \mathbf{X_i^{0\sigma}} + \mathbf{X_i^{-\sigma 2}}, \quad n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$$

Two subbands:

LHB – one-hole d - like state $|\sigma>$: $\varepsilon_1 = \varepsilon_d - \mu$

UHB – two-hole (p - d) ZR singlet state: $|\uparrow\downarrow>$: $\varepsilon_2 = 2\,\varepsilon_1 + \Delta$

For these 4 states we introduce the Hubbard operators:

$$X_i^{\alpha\beta} = |\, i\alpha > < i\beta\,|$$

where $|\,\alpha> = |\,0>,\ |\,\sigma> = |\uparrow>,\ |\downarrow>$, and $|\,2> = |\uparrow\downarrow>$

Hubbard operators rigorously obey the constraint:

$$X_i^{00} + X_i^{\uparrow\uparrow} + X_i^{\downarrow\downarrow} + X_i^{22} = 1$$

- only one quantum state can be occupied at any site $|\, i>$

Commutation relations for the Hubbard operators:

anticommutator for the Fermi-like operators

$$\{ X_i^{0\sigma} , X_j^{\sigma' 0} \} = \delta_{ij} \, (\delta_{\sigma' \sigma} X_i^{00} + X_i^{\sigma' \sigma}),$$

commutator for the Bose-like operators

$$[X_i^{\sigma\sigma'}, X_j^{\sigma''\sigma}] = \delta_{ij} (\delta_{\sigma' \sigma''} X_i^{\sigma\sigma} - X_i^{\sigma'' \sigma'})$$

These commutation relations result in the kinematic interaction.

Spin operators in terms of HOs:

$$S_i^z = (1/2) (X_i^{++} - X_i^{--}), \; S_i^+ = X_i^{+-}, \; S_i^- = X_i^{-+},$$

Number operator

$$N_i = (X_i^{++} + X_i^{--}) + 2 X_i^{22}$$

The two-subband effective Hubbard model for holes

$$\mathrm{H} = \varepsilon_1 \sum_{i,\sigma} X_i^{\sigma\sigma} + \varepsilon_2 \sum_{i} X_i^{22} + \sum_{i\neq j,\sigma} \{ t_{ij}^{11} X_i^{\sigma 0} X_j^{0\sigma} + t_{ij}^{22} X_i^{2\sigma} X_j^{\sigma 2} + 2\sigma t_{ij}^{12} (X_i^{2\bar{\sigma}} X_j^{0\sigma} + \mathrm{H.c.}) \},$$

One-hole and two-hole single-site energies

$$\varepsilon_1 = \varepsilon_d - \mu, \quad \varepsilon_2 = 2\varepsilon_1 + U_{\mathrm{eff}}, \quad U_{\mathrm{eff}} = \Delta = \epsilon_p - \epsilon_d$$

Hopping parameters for n.n. t and n.n.n sites t', t'':

$$t(\mathbf{k}) = 4t\,\gamma(\mathbf{k}) + 4t'\,\gamma'(\mathbf{k}) + 4t''\,\gamma''(\mathbf{k})$$

Average number of holes is defined by the chemical potential μ:

$$n = \langle N_i \rangle = \langle \sum_{\sigma} X_i^{\sigma\sigma} + 2X_i^{22} \rangle = 1 + \delta \leq 2$$

Single-particle two-subband thermodynamic (retarded) Green functions

$$\hat{G}_{ij\sigma}(t-t') = \langle\langle \hat{X}_{i\sigma}(t) \mid \hat{X}^{\dagger}_{j\sigma}(t')\rangle\rangle = \langle\langle \begin{pmatrix} X_i^{\sigma 2} \\ X_i^{0\bar{\sigma}} \end{pmatrix} \mid (X_i^{2\sigma}\; X_i^{\bar{\sigma}0})\rangle\rangle$$

$$= -i\theta(t-t')\langle\{\hat{X}_{i\sigma}(t), \hat{X}^{\dagger}_{j\sigma}(t')\}\rangle$$

Mori-type projection technique for equations of motion:

$$i\, d X_{i\sigma}/dt = \hat{Z}_{i\sigma} = [\hat{X}_{i\sigma}, H] = \sum_j \hat{\varepsilon}_{ij\sigma}\hat{X}_{j\sigma} + \hat{Z}^{(ir)}_{i\sigma},$$

orthogonality condition:

$$\langle\{\hat{Z}^{(ir)}_{i\sigma}, \hat{X}^{\dagger}_{j\sigma}\}\rangle = \langle \hat{Z}^{(ir)}_{i\sigma}\, \hat{X}^{\dagger}_{j\sigma} + \hat{X}^{\dagger}_{j\sigma}\, \hat{Z}^{(ir)}_{i\sigma}\rangle = 0$$

Frequency matrix – QP spectra in MFA:

$$\hat{\varepsilon}_{ij} = \langle\{[\hat{X}_{i\sigma}, H], \hat{X}^{\dagger}_{j\sigma}\}\rangle\, \hat{Q}^{-1}$$

$$\hat{Q} = \langle\{\hat{X}_{i\sigma}, \hat{X}^{\dagger}_{i\sigma}\}\rangle = \begin{pmatrix} Q_2 & 0 \\ 0 & Q_1 \end{pmatrix}$$

where spectral weights for Hubbard subbands:

$$Q_2 = n/2$$

$$Q_1 = 1 - n/2$$

Eqution for GF: $\hat{G}_\sigma(\mathbf{k},\omega) = \hat{G}^0_\sigma(\mathbf{k},\omega) + \hat{G}^0_\sigma(\mathbf{k},\omega)\,\hat{Q}^{-1}\langle\langle \hat{Z}^{irr}_{\mathbf{k}\sigma} \mid \hat{X}^\dagger_{\mathbf{k}\sigma}\rangle\rangle_\omega$

where GF in MFA: $\hat{G}^0_\sigma(\mathbf{k},\omega) = \left(\omega\hat{\tau}_0 - \hat{\varepsilon}(\mathbf{k})\right)^{-1}\hat{Q},$

Differentiation of the many-particle GF $\langle\langle \hat{Z}^{irr}_{i\sigma}(t) \mid \hat{X}^\dagger_{j\sigma}(t')\rangle\rangle$ over t' and carrying-out the projection results in the Dyson equation:

$$G_\sigma(\mathbf{k},\omega) = \left\{\omega\hat{\tau}_0 - \hat{\varepsilon}(\mathbf{k}) - \hat{\Sigma}_\sigma(\mathbf{k},\omega)\right\}^{-1}\hat{Q}$$

where the self-energy (SE) is the many-particle GF $\hat{\Sigma}_\sigma(\mathbf{k},\omega) = \langle\langle \hat{Z}^{(ir)}_\sigma \mid \hat{Z}^{(ir)\dagger}_\sigma\rangle\rangle^{(prop)}_{\mathbf{k},\omega}\,\hat{Q}^{-1}$

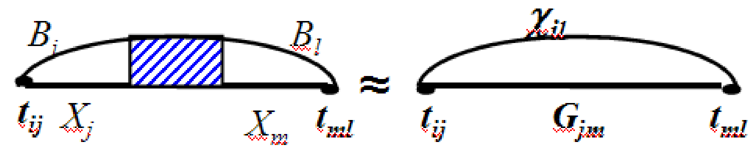
Kinematic interaction: $(id/dt)\,X_i^{\sigma 2} = [X_i^{\sigma 2}, H] = (\varepsilon_1 + \Delta)X_i^{\sigma 2}$

$$+ \sum_{l\neq i,\sigma'}\left(t^{22}_{il}B^{22}_{i\sigma\sigma'}X_l^{\sigma' 2} - 2\sigma t^{21}_{il}B^{21}_{i\sigma\sigma'}X_l^{0\bar{\sigma}'}\right) - \sum_{l\neq i} X_i^{02}\left(t^{11}_{il}X_l^{\sigma 0} + 2\sigma t^{21}_{il}X_l^{2\bar{\sigma}}\right)$$

$B^{22}_{i\sigma\sigma'} = (N_i/2 + S_i^z)\delta_{\sigma'\sigma} + S_i^\sigma\delta_{\sigma'\bar{\sigma}}$ $\quad B^{21}_{i\sigma\sigma'} = (N_i/2 + S_i^z)\delta_{\sigma'\sigma} - S_i^\sigma\delta_{\sigma'\bar{\sigma}}$

Self-consistent system of equations for GF and SE

Non-crossing approximation (NCA) for SE is given by the decoupling



for Fermi and Bose-like operators in the two-time correlation functions:

$$\langle B_{1'}(t)X_1(t) \mid B_{2'}X_2\rangle \simeq \langle X_1(t)X_2\rangle \; \langle B_{1'}(t)B_{2'}\rangle_{(1' \neq 1)}$$

SE in NCA for two Hubbard subbands reads:

$$\tilde{\Sigma}(\mathbf{k},\omega) = \frac{1}{N}\sum_{\mathbf{q}} |t(\mathbf{q})|^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{d\nu\, dz}{\omega - z - \nu}\, \frac{1}{2}\left(\tanh\frac{z}{2T} + \coth\frac{\nu}{2T}\right)$$
$$\times (1/\pi)\mathrm{Im}\chi_{sc}(\mathbf{k}-\mathbf{q},\nu)\; (1/\pi)\mathrm{Im}\left\{\tilde{G}_1(\mathbf{q},z) + \tilde{G}_2(\mathbf{q},z)\right\}$$

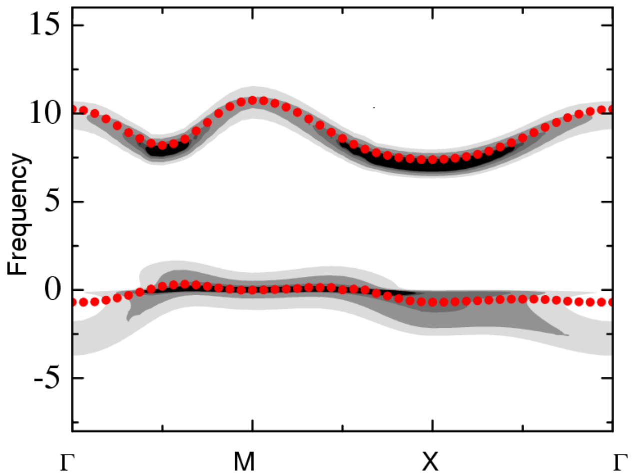
The interaction is specified by the hopping parameter **t(q)** and the

spin-charge susceptibility $\chi_{sc}(\mathbf{q},\nu) = (1/4)\langle\langle N_{\mathbf{q}}|N_{-\mathbf{q}}\rangle\rangle_\nu + \langle\langle \mathbf{S}_{\mathbf{q}}|\mathbf{S}_{-\mathbf{q}}\rangle\rangle_\nu$

where the GFs for two subbands $\tilde{G}_{1(2)}(\mathbf{q},\omega) = \dfrac{1}{\omega - \tilde{\varepsilon}_{1(2)}(\mathbf{q}) - \tilde{\Sigma}(\mathbf{q},\omega)}$

Spectrum in MFA

$$\hat{G}^{0}_{\sigma}(\mathbf{k},\omega) = \left(\omega\hat{\tau}_0 - \hat{\varepsilon}(\mathbf{k})\right)^{-1}\hat{Q},$$



Dispersion curves ($\delta = 0.1$) along the symmetry directions $\Gamma\,(0,0) \to M(\pi,\pi) \to X(\pi,0) \to \Gamma\,(0,0)$ in MFA (●●●) and with SE corrections (contour plot) for U=8t

$$\tilde{\varepsilon}_{1,2}(\mathbf{k}) = (1/2)[\omega_2(\mathbf{k}) + \omega_1(\mathbf{k})] \mp (1/2)\Lambda(\mathbf{k}),$$
$$\Lambda(\mathbf{k}) = \{[\omega_2(\mathbf{k}) - \omega_1(\mathbf{k})]^2 + 4|W(\mathbf{k})|^2\}^{1/2},$$
$$\omega_1(\mathbf{k}) = 4t\,\alpha_1\gamma(\mathbf{k}) + 4t'\,\beta_1\gamma'(\mathbf{k}) - \mu,$$
$$\omega_2(\mathbf{k}) = \Delta + 4t\,\alpha_2\gamma(\mathbf{k}) + 4t'\,\beta_2\gamma'(\mathbf{k}) - \mu,$$
$$|W(\mathbf{k})| = 4t\,\alpha_{12}\gamma(\mathbf{k}) + 4t'\,\beta_{12}\gamma'(\mathbf{k})$$

where

$$\gamma(\mathbf{k}) = (1/2)(\cos k_x + \cos k_y),$$
$$\gamma'(\mathbf{k}) = \cos k_x \cos k_y,$$

Renormalization parameters

$$\alpha_{1(2)} = Q_{1(2)}[1 + C_1/Q^2_{1(2)}],$$
$$\alpha_{12} = \sqrt{Q_1 Q_2}[1 - C_1/Q_1 Q_2],$$
$$\beta_{1(2)} = Q_{1(2)}[1 + C_2/Q^2_{1(2)}],$$
$$\beta_{12} = \sqrt{Q_1 Q_2}[1 - C_2/Q_1 Q_2]$$

$$C_1 = \langle \mathbf{S}_i \mathbf{S}_{i\pm a_x/a_y}\rangle, \quad C_2 = \langle \mathbf{S}_i \mathbf{S}_{i\pm a_x \pm a_y}\rangle$$

1. Strong spectrum renormalization by the short-range static antiferromagnetic correlations (missed in DMFT)

$$\omega_2(\mathbf{k}) \;=\; \Delta + 4\mathrm{t}\,\alpha_2\gamma(\mathbf{k}) + 4\mathrm{t}'\,\beta_2\gamma'(\mathbf{k}) - \mu,$$

where $\gamma(\mathbf{k}) = (1/2)(\cos \mathrm{k_x} + \cos \mathrm{k_y}),\ \gamma'(\mathbf{k}) = \cos \mathrm{k_x} \cos \mathrm{k_y}$,

$$\alpha_{1(2)} = \mathrm{Q}_{1(2)}[1 + \mathrm{C}_1/\mathrm{Q}^2_{1(2)}], \quad \beta_{1(2)} = \mathrm{Q}_{1(2)}[1 + \mathrm{C}_2/\mathrm{Q}^2_{1(2)}],$$

AF spin correlation functions: $\mathrm{C}_1 = \langle \mathbf{S}_i \mathbf{S}_{i\pm a_x/a_y} \rangle, \quad \mathrm{C}_2 = \langle \mathbf{S}_i \mathbf{S}_{i\pm a_x \pm a_y} \rangle$

Close to half-filling, n = 1.05, Q_2= n/2, $C_1 \approx -0.26$, $C_2 \approx 0.16$

hopping for the nearest neighbor sites is suppressed:

$\alpha_2 \approx 0.1$, $t_{ren} = 0.1\, t << t$

So, the dispersion is given by the next nearest neighbor hopping

$\omega_1(\mathbf{k}) = 4\, t' \,\beta_1 \cos k_x \cos k_y$, $\beta_1 \approx 1.6$, $t'_{ren} = 1.6\, t' > t_{ren}$

2. Self-energy in a static approximation *(Pines et al., Sadovskii et al.)*
In the classical limit $kT >> \omega_s$ we get for the self-energy

$$\Sigma(\mathbf{k}, i\omega_n) \simeq |g(\mathbf{k}-\mathbf{Q})|^2 \frac{T}{N} \sum_{\mathbf{p}} \frac{1}{\kappa^2 + p^2}$$
$$\times [G_1(\mathbf{k}-\mathbf{Q}-\mathbf{p}, i\omega_n) + G_2(\mathbf{k}-\mathbf{Q}-\mathbf{p}, i\omega_n)]$$

For $\kappa = 1/\xi \to 0$ for the GF we get equation (in one subband)

$$[G(k,\omega)]^{-1} \approx \{ \omega - \varepsilon(k) - |g(k-Q)|^2 / [\omega - \varepsilon(k-Q) - \Sigma(k-Q,\omega)] \}$$

This results in the AF gap in the spectrum (neglecting $\Sigma(k-Q,\omega)$)

$$E_{1,2} = (1/2)\,[\varepsilon(k) + \varepsilon(k-Q)] \pm (1/2)\,\{[\varepsilon(k) - \varepsilon(k-Q)]^2 + 4\,|g(k-Q)|^2\}^{1/2}$$

or a pseudogap for finite ξ and finite $\Sigma(k-Q,\omega)$ close to X $(\pi,0)$ region.

Thus, the pseudogap appears due to AF short-range correlations
in our theory -- dynamical short-range spin fluctuations

Numerical Results

The system of equations for GFs and SE was solved self-consistently by using imaginary frequency representation .

Model for the dynamical spin-susceptibility function in SE

$$\mathrm{Im}\,\chi_s(\mathbf{q},\nu) = \frac{\chi_0}{1+\xi^2(1+\gamma(\mathbf{q}))}\tanh\frac{\nu}{2T}\frac{1}{1+(\nu/\omega_s)^2}$$

$$\chi_0 = \frac{3(1-|\delta|)}{2\omega_s}\left\{\frac{1}{N}\sum_{\mathbf{q}}\frac{1}{1+\xi^2[1+\gamma(\mathbf{q})]}\right\}^{-1}$$

Spin-susceptibility shows a maximum at AF wave-vector $\mathbf{Q}_{AF} = (\pi,\pi)$.

where $\gamma(\mathbf{q}) = (1/2)(\cos q_x + \cos q_y)$ = – 1

Two fitting parameters: AF correlation length ξ and energy $\omega_s \sim J = 0.4\,t$

,while constant χ_0 is defined by the equation: $\langle \mathbf{S}_i\mathbf{S}_i\rangle = (3/4)(1-|\delta|)$

Static AF correlation functions C_1,C_2 and correlation length **ξ**

$\delta =$	0.03	0.05	0.10	0.15	0.20	0.30
C_1	-0.36	-0.26	-0.21	-0.18	-0.14	-0.10
C_2	0.27	0.16	0.11	0.09	0.06	0.04
$C(\xi)$	22.0	5.91	3.58	2.67	1.93	1.40
ξ	8.0	3.40	2.50	2.10	1.70	1.40

where $$\mathrm{C}_1 = \langle \mathbf{S}_{\mathrm{i}} \mathbf{S}_{\mathrm{i} \pm \mathrm{a_x}/\mathrm{a_y}} \rangle, \quad \mathrm{C}_2 = \langle \mathbf{S}_{\mathrm{i}} \mathbf{S}_{\mathrm{i} \pm \mathrm{a_x} \pm \mathrm{a_y}} \rangle$$

$$C_1 = \frac{1}{N} \sum_{\mathbf{q}} C_{\mathbf{q}} \, \gamma(\mathbf{q}), \quad C_2 = \frac{1}{N} \sum_{\mathbf{q}} C_{\mathbf{q}} \, \gamma'(\mathbf{q}).$$

$$C_{\mathbf{q}} = \langle \mathbf{S}_{\mathbf{q}} \mathbf{S}_{-\mathbf{q}} \rangle = \frac{C(\xi)}{1 + \xi^2 [1 + \gamma(\mathbf{q})]}, \qquad C(\xi) = \chi_0 \, (\omega_s/2).$$

Spectral function for electrons $A_{el}(k,\omega) = A_h(k, -\omega)$ where

$$
\begin{aligned}
A_{(h)}(\mathbf{k},\omega) &= \{1/2 - P(\mathbf{k})\}\,\tilde{A}_1(\mathbf{k},\omega) + \{1/2 + P(\mathbf{k})\}\,\tilde{A}_2(\mathbf{k},\omega),\\
\tilde{A}_{1(2)}(\mathbf{k},\omega) &= -(1/\pi)\,\mathrm{Im}\,\tilde{G}_{1(2)}(\mathbf{k},\omega + i0^+)
\end{aligned}
$$

where $P(\mathbf{k})$ is the hybridization contribution.

Electron occupation numbers $n_\sigma^{(el)}(\mathbf{k}) = 1 - n_\sigma^{(hole)}(\mathbf{k})$

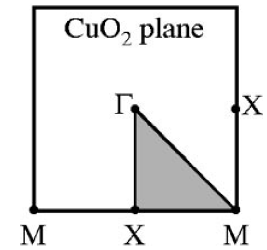
where hole numbers

$$
\begin{aligned}
n_\sigma^{hole}(\mathbf{k}) &= \int_{-\infty}^{\infty} \frac{d\omega}{e^{\omega/T}+1} A_{(h)}(\mathbf{k},\omega)\\
&= \{1/2 - P(\mathbf{k})\}\,\tilde{N}_1(\mathbf{k}) + \{1/2 + P(\mathbf{k})\}\,\tilde{N}_2(\mathbf{k})
\end{aligned}
$$

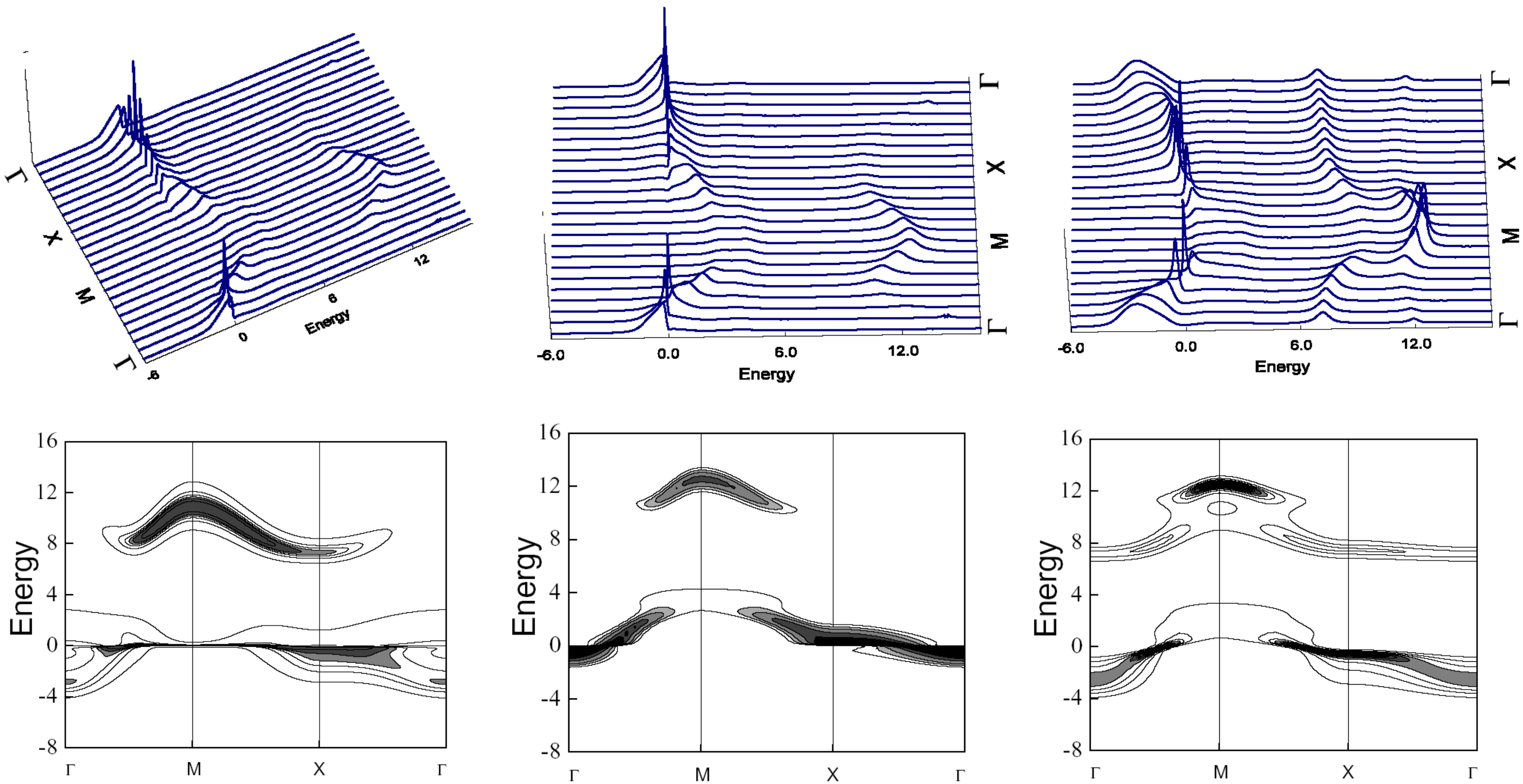
Parameters: $t \approx 0.4$ eV, $t' = -0.3\,t$, $U_{eff} = 8\,t$

$t \approx 0.6$ eV, $t' = -0.13\,t$, $t'' = 0.16\,t$, $U_{eff} = 4\,t$

Spectral functions A(k, ω) and dispersion curves along symmetry directions Γ (0,0) → M(π,π) → X(π,0) → Γ (0,0)

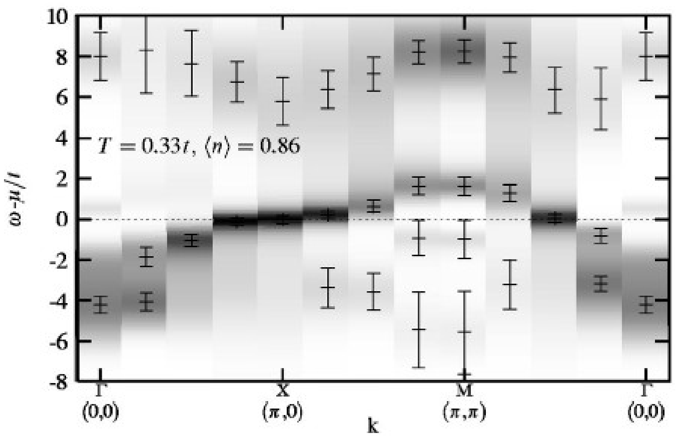


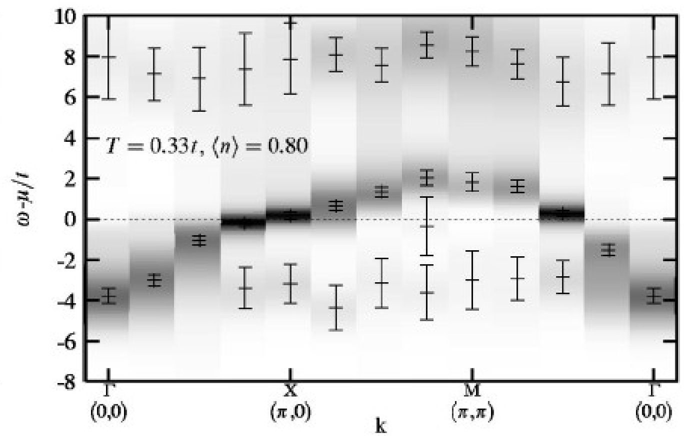
δ = 0.1 (T ≈ 0.03 t) δ = 0.3 (T ≈ 0.03 t) δ = 0.1 (T ≈ 0.3 t)



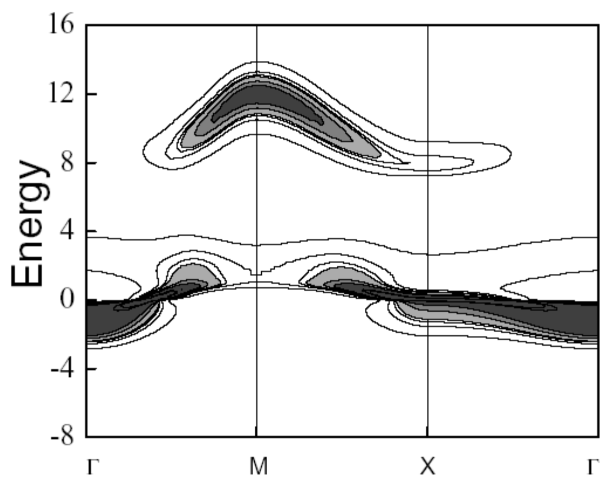
MC study of A(k, ω) for 8x8 cluster at T=0.33 t, U =8t *[Grober et al. (2000)]*

δ = 0.14

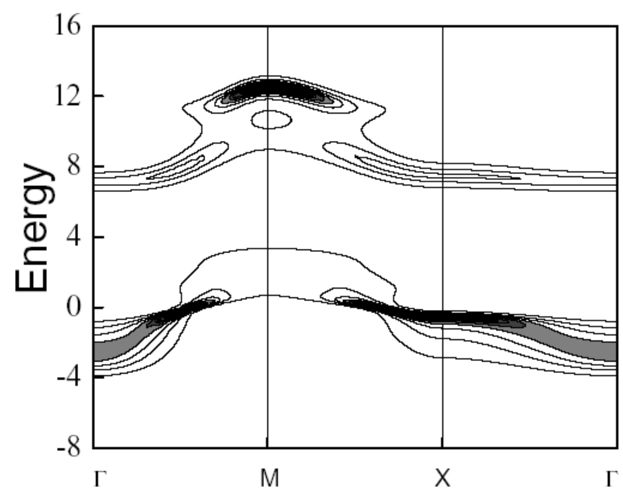




δ = 0.20



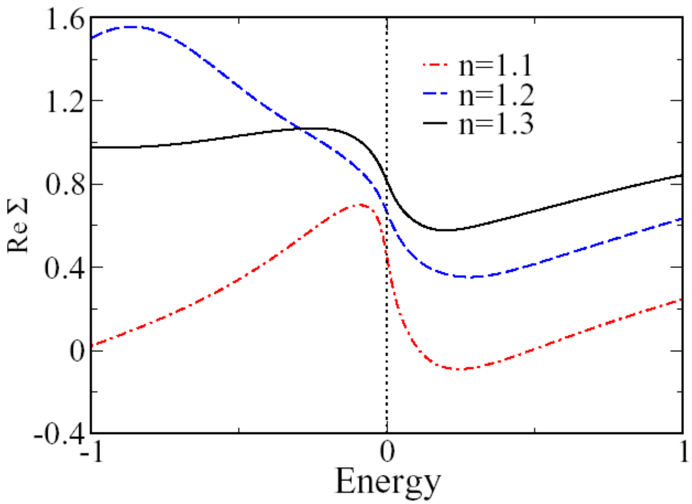
δ = 0.2 (T ≈ 0.03 t)



δ = 0.1 (T ≈ 0.3 t)

Coupling constant

$$\lambda(\mathbf{k}) = -(\partial\, \mathrm{Re}\Sigma(\mathbf{k},\omega)/\partial\omega)_{\omega=0}$$

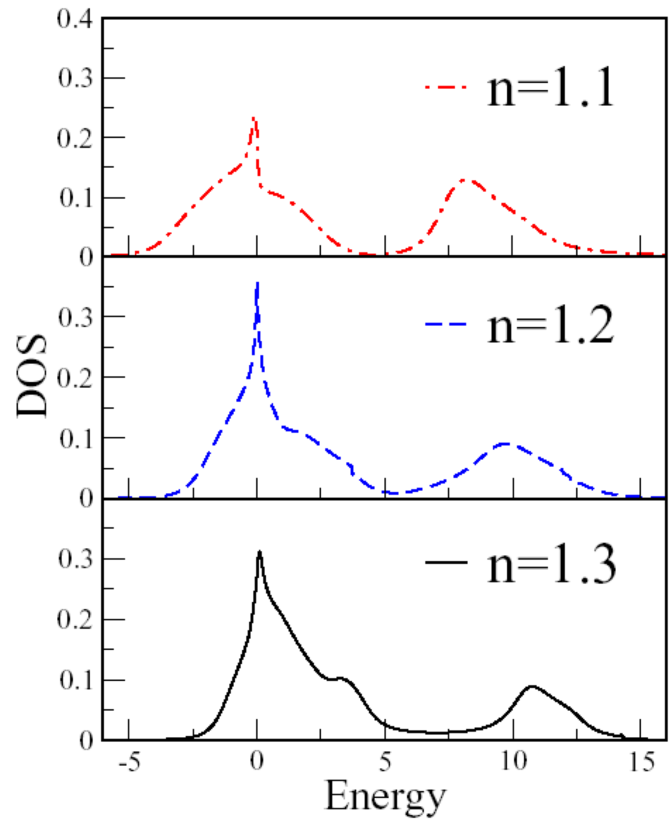


$\lambda(k_F)$ = 7.86 at δ = 0.1

$\lambda(k_F)$ = 3.3 at δ = 0.3

Density of states $A(\omega)$:

Spectral weight transfer with doping

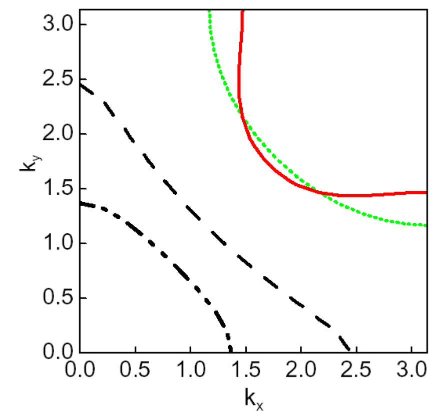


Fermi surface: contour plot of equation

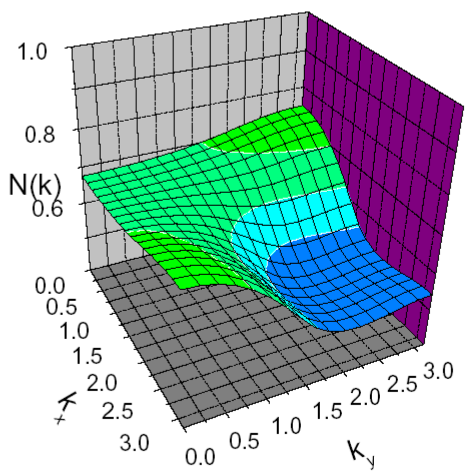
$$\tilde{\varepsilon}_2(\mathbf{k}_\mathrm{F}) + \tilde{\Sigma}(\mathbf{k}_\mathrm{F}, \omega = 0) = 0$$

(T ≈ 0.03 t): δ = 0.1 —— δ = 0.2 -- δ = 0.3 - - - -

(T ≈ 0. 3 t): δ = 0.1 ——

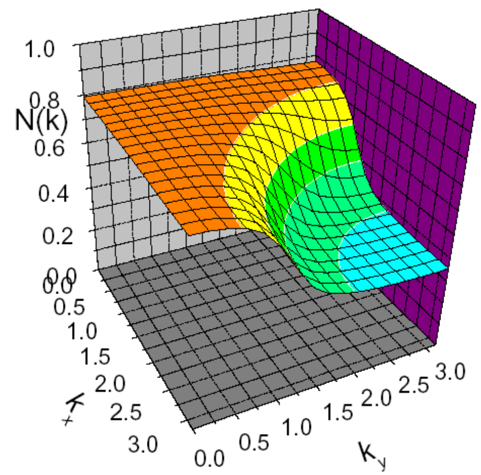


Electron occupation numbers $n_{el}(\mathbf{k}) = 1 - n_h(\mathbf{k})$



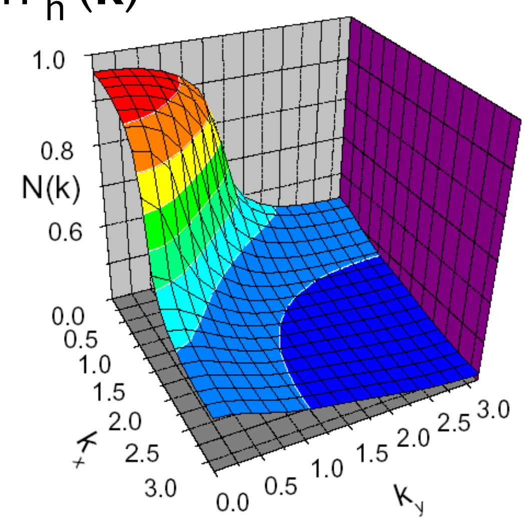
δ = 0.1 (T ≈ 0.03 t)

Δ n ≈ 0.15



δ = 0.1 (T ≈ 0.3 t)

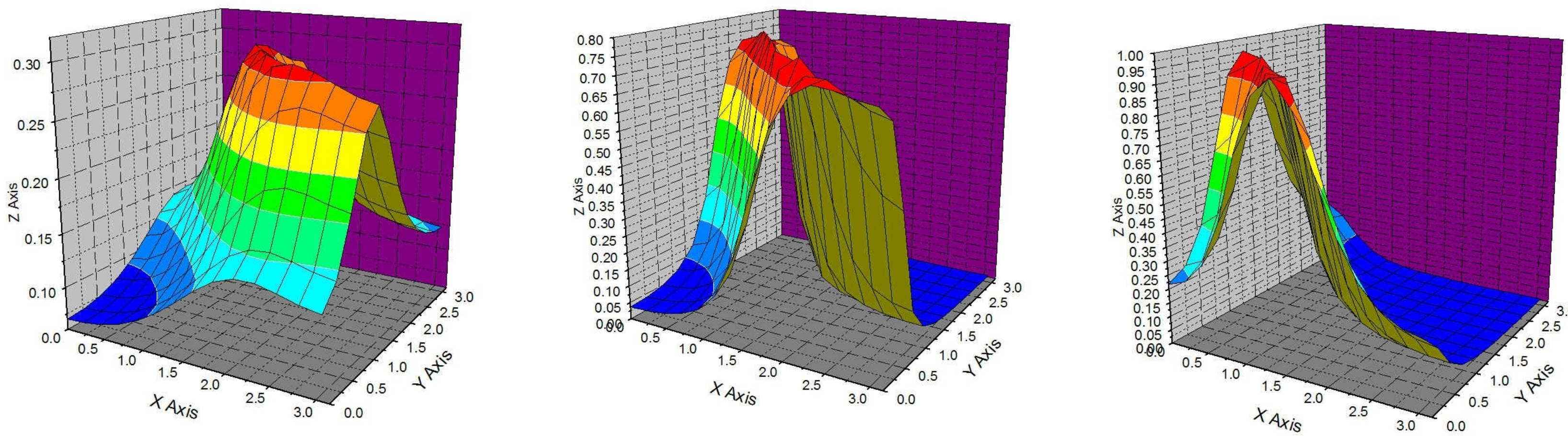
Δ n ≈ 0.45

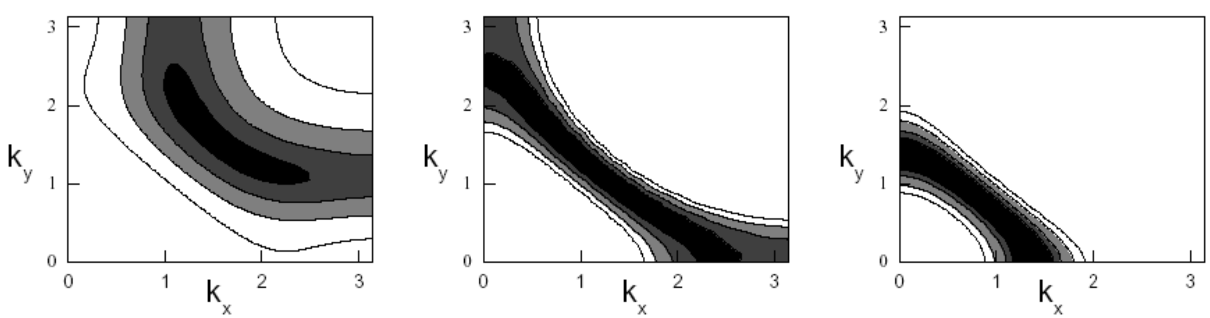


δ = 0.3 (T ≈ 0.03 t)

Δ n ≈ 0.55

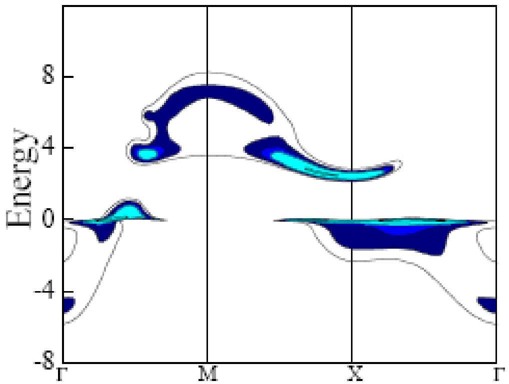
Fermi surface: maximum values of $A_{(el)}(k_F, \omega = 0)$



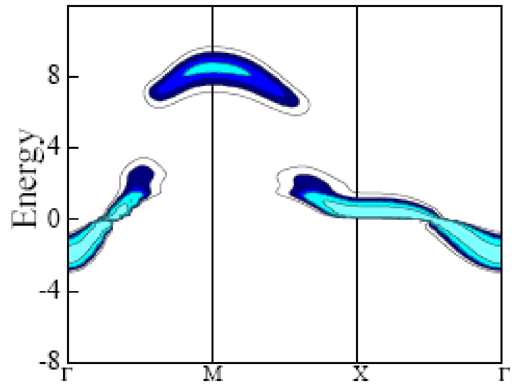


(T ≈ 0.03 t): δ = 0.1 δ = 0.2 δ = 0.3

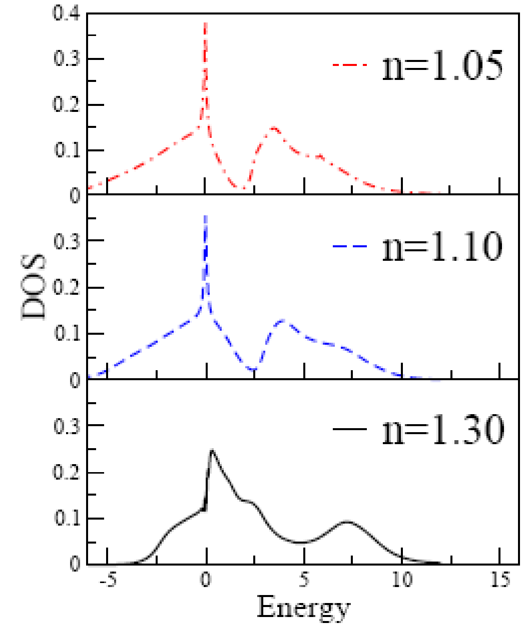
Numerical solution for $U_{eff} = 4t$

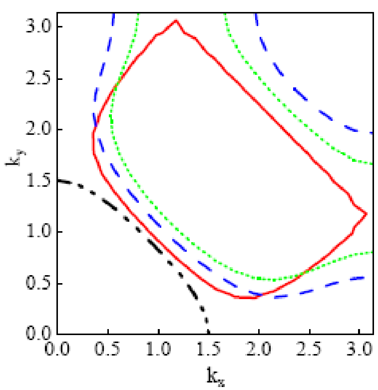


$\delta = 0.05$ (T ≈ 0.03 t)



$\delta = 0.3$ (T ≈ 0.03 t)

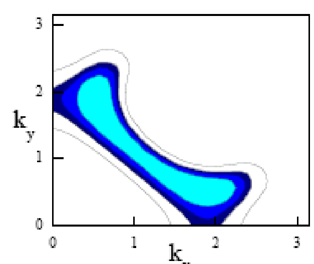




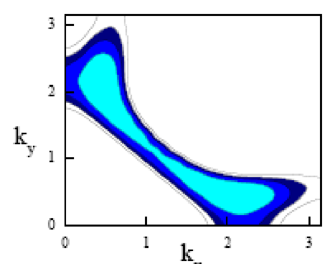
(T ≈ 0.03 t):
$\delta = 0.1$ —
$\delta = 0.2$ - -
$\delta = 0.3$ — - -

(T ≈ 0. 3 t):
$\delta = 0.1$ —

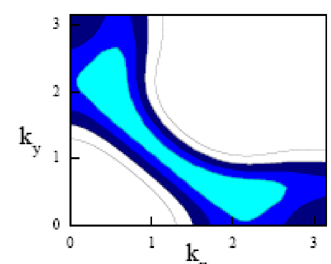
Fermi surface: A(k, 0)=0



$\delta = 0.05$
(T ≈ 0.03 t)

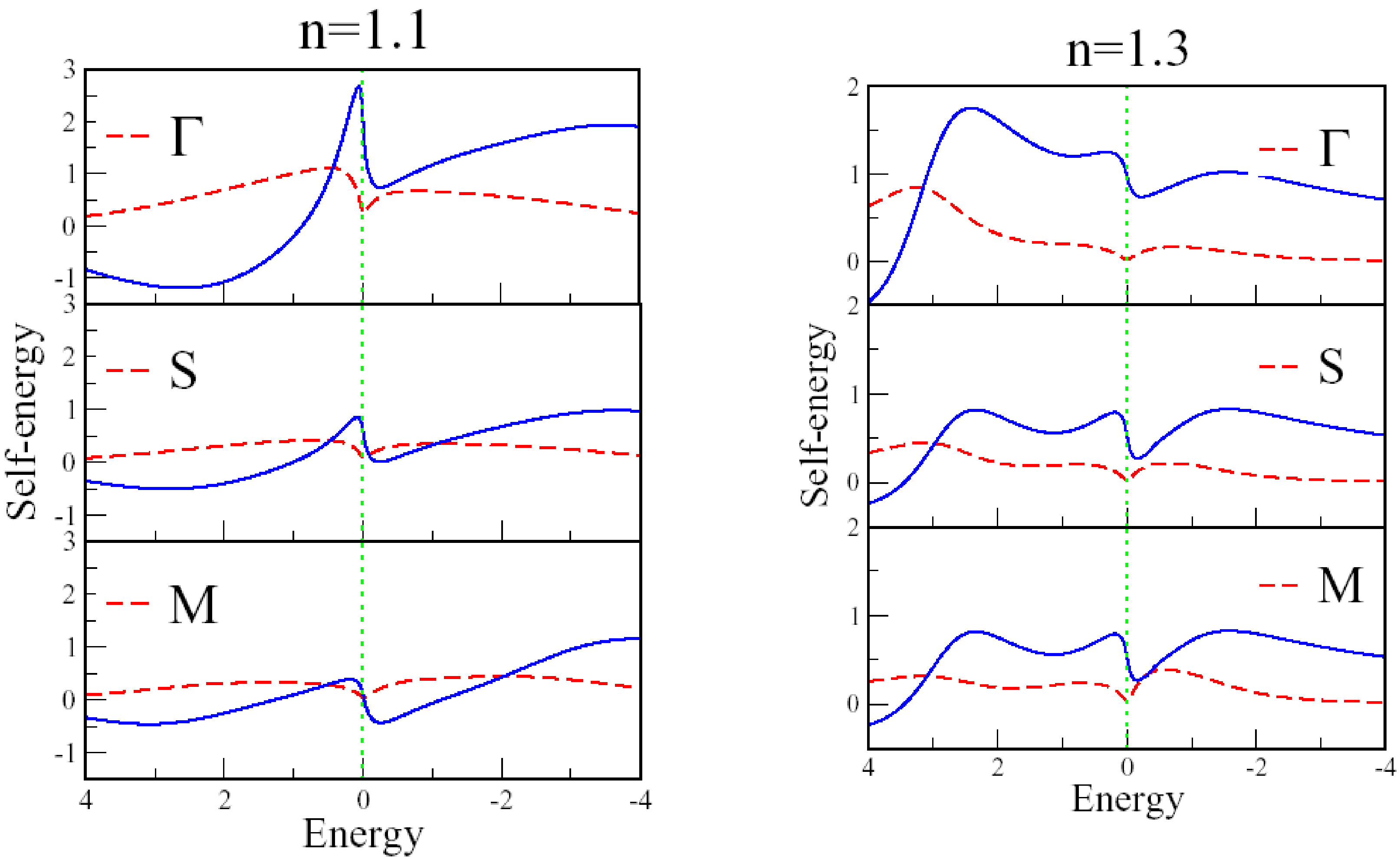


$\delta = 0.1$
(T ≈ 0.03 t)

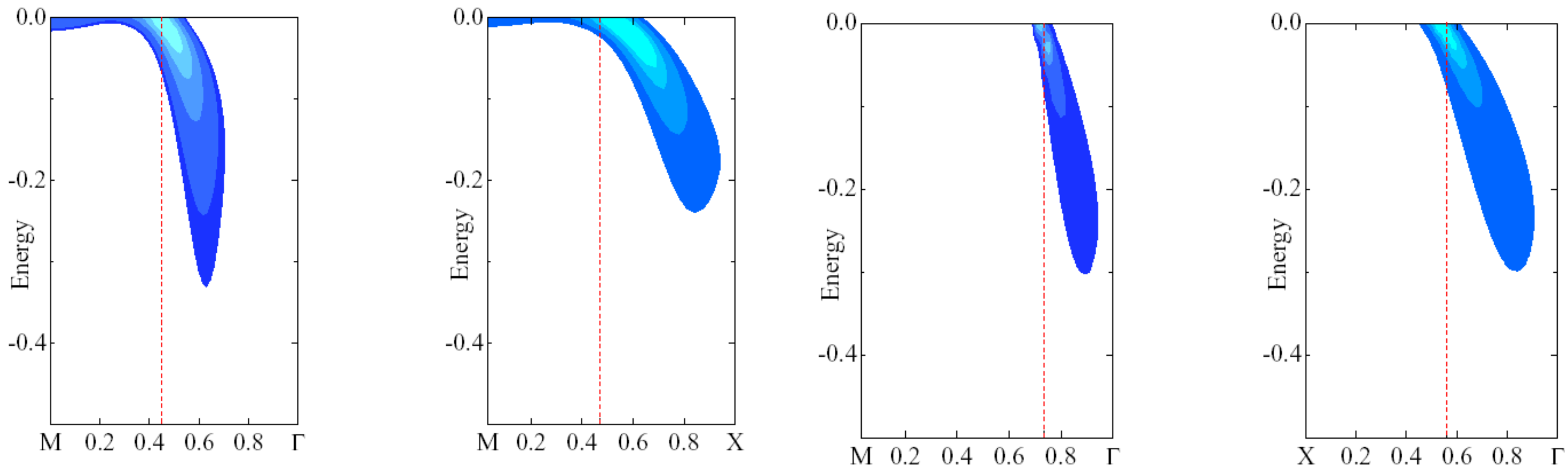


$\delta = 0.1$
(T ≈ 0.3 t)

Self-energy: real (---) and imaginary (---) parts at Γ(0,0), S(π/2,π/2), and M(π, π) points of BZ



“Kink” in the dispersion curves



M(π,π) ⟶ Γ(0,0)   M(π,π) ⟶ X(0, π)
Dispersion along symmetry directions
at doping δ = 0.1

M(π,π) ⟶ Γ(0,0)   X(0, π) ⟶ Γ(0,0)
Dispersion along symmetry directions
at doping δ = 0.3

No well defined kink energy due a continuum spectrum of spin fluctuations up to ω_s~ J = 0.4 t ~ 160 meV

Numerical solution (direct diagonalization) of the SC gap equation

$$\phi(\mathbf{k}, i\omega_n) = -T \sum_{\mathbf{q}} \sum_m K(\mathbf{k}-\mathbf{q}, \mathbf{q} \mid i\omega_n, i\omega_m)\, F(\mathbf{q}, i\omega_m)$$

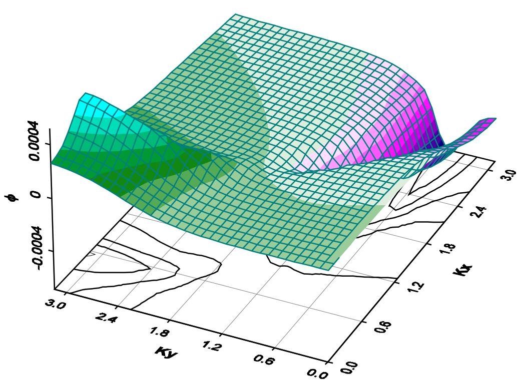
$$K(\mathbf{k}-\mathbf{q}, \mathbf{q} \mid i\omega_n, i\omega_m) = [\, J(\mathbf{k}-\mathbf{q}) + \lambda(\mathbf{q}, \mathbf{k}-\mathbf{q} \mid i\omega_n - i\omega_m)\,]\, F(\mathbf{q}, i\omega_m)$$

with interaction $\lambda(\mathbf{q}, \mathbf{k}-\mathbf{q} \mid i\omega_n) = -|t(\mathbf{q})|^2\, \chi_s(\mathbf{k}-\mathbf{q} \mid i\omega_n)$

for the linearized anomalous GF

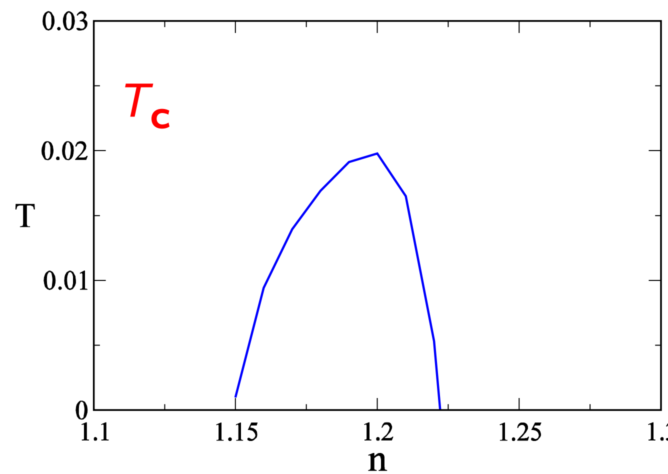
$$F(\mathbf{q}, i\omega_m) = -G(\mathbf{q}, -i\omega_m)\, \phi(\mathbf{q}, i\omega_m)\, G(\mathbf{q}, i\omega_m)$$

results in *d*-wave pairing:



$T_c \sim 0.02t$

~ 100 K



Conclusion

- The proposed microscopic theory provides an explanation for doping and temperature dependence of electronic spectrum in cuprates as controlled by the AF spin correlations.

- Self-consistent solution of the Dyson equation for GF and SE in NCA reproduces the gross features of the electronic spectra:
  -- pseudogap formation and arc-type FS in the underdoped region,
  -- doping dependence of the dispersion and QP weight at the FS,
  -- weight transfer of the subband spectral density with doping

- To perform quantitative comparison with ARPES data contributions from charge fluctuations and electron-phonon interaction should be taken into account

Publications: *N.M. Plakida, et al. JETP **97**, 331 (2003). Exchange and spin-fluctuation mechanisms of superconductivity in cuprates.*
*N. M. Plakida, V. S. Oudovenko, JETP **104**, 230 (2007): Electronic spectrum in high-temperature cuprate superconductors.*

M.V.Sadovskii (1974): “Toy” 1D pseudogap model (2D -- hot spots)

$$\Sigma(\varepsilon_n p) = \int \frac{dQ}{2\pi} V_{eff}(Q) \frac{1}{i\varepsilon_n - \xi_{p-Q}} \approx 2W^2 \int_{-\infty}^{\infty} \frac{dx}{2\pi} \frac{\kappa}{x^2+\kappa^2} \frac{1}{i\varepsilon_n + \xi_p - v_F x} =$$

$$= 2W^2 \int_{-\infty}^{\infty} \frac{dx}{2\pi} \frac{\kappa}{(x-i\kappa)(x+i\kappa)} \frac{1}{i\varepsilon_n + \xi_p - v_F x} =$$

where

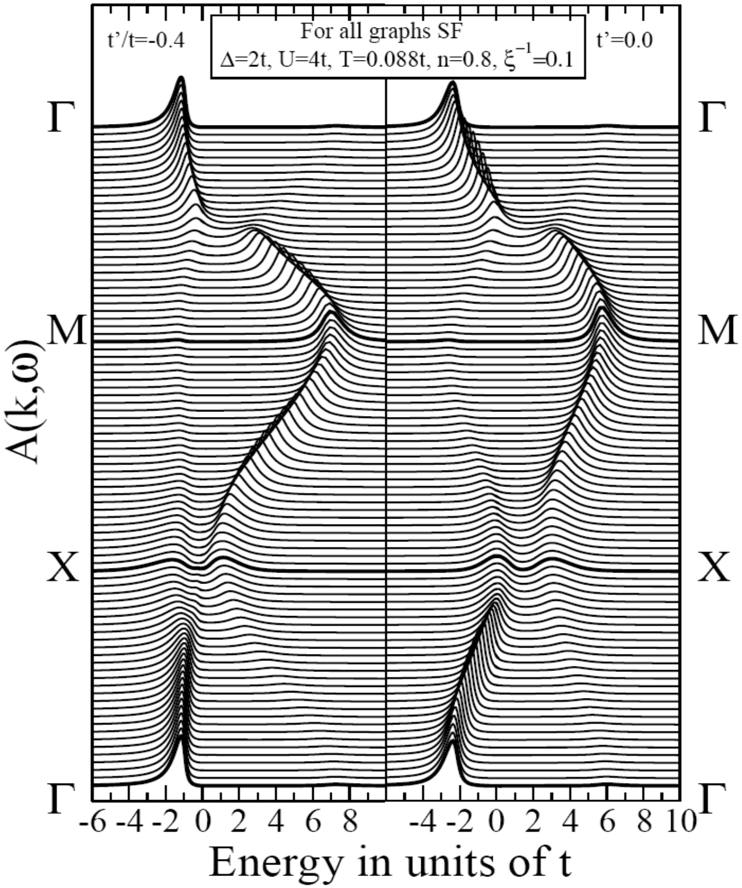
$$V_{eff}(Q) = 2W^2 \left\{ \frac{\kappa}{(Q-2p_F)^2+\kappa^2} + \frac{\kappa}{(Q+2p_F)^2+\kappa^2} \right\}$$

$$= \frac{W^2}{i\varepsilon_n + \xi_p + i v_F \kappa}$$

M.V.Sadovskii et al. (2005): DMFT + Σ_k approach

$$G_{\mathbf{k}}(i\omega) = \frac{1}{i\omega + \mu - \varepsilon(\mathbf{k}) - \Sigma(i\omega) - \Sigma_{\mathbf{k}}(i\omega)}$$

$$\Sigma_n(i\omega, \mathbf{k}) = \Delta^2 \frac{s(n)}{i\omega + \mu - \Sigma(i\omega) - \varepsilon_n(\mathbf{k}) + inv_n\kappa - \Sigma_{n+1}(i\omega, \mathbf{k})}$$



DMFT + $\Sigma_{\mathbf{k}}$ calculations for

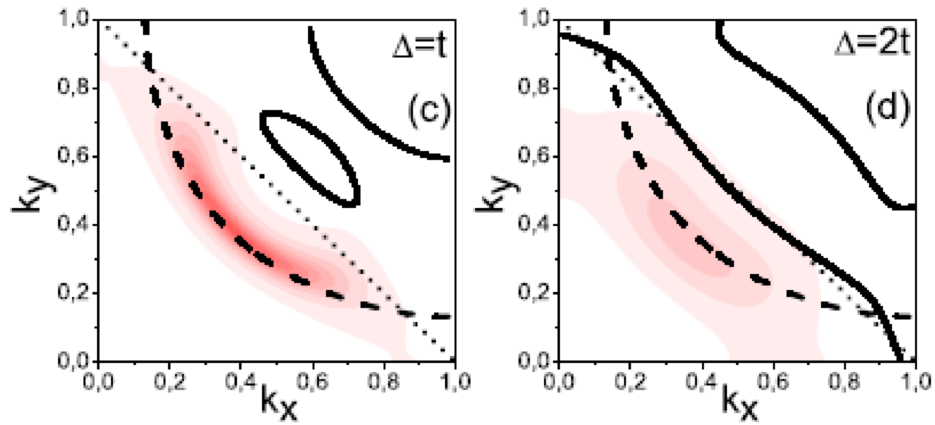
U = 4t and n = 0.8

(ξ = 10, Δ = 2t)

Sadovskii et al.
*Phys. Rev. B **72**, 155105 (2005)*

Pseudogaps in strongly correlated metals: A generalized dynamical mean-field theory approach

E. Z. Kuchinskii et al.,
*JETP Letters, **82**, 198 (2005)*



DMFT + $\Sigma_{\mathbf{k}}$ calculations for

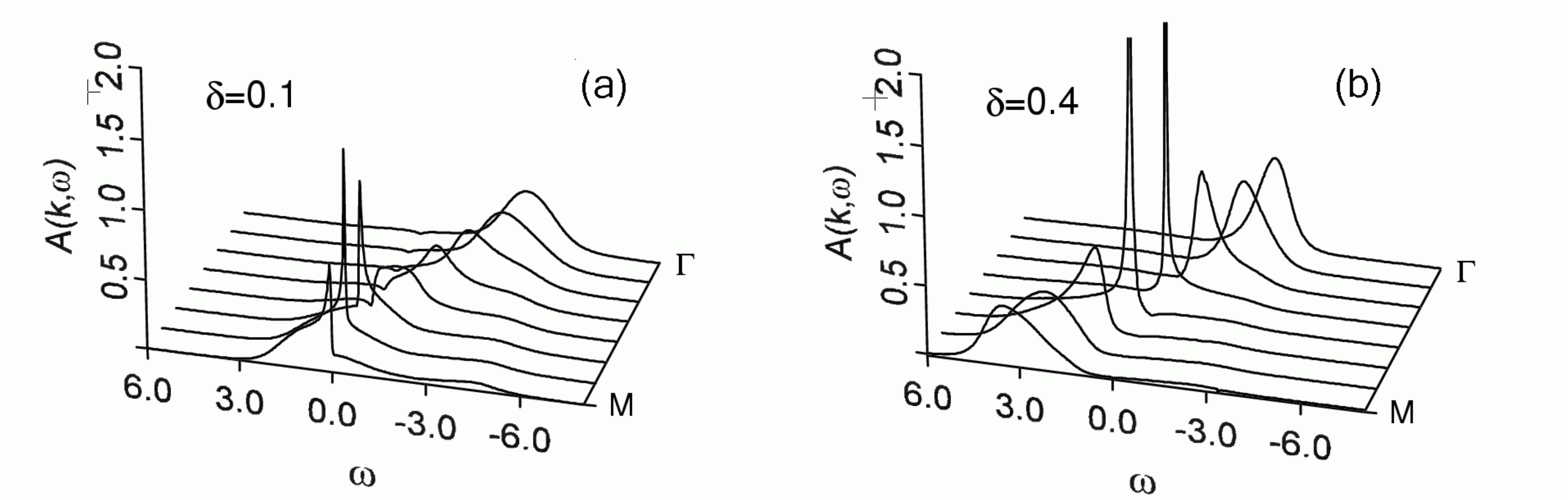
U = 4t and n = 0.8.

Comparison with t-J model

*N.M. Plakida, V.S. Oudovenko, Phys. Rev. B **59**, 11949 (1999)*

Electron spectrum and superconductivity in the **t-J** model at moderate doping.

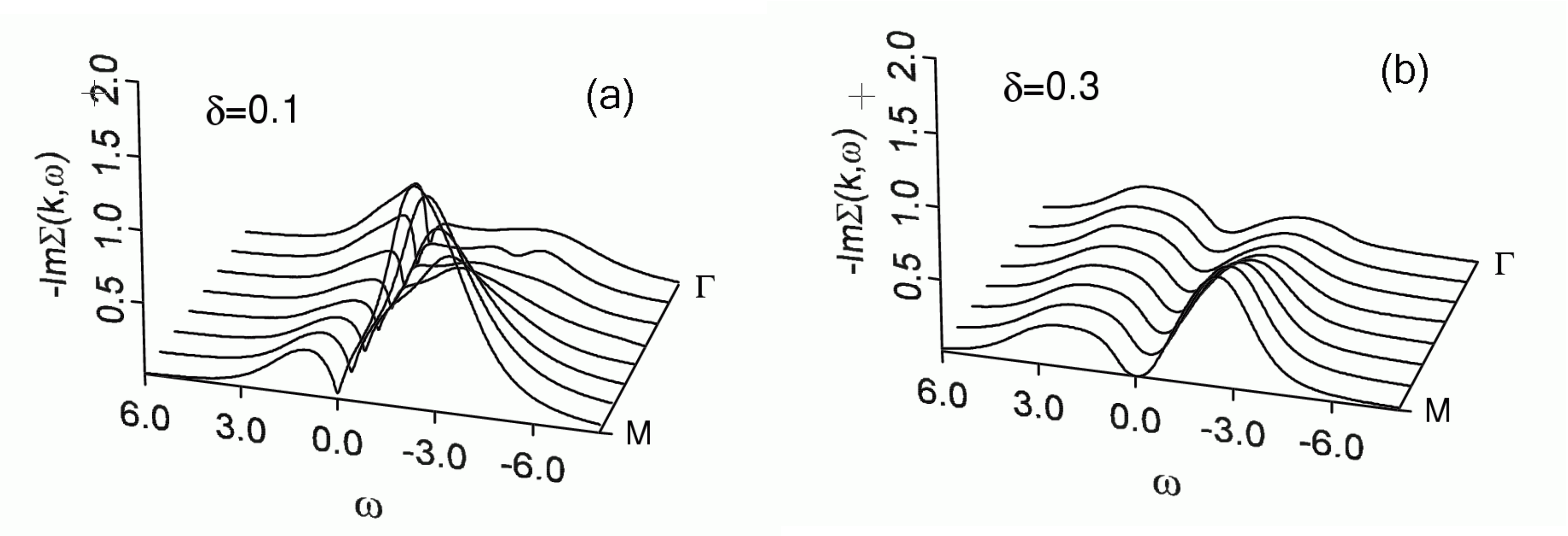
1. Spectral functions A(k, ω)



Spectral function for the t-J model in the symemtry direction

Γ(0,0) → M(π,π) at doping δ = 0.1 (a) and δ = 0.4 (b) .

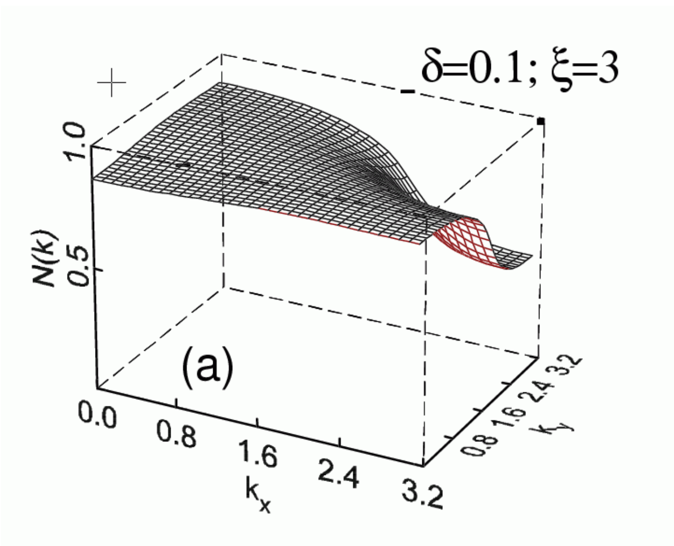
2. Self-energy, Im Σ(k, ω)

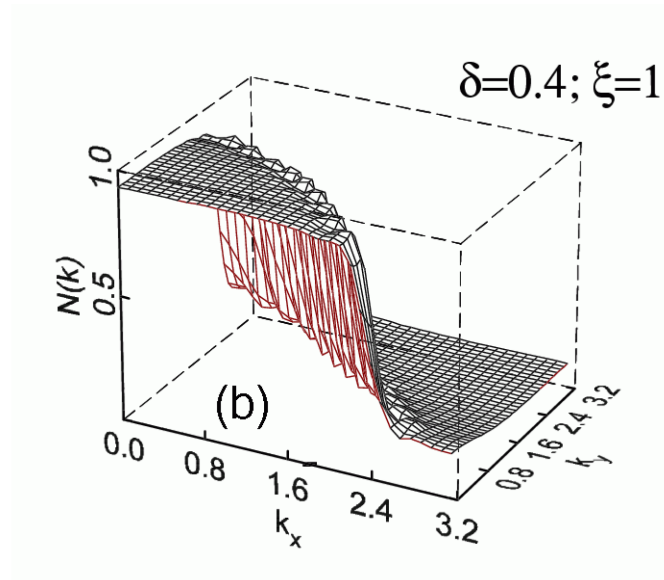


Self-energy for the t-J model in the symemtry direction

Γ(0,0) → M(π,π) at doping $\delta = 0.1$ (a) and $\delta = 0.4$ (b) .

3. Electron occupation numbers N(k) = n(k)/2





Electron occupation numbers for the t-J model in the quarter of BZ, ($0 < k_x, k_y < \pi$) at doping $\delta = 0.1$ (a) and $\delta = 0.4$ (b) .