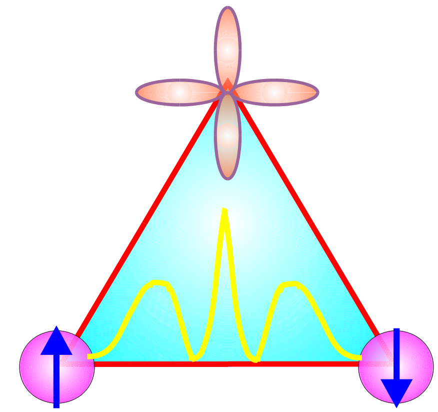


Non-local Correlations in Electronic Structure Scheme: Beyond DMFT

A. Lichtenstein
University of Hamburg

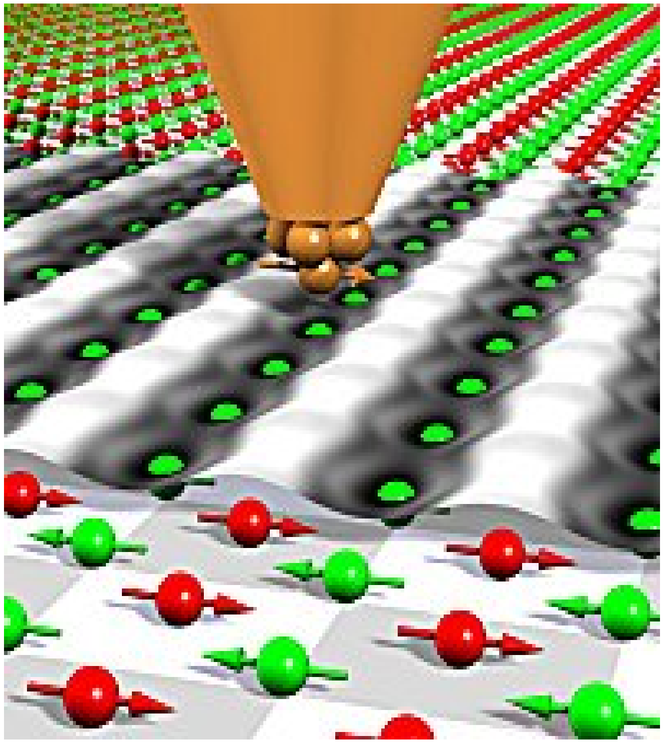
In collaborations with:

A. Rubtsov (Moscow), M. Katsnelson (Nijmegen)
H. Monien and G. Li (Bonn)
H. Hafermann, C. Jung and S. Brener (Hamburg)

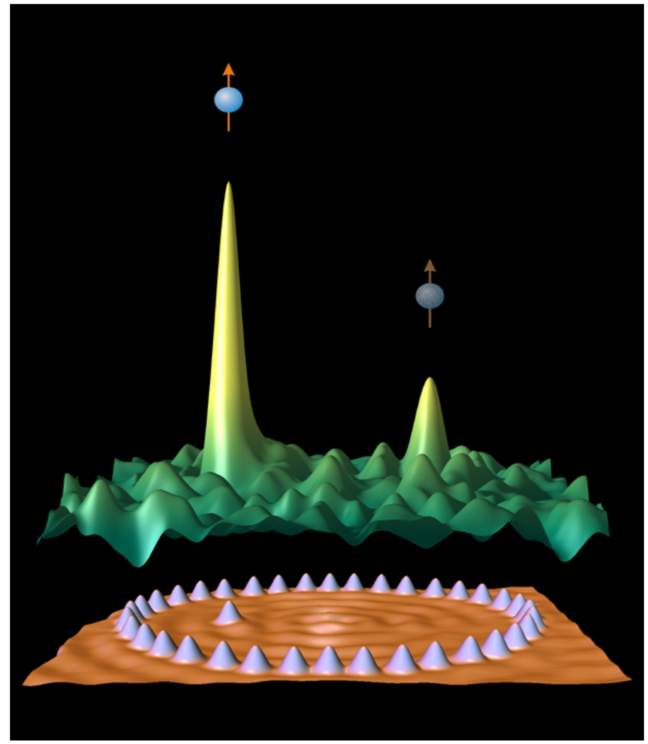
Outline

- Correlated systems: Non-local effects
- ‘Good’ Cluster-DMFT = Double-Bethe
- Magnetic nanosystems: CTQMC
- Beyond DMFT – Dual Fermions
- Superperturbation on real axes
- Conclusions

STM: non-local spin-nanostructures

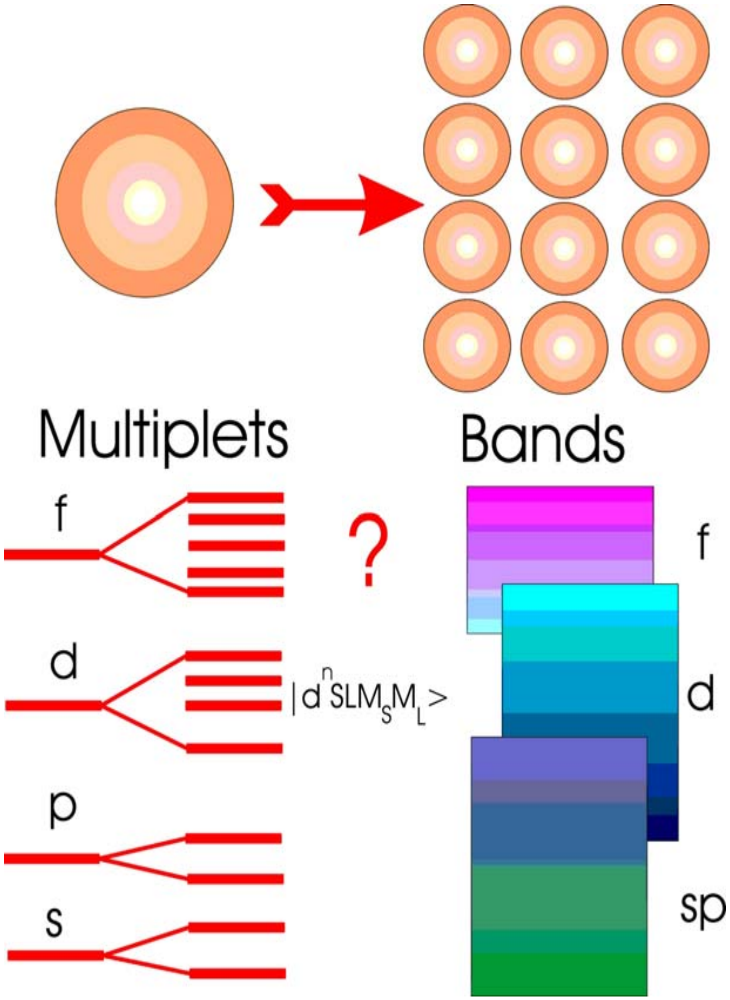


2d-AMF structure
R. Wiesendanger
(UH)



Quantum corral
D. Eigler
(IBM)

From Atom to Solids

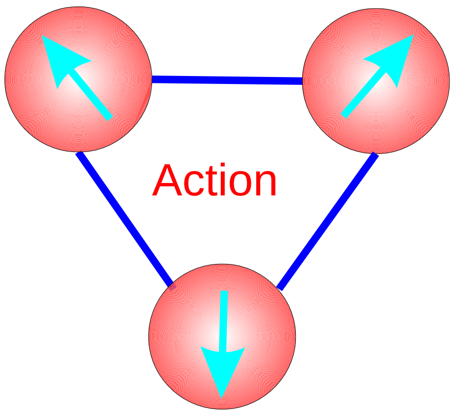


- How to incorporate atomic physics in the band structure ?
- How good is a local approximation ?
- What is a best solution for atomic problem in effective medium ?
- What is different from one band Hubbard model?
- How to solve a complicated Quantum multiorbital problem ?
- What is the best Tight-Binding scheme for realistic Many-Body calculation for solids?

Model: correlated exchange-triangle

a) Is the difference between Heisenberg and Ising types of the exchange interaction essential?

b) How does geometry of the problem affect on Kondo response of the system?



Bath Green function

Interaction W

$$S = S_0 + W$$

$$S_0 = -\int_0^\beta \int_0^\beta d\tau d\tau' \sum_{i,j;\sigma} c^\dagger_{i\sigma}(\tau) \mathcal{G}^{-1}_{ij}(\tau - \tau') c_{j\sigma}(\tau')$$

$$W = \int_0^\beta d\tau \left(U \sum_i n_{i\uparrow}(\tau) n_{i\downarrow}(\tau) + \sum_{i,j} J_{ij} \mathbf{S}_i(\tau) \mathbf{S}_j(\tau) \right)$$

$$\mathcal{G}^{-1}_{ij} = \mathcal{G}^{-1}_i \delta_{ij} - t_{ij}$$

$$\mathcal{G}^{-1}_i(i\omega_n) = \mu + i(\omega_n + \sqrt{\omega_n^2 + 1})/2$$

First term – Hubbard repulsion

Second term – intersite exchange interaction

Continuous Time QMC formalism

Formal perturbation-series:

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

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

$$D_{r'_1 ... r'_{2k}}^{r_1 ... r_{2k}} = \left\langle T \left(c_{r'_1}^{+} c^{r_1} - \alpha_{r'_1}^{r_1} \right) ... \left(c_{r'_{2k}}^{+} c^{r_{2k}} - \alpha_{r'_{2k}}^{r_{2k}} \right) \right\rangle$$

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

$$g_{r'}^{r}(k) = \frac{\left\langle T c_{r'}^{+} c^{r} \left(c_{r'_1}^{+} c^{r_1} - \alpha_{r'_1}^{r_1} \right) ... \left(c_{r'_{2k}}^{+} c^{r_{2k}} - \alpha_{r'_{2k}}^{r_{2k}} \right) \right\rangle}{\left\langle T \left(c_{r'_1}^{+} c^{r_1} - \alpha_{r'_1}^{r_1} \right) ... \left(c_{r'_{2k}}^{+} c^{r_{2k}} - \alpha_{r'_{2k}}^{r_{2k}} \right) \right\rangle}$$

↓

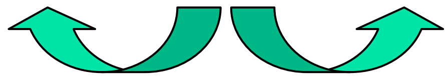
ratio of determinants → In practice efficient calculation of a ratio is possible due to fast-update formulas

α – *for sign problem !*

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

Random walks in the *k* space

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



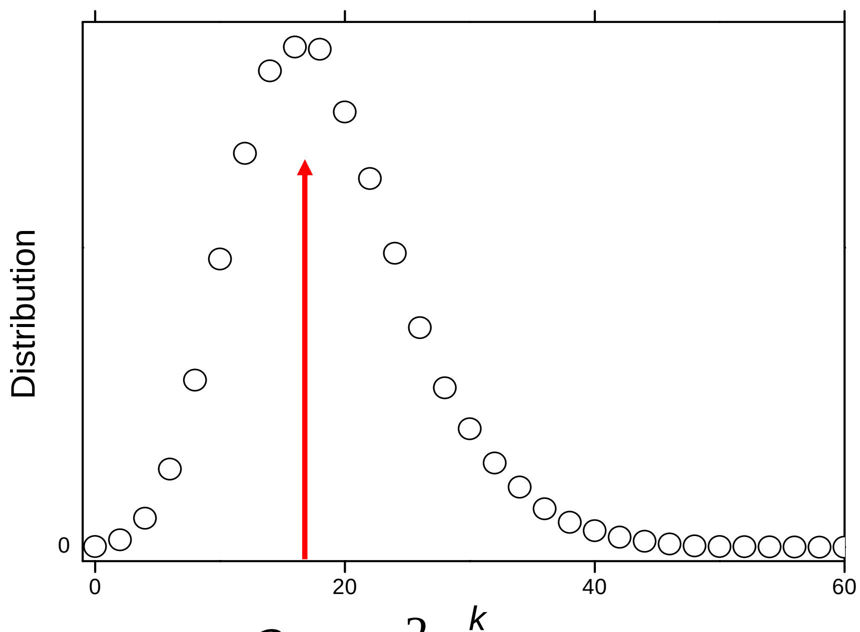
k-1 *k*+1

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 $\beta U N^2$

CT-QMC: fast update k -> k+1

$$G^{(k)} = \begin{pmatrix} G_{1,1} & G_{1,2} & \dots & G_{1,k} & 0 \\ G_{2,1} & G_{2,2} & \dots & G_{2,k} & 0 \\ \dots & \dots & \dots & \dots & \dots \\ G_{k,1} & G_{k,2} & \dots & G_{k,k} & 0 \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix} \quad G^{(k+1)} = \begin{pmatrix} G_{1,1} & G_{1,2} & \dots & G_{1,k} & G_{1,k+1} \\ G_{2,1} & G_{2,1} & \dots & G_{2,k} & G_{2,k+1} \\ \dots & \dots & \dots & \dots & \dots \\ G_{k,1} & G_{k,2} & \dots & G_{k,k} & G_{k,k+1} \\ G_{k+1,1} & G_{k+1,2} & \dots & G_{k+1,k} & G_{k+1,k+1} \end{pmatrix}$$

$$M_{(k+1)} = M_{(k)}[1 + \Delta M_{(k)}]^{-1}$$

$$\begin{aligned} M_{(k)} &= G^{-1}_{(k)} \\ M_{(k+1)} &= G^{-1}_{(k+1)} \\ \Delta &= G_{(k+1)} - G_{(k)} \end{aligned}$$

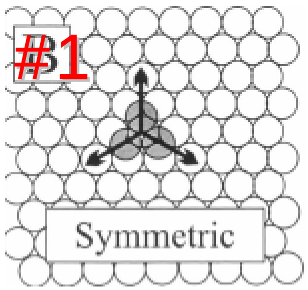
$$M_{k+1} = \begin{pmatrix} M_{i,j} + L_{i,k+1}\alpha R_{k+1,j} & -L_{i,k+1}\alpha \\ -\alpha R_{k+1,j} & \alpha \end{pmatrix}$$

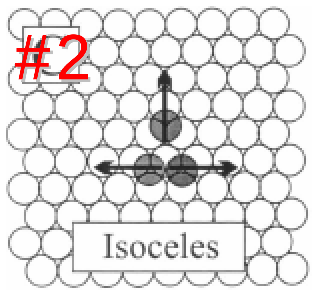
$$\begin{aligned} R_{i,j} &= G_{in} M_{nj} \\ L_{i,j} &= M_{in} G_{nj} \end{aligned}$$

$$\alpha^{-1} = G_{k+1,k+1} - G_{k+1n} M_{nm} G_{mk+1}$$

N^2 operations

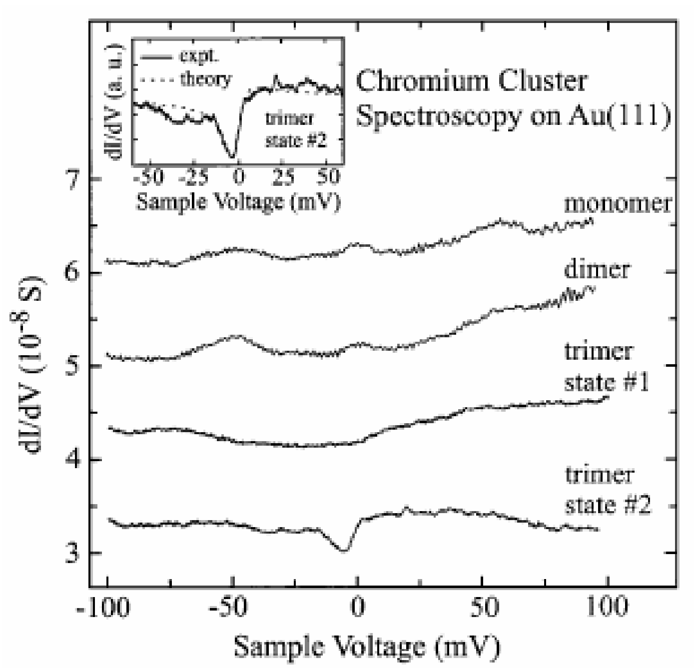
Magnetism vs. Kondo resonance

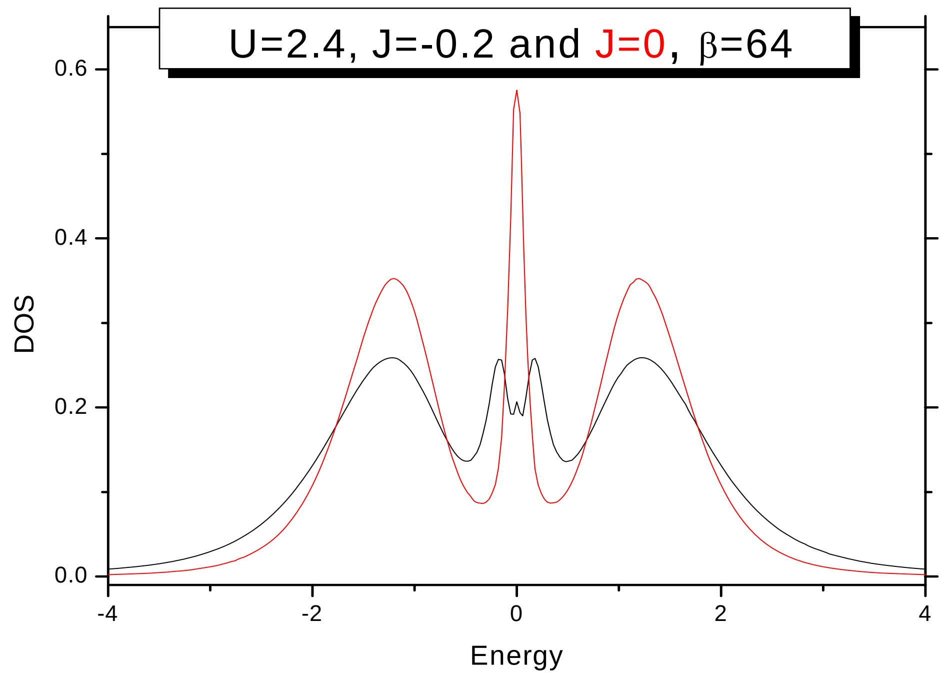




Three impurity atoms with Hubbard repulsion and exchange interaction

$$U n_{i\uparrow} n_{i\downarrow} + J_{ij} \vec{S}_i \vec{S}_j$$





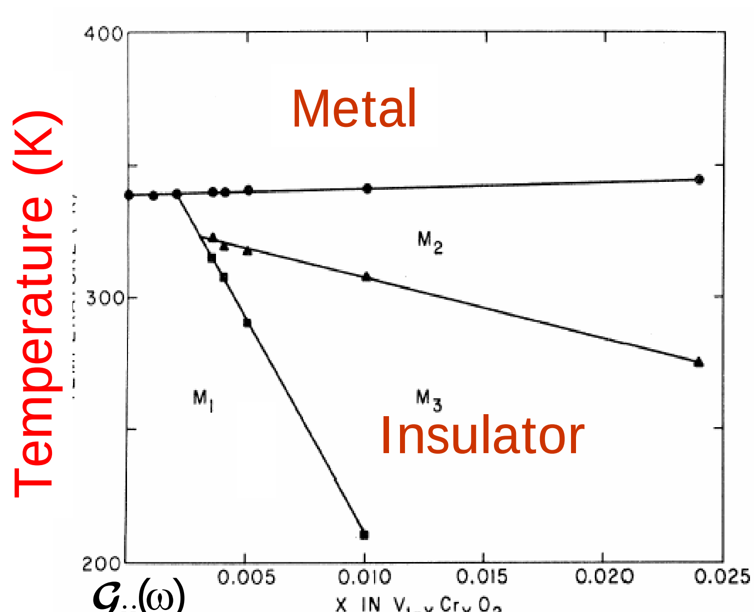
M. Crommie, PRL(2001)

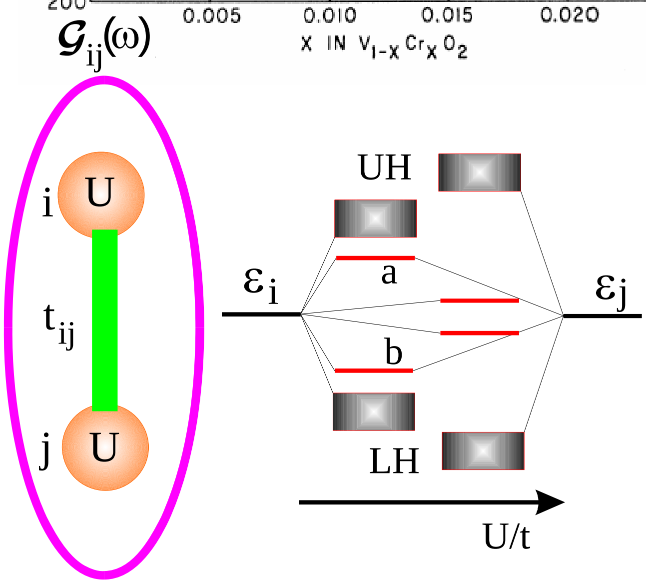
CT-QMC: single vs. trimer

V. Savkin et al, PRL (2005)

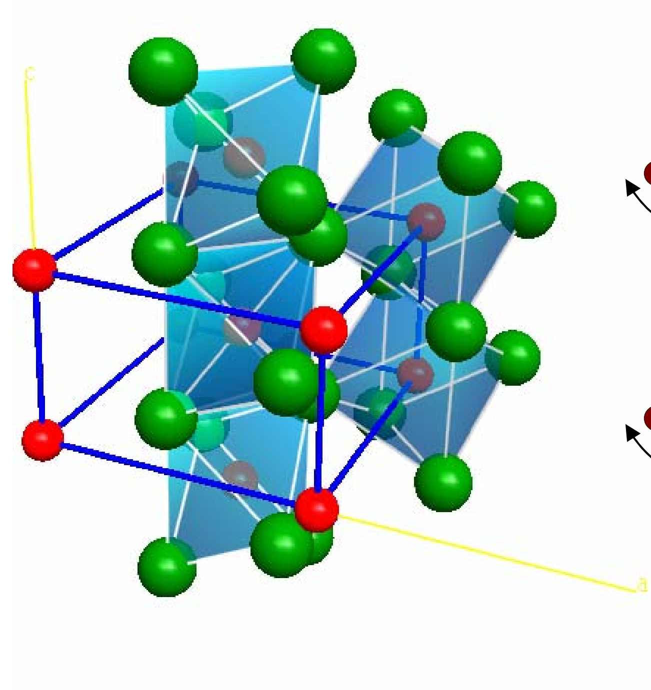
'Good' Cluster - VO_2: singlet formation

M. Marezio et al., (1972)

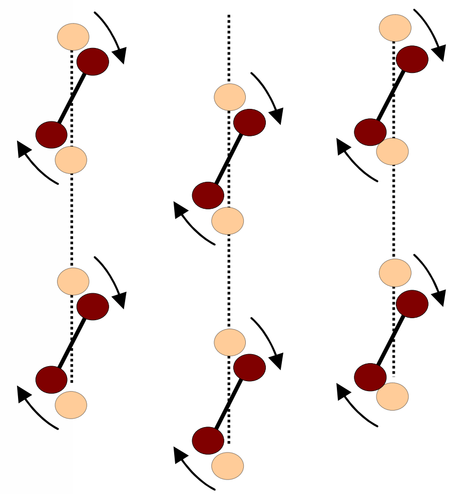




Rutile structure

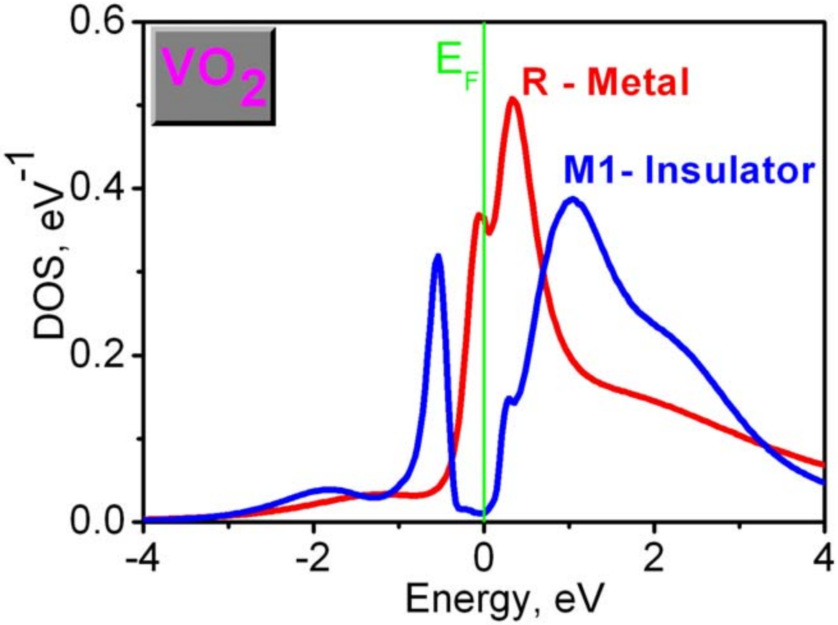


Monoclinic distortion in the insulating phase

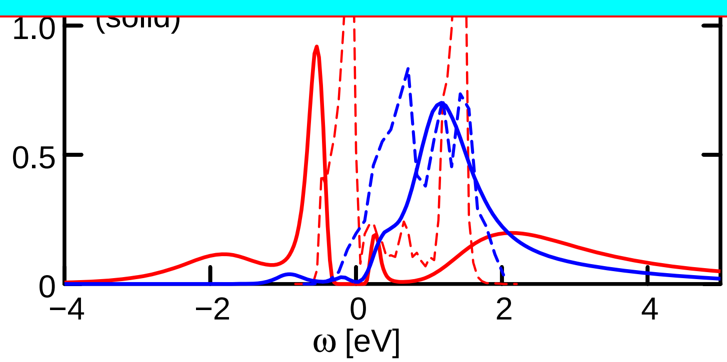


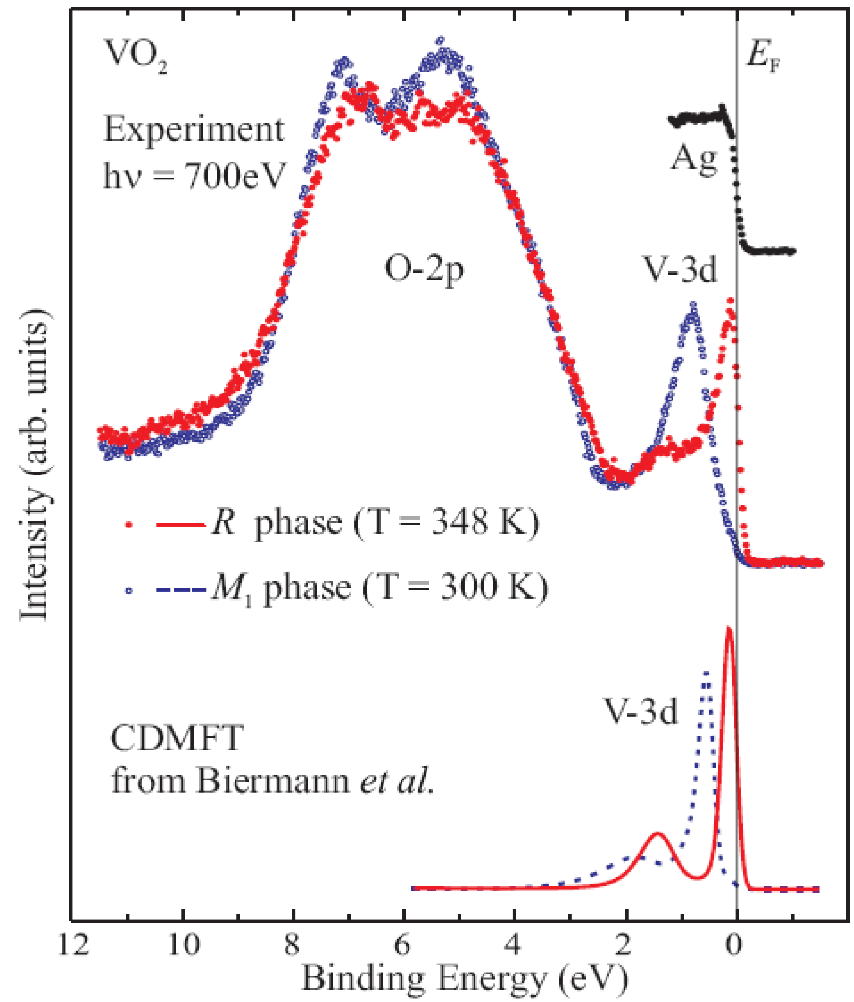
Correlation vs. Bonding

Cluster-DMFT results for VO_2



Sharp peak below the gap is NOT a Hubbard band !





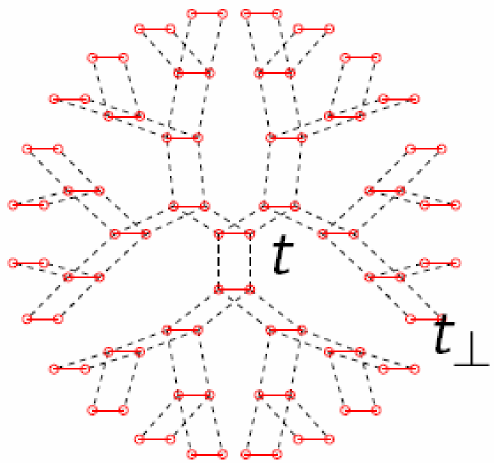
New photoemission from Tjeng's group
T. C. Koethe, et al. PRL (2006)

S. Biermann, et al, PRL **94**, 026404 (2005)

Double-Bethe Lattice: exact C-DMFT

bilayer Hubbard model on the Bethe lattice
(for coordination $z = 3$)

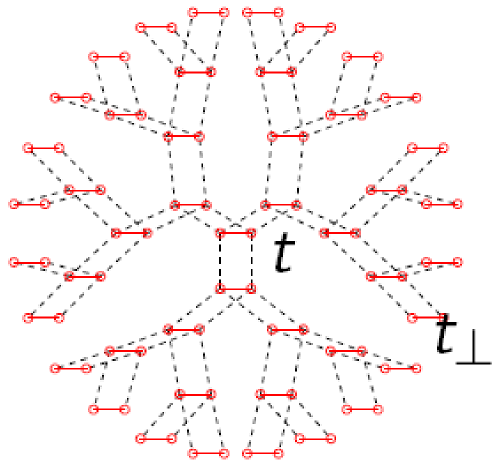
G. Moeller ,
V. Dobrosavljevic,
and A. Ruckenstein
PRB (1999)



$$H = -t \sum_{\langle ij \rangle, \sigma} (a^\dagger_{i\sigma} a_{j\sigma} + b^\dagger_{i\sigma} b_{j\sigma}) - t_\perp \sum_{i\sigma} (a^\dagger_{i\sigma} b_{i\sigma} + b^\dagger_{i\sigma} a_{i\sigma})$$

$$+ U \sum_{i\sigma} (n_{ai\uparrow} n_{ai\downarrow} + n_{bi\uparrow} n_{bi\downarrow})$$

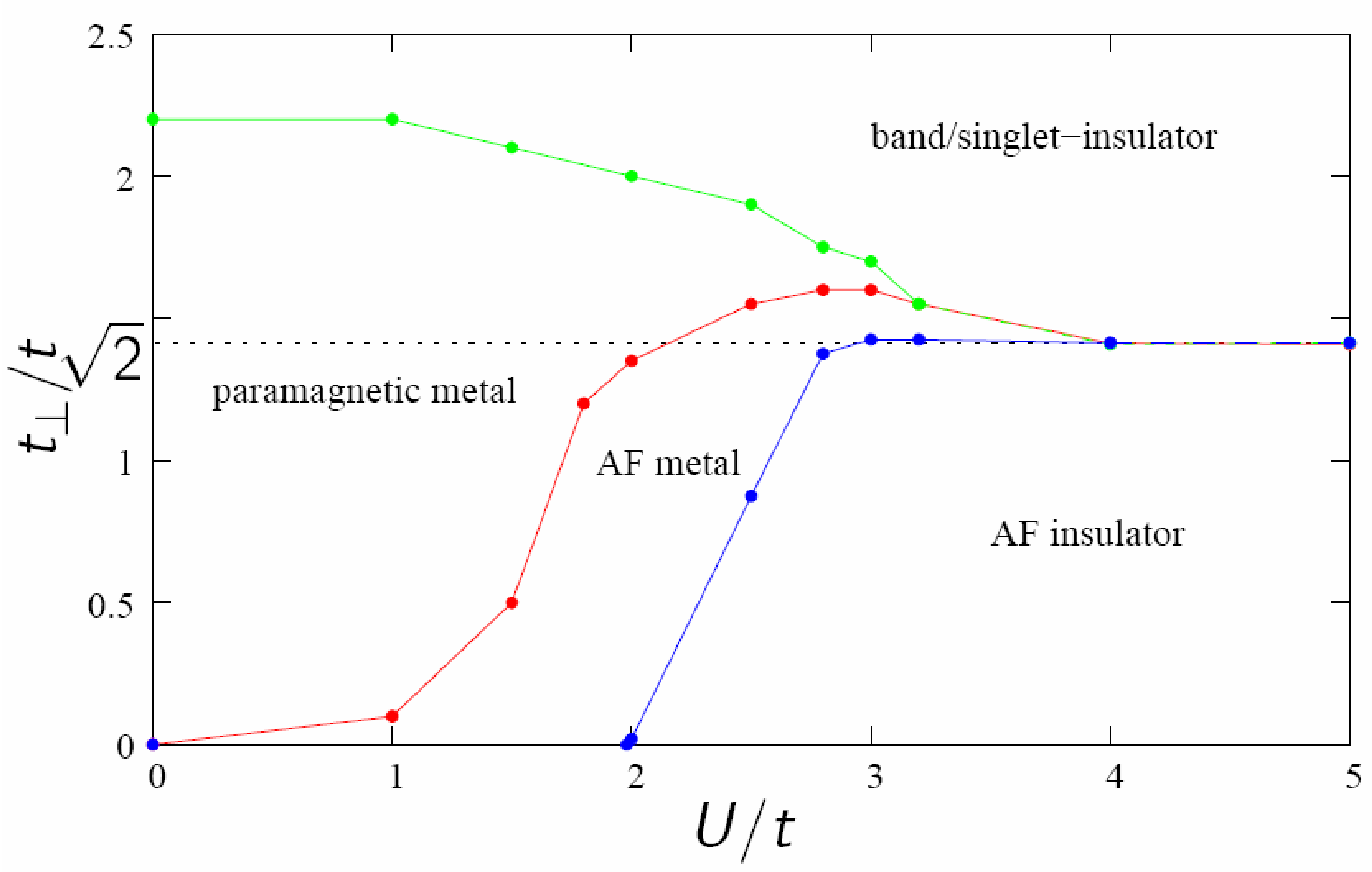
Self-consistent condition: C-DMFT



$$\mathcal{G}_\sigma^{-1}(i\omega_n) = \begin{pmatrix} i\omega_n + \mu - h\sigma & -t_\perp \\ -t_\perp & i\omega_n + \mu + h\sigma \end{pmatrix} - t^2 \mathbf{G}_{-\sigma}(i\omega_n) \; ,$$

AF-between plane *AF-plane*

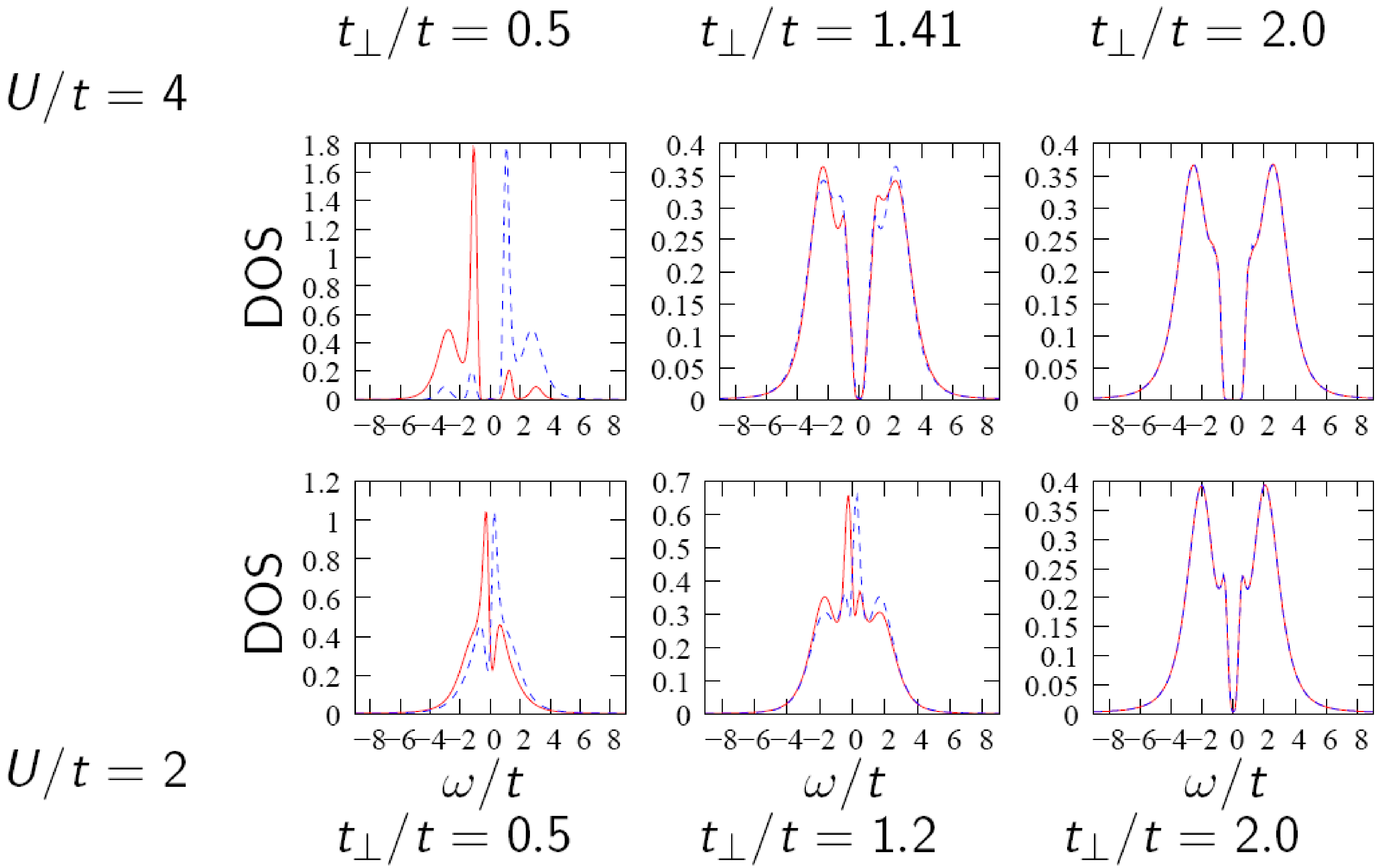
Finite temperature phase diagram



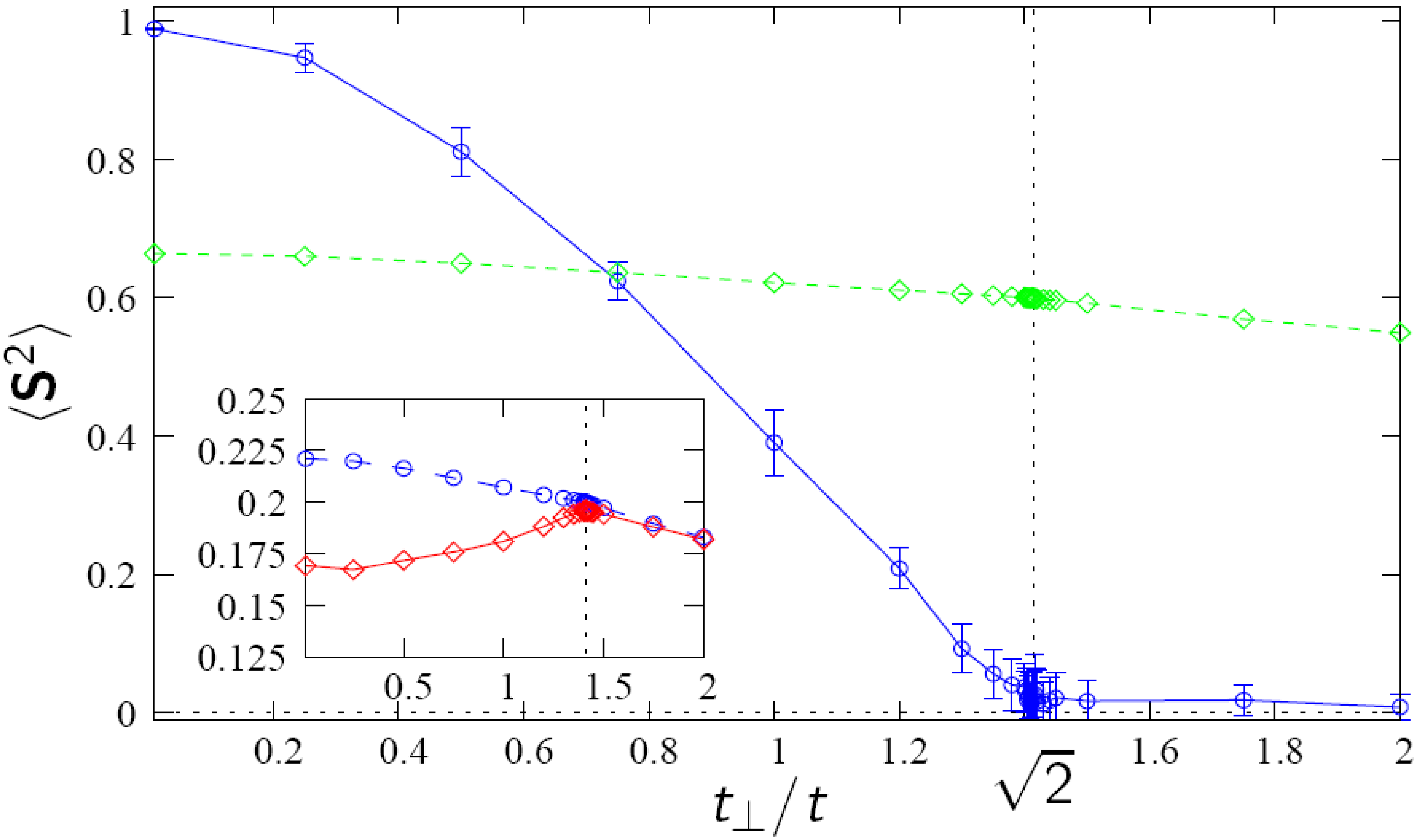
- order-disorder transition at $t_\perp / t = \sqrt{2}$ for large U
- MIT for intermediate U

H. Hafermann EPL(2009)

Density of States: large U



Spin-correlations: large U

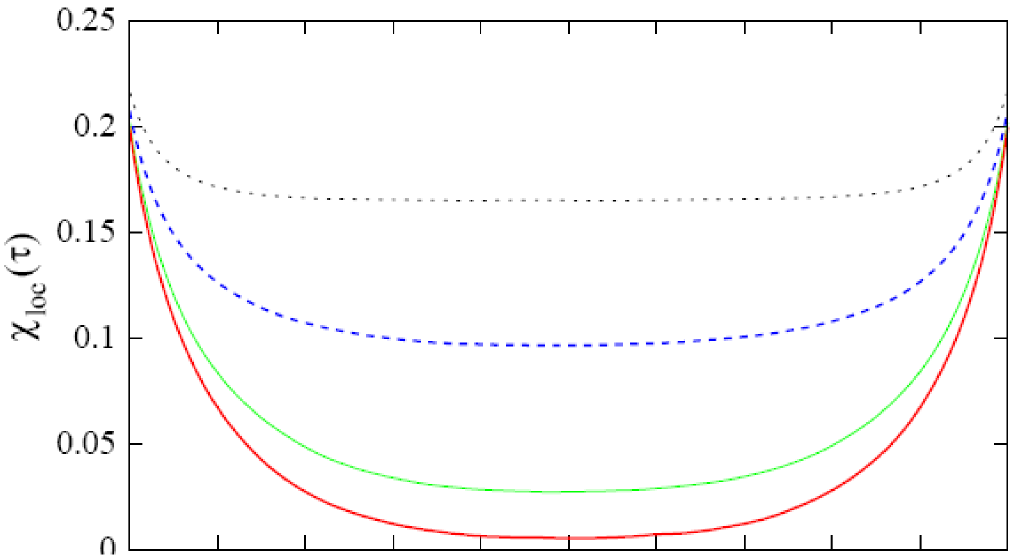


- formation of a coherent state for $t_\perp / t > \sqrt{2}$
- magnetic order is supressed by singlet formation

CT-QMC measuring χ in imaginary time

$$\chi_{\text{loc}}(\tau) = \langle S^z(\tau) S^z(0) \rangle$$

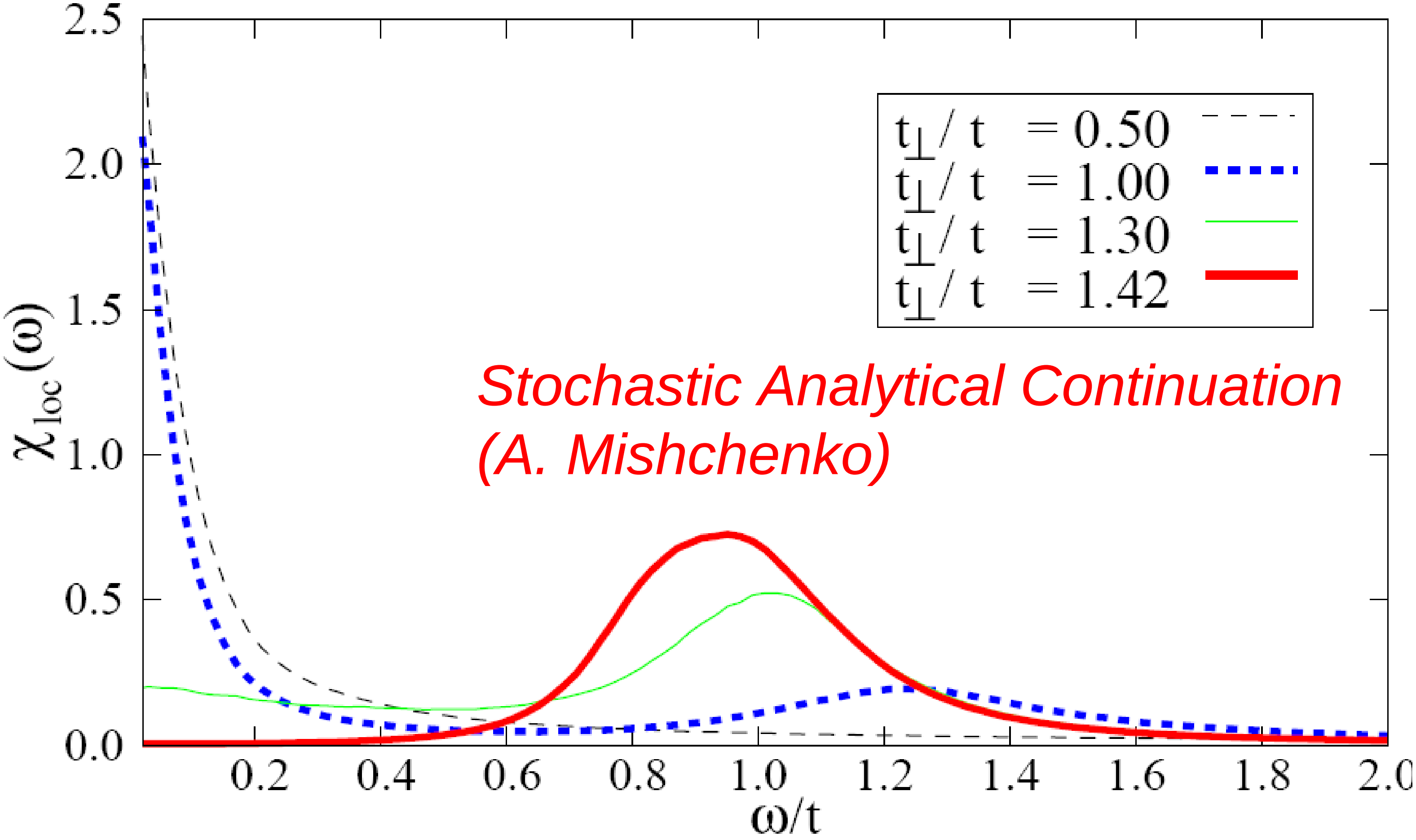
$$\langle c_\sigma^\dagger(\tau) c_\sigma(\tau) c_\sigma^\dagger(0) c_\sigma(0) \rangle = \langle \tilde{g}_\sigma(\tau,\tau) \tilde{g}_{\sigma'}(0,0) \rangle - \delta_{\sigma,\sigma'} \langle \tilde{g}_\sigma(\tau,0) \tilde{g}_{\sigma'}(0,\tau) \rangle$$



$$\tilde{g}(\tau,\tau') = G_0(\tau-\tau') - \sum_{ij=1}^{k} G_0(\tau-\tau_i) \hat{M}_{ij} G_0(\tau_j-\tau')$$

$$G(\tau-\tau') = \langle \tilde{g}(\tau,\tau') \rangle$$

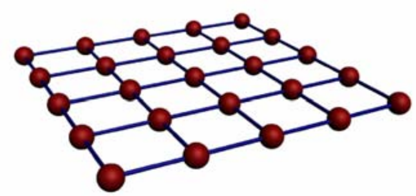
Dynamical susceptibility



- Goldstone mode for small $t_\perp$
- singlet-triplet excitation at $\sim J_{||} = 4t^2/U = 0.5$

Beyond DMFT: Dual Fermion scheme

General Lattice Action $H = h + U$

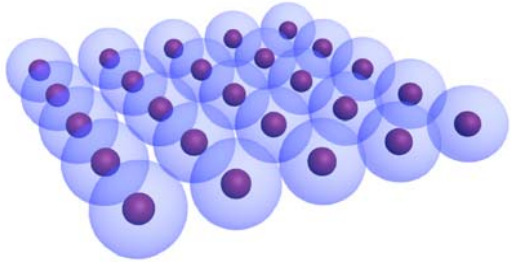


$$S[c^*, c] = \sum_{\omega k m m' \sigma} \left[h_k^{mm'} - (i\omega + \mu) 1 \right] c^*_{\omega k m \sigma} c_{\omega k m' \sigma} + \frac{1}{4} \sum_{i\{m,\sigma\}} \int_0^\beta U_{1234} c_1^* c_2^* c_3 c_4 d\tau$$

Optimal Local Action with hybridization Δ_ω

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

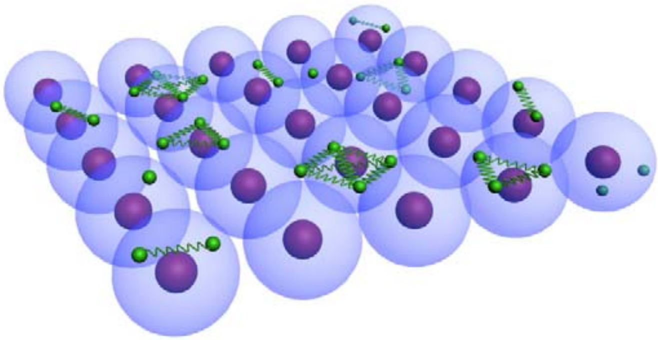
Lattice-Impurity connection:



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

A. Rubtsov, et al, *Phys. Rev. B (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
$$A = g_\omega^{-1}(\Delta_\omega - h_k)g_\omega^{-1}$$
$$B = g_\omega^{-1}$$

new Action:

$$S_d[f^*,f] = -\sum_{k\omega\sigma}\mathcal{G}_{k\omega\sigma}^{-1}f_{k\omega\sigma}^*f_{k\omega\sigma}+\frac{1}{4}\sum_{1234}\gamma_{1234}^{(4)}f_1^*f_2^*f_4f_3+\gamma^{(6)}\ldots$$

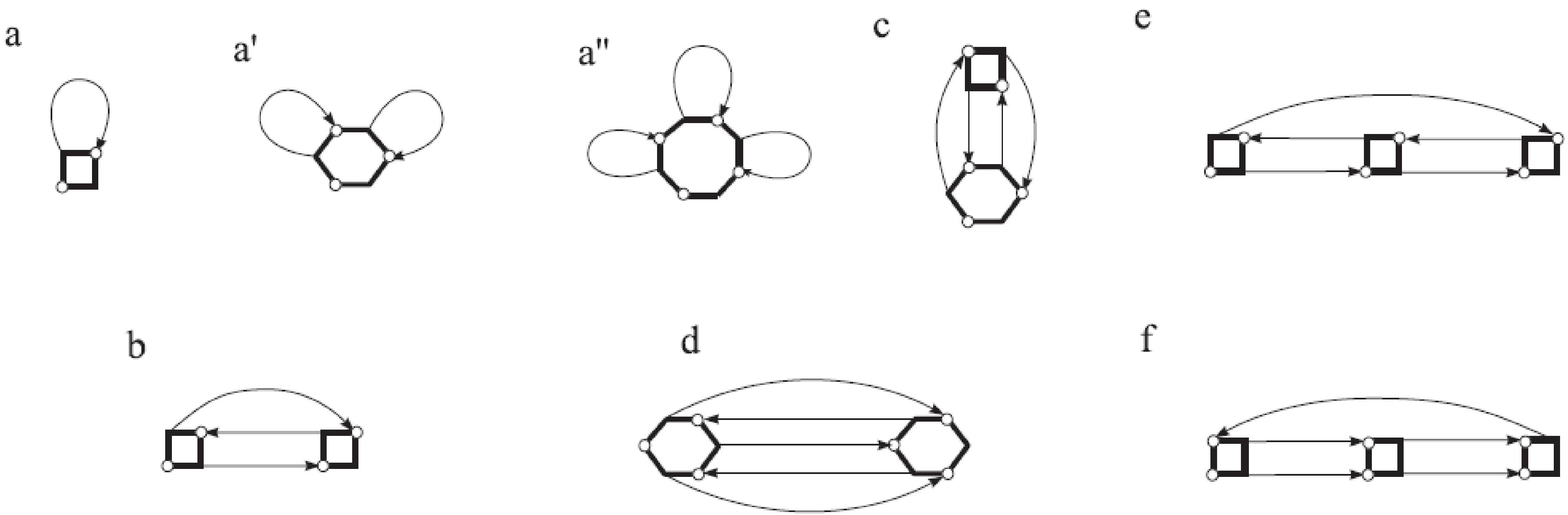
here:

$$\mathcal{G}_{k\omega}^{-1} = [g_\omega(h_k-\Delta_\omega)g_\omega]^{-1}-g_\omega^{-1}$$

$$\gamma_{1234}^{(4)} = g_{11'}^{-1}g_{22'}^{-1}\left(\chi_{1'2'3'4'}-\chi_{1'2'3'4'}^{0}\right)g_{3'3}^{-1}g_{4'4}^{-1}$$

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

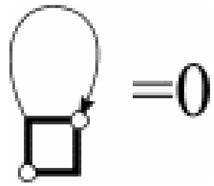
Basic diagrams for dual self-energy



Lines denote the renormalized Green's function.

Condition for Δ and relation with DMFT

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

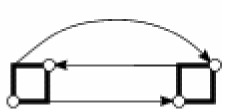


To determine Δ, we require that Hartree correction in dual variables vanishes. If no higher diagrams are taken into account, one obtains DMFT:

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

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

b



$\Sigma(k,\omega)$

Dual and Lattice Green's Functions

The partition function can be written in two equivalent forms:

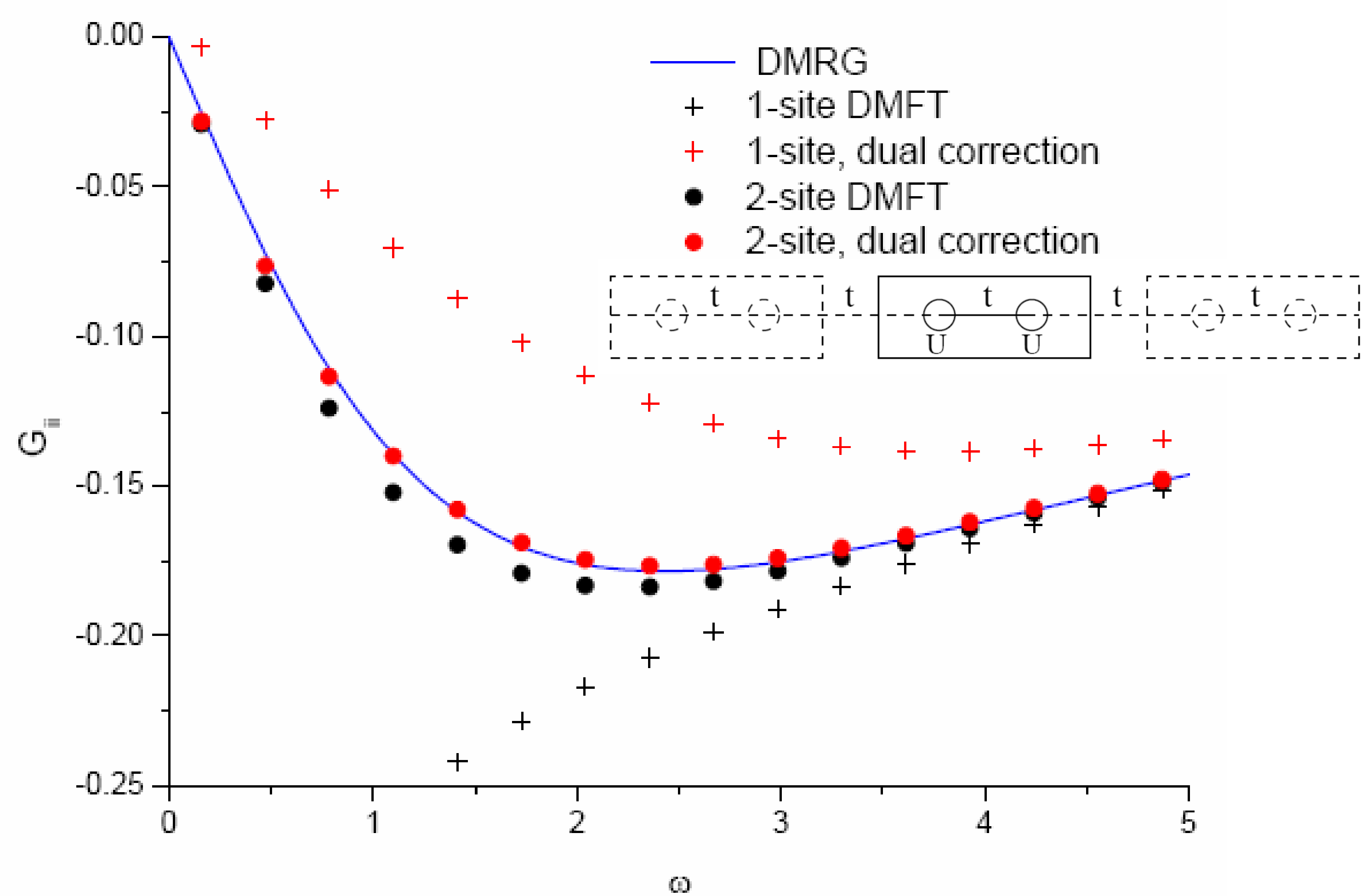
$$
\begin{aligned}
Z &= \int \exp\left(-S[c^*, c]\right) \mathcal{D}[\mathbf{c}, \mathbf{c}^*] = \\
& \prod_{\omega \mathbf{k} \sigma} \det\left[g_{\omega\sigma}\left(\Delta_{\omega\sigma} - H_\sigma(\mathbf{k})\right) g_{\omega\sigma}\right] \times \\
& \int\int \exp\left(-S[\mathbf{c}^*, \mathbf{c}, \mathbf{f}^*, \mathbf{f}]\right) \mathcal{D}[\mathbf{f}, \mathbf{f}^*] \mathcal{D}[\mathbf{c}, \mathbf{c}^*]
\end{aligned}
$$

- the dual transformation ensures an*exact* relation between $G^{\mathrm{dual}}_{\omega \mathbf{k} \sigma} = -\langle T \mathbf{f}_{\omega \mathbf{k} \sigma} \mathbf{f}^*_{\omega \mathbf{k} \sigma} \rangle$ and $G_{\omega \mathbf{k} \sigma} = -\langle T \mathbf{c}_{\omega \mathbf{k} \sigma} \mathbf{c}^*_{\omega \mathbf{k} \sigma} \rangle$

$$
\begin{aligned}
G_{\omega \mathbf{k} \sigma} &= \left(\Delta_{\omega\sigma} - H_\sigma(\mathbf{k})\right)^{-1} \; g^{-1}_{\omega\sigma} \; G^{\mathrm{dual}}_{\omega \mathbf{k} \sigma} \; g^{-1}_{\omega\sigma} \; \left(\Delta_{\omega\sigma} - H_\sigma(\mathbf{k})\right)^{-1} \\
&+ \left(\Delta_{\omega\sigma} - H_\sigma(\mathbf{k})\right)^{-1}
\end{aligned}
$$

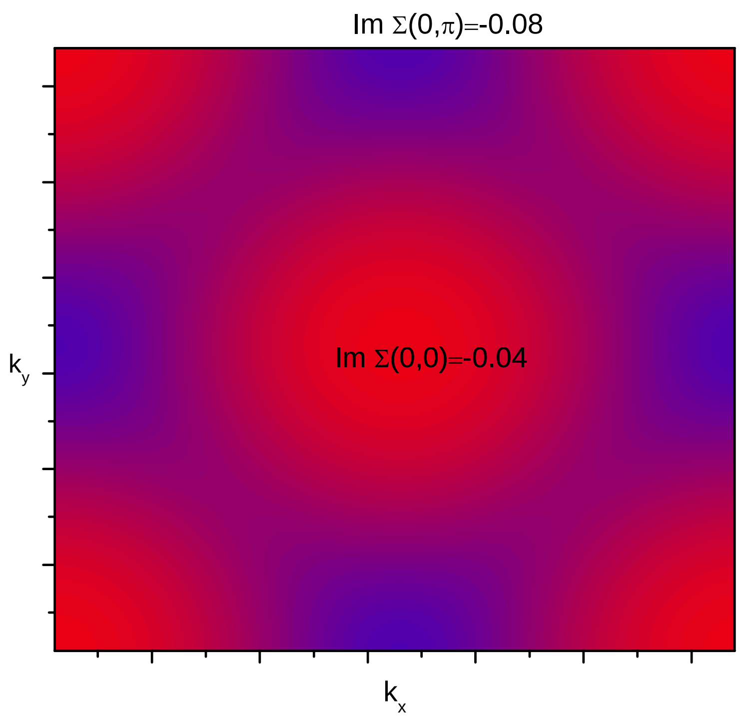
Cluster Dual Fermions: 1d-test, n=1

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

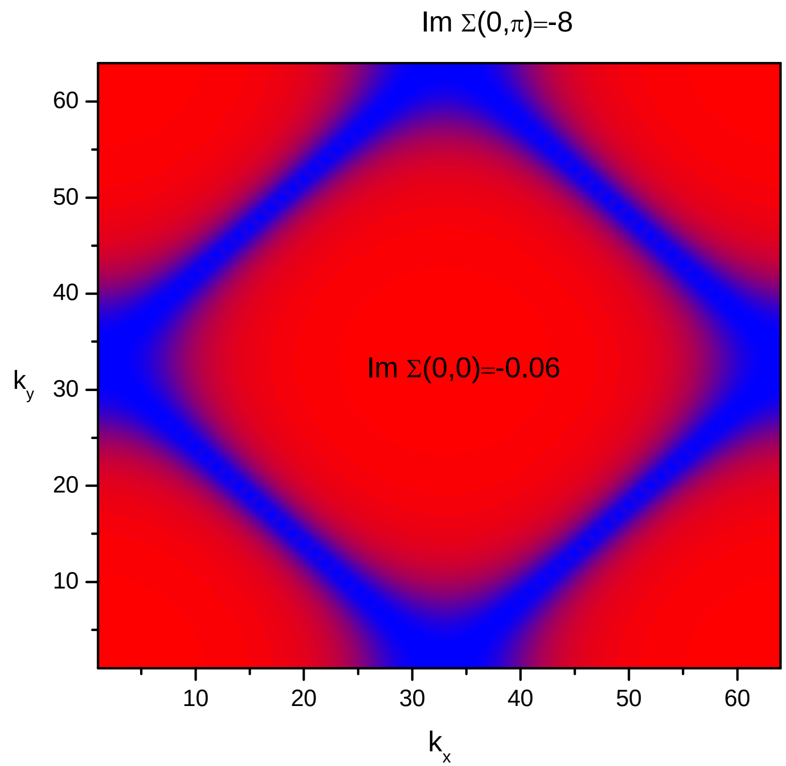


H. Hafermann, *et al.* JETP Lett (2007),

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



U=1



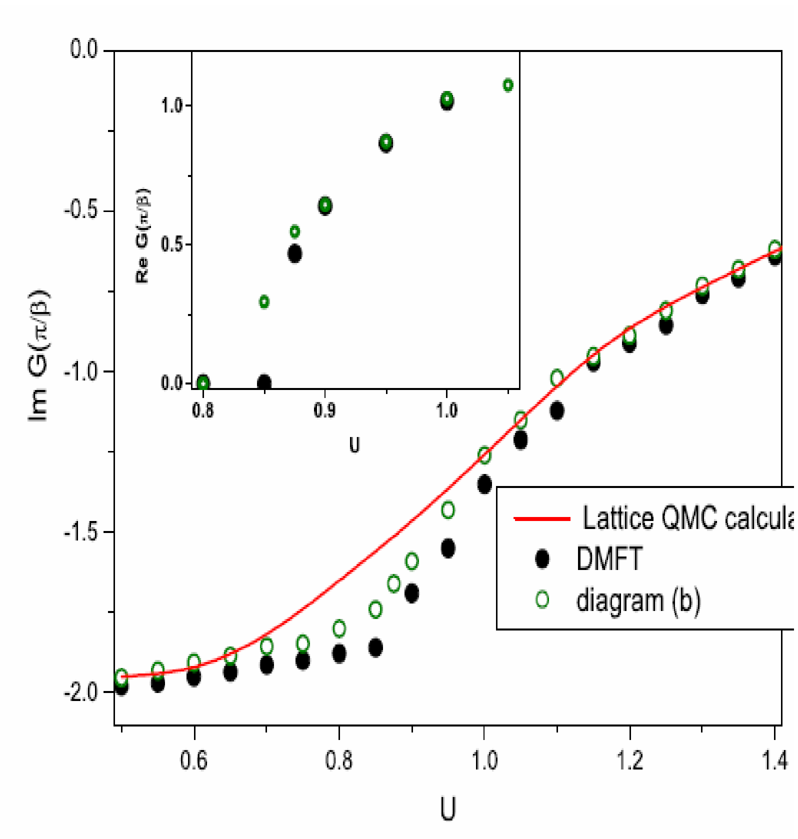
U=2

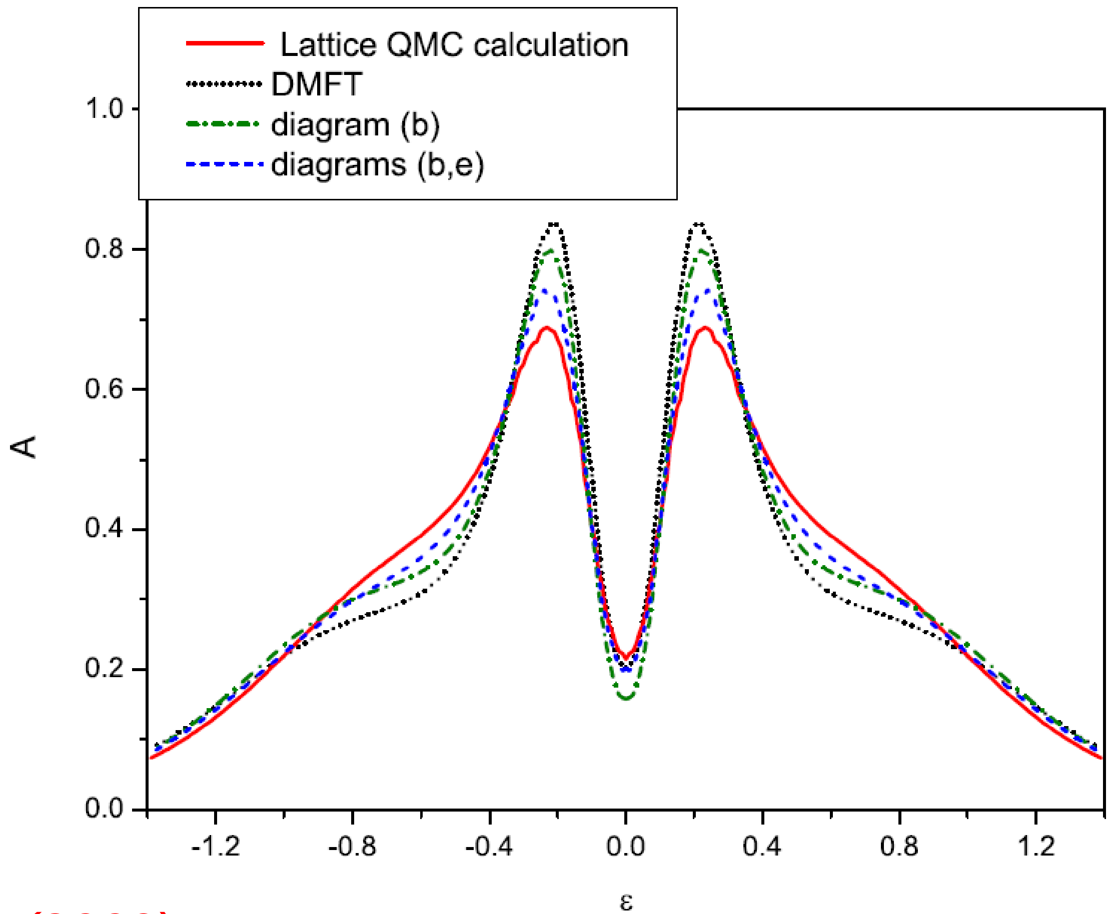
Hubbard model with $8t = 2, \beta = 20$ at half-filling.
Data for Im Σ_k at $\omega = 0$.

A. Rubtsov, et al, *Phys. Rev. B (2008)*

AFM – symmetry breaking

$$\begin{pmatrix} G_k^{dual(0)} & G_k^{dual(AF)} \\ G_k^{dual(AF)} & G_{k+Q}^{dual(0)} \end{pmatrix}$$



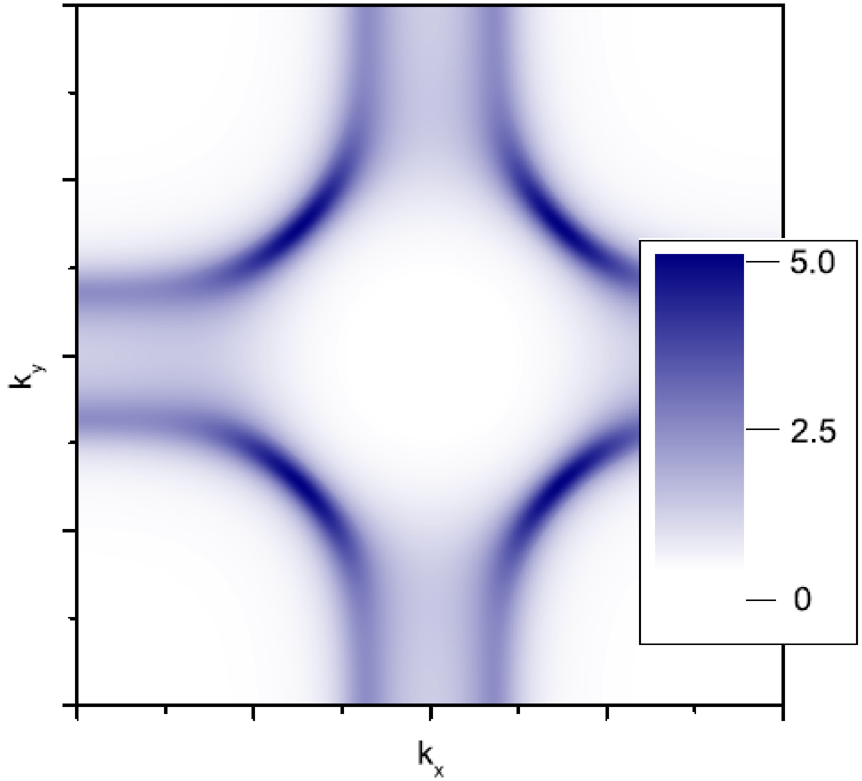


A. Rubtsov, et al, *Phys. Rev. B (2009)*

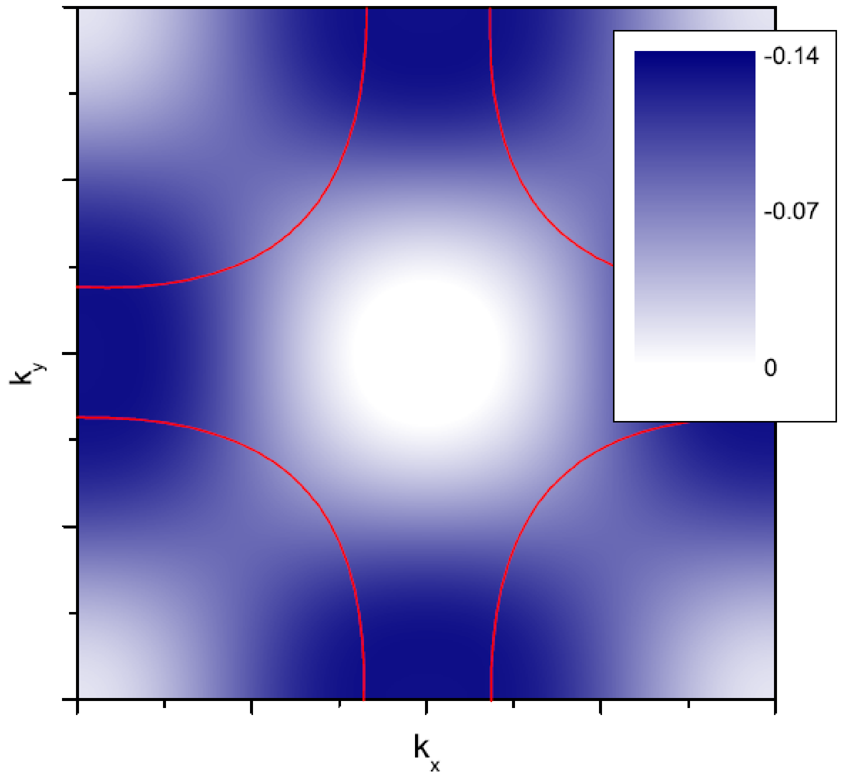
U=1 W=2 β=20

Pseudogap in HTSC: dual fermions

$$S[f,f^*] = \sum_{\omega k \sigma} g_\omega^{-2}\left((\Delta_\omega - \epsilon_k)^{-1} + g_\omega\right) f^*_{\omega k \sigma} f_{\omega k \sigma} + \sum_i V_i$$



FS



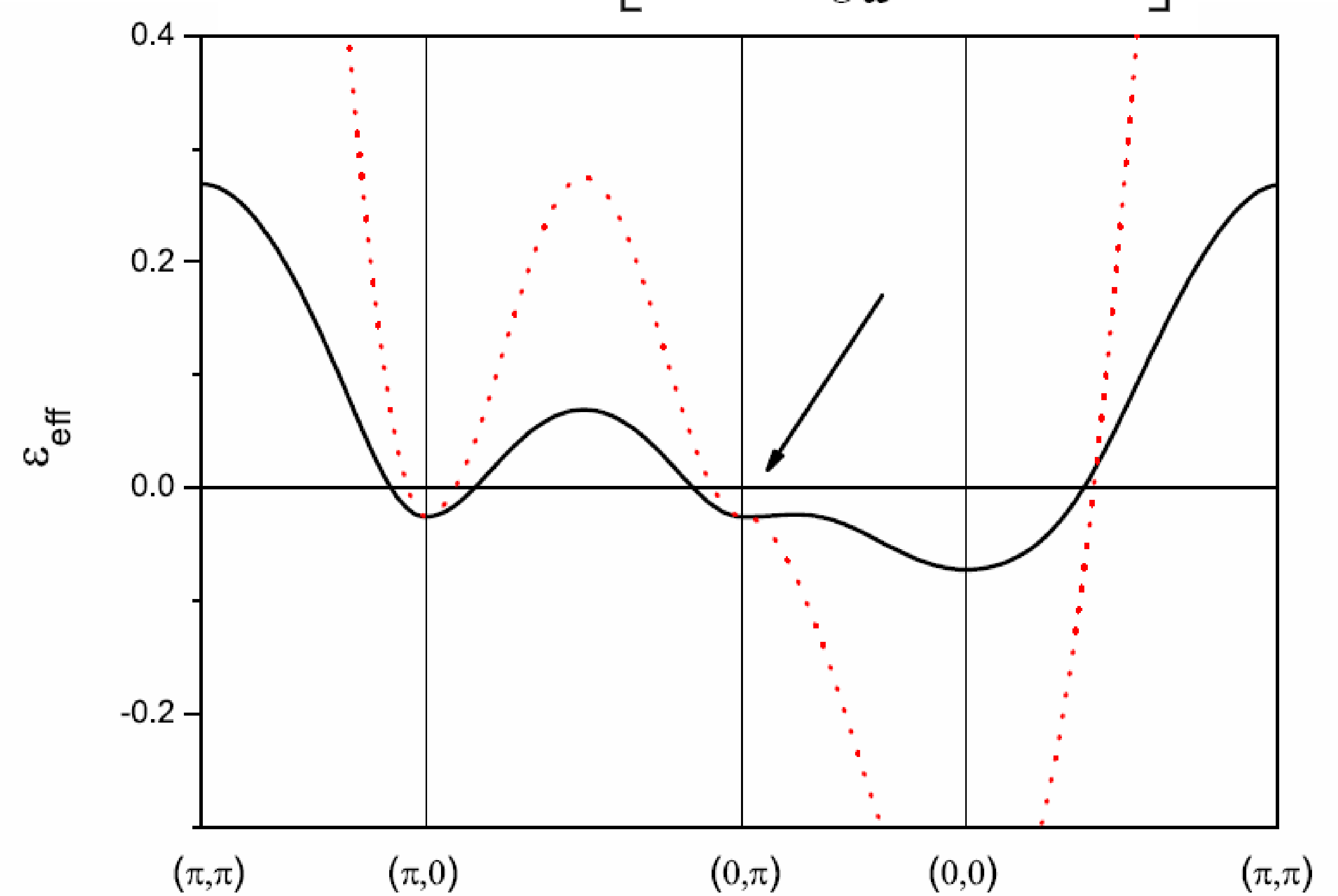
Σ

2d: U=4 W=2 t'/t=-0.3 δ=14% β=80

A. Rubtsov et al, PRB (2009)

Quasiparticle dispersion

$$\epsilon_k^{eff} = \mathrm{Re}\left[\frac{\epsilon_k - \mu + \Sigma_{\omega=0,k}}{1 + i\frac{\partial}{\partial\omega}\Sigma_{k,\omega=0}}\right]$$



A. Rubtsov, et al, *Phys. Rev. B (2009)*

Two-particle Green-Functions

- Exact relation between dual and lattice two-particle Green functions (symbolically):

$$\chi(k,k';q) = \langle T \mathbf{c}_{k+q} \mathbf{c}^*_k \mathbf{c}_{k'} \mathbf{c}^*_{k'+q} \rangle$$

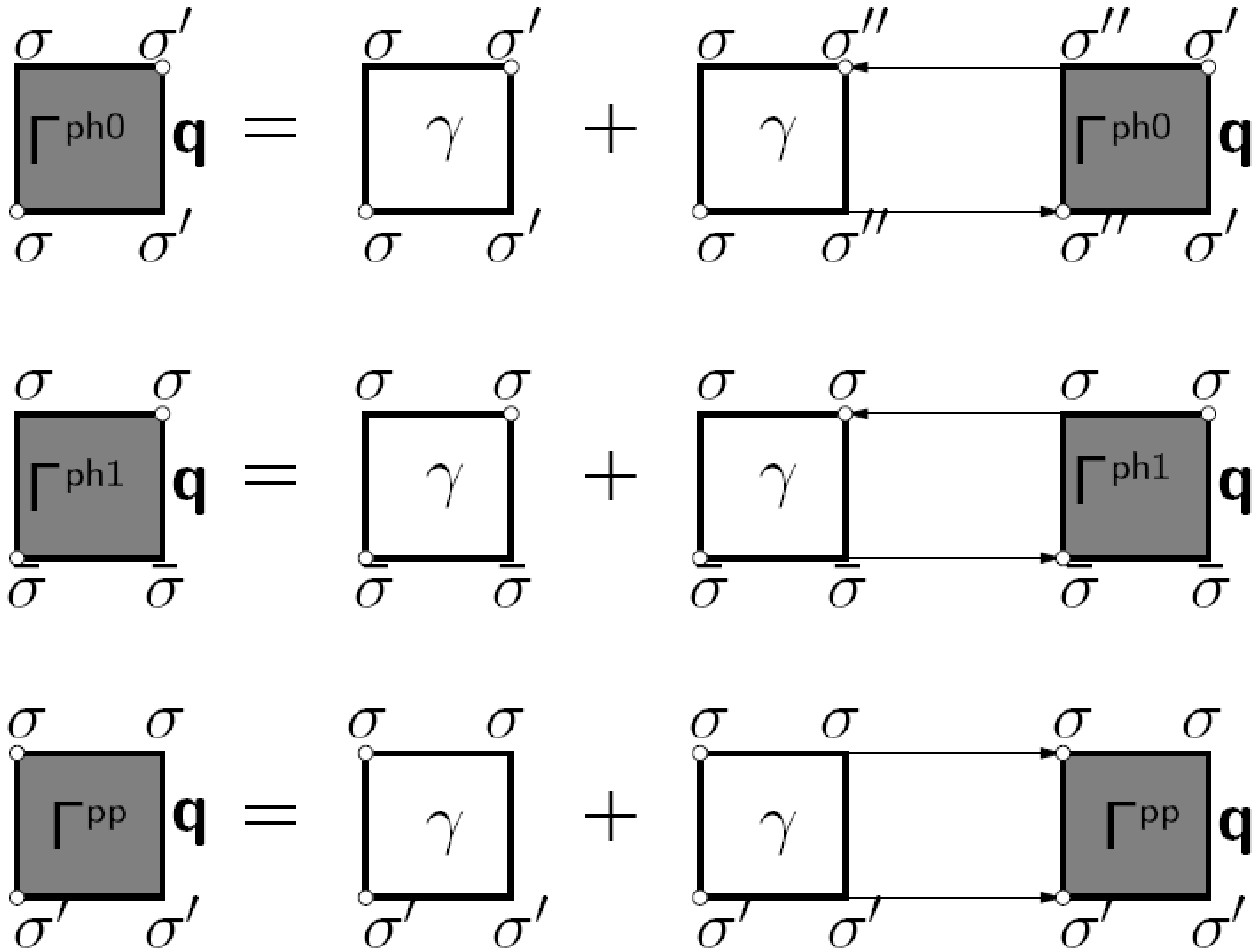
$$\chi - G \otimes G = \left[(\Delta - H)^{-1} g^{-1} \right] \left[(\Delta - H)^{-1} g^{-1} \right] (\chi^d - G^d \otimes G^d) \times \\ \left[g^{-1} (\Delta - H)^{-1} \right] \left[g^{-1} (\Delta - H)^{-1} \right]$$

- two-particle excitations for dual and original fermions are the same!

S. Brener et al. PRB (2008)

Bethe-Salpeter Equations

- Three channels:



Susceptibility: DF vs.DMFT

- DMFT approximation for 2PGF:

$$\chi - G^{\mathrm{D}} \otimes G^{\mathrm{D}} = G^{\mathrm{D}} G^{\mathrm{D}} \gamma^{\mathrm{ir}} \chi$$

with

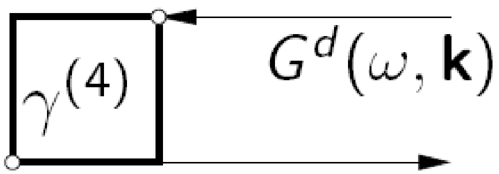
$$\gamma^{(4)} = \gamma^{\mathrm{ir}} + \gamma^{\mathrm{ir}} g\, g\, \gamma^{(4)}$$

- Not recovered completely in the lowest non-trivial order of DF:

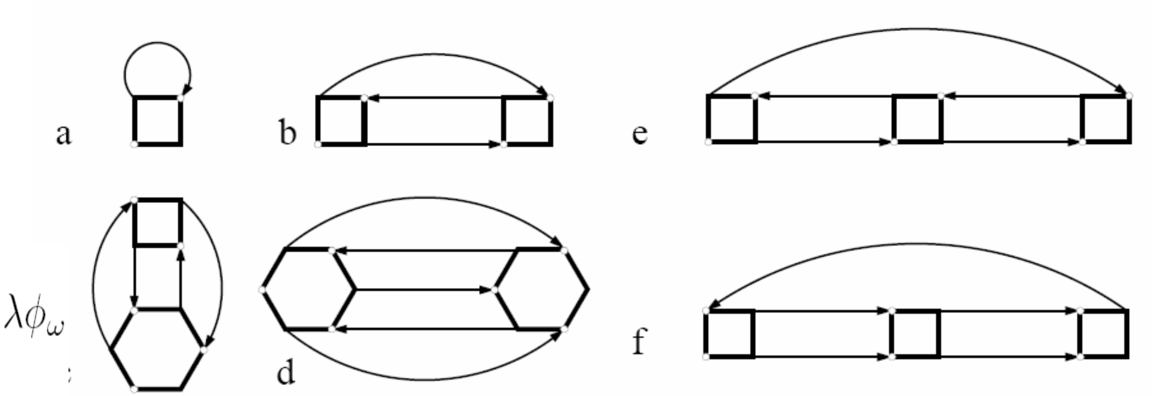
$$\chi - G^{\mathrm{D}} \otimes G^{\mathrm{D}} = G^{\mathrm{D}} G^{\mathrm{D}} \gamma^{(4)} G^{\mathrm{D}} G^{\mathrm{D}}$$

$$g = G^{\mathrm{D}} - G^{\mathrm{d},0}$$

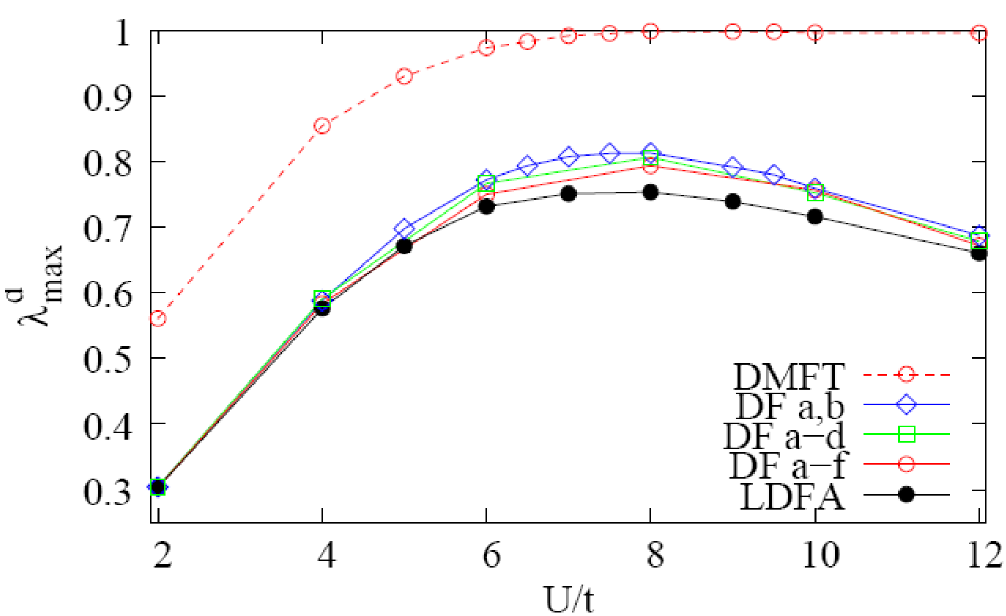
Convergence of Dual Fermions: 2d

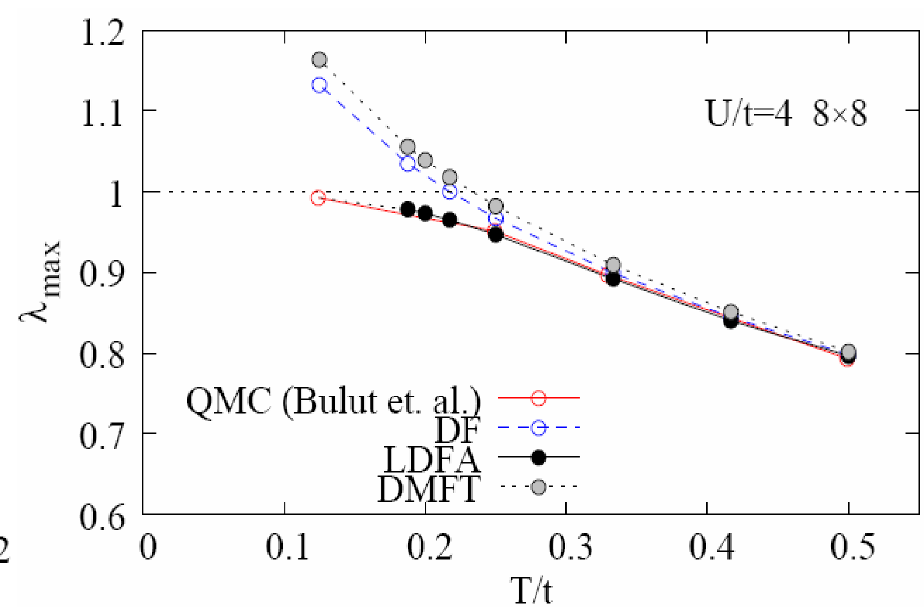


=1



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

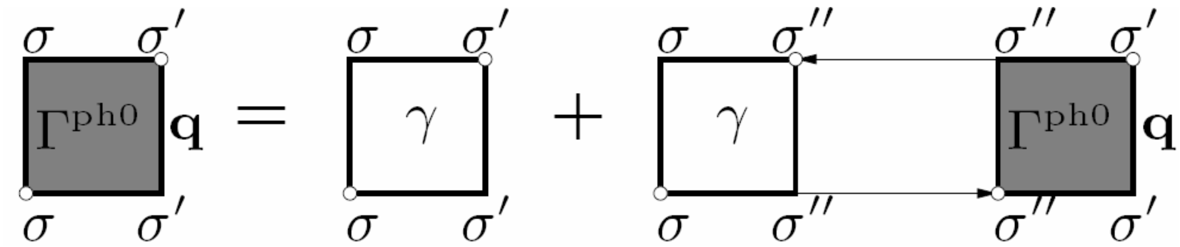




H. Hafermann, arXiv:0812.2456

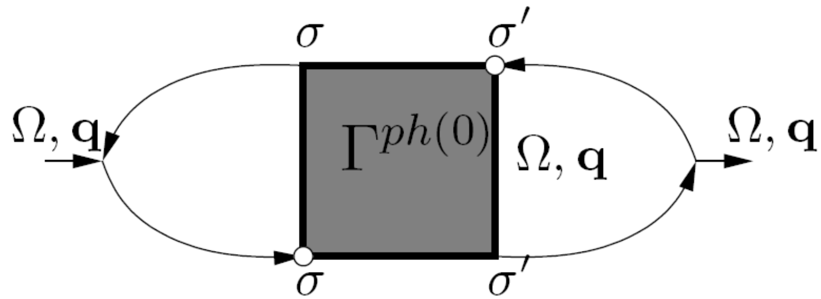
Magnetic susceptibility: exact results

Bethe-Salpeter Equation:

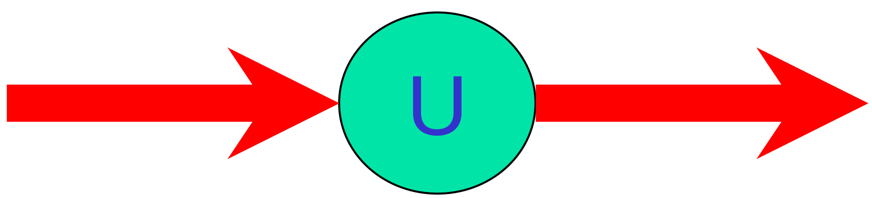


Susceptibility:

$$\tilde{\chi}^{\sigma\sigma'}(\Omega, \mathbf{q})$$

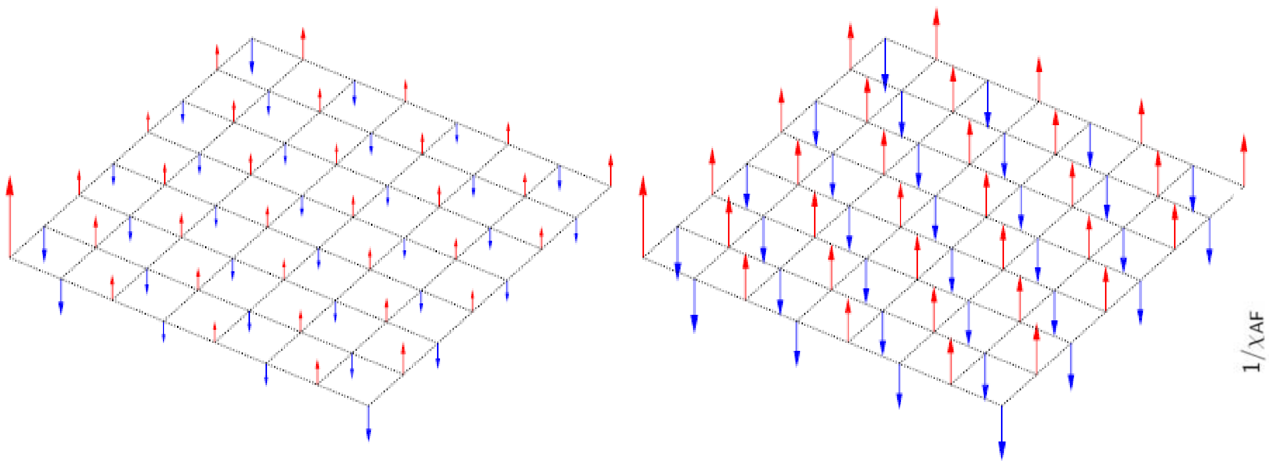


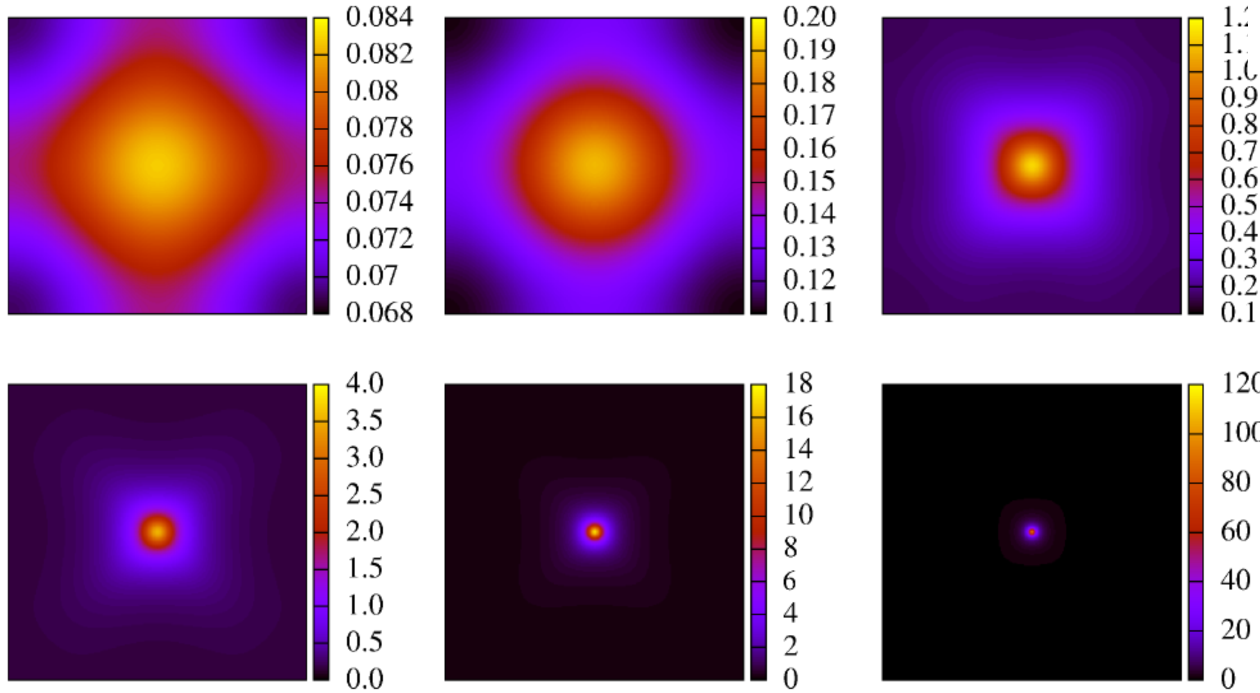
For local correlated system - exact separation:

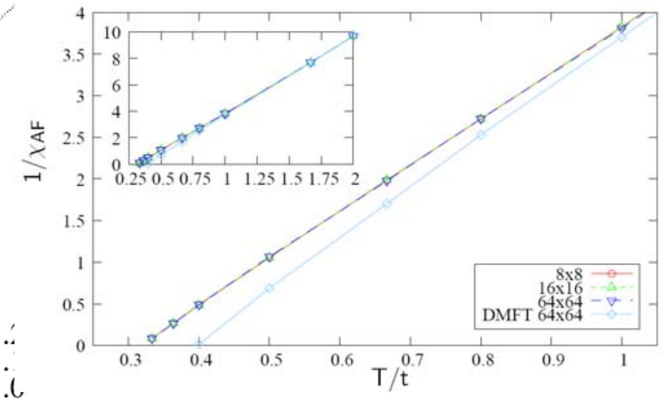


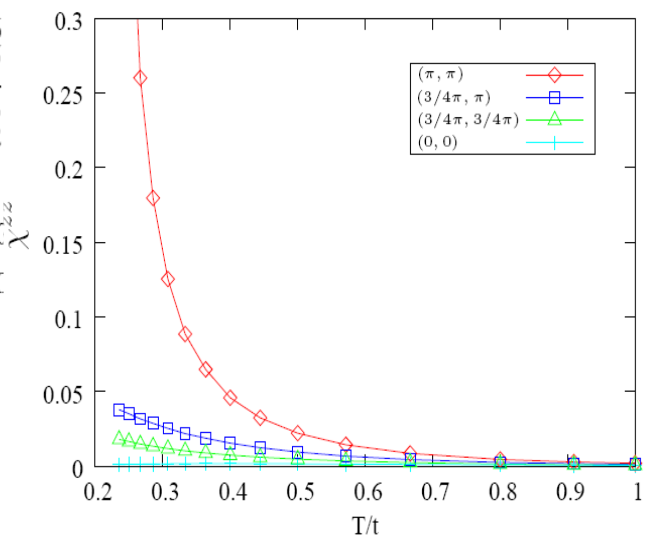
$$\chi^{-1}_{\nu,\nu'}(\vec{q},\omega) = \chi^{-1}_{0,\nu,\nu'}(\vec{q},\omega) - \gamma_{\nu,\nu'}(\omega)$$

Susceptibility: 2d – Hubbard model

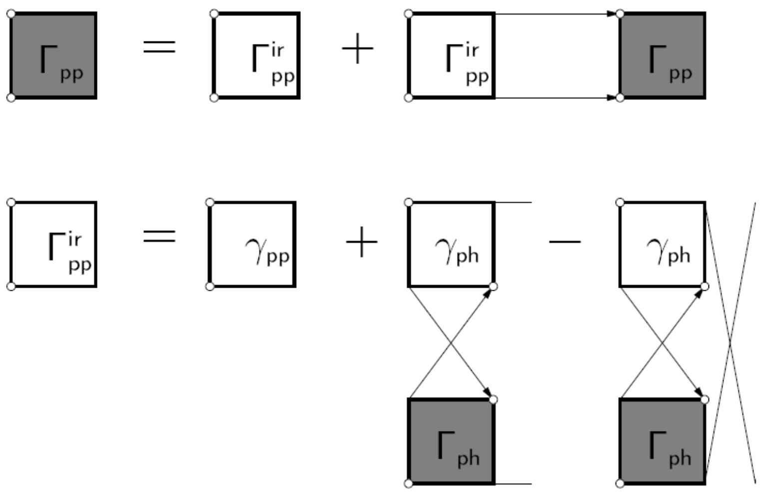


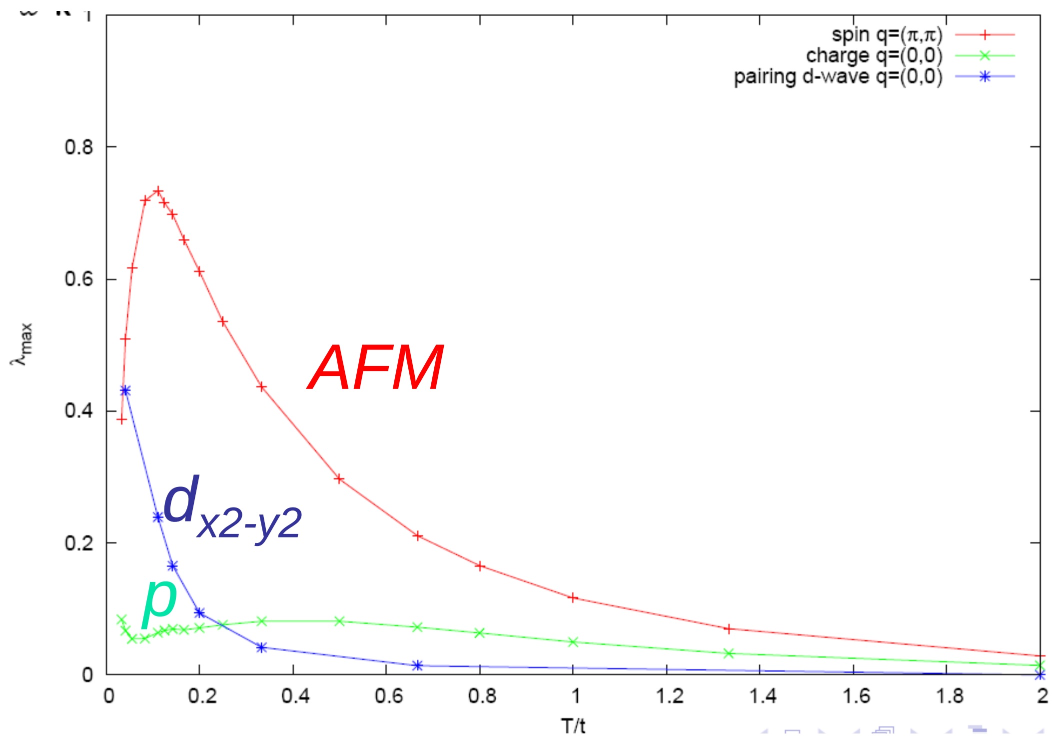






Bethe-Salpeter equation: pp-channel

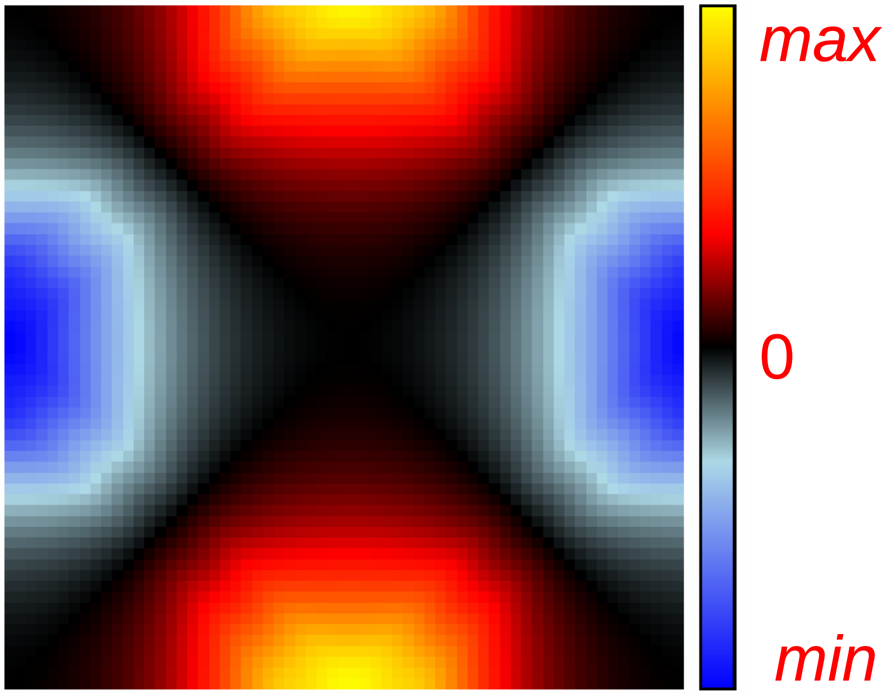


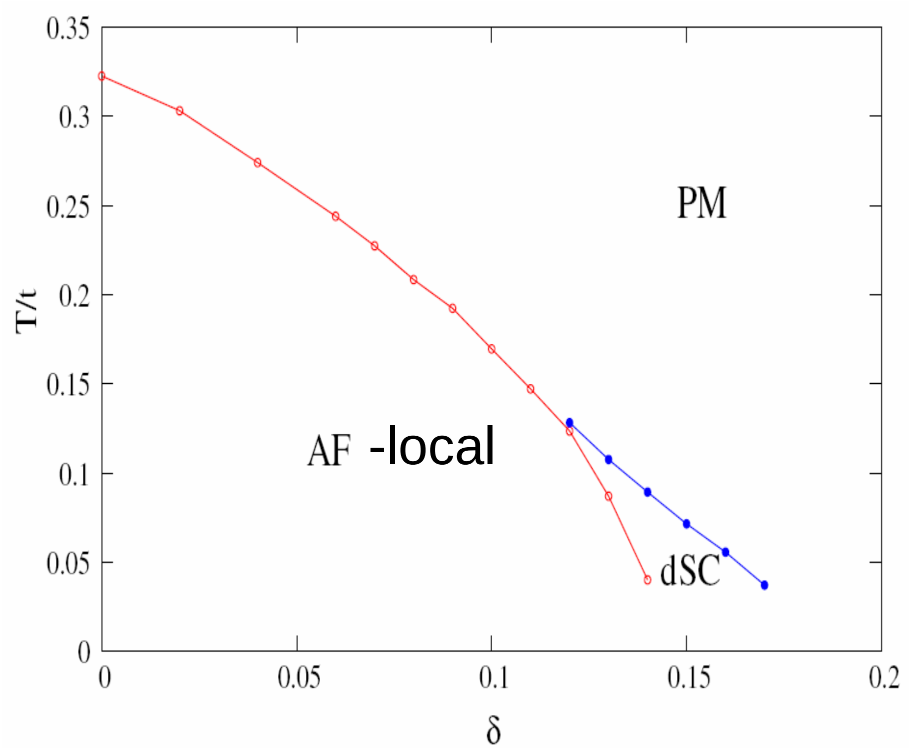


U=W t'/t=-0.3 x=15%

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

d-wave symmetry of the eigenfunction

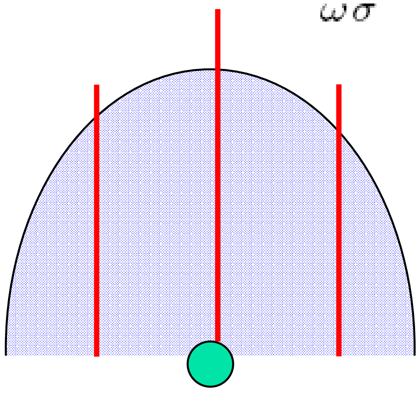




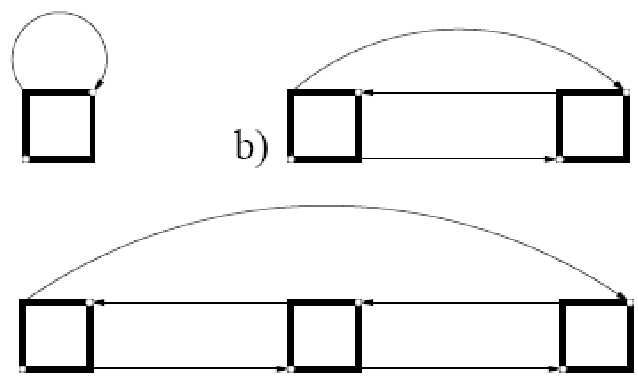
H. Hafermann et al. J. Supercond. Novel Mag. ***22****, 45 (2009)*

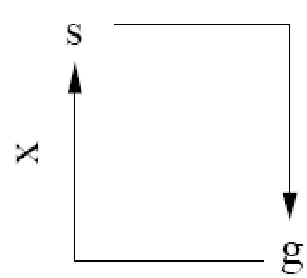
Superperturbation around ED

$$S[c^*,c] = -\sum_{\omega\sigma} c^*_{\omega\sigma}\left((i\omega+\mu)-\Delta^{(n)}_{\omega\sigma}\right)c_{\omega\sigma} + H_{\text{int}}[c^*,c] - \sum_{\omega\sigma} c^*_{\omega\sigma}(\Delta^{(n)}_{\omega\sigma} - \Delta_{\omega\sigma})c_{\omega\sigma}$$



$$\Delta^{(n)}_{\omega\sigma} = \sum_{p=1}^{n} \frac{|V_p^\sigma|^2}{i\omega - \epsilon_p^\sigma}$$





$$D_{\omega\sigma} = \Delta^{(n)}_{\omega\sigma} - \Delta_{\omega\sigma}$$

$$\begin{aligned} G_{12} &= [g(Dg+1)^{-1}]_{12} - [(1+gD)^{-1}]_{11'} \times \\ &\times (\chi - \chi^0)_{1'2'3'4'}[(g+D^{-1})^{-1}]_{4'3'}[(Dg+1)^{-1}]_{2'2} \end{aligned}$$

H. Hafermann et al, arXiv:0809.1051

Two-particle GF: H. Lehmann

$$\chi^{\sigma\sigma'}_{\omega_1\omega_2\omega_3} = \frac{1}{\beta^2}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \int_0^\beta d\tau_3\, e^{i(\omega_1\tau_1+\omega\tau_2+\omega_3\tau_3)} \langle T_\tau c_\sigma(\tau_1) c^\dagger_\sigma(\tau_2) c_{\sigma'}(\tau_3) c^\dagger_{\sigma'}(0)\rangle$$

$$\chi^{\sigma\sigma'}_{\omega_1\omega_2\omega_3} = \frac{1}{Z}\sum_{ijkl}\sum_{\Pi}\phi(E_i,E_j,E_k,E_l,\omega_{\Pi_1},\omega_{\Pi_2},\omega_{\Pi_3})\ \mathrm{sgn}(\Pi)\langle i|\mathcal{O}_{\Pi_1}|j\rangle\,\langle j|\mathcal{O}_{\Pi_2}|k\rangle\,\langle k|\mathcal{O}_{\Pi_3}|l\rangle\,\langle l|c^\dagger_{\sigma'}|i\rangle$$

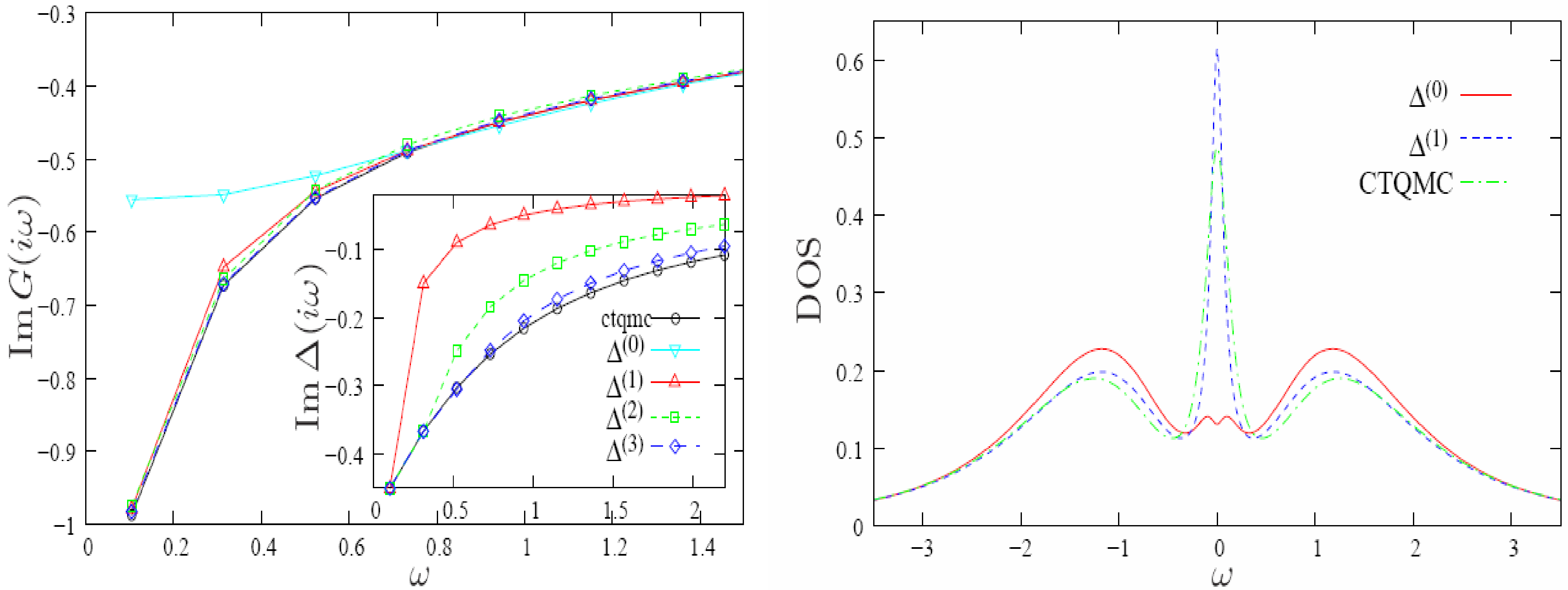
$$\phi(E_i,E_j,E_k,E_l,\omega_1,\omega_2,\omega_3) = \frac{1}{i\omega_3+E_k-E_l}\times$$

$$\Bigg[\frac{1-\delta_{\omega_2,-\omega_3}\delta_{E_j,E_l}}{i(\omega_2+\omega_3)+E_j-E_l}\left(\frac{e^{-\beta E_i}+e^{-\beta E_j}}{i\omega_1+E_i-E_j}-\frac{e^{-\beta E_i}+e^{-\beta E_l}}{i(\omega_1+\omega_2+\omega_3)+E_i-E_l}\right)$$

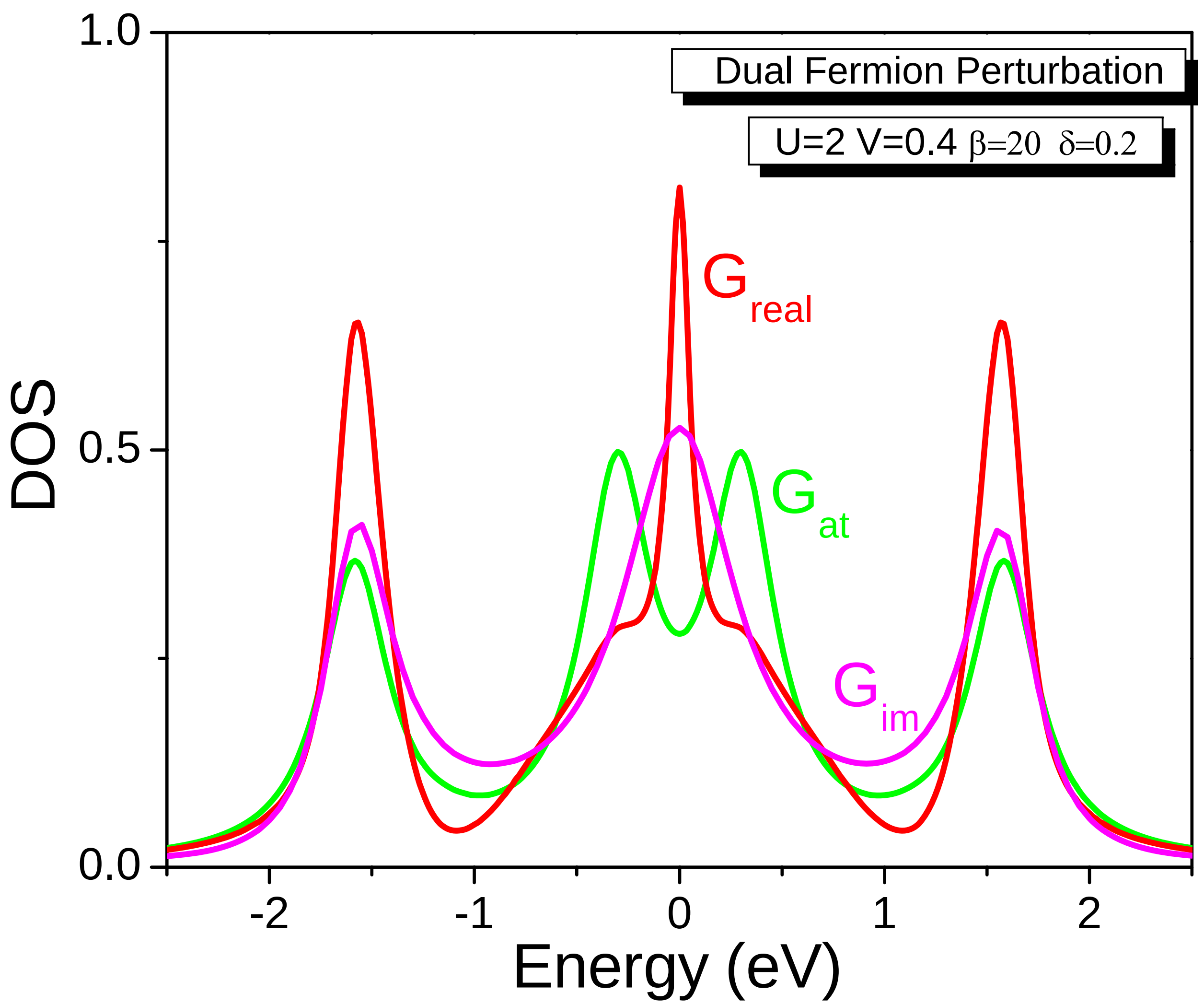
$$+\delta_{\omega_2,-\omega_3}\delta_{E_j,E_l}\left(\frac{e^{-\beta E_i}+e^{-\beta E_j}}{(i\omega_1+E_i-E_j)^2}-\beta\frac{e^{-\beta E_j}}{i\omega_1+E_i-E_j}\right)-\frac{1}{i\omega_2+E_j-E_k}\times$$

$$\left(\frac{e^{-\beta E_i}+e^{-\beta E_j}}{i\omega_1+E_i-E_j}-(1-\delta_{\omega_1,-\omega_2}\delta_{E_i,E_k})\frac{e^{-\beta E_i}-e^{-\beta E_k}}{i(\omega_1+\omega_2)+E_i-E_k}+\beta e^{-\beta E_i}\delta_{\omega_1,-\omega_2}\delta_{E_i,E_k}\right)\Bigg]$$

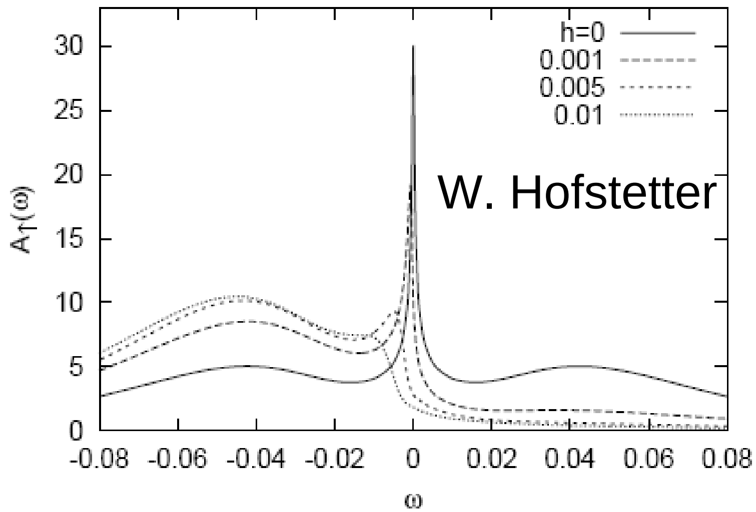
Impurity test: semirsircular DOS



Real-axis scheme: First Diagram



SIAM in Magnetic field



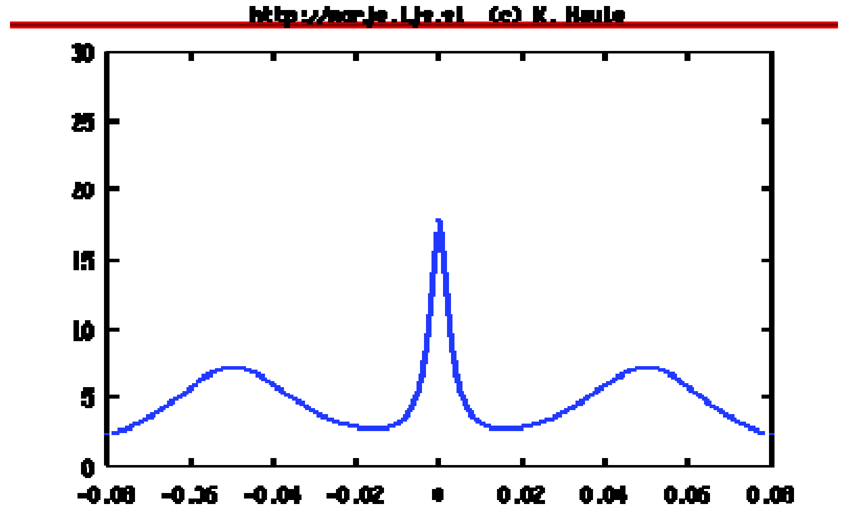
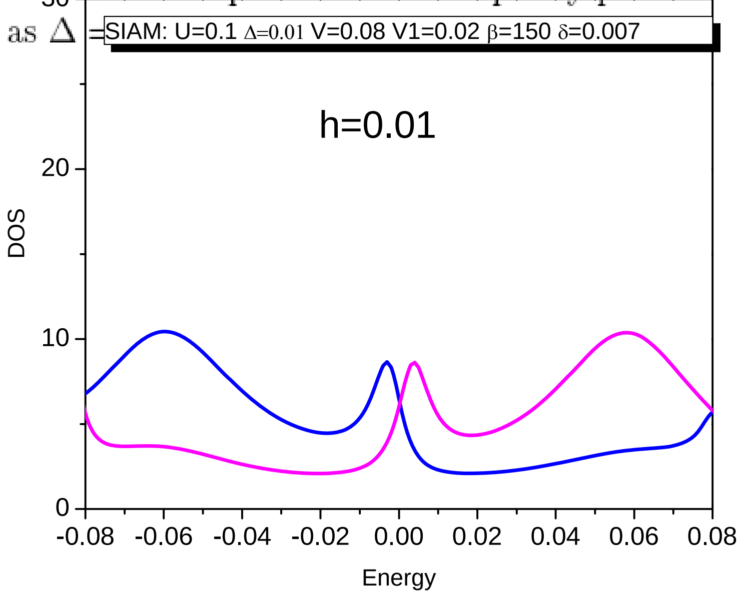
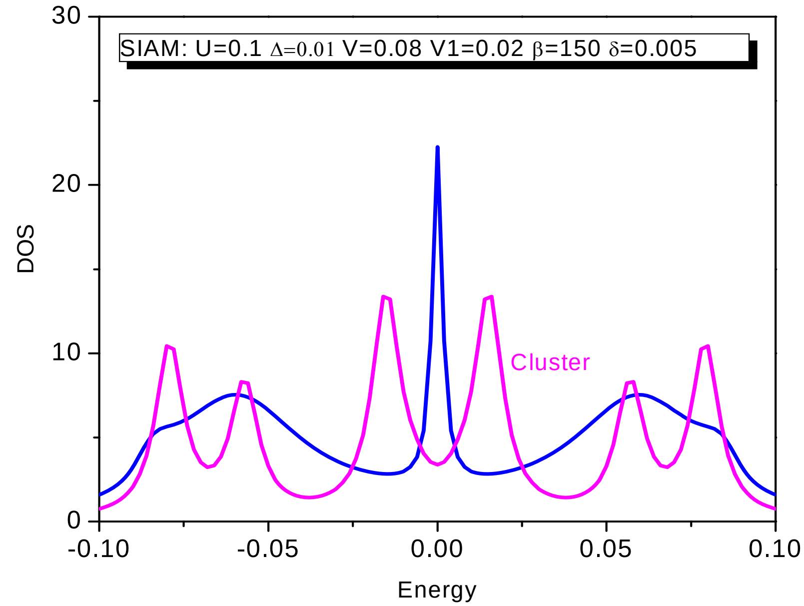


FIG. 4. Shift of the spectral function with increasing magnetic field at zero temperature. The impurity parameters are chosen as Δ =



NCA-K. Haule Δ=0.01



Conclusions

- Electronic Structure and Magnetism of non-local correlated systems can be described in CTQMC + DF scheme

- Exact Spin Dynamics for magnetic nanosystems with vertex corrections can be calculated within CTQMC