Correlated Matter: DMFT and Beyond

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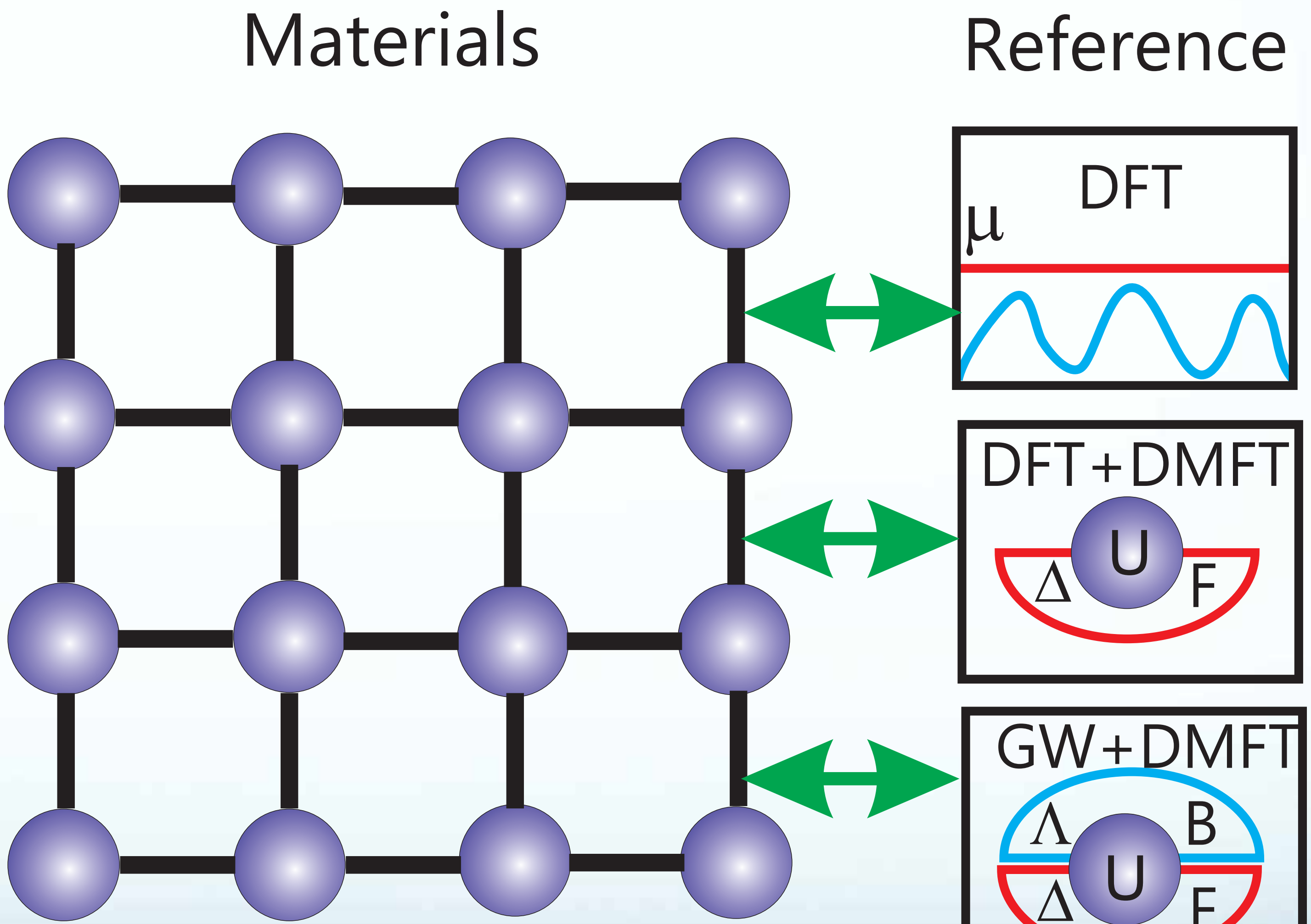
Outline

- Introduction: Reference system
- Path integral for fermions
- Functional approach: Route to fluctuations
- Dual Fermion scheme: beyond DMFT
- Numerical examples

Real Materials: Reference Systems



Reference system is important: Archimedes
„Give me the place to stand, and I shall move the earth.“

QM-Alphabet

1-Q

$$\left(-\frac{1}{2}\Delta + V_{eff}(\vec{r})\right)\psi(\vec{r}) = \varepsilon\psi(\vec{r})$$

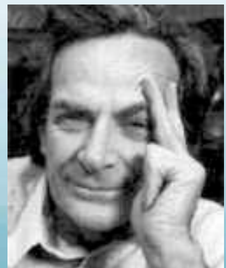
2-Q

$$\hat{H} = \sum_{ij\sigma} t_{ij}\hat{c}^{+}_{i\sigma}\hat{c}_{j\sigma} + \sum_{i} U\hat{n}_{\uparrow}\hat{n}_{\downarrow}$$

3-PI

$$Z = Sp(e^{-\beta\hat{H}}) = \int D[c^*,c]\, e^{-\int_0^\beta d\tau\left[c^*_\tau\partial_\tau c_\tau + H(c^*_\tau, c_\tau)\right]}$$

Richard Feynman
1948



x_1

x_2

Paul Dirac
1933

References

- John W. Negele and Henri Orland „Quantum Many-particle Systems“ (Addison Wesley 1988)
- Piers Coleman „Introduction to Many-Body Physics“ (Cambridge Uni Press 2015)
- Eduardo Fradkin „Field Theories of Condensed Matter Physics“ (Cambridge Uni Press 2013)
- Alexander Altland and Ben D. Simons „Condensed Matter Field Theory“ (Cambridge Uni Press 2010)
- Alexey Kamenev „Field Theory of Non-Equilibrium Systems“ (Cambridge Uni Press 2011)

Summary for Fermions $\{\hat{c}_i, \hat{c}_j^+\} = \delta_{ij}$

$$\hat{c}_i |1\rangle = |0\rangle \qquad \hat{c}_i |0\rangle = 0$$

$$\hat{c}_i^+ |0\rangle = |1\rangle \qquad \hat{c}_i^+ |1\rangle = 0$$

Pauli principle

$$\begin{aligned} \hat{c}_i^+ \hat{c}_i |n\rangle &= n_i |n\rangle \\ \hat{c}_i^2 = (\hat{c}_i^+)^2 &= 0 \,. \end{aligned}$$

Fermionic coherent states $|c\rangle$

$$\hat{c}_i |c\rangle = c_i |c\rangle$$

Left-eigenbasis has only annihilation operator - bounded from the bottom:

$$\hat{c}_i |0\rangle = 0 |0\rangle$$

Grassmann numbers c_i

F. A. Berezin: Method of Second Quantization (Academic Press , New York, 1966)

Eigenvalues of coheren states

$$c_i c_j = -c_j c_i$$
$$c_i^2 = 0$$

Exact representation

$$|c\rangle = e^{-\sum_i c_i \hat{c}_i^+} |0\rangle$$

Proof for one fermionic states

$$\hat{c}\,|c\rangle = \hat{c}(1 - c\hat{c}^+)\,|0\rangle = \hat{c}\,(|0\rangle - c\,|1\rangle) = -\hat{c}c\,|1\rangle = c\,|0\rangle = c\,|c\rangle$$

Left coherent state ⟨c| :

$$\langle c|\,\hat{c}_i^+ = \langle c|\,c_i^*$$

$$\langle c| = \langle 0|\,e^{-\sum_i \hat{c}_i c_i^*}$$

general function of two Grassmann variables

$$f(c^*, c) = f_{00} + f_{10}c^* + f_{01}c + f_{11}c^*c$$

Grassmann calculus

Formal definition of derivative $$\frac{\partial c_i}{\partial c_j} = \delta_{ij}$$

Due to anti-commutation rule: $$\frac{\partial}{\partial c_2} c_1 c_2 = -c_1$$

Example: $$f(c^*, c) = f_{00} + f_{10} c^* + f_{01} c + f_{11} c^* c$$

$$\frac{\partial}{\partial c^*}\frac{\partial}{\partial c} f(c^*, c) = \frac{\partial}{\partial c^*}(f_{01} - f_{11} c^*) = -f_{11} = -\frac{\partial}{\partial c}\frac{\partial}{\partial c^*} f(c^*, c)$$

Formal definition of integration over Grassmann variables

$$\int ... dc \to \frac{\partial}{\partial c} ...$$

$$\int 1 dc = 0 \qquad \int c dc = 1$$

Resolution of unity operator

Overlap of any two coherent fermionic states $\langle c|c\rangle = e^{\sum_i c_i^* c_i}$

Proof for single particle

$$\langle c|c\rangle = (\langle 0| - \langle 1|\, c^*)\,(|0\rangle - c\,|1\rangle) = 1 + c^* c = e^{c^* c}$$

Unity operator

$$\int dc^* \int dc\; e^{-\sum_i c_i^* c_i}\, |c\rangle\,\langle c| = \hat{1} = \int\!\!\int dc^* dc\, \frac{|c\rangle\,\langle c|}{\langle c|c\rangle}$$

Proof for single particle

$$\int\!\!\int dc^* dc\; e^{-c^* c}\, |c\rangle\,\langle c| = \int\!\!\int dc^* dc\,(1 - c^* c)\,(|0\rangle - c\,|1\rangle)\,(\langle 0| - \langle 1|\, c^*) =$$

$$- \int\!\!\int dc^* dc\; c^* c\,(|0\rangle\,\langle 0| + |1\rangle\,\langle 1|) = \sum_n |n\rangle\,\langle n| = \hat{1}$$

Trace Formula

Matrix elements of normally ordered operators

$$\langle c^*| \hat{H}(\hat{c}^+, \hat{c}) |c\rangle = H(c^*, c) \langle c^*|c\rangle = H(c^*, c)\, e^{\sum_i c_i^* c_i}$$

Trace of fermionic operators in normal order

$$Tr\left(\widehat{O}\right) = \sum_{n=0,1} \langle n|\, \widehat{O}\, |n\rangle = \sum_{n=0,1} \int\int dc^* dc\; e^{-c^* c} \langle n|\, c\rangle \langle c|\, \widehat{O}\, |n\rangle =$$
$$= \int\int dc^* dc\; e^{-c^* c} \sum_{n=0,1} \langle -c|\, \widehat{O}\, |n\rangle \langle n|\, c\rangle = \int\int dc^* dc\; e^{-c^* c} \langle -c|\, \widehat{O}\, |c\rangle$$

„Minus" fermionic sign due to commutations:

$$\langle n|c\rangle \langle c|n\rangle = \langle -c|n\rangle \langle n|c\rangle$$

Mapping: $$(\hat{c}_i^+, \hat{c}_i) \to (c_i^*, c_i)$$

Partition function

Grand-canonical quantum ensemble $H = \widehat{H} - \mu\widehat{N}$

N-slices Trotter decomposition [0,β)

$$\tau_n = n\Delta\tau = n\beta/N \; (n = 1, ..., N).$$

$$e^{-\beta H} = \lim_{N\to\infty} (e^{-\Delta\tau H})^N$$

Insert N-times the resolution of unity:

$$\begin{aligned} Z &= Tr\left[e^{-\beta H}\right] = \int\int dc^* dc e^{-c^* c} \langle -c| e^{-\beta H} |c\rangle \\ &= \int \Pi_{n=1}^N dc_n^* dc_n e^{-\sum_n c_n^* c_n} \langle c_N| e^{-\Delta\tau H} |c_{N-1}\rangle \langle c_{N-1}| e^{-\Delta\tau H} |c_{N-2}\rangle ... \langle c_1| e^{-\Delta\tau H} |c_0\rangle \\ &= \int \Pi_{n=1}^N dc_n^* dc_n e^{-\Delta\tau \sum_{n=1}^N [c_n^*(c_n - c_{n-1})/\Delta\tau + H(c_n^*, c_{n-1})]} \end{aligned}$$

In continuum limit (N → ∞)

$$\Delta\tau \sum_{n=1}^N ... \mapsto \int_0^\beta d\tau ...$$

$$\frac{c_n - c_{n-1}}{\Delta\tau} \mapsto \partial_\tau$$

$$\Pi_{n=0}^{N-1} dc_n^* dc_n \mapsto D\left[c^*, c\right]$$

$$Z = \int D\left[c^*, c\right] e^{-\int_0^\beta d\tau [c^*(\tau)\partial_\tau c(\tau) + H(c^*(\tau), c(\tau))]}$$

Antiperiodic boundary condition $c(\beta) = -c(0), \quad c^*(\beta) = -c^*(0)$

Gaussian path integral

Non-interacting "quadratic" fermionic action

$$Z_0\left[J^*,J\right] = \int D\left[c^*c\right]\, e^{-\sum_{i,j=1}^N c_i^* M_{ij} c_j + \sum_{i=1}^N \left(c_i^* J_i + J_i^* c_i\right)} = \det\left[M\right] e^{-\sum_{i,j=1}^N J_i^* \left(M^{-1}\right)_{ij} J_j}$$

Hint for proof: $$e^{-\sum_{i,j=1}^N c_i^* M_{ij} c_j} = \frac{1}{N!}\left(-\sum_{i,j=1}^N c_i^* M_{ij} c_j\right)^N$$

Exercise for N=1 and 2: $$\int D\left[c^*c\right] e^{-c_1^* M_{11} c_1} = \int D\left[c^*c\right]\left(-c_1^* M_{11} c_1\right) = M_{11} = \det M$$

$$\int D\left[c^*c\right] e^{-c_1^* M_{11} c_1 - c_1^* M_{12} c_1 - c_2^* M_{21} c_1 - c_2^* M_{22} c_2} =$$

$$\frac{1}{2!}\int D\left[c^*c\right]\left(-c_1^* M_{11} c_1 - c_1^* M_{12} c_1 - c_2^* M_{21} c_1 - c_2^* M_{22} c_2\right)^2 = M_{11}M_{22} - M_{12}M_{21} = \det M$$

Shift of Grassmann variable: $$c^* M c - c^* J - J^* c = \left(c^* - J^* M^{-1}\right) M \left(c - M^{-1} J\right) - J^* M^{-1} J$$

correlation functions for a non- interaction action (Wick-theorem)

$$\left\langle c_i c_j^* \right\rangle_0 = -\frac{1}{Z_0}\frac{\delta^2 Z_0\left[J^*,J\right]}{\delta J_i^*\, \delta J_j}\Big|_{J=0} = M_{ij}^{-1}$$

$$\left\langle c_i c_j c_k^* c_l^* \right\rangle_0 = \frac{1}{Z_0}\frac{\delta^4 Z_0\left[J^*,J\right]}{\delta J_i^* \delta J_j^* \delta J_l \delta J_k}\Big|_{J=0} = M_{il}^{-1} M_{jk}^{-1} - M_{ik}^{-1} M_{jl}^{-1}$$

Path Integral for Everything

Euclidean action

$$
\begin{aligned}
Z &= \int \mathcal{D}[c^*, c] e^{-S} \\
S &= \sum_{12} c_1^* \left(\partial_\tau + t_{12}\right) c_2 + \frac{1}{4} \sum_{1234} c_1^* c_2^* \, U_{1234} \, c_4 c_3
\end{aligned}
$$

One- and two-electron matrix elements:

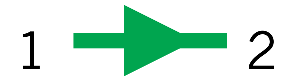
$$
\begin{aligned}
t_{12} &= \int d\mathbf{r} \, \phi_1^*(\mathbf{r}) \left(-\frac{1}{2} \nabla^2 + V(\mathbf{r}) - \mu \right) \phi_2(\mathbf{r}) \\
U_{1234} &= \int d\mathbf{r} \int d\mathbf{r}' \, \phi_1^*(\mathbf{r}) \phi_2^*(\mathbf{r}') \, U(\mathbf{r} - \mathbf{r}') \, \phi_3(\mathbf{r}) \phi_4(\mathbf{r}')
\end{aligned}
$$

Shot notation:

$$
\sum_1 \ldots \equiv \sum_{im} \int d\tau \ldots
$$

One- and Two-particle Green Functions

One-particle Green function



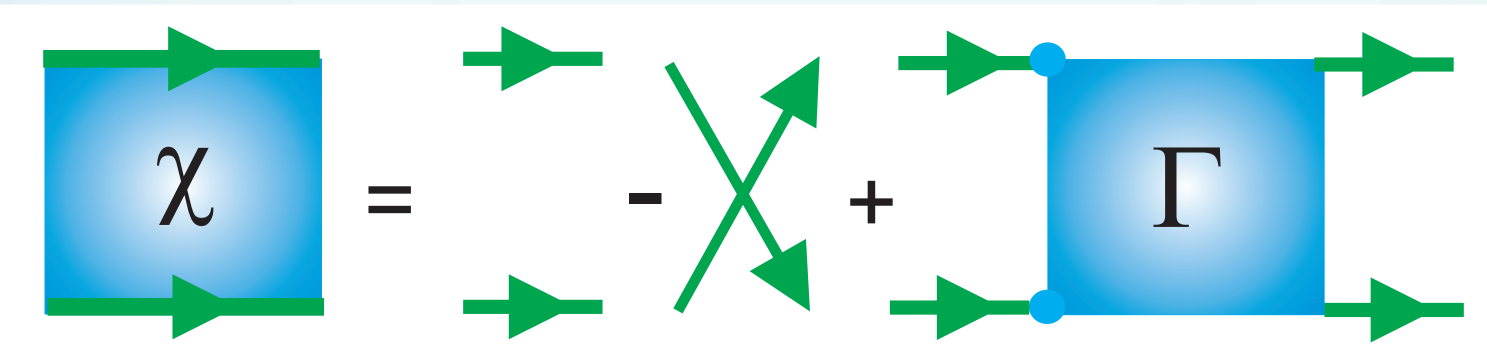
$$G_{12} = -\langle c_1 c_2^* \rangle_S = -\frac{1}{Z} \int \mathcal{D}[c^*, c]\, c_1 c_2^*\, e^{-S}$$

Two-particle Green function (generalized susceptibilities)

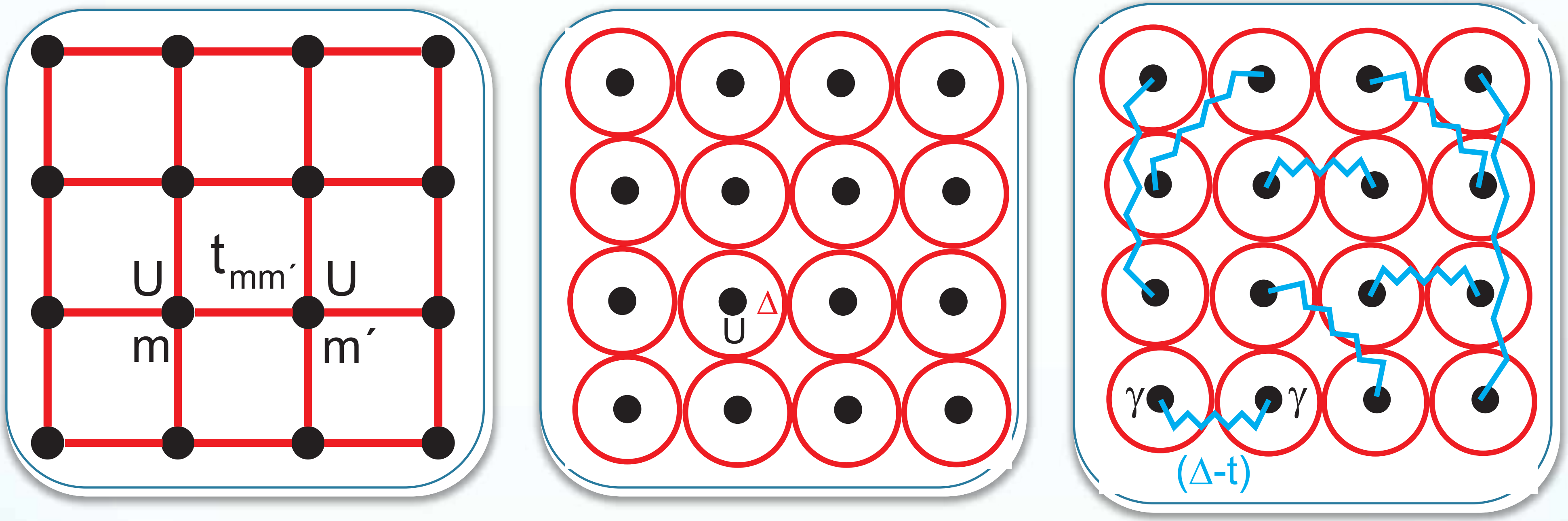
$$\chi_{1234} = \langle c_1 c_2 c_3^* c_4^* \rangle_S = \frac{1}{Z} \int \mathcal{D}[c^*, c]\, c_1 c_2 c_3^* c_4^*\, e^{-S}$$

Vertex function:

$$X_{1234} = G_{14} G_{23} - G_{13} G_{24} + \sum_{1'2'3'4'} G_{11'} G_{22'} \mathit{\Gamma}_{1'2'3'4'} G_{3'3} G_{4'4}$$



How to find “optimal”-functional?



Dual Fermions: Basic

Start from
Correlated Lattice

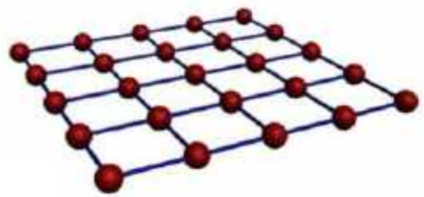
Find the optimal
Reference System
Bath hybridization

Expand around
DMFT solution

Dual Fermion scheme

General Lattice Action

$$Z = \int \mathcal{D}[c^*, c] \exp\left(-S_L[c^*, c]\right)$$

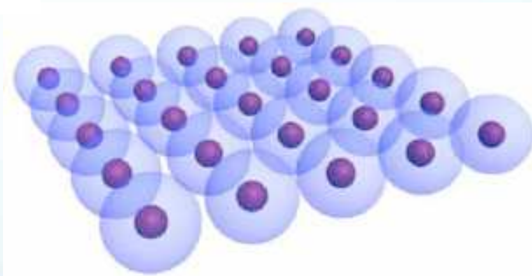


$$S_L[c^*, c] = -\sum_{\mathbf{k}\nu\sigma} c^*_{\mathbf{k}\nu\sigma} \left(i\nu + \mu - t_{\mathbf{k}}\right) c_{\mathbf{k}\nu\sigma} + \sum_i \int_0^\beta d\tau \, U \, n^*_{i\tau\uparrow} n_{i\tau\downarrow}$$

Reference system: Local Action with hybridization Δ_ν

$$S_\Delta[c_i^*, c_i] = -\sum_{\nu,\sigma} c^*_{i\nu\sigma} \left(i\nu + \mu - \Delta_\nu\right) c_{i\nu\sigma} + \sum_\nu U n^*_{i\nu\uparrow} n_{i\nu\downarrow}$$

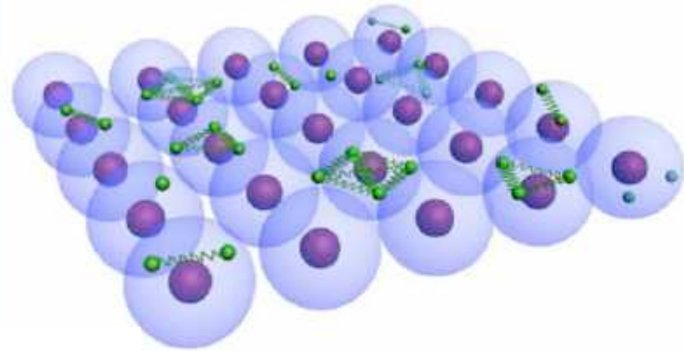
Lattice-Impurity connection:



$$S_L[c^*, c] = \sum_i S_\Delta[c_i^*, c_i] - \sum_{\mathbf{k}\nu\sigma} c^*_{\mathbf{k}\nu\sigma} \left(\Delta_\nu - t_{\mathbf{k}}\right) c_{\mathbf{k}\nu\sigma}$$

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

Dual Transformation



Gaussian path-integral

$$e^{c_1^* \,\widetilde{\Delta}_{12}\, c_2} = \det \widetilde{\Delta} \int \mathcal{D}\left[d^*, d\right] \, e^{-d_1^* \widetilde{\Delta}_{12}^{-1} d_2 - d_1^* c_1 - c_1^* d_1}$$

new Action:

With $\widetilde{\Delta}_{\mathbf{k}\nu} = (\Delta_\nu - t_{\mathbf{k}})$

$$\tilde{S}[d^*, d] = -\sum_{\mathbf{k}\,\nu\sigma} d^*_{\mathbf{k}\nu\sigma}\, \tilde{G}^{-1}_{0\mathbf{k}\nu}\, d_{\mathbf{k}\nu\sigma} + \sum_i V_i[d_i^*, d_i]$$

Diagrammatic:

$$g_{12} = -\langle c_1 c_2^* \rangle_\Delta$$

$\longrightarrow$ $$\tilde{G}^0_{\mathbf{k}\nu} = \left(\left(t_{\mathbf{k}} - \Delta_\nu \right)^{-1} - g_\nu \right)^{-1}$$

$$V[d^*, d] = \frac{1}{4} \sum_{1234} \gamma_{1234}\, d_1^* d_2^* d_4 d_3$$

$\square$ $$\gamma_{1234} = \chi_{1234} - \chi^0_{1234}$$

$$\chi_{1234} = \langle c_1 c_2 c_3^* c_4^* \rangle_\Delta$$

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

Dual Fermion Action: Details

Lattice - dual action $$\frac{Z}{Z_d} = \int \mathcal{D}[c^*, c, d^*, d] \exp\big(-S[c^*, c, d^*, d]\big) \qquad Z_d = \det \widetilde{\Delta}$$

$$S[c^*, c, d^*, d] = \sum_i S_\Delta^i + \sum_{\mathbf{k},\nu,\sigma} d^*_{\mathbf{k}\nu\sigma} \big(\Delta_\nu - t_k\big)^{-1} d_{\mathbf{k}\nu\sigma}$$

$$S_\Delta^i[c_i^*, c_i, d_i^*, d_i] = S_\Delta[c_i^*, c_i] + \sum_{\nu,\sigma} \big(d^*_{i\nu\sigma}\, c_{i\nu\sigma} + c^*_{i\nu\sigma}\, d_{i\nu\sigma}\big)$$

For each site (i) integrate-out original c-Fermions:

$$\frac{1}{Z_\Delta} \int \mathcal{D}[c^*, c] \exp\big(-S_\Delta^i[, c_i^*, c_i, d_i^* d_i]\big) = \exp\Big(-\sum_{\nu\,\sigma} d^*_{i\nu\sigma}\, g_\nu d_{i\nu\sigma} - V_i[d_i^* d_i]\Big)$$

Dual potential: $$V[d^*, d] = \frac{1}{4} \sum_{1234} \gamma_{1234}\, d_1^* d_2^* d_4 d_3 \ + \ldots \qquad \gamma_{1234} = \chi_{1234} - \chi^0_{1234}$$

$$\chi_{1234} = \langle c_1 c_2 c_3^* c_4^* \rangle_\Delta = \frac{1}{Z_\Delta} \int \mathcal{D}[c^*, c]\, c_1 c_2 c_3^* c_4^*\, e^{-S_\Delta[c^*, c]} \qquad \chi^0_{1234} = g_{14} g_{23} - g_{13} g_{24}$$

$$g_{12} = -\langle c_1 c_2^* \rangle_\Delta = \frac{1}{Z_\Delta} \int \mathcal{D}[c^*, c]\, c_1 c_2^*\, e^{-S_\Delta[c^*, c]}$$

Dual and Lattice Green's Functions

Two equivalent forms for partition function:

$$e^{F[J^*J,L^*L]} = \mathcal{Z}_d \int \mathcal{D}[c^*c, d^*d]\, e^{-S[c^*c,d^*,d]+J_1^*c_1+c_2^*J_2+L_1^*d_1+d_2^*L_2}$$

$$e^{F[L^*,L]} = \tilde{\mathcal{Z}}_d \int \mathcal{D}[d^*, d]\, e^{-S_{\mathrm{d}}[d^*,fd+L_1^*d_1+d_2^*L_2}$$

$$\tilde{\mathcal{Z}}_d = \mathcal{Z}/\tilde{\mathcal{Z}}$$

Hubbard-Stratanovich transformation:

$$F[J^*J, L^*L] = L_1^*(\Delta - t)_{12}L_2 + \ln \int \mathcal{D}[c^*, c] \exp\Big(-S[c^*, c] + J_1^*c_1 + c_2^*J_2 + L_1^*(\Delta{-}t)_{12}c_2 + c_1^*(\Delta{-}t)_{12}L_2\Big)$$

Relation between Green functions:

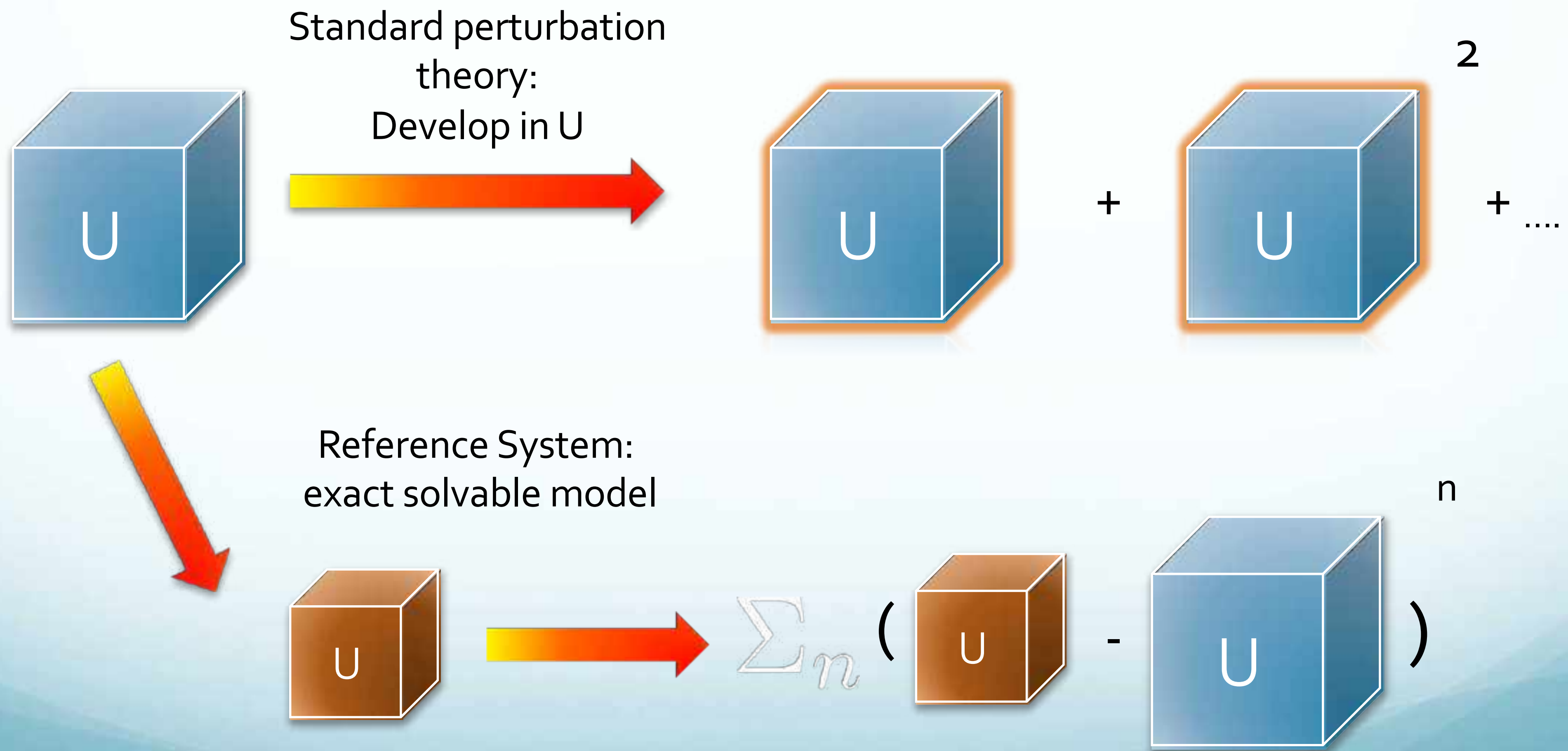
$$\tilde{G}_{12} = -\frac{\delta^2 F}{\delta L_2 \delta L_1^*}\bigg|_{L^*=L=0}$$

$$\tilde{G}_{12} = -(\Delta{-}t)_{12} + (\Delta{-}t)_{11'}G_{1'2'}(\Delta{-}t)_{2'2}$$

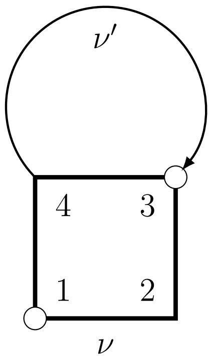
T-matrix like relations via dual self-energy

$$G_{\mathbf{k}\nu} = \left(\left(g_\nu + \widetilde{\Sigma}_{\mathbf{k}\nu}\right)^{-1} - \widetilde{\Delta}_{\mathbf{k}\nu}\right)^{-1}$$

Super-perturbation



1-st order diagram for dual self-energy



$$\tilde{\Sigma}^{(1)i}_{12}(\nu) = \sum_{\nu',3,4} \gamma^{d}_{1234}(\nu, \nu', 0)\, \tilde{G}^{ii}_{43}(\nu')$$

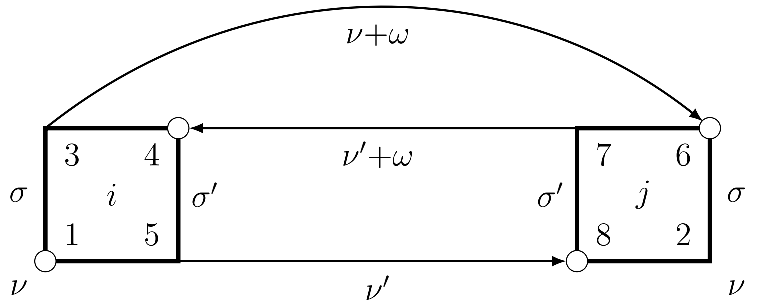
Density (d) and Magnetic (m) Vertices:

$$\gamma^{d/m}_{1234}(\nu, \nu', \omega) = \gamma^{\uparrow\uparrow}_{1234}(\nu, \nu', \omega) \pm \gamma^{\uparrow\downarrow}_{1234}(\nu, \nu', \omega)$$

Connected 2-particle GF:

$$\gamma^{\sigma\sigma'}_{1234}(\tau_1, \tau_2, \tau_3, \tau_4) = -\left\langle c_{1\sigma} c^{*}_{2\sigma} c_{3\sigma'} c^{*}_{4\sigma'} \right\rangle_{\Delta} + g^{\sigma}_{12} g^{\sigma'}_{34} - g^{\sigma}_{14} g^{\sigma}_{32} \delta_{\sigma\sigma'}$$

2-nd order diagram for dual self-energy



$c_d = -1/4$ and $c_m = -3/4$

$$\widetilde{\Sigma}_{12}^{(2)ij}(\nu) = \sum_{\nu'\omega} \sum_{3\text{-}8} \sum_{\alpha=d,m} c_\alpha \gamma_{1345}^{\alpha,i}(\nu,\nu',\omega)\, \widetilde{G}_{36}^{ij}(\nu+\omega) \widetilde{G}_{74}^{ji}(\nu'+\omega)\, \widetilde{G}_{58}^{ij}(\nu')\, \gamma_{8762}^{\alpha,j}(\nu',\nu,\omega)$$

Lattice Self-Energy:

$$\Sigma_{\mathbf{k}\nu} \quad = \quad \Sigma_\nu^0 + \Sigma'_{\mathbf{k}\nu}$$

Non-Local DF-correction:

$$\Sigma'_{\mathbf{k}\nu} \quad = \quad g_\nu^{-1} - \left(g_\nu + \widetilde{\Sigma}_{\mathbf{k}\nu}\right)^{-1}$$

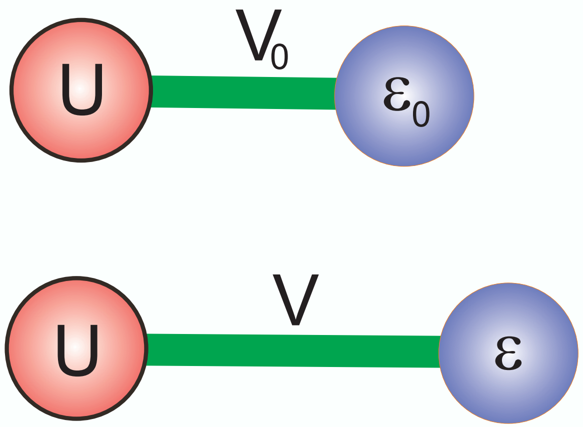
Lattice Green Function:

$$G_{\mathbf{k}\nu} = \left(\left(g_\nu + \widetilde{\Sigma}_{\mathbf{k}\nu}\right)^{-1} - \widetilde{\Delta}_{\mathbf{k}\nu}\right)^{-1}$$

Two site test

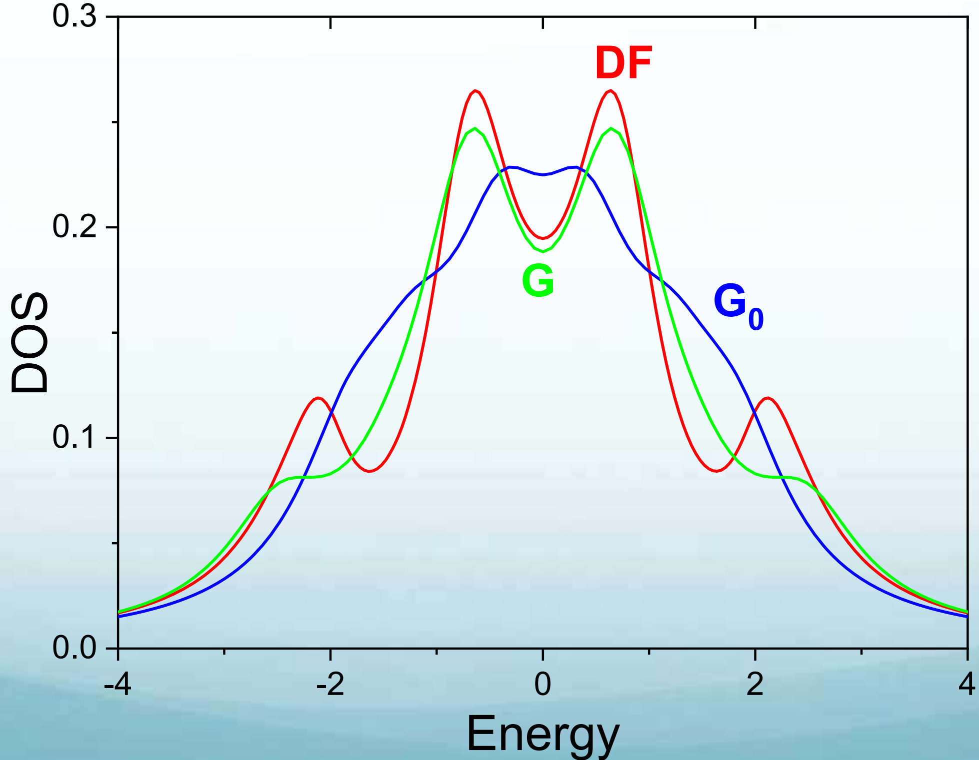
$U=2,\ \varepsilon_0=0$ $\quad V_0=0.5$

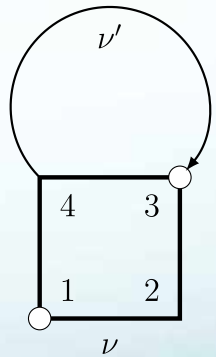
Fixed $\quad V=1.5V_0$



Ref.

Sys.



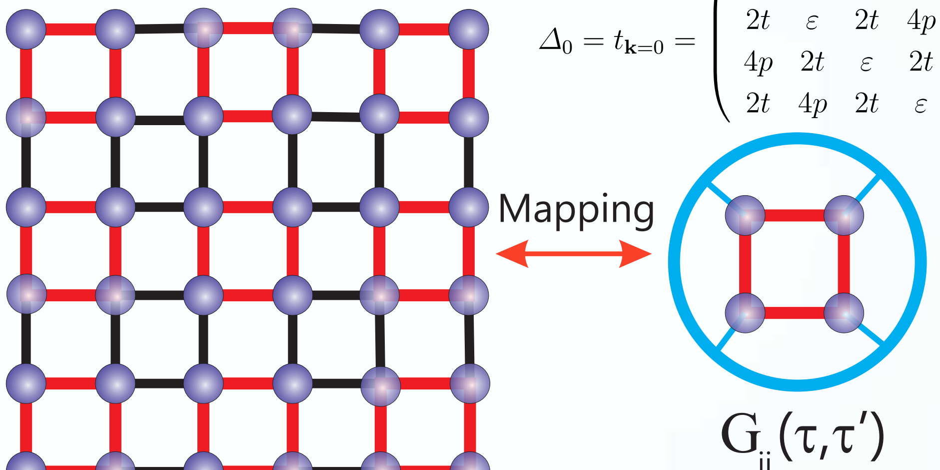


Plaquette DF-perturbation

$$t_{\mathbf{k}} = \begin{pmatrix} \varepsilon & tK^{0+} & pL^{-+} & tK^{-0} \\ tK^{0-} & \varepsilon & tK^{-0} & pL^{--} \\ pL^{+-} & tK^{+0} & \varepsilon & tK^{0-} \\ tK^{+0} & pL^{++} & tK^{0+} & \varepsilon \end{pmatrix}$$

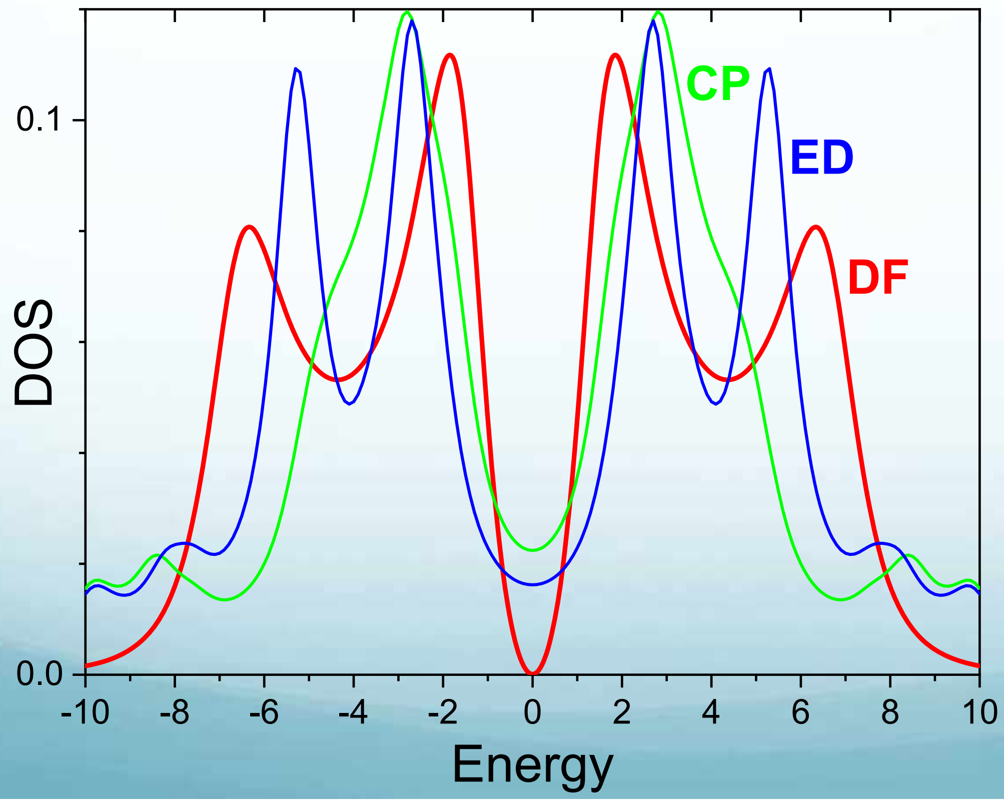
$$\begin{aligned} K_{\mathbf{k}}^{mn} &= 1 + e^{i(mk_x + nk_y)} \\ L_{\mathbf{k}}^{mn} &= 1 + e^{i(mk_x + nk_y)} + e^{imk_x} + e^{ink_y} \end{aligned}$$

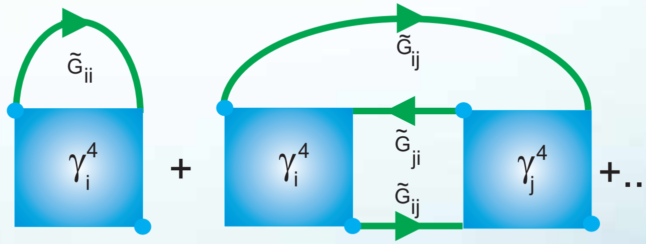
$$[m(n)] = -(1), 0, +(1)$$



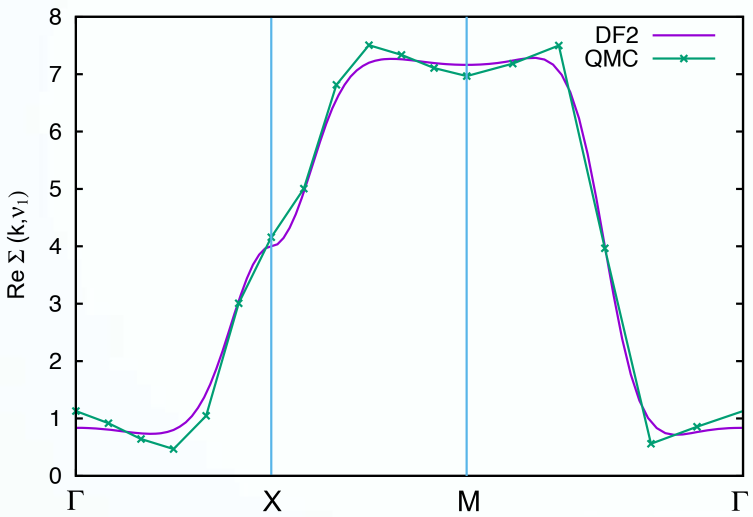
$$\Delta_0 = t_{\mathbf{k}=0} = \begin{pmatrix} \varepsilon & 2t & 4p & 2t \\ 2t & \varepsilon & 2t & 4p \\ 4p & 2t & \varepsilon & 2t \\ 2t & 4p & 2t & \varepsilon \end{pmatrix}$$

U=8
t=1
T=t/3

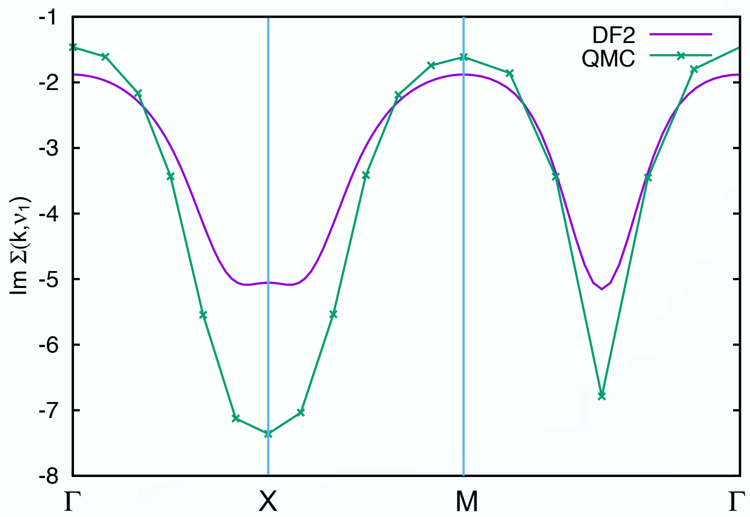




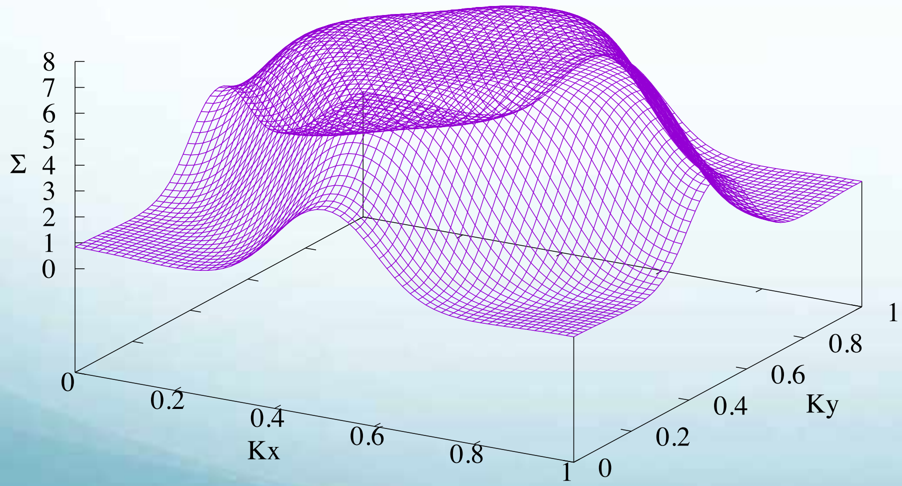
Self-energy: Plaquette DF

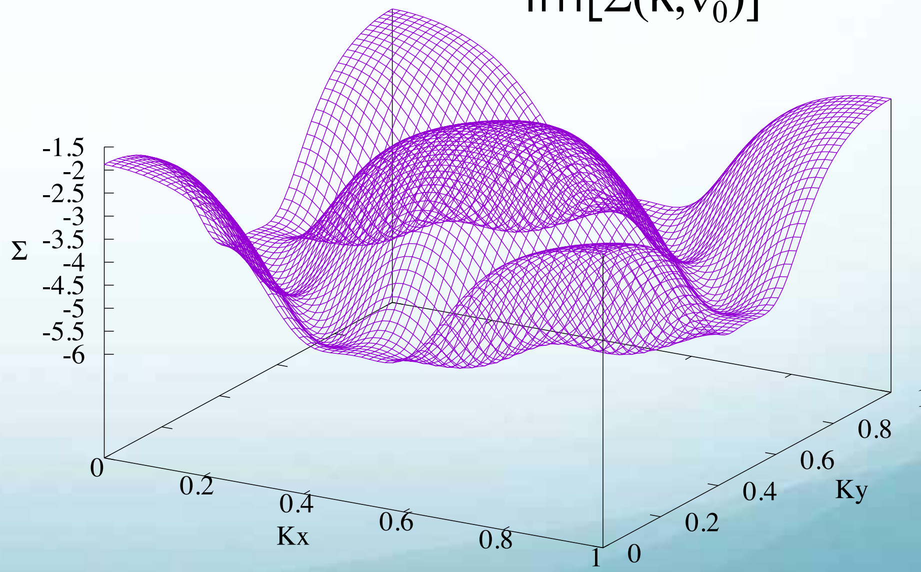


$\mathrm{Re}[\Sigma(\mathbf{k},\nu_0)]$



$\mathrm{Im}[\Sigma(\mathbf{k},\nu_0)]$

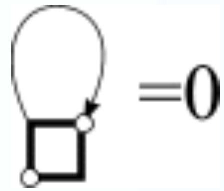




QMC: J. Gukelberger, E. Kozik, H. Hafermann, PRB **96**, 035152 (2017)

Condition for Δ and relation with DMFT

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

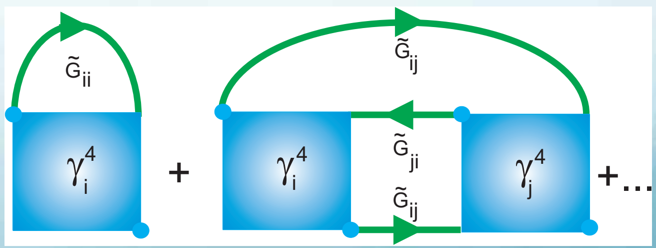


To determine Δ, we require
that Hartree correction in dual variables vanishes.
If no higher diagrams are taken into account, one obtains DMFT:

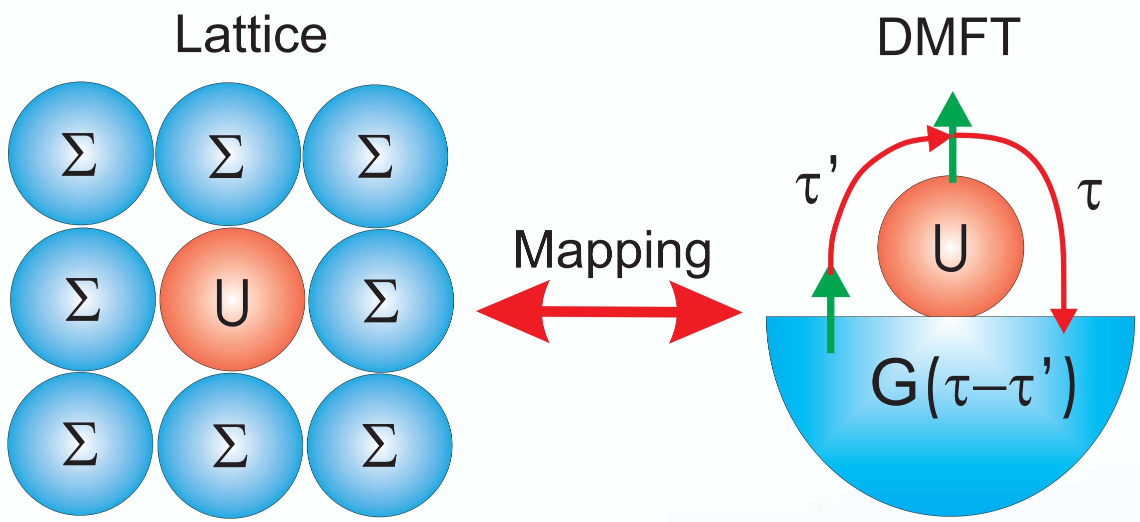
$$G_d = g\,\widetilde{G}\,g = G_{DMFT} - g \qquad G_{DMFT} = \left(g_\nu + \Delta_\nu - t_{\mathbf{k}}\right)^{-1}$$

$$\frac{1}{N}\sum_{\mathbf{k}} \tilde{G}^0_\omega(\mathbf{k}) = 0 \quad \Longleftrightarrow \quad \frac{1}{N}\sum_{\mathbf{k}} G^{\mathrm{DMFT}}_\omega(\mathbf{k}) = g_\omega$$

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



Dinamical Mean Field Theory



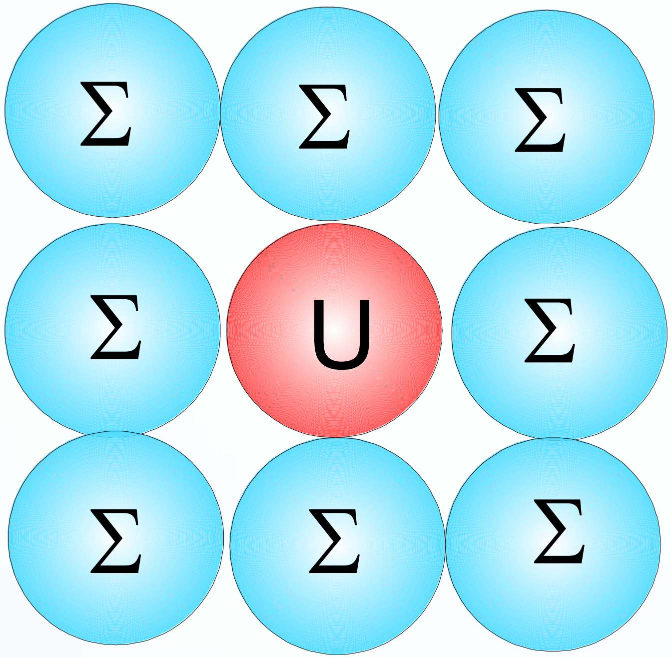
Self-consistent condition:

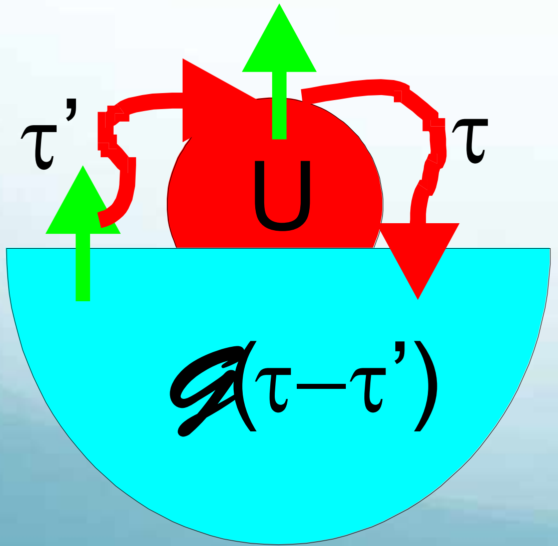
$$\sum_{\mathbf{k}} \left(g_\nu^{-1} + \Delta_\nu - t_{\mathbf{k}}\right)^{-1} = g_\nu$$

DMFT minimize “distance”:

$$|t_{\mathbf{k}} - \Delta_\nu|$$

Quantum Impurity Solver





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

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

What is a best scheme?
Quantum Monte Carlo !

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)

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

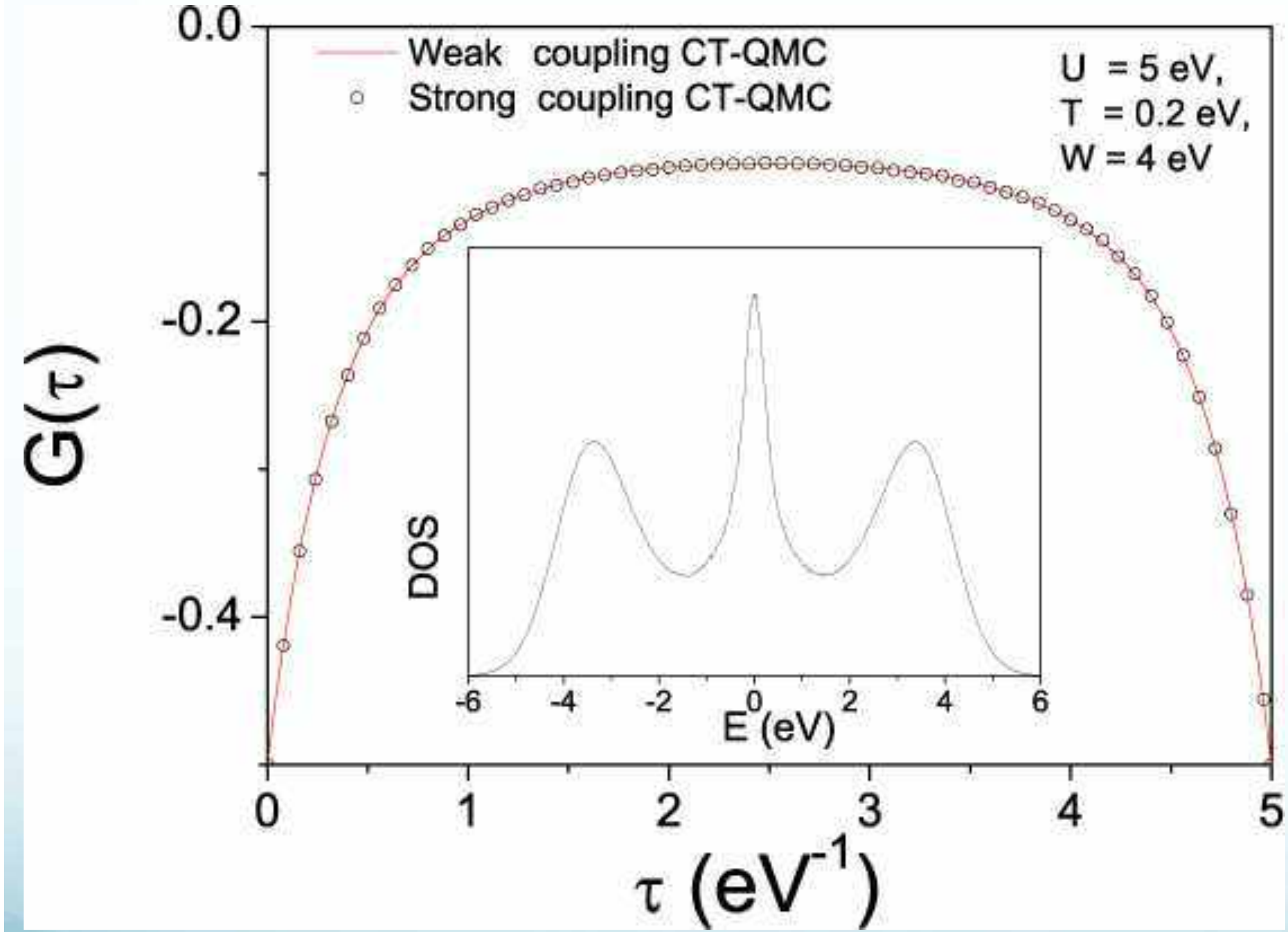
Hybridization expansion CT-HYB: P. Werner et al, PRL (2006)

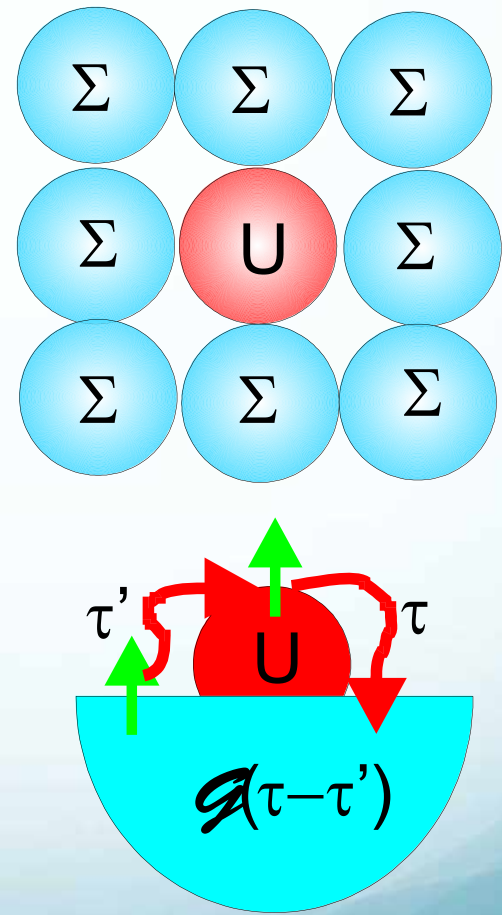
$$Z=Z_0\sum_{k=0}^{\infty}\frac{1}{k!}Tr\left\langle c_\sigma^+(\tau)c_\sigma(\tau')...c_{\sigma'}^+(\tau)c_{\sigma'}(\tau')\right\rangle_0\det[\Delta(\tau-\tau')]$$

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

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

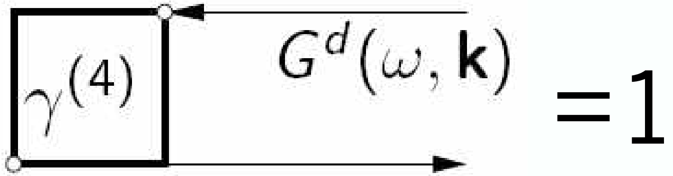
Comparison of different CT-QMC

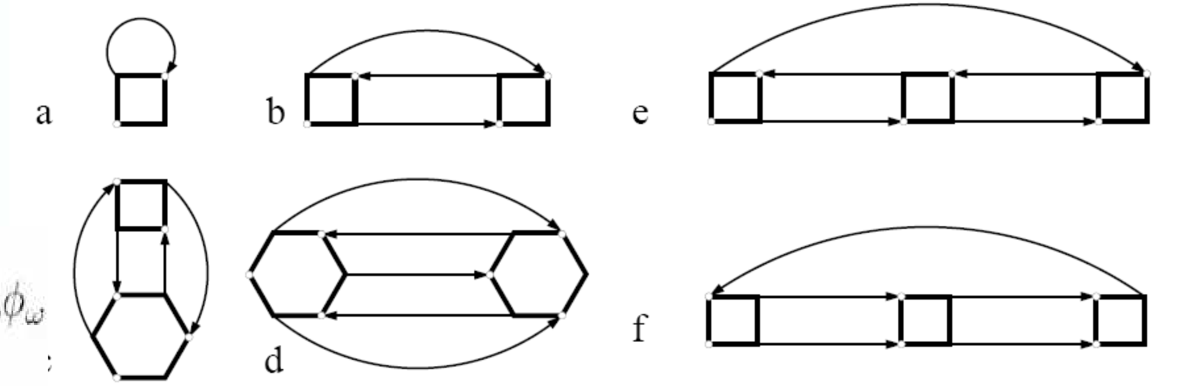




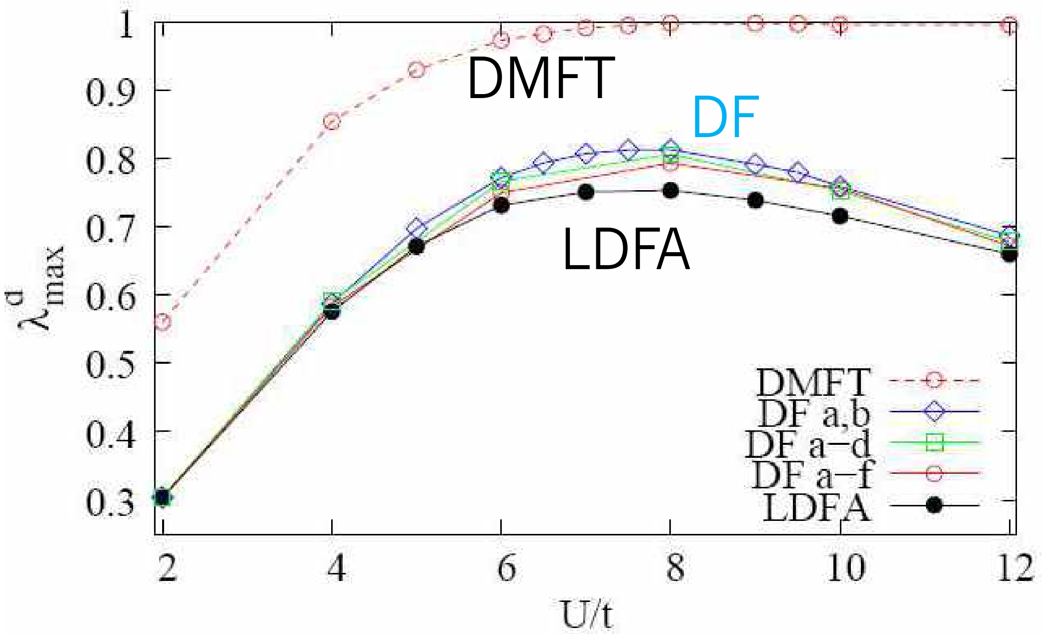
Ch. Jung, unpublished

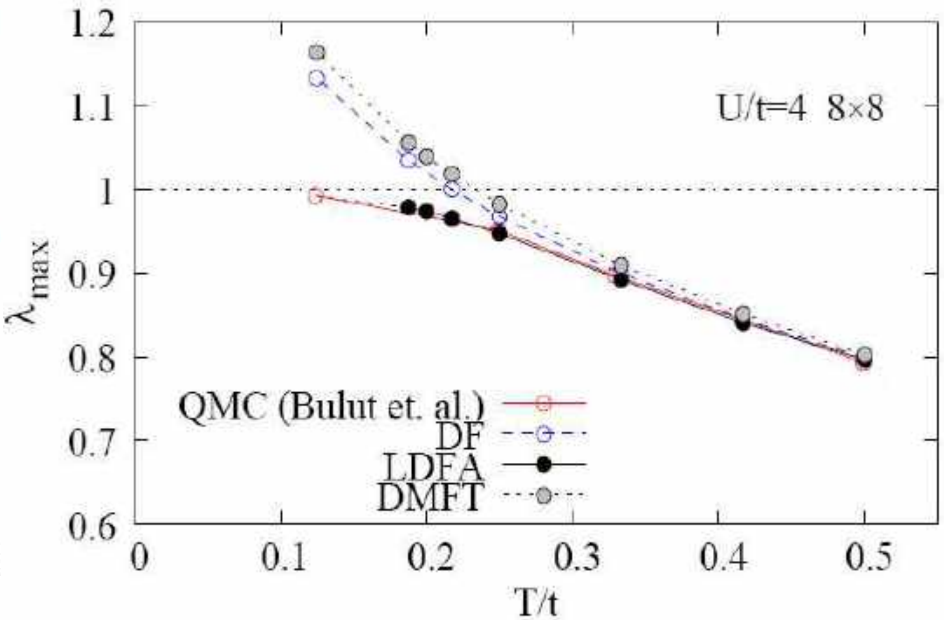
Convergence of Dual Fermions: 2d





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



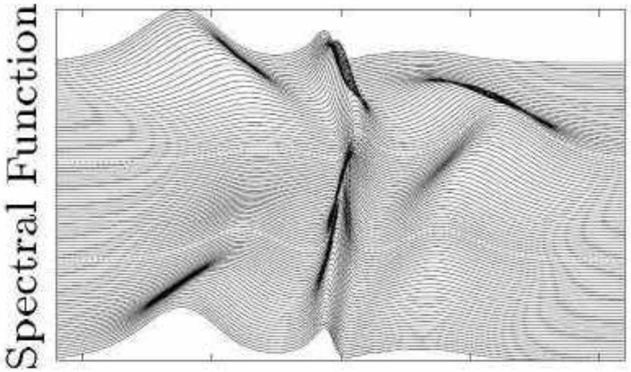


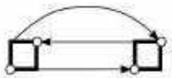
H. Hafermann, et al. PRL**102**, 206401 (2009)

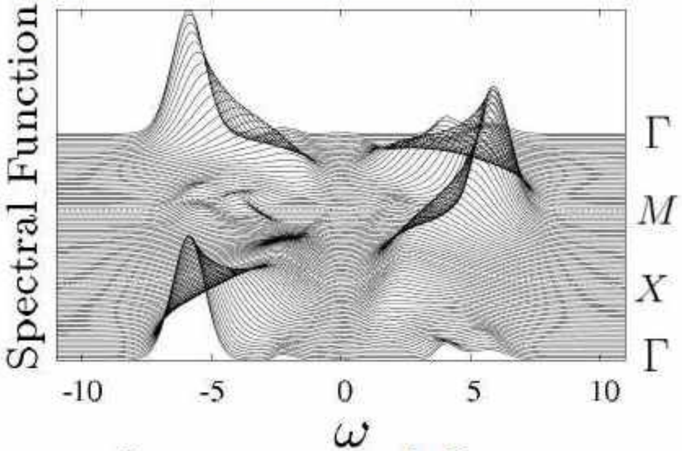
2d-Hubbard: Spectral Function

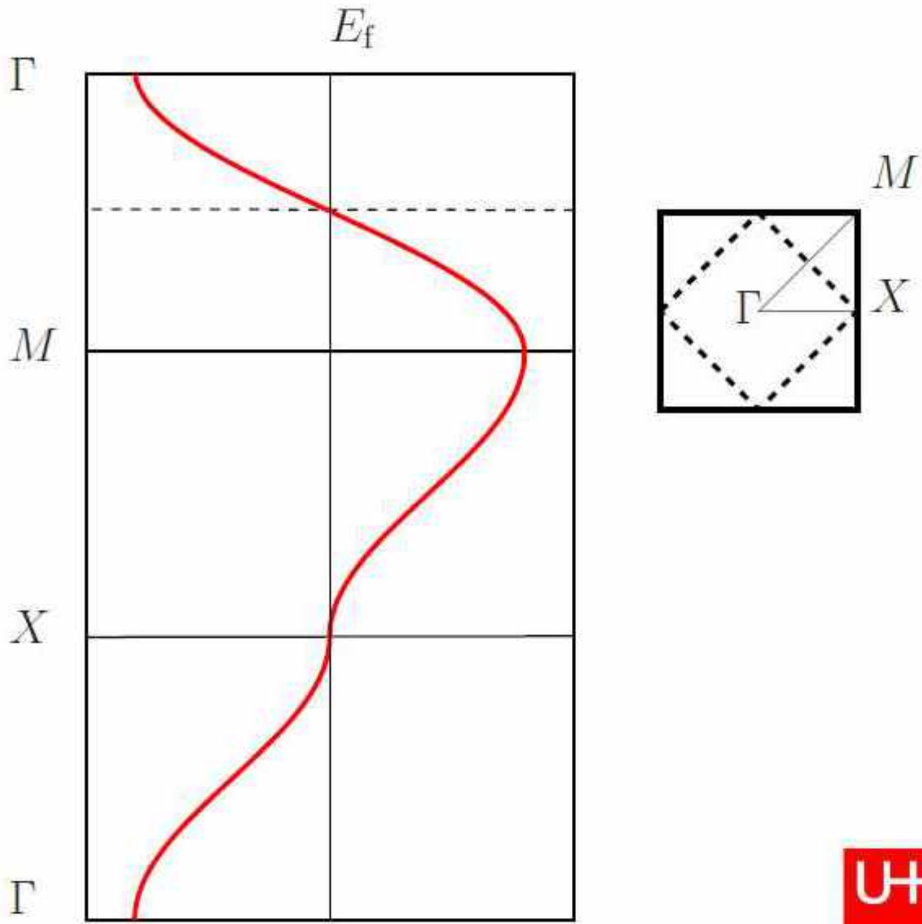
paramagnetic calculation $U/t = 8$, $T/t = 0.235$

DMFT



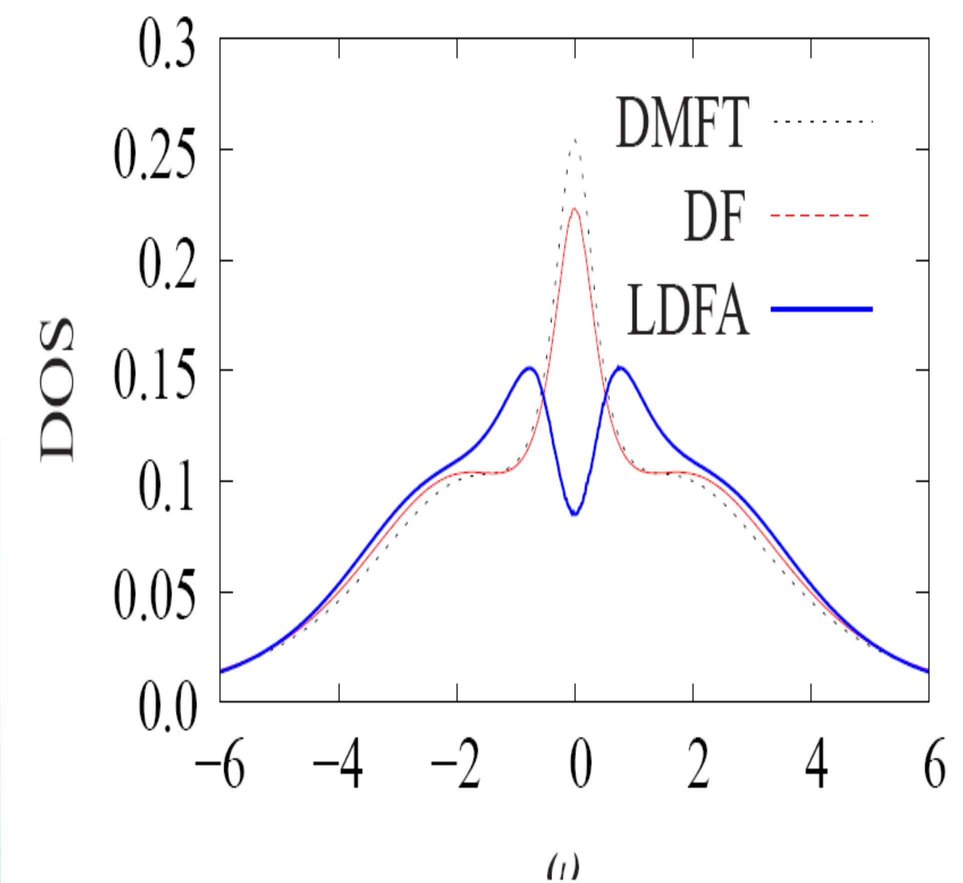
Dual Fermion $\Sigma^{d} =$ 

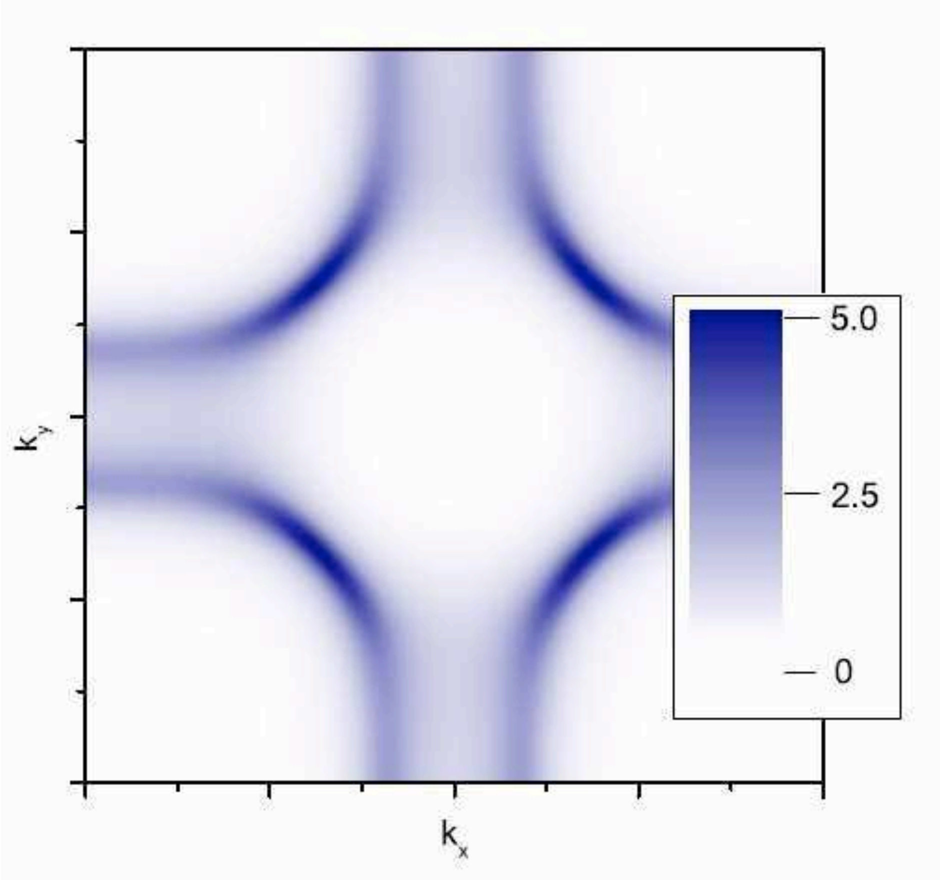




- Strong modifications through AF short-range correlations

Pseudogap in HTSC: dual fermions



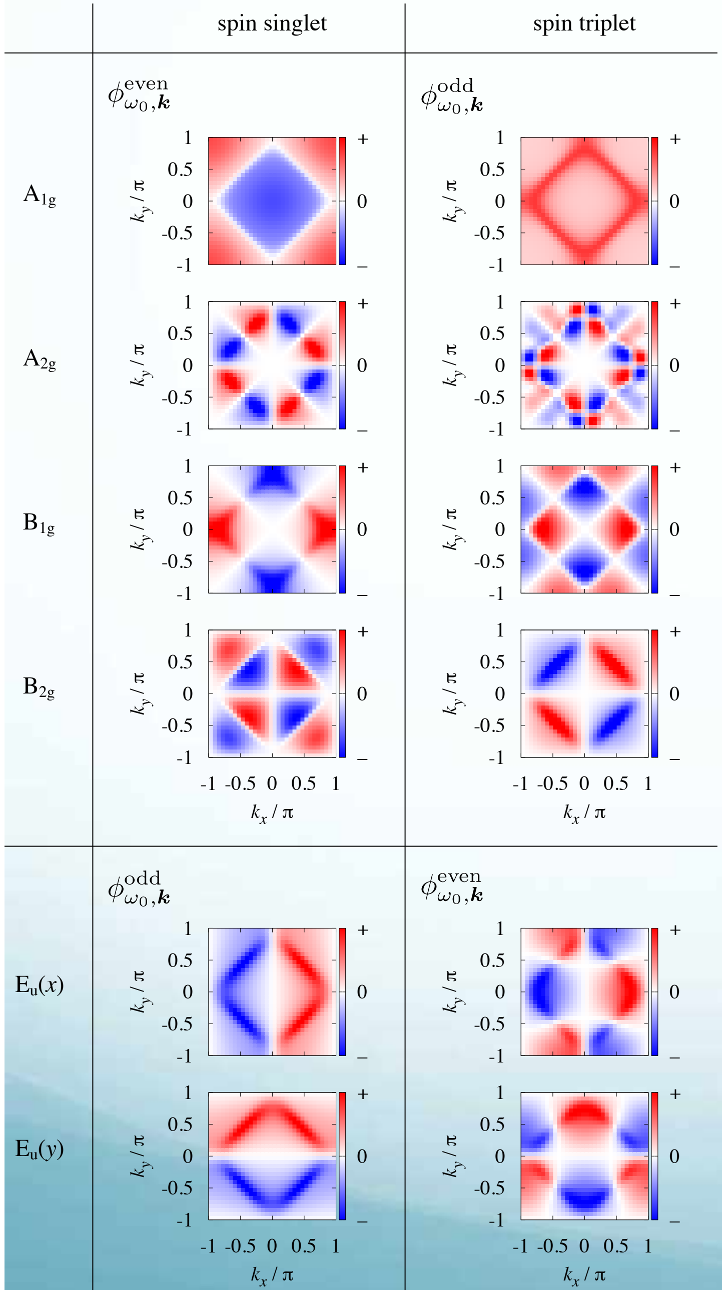


n=1

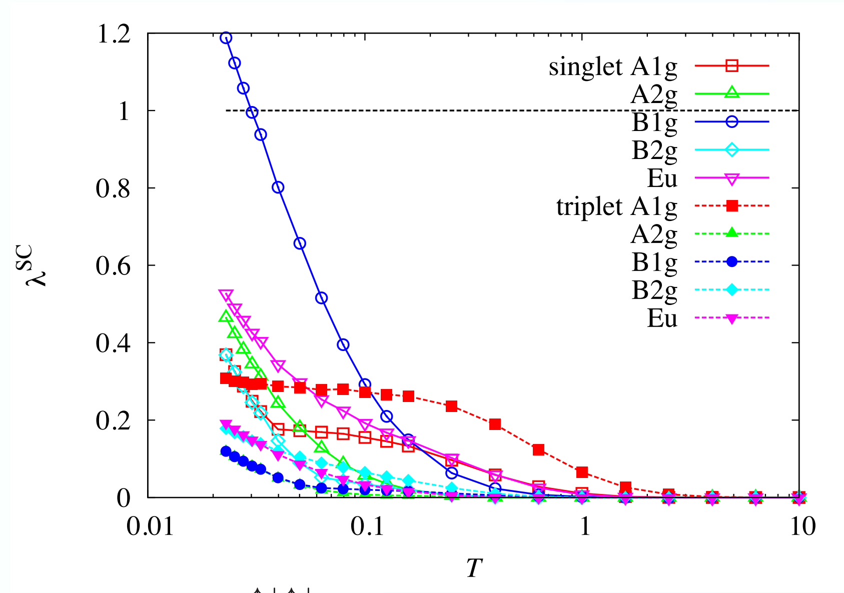
FS, n=0.85

2d: U=W=2

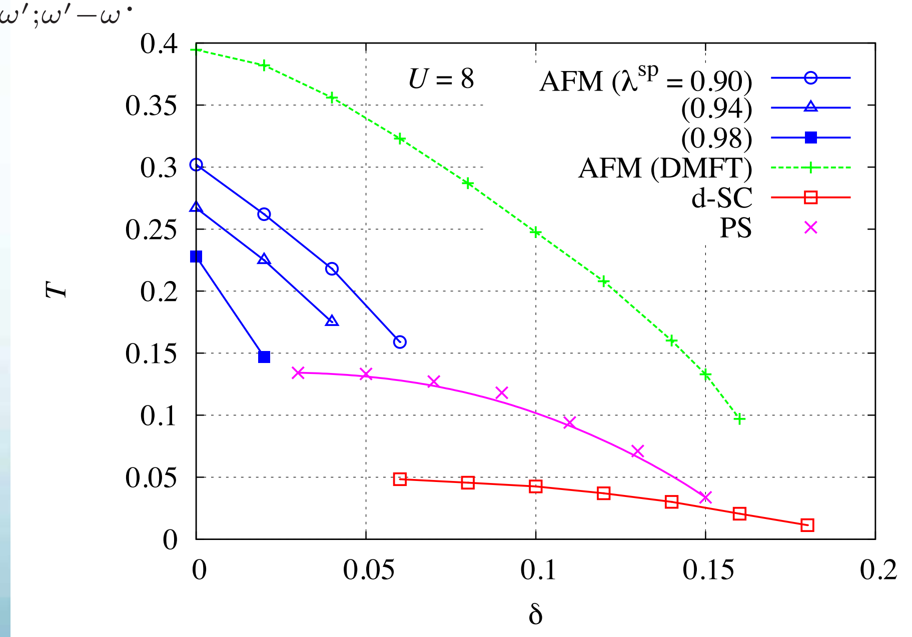
DF: AFM and SC instabilities



U=8
δ=0.15



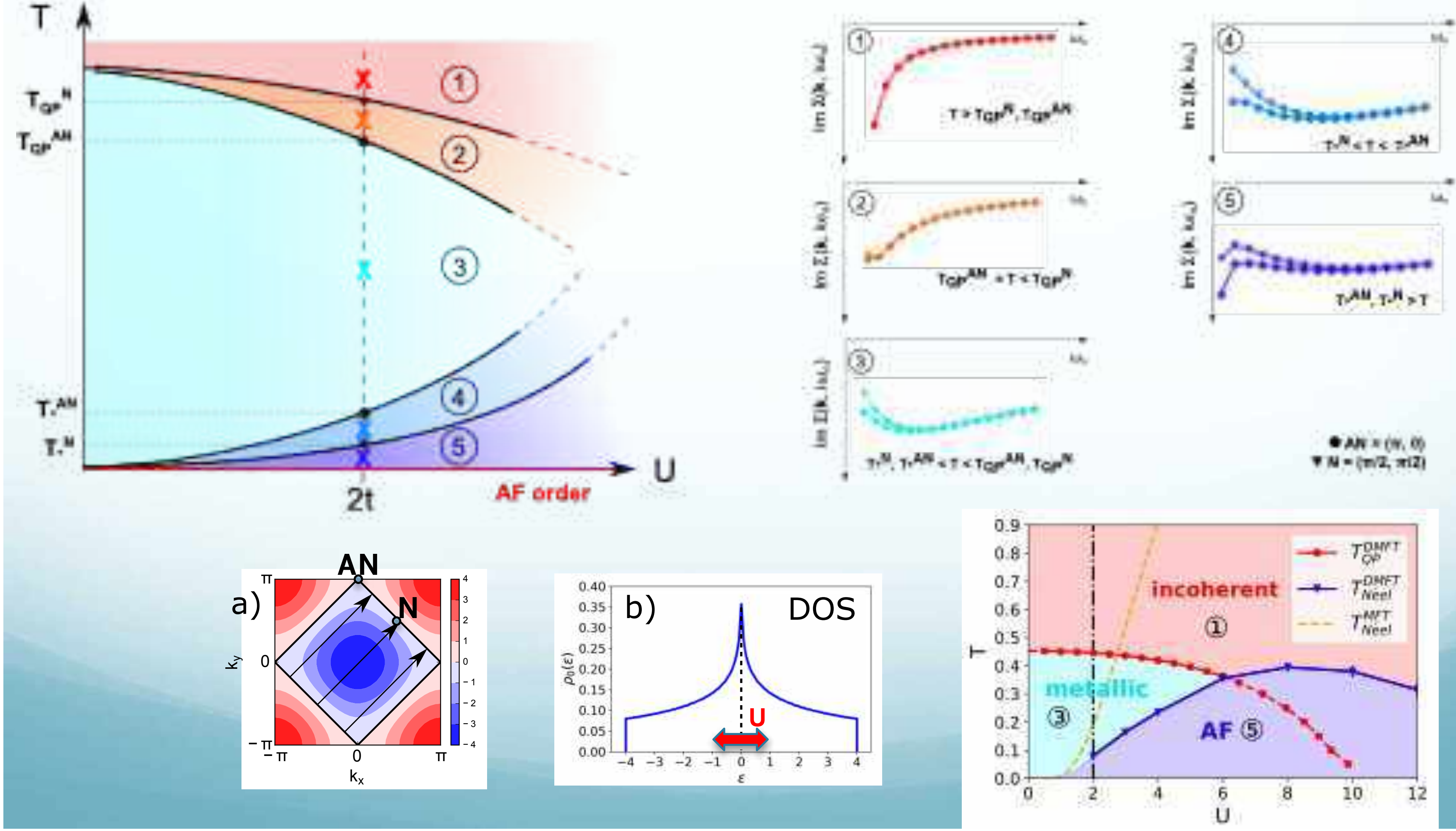
$$\Gamma^{\mathrm{pp}}_{kk'} = -\Gamma^{\uparrow\downarrow\downarrow\uparrow}_{\omega,-\omega';\omega'-\omega,\boldsymbol{k}'-\boldsymbol{k}} + \Gamma^{\uparrow\downarrow\uparrow\downarrow}_{\omega,\omega';-\omega-\omega',-\boldsymbol{k}-\boldsymbol{k}'} + \gamma^{\uparrow\downarrow\downarrow\uparrow}_{\omega,-\omega';\omega'-\omega}.$$



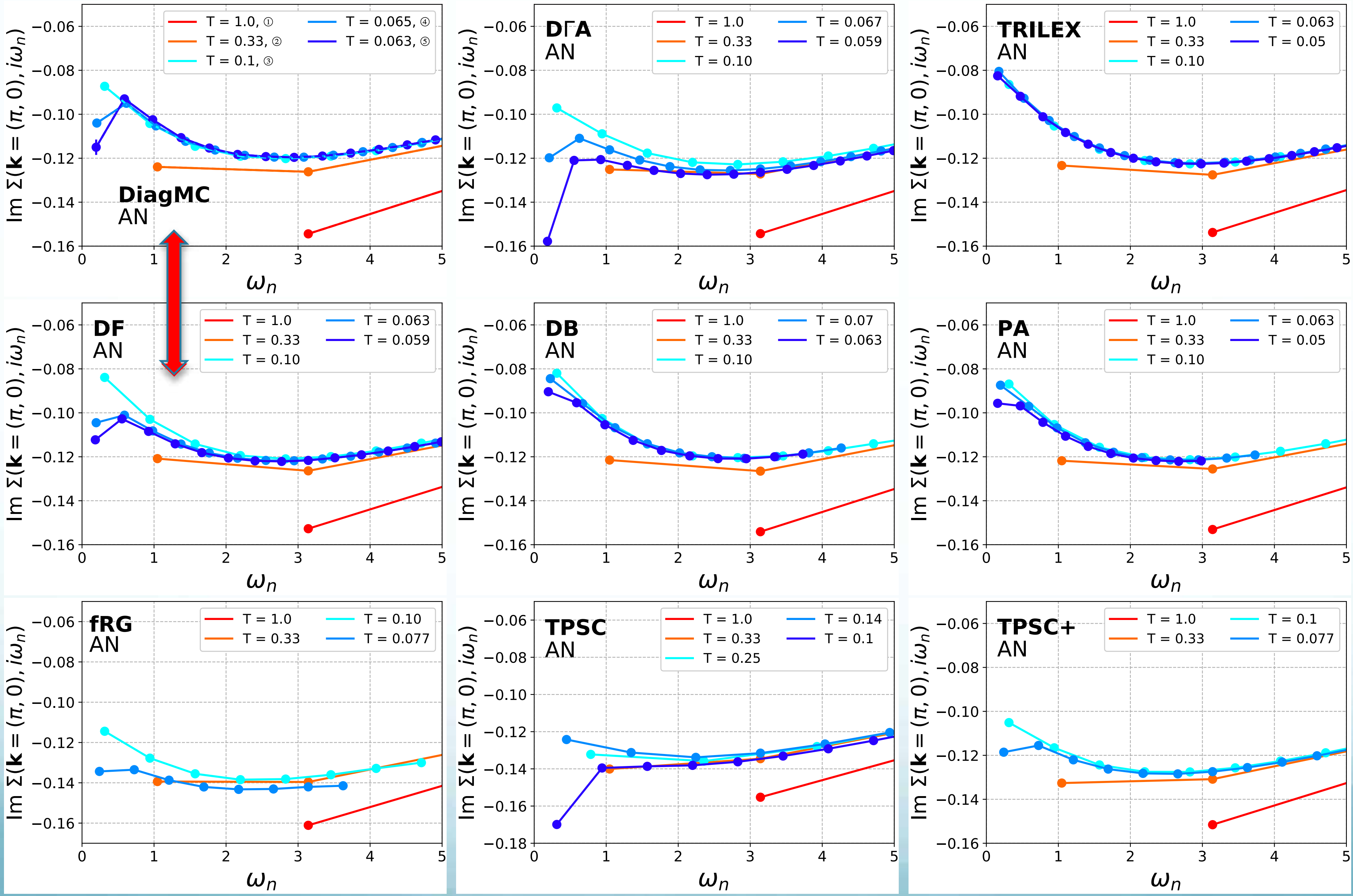
J. Otsuki, H. Hafermann, and A.L. Phys. Rev. B 90, 235132 (2014)

Test: Tracking the Footprints of Spin Fluctuations: A Multi-Method, Multi-Messenger Study of the Two-Dimensional Hubbard Model

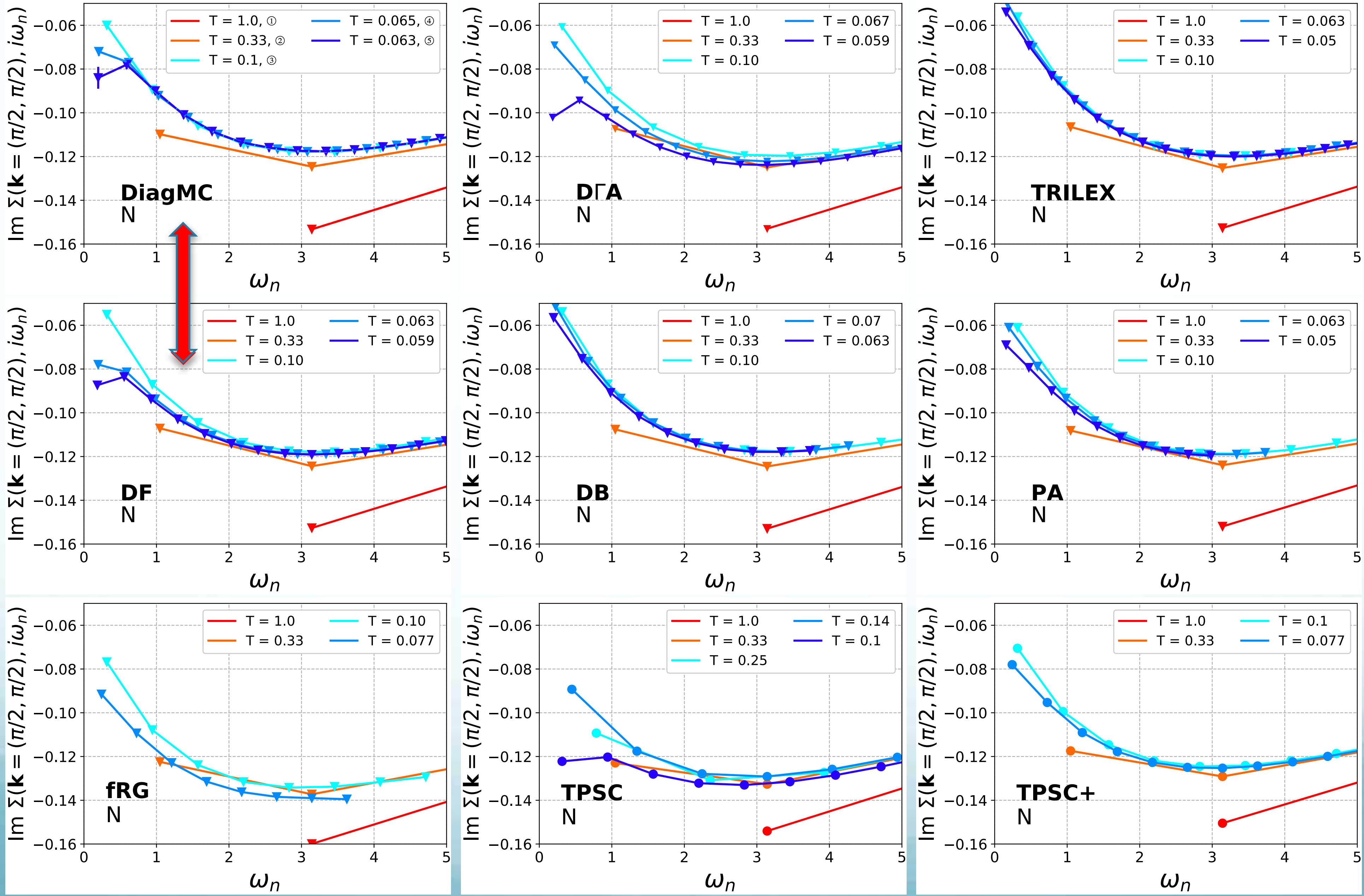
Thomas Schäfer[a,b],* Nils Wentzell[c], Fedor Šimkovic IV[a,b], Yuan-Yao He[c,d],
Cornelia Hille[e], Marcel Klett[e], Christian J. Eckhardt[f,g], Behnam Arzhang[h], Viktor Harkov[i,j],
François-Marie Le Régent[b], Alfred Kirsch[b], Yan Wang[k], Aaram J. Kim[l], Evgeny Kozik[l], Evgeny A. Stepanov[i],
Anna Kauch[f], Sabine Andergassen[e], Philipp Hansmann[m,n], Daniel Rohe[o], Yuri M. Vilk[k], James P. F. LeBlanc[h],
Shiwei Zhang[c,d], A.-M. S. Tremblay[k], Michel Ferrero[a,b], Olivier Parcollet[c,p], and Antoine Georges[a,b,c,q]



Comparisson with other methods: AN

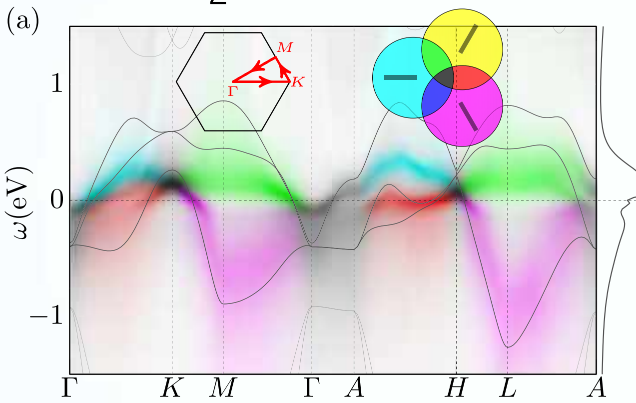


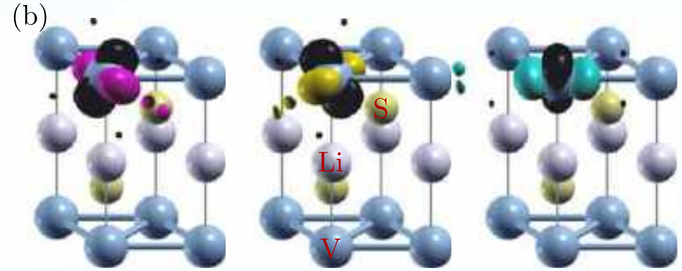
Comparisson with other methods: N

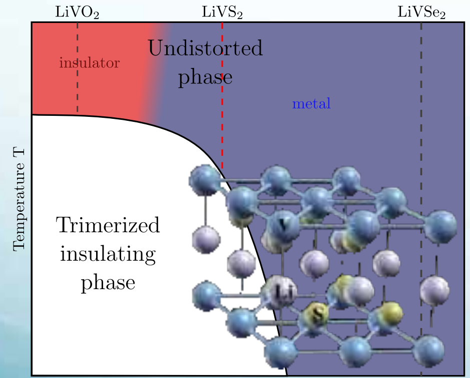


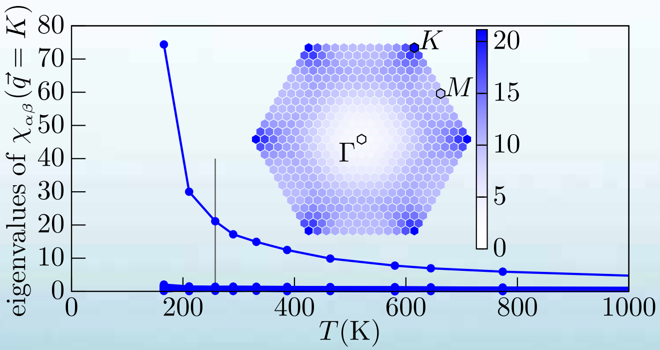
Realistic systems

$LiVS_2$

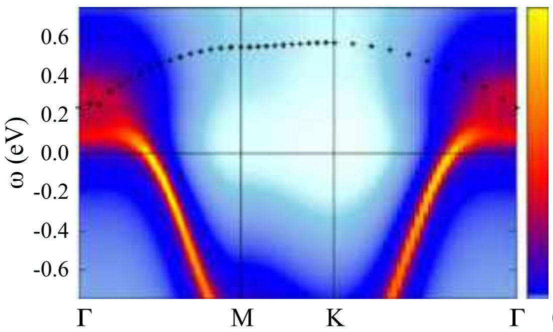


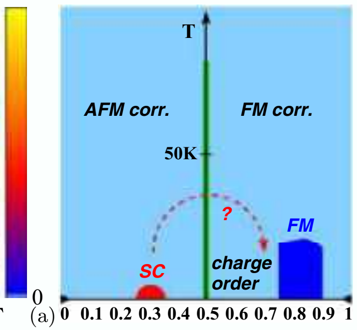


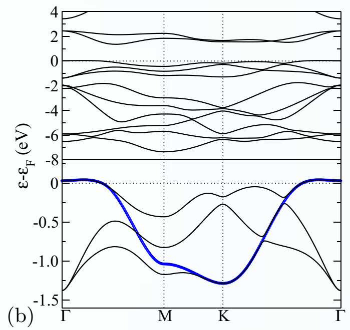


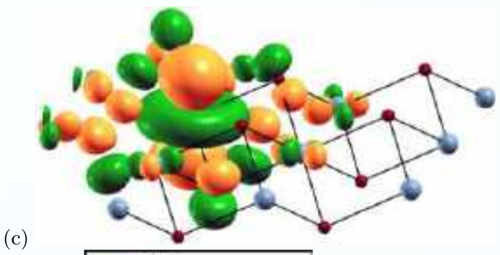


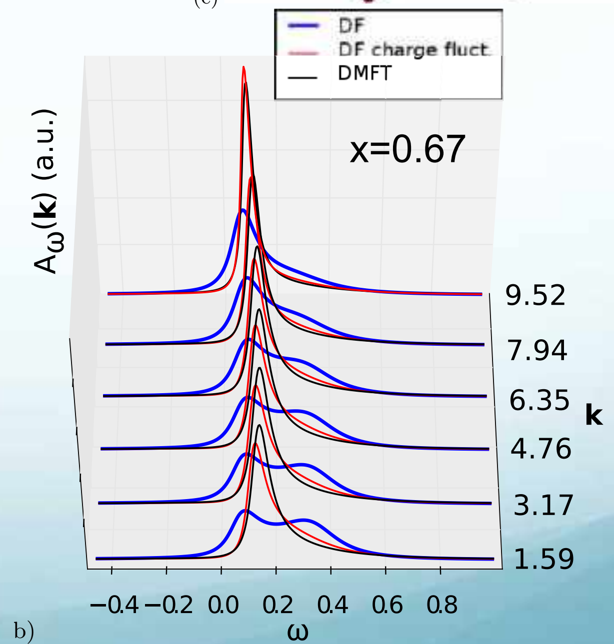
Na_xCoO_2











L. Boehnke, A.L., M. Katsnelson, and F. Lechermann
Phys. Rev. B **102**, 115118 (2020)

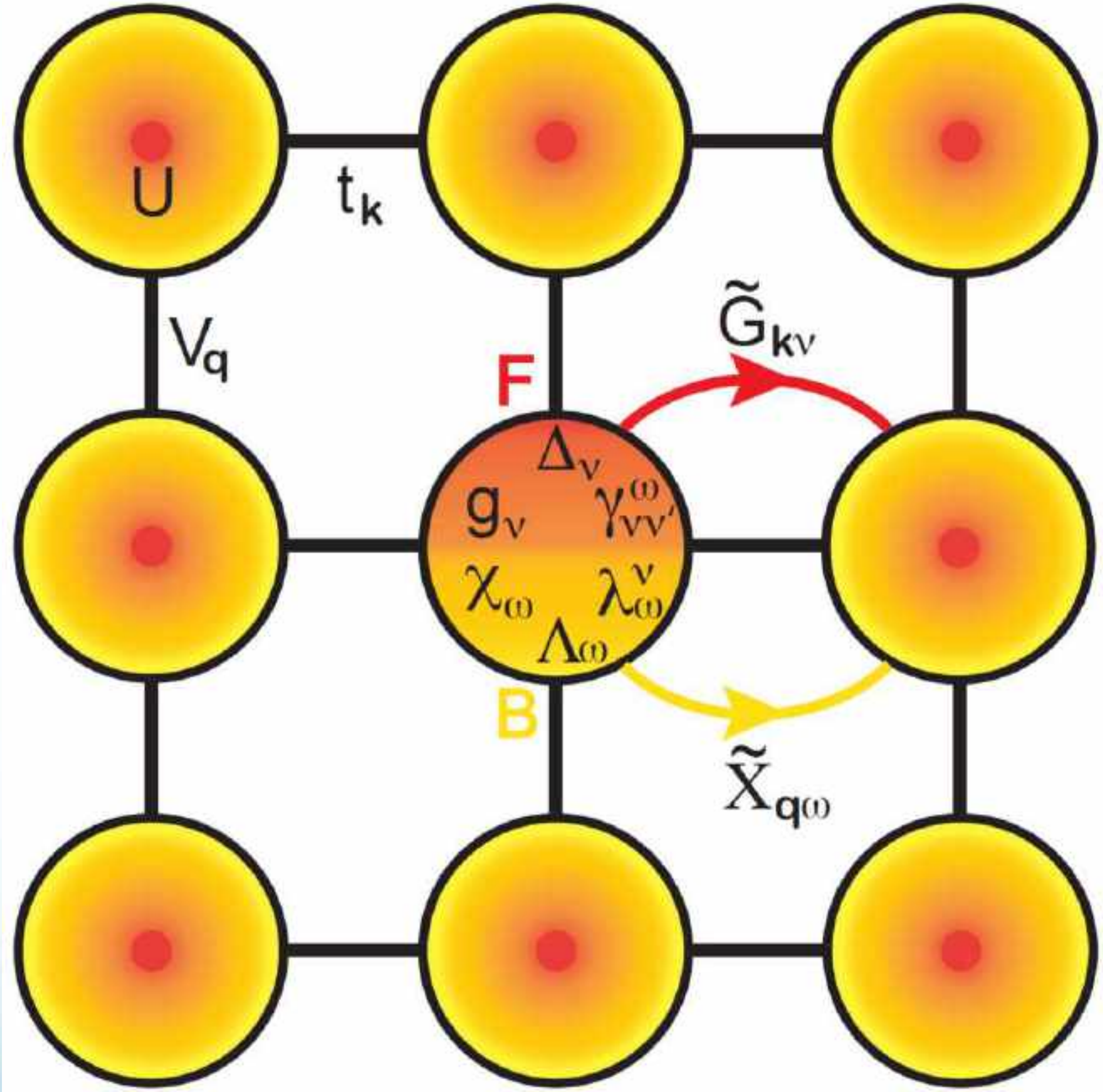
A. Wilhelm F. Lechermann, et al.
Phys. Rev. B **91**, 155114 (2015)

Non-local Interactions: Dual Boson

HTSC

$\Lambda_\omega \sim$

$J_{\tau\tau'} \vec{S}_\tau \cdot \vec{S}_{\tau'}$



A. Rubtsov, M. Katsnelson, A.L., Ann. Phys. **327**, 1320 (2012)
G. Rohringer, et al, Rev. Mod. Phys. **90**, 025003 (2018)

Summary

- Path-Integral DF-perturbation based on DMFT as the reference system
- DMFT corresponds to the Zero-order DF-approximation or „free dual fermions“
- DF-theory is in a good agreement with QMC results