Spectral functions and Luttinger sum sule in models of strongly correlated electrons

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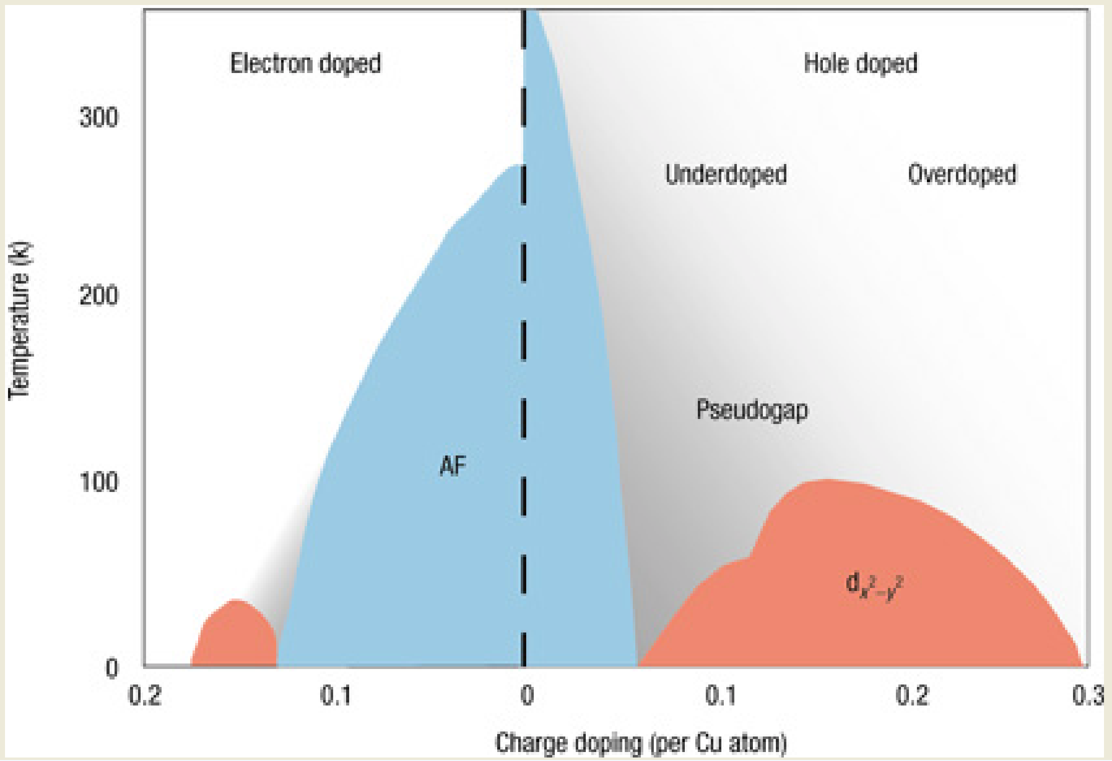
Outline

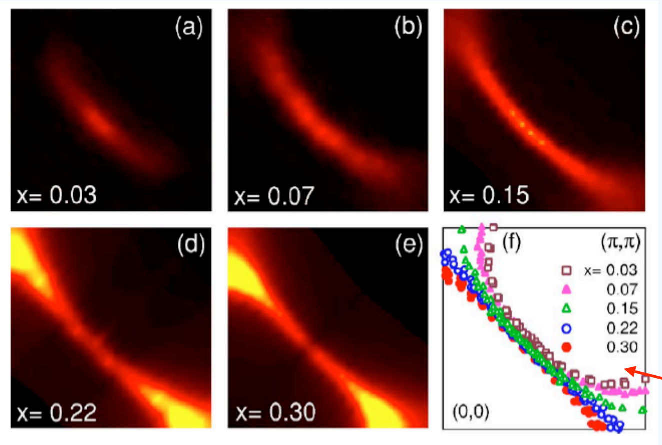
- **Cuprates: ARPES results – theoretical challenges:** pseudogap, asymmetry electron-hole doping, waterfall dispersion, Luttinger sum rule
- **Exact diagonalization T>0 (FTLM) method**
- **Hole-doping:** Fermi surface evolution, anomalous QP relaxation rate, pseudogap
- **Electron-doping:** Fermi surface from pocket to large FS
- **High-energy kink and waterfall** dispersion: origin due to strong correlations
- **Luttinger sum rule:** valid for finite systems, violated for t-J model and Mott-Hubbard insulator ?

Cuprates: phase diagram

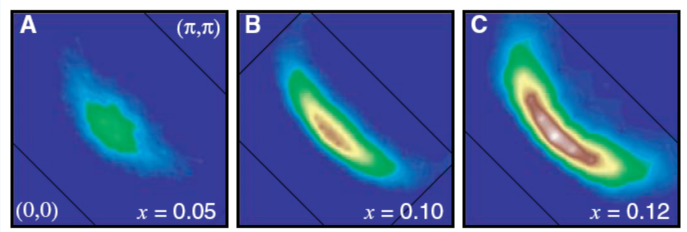


Hole-doped cuprates: ARPES

Fermi surface reconstruction: from arc to large FS



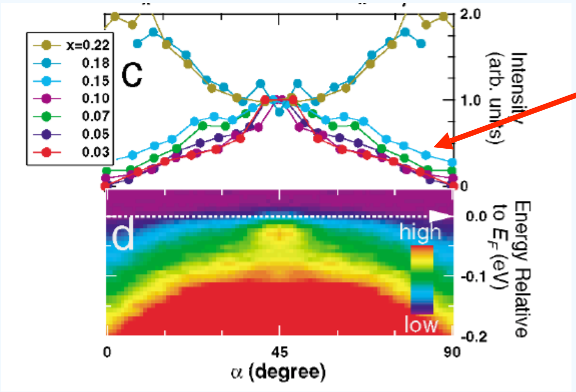
$La_{2-x}Sr_xCuO_4$: Yoshida et al 06



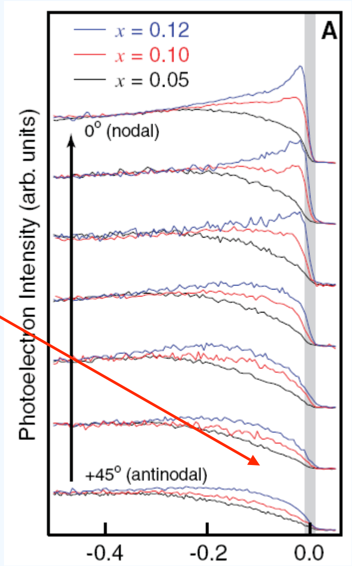
Na-CCOC : K.Shen et al 05

Luttinger sum rule ?

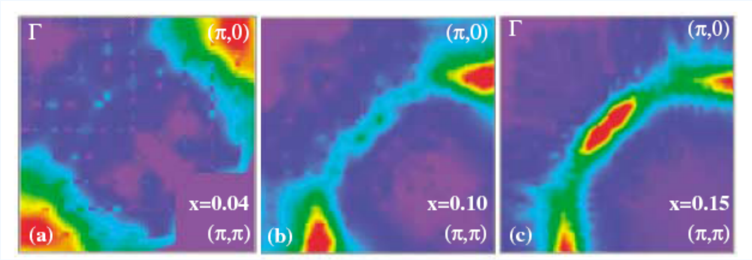
Pseudogap:



Yoshida et al 03

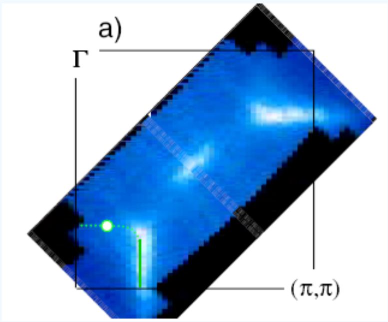


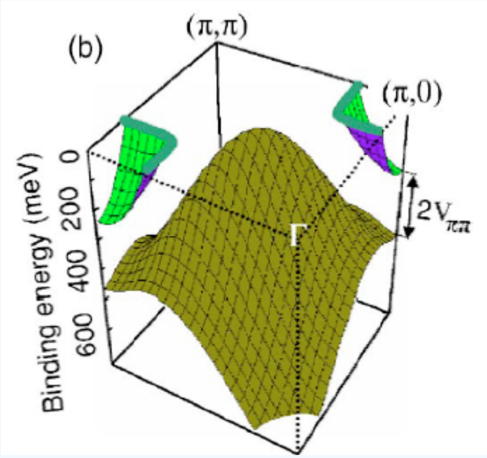
Electron-doped cuprates: ARPES



$Nd_{2-x}Ce_xCuO_{4\pm\delta}$: Armitage et al. 02

electron pockets at low doping
closing of Mott-Hubbard gap with doping ?



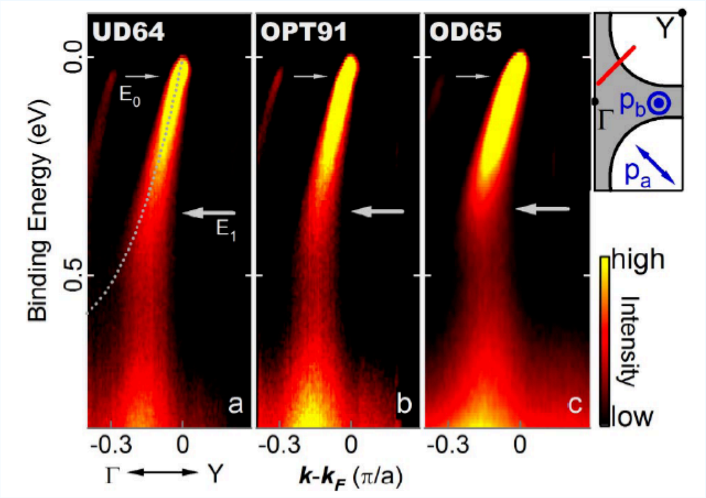


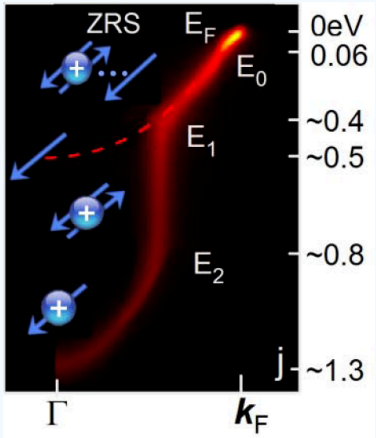
$Sm_{1.86}Ce_{0.14}CuO_4$: Park et al 07

band splitting: due to SDW, AFM ?
Mott-Hubbard gap remains
pseudogap (splitting) the same as in $\sigma(\omega)$?

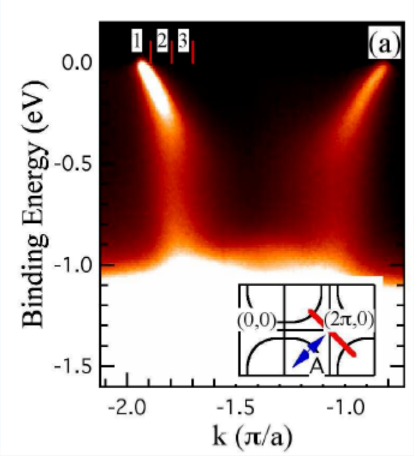
High energy kink - waterfall

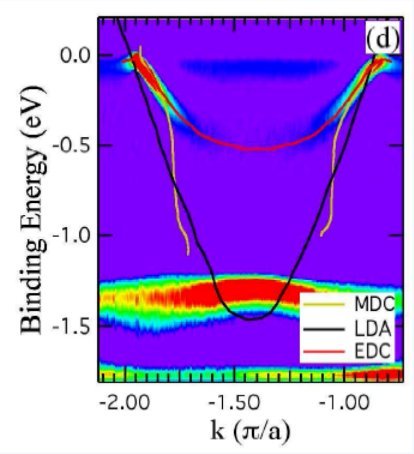
ARPES:





Graf et al (07)



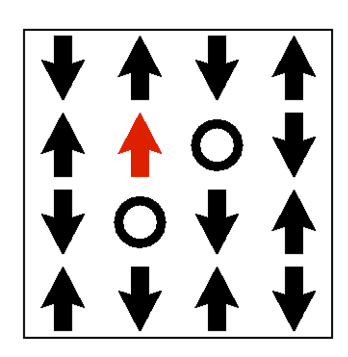


Pb-Bi2201

Pan et al

t – J model

interplay : electron hopping + spin exchange
single band model for **strongly correlated electrons**



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

$t_{ij} = t$ n.n. hopping

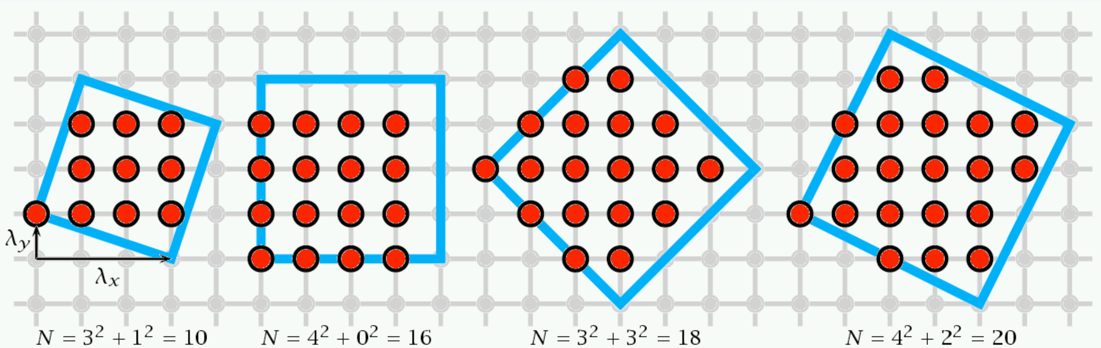
$\tilde{c}^{\dagger}_{is} = (1 - n_{i,-s}) c^{\dagger}_{is}$

$t_{ij} = t'$ n.n.n. hopping

etc.

projected fermionic operators:
no double occupation of sites

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



$T > T_{fs}$

finite size temperature

T > 0 Lanczos method (FTLM) for dynamical quantities

$$
\begin{aligned}
H|\phi_0\rangle &= a_0|\phi_0\rangle + b_1|\phi_1\rangle \\
H|\phi_i\rangle &= b_i|\phi_{i-1}\rangle + a_i|\phi_i\rangle + b_{i+1}|\phi_{i+1}\rangle, \\
H|\phi_M\rangle &= a_0|\phi_M\rangle + b_{M-1}|\phi_{M-1}\rangle
\end{aligned}
$$

Jaklič, Prelovšek (1994)

M Lanczos steps started with normalized

$$
\begin{aligned}
|\phi_0\rangle = |n\rangle \quad &\Longrightarrow L_M = \{|\phi_j\rangle,\ j = 0 \dots M\} \Longrightarrow |\psi_j\rangle \\
|\tilde{\phi}_0\rangle = \frac{A|\phi_0\rangle}{\sqrt{\langle\phi_0|A^\dagger A|\phi_0\rangle}} \quad &\Longrightarrow \tilde{L}_M = \{|\tilde{\phi}_j\rangle,\ j = 0 \dots M\} \Longrightarrow |\tilde{\psi}_j\rangle
\end{aligned}
$$

$$
\langle B(t)A\rangle \approx Z^{-1} \sum_{n=1}^{N_{st}} \sum_{i=0}^{M} \sum_{j=0}^{M} e^{-\beta\epsilon_i^n} e^{it(\epsilon_i^n - \tilde{\epsilon}_j^n)} \langle n|\psi_i^n\rangle \langle\psi_i^n|B|\tilde{\psi}_j^n\rangle \langle\tilde{\psi}_j^n|A|n\rangle
$$

Short - t (high - ω), high - T expansion: exact k,l < M

+ random sampling: $r << N_{st}$

Spectral functions

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

projected operators

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

$$|\Sigma(\mathbf{k},\omega \rightarrow \pm\infty)| \propto 1/\omega$$

$\alpha = (1 + c_h)/2$ normalization

$$\zeta_{\mathbf{k}} = \int d\omega\omega A(\mathbf{k},\omega)/\alpha = \bar{\zeta} - 4\sum_j r_j t_j \gamma_j(\mathbf{k})$$

$$r_j = \alpha + \frac{1}{\alpha}\langle \mathbf{S}_0 \cdot \mathbf{S}_j \rangle$$

'free' term

Finite size lattice:

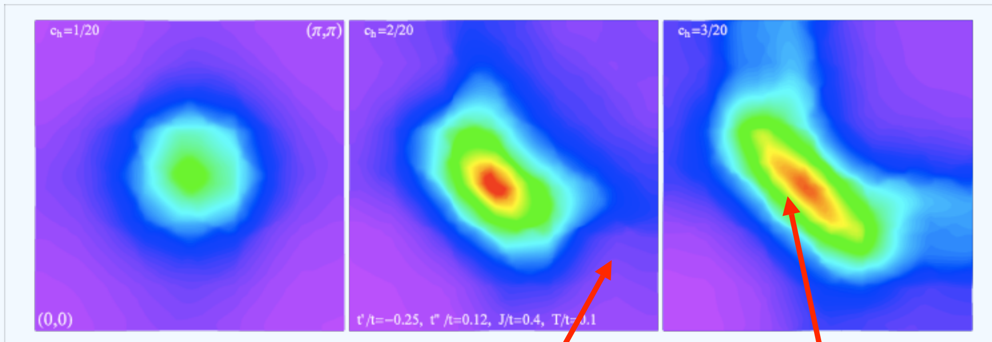
Continuous **k:** $t_{ij} \rightarrow \tilde{t}_{ij} = t_{ij}\exp(i\vec{\theta}\cdot\vec{r}_{ij})$ $\mathbf{k} = \mathbf{k}_l + \vec{\theta}$

Regularization: with FTLM calculate $G(\mathbf{k},\omega)$ → $\Sigma(\mathbf{k},\omega)$

→ average $\Sigma(\mathbf{k},\omega)$ over $\delta k \sim 0.3$ → $G(\mathbf{k},\omega)$

Hole-doped case

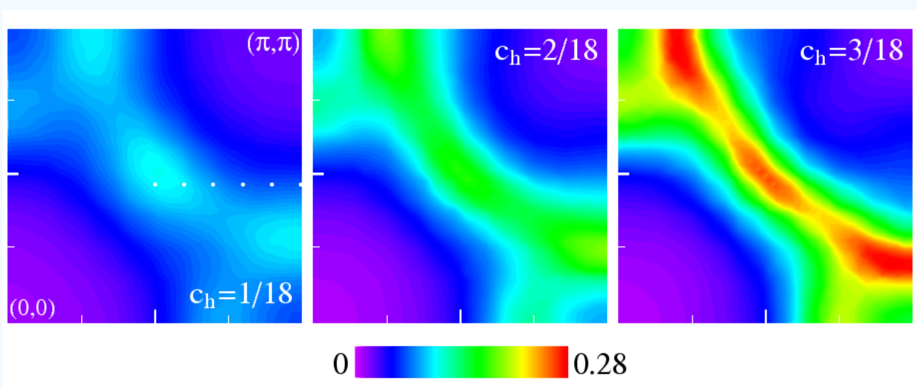
Fermi surface evolution: A(k,ω=0)   Zemljič, Prelovšek PRB (07)



t - t'- t''- J model:
t'= - 0.3 t,   t''=0.12 t,
J=0.4 t

c_h = 1/20, 2/20, 3/20

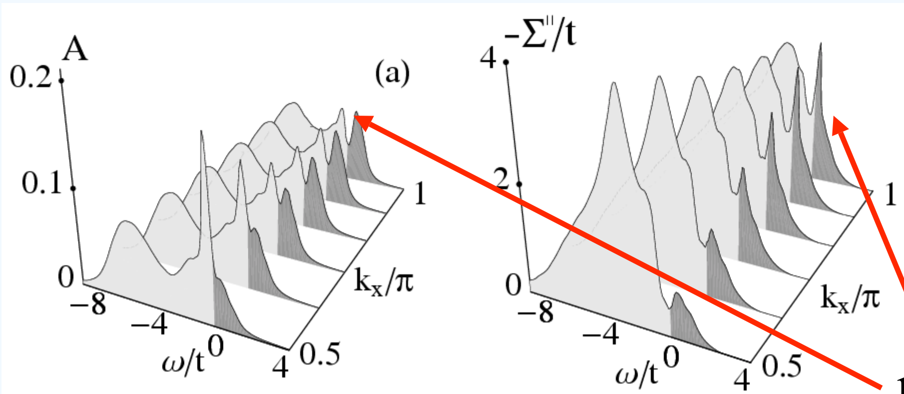
pseudogap   Fermi arc



t - J model:
J=0.3 t

c_h = 1/18, 2/18, 3/18

Pseudogap: spectral function and self energy along the 'Fermi line'



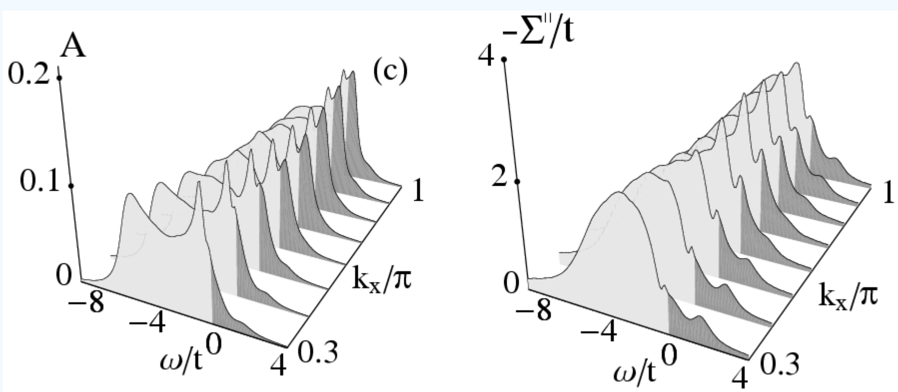
t - t' - J model:
low doping: $c_h = 0.05$

pseudogap contribution

$$\Sigma(\mathbf{k},\omega) \sim \Sigma_{MFL}(\mathbf{k},\omega) + \Delta^2_{\mathbf{k}}/(\omega - \omega^*_{\mathbf{k}} + i\Gamma_{\mathbf{k}})$$

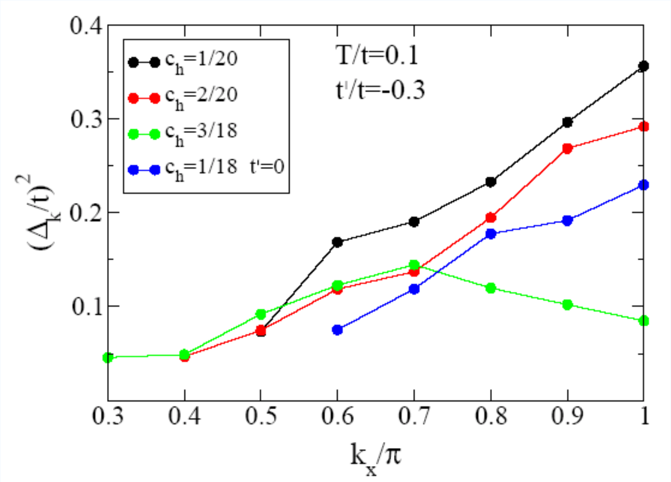
$$-\Sigma''_{MFL}(\mathbf{k},\omega\sim 0) \sim a_{\mathbf{k}} + b_{\mathbf{k}}|\omega|$$

marginal FL damping



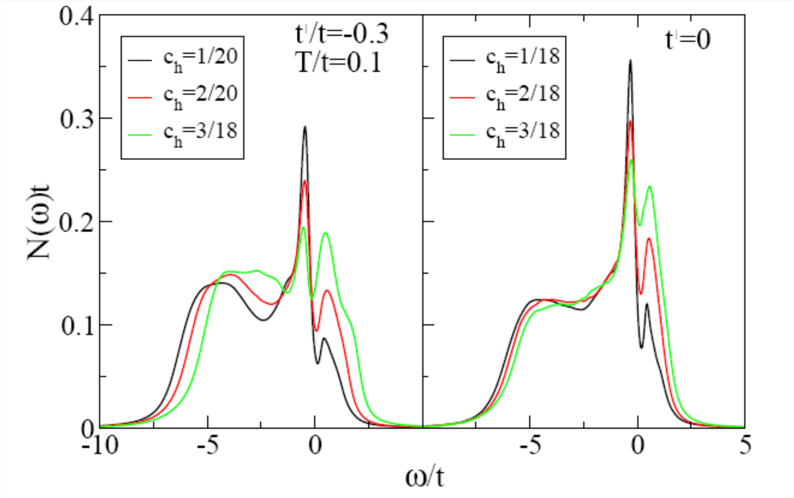
intermediate (optimum) doping:
$c_h = 0.17$

Pseudogap evolution:



pseudogap large:

a) antinodal region
b) low doping

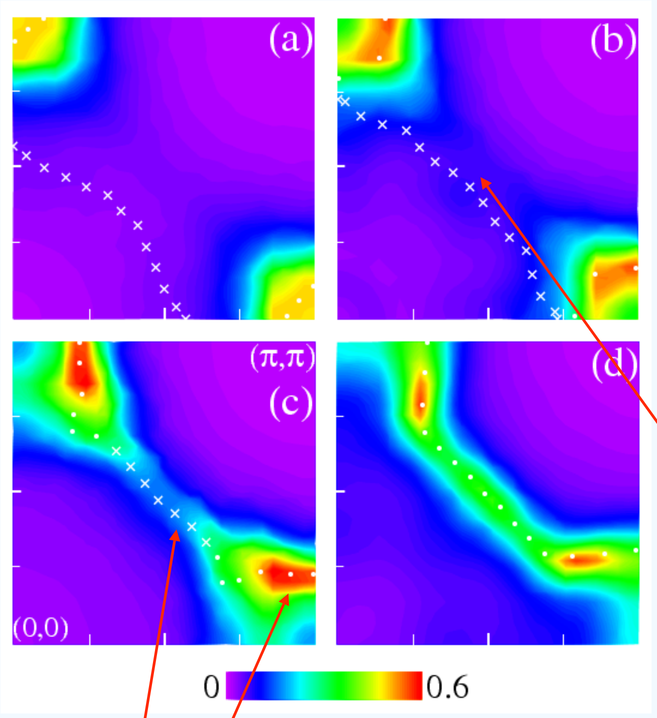


density of states:
integrated pseudogap

Electron-doped case

t – t' – J model: t' = 0.3 t, J=0.3 t

Zemljic, PP, Tohyama, PRB (07)



c_e = 1/20, 2/20, 3/20, 4/18

Fermi surface evolution:

a) electron pockets at low doping

b) large FS at OD

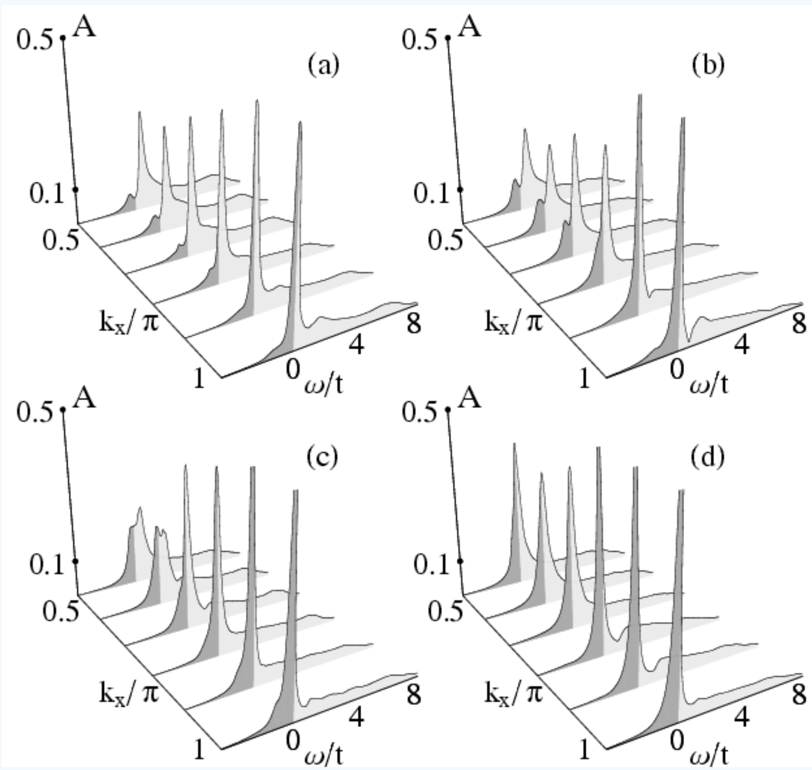
no closing of Mott-Hubbard gap !

pseudogap along zone diagonal

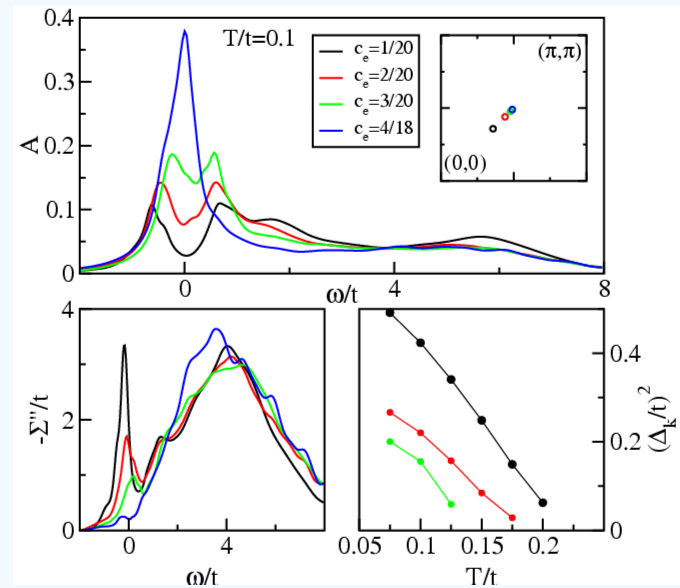
Luttinger line - GF zero : pole

Pseudogap evolution:

SF along the AFM zone boundary

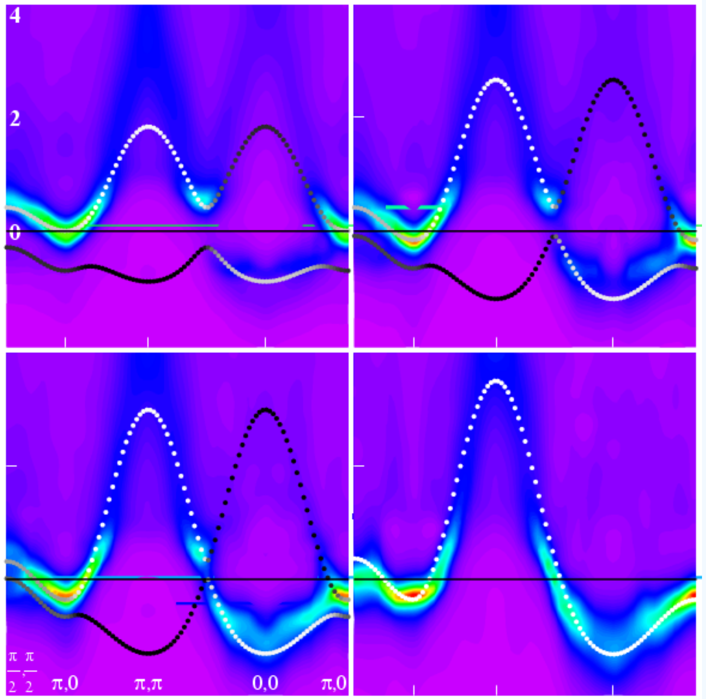


$c_e = 1/20, 2/20, 3/20, 4/18$



pseudogap closing with doping and T

Effective bands:



$c_e = 1/20,\ 2/20,\ 3/20,\ 4/18$

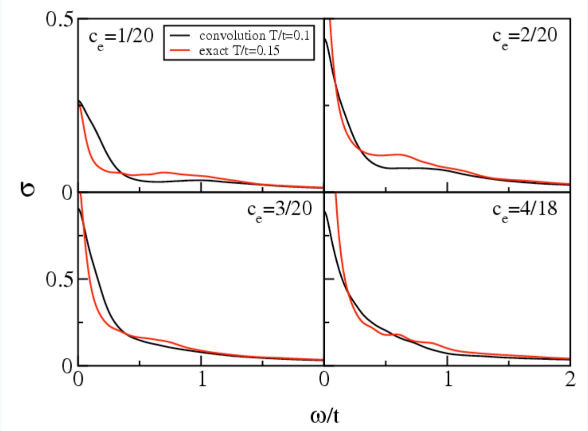
$$\epsilon_{\pm}(\mathbf{k}) = -4\tilde{t}'\gamma'_{\mathbf{k}} \pm \sqrt{(4\tilde{t}\gamma_{\mathbf{k}})^2 + w\bar{s}^2}$$

two effective bands:

a) splitting vanishes in overdoped

b) splitting due to AFM order ?

c) band renormalization smaller relative to hole-doped case

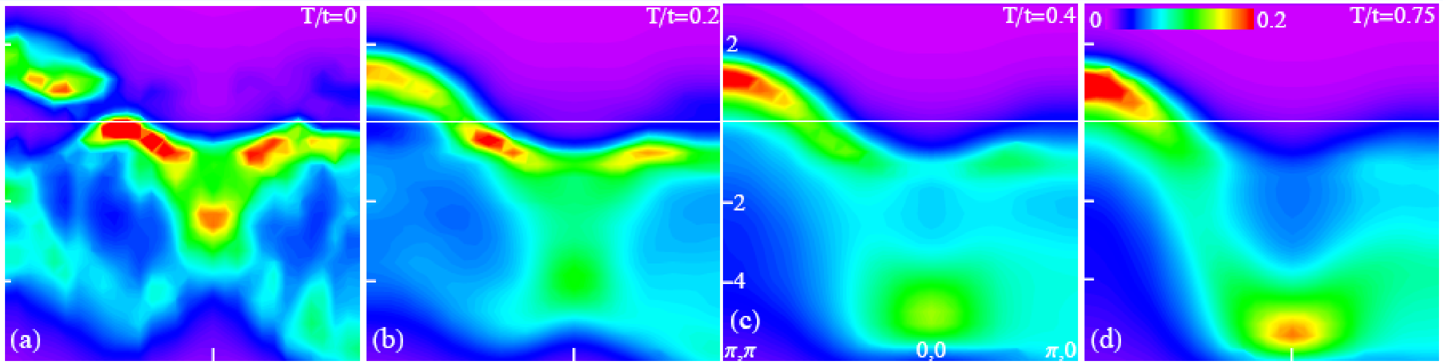


the same pseudogap shows up in optical conductivity

High energy kink - waterfall

extended t-J model: t'= - 0.3 t, t''=0.12 t, J=0.4 t

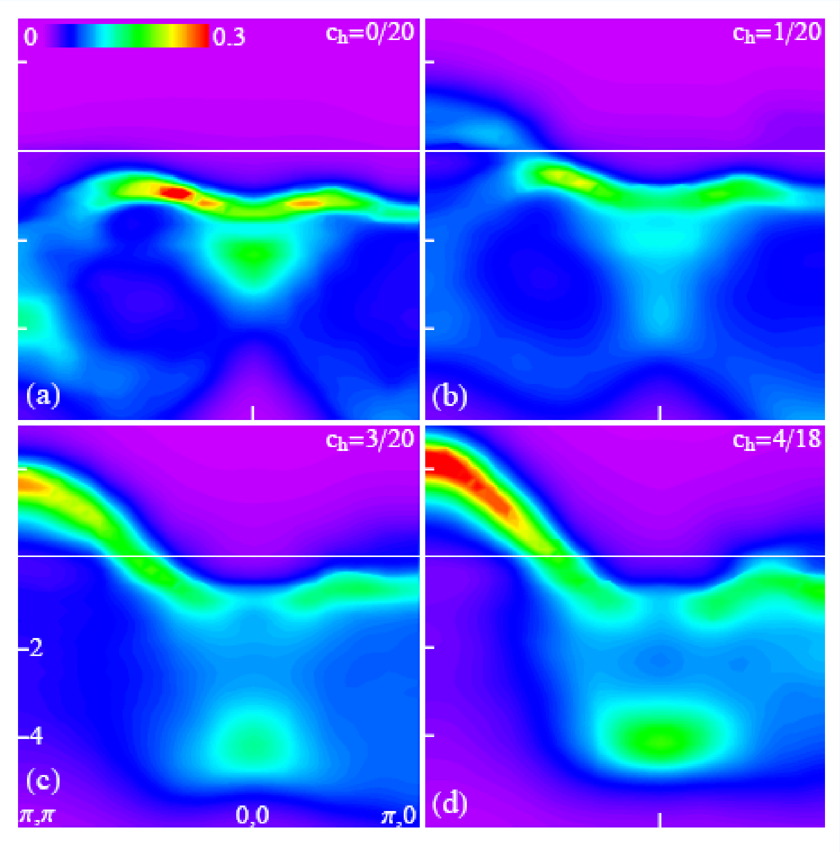
low hole doping: c_h = 2/20 = 0.1 Zemljic, PP, Tohyama, cond-mat/07..



T – dependence : T/t = 0, 0.2, 0.4, 0.75

- **waterfall even at T = t >> J:** eliminates several scenarios ?
- at low T < J coexisting band: renormalized QP band + bottom band
- no waterfall in the IPES part

doping dependence: t – J model



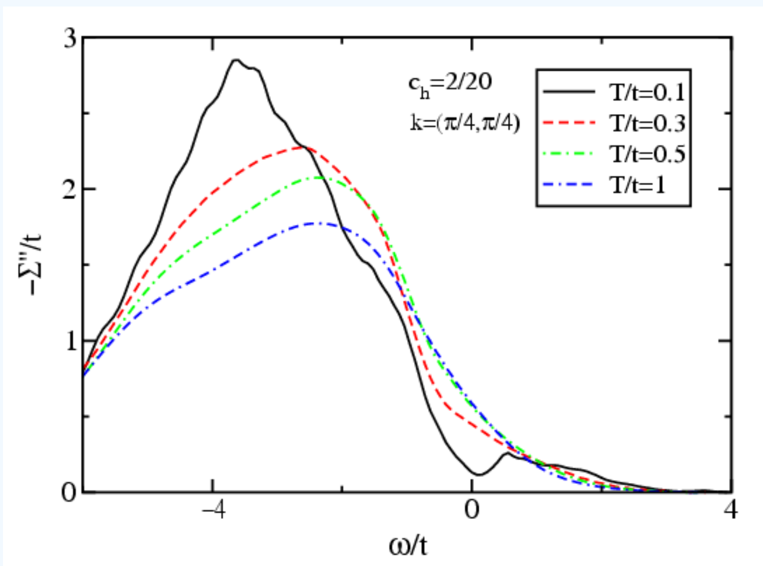
J = 0.3 t, T = 0.1 t

c_h = 0.05, 0.1, 0.15, 0.22

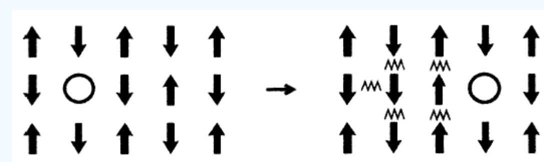
similarity to T dependence

origin of high-energy kink and waterfall:

anomalous self energy, characteristic for strong correlation
correlated motion of hole: **Brinkman – Rice incoherent band**



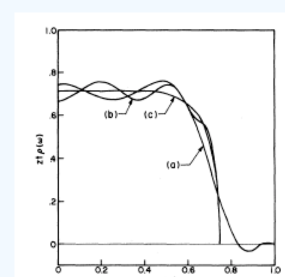
- weakly dependent on T, except at T ~ 0
- weakly dependent on c_h
- magnitude and shape close to BR retreacable path app.



$$\Sigma^A(\omega) = \tfrac{1}{2} \pm \left[\tfrac{1}{4} - (z-1)t^2/\omega^2\right]^{1/2}$$

$$\omega_{\mathbf{k}} - \zeta_{\mathbf{k}} + \frac{1}{\pi}\int d\omega' \frac{\Sigma''(\mathbf{k},\omega')}{\omega_{\mathbf{k}} - \omega'} = 0$$

$$\eta_{\mathbf{k}}^2 = -\int \Sigma''(\mathbf{k},\omega) d\omega/\pi \sim 3 - 4\, t^2$$



Luttinger sum rule

$$N = \sum_{\mathbf{k}s, G_s(\mathbf{k},0)>0} 1$$

T=0: determines Fermi (Luttinger) surface $\mathbf{k_F}$

a) metal: $G_s(\mathbf{k}, \omega = 0)$ has poles (changes sign) at chem. potential μ and k = k_F on Fermi surface

b) insulator: $G_s(\mathbf{k}, \omega = 0)$ has zeroes at k = k_F - Luttinger surface

Validity of LSR:

a) existence of functional for skeleton diagrams: validity of perturbation expansion – adiabatic connection to noninteracting fermions
b) valid also for finite systems
c) can be generalized for inhomogeneous systems etc.

Basic steps to LSR:

$$N = \frac{1}{\beta}\sum_{l}\sum_{\mathbf{k}s}\mathcal{G}_s(\mathbf{k},\omega_l)e^{i\omega_l 0^+}$$

$$N = I_1 + I_2$$

$$I_1 = -\frac{1}{2\pi i}\sum_{\mathbf{k}s}\int_\Gamma \frac{\partial}{\partial\zeta}\ln(\mathcal{G}_s(\mathbf{k},\zeta))e^{\zeta 0^+}\frac{1}{e^{\beta\hbar\zeta}+1}d\zeta$$

$$I_2 = \frac{1}{2\pi i}\sum_{\mathbf{k}s}\int_\Gamma \mathcal{G}_s(\mathbf{k},\zeta)\frac{\partial}{\partial\zeta}\Sigma_s(\mathbf{k},\zeta)e^{\zeta 0^+}\frac{1}{e^{\beta\hbar\zeta}+1}d\zeta$$

construction of functional Y' – closed linked skeleton diagrams:

$T \to 0$ $\quad$ $I_2 = \partial Y'/\partial\delta\epsilon = 0$

→ $$N = -\frac{1}{2\pi i}\sum_{\mathbf{k}s} 2\mathrm{Im}[\int_{-\infty}^{0} d\zeta\{\frac{\partial}{\partial\zeta}\ln(G_s(\mathbf{k},\zeta))\}]$$

counting poles and zeroes of Green's function
valid also for finite systems

$$N = \sum_{\mathbf{k}s, G_s(\mathbf{k},0)>0} 1$$

LSR on finite systems

Kokalj, PP, PRB (07)

$$H = -\sum_{i,j,s} t_{ij} c^{\dagger}_{js} c_{is} + H_{int}$$

tight binding models: Hubbard, t-J,...

$$\mu_N = (E_0^{N+1} - E_0^{N-1})/2$$

from: $N = T\partial(\ln\Omega)/\partial\mu$ $\quad T \to 0$

$$G_s(\mathbf{k},\zeta) = \sum_m \frac{\left|\langle m_{N-1}|c_{\mathbf{k}s}|0_N\rangle\right|^2}{\zeta + \mu_N - (E_0^N - E_m^{N-1})} + \sum_l \frac{\left|\langle l_{N+1}|c^{\dagger}_{\mathbf{k}s}|0_N\rangle\right|^2}{\zeta + \mu_N - (E_l^{N+1} - E_0^N)}$$

$G_s(\mathbf{k},\omega = 0)$ calculated on small system:
full diagnalisation or Lanczos method

Small system results

excluding 'trivial' violations of LSR:

- level crossing – change of g.s. character, quantum numbers: FM, LRO..
- degenerate g.s.
- level crossing of $|0_{N+1}>$ or $|0_{N-1}>$

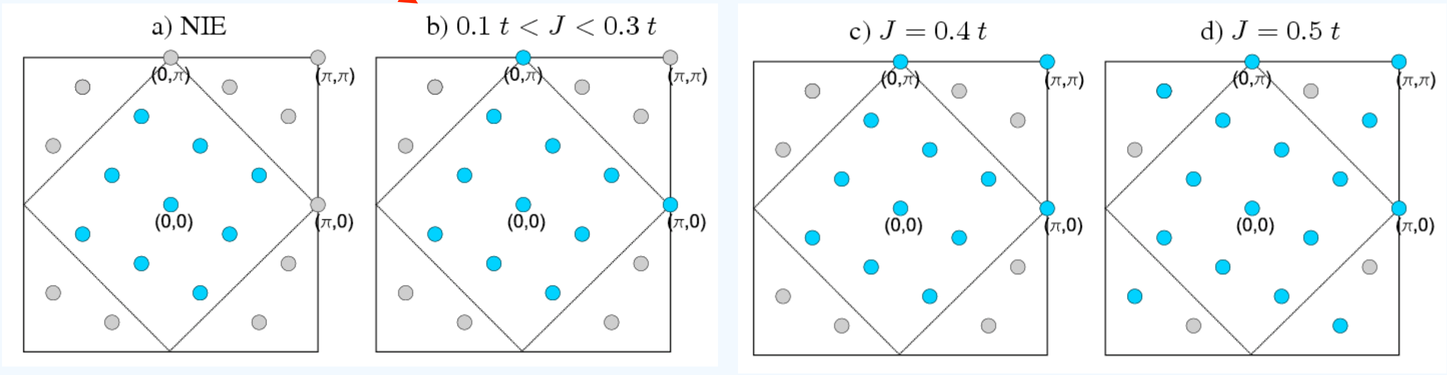
a) 2D t - U Hubbard model: U/t = 0 – 50, sites N_0 = 8, 10, 16

no evident LSR violation (for small systems)

b) 2D t – J model:

LSR violation - $N_0 = 20$ with N = 18 fermions (2 holes)

origin – model in restricted basis – nonperturbative ?



LSR in Mott – Hubbard insulator

Example: **2D Hubbard model**

μ inside the MH gap: possible moment expansion in t/U

$$G(\mathbf{k},\omega) = \int_{-\infty}^{\infty} \frac{A(\mathbf{k},\omega')}{\omega+\mu-\omega' \pm i\eta} d\omega'$$

Kokalj, PP, cond-mat/07..

$$G(\mathbf{k},0) = G^-(\mathbf{k},0) + G^+(\mathbf{k},0)$$

$$G^-(\mathbf{k},0) = \sum_{n=0}^{\infty} \left(\frac{2}{U}\right)^{n+1} \sum_{m=0}^{n} M^-_{n-m}(\mathbf{k}) \binom{n}{m} (-\tilde{\mu})^m$$

$$\tilde{\mu} = \mu - U/2$$

$$M^-_l(\mathbf{k}) = \langle [H, \dots [H, c^\dagger_{\mathbf{k}s}]] c_{\mathbf{k}s} \rangle$$

$$M_0^{\mp}(\mathbf{k}) = \frac{1}{2} \pm \frac{2}{U} \sum_\delta \varepsilon_\delta(\mathbf{k}) [\langle \mathbf{S}_\delta \cdot \mathbf{S}_0 \rangle - \frac{1}{4}] + O(\frac{t_{ij}^2}{U})$$

$$\varepsilon_\delta(\mathbf{k}) = -t_\delta \sum_{i_\delta} \mathrm{e}^{i\mathbf{k}\mathbf{r}_{i\delta}}$$

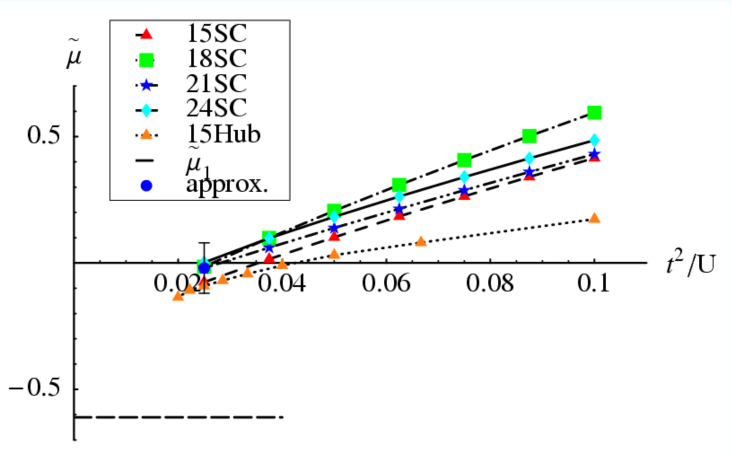
$$G(\mathbf{k},0) = \frac{4}{U^2} \left(\sum_\delta 4\varepsilon_\delta(\mathbf{k}) \langle \mathbf{S}_\delta \cdot \mathbf{S}_0 \rangle - \tilde{\mu} \right) + O(\frac{t_{ij}^2}{U^3})$$

Results

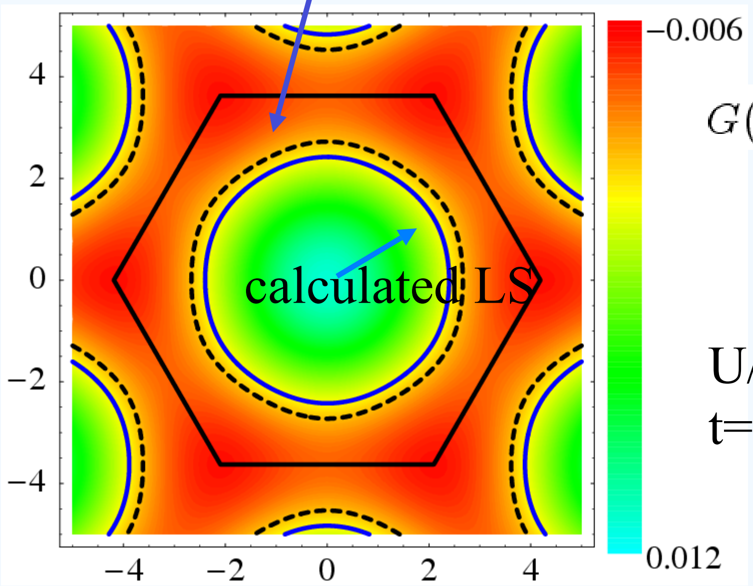
a) LSR satisfied for model with particle – hole symmetry:
Hubbard on bipartite lattice

b) (generally ?) violated on lattices without p-h symmetry:

Hubbard on triangular lattice



noninteracting FS



Summary

Hole – doped cuprates:

- Fermi surface evolution with doping: hole pocket – large FS

H

- self energy: MFL part + pseudogap contribution

o

- pseudogap vanishes in OD regime and for T>T* ~J

le

Electron – doped cuprates:

- Fermi surface: electron pocket – large FS: no vanishing of MH gap
- pseudogap along zone diagonal
- double band: sue to SDW-like splitting

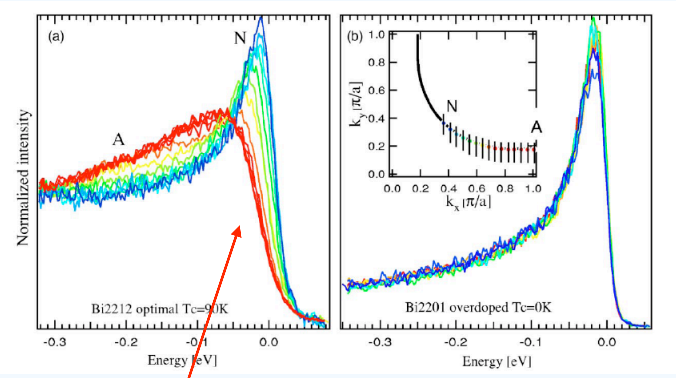
High – energy kink, waterfall:

- general feature in hole-dispersion for $\omega < 0$, not for EDC for $\omega < 0$!
- persists up to T ~ t, origin incoherent motion a la Brinkman-Rice

Luttinger sum rule:

- (in principle) valid also for finite systems, violated for t - J model
- violated for Mott – Hubbard insulator without p – h symmetry

QP relaxation rate: momentum dependence



Kaminski et al (05)

pseudogap