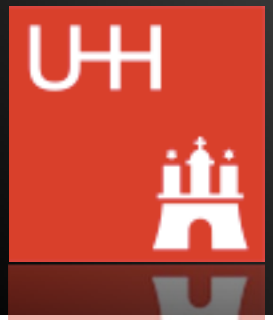
Electronic structure, non-local correlation effects and superconductivity in cuprates

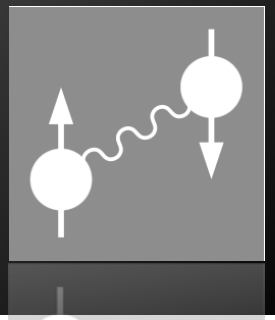
Alexander Lichtenstein

University of Hamburg

In collaboration with

H. Hafermann, A. Rubtsov, and M. Katsnelson

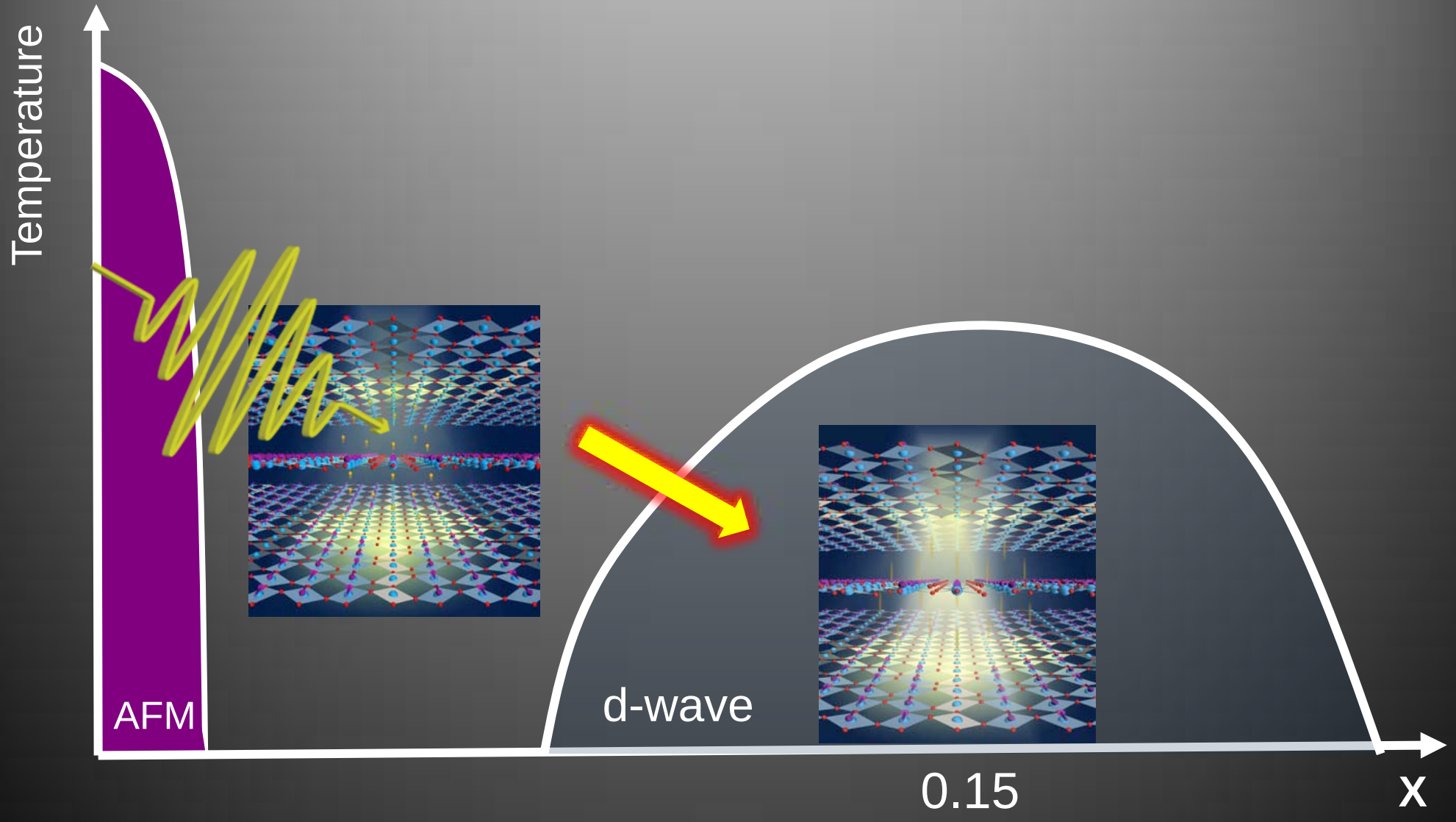




Outline

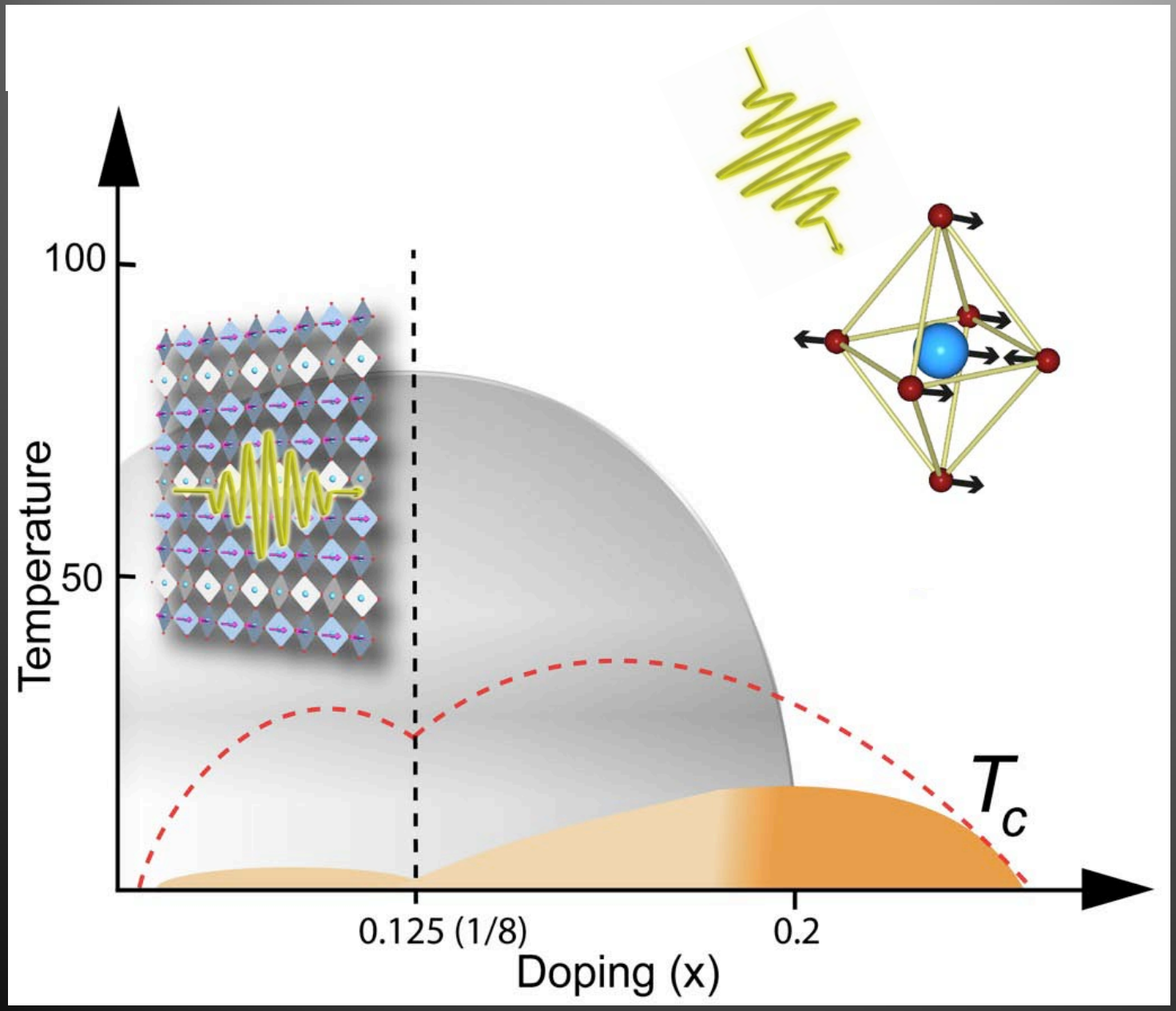
- What is new in HTSC?
- From electronic structure to Hubbard model
- Antiferromagnetism and Superconductivity
- d-wave: BSE
- Conclusions

Can we control superconductivity with light ?



Yes - Andrea Cavalleri, MPI Hamburg

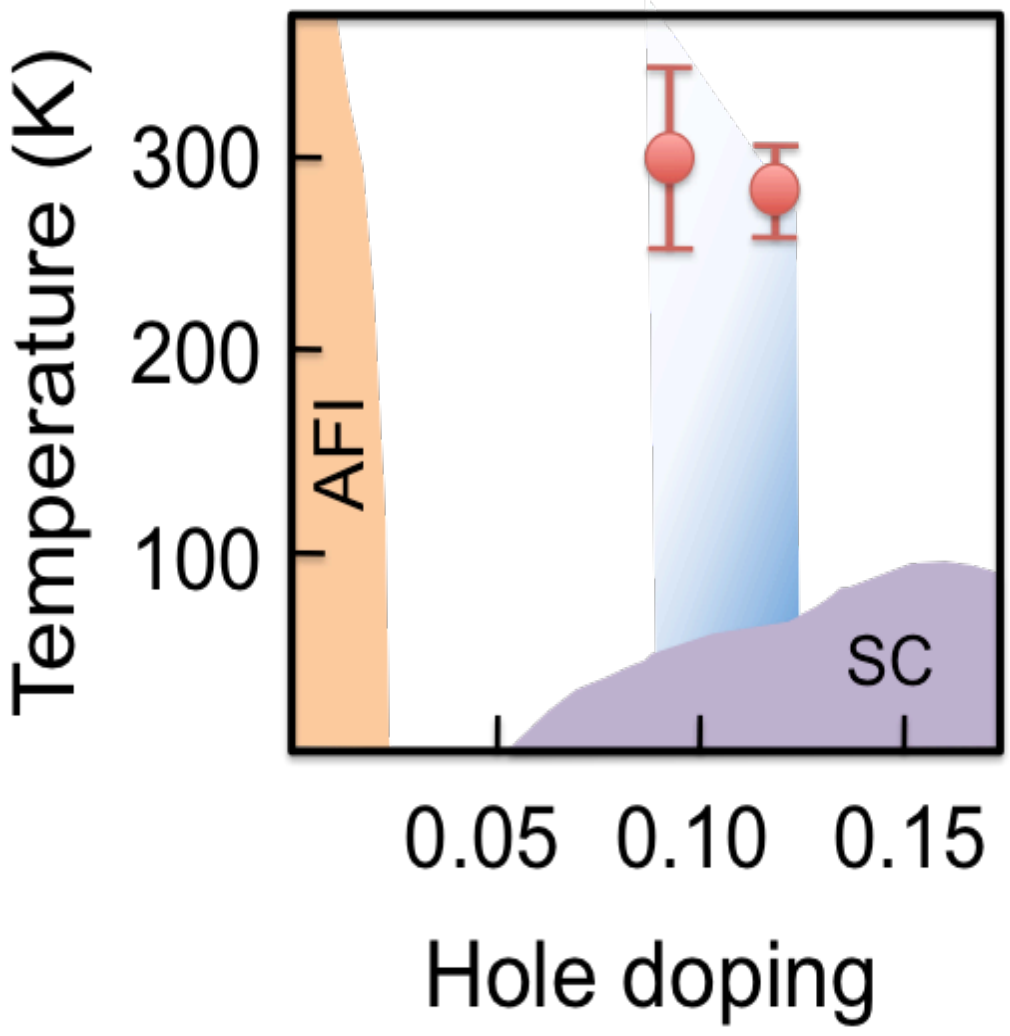
Can we selectively quench stripes distortion?

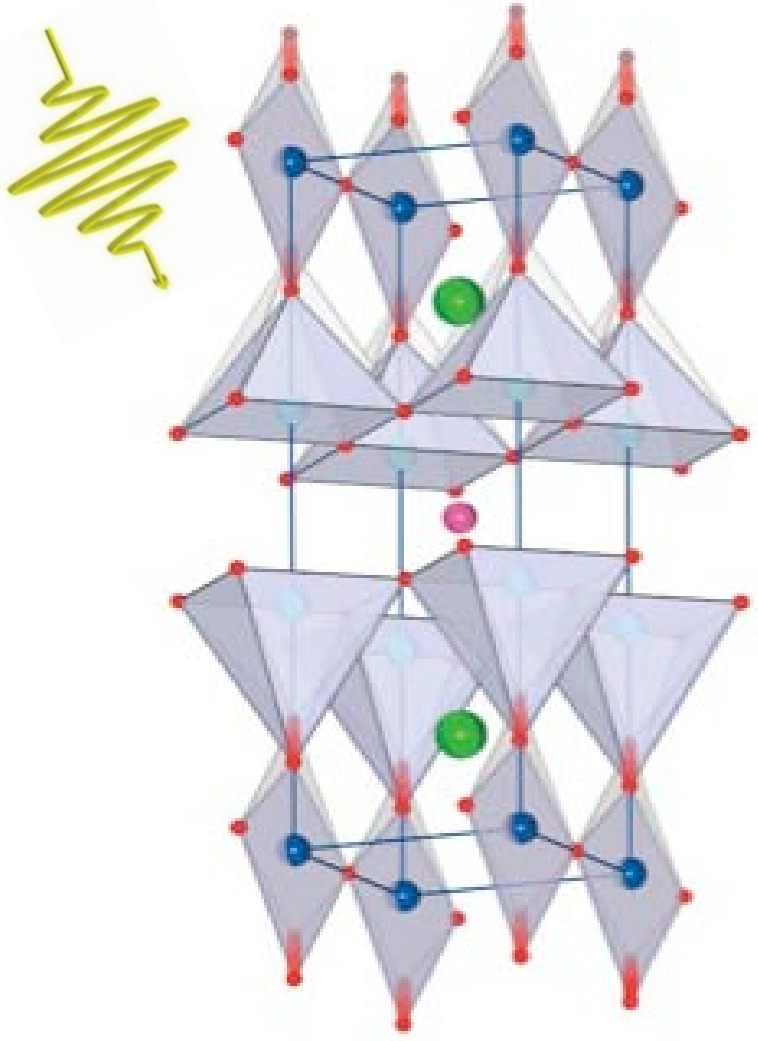


Andrea Cavalleri
MPI Hamburg

D. Fausti, Science, 331, 189 (2011)

YBCO: Driving Apical Oxygen Motion

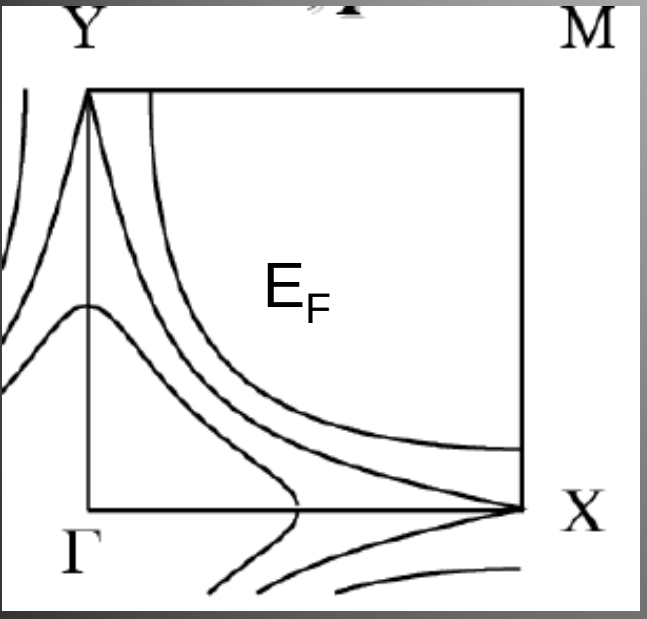




Andrea Cavalleri
MPI Hamburg

S. Kaiser, et al.,
arXiv:1205.4661

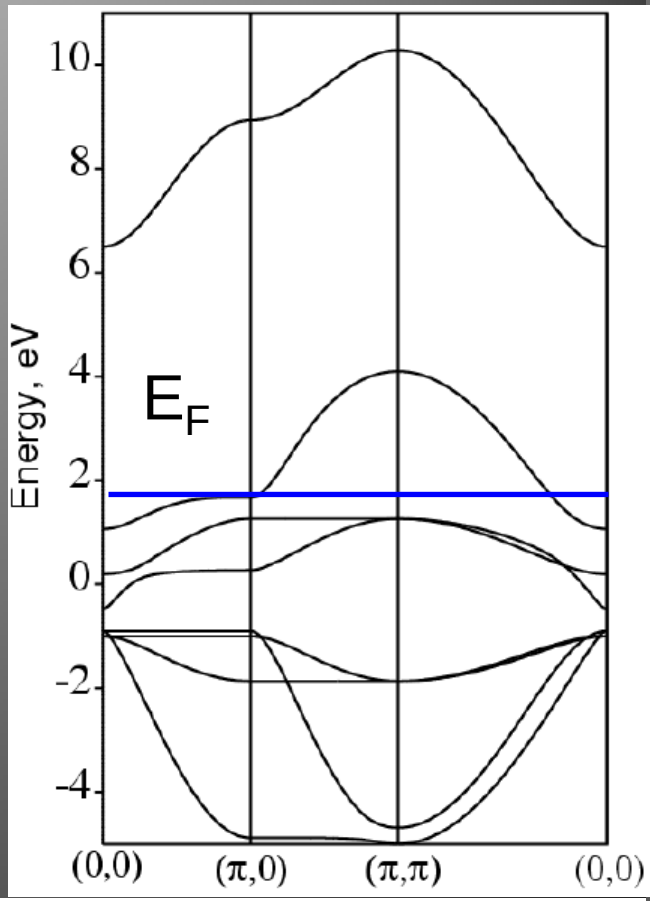
HTSC: from LDA to 1-band model

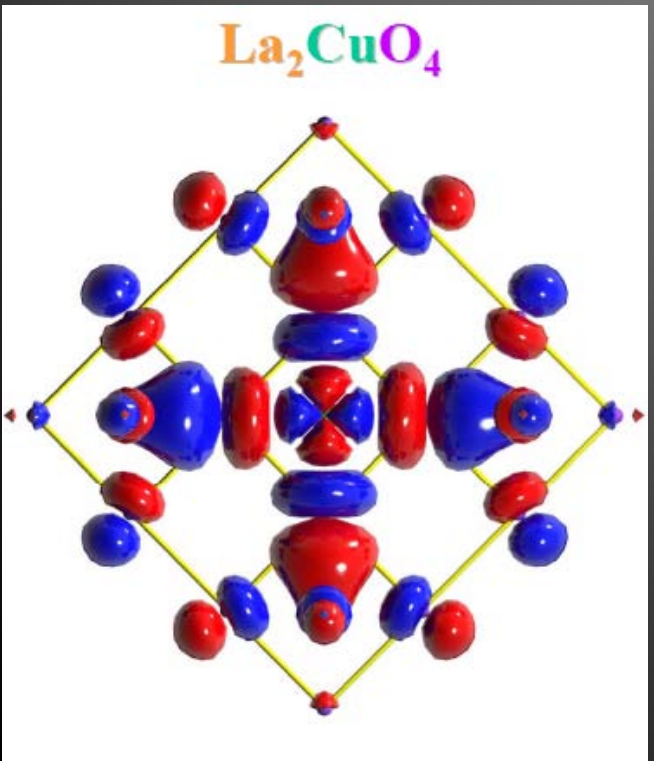


From LDA "Chemistry"
to
Low-energy TB-model

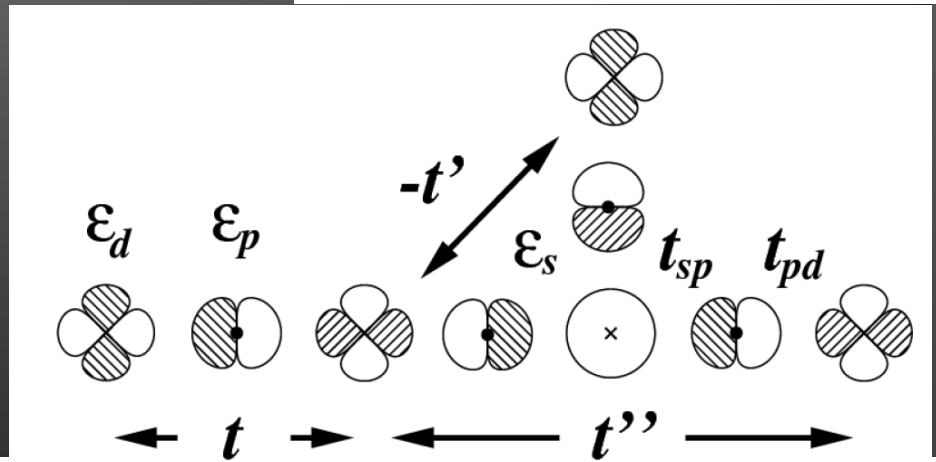
t'/t= -0.3 for YBCO

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





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



General Cluster Idea

One-band Habbard model on Lattice

$$H = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

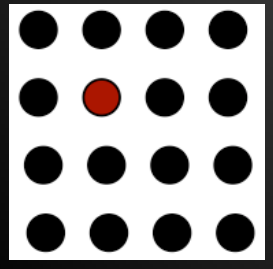
Exact solurion:

$$G(\mathbf{k}, i\omega) = (i\omega + \mu - t(\mathbf{k}) - \Sigma(\mathbf{k}, i\omega))^{-1}$$

Approximate self-energy:

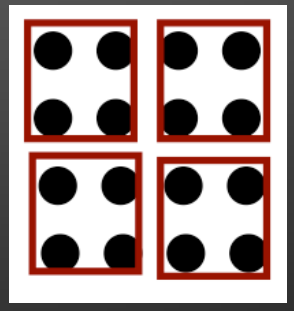
$$\Sigma(\mathbf{k}, i\omega) \approx \sum_{i=1}^{N} \phi_i(\mathbf{k}) \Sigma_i(\omega)$$

N=1 ⇔ single-site DMFT



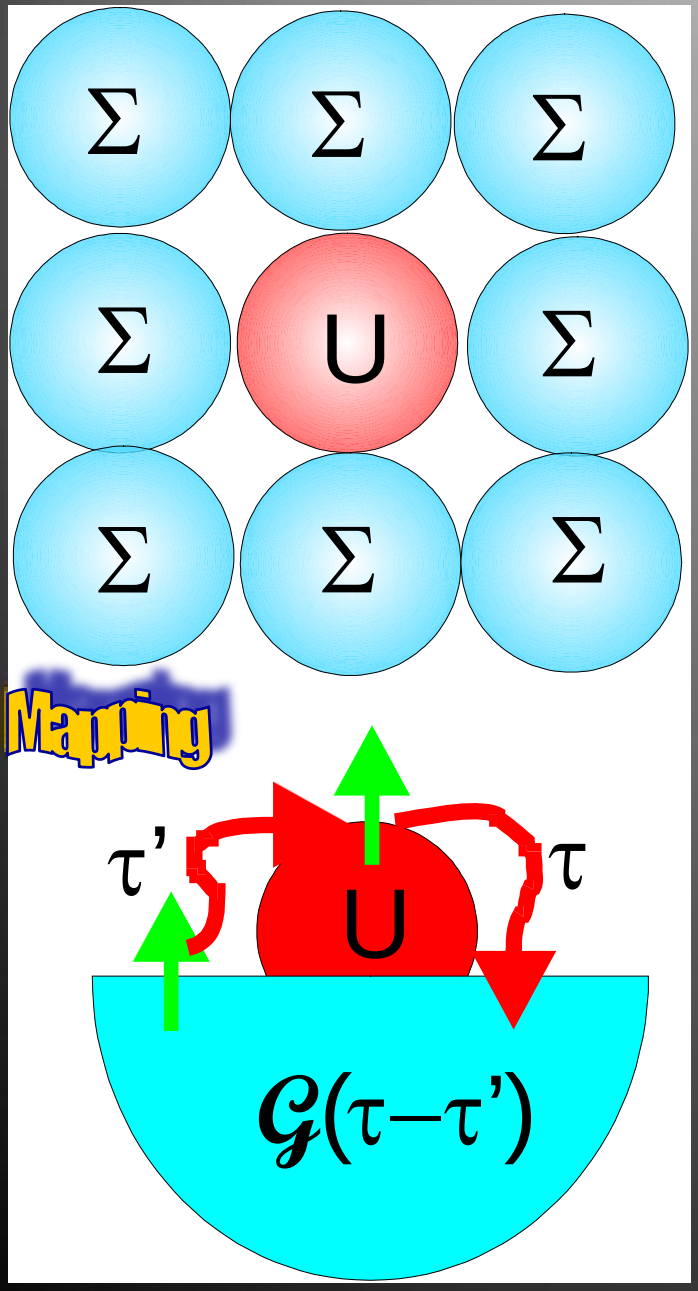
MIT
Mott Transition
Paramagnetic Insulator

N=4 ⇔ plaquette CDMFT



d-wave HTSC
Antiferromagnetism
CDW

Dynamical Mean Field Theory



$$\hat{G}(i\omega_n) = \frac{1}{\Omega}\sum_{k}^{BZ}\left[\hat{I}(\mu + i\omega_n) - \hat{H}_0(k) - \hat{\Sigma}(i\omega_n)\right]^{-1}$$

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

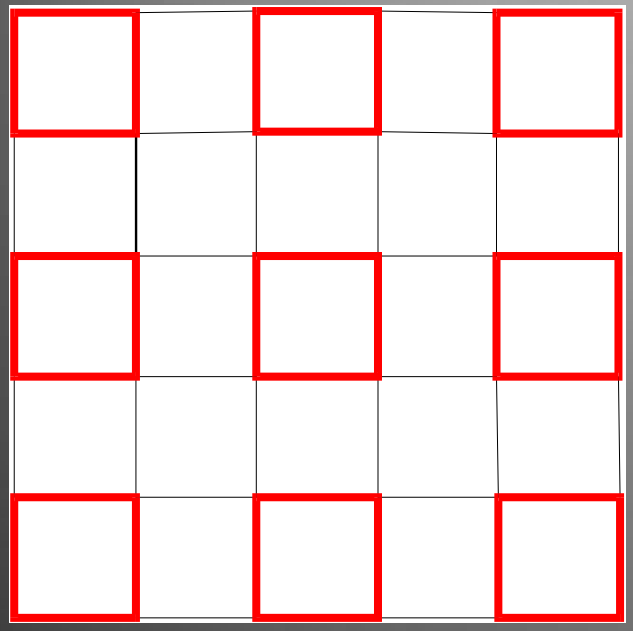
$$S_{eff} = -\iint d\tau d\tau' c_\sigma^+(\tau)\mathcal{G}_0^{-1}(\tau-\tau')c_\sigma(\tau') + \int d\tau U n^\uparrow(\tau)n^\downarrow(\tau)$$

$$\hat{G}(\tau-\tau') = -\frac{1}{Z}\int D[c,c^+]c(\tau)c^+(\tau')e^{-S_{eff}}$$

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

W. Metzner and D. Vollhardt, PRL(1989)
A. Georges et al., RMP 68, 13 (1996)

Cluster DMFT scheme

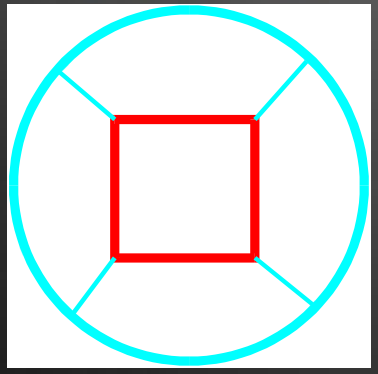


$$\hat{G}(i\omega_n) = \frac{1}{\Omega}\sum_{k}^{BZ}\left[\hat{I}(\mu + i\omega_n) - \hat{H}_0(k) - \hat{\Sigma}(i\omega_n)\right]^{-1}$$

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

$$S_{eff} = -\iint d\tau d\tau' c^{+}_{I\sigma}(\tau)\mathcal{G}^{-1}_{IJ}(\tau - \tau')c_{J\sigma}(\tau') + \int d\tau U n_{I\uparrow}(\tau)n_{J\downarrow}(\tau)$$

Mapping



$$\hat{G}_{IJ}(\tau - \tau') = -\frac{1}{Z}\int D[c,c^{+}]c_I(\tau)c_J^{+}(\tau')e^{-S_{eff}}$$

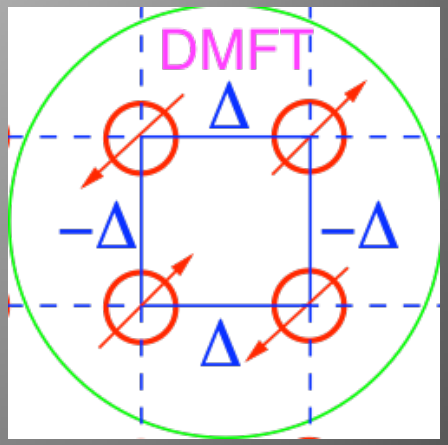
$$\hat{\Sigma}_{new}(i\omega_n) = \hat{\mathcal{G}}_0^{-1}(i\omega_n) - \hat{G}^{-1}(i\omega_n)$$

A.L., M. Katsnelson, PRB ***62****, R928368, (2000)*
G. Kotliar, et al RMP ***78****, 865 (2006)*

Cluster Impurity Problem

Super-impurity partition function:

$$Z = \int \mathcal{D}[c^*, c] e^{-S_{simp}}$$



$$\Psi_I^+(\tau) = \left(c_{I\uparrow}^\dagger, c_{I\downarrow}^\dagger, c_{I\uparrow}, c_{I\downarrow} \right)$$

I=(1,2,3,4)

$$S_{simp} = -\sum_{I,J=0}^{N} \int_0^\beta d\tau \int_0^\beta d\tau'\, c_{I\sigma}^*(\tau) \left[\mathcal{G}_\sigma^{-1}(\tau - \tau') \right]_{IJ} c_{J\sigma}(\tau') + \sum_{I=1}^{N} \int_0^\beta d\tau U n_{I,\uparrow}(\tau) n_{I,\downarrow}(\tau)$$

Local plaquette Green-function:

$$G_{IJ}(i\omega) = \sum_{\mathbf{K}} G_{IJ}(\mathbf{K}, i\omega)$$

Bath Green-fanction matrix:

$$\mathcal{G}^{-1}(i\omega) = G^{-1}(i\omega) + \Sigma(i\omega)$$

CTQMC: Exact solution of S-imp:

$$G_{IJ}^{simp}(\tau) = -\langle c_{I\sigma}(\tau) c_{J\sigma}^\dagger(0) \rangle_{simp}$$

New self-energy matrix:

$$\Sigma_{new}(i\omega) = \mathcal{G}^{-1}(i\omega) - G_{simp}^{-1}(i\omega)$$

CDMFT: Self-consistent condition:

$$G_{IJ}^{simp}(i\omega) = G_{IJ}(i\omega)$$

Imputity solver: miracle of CT-QMC

$$S = \sum_{\sigma\sigma'} \int_0^\beta d\tau \int_0^\beta d\tau [-G_0^{-1}(\tau-\tau') c_\sigma^+(\tau) c_\sigma(\tau') + \frac{1}{2} U \delta(\tau-\tau') c_\sigma^+(\tau) c_{\sigma'}^+(\tau) c_{\sigma'}(\tau') c_\sigma(\tau')]$$

$$G_0^{-1}(\tau - \tau') = \delta(\tau - \tau')[\frac{\partial}{\partial \tau} + \mu] - \Delta(\tau - \tau')$$

Interaction expansion CT-INT: A. Rubtsov et al, JETP Lett (2004)

$$Z = Z_0 \sum_{k=0}^{\infty} \frac{(-U)^k}{k!} Tr \det[G_0(\tau - \tau')]$$

Hybridization expansion CT-HYB: P. Werner et al, PRL (2006)

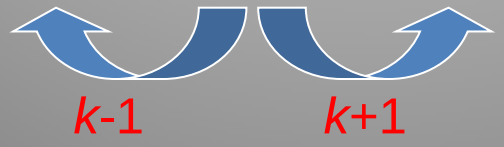
$$Z = Z_0 \sum_{k=0}^{\infty} \frac{1}{k!} Tr \left\langle c_\sigma^+(\tau) c_\sigma(\tau') ... c_{\sigma'}^+(\tau) c_{\sigma'}(\tau') \right\rangle_0 \det[\Delta(\tau-\tau')]$$

Efficient Krylov scheme: A. Läuchli and P. Werner, PRB (2009)

E. Gull, et al, RMP **83**, 349 (2011)

CT-QMC: random walks in the *k* space

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



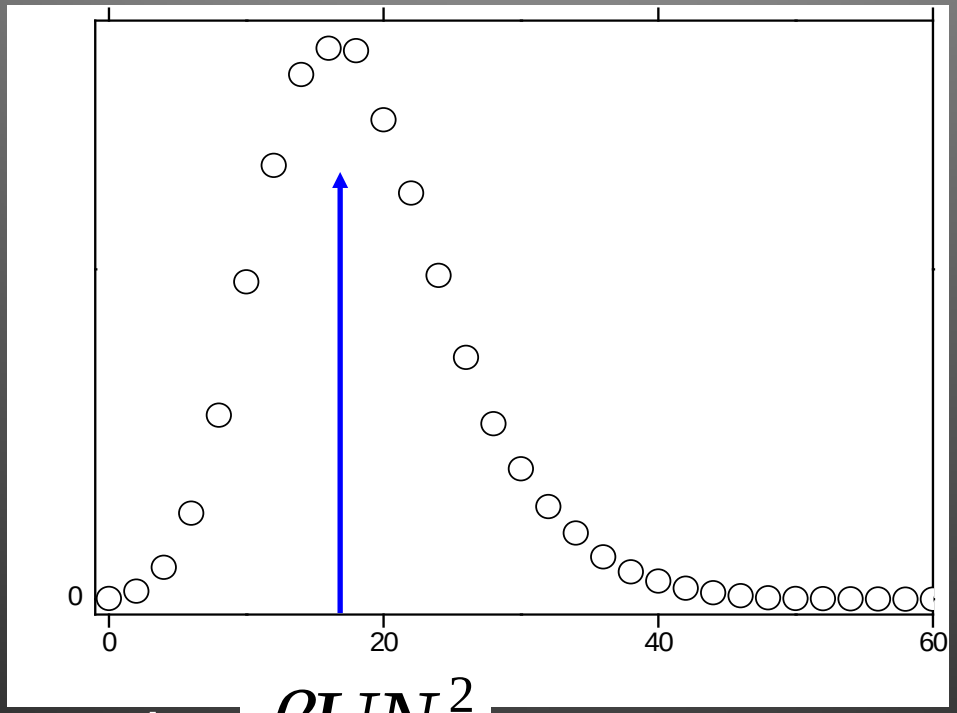
Acceptance ratio

decrease

increase

Step *k*-1

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

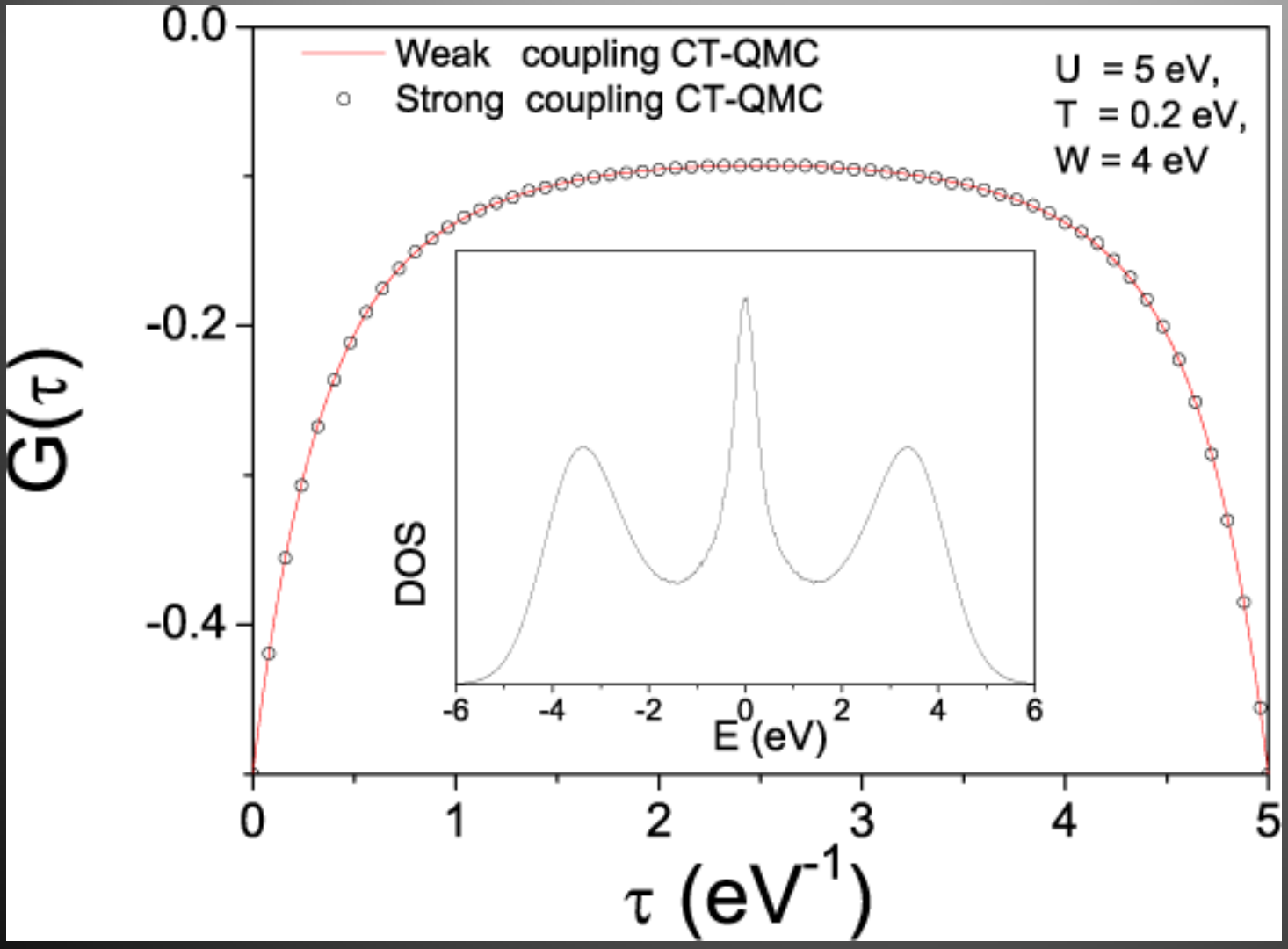


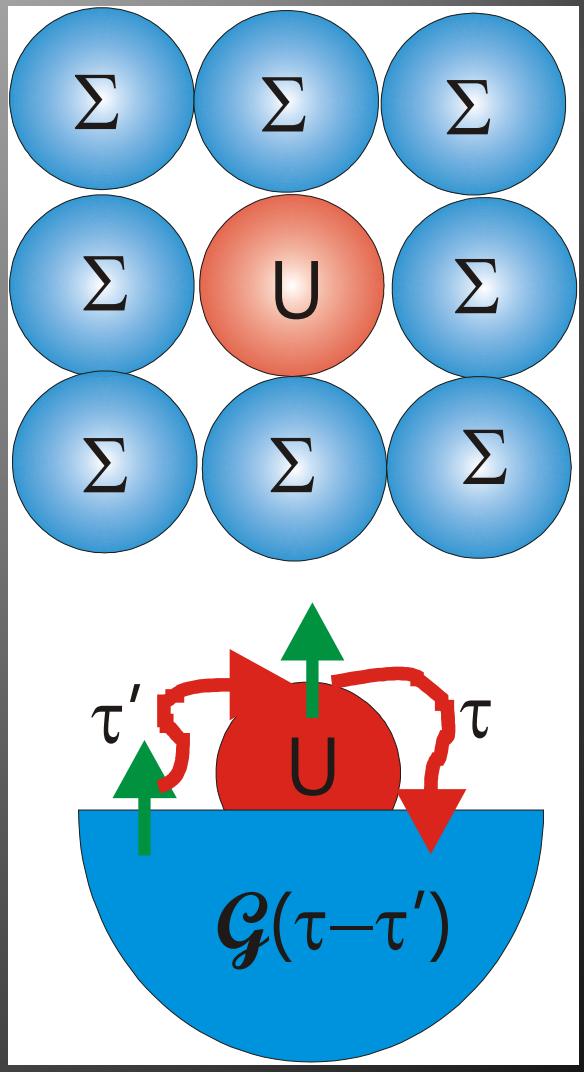
Step *k*+1

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

Maximum at $\beta U N^2$

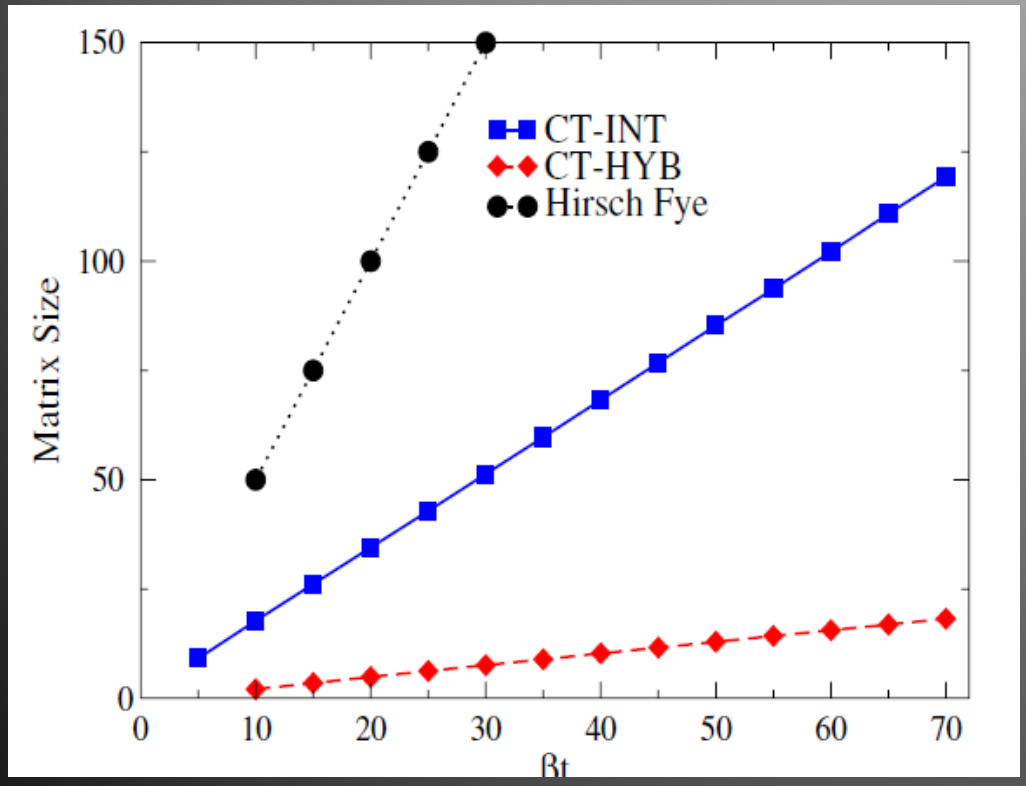
Comparison of different CT-QMC



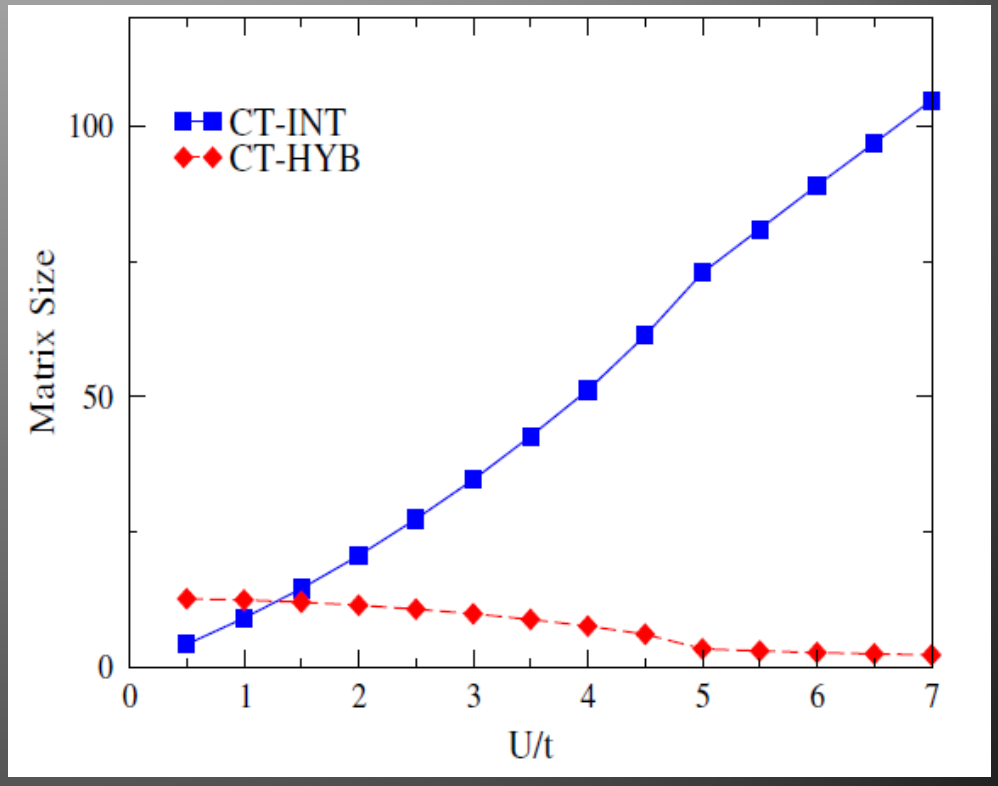


Ch. Jung, unpublished

Scaling of CT-QMC



Temperature

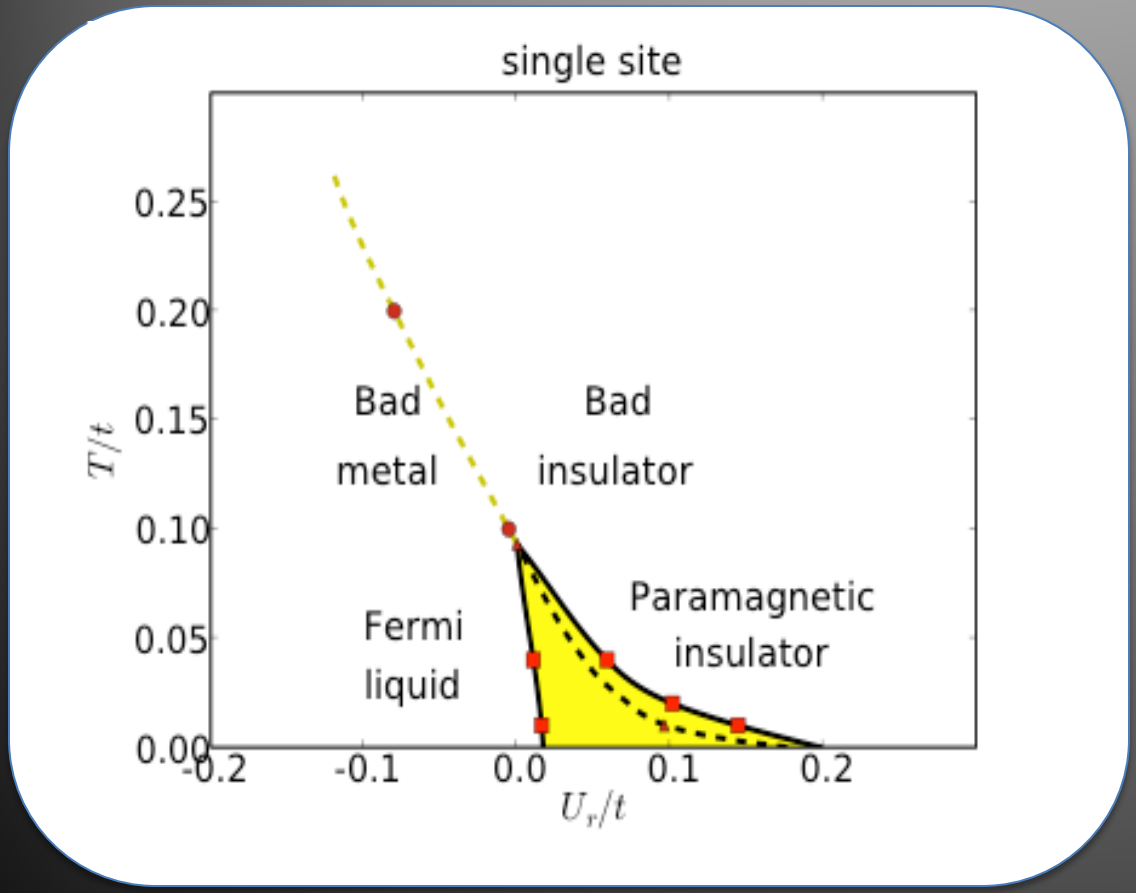


Interactions

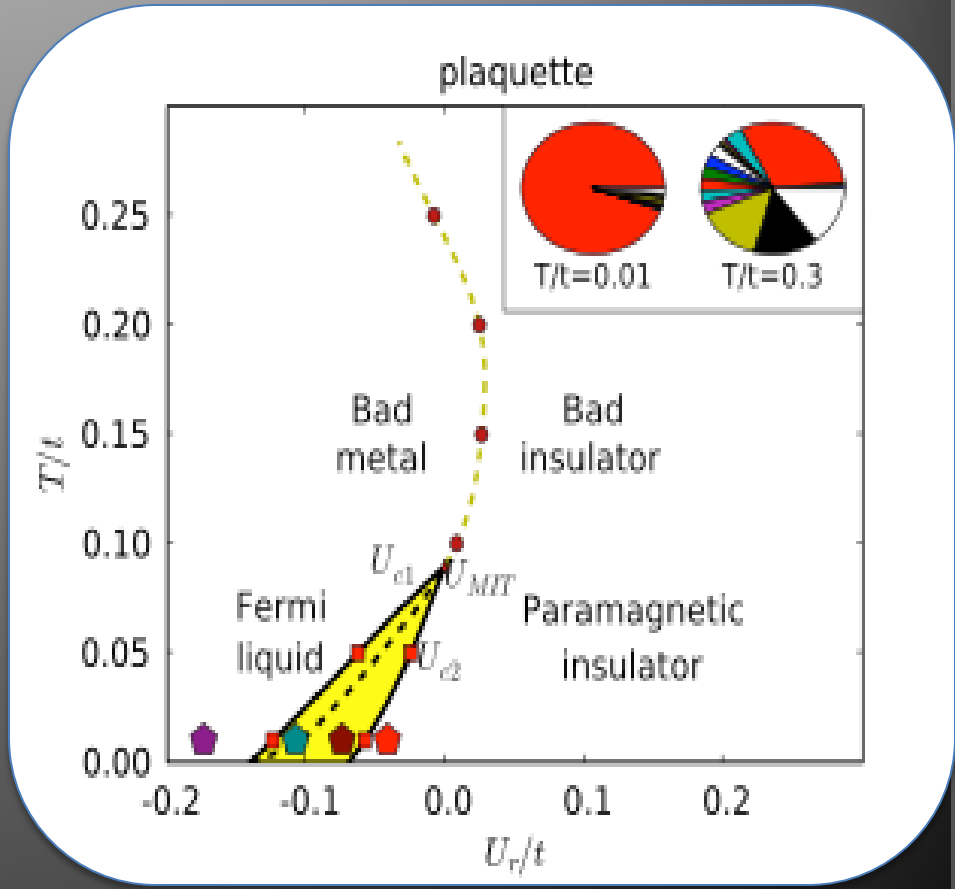
CT-QMC review :E. Gull et al. RMP (2011)

Phase diagram of Hubbard model

Uc=9.35t



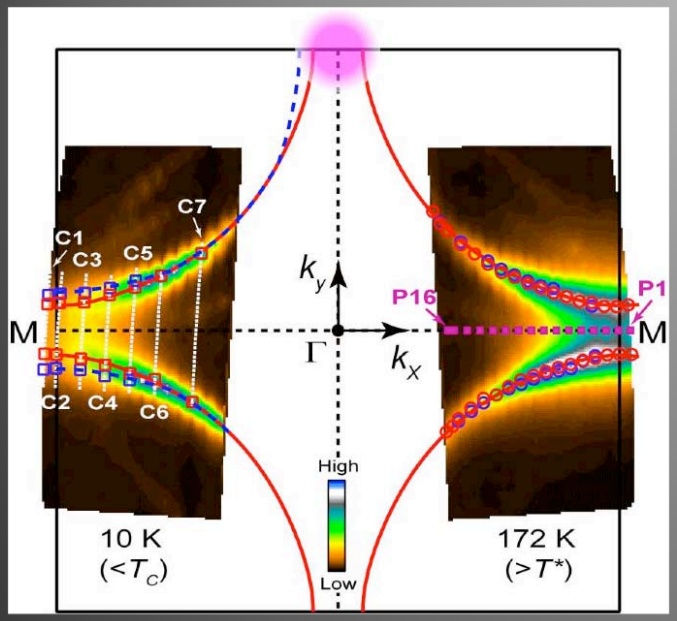
Uc=6.05t

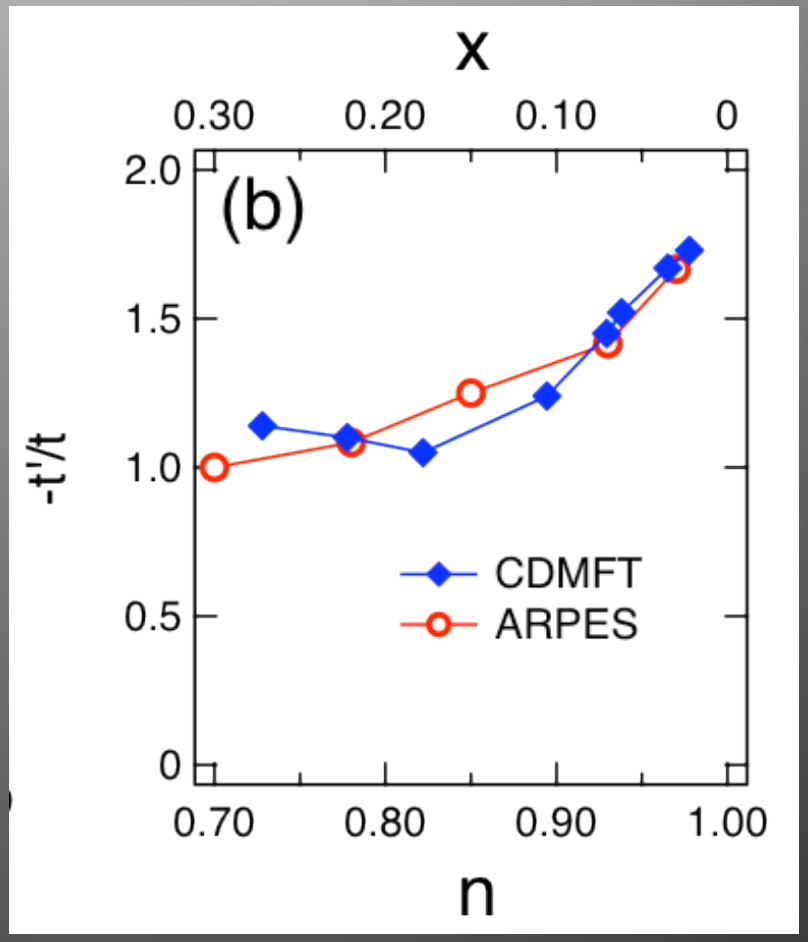


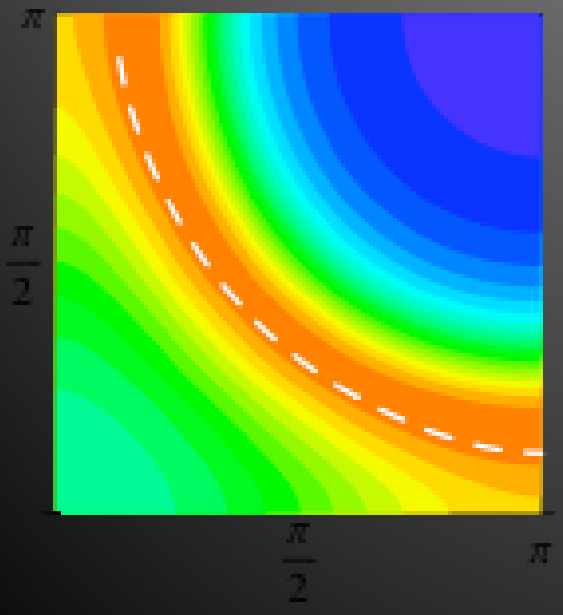
H. Park et al PRL (2008)
C-DMFT with CT-QMC

ARPES of HTSC

Z.X. Shen (Stanford)







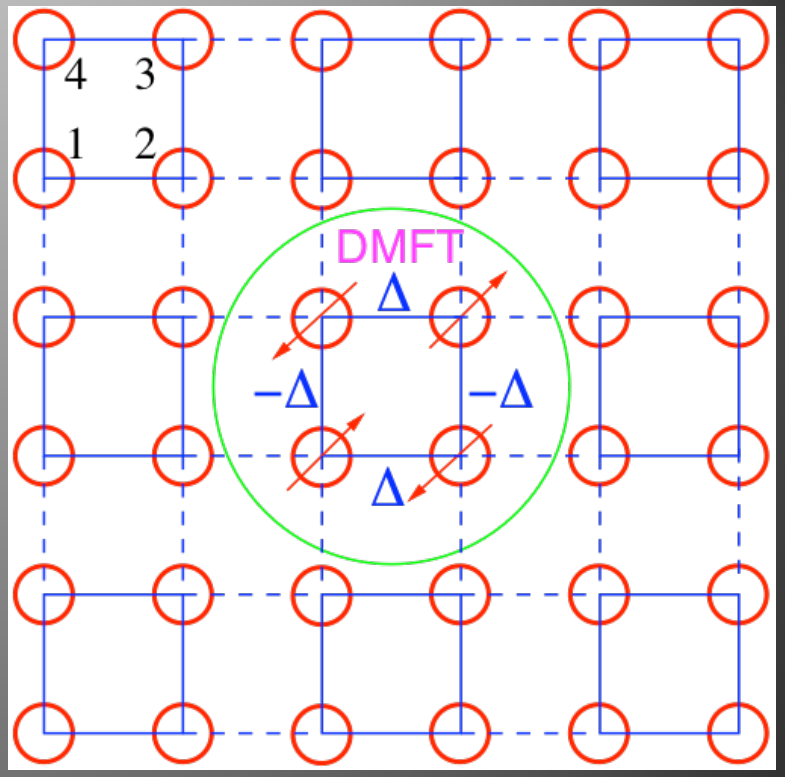
M. Civelli et al PRL (2005) CDMFT

Cluster-DMFT

Plaquette hopping matrix

$$T_{I,J}(\mathbf{K}) = \begin{pmatrix} 0 & t_x K_x^+ & 0 & t_y K_y^+ \\ t_x K_x^- & 0 & t_y K_y^+ & 0 \\ 0 & t_y K_y^- & 0 & t_x K_x^- \\ t_y K_y^- & 0 & t_x K_x^+ & 0 \end{pmatrix}$$

where $K_{x(y)}^{\pm} \equiv 1 + \exp\left(\pm i K_{x(y)} a\right)$



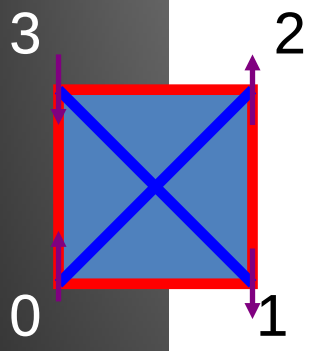
Supercell Green Function

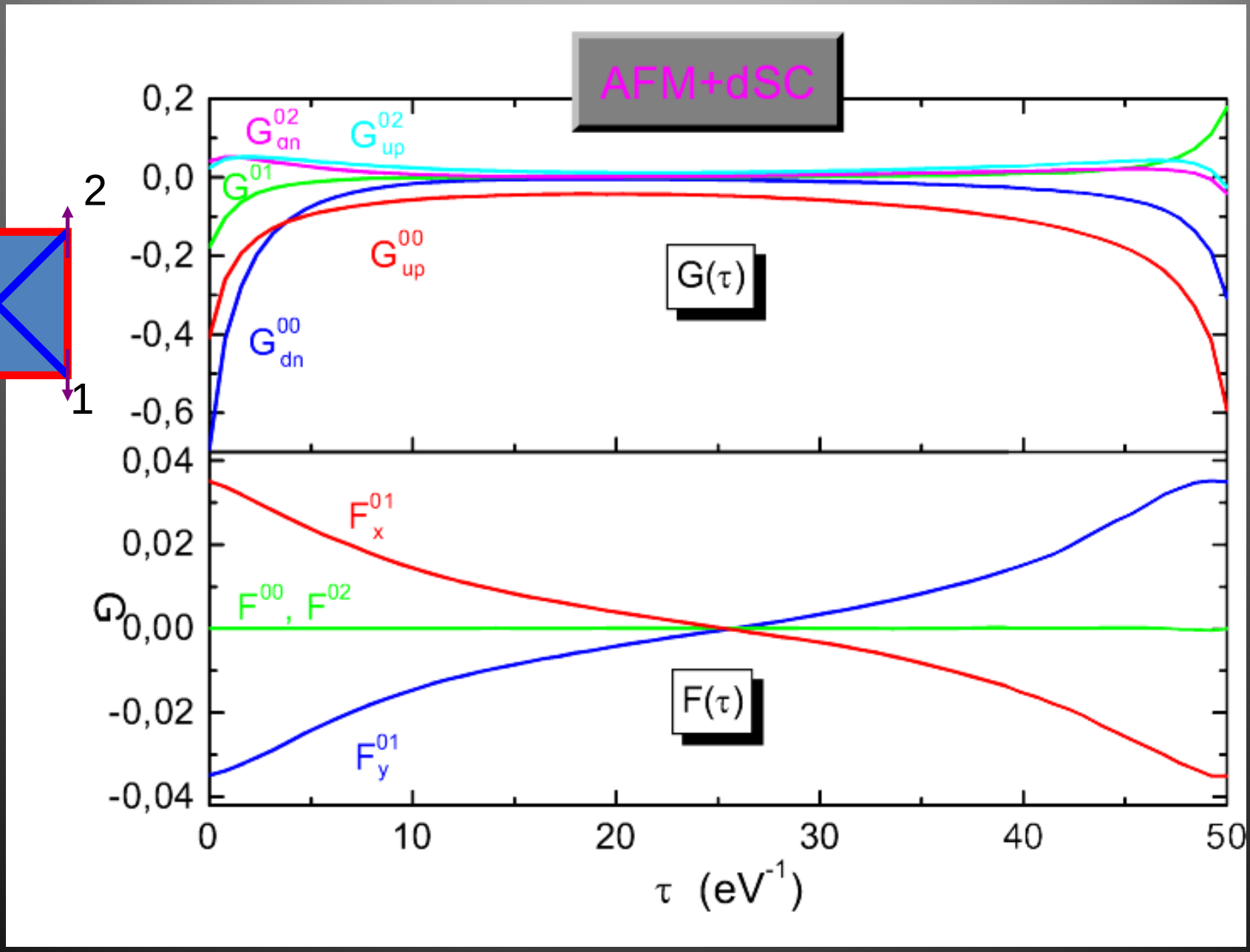
$$G(\mathbf{K}, i\omega) = \left[(i\omega + \mu)\mathbf{1} - T(\mathbf{K}) - \Sigma(i\omega)\right]^{-1}$$

Where Self-energy matrix for plaquette has the form:

$$\Sigma_{I,J}(i\omega) = \begin{pmatrix} \Sigma_0 & \Sigma_x & \Sigma_{xy} & \Sigma_y \\ \Sigma_x & \Sigma_0 & \Sigma_y & \Sigma_{xy} \\ \Sigma_{xy} & \Sigma_y & \Sigma_0 & \Sigma_x \\ \Sigma_y & \Sigma_{xy} & \Sigma_x & \Sigma_0 \end{pmatrix}$$

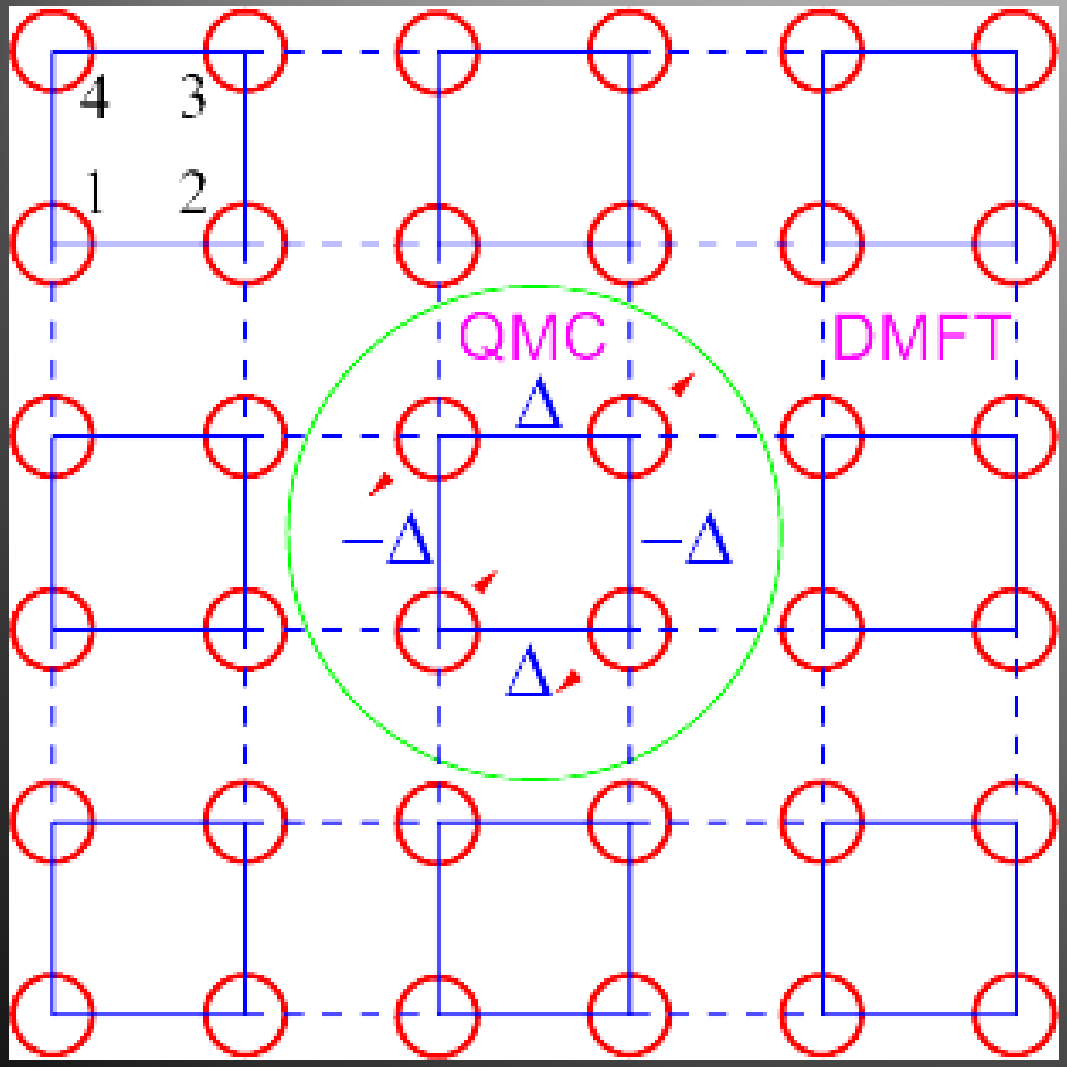
Coexistence of AFM and d-wave

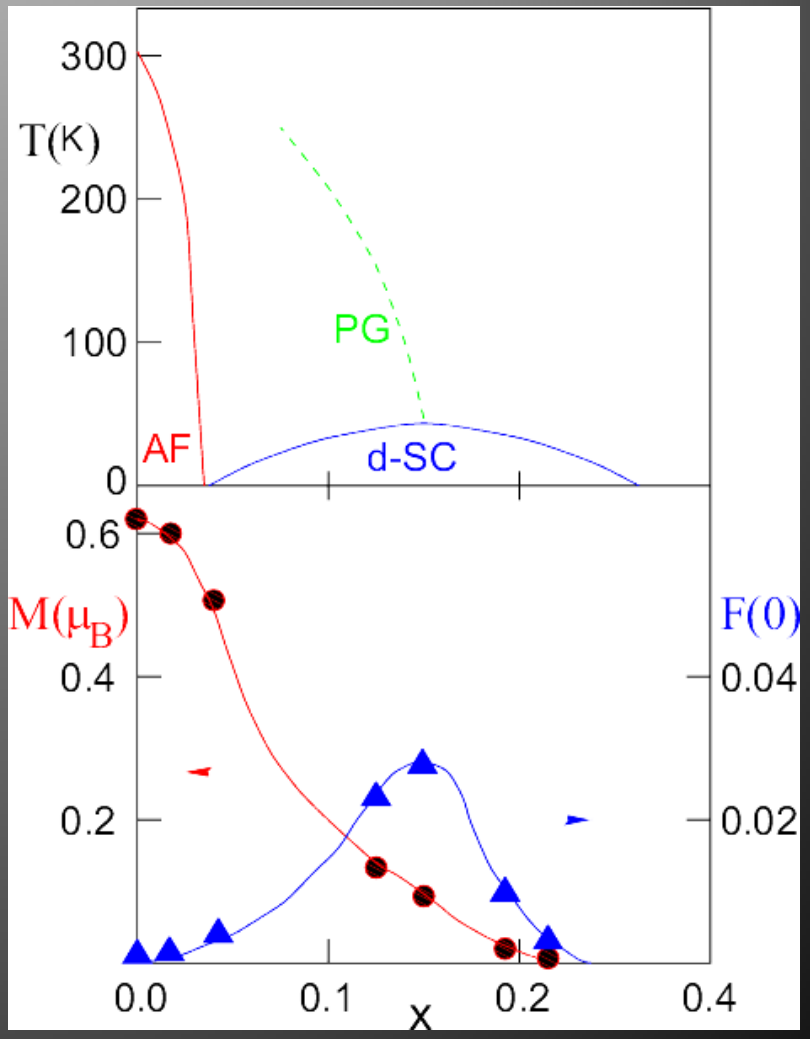




A.L. and M.Katsnelson, PRB (2000)

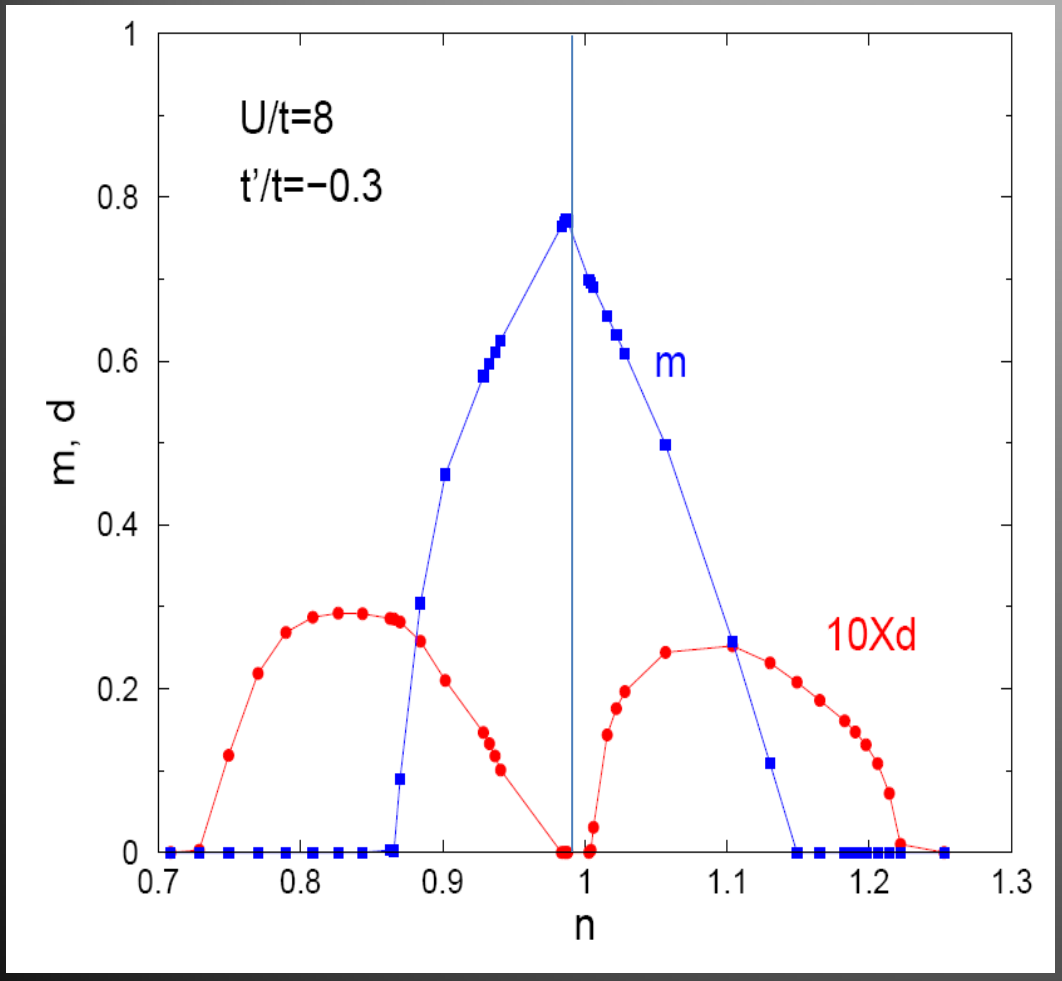
AFM and d-wave in HTSC





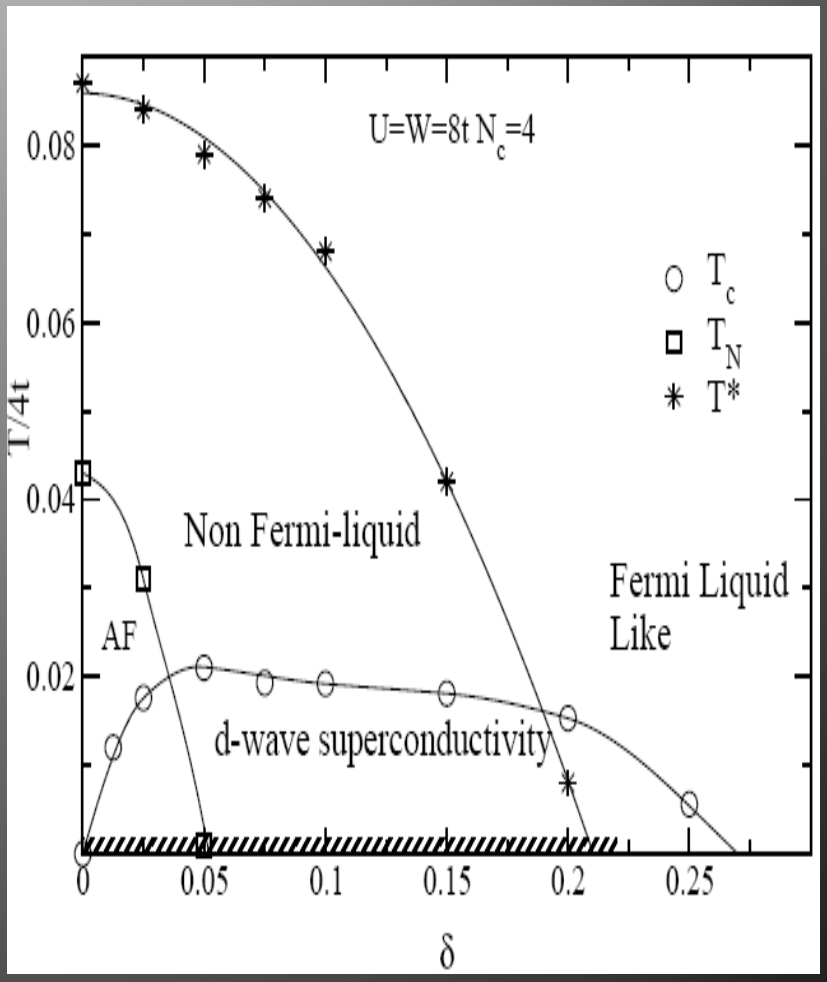
A.L. and M.Katsnelson, PRB **62**, R9283 (2000)

CDMFT and DCA: phase diagram



S. Kancharla et al, PRB (2008)

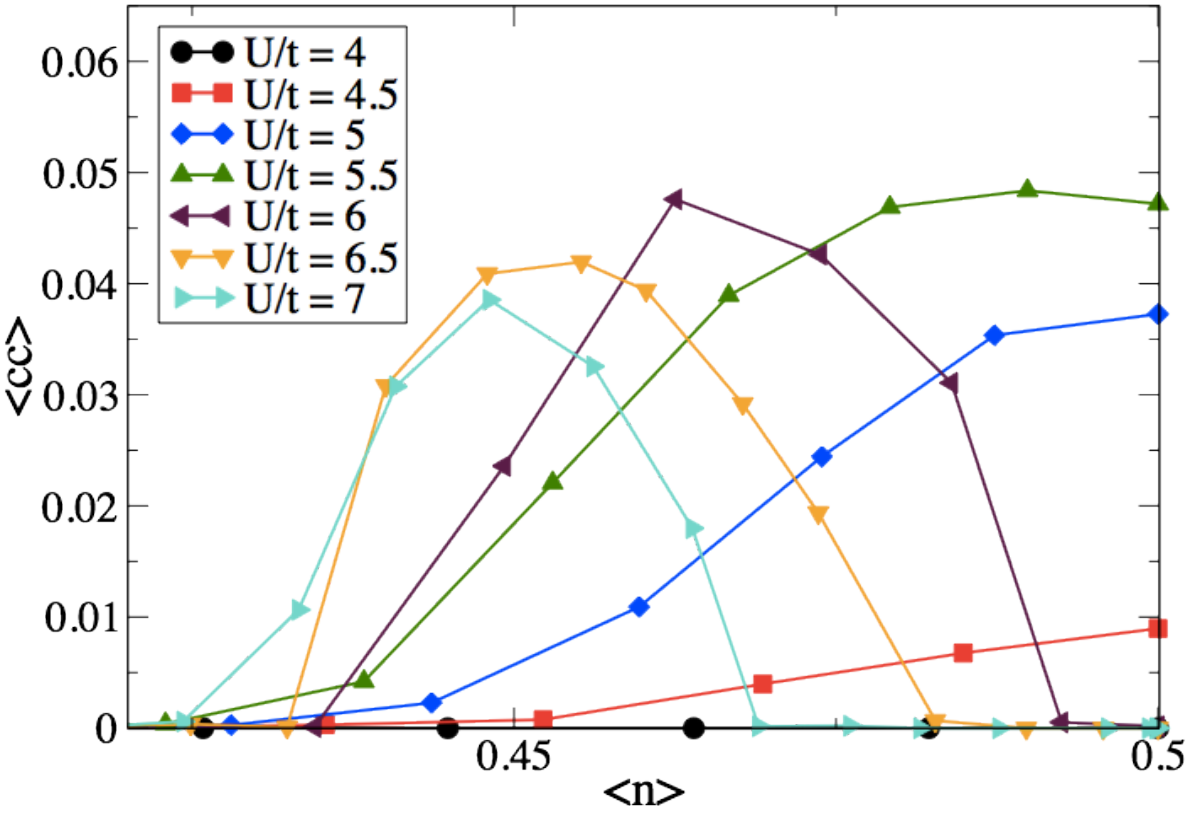
CDMFT

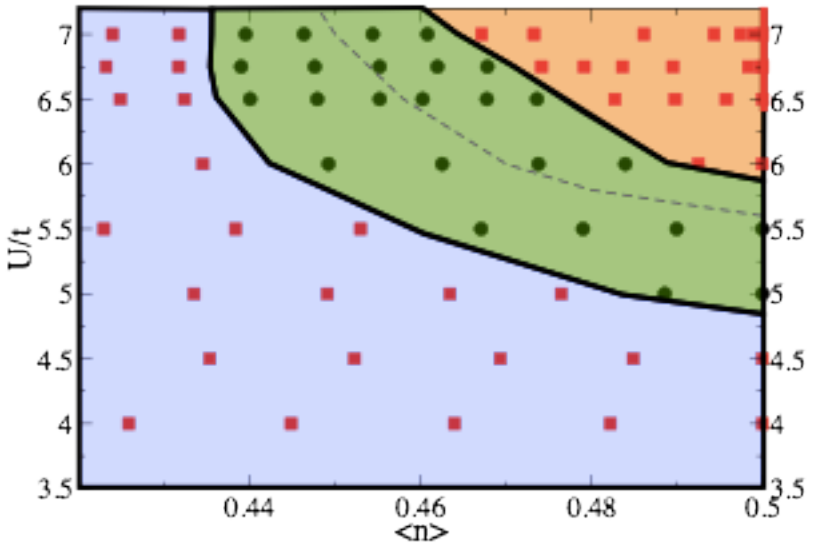


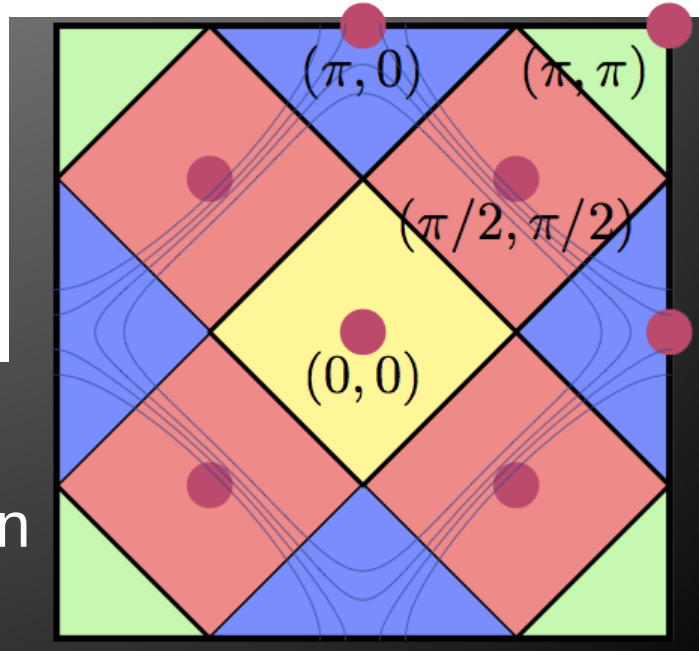
M. Jarrell et al, EPL (2001)

DCA

Superconducting order parameter



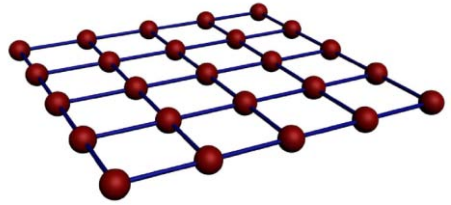




Emanuel Gull et al. to be published,
CT-QMC and Dynamical Cluster Approximation

Beyond DMFT: Dual Fermion scheme

General Lattice Action $H = h + U$

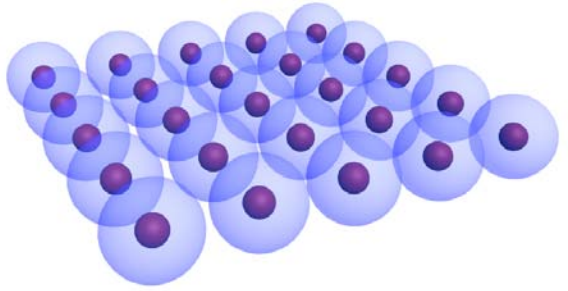


$$S[c^*,c] = \sum_{\omega k m m' \sigma} \left[h_k^{mm'} - (i\omega + \mu)1 \right] c^*_{\omega k m \sigma} c_{\omega k m' \sigma} + \frac{1}{4} \sum_{i\{m,\sigma\}} \int_0^\beta U_{1234} c_1^* c_2^* c_3 c_4 d\tau$$

Reference system: Local Action with hybridization Δ_ω

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

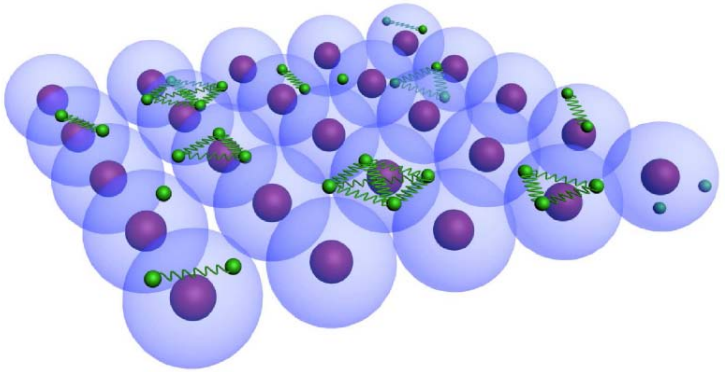
Lattice-Impurity connection:



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

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:

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

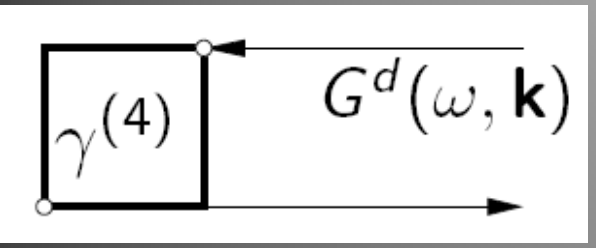
Diagrammatic:

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

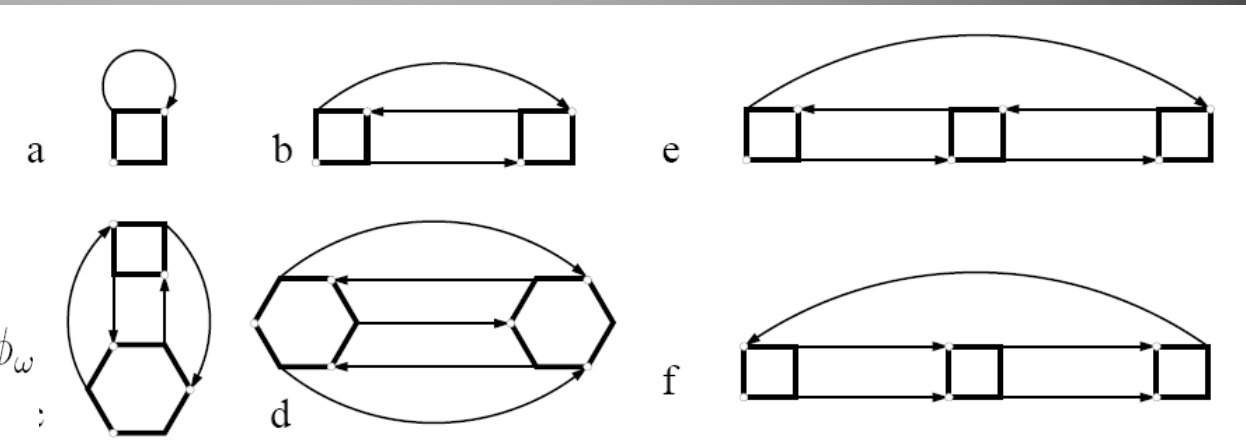
□ $$\gamma^{(4)}_{1234} = g^{-1}_{11'}g^{-1}_{22'}\left(\chi_{1'2'3'4'}-\chi^0_{1'2'3'4'}\right)g^{-1}_{3'3}g^{-1}_{4'4}$$

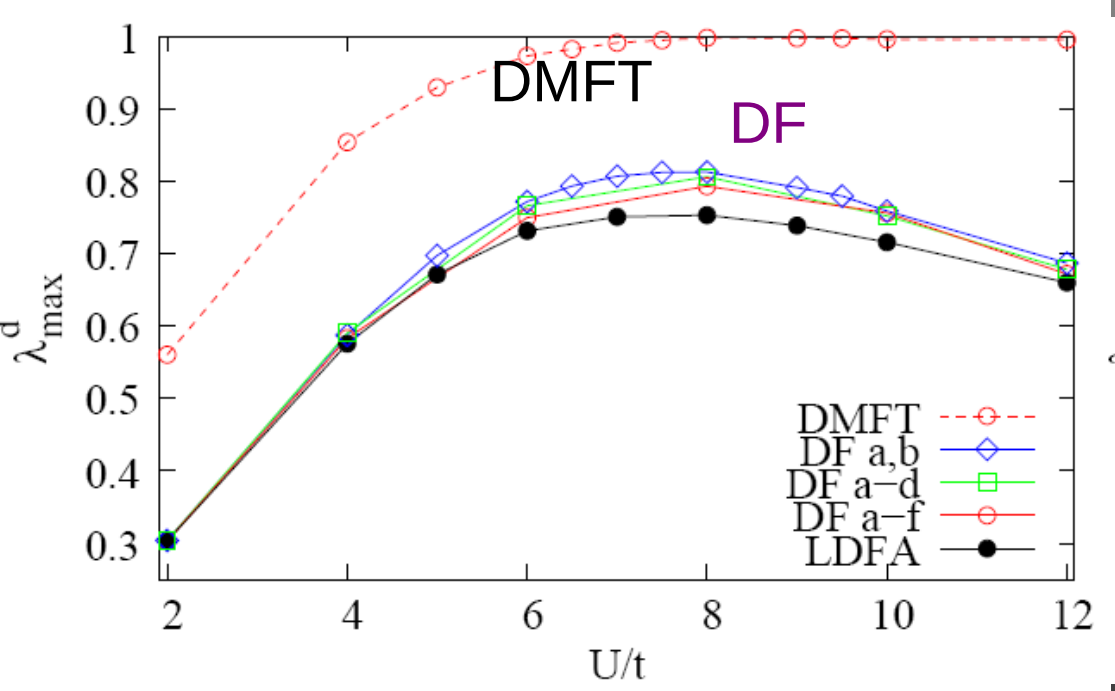
g_ω and $\chi_{\nu,\nu',\omega}$ from DMFT impurity solver

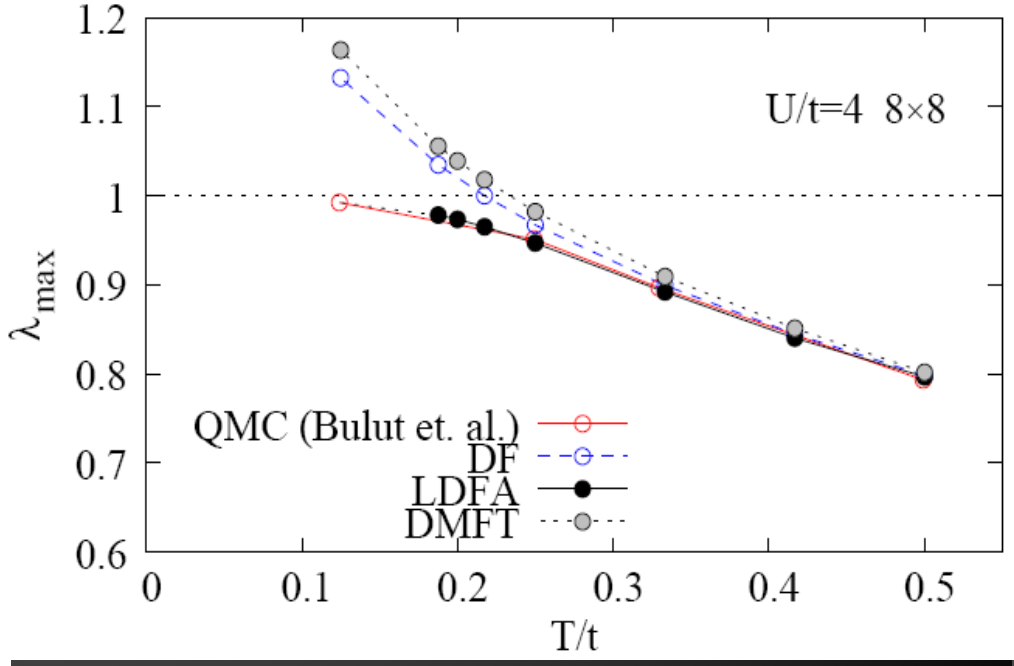
Convergence of Dual Fermions: 2d



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



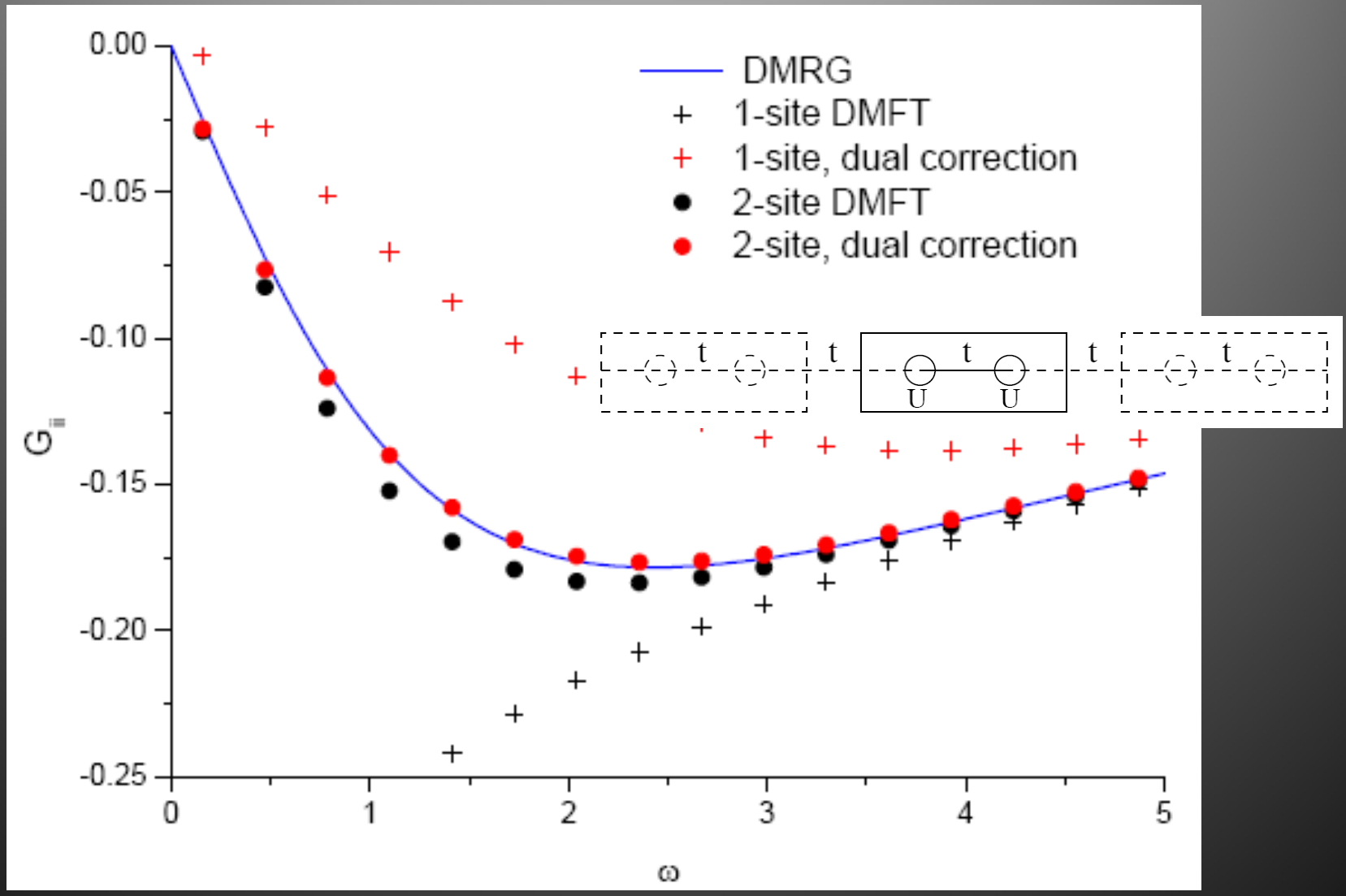




H. Hafermann, et al. PRL**102**, 206401 (2009)

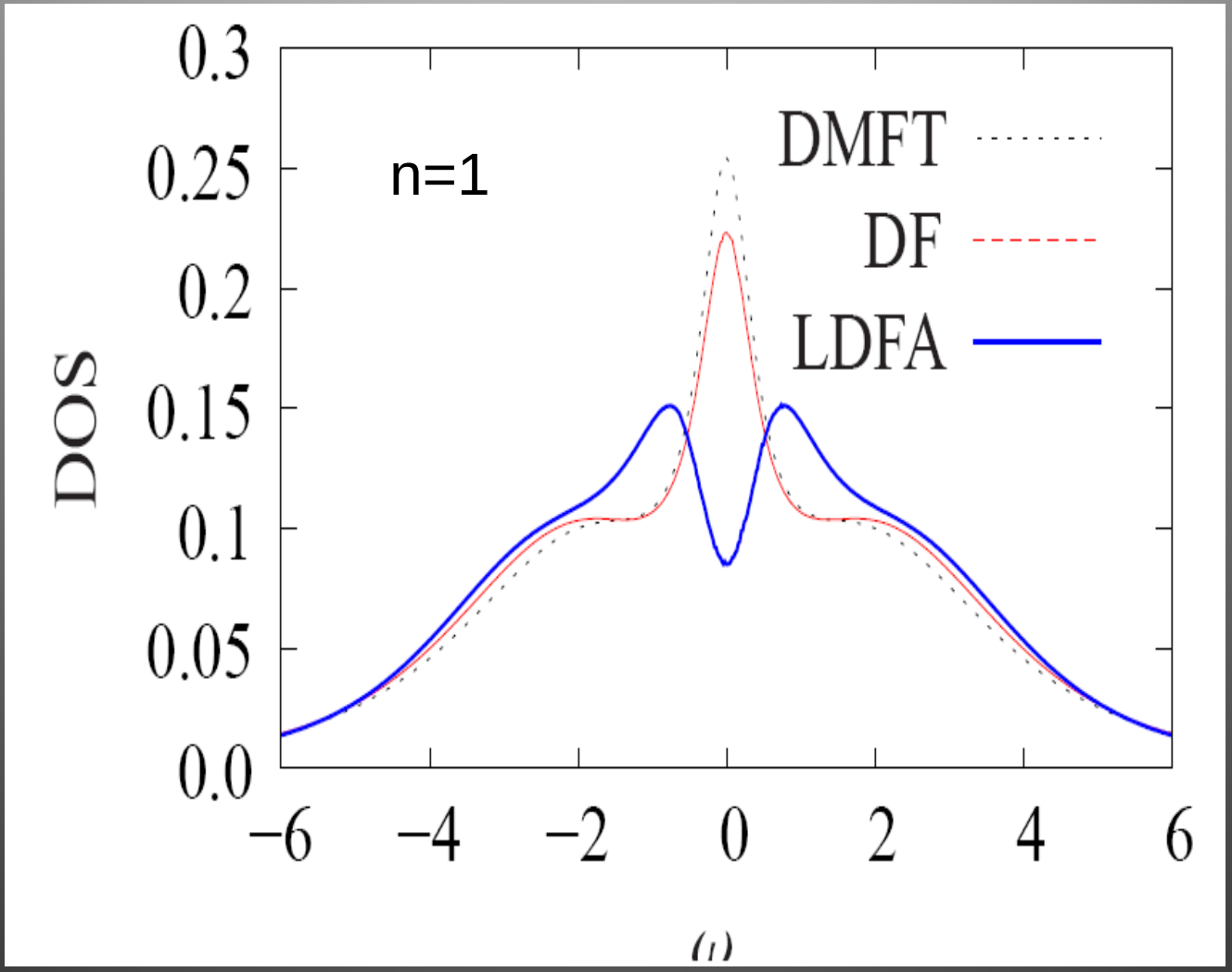
Cluster Dual Fermions: 1d-test, n=1

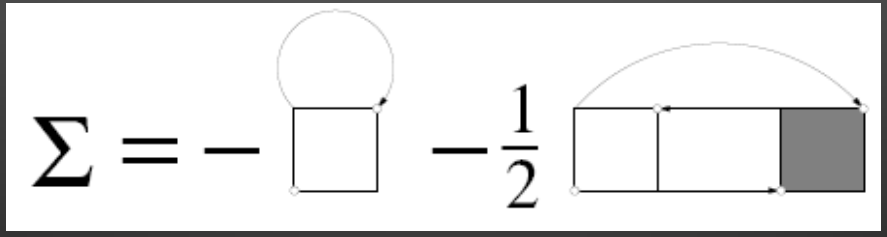
1D Hubbard chain $U/t = 6,\ \beta = 10,\ \epsilon(\mathbf{k}) = -2t\cos(ka)$



H. Hafermann, et al. JETP Lett (2007)

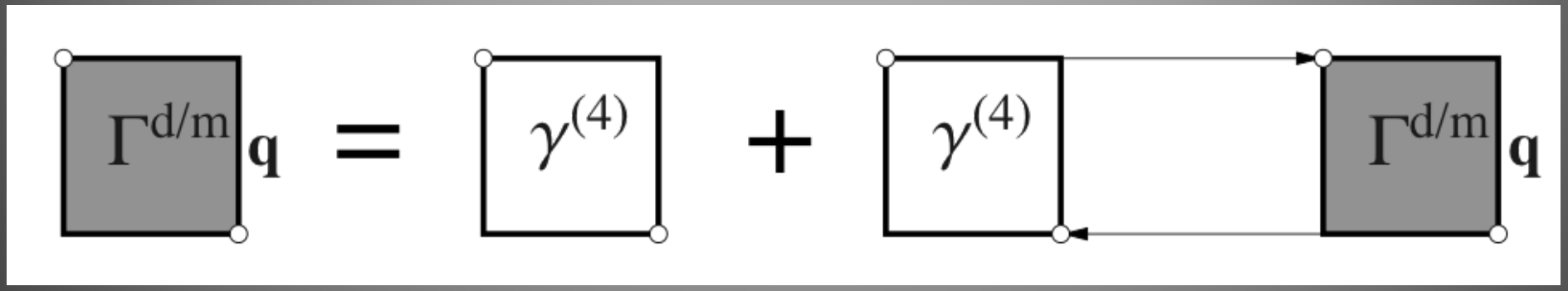
Pseudogap in HTSC: Ladder-DF



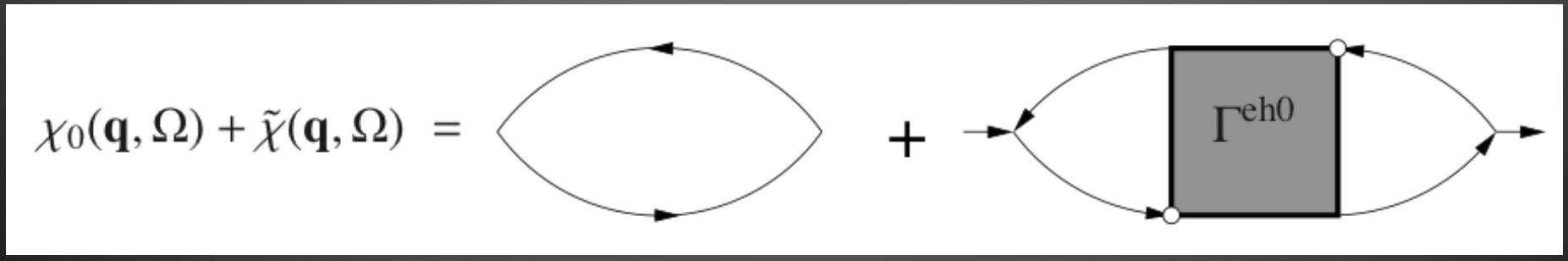


H. Hafermann, et al. PRL**102**, 206401 (2009)

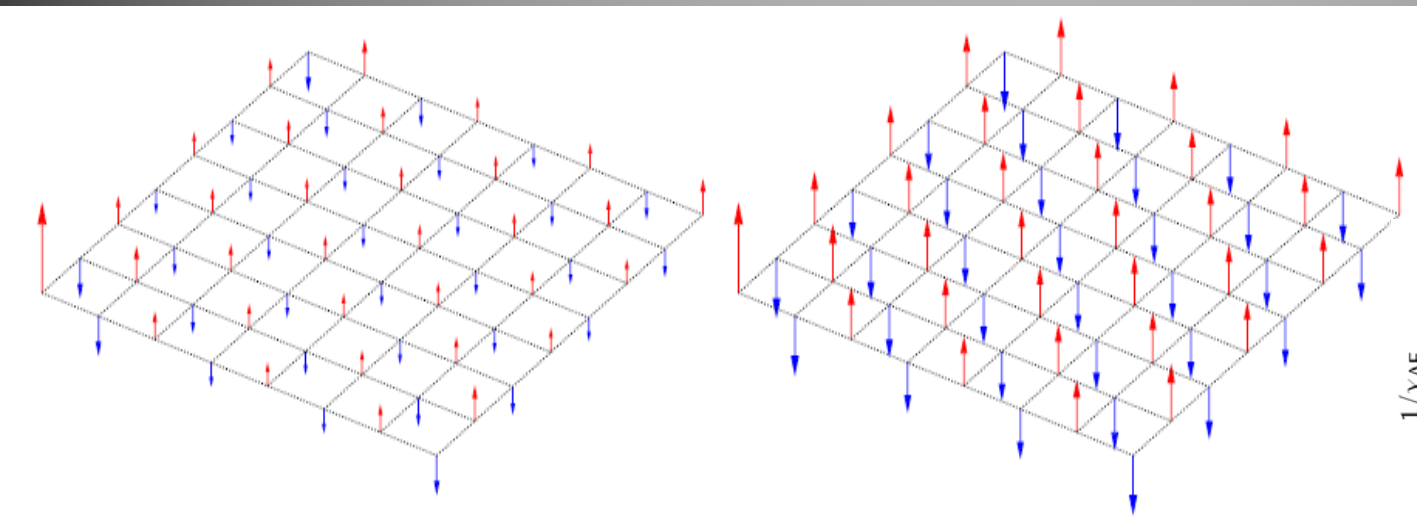
Bethe-Salpeter Equations

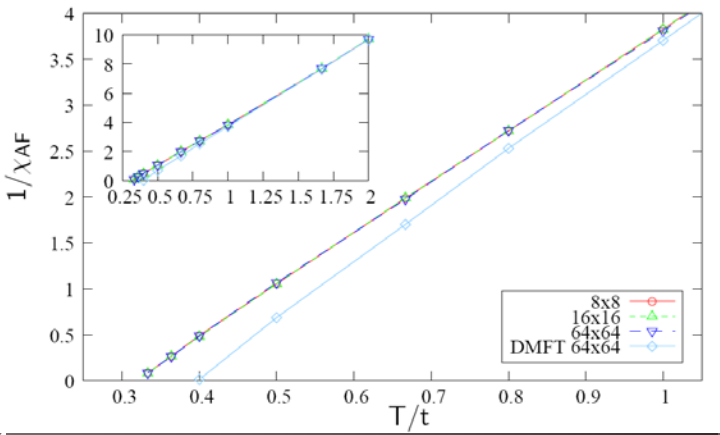


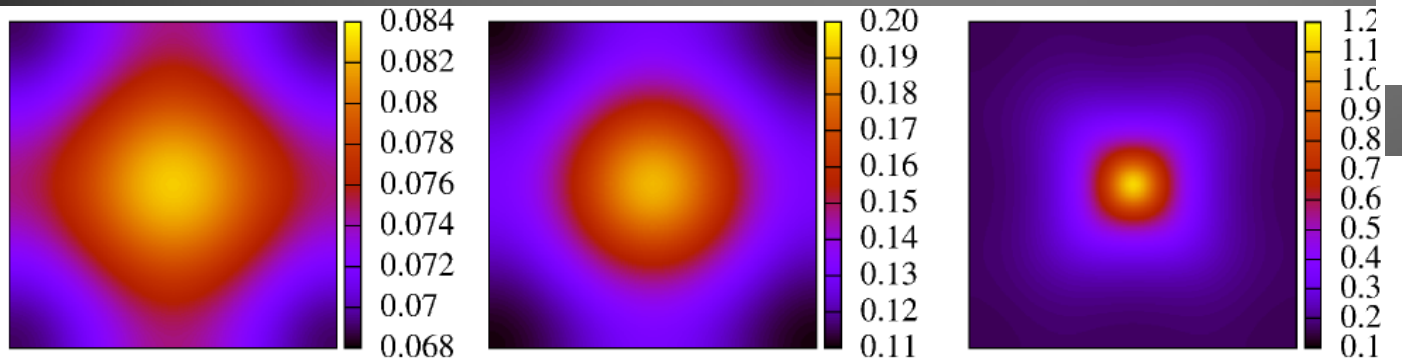
Non-local susceptibility with vertex corrections

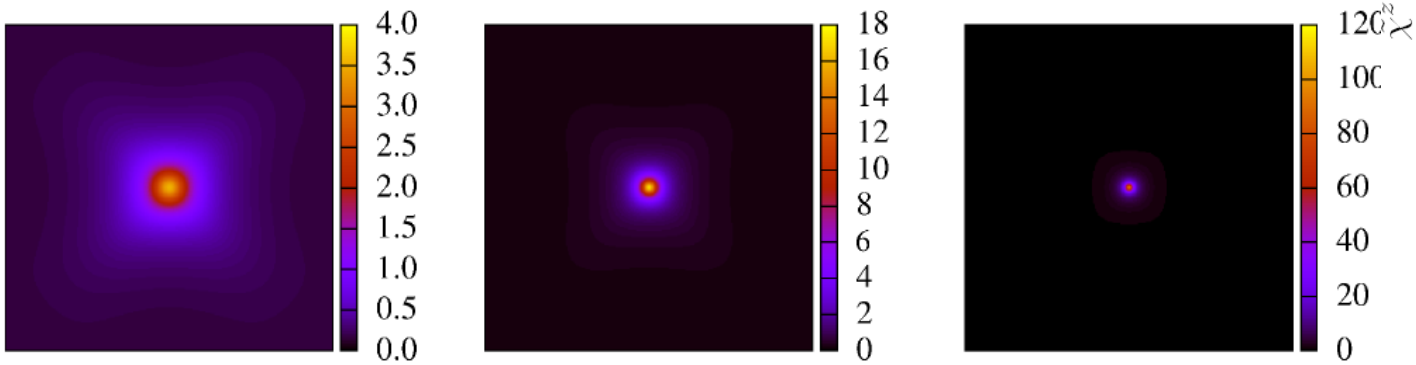


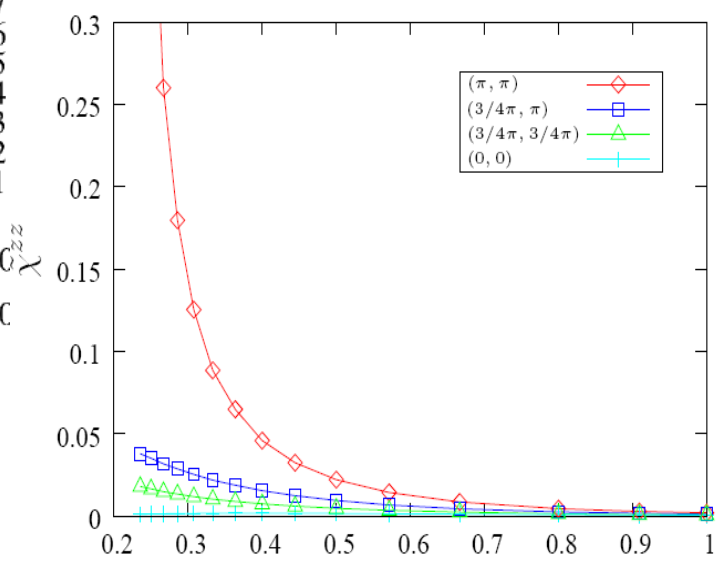
Susceptibility: 2d – Hubbard model





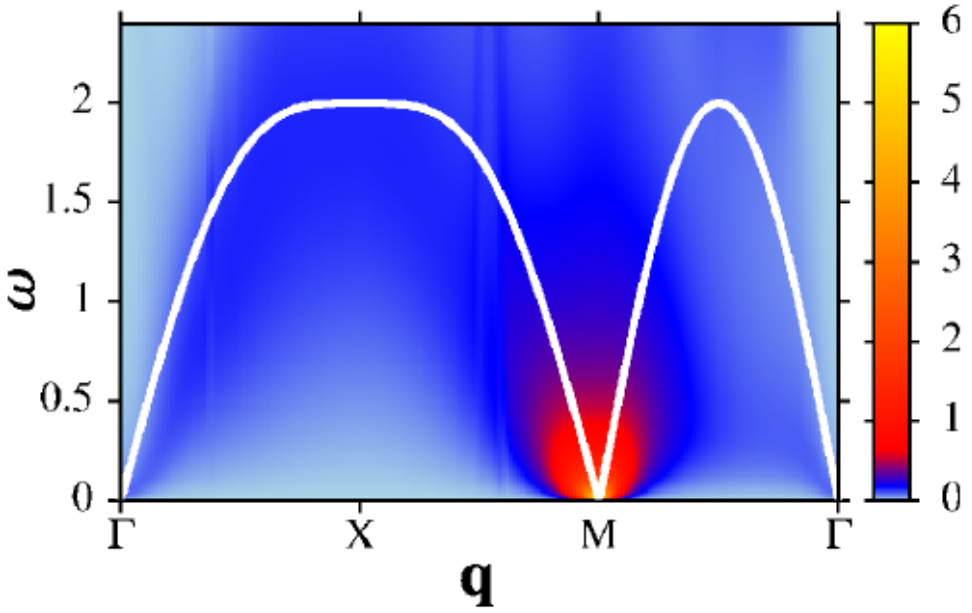


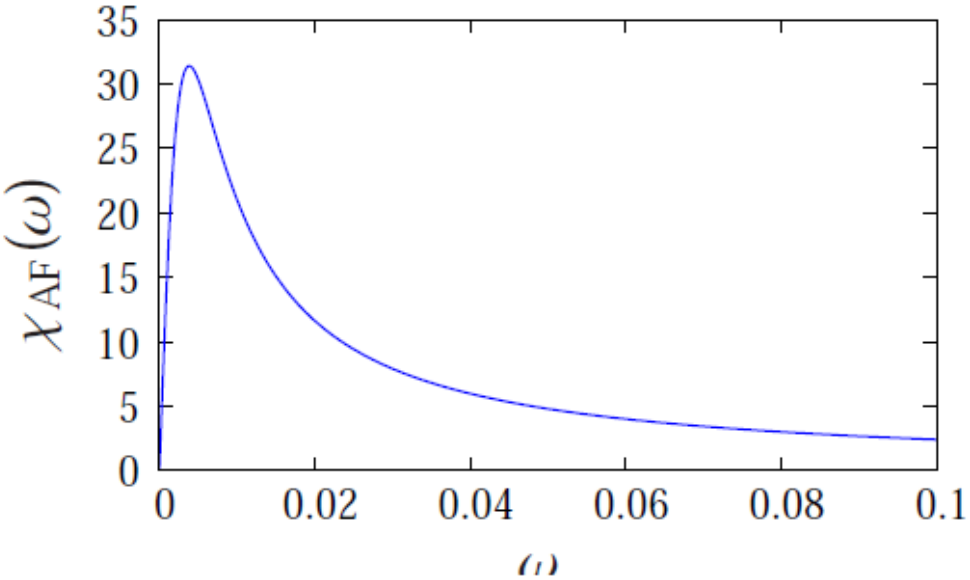




DF: Ladder Approximation

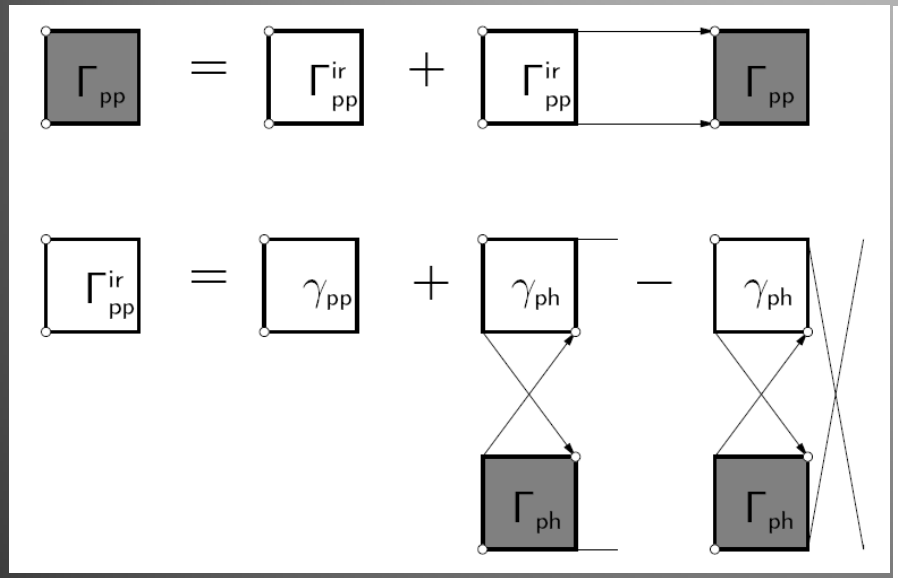
dynamical susceptibility



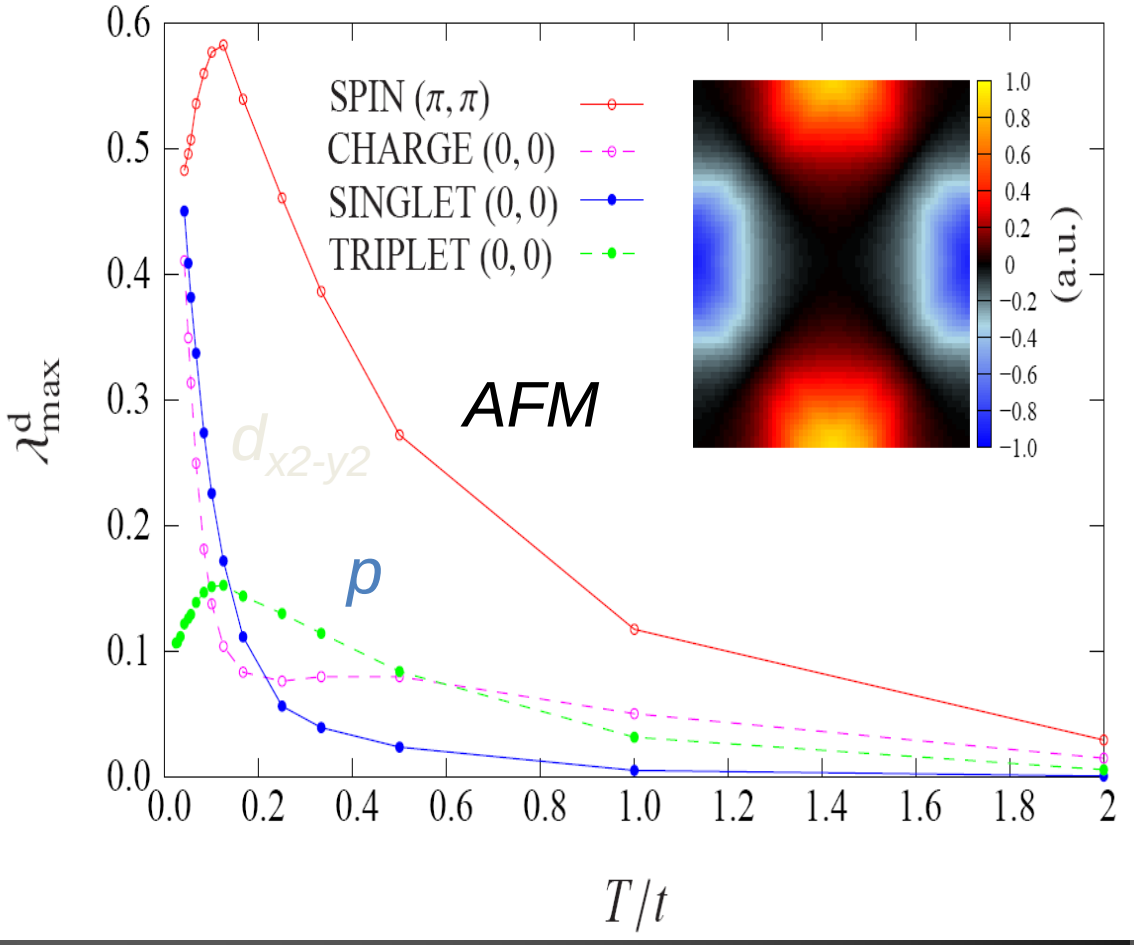


- magnon spectrum in the paramagnetic state
- compare to spin wave theory with $J = 4t^2/U$
- strong enhancement at $\mathbf{Q} = (\pi, \pi)$
- Heisenberg-like with large correlation length ξ and small energy scale $\sim Ja/\xi$

Bethe-Salpeter equation: pp-channel



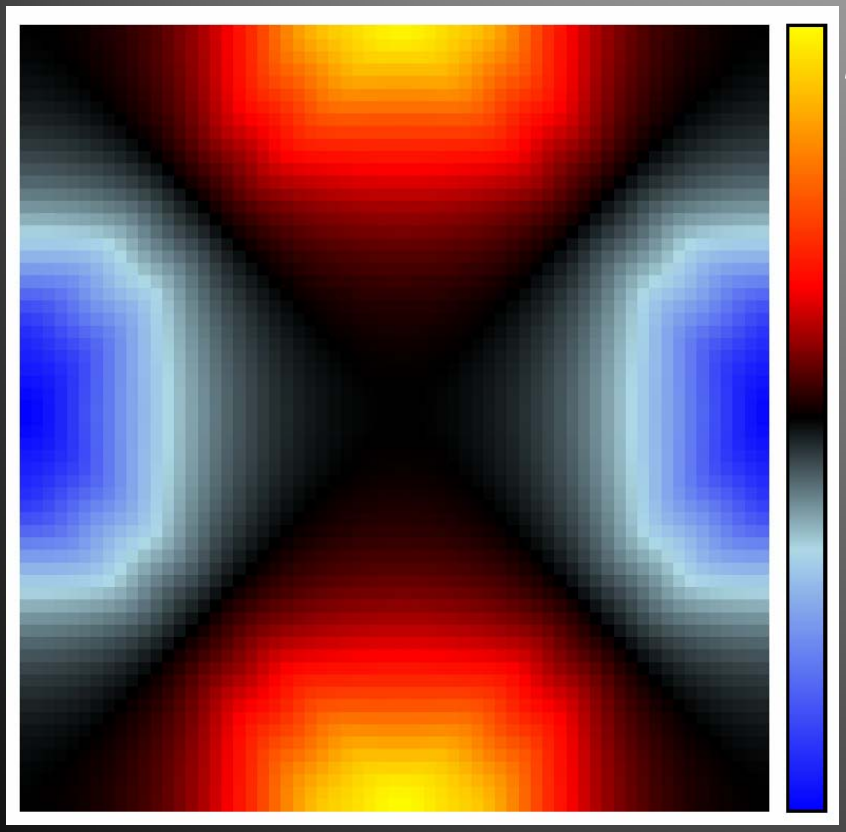
U=W t'/t=-0.3 x=15%

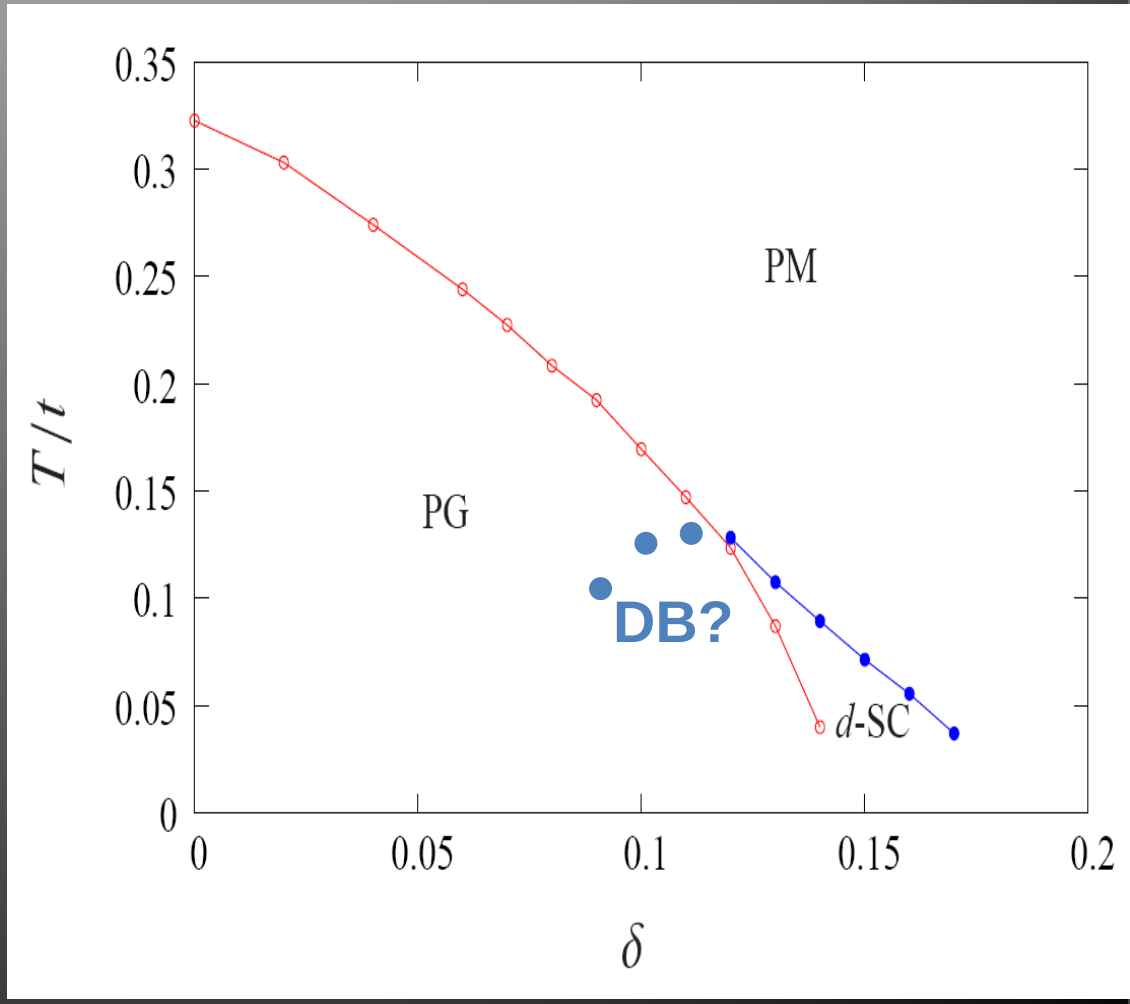


$$\frac{1}{2\beta N^d}\sum_{\omega' \mathbf{k}'_1}\gamma^{\mathrm{irr},s/t}_{p\omega\omega'\Omega=0}(\mathbf{k},\mathbf{k}',\mathbf{q}=0)\,G^{\mathrm{d}}_{-\omega'}(-\mathbf{k}')\,G^{\mathrm{d}}_{\omega'}(\mathbf{k}')\phi_{\omega'}(\mathbf{k}')=\lambda\phi_{\omega}(\mathbf{k})$$

d-wave symmetry of the eigenfunction

U/W=1 t'/t=-0.3





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

Conclusions

- Antiferromagnetism and d-wave superconductivity obtained in cluster-DMFT
- Pseudogap and Fermi-arcs describe well in ladder DF-scheme
- Realistic multiorbital LDA+DF for correlated higher-T_c materials is a next challenge