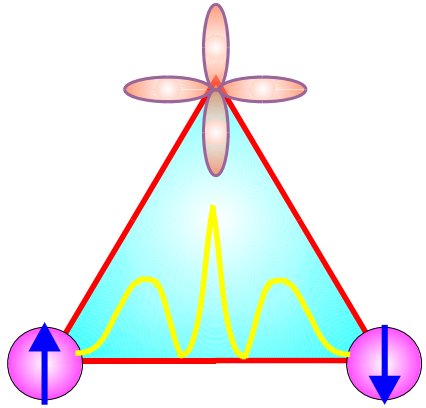
$U+t \Rightarrow J \Rightarrow \Delta$?



Efficient Perturbation Theory for Correlated Higher T_c Materials

A. Lichtenstein

University of Hamburg

In collaborations with:

H. Hafermann, M. Kecker, F. Lechermann, S. Brener (Hamburg)

A. Rubtsov (Moscow)

M. Katsnelson, I. Di Marco (Nijmegen)

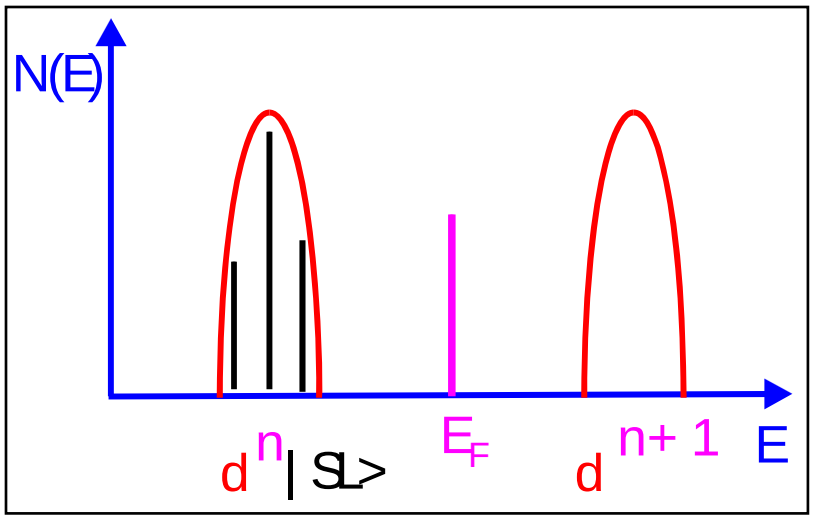
Outline

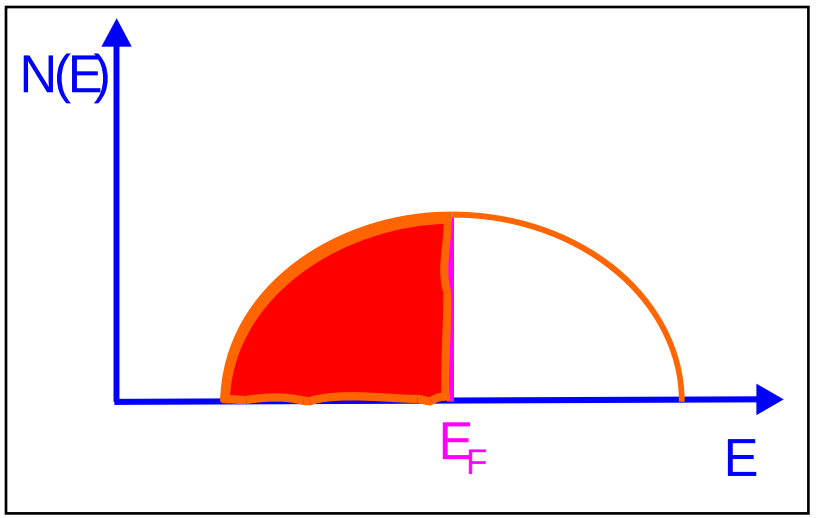
- Correlated systems: non-perturbative DMFT
- Beyond DMFT: Dual Fermion approach
- Antiferromagnetic pseudogap
- d-wave: BSE
- Conclusions

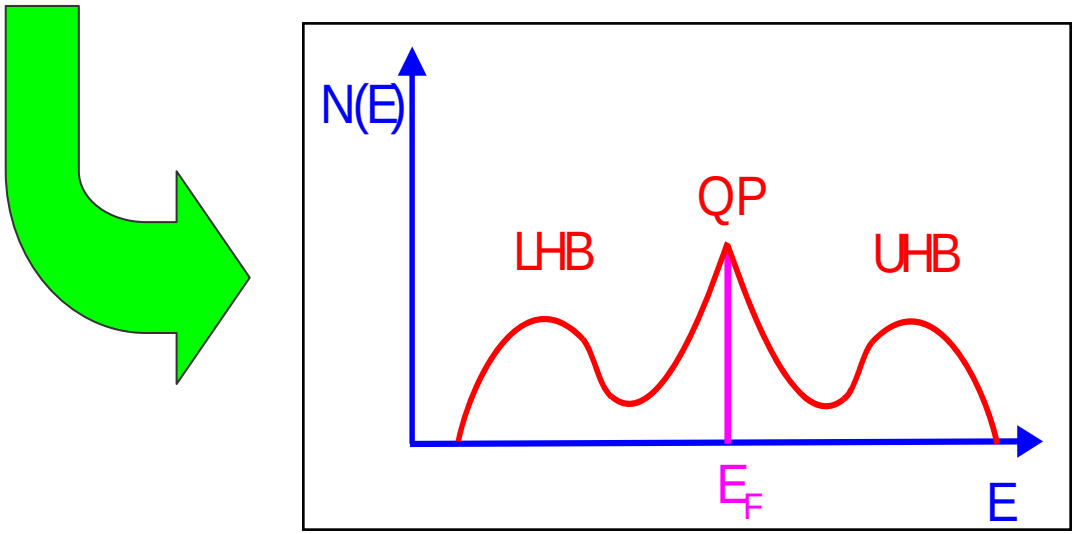
From Atom to Solid: DMFT

Atomic physics

Bands effects (LDA)

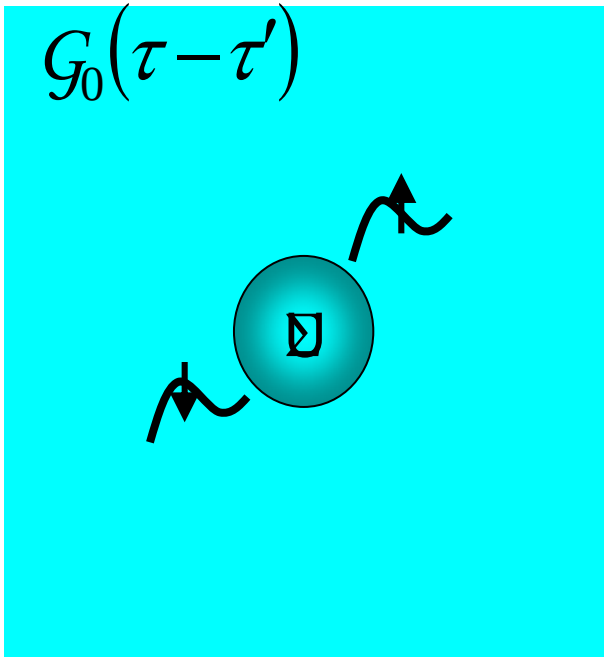






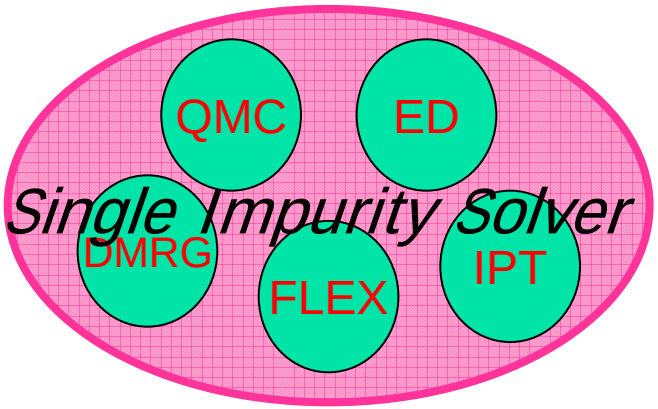
LDA+DMFT

DMFT: Self-Consistent Set of Equations



$$\hat{G}(i\omega_n)=\frac{1}{\Omega}\sum_{\vec{k}}^{BZ}\hat{G}(\vec{k},i\omega_n)$$

$$\hat{\mathcal{G}}_0^{-1}(i\omega_n)=\hat{G}^{-1}(i\omega_n)+\hat{\Sigma}(i\omega_n)$$



$$\hat{\Sigma}_{new}(i\omega_n)=\hat{\mathcal{G}}_0^{-1}(i\omega_n)-\hat{G}^{-1}(i\omega_n)$$

A. Georges and G. Kotliar (1992)
W. Metzner and D. Vollhardt (1987)

Real Materials: LDA+DMFT

V. Anisimov, et al. J. Phys. CM **9**, 7359 (1997)
A. L. and M. Katsnelson PRB, **57**, 6884 (1998**)**

LDA+U
Static mean-field approximation
Energy-independent potential

$$\hat{V} = \sum_{mm'\sigma} | inlm\,\sigma > V^{\sigma}_{mm'} < inl\,m'\sigma |$$

Applications:
Insulators with long-range
spin-,orbital- and charge order

LDA+DMFT
Dynamic mean-field approximation
Energy-dependent self-energy operator

$$\hat{\Sigma}(\varepsilon) = \sum_{mm'\sigma} | inlm\sigma > \Sigma(\varepsilon)^{\sigma}_{mm'} < inlm'\sigma |$$

Applications:
Paramagnetic, paraorbital
strongly correlated metals

short range spin and orbital order

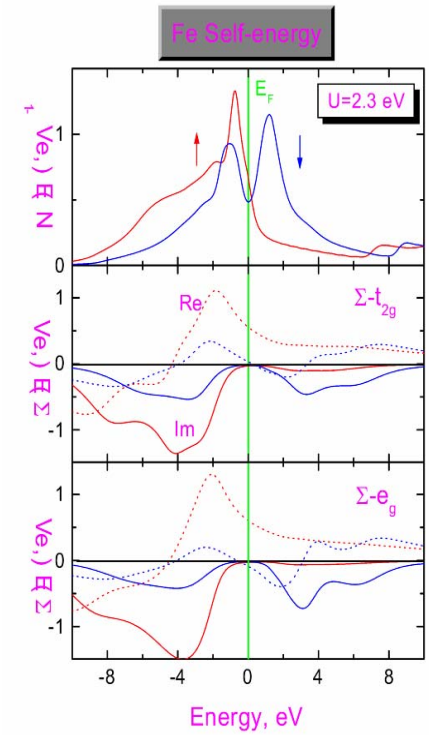
Cluster LDA+DMFT approximation

A. Poteryaev, A. L., and G. Kotliar, PRL **93**, 086401 (2004)

Spectral Function Fe: ARPES vs. DMFT

Vertical Pol.

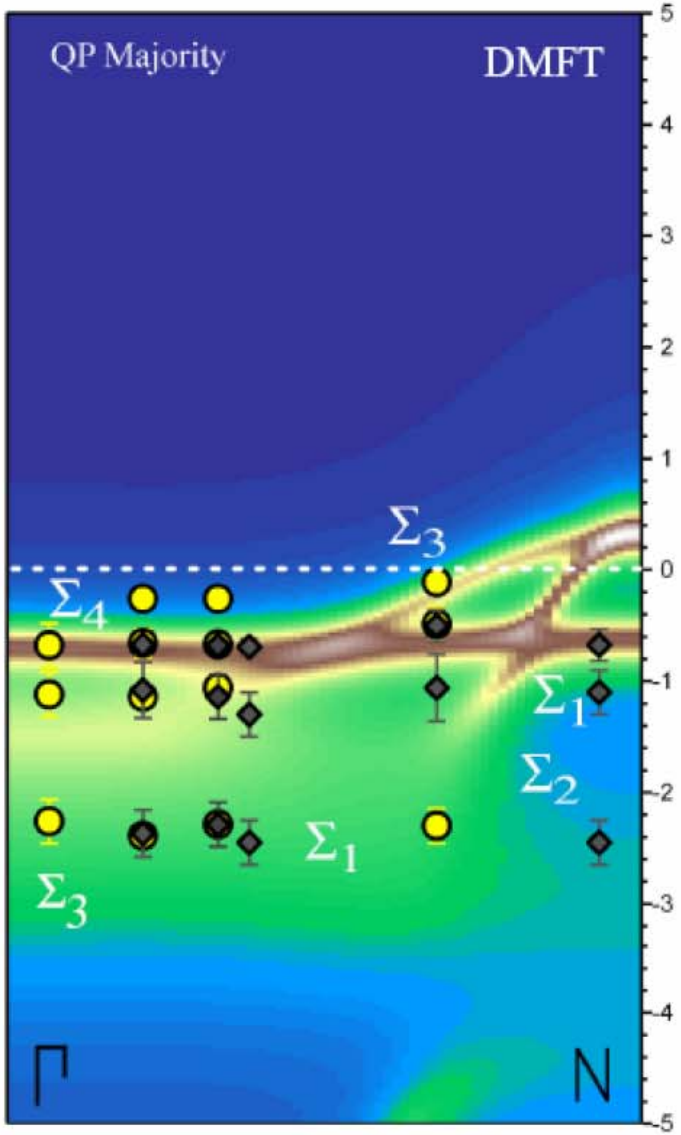
Horizontal Pol.

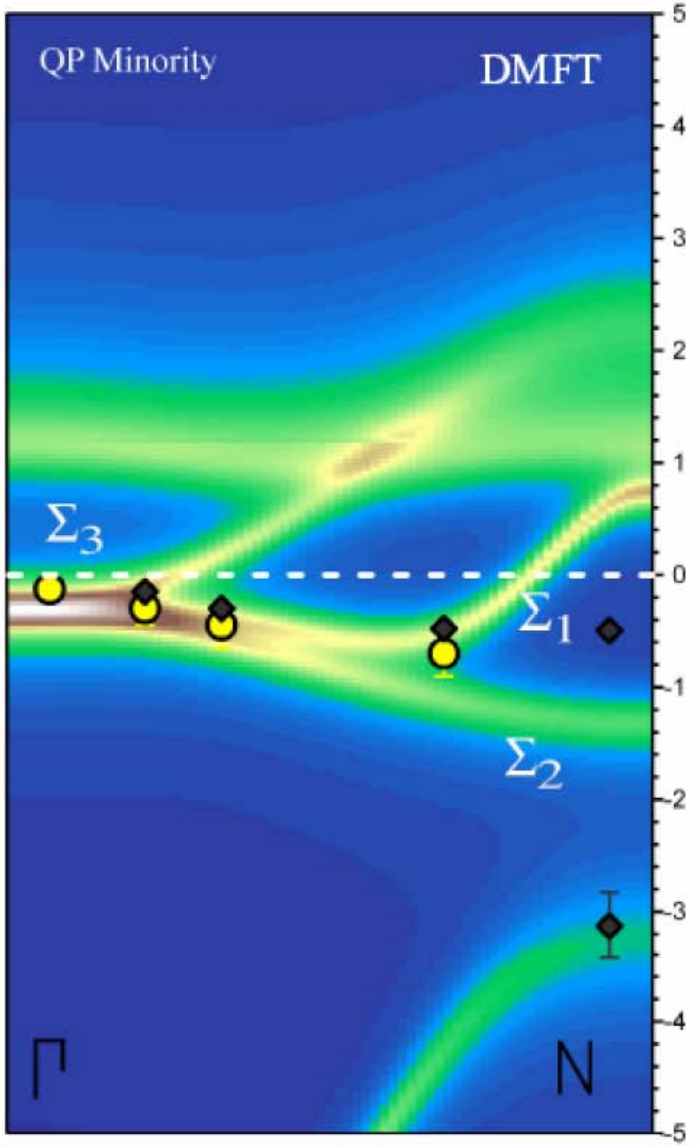


SP-ARPES:

J. Sánchez-Barriga, et al,

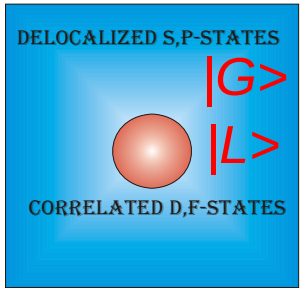
BESSY





General Projection formalism for LDA+DMFT

$$|L\rangle = |ilm\sigma\rangle \qquad \langle L_i|L_j\rangle = \delta_{ij}$$
$$|G\rangle = \left|n\,\vec{k}\,\sigma\right\rangle \qquad P_c = \langle L|G\rangle$$



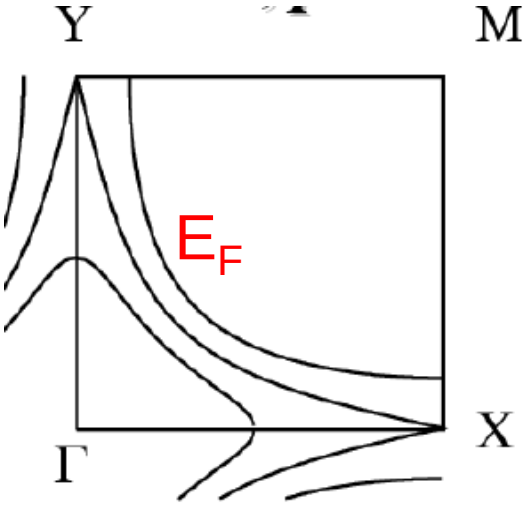
$$G^c_{mm'}(i\omega) = \sum_{\vec{k}\,nn'} \langle L_m|G_n\rangle \left[(i\omega+\mu)\,\hat{1} - \widehat{H}_{KS}(\vec{k}) - \Delta\Sigma(i\omega)\right]^{-1}_{nn'} \langle G_{n'}|L_{m'}\rangle$$

$$\Delta\Sigma_{nn'}(i\omega) = \sum_{mm'} \langle G_n|L_m\rangle\, \Delta\Sigma_{mm'}(i\omega)\, \langle L_{m'}|G_{n'}\rangle$$

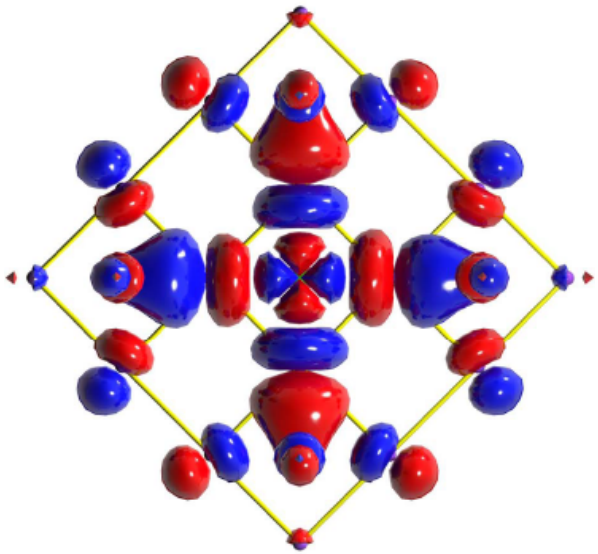
$$\Sigma_{mm'}(i\omega) = \left(G_0^{-1} - G^{-1}\right)_{mm'}$$
$$\Delta\Sigma_{mm'}(i\omega) = \Sigma_{mm'}(i\omega) - \Sigma_{dc}$$

G. Trimarchi *et al*. JPCM **20**,135227 (2008)
B. Amadon *et al*. PRB **77**, 205112 (2008)

HTSC: from LDA to 1-band model

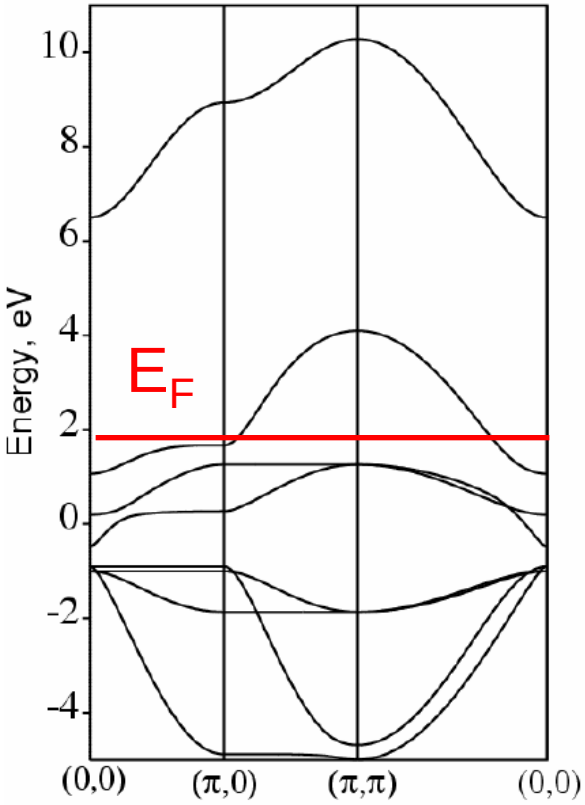


La_2CuO_4

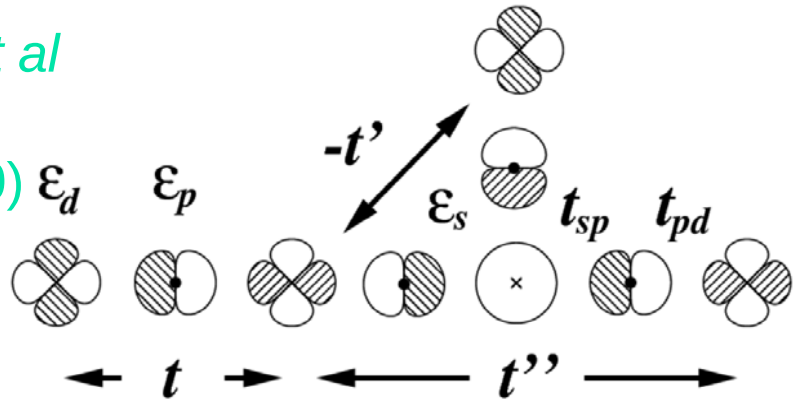


O.K. Andersen, *at al*
J. Phys. Chem. Solids
56, 1573 (1995)

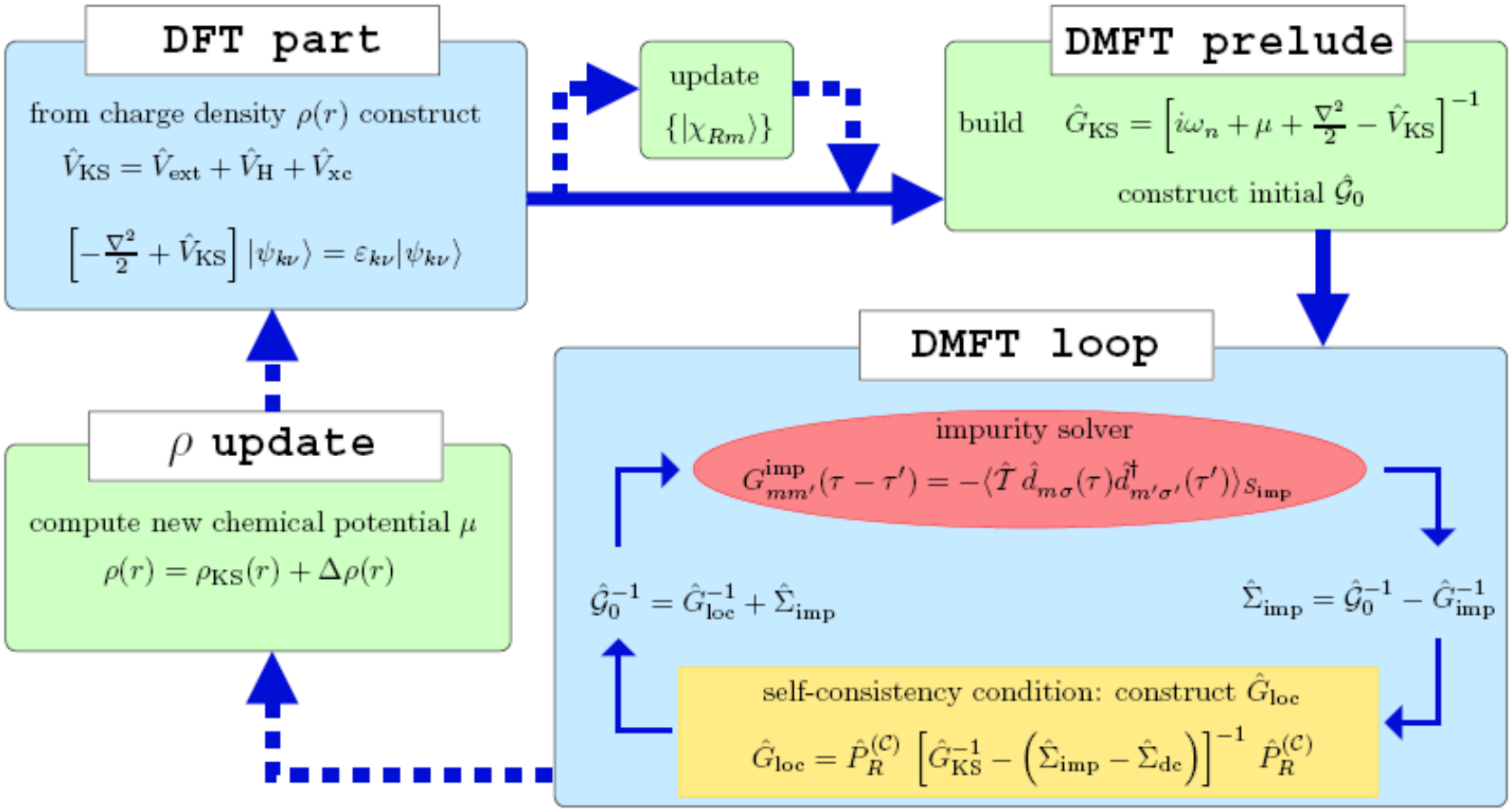
From LDA "Chemistry"
to
Low-energy TB-model
t'/t=r (-0.3 for YBCO)
$t_\perp \sim (\cos k_x - \cos k_y)^2$



NMTO-orbitals
O.K. Andersen, *et al*
Phys. Rev. B
62, R16219 (2000)



SCF-LDA+DMFT



F. Lechermann, et al, PRB (2007)

Continuous Time QMC formalism

Partition function and action for fermionic system with pair interactions

$$Z = \mathrm{Tr}(Te^{-S})$$

$$S = \int\int t_r^{r'} c_{r'}^{+} c^r dr dr' + \int\int\int\int w_{r_1 r_2}^{r'_1 r'_2} c_{r'_1}^{+} c^{r_1} c_{r'_2}^{+} c^{r_2} dr_1 dr'_1 dr_2 dr'_2$$

$$r = \{\tau, i, s\}$$

$$\int dr = \int_0^\beta d\tau \sum_i \sum_s$$

Splitting of the action into Gaussian part and interaction

$$S = S_0 + W$$

$$S_0 = \int\int \left(t_r^{r'} + \int\int \alpha_{r'_2}^{r_2} \left(w_{r_1 r_2}^{r'_1 r'_2} + w_{r_2 r_1}^{r'_2 r'_1} \right) dr_2 dr'_2 \right) c_{r'}^{+} c^r dr dr'$$

$$W = \int\int\int\int w_{r_1 r_2}^{r'_1 r'_2} \left(c_{r'_1}^{+} c^{r_1} - \alpha_{r'_1}^{r_1} \right) \left(c_{r'_2}^{+} c^{r_2} - \alpha_{r'_2}^{r_2} \right) dr_1 dr'_1 dr_2 dr'_2$$

$\alpha_{r'}^{r}$ -- additional parameters, which are necessary to minimize the sign problem

A. Rubtsov *"Quantum Monte Carlo determinantal algorithm without Hubbard-Stratonovich transformation: a general consideration "*

arXiv: 0302228

Continuous Time QMC formalism

Formal perturbation-series:

$$Z = \sum_{k=0}^{\infty} \int dr_1 \int dr'_1 \ldots \int dr_{2k} \int dr'_{2k} \Omega_k (r_1, r'_1, \ldots, r_{2k}, r'_{2k})$$

$$\Omega_k (r_1, r'_1, \ldots, r_{2k}, r'_{2k}) = Z_0 \frac{(-1)^k}{k!} w^{r'_1 r'_2}_{r_1 r_2} \ldots w^{r'_{2k-1} r'_{2k}}_{r_{2k-1} r_{2k}} D^{r_1 \ldots r_{2k}}_{r'_1 \ldots r'_{2k}}$$

$$D^{r_1 \ldots r_{2k}}_{r'_1 \ldots r'_{2k}} = \left\langle T \left(c^+_{r'_1} c^{r_1} - \alpha^{r_1}_{r'_1} \right) \ldots \left(c^+_{r'_{2k}} c^{r_{2k}} - \alpha^{r_{2k}}_{r'_{2k}} \right) \right\rangle$$

Since S_0 is Gaussian one can apply the Wick theorem → *D* can be presented as a determinant g0

The Green function can be calculated as follows

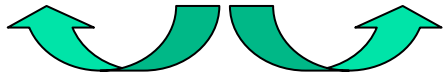
$$g^r_{r'}(k) = \frac{\left\langle T c^+_{r'} c^r \left(c^+_{r'_1} c^{r_1} - \alpha^{r_1}_{r'_1} \right) \ldots \left(c^+_{r'_{2k}} c^{r_{2k}} - \alpha^{r_{2k}}_{r'_{2k}} \right) \right\rangle}{\left\langle T \left(c^+_{r'_1} c^{r_1} - \alpha^{r_1}_{r'_1} \right) \ldots \left(c^+_{r'_{2k}} c^{r_{2k}} - \alpha^{r_{2k}}_{r'_{2k}} \right) \right\rangle}$$

ratio of determinants → In practice efficient calculation of a ratio is possible due to fast-update formulas

A. Rubtsov and A.L., JETP Lett. **80**, 61 (2004)

Random walks in the *k* space

$Z = \ldots Z_{k-1} + Z_k + Z_{k+1} + \ldots$



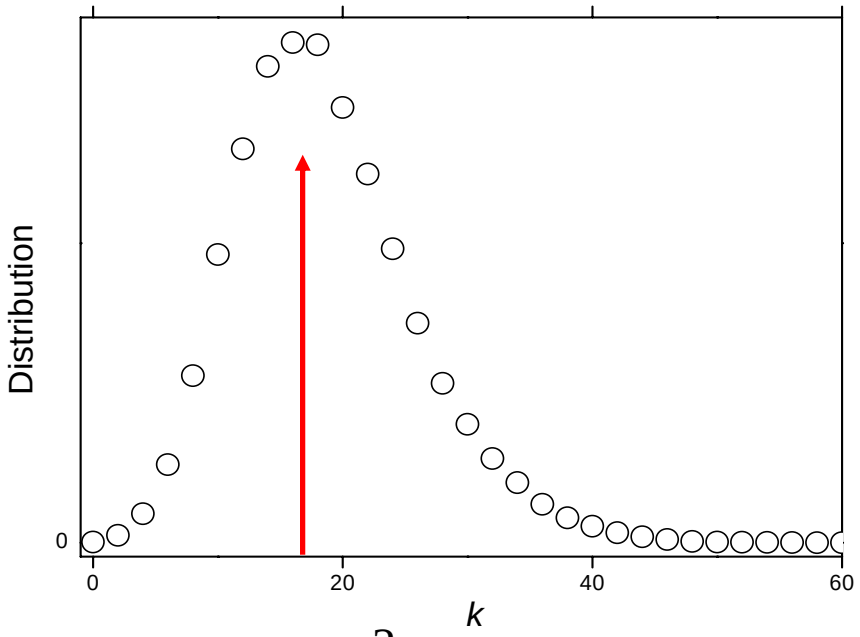
k-1 *k*+1

Acceptance ratio

decrease

Step *k*-1

$$\frac{k}{|w|}\frac{D^{k-1}}{D^k}$$



increase

Step *k*+1

$$\frac{|w|}{k+1}\frac{D^{k+1}}{D^k}$$

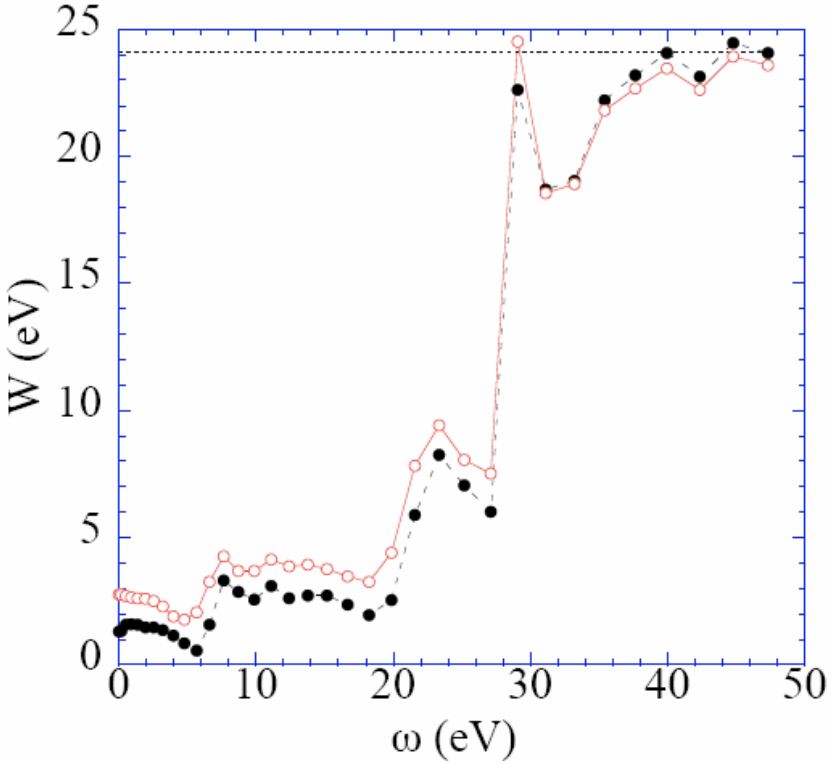
Maximum at $\beta U N^2$

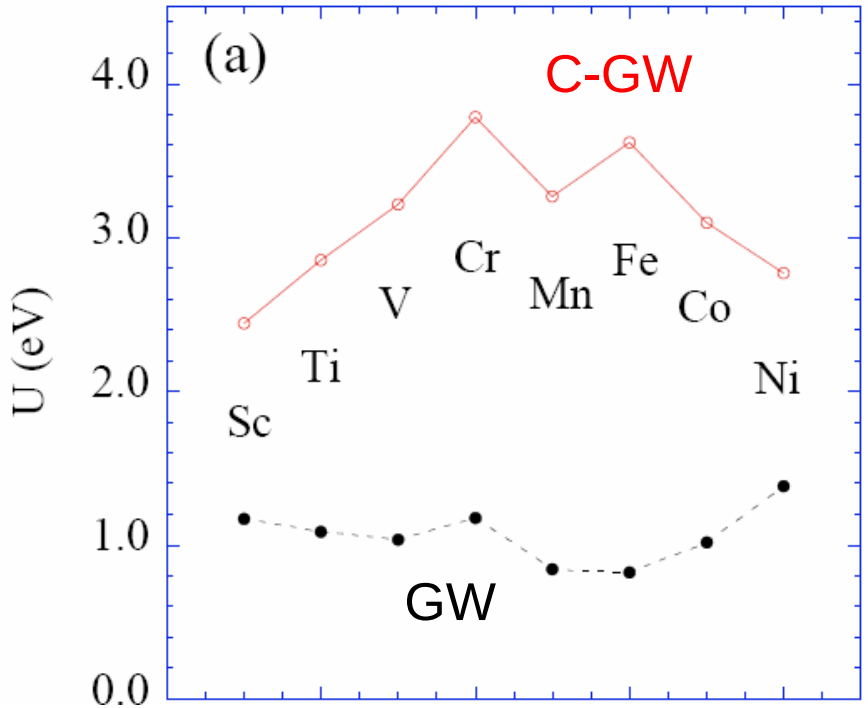
Wannier - GW and effective U(ω)

$$|\varphi_{n\mathbf{R}}\rangle = \frac{V}{(2\pi)^3}\int e^{-i\mathbf{k}\cdot\mathbf{R}}|\psi^{(\mathrm{w})}_{n\mathbf{k}}\rangle d^3k$$

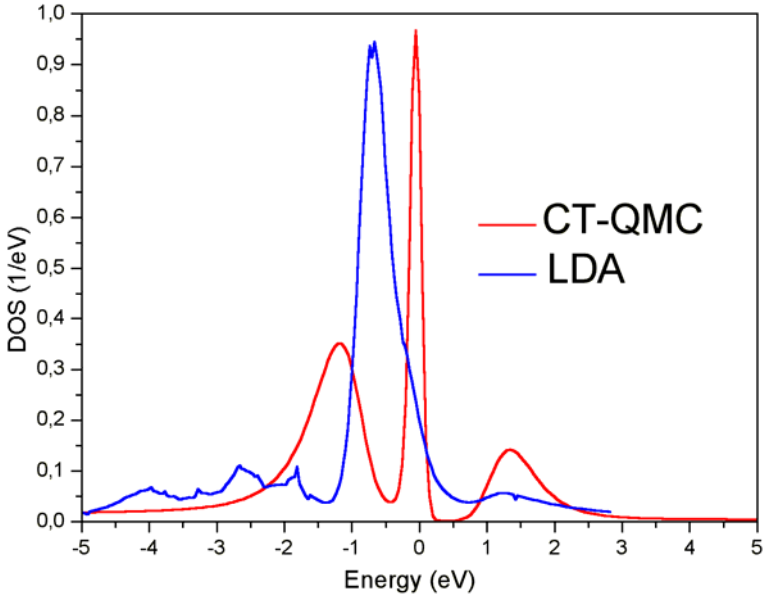
$$|\psi^{(\mathrm{w})}_{n\mathbf{k}}\rangle = \sum_m \mathcal{U}_{mn}(\mathbf{k})|\psi_{m\mathbf{k}}\rangle$$

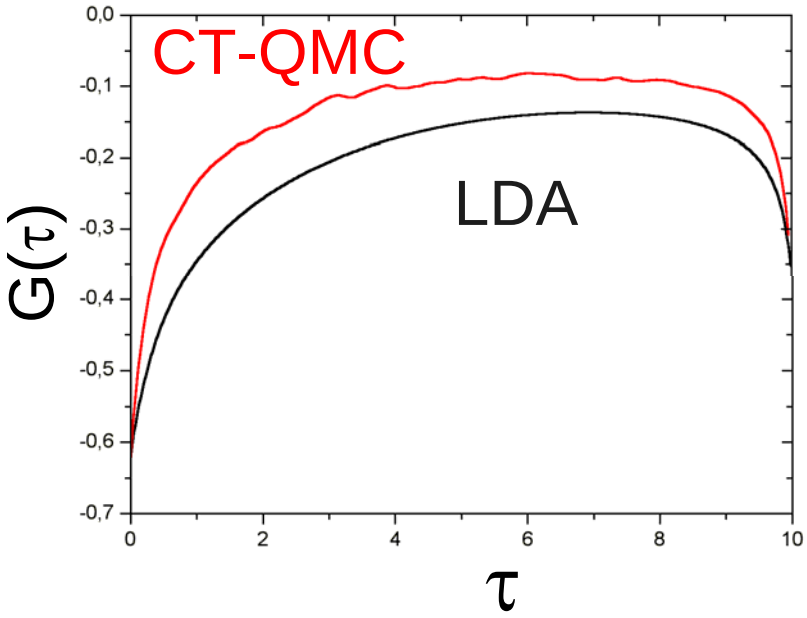
T. Miyake and F. Aryasetiawan
Phys. Rev. B 77, 085122 (2008)





Co on Cu: 5d-orbitals QMC calculation

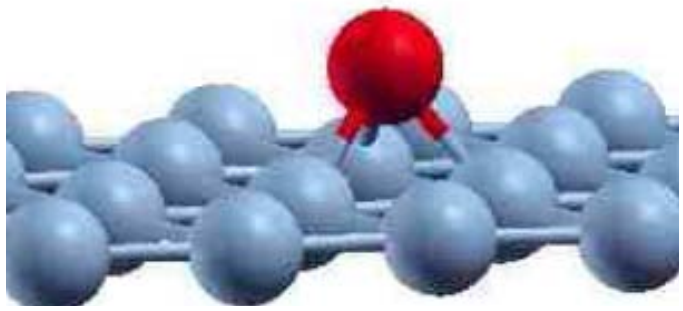




DOS for Co atom in Cu

U=4, b = 10 (T ~ 1/40 W)

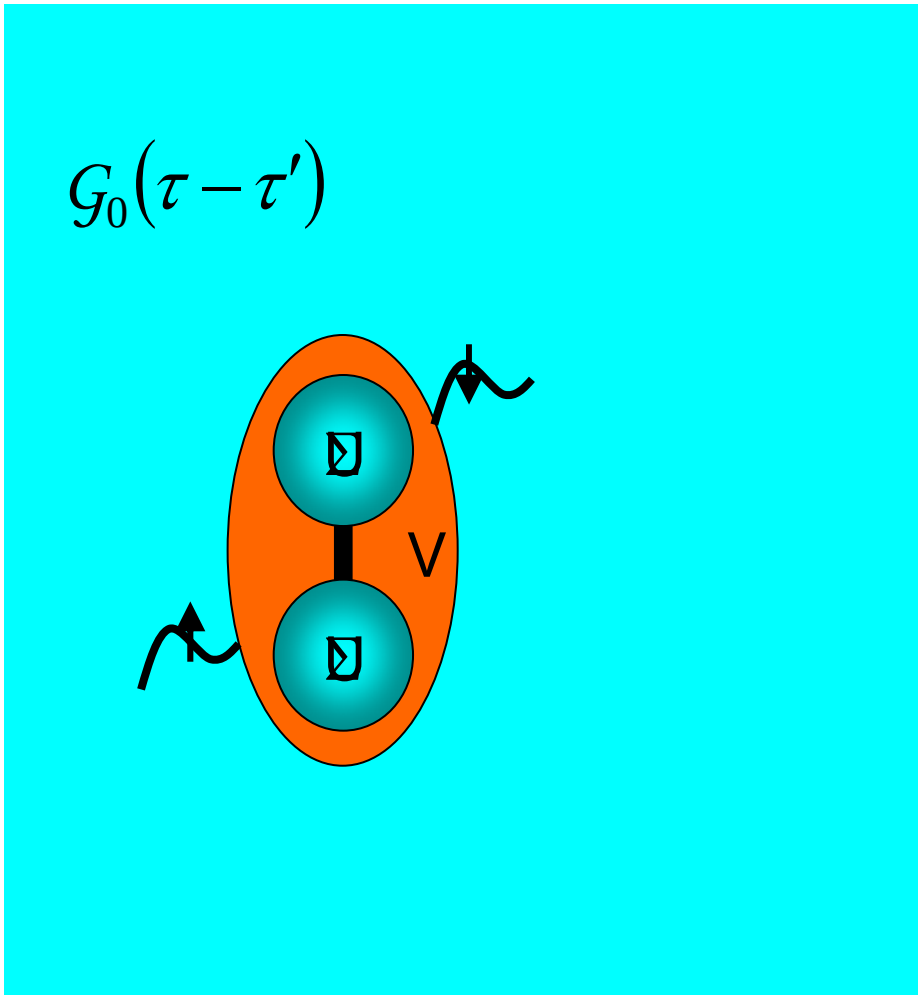
E. Gorelov et al, arXiv:0905.3581



Beyond single-site DMFT

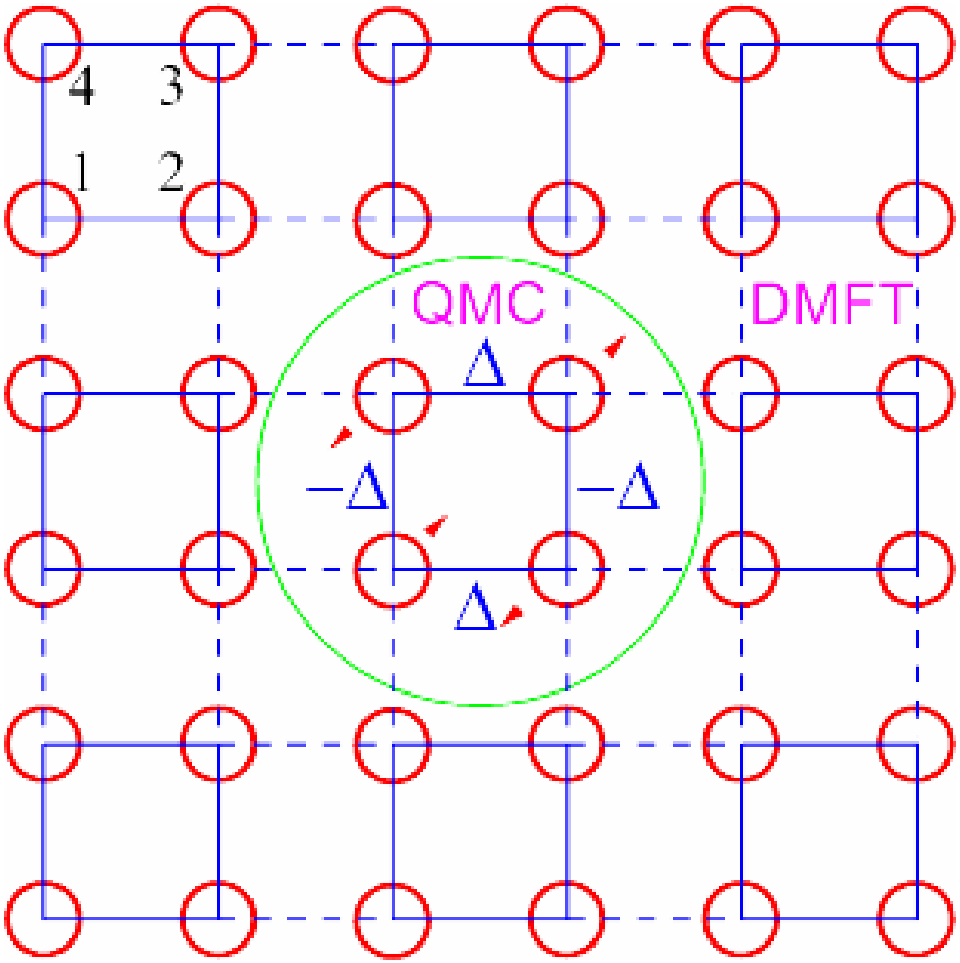
- 1/d expansion: A. Schiller and K. Ingersent PRL'95;
- A. Georges and G. Kotliar, et. al. RMP'96
- 2-site Bethe lattice: G. Moeller, PhD'94, et. al. , PRB'99
- DCA k-space: M. Jarrell: H. Hettler et. al. , PRB'98
- Cluster DMFT: A. L. and M. Katsnelson, PRB'00
- CDMFT: G. Kotliar et al. PRL'01
- Chain-DMFT: A. Georges, PRB'00, S. Biermann et al, PRL'01

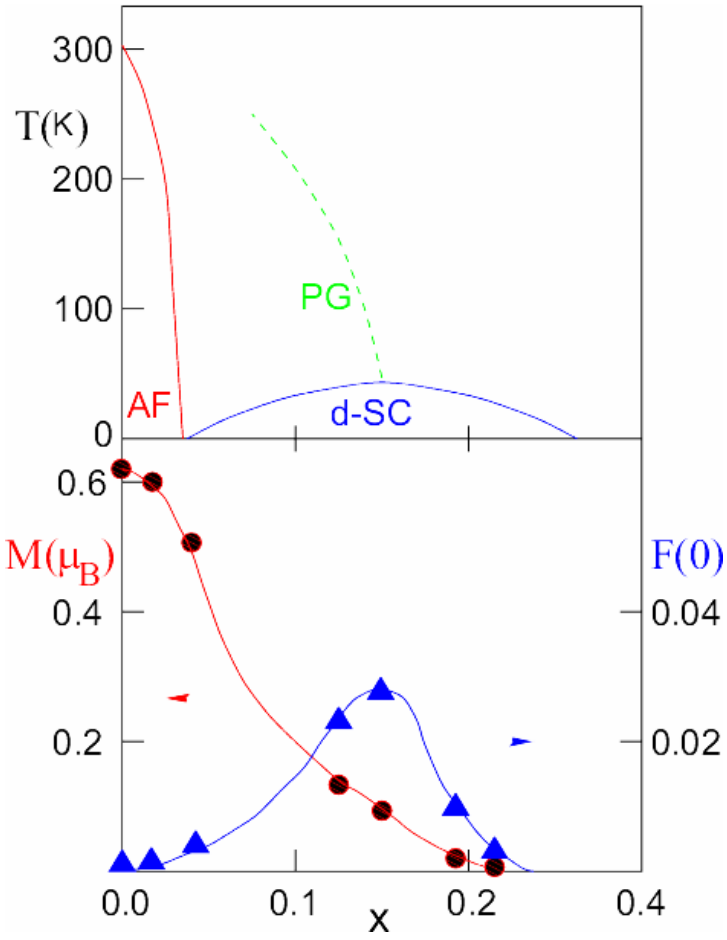
Cluster DMFT



M. Hettler et al, PRB **58**, 7475 (1998)
A. L. and M. Katsnelson, PRB **62**, R9283 (2000)
G. Kotliar, et al, PRL **87**, 186401 (2001)

AFM and d-wave in HTSC





A.L. and M.Katsnelson, PRB **62**, R9283 (2000)

AFM and d-wave in CDMFT (2x2)

$$G(\mathbf{k},i\omega) = [i\omega + \mu - h(\mathbf{k},i\omega)]^{-1}$$

$$h(\mathbf{k},i\omega) = \begin{pmatrix} \Sigma_0 & t_x K_x^+ & 0 & t_y K_y^+ \\ t_x^* K_x^- & \Sigma_0 & t_y K_y^+ & 0 \\ 0 & t_y^* K_x^- & \Sigma_0 & t_x^* K_x^- \\ t_y^* K_y^- & 0 & t_x K_x^+ & \Sigma_0 \end{pmatrix}$$

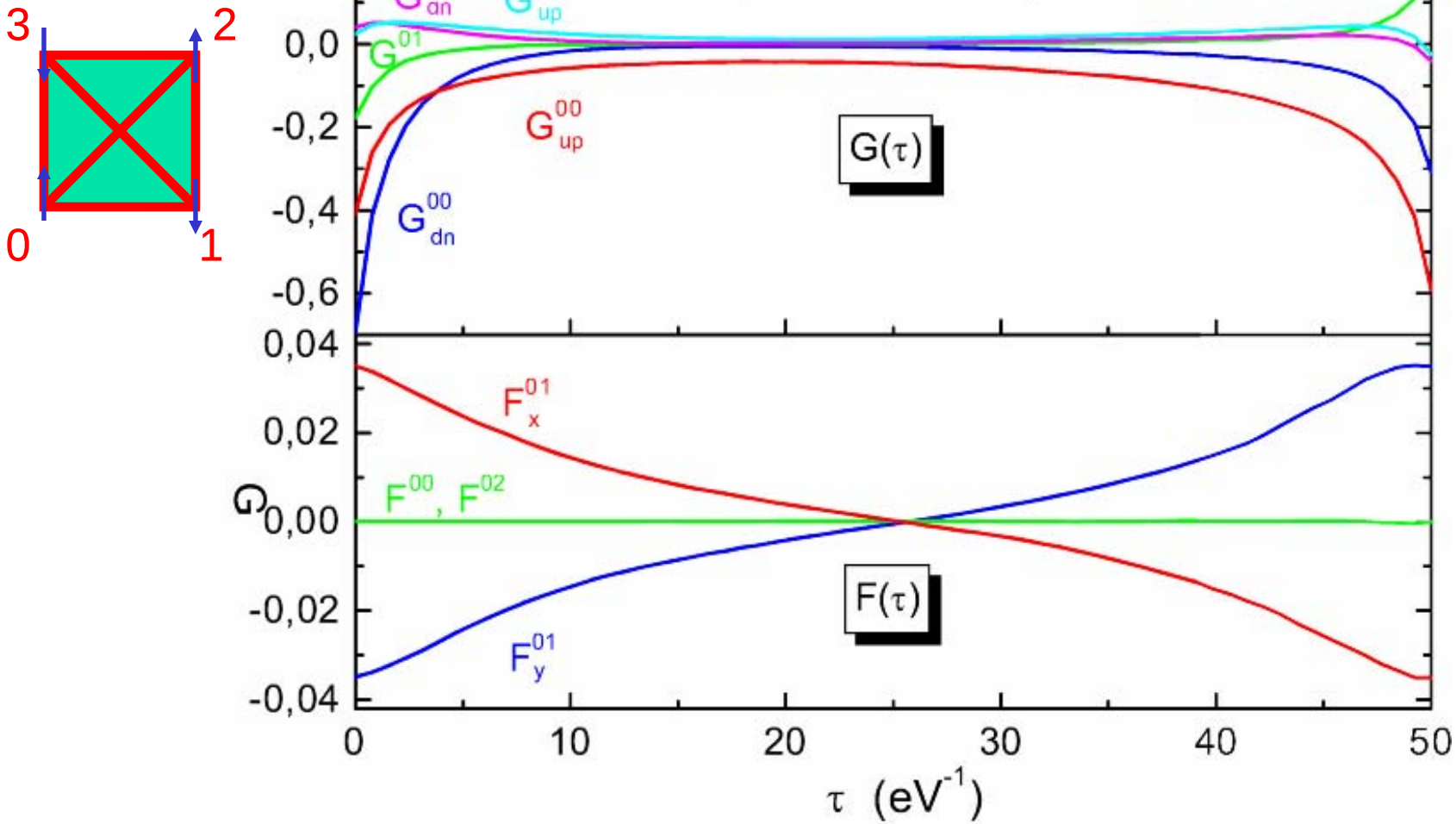
$$K_{x(y)}^{\pm} = 1 + \exp\left(\pm i k_{x(y)} a\right) \quad t_x = t + \Sigma_x,\ t_y = t + \Sigma_y$$

In superconducting state:

$$G(i\omega) = \begin{pmatrix} G_\uparrow(i\omega) & F(i\omega) \\ F(i\omega) & G_\downarrow^*(-i\omega) \end{pmatrix}$$

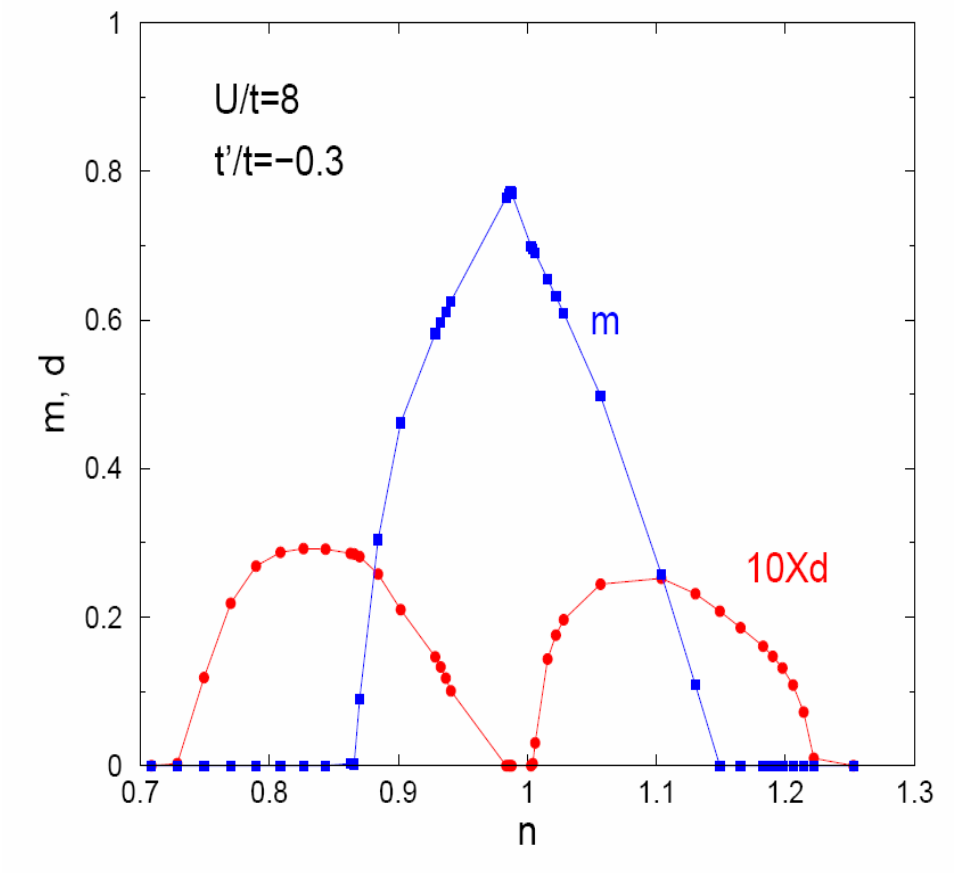
$$\mathcal{G}^{-1}(i\omega) - G^{-1}(i\omega) = \begin{pmatrix} \Sigma_\uparrow(i\omega) & S(i\omega) \\ S(i\omega) & \Sigma_\downarrow^*(-i\omega) \end{pmatrix},$$

Coexistence of AFM and d-wave



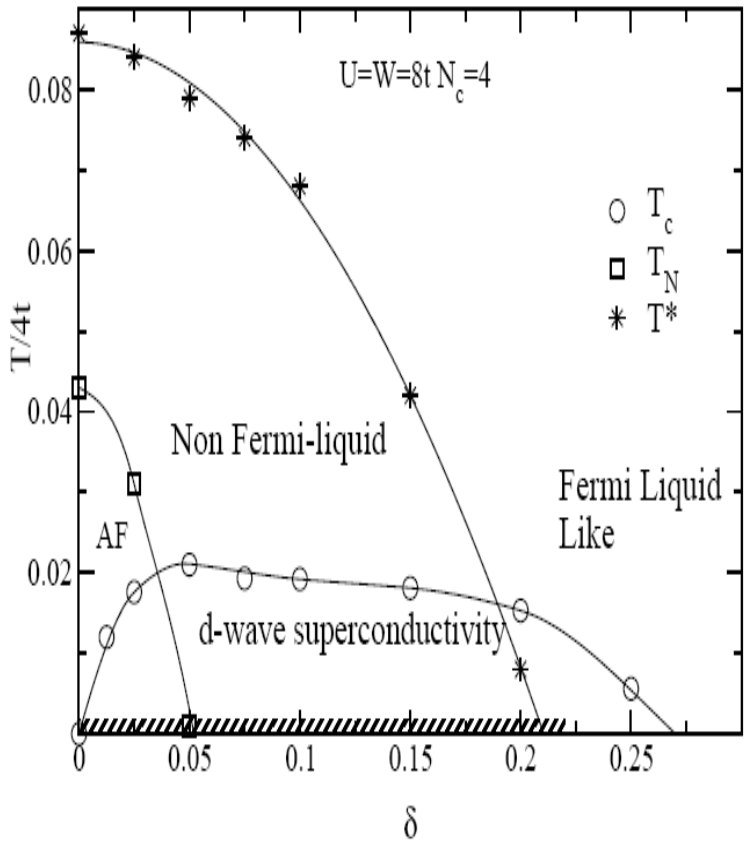
A.L. and M.Katsnelson, PRB (2000)

CDMFT and DCA: phase diagram



S. Kancharla et al, PRB (2008)

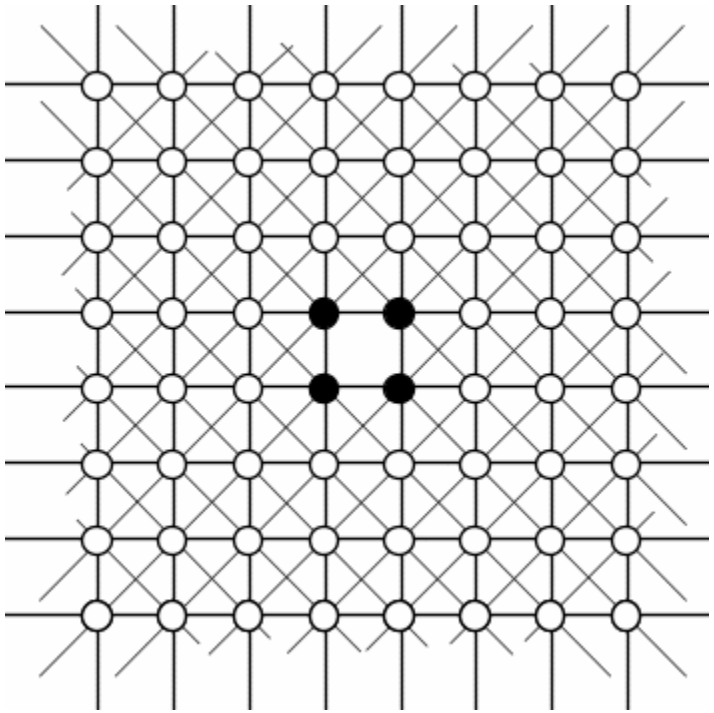
CDMFT



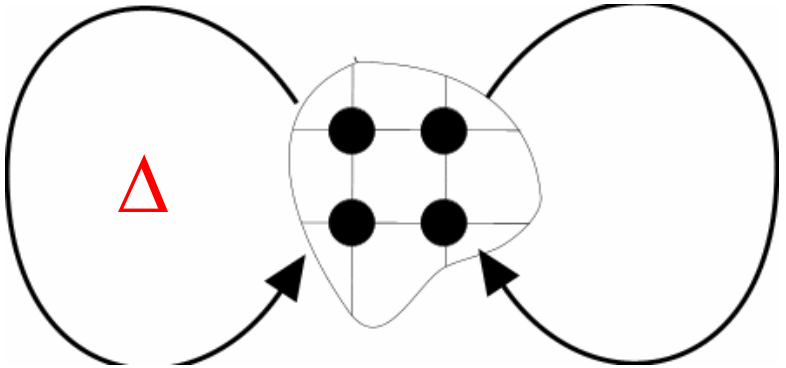
M. Jarrell et al, EPL (2001)

DCA

Cluster DMFT and beyond



short-range fluctuations

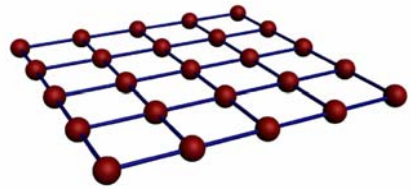


How to include exact k-dependence for correlated systems?

- Dynamical Vertex Approximation (K. Held, M. Jarrell)
- Dual Fermion Approximation (A. Rubtsov)

Beyond DMFT: Dual Fermion scheme

General Lattice Action $H = h + U$

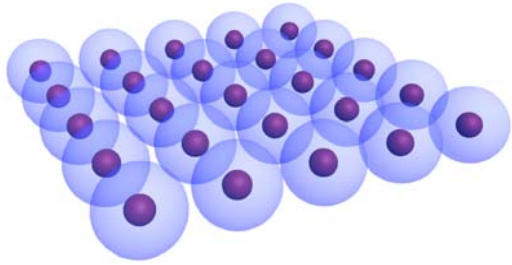


$$S[c^*,c] = \sum_{\omega k m m' \sigma} \left[h_k^{mm'} - (i\omega+\mu)1\right] c^*_{\omega k m\sigma} c_{\omega k m'\sigma} + \frac{1}{4}\sum_{i\{m,\sigma\}} \int_0^\beta U_{1234} c_1^* c_2^* c_3 c_4 d\tau$$

Optimal Local Action with hybridization Δ_ω

$$S_{loc} = \sum_{\omega m m' \sigma} \left[\Delta_\omega^{mm'} - (i\omega+\mu)1\right] c^*_{\omega m\sigma} c_{\omega m'\sigma} + \frac{1}{4}\sum_{i\{m,\sigma\}} \int_0^\beta U_{1234} c_1^* c_2^* c_3 c_4 d\tau$$

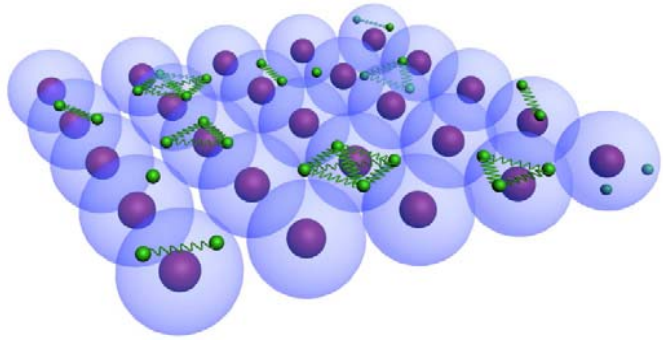
Lattice-Impurity connection:



$$S[c^*,c] = \sum_i S_{loc}[c_i^*, c_i] + \sum_{\omega k m m' \sigma} \left(h_k^{mm'} - \Delta_\omega^{mm'}\right) c^*_{\omega k m\sigma} c_{\omega k m'\sigma}.$$

A. Rubtsov, et al, PRB **77**, 033101 (2008)

Dual Fermions



Gaussian path-integral

$$\int D[\vec{f}^*,\vec{f}]\exp(-\vec{f}^*\hat{A}\vec{f}+\vec{f}^*\hat{B}\vec{c}+\vec{c}^*\hat{B}\vec{f})=\det(\hat{A})\exp(\vec{c}^*\hat{B}\hat{A}^{-1}\hat{B}\vec{c})$$

With $\begin{aligned} A &= g_\omega^{-1}(\Delta_\omega - h_k)g_\omega^{-1} \\ B &= g_\omega^{-1} \end{aligned}$

new Action:

$$S_d[f^*,f]=-\sum_{k\omega}\mathcal{G}^{-1}_{k\omega}f^*_{k\omega}f_{k\omega}+\frac{1}{4}\sum_{1234}\gamma^{(4)}_{1234}f^*_1f^*_2f_4f_3+\ldots$$

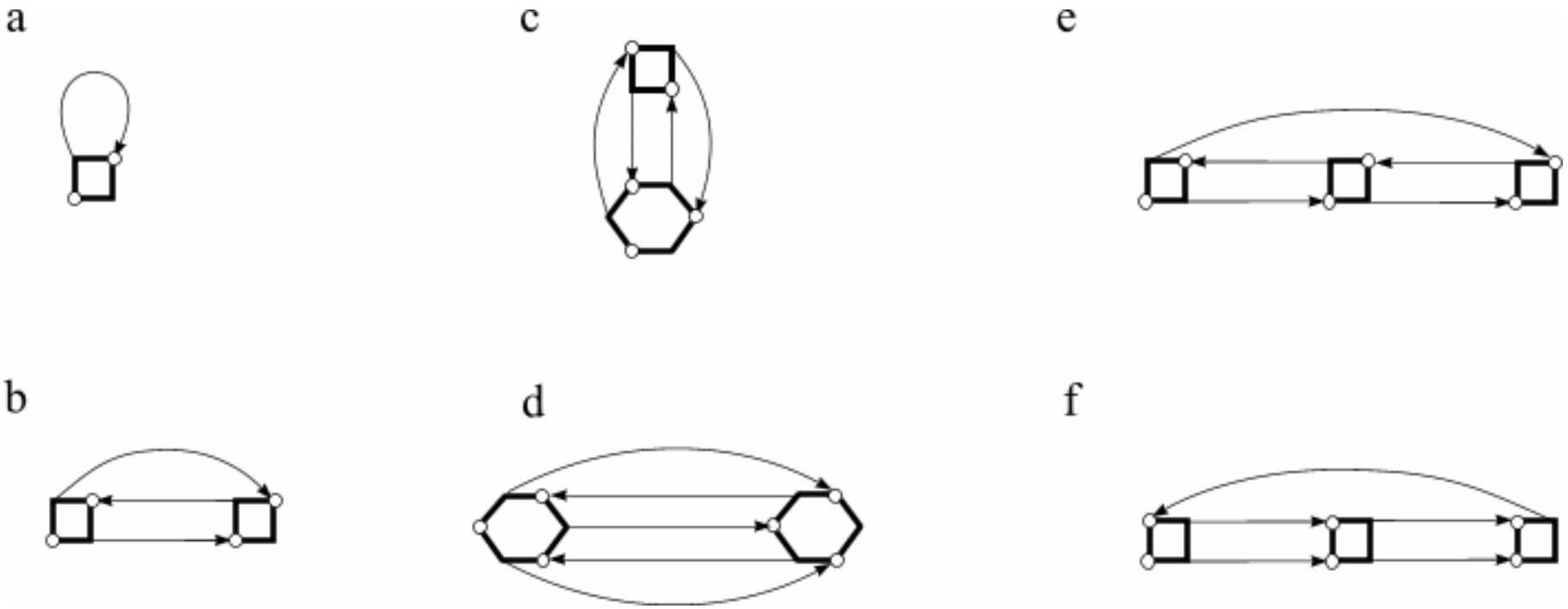
Diagrammatic:

$$\longrightarrow \quad \mathcal{G}_{k\omega}=G^{DMFT}_{k\omega}-g_\omega$$

$$\square \quad \gamma^{(4)}_{1234} = g^{-1}_{11'}g^{-1}_{22'}\left(\chi_{1'2'3'4'}-\chi^0_{1'2'3'4'}\right)g^{-1}_{3'3}g^{-1}_{4'4}$$

g_ω and $\chi_{\nu,\nu',\omega}$ from DMFT

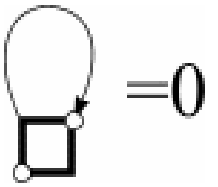
Basic diagrams for dual self-energy



Lines denote the renormalized Green's function.

Condition for Δ and relation with DMFT

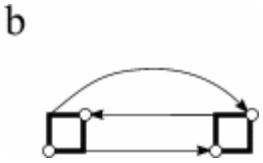
$G^d = G^{DMFT} - g$



To determine Δ, we require
that Hartree correction in dual variables vanishes.
If no higher diagrams are taken into account, one obtains DMFT:

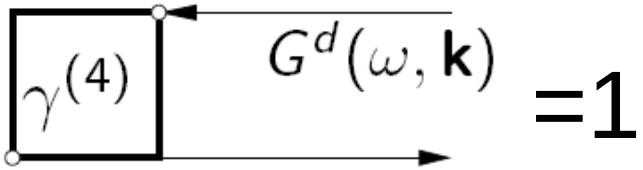
$$\sum_k \mathcal{G}^d_{k\omega} = 0 \longrightarrow \sum_k \left[g_\omega - (h_k - \Delta_\omega)^{-1} \right]^{-1} = 0$$

Higher-order diagrams give corrections to the DMFT self-energy,
and already the leading-order correction is nonlocal.

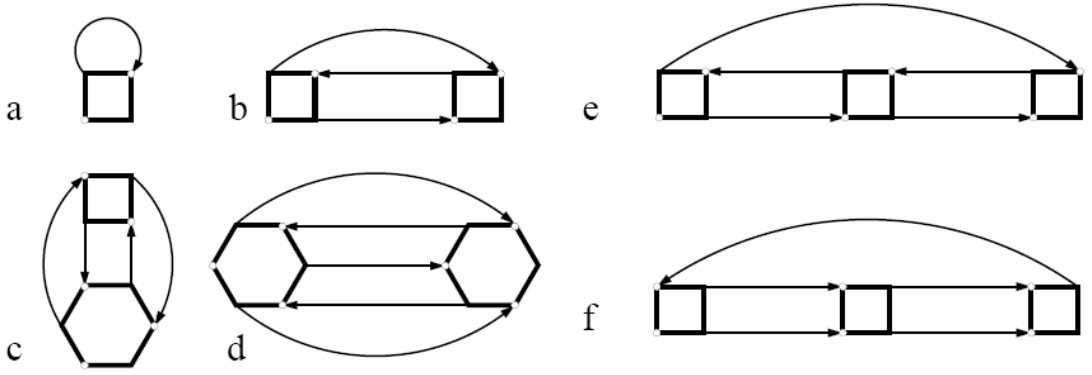


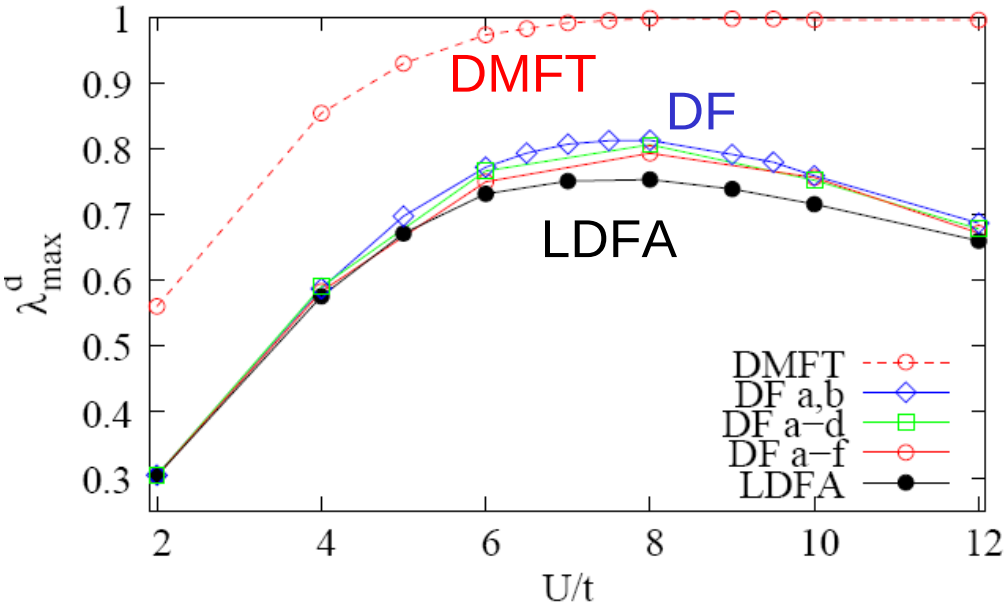
$\Sigma(k,\omega)$

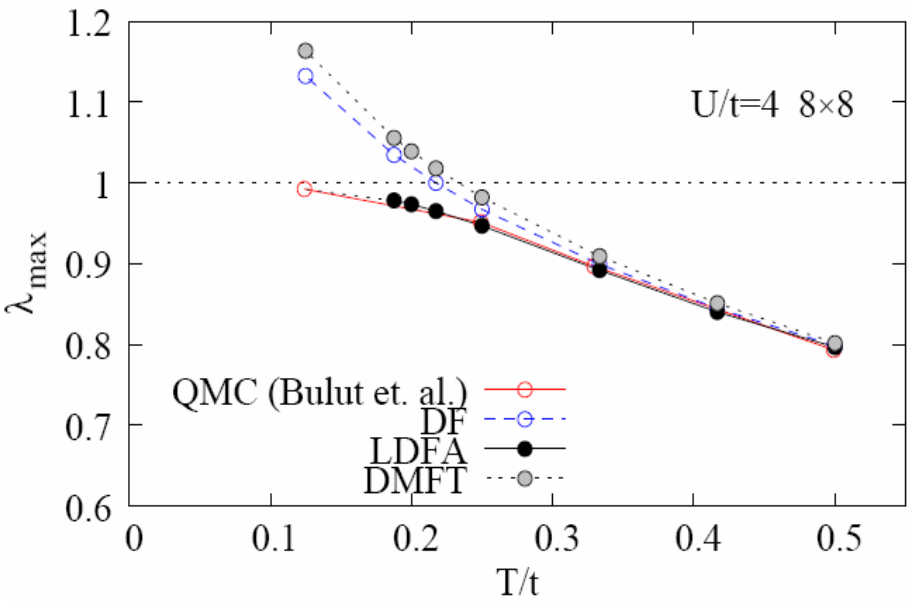
Convergence of Dual Fermions: 2d



$$-\frac{T}{N}\sum_{w'\mathbf{k}'}\Gamma^{d\,\mathrm{irr},s}_{\omega\omega'\Omega}\,G^d_{\omega'}(\mathbf{k}')\,G^d_{\omega'+\Omega}(\mathbf{k}'+\mathbf{q})\phi_{\omega'}=\lambda\phi_\omega$$

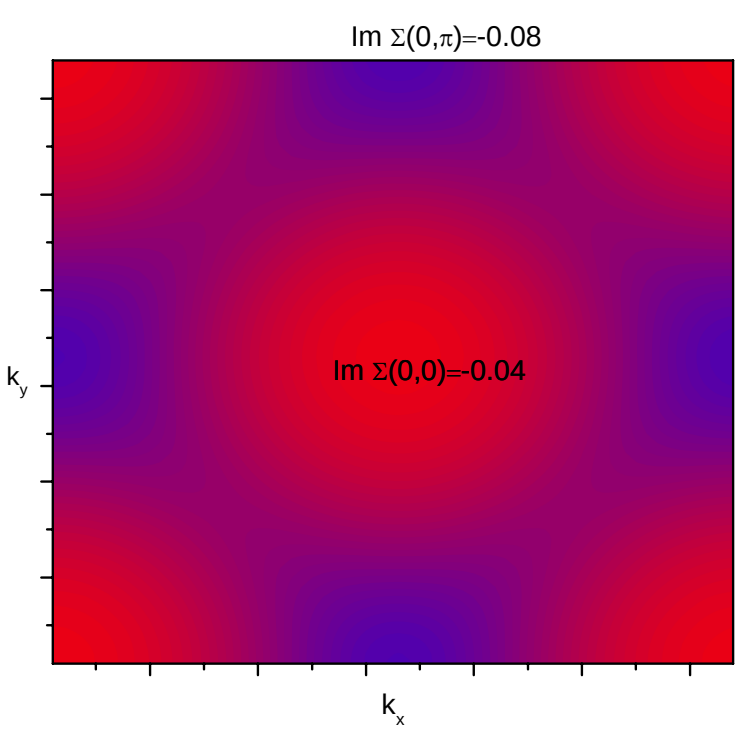




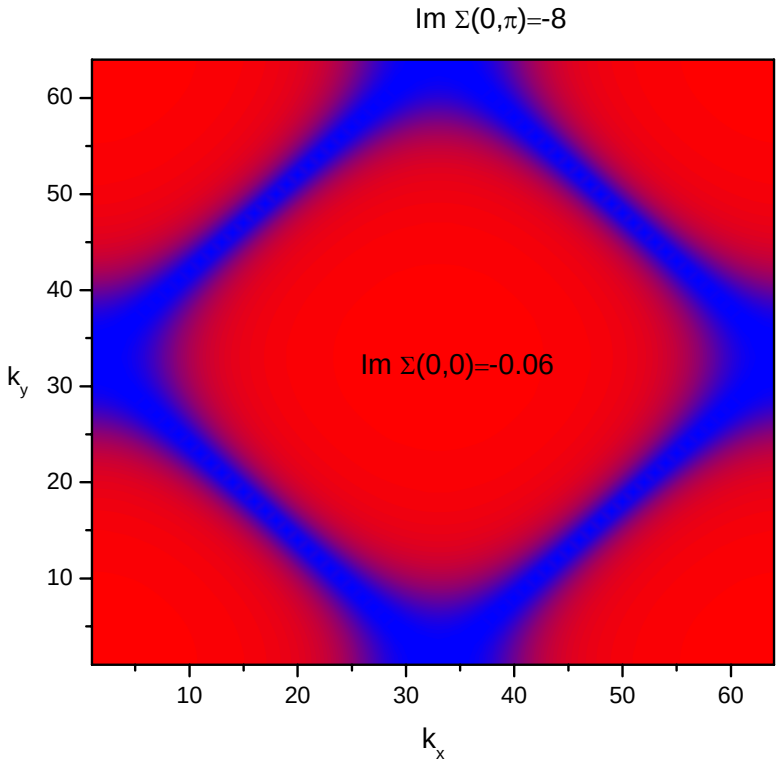


H. Hafermann, et al. PRL**102**, 206401 (2009)

2d: Im $\Sigma(k, \omega=0)$



U=1



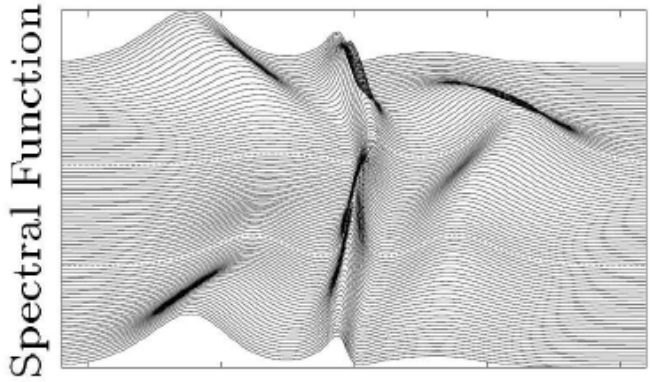
U=2

Hubbard model with $8t = 2, \beta = 20$ at half-filling.
Data for Im Σ_k at $\omega = 0$.

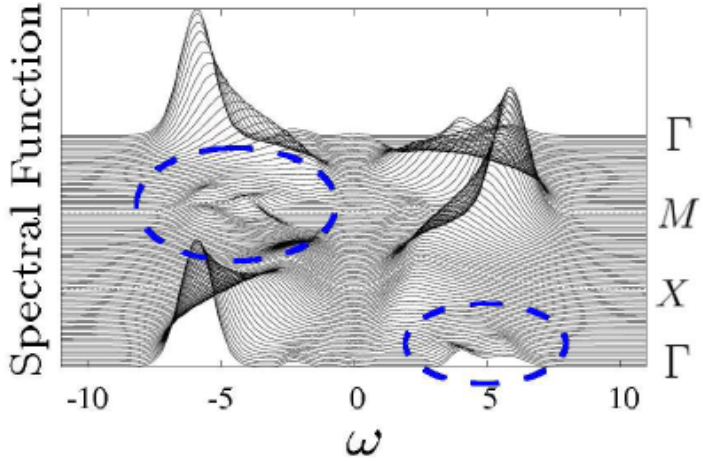
A. Rubtsov, et al, PRB **79**, 045133 (2009)

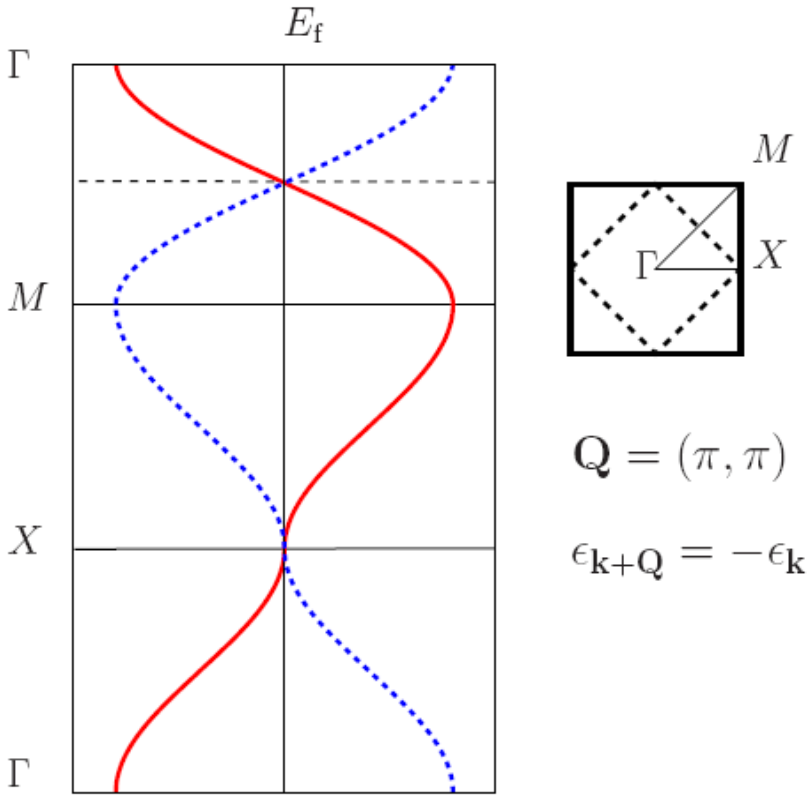
Dynamical AF correlations: shadow bands

DMFT



Dual Fermion $\Sigma^{\mathrm{d}} =$

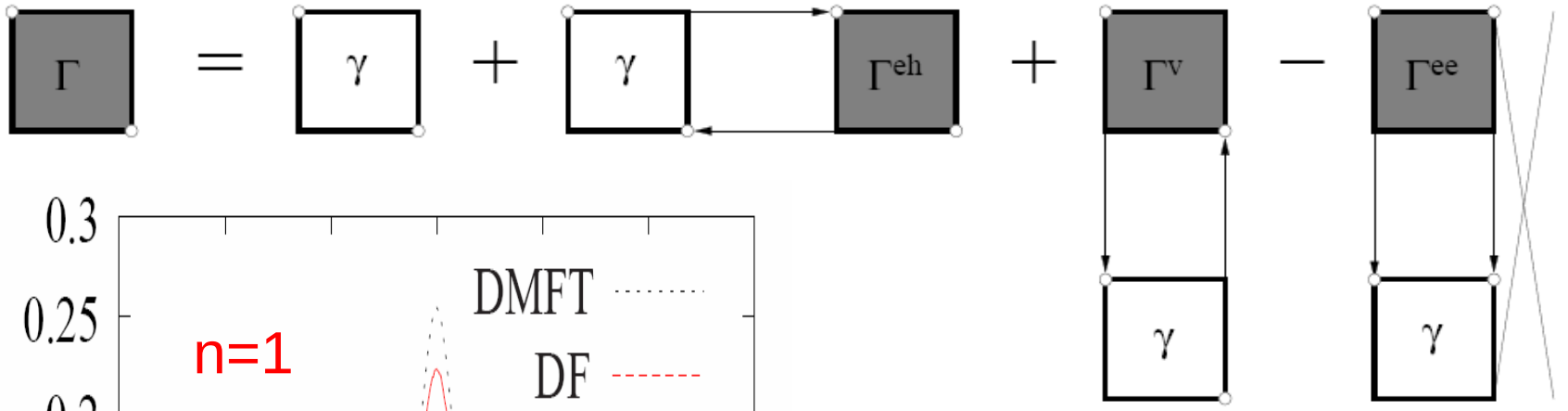


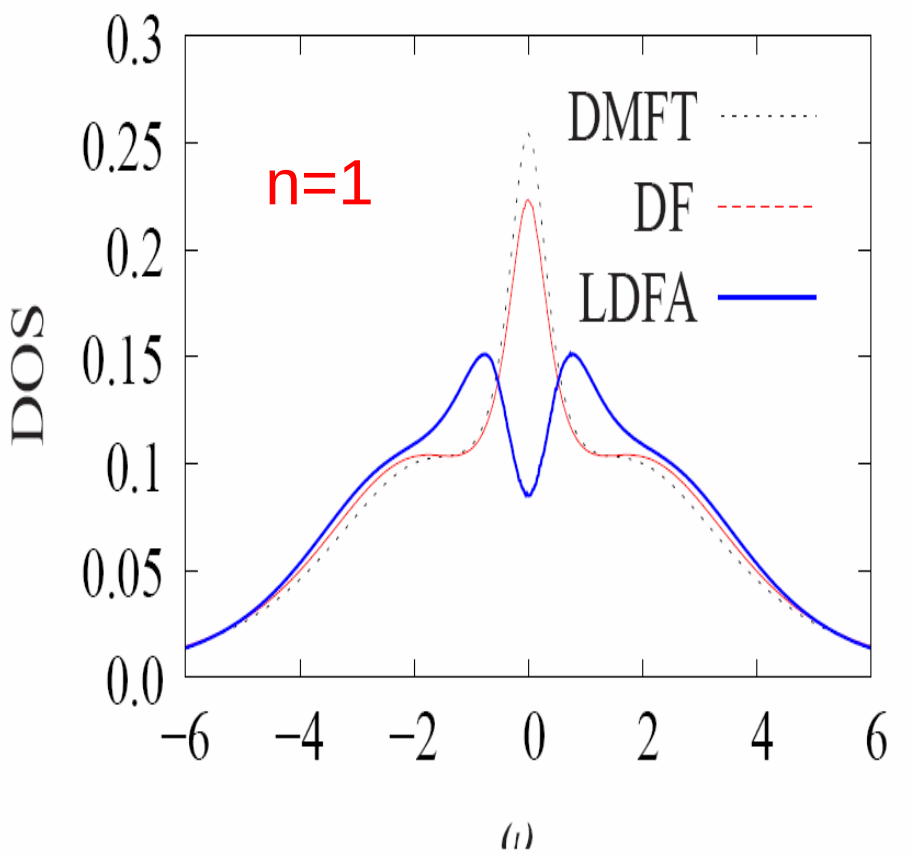


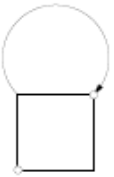
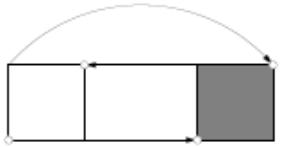
U=8t=W, T=0.2t, n=1

H. Hafermann, PhD (2009)

Pseudogap in HTSC: Ladder-DF

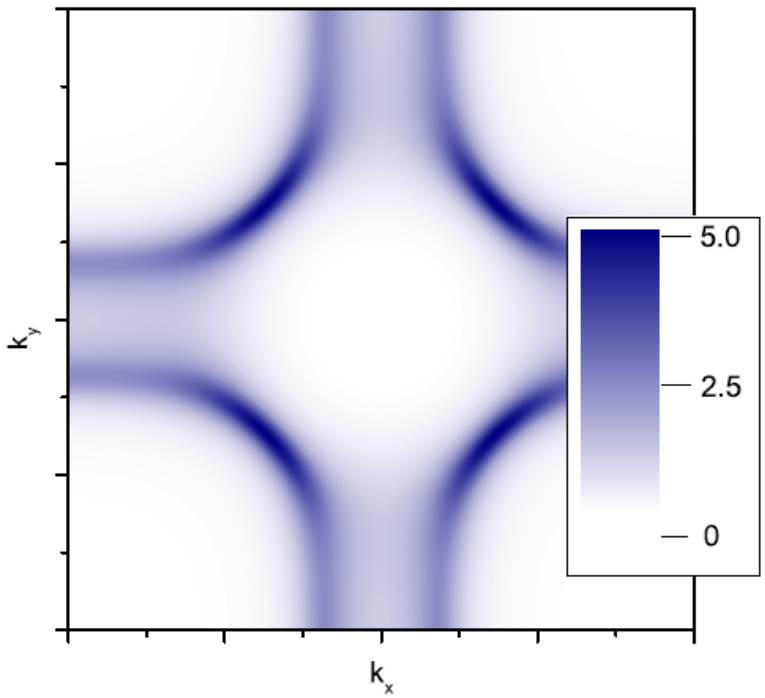


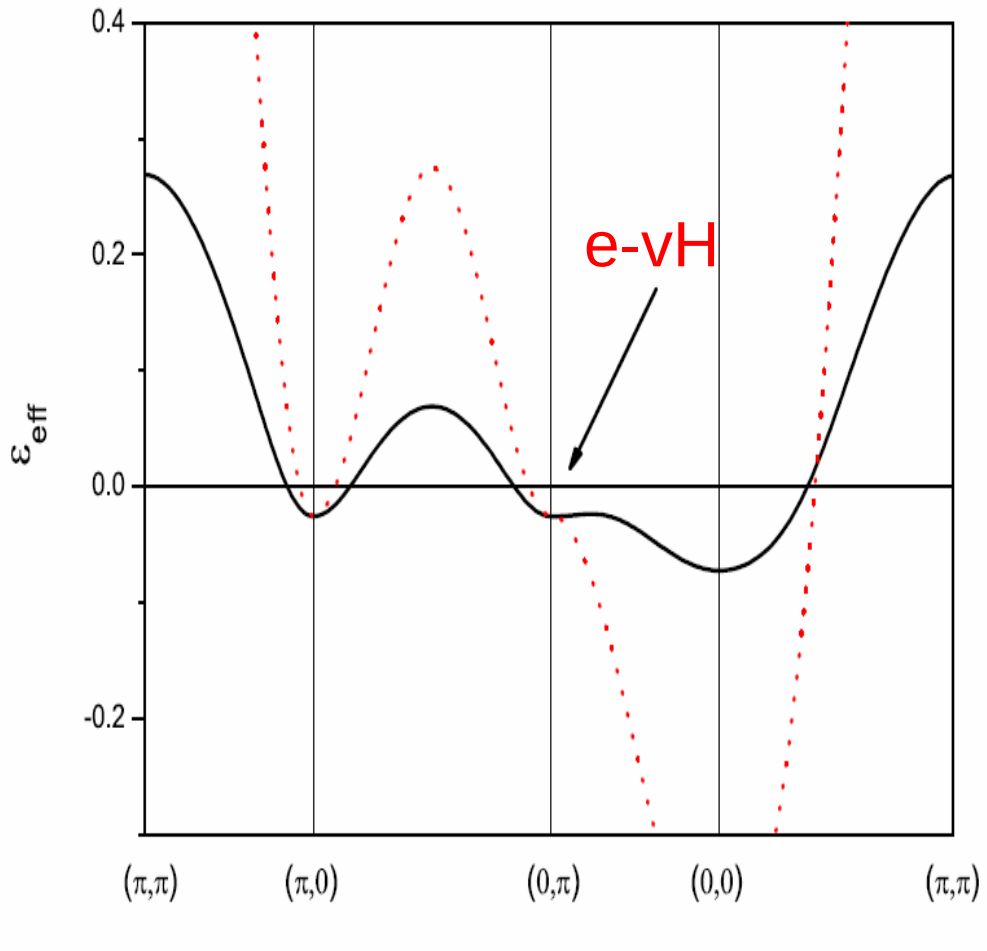


$$\Sigma = -$$  $$-\frac{1}{2}$$ 

H. Hafermann, et al. PRL**102**, 206401 (2009)

Arcs in HTSC: Dual Fermions





FS, n=0.85

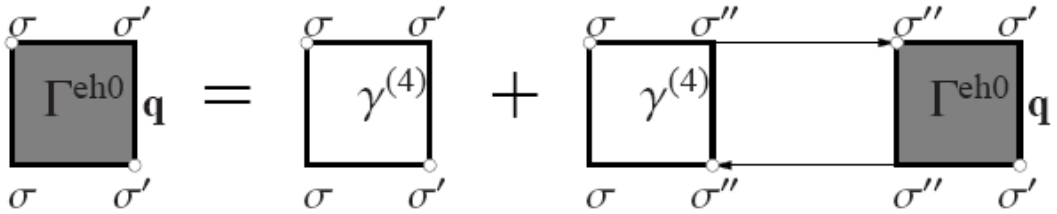
QP-dispersion

A. Rubtsov, et al, PRB **79**, 045133 (2009)

2d: U=W=2

Bethe-Salpeter Equation

Electron-hole channel

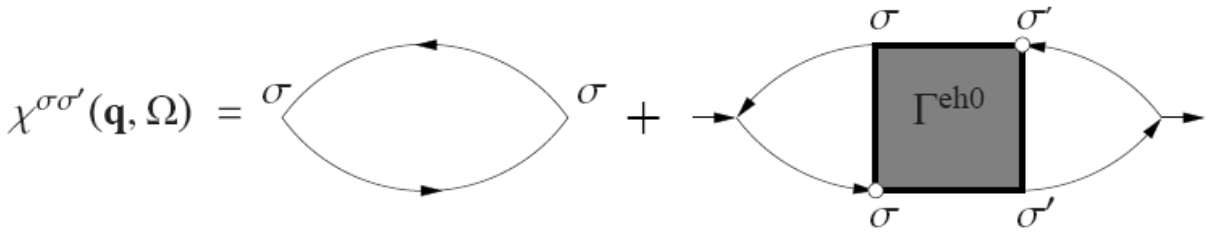


Exact transformation to original fermions

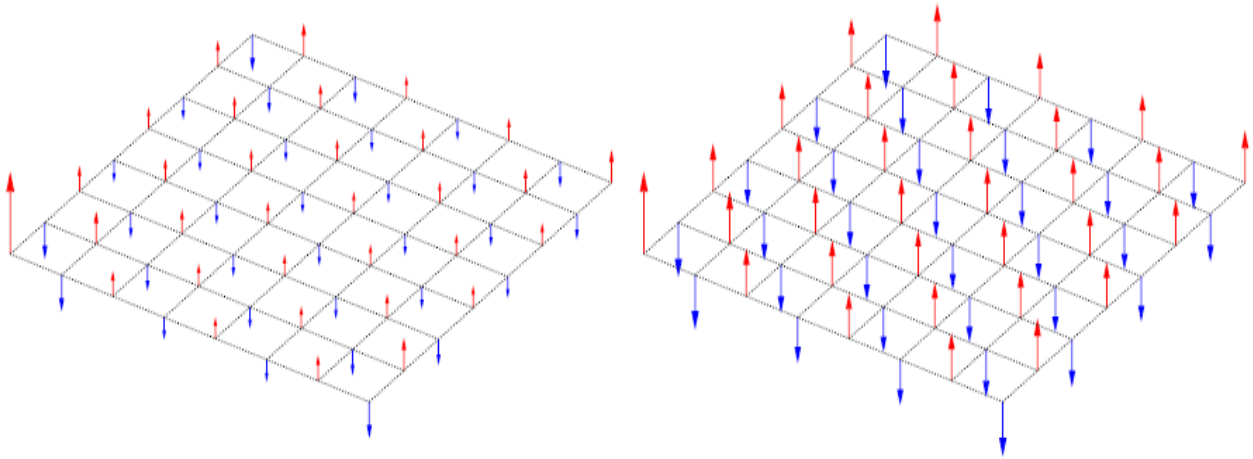
$$\Gamma_{1234} = L_{11'} L_{33'} \Gamma^{\mathrm{d}}_{1'2'3'4'} R_{2'2} R_{4'4}$$

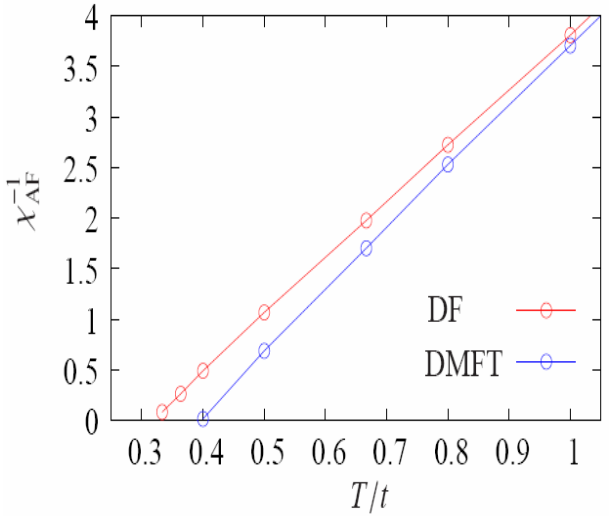
$$L_{12} = -[\mathbb{1} + \Sigma^{\mathrm{d}} g]^{-1}_{12} \qquad R_{12} = -[\mathbb{1} + g\Sigma^{\mathrm{d}}]^{-1}_{12}$$

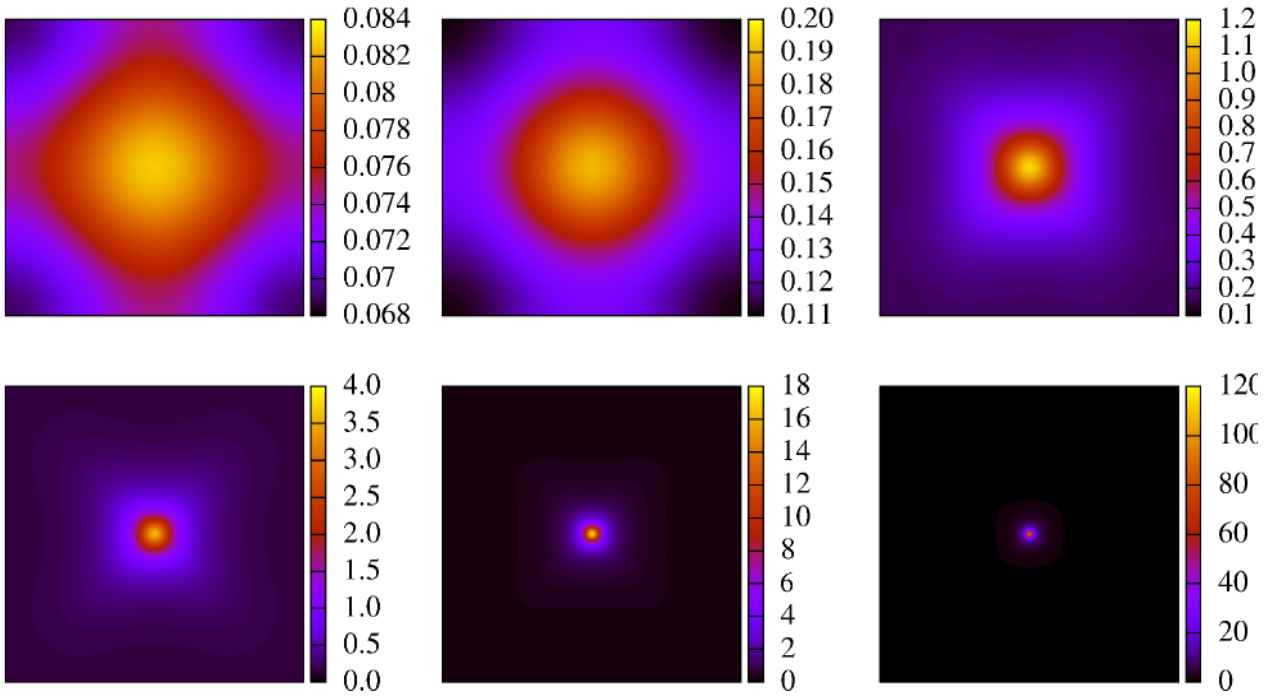
Magnetic susceptibility

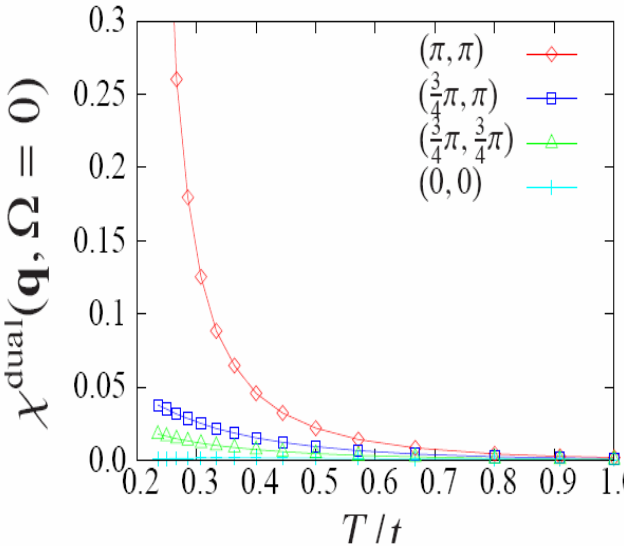


Susceptibility: 2d – Hubbard model

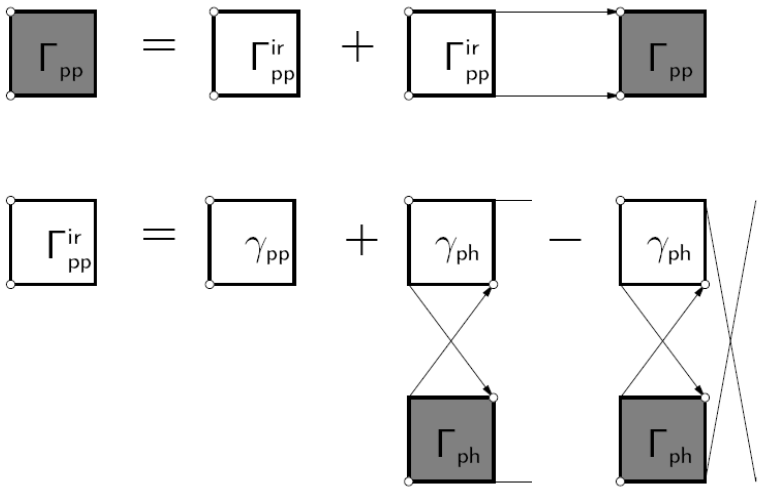


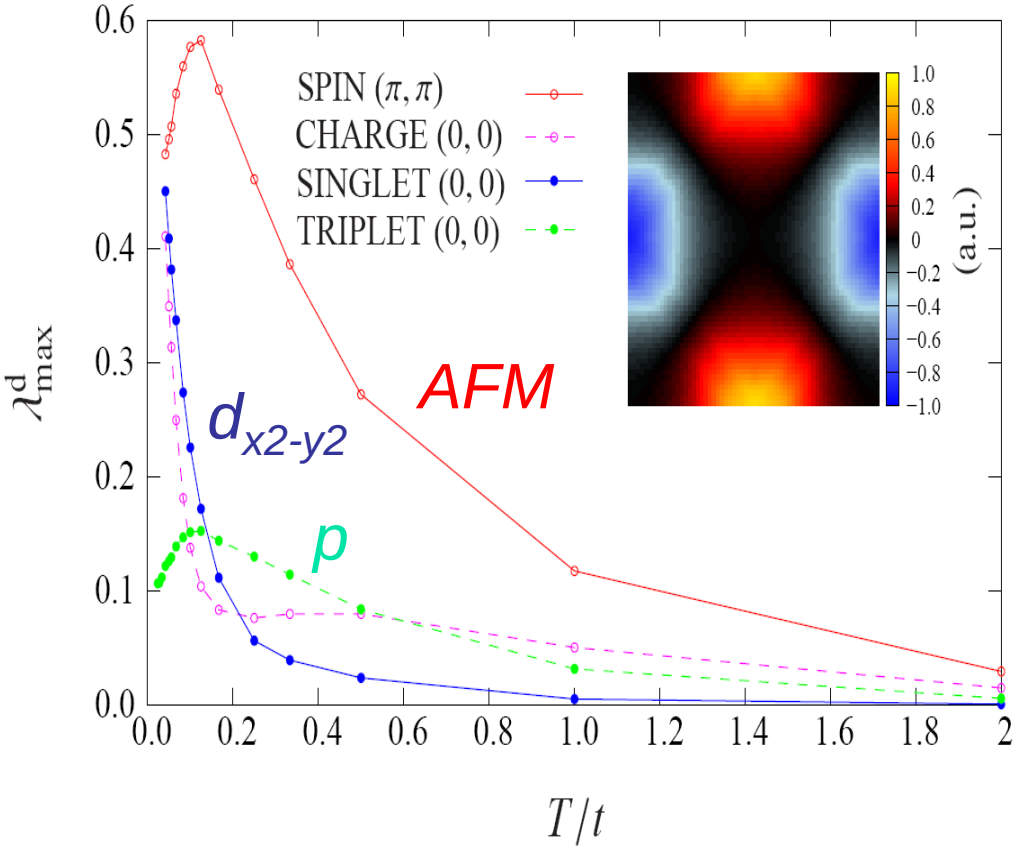






Bethe-Salpeter equation: pp-channel

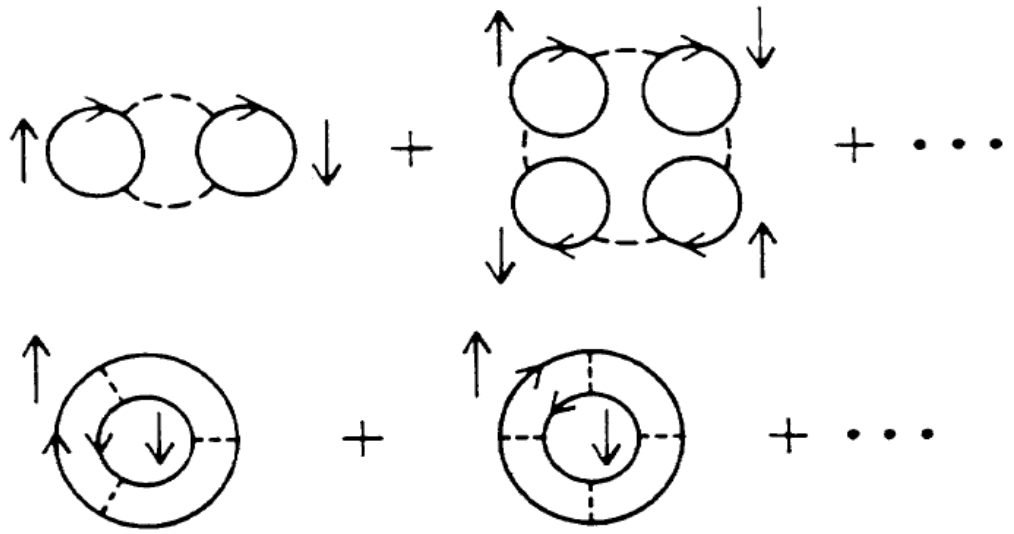




U=W/2 t'/t=-0.3 x=15%

$$\frac{1}{2\beta N^d}\sum_{\omega'\mathbf{k}'_1}\gamma^{\mathrm{irr},s/t}_{p\omega\omega'\Omega=0}(\mathbf{k},\mathbf{k}',\mathbf{q}=0)\,G^{\mathrm{d}}_{-\omega'}(-\mathbf{k}')\,G^{\mathrm{d}}_{\omega'}(\mathbf{k}')\phi_{\omega'}(\mathbf{k}')=\lambda\phi_{\omega}(\mathbf{k})$$

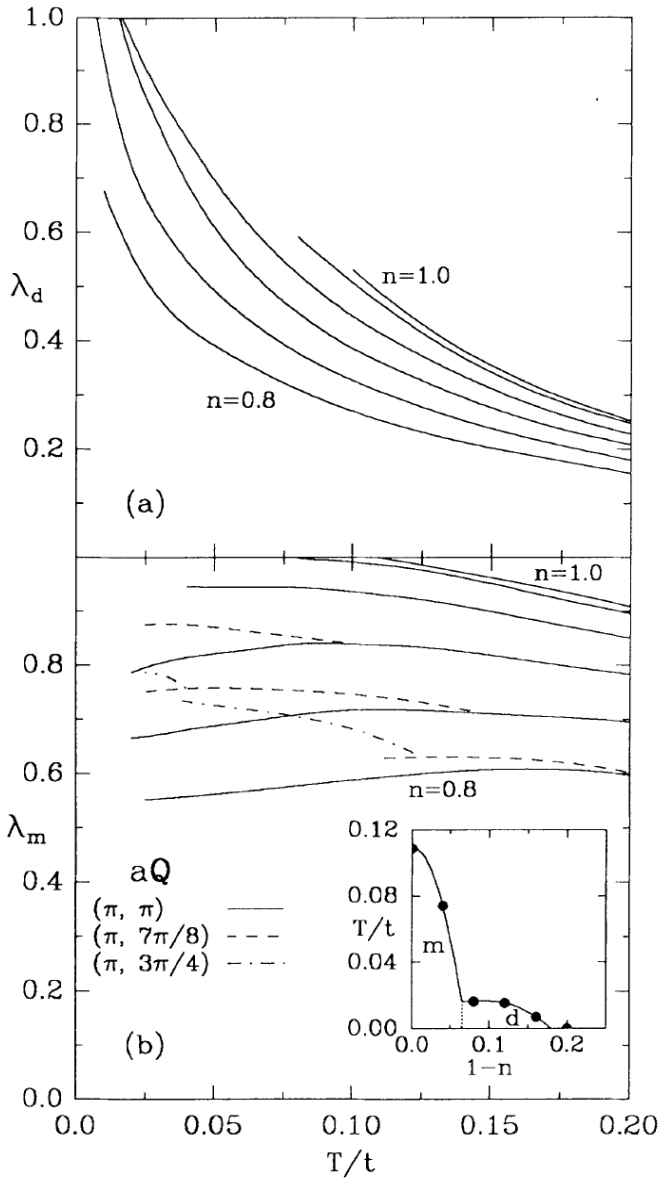
Weak-coupling perturbation: FLEX



U/W=0.5 t'=0

N. Bickers, D. Scalapino and S. White, PRL (1988)

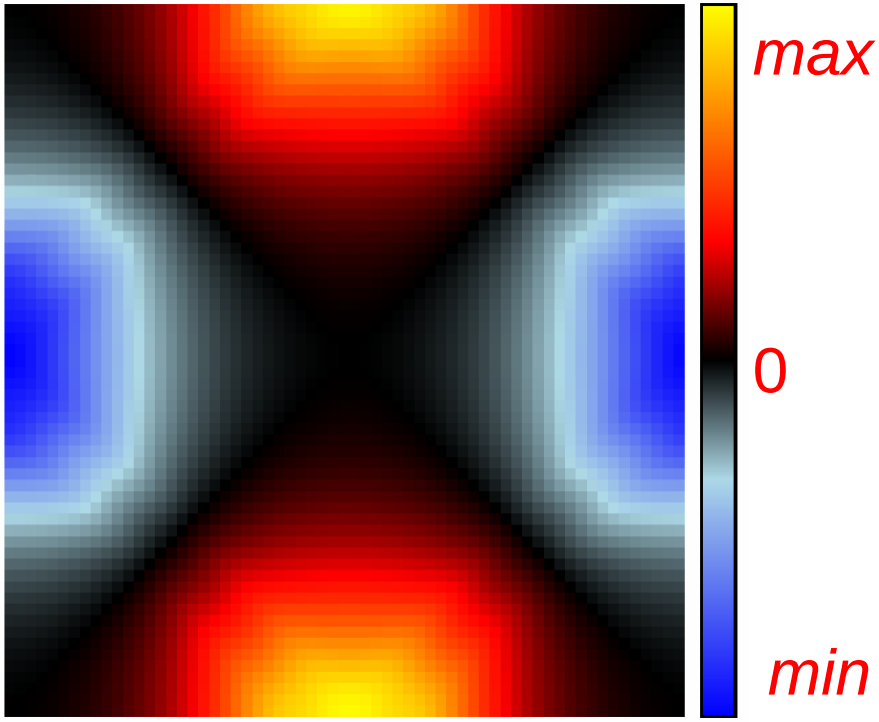
LDFA – strong coupling analog of FLEX

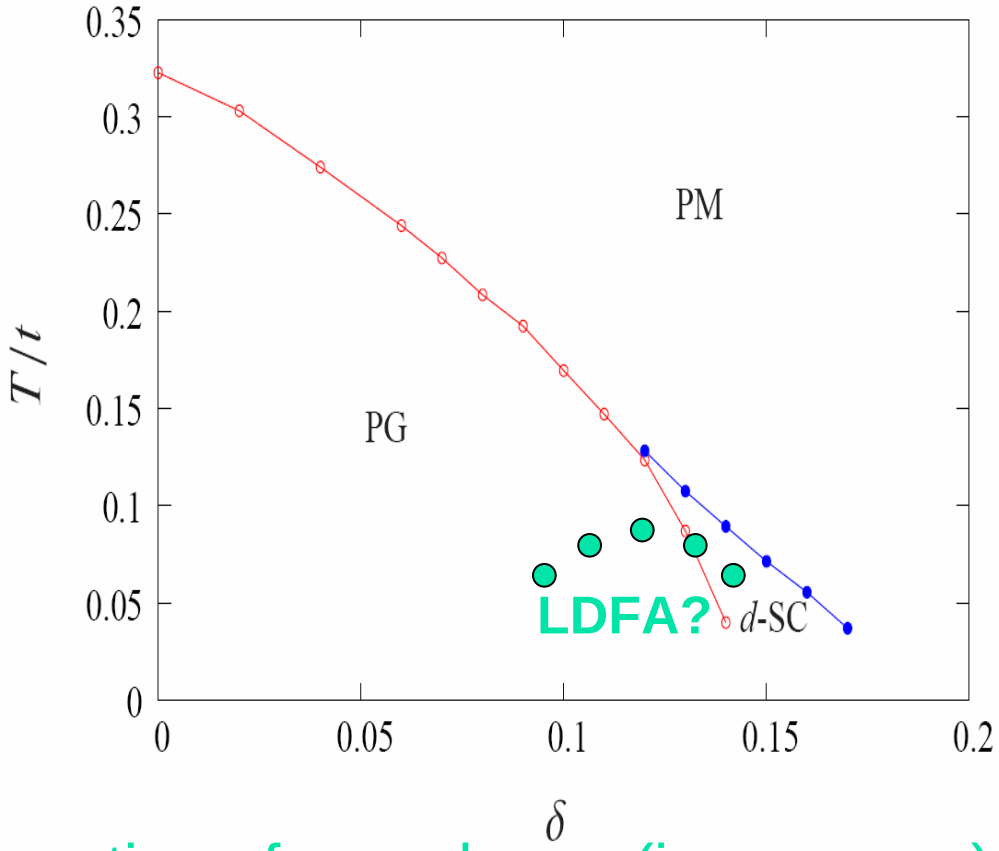


d-wave symmetry of the eigenfunction: DF

H. Hafermann, et al, J. Supercond. Nov. Magn. **22**, 45 (2008)

U/W=1 t'=0





LDFA can reduce Tc due to formation of pseudogap (in progress)

Conclusions

- Dual Fermion expansion around DMFT can efficiently interpolate between weak and strong coupling
- Antiferromagnetic pseudo-gap and Fermi-arcs describe well in ladder DF-scheme
- d-wave pairing for overdoped regime can be analysed in simple DF, while for underdoped limit the cluster-DF or ladder-DF is needed
- Realistic multiorbital LDA+DF for correlated higher-T_c materials (Fe-As) is a next challenge: work in progress.