Path Integrals and Dual Fermions

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In collaboration with

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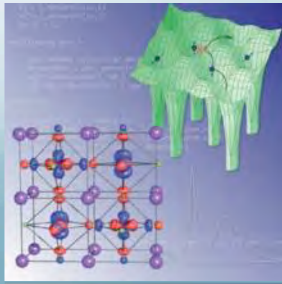
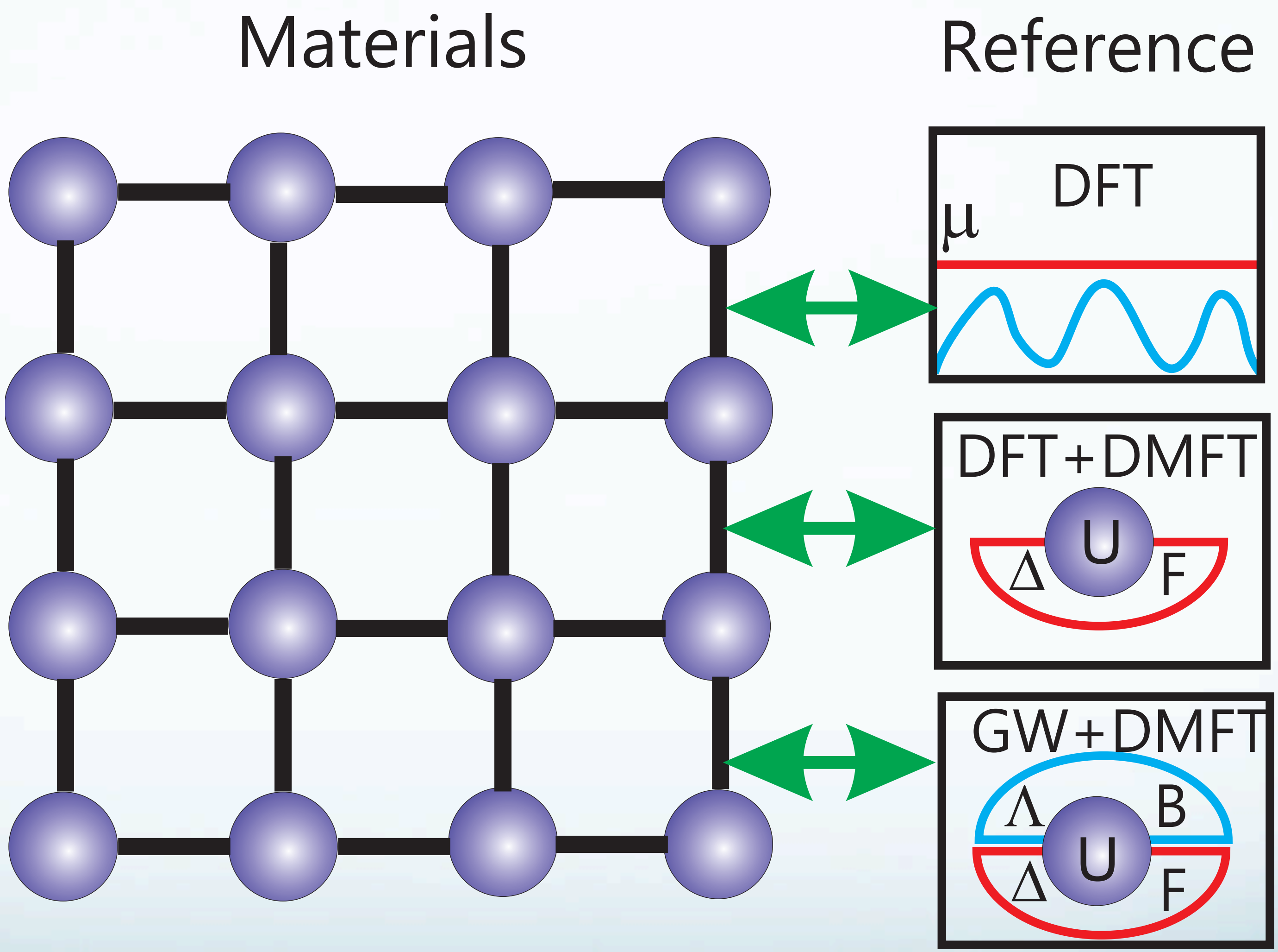


Outline

- Introduction: Reference System
- Path integral for fermions
- Functional approach: Route to fluctuations
- Dual Fermion approach: beyond DMFT
- Solving quantum impurity problems
- Non-Local screened interactions: cRPA
- Dual Boson approach for non-local interactions
- Plasmons in Correlated Materials
- Outlook

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

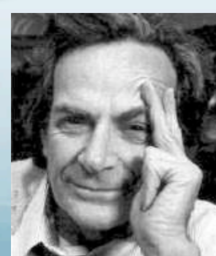
$$\left(-\frac{1}{2}\Delta + V_{eff}(\vec{r})\right)\psi(\vec{r}) = \varepsilon\psi(\vec{r})$$

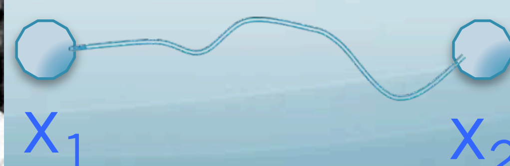
2-Q

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

3-PI

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





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

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

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

Pauli principle

$$\hat{c}_i^+ \hat{c}_i \left|n\right\rangle = n_i \left|n\right\rangle$$

$$\hat{c}_i^2 = (\hat{c}_i^+)^2 = 0\,.$$

Fermionic coherent states $|c\rangle$

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

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

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

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

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

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

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

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

„Minus“ fermionic sign deu to commutations:

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

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

Partition function

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

N-slices Trotter decomposition $[0, \beta)$

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

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 → ∞)

$$\begin{aligned} \Delta\tau \sum_{n=1}^{N} ... &\mapsto \int_0^\beta d\tau ... \\ \frac{c_n - c_{n-1}}{\Delta\tau} &\mapsto \partial_\tau \\ \Pi_{n=0}^{N-1} dc_n^* dc_n &\mapsto D[c^*, c] \end{aligned}$$

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

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

Gaussian path integral

Non-interacting "quadratic" fermionic action

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

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: $c^*Mc-c^*J-J^*c=\left(c^*-J^*M^{-1}\right)M\left(c-M^{-1}J\right)-J^*M^{-1}J$

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

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

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

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:

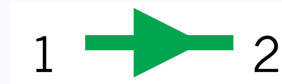
$$
\begin{aligned}
t_{12} &= \int d\mathbf{r}\, \phi_1^*(\mathbf{r}) \left(-\frac{1}{2}\nabla^2 + V(\mathbf{r}) - \mu\right) \phi_2(\mathbf{r}) \\
U_{1234} &= \int d\mathbf{r} \int d\mathbf{r}'\, \phi_1^*(\mathbf{r})\phi_2^*(\mathbf{r}')\, U(\mathbf{r} - \mathbf{r}')\, \phi_3(\mathbf{r})\phi_4(\mathbf{r}')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

Shot notation:

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

One- and Two-particle Green Functions

One-particle Green function



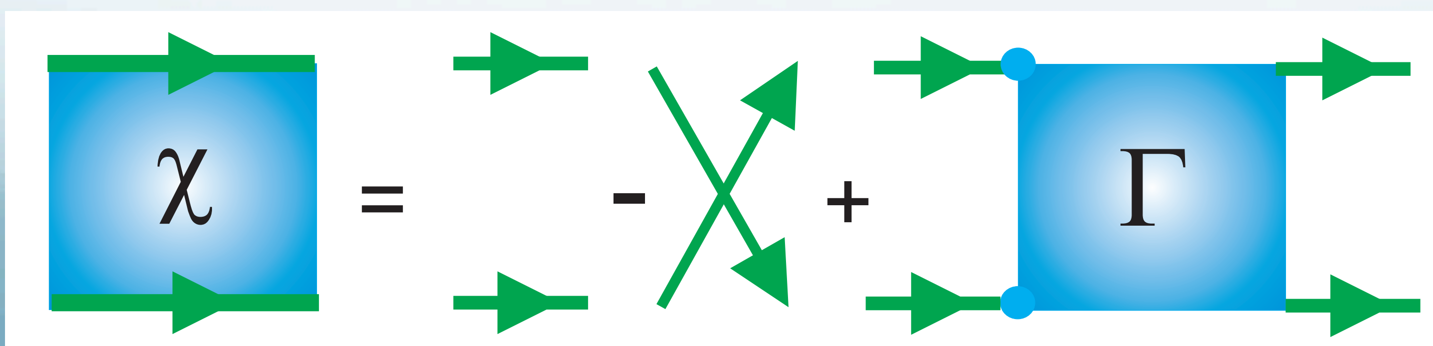
$$G_{12} = -\langle c_1 c_2^* \rangle_S = -\frac{1}{Z} \int \mathcal{D}[c^*, c]\, c_1 c_2^*\, e^{-S}$$

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:

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



Baym-Kadanoff functional

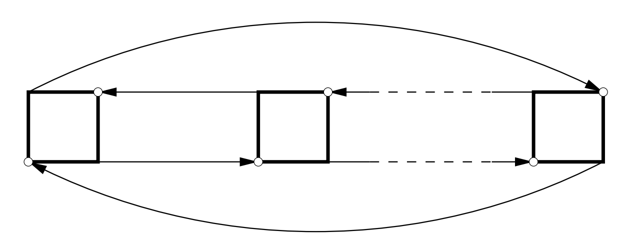
Source term
$$S[J] = S + \sum_{ij} c_i^* J_{ij} c_j$$

Partition function and Free-energy:
$$Z[J] = e^{-F[J]} = \int \mathcal{D}[c^*, c]\, e^{-S[J]}$$

Legendre transforming from J to G:
$$F[G] = F[J] - \mathrm{Tr}(JG)$$
$$G_{12} = \frac{1}{Z[J]} \frac{\delta Z[J]}{\delta J_{12}}\bigg|_{J=0} = \frac{\delta F[J]}{\delta J_{12}}\bigg|_{J=0}$$

Decomposition into the single particle part and correlated part
$$F[G] = \mathrm{Tr}\ln G - \mathrm{Tr}\,(\Sigma G) + \Phi[G]$$

$$\Phi[G] = \sum_i$$



Baym-Kadanoff Functional

$$F[G] = -Tr\ln[-(G_0^{-1} - \Sigma[G])] - Tr(\Sigma[G]G) + \Phi[G]$$

Exact representation of Φ: $V^{\alpha}_{ee} = \alpha\, V_{ee}$

$$\Phi = \frac{1}{2}\int_0^1 d\alpha Tr[V_{ee}^{\alpha} < \psi^{+}\psi^{+}\psi\psi >]$$

Different Functionals:

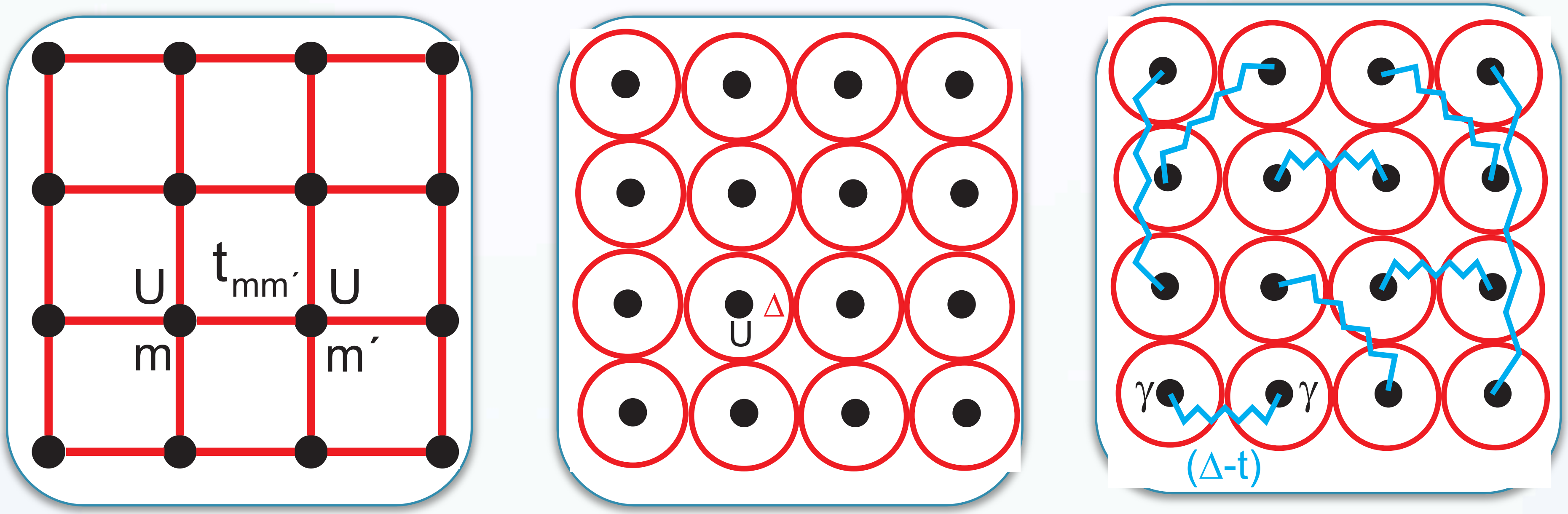
DFT:	$G = \rho$	$J = V = V_h + V_{xc}$
DMFT:	$G = G(i\omega)$	$J = \Sigma_{loc}(i\omega)$
BKF:	$G = G(k, i\omega)$	$J = \Sigma(k, i\omega)$

Functionals: MFT- DFT- DMFT-BK

G. Kotliar et. al. RMP (2006), A. Georges (2004)

- Weiss Mean-Field Theory (MFT) of classical magnets
- Kohn Density Functional Theory (DFT) of inhomogeneous electron gas in solids
- Dynamical Mean-Field Theory (DMFT) of strongly correlated electron systems
- Baym-Kadanoff Functional

How to find DMFT-functional?



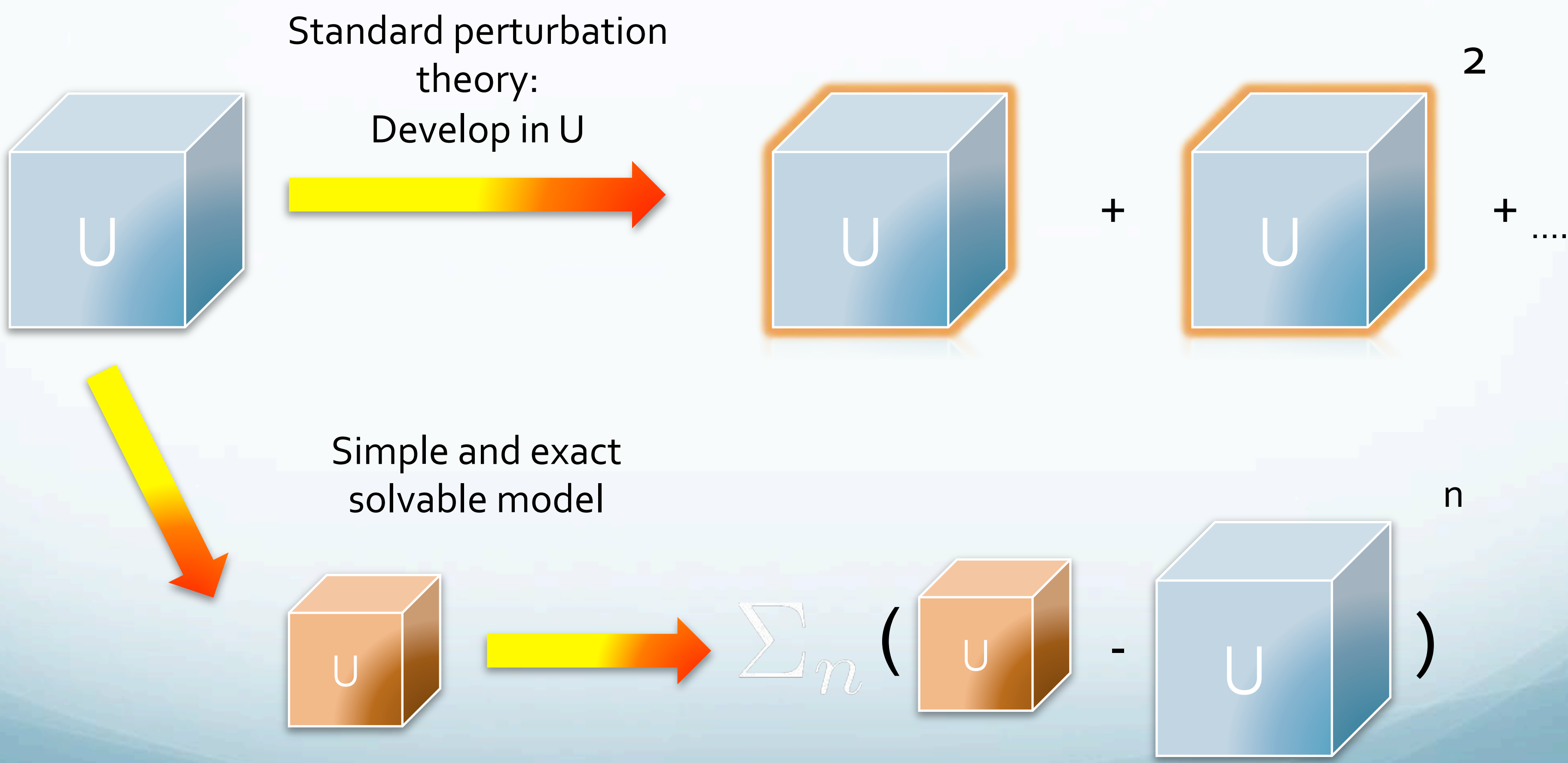
Dual Fermions: Basic

Start from
Correlated Lattice

Find the optimal
Reference System
Bath hybridization

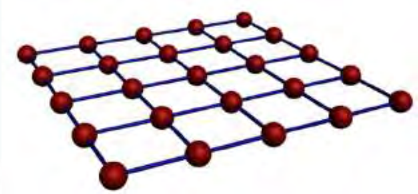
Expand around
DMFT solution

Superperturbation



Dual Fermion scheme

General Lattice Action $H = h + U$

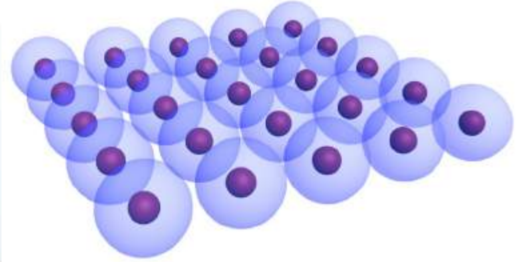


$$S[c^*, c] = \sum_{\omega k m m' \sigma} \left[h_k^{mm'} - (i\omega + \mu) 1 \right] c^*_{\omega k m \sigma} c_{\omega k m' \sigma} + \frac{1}{4} \sum_{i\{m,\sigma\}} \int_0^\beta U_{1234} c_1^* c_2^* c_3 c_4 d\tau$$

Reference system: Local Action with hybridization Δ_ω

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

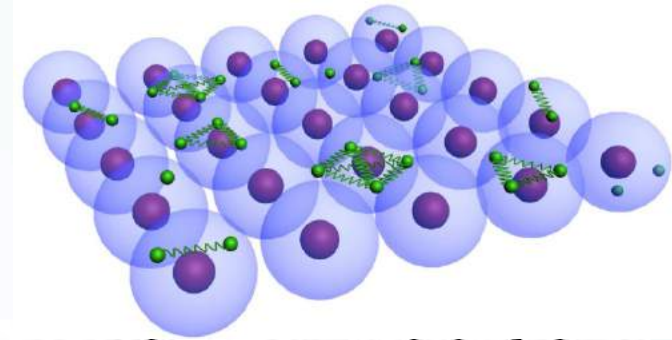
Lattice-Impurity connection:



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

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

Dual Transformation



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

new Action:

$$S_d[f^*,f] = -\sum_{k\omega} \tilde{\mathcal{G}}_{k\omega}^{-1} f_{k\omega}^* f_{k\omega} + \frac{1}{4}\sum_{1234} \gamma_{1234}^{(4)} f_1^* f_2^* f_4 f_3 + \ldots$$

Diagramatic:

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

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

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

Dual Fermion Action: Details

Lattice - dual action

$$S[c^*, c, f^*, f] = \sum_i S_{\text{site},i} + \sum_{\omega\mathbf{k}\,\alpha\beta} f^*_{\omega\mathbf{k}\alpha}[g_\omega^{-1}\left(\Delta_\omega - t_\mathbf{k}\right)^{-1} g_\omega^{-1}]_{\alpha\beta} f_{\omega\mathbf{k}\beta}$$

$$S_{\text{site},i}[c_i^*, c_i, f_i^*, f_i] = S_{\text{loc}}[c_i^*, c_i] + \sum_{\alpha\beta} f^*_{\omega i\alpha}\, g^{-1}_{\omega\,\alpha\beta} c_{\omega i\beta} + c^*_{\omega i\alpha}\, g^{-1}_{\omega\,\alpha\beta} f_{\omega i\beta}$$

For each site I integrate-out c-Fermions:

$$\int \mathcal{D}[c^*, c] \exp\left(-S_{\text{site}}[c_i^*, c_i, f_i^*, f_i]\right) =$$

$$\mathcal{Z}_{\text{loc}} \exp\left(-\sum_{\omega\,\alpha\beta} f^*_{\omega i\alpha}\, g^{-1}_{\omega\,\alpha\beta} f_{\omega i\beta} - V_i[f_i^*, f_i]\right)$$

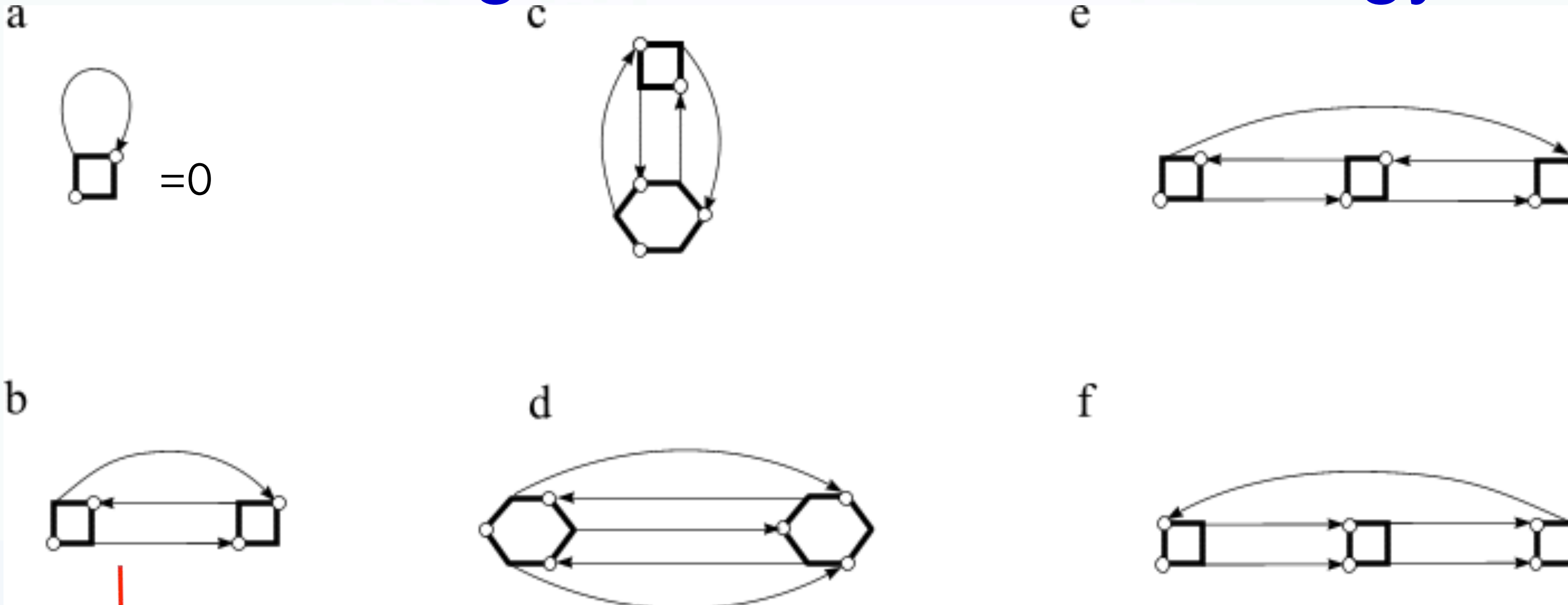
Dual potential:

$$V[f^*, f] = \frac{1}{4}\gamma_{1234} f_1^* f_2^* f_4 f_3 \; + \ldots$$

$$\gamma_{1234} = g^{-1}_{11'} g^{-1}_{22'} \left[\chi_{1'2'3'4'} - \chi^0_{1'2'3'4'}\right] g^{-1}_{3'3} g^{-1}_{4'4} \qquad \chi^0_{1234} = g_{14}g_{23} - g_{13}g_{24}$$

$$\chi^{1234} = \langle c_1 c_2 c_3^* c_4^* \rangle_{\text{loc}} = \frac{1}{\mathcal{Z}_{\text{loc}}} \int \mathcal{D}[c^*, c] c_1 c_2 c_3^* c_4^* \exp\left(-S_{\text{loc}}[c^*, c]\right)$$

Basic diagrams for dual self-energy



Lines - dual Green's function. $\tilde{G}^0_\omega(\mathbf{k}) = \left[g_\omega^{-1} + \Delta_\omega - t_\mathbf{k}\right]^{-1} - g_\omega$

$$\tilde{\Sigma}^{(b)}_{12}(\mathbf{k}) = -\frac{1}{2}\left(\frac{T}{N}\right)^2 \sum_{\mathbf{k}_1\mathbf{k}_2}\sum_{345678} \gamma_{1345}\tilde{G}_{57}(\mathbf{k}_1)\tilde{G}_{83}(\mathbf{k}_2)\tilde{G}_{46}(\mathbf{k}+\mathbf{k}_2-\mathbf{k}_1)\gamma_{6728}$$

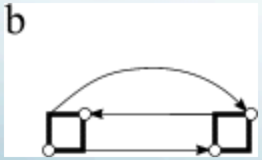
Condition for Δ and relation with DMFT

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

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

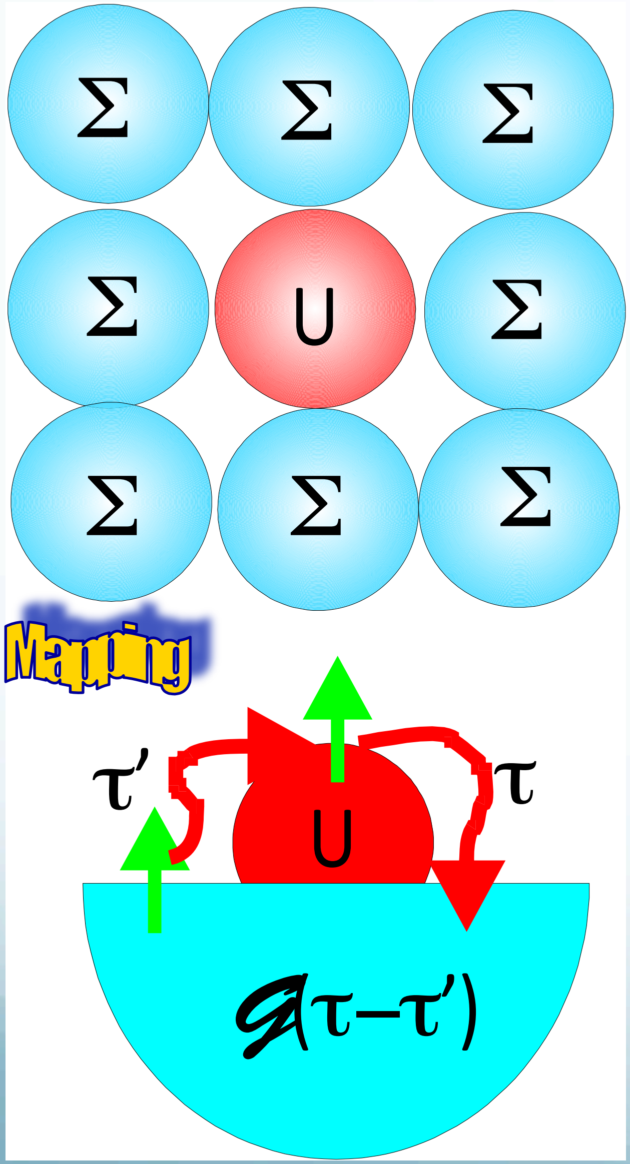
$$\frac{1}{N}\sum_{\mathbf{k}} \tilde{G}^0_\omega(\mathbf{k}) = 0 \quad \Longleftrightarrow \quad \frac{1}{N}\sum_{\mathbf{k}} G^{\mathrm{DMFT}}_\omega(\mathbf{k}) = g_\omega$$

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



$$\Sigma(k,\omega) = \Sigma_{\mathrm{DMFT}}(\omega) + \Sigma_d(k,\omega)/[1 + g\Sigma_d(k,\omega)]$$

Dynamical Mean Field Theory



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

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

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

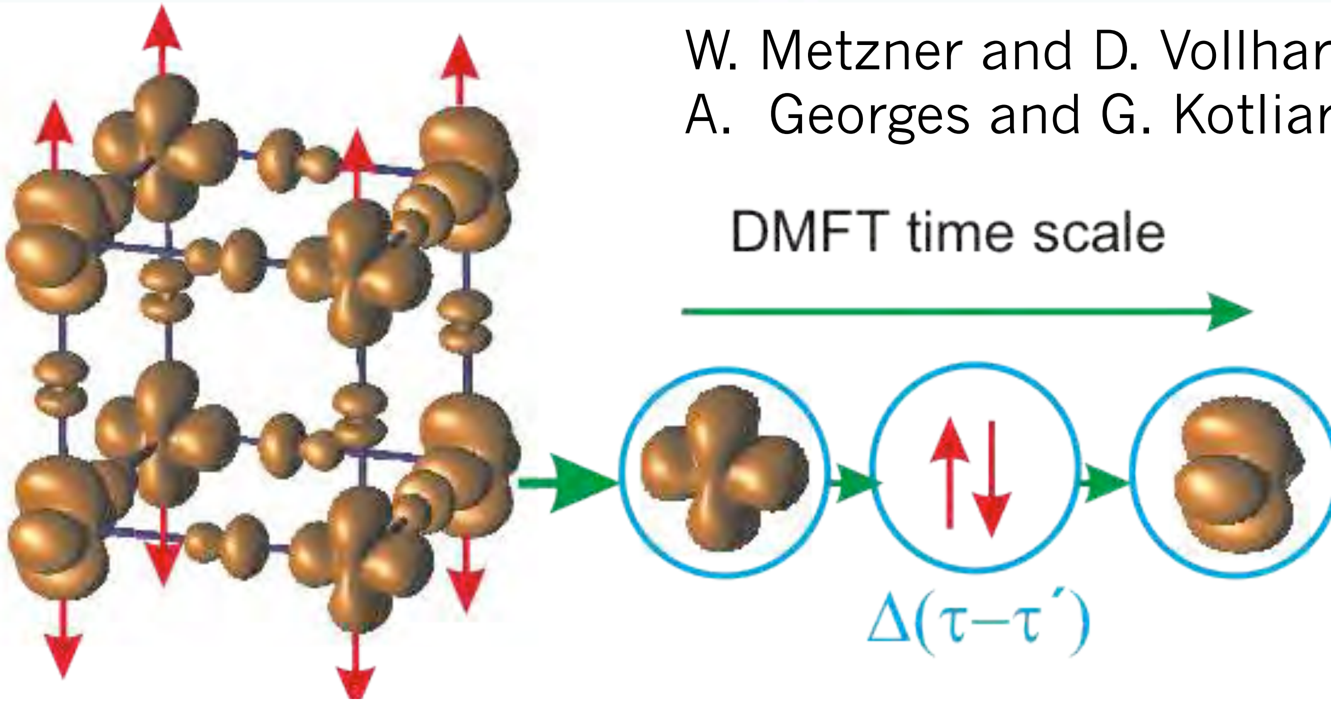
$$\hat{G}(\tau - \tau') = -\frac{1}{Z}\int D[c, c^+] c(\tau) c^+(\tau') e^{-S_{eff}}$$

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

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

Realistic DMFT: Charge+Spin+Orbital Fluctuations

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



$$S[c^*,c] = -\sum_{\omega \mathbf{k}\sigma\, mm'} c^*_{\omega\mathbf{k}\sigma m}\left[(i\omega+\mu)\mathbf{1} - t^{mm'}_{\mathbf{k}\sigma}\right] c_{\omega\mathbf{k}\sigma m'} + \sum_i S_{\mathrm{U}}[c_i^*, c_i]$$

$$S_{\mathrm{loc}}[c^*,c] = -\sum_{\omega\,\alpha\beta} c^*_{\omega\alpha}\left[(i\omega+\mu)\mathbf{1} - \Delta^{\alpha\beta}_{\omega}\right] c_{\omega\beta} + S_{\mathrm{U}}[c^*,c]$$

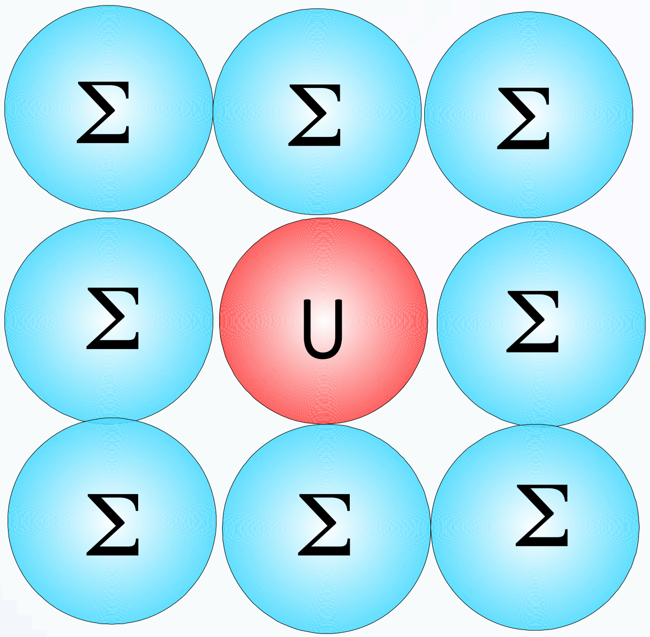
$$g_{12} = -\langle c_1 c_2^* \rangle_{\mathrm{loc}}$$

$$\sum_{\mathbf{k}} \left[g_\omega^{-1} + \Delta_\omega - t_{\mathbf{k}}\right]^{-1} = g_\omega$$

DMFT
self-consistensy

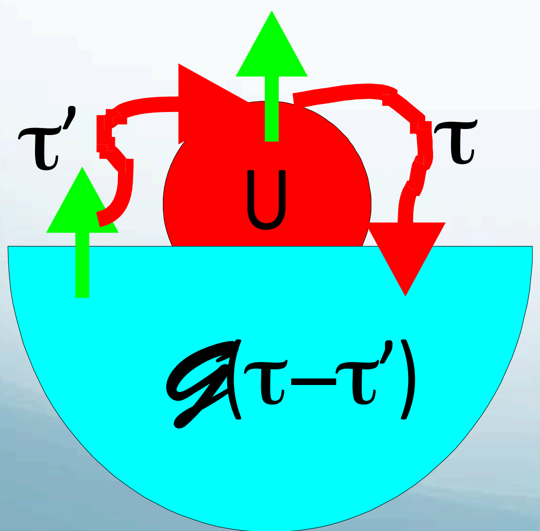
DMFT
Impurity solver
TRIQS, ALPS

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)

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

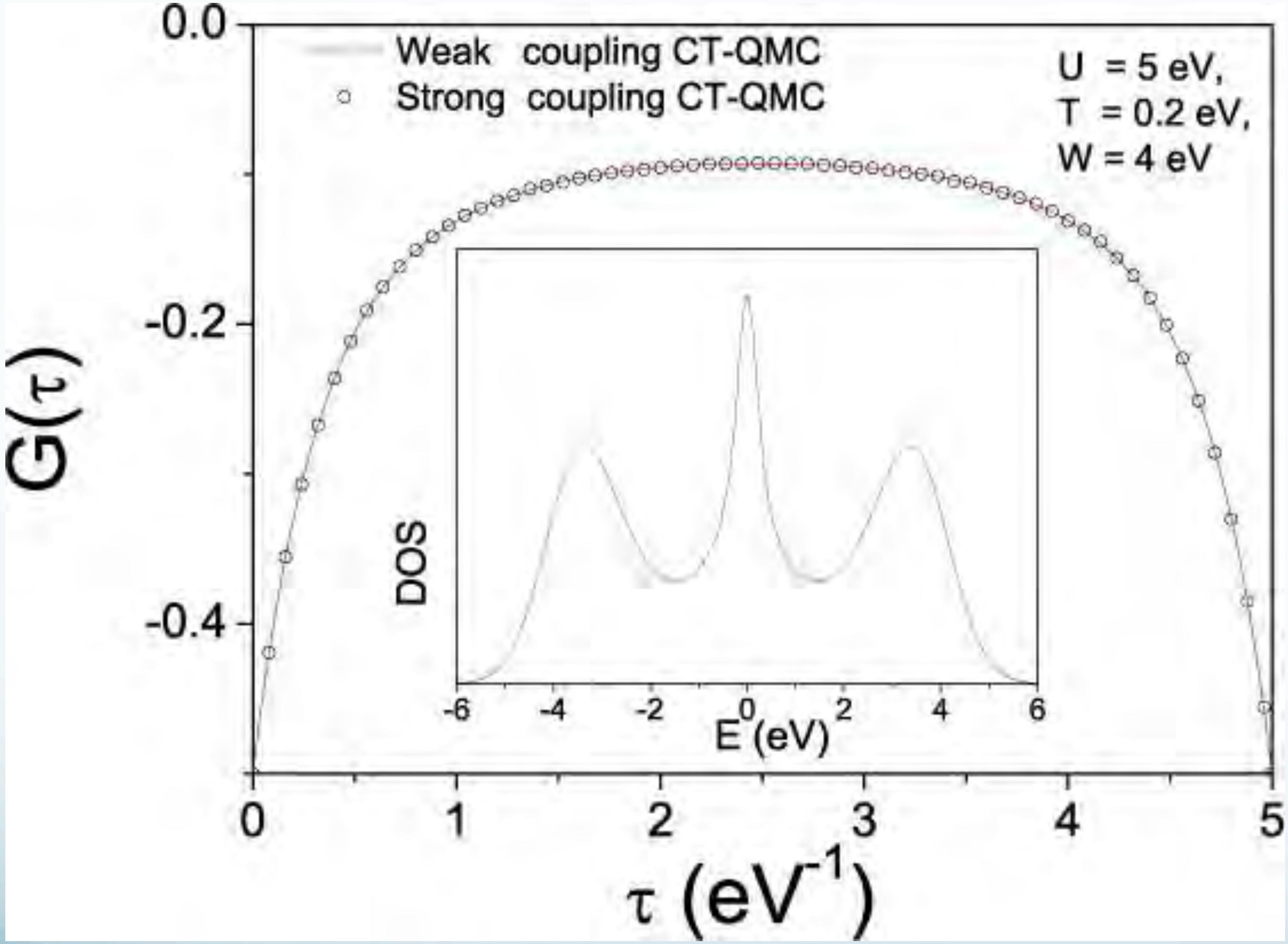
Hybridization expansion CT-HYB: P. Werner et al, PRL (2006)

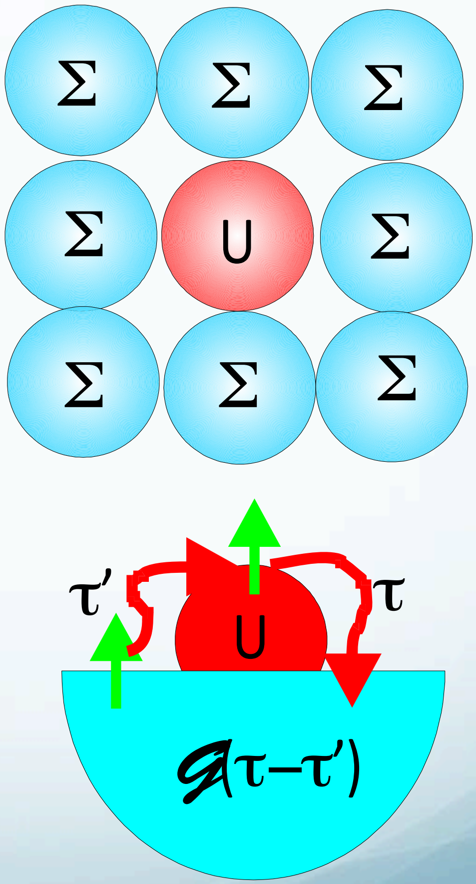
$$Z = Z_0 \sum_{k=0}^{\infty} \frac{1}{k!} Tr \left\langle c_\sigma^+(\tau)c_\sigma(\tau')\ldots c_{\sigma'}^+(\tau)c_{\sigma'}(\tau')\right\rangle_0 \det[\Delta(\tau-\tau')]$$

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

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

Comparison of different CT-QMC

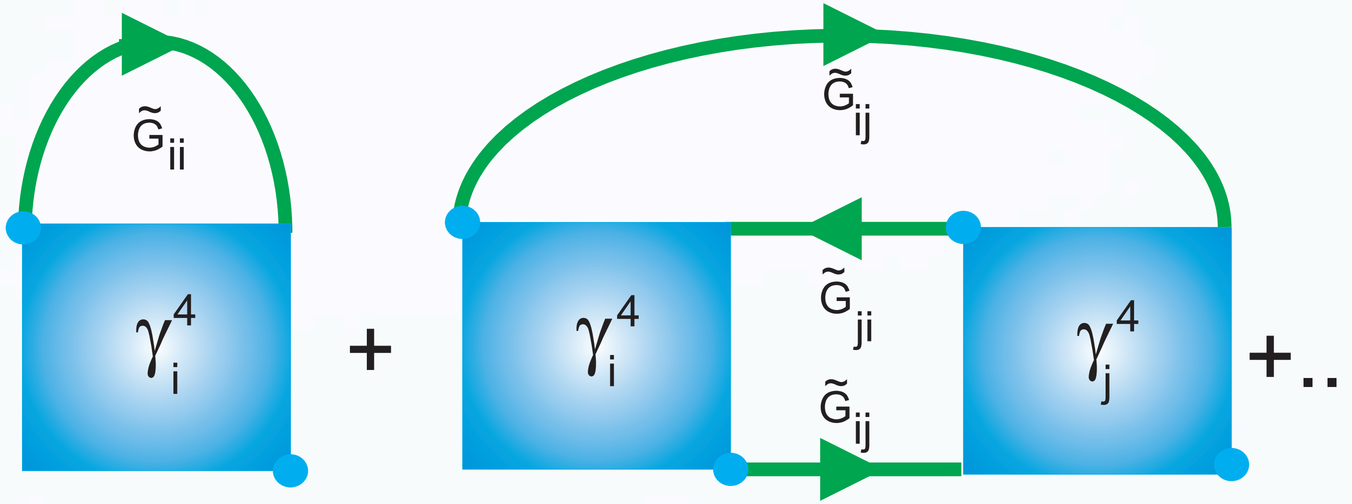




Ch. Jung, unpublished

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

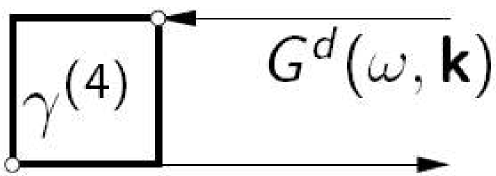
Dual Fermions: Diagrams



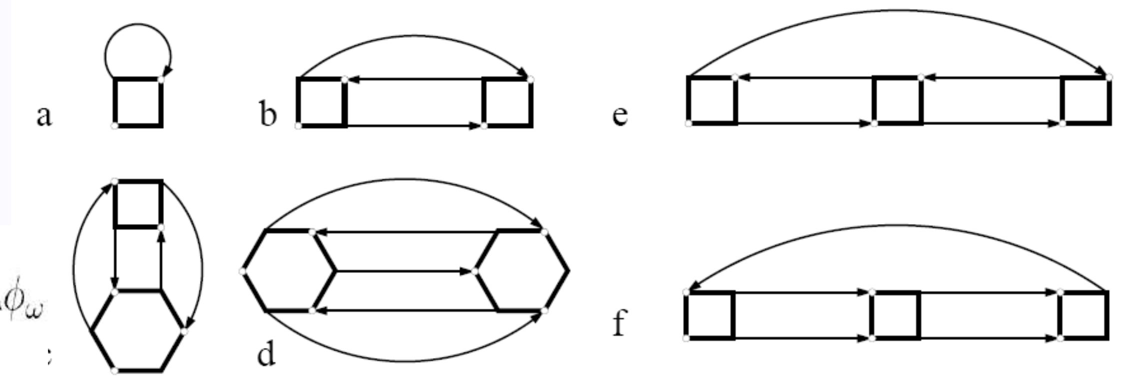
$$\tilde{\Sigma}^{(1)}_{12} = -T \sum_{34} \gamma_{1324}\, \tilde{G}^{\mathrm{loc}}_{43}$$

$$\tilde{\Sigma}^{(2)}_{12}(\mathbf{k}) = -\frac{1}{2}\left(\frac{T}{N_k}\right)^2 \sum_{\mathbf{k}_1\mathbf{k}_2} \sum_{345678} \gamma_{1345}\, \tilde{G}_{57}(\mathbf{k}_1)\, \tilde{G}_{83}(\mathbf{k}_2)\, \tilde{G}_{46}(\mathbf{k}+\mathbf{k}_2-\mathbf{k}_1)\, \gamma_{6728}$$

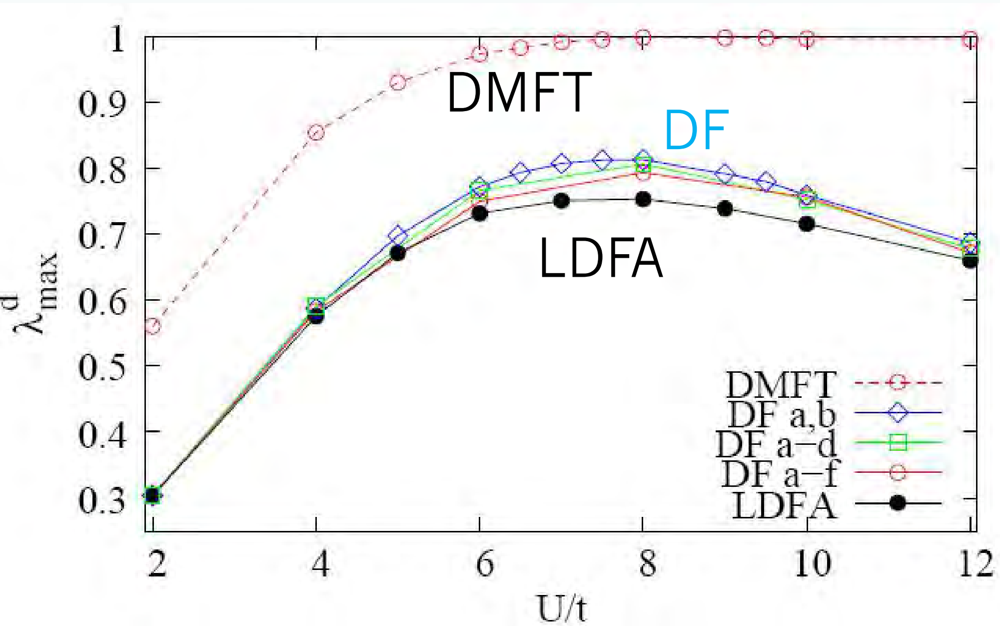
Convergence of Dual Fermions: 2d

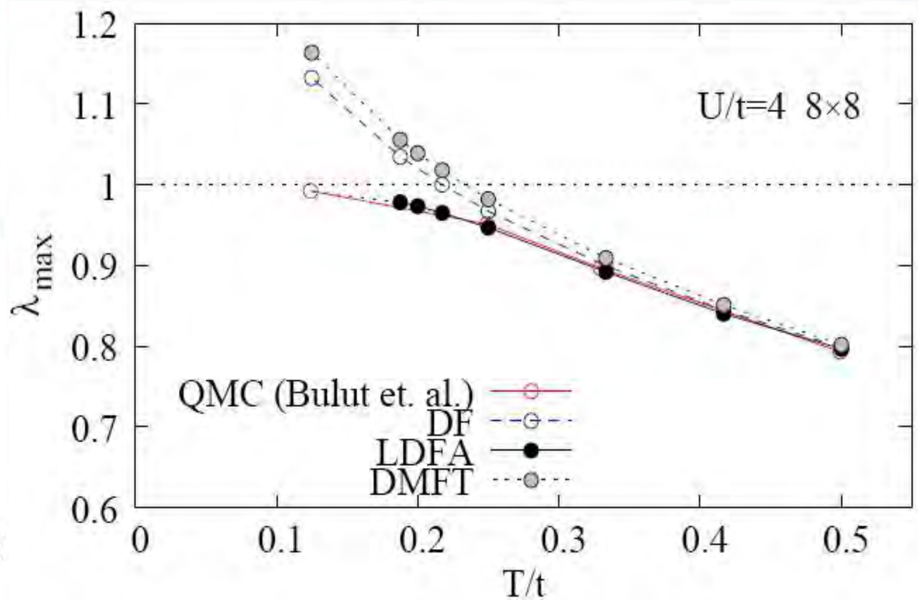


$=1$



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





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

Dual and Lattice Green's Functions

Two equivalent forms for partition function:

$$F[J^*,J;L^*,L] = \ln \mathcal{Z}_f \int \mathcal{D}[c^*,c;f^*,f] \exp\Big(-S[c^*,c;f^*,f] + J_1^* c_1 + c_2^* J_2 + L_1^* f_1 + f_2^* L_2\Big)$$

$$F[L^*,L] = \ln \tilde{\mathcal{Z}}_f \int \mathcal{D}[f^*,f] \exp\left(-S_{\mathrm{d}}[f^*,f] + L_1^* f_1 + f_2^* L_2\right)$$

Hubbard-Stratanovich transformation:

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

Relation between Green functions:

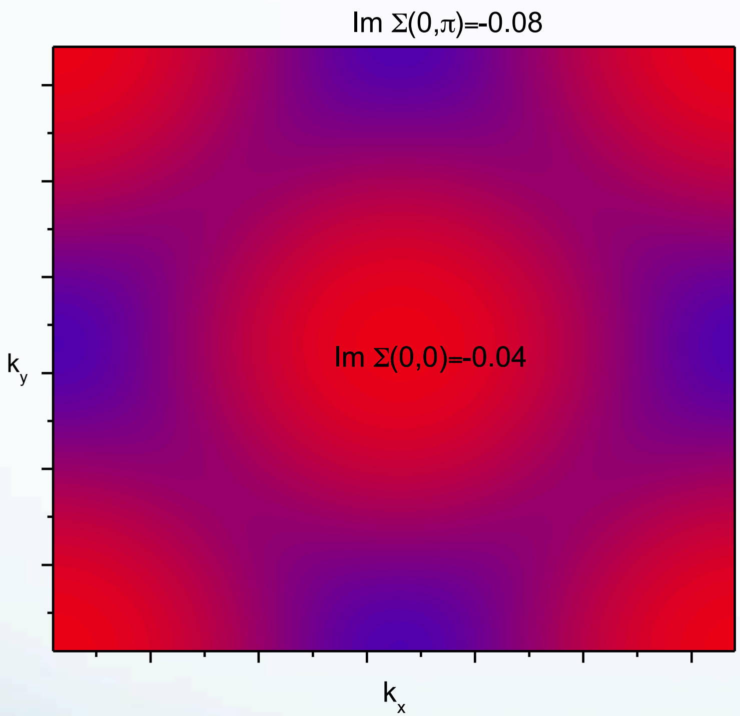
$$\tilde{G}_{12} = - \frac{\delta^2 F}{\delta L_2 \delta L_1^*}\Big|_{L^*=L=0}$$

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

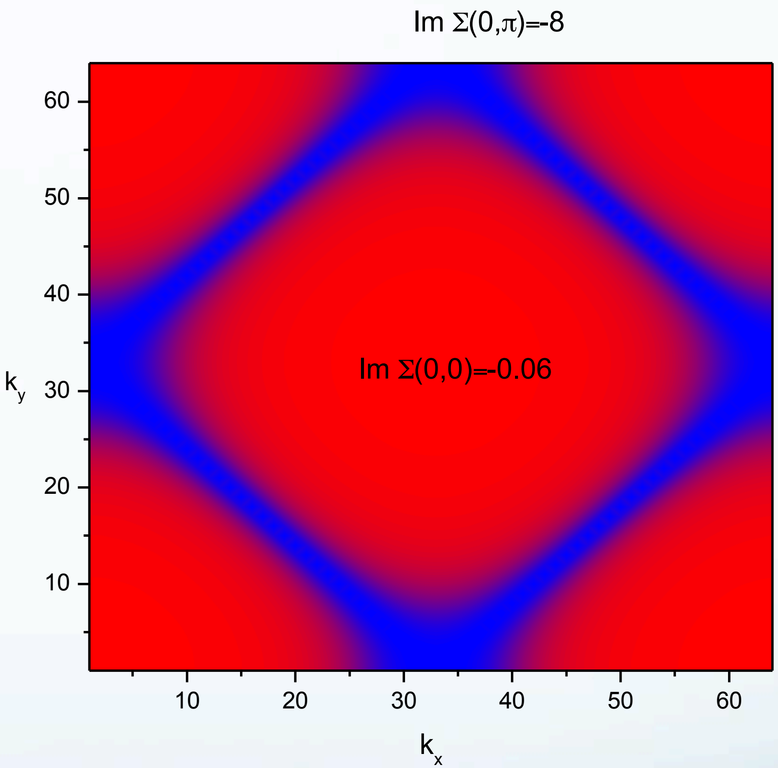
T-matrix like relations via dual self-energy

$$G_\omega(\mathbf{k}) = \left[\Big(g_\omega + g_\omega \tilde{\Sigma}_\omega(\mathbf{k}) g_\omega \Big)^{-1} + \Delta_\omega - t_k \right]^{-1}$$

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



U=1



U=2

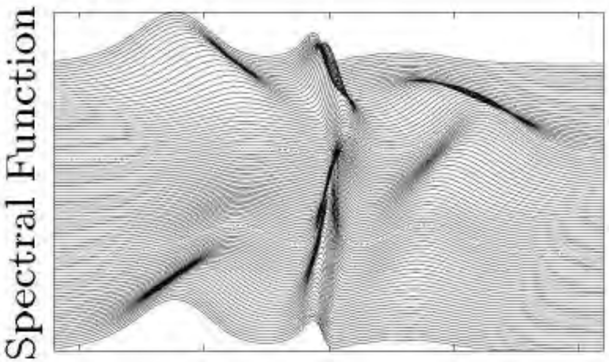
Hubbard model with $8t = 2, \beta = 20$ at half-filling.
Data for Im Σ_k at $\omega = 0$.

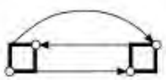
A. Rubtsov, et al, PRB **79**, 045133 (2009)

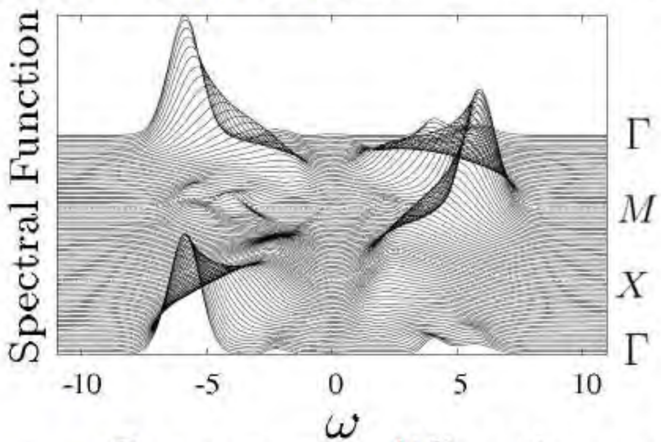
2d-Hubbard: Spectral Function

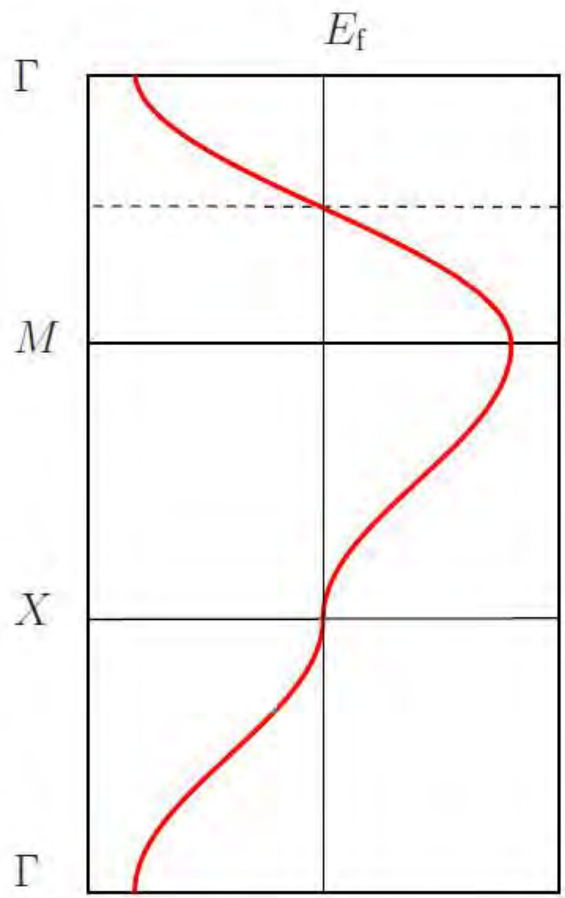
paramagnetic calculation $U/t = 8$, $T/t = 0.235$

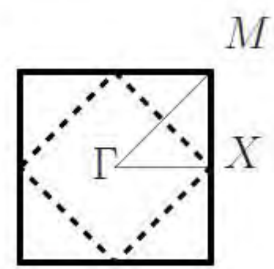
DMFT



Dual Fermion $\Sigma^{d} =$ 



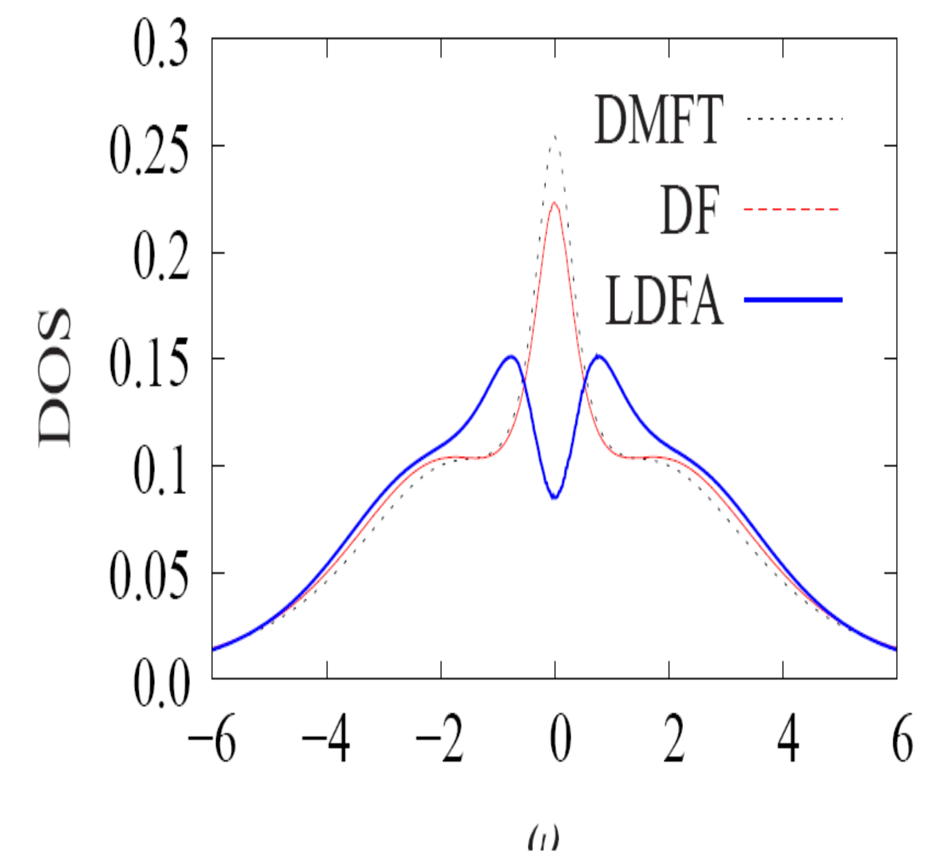




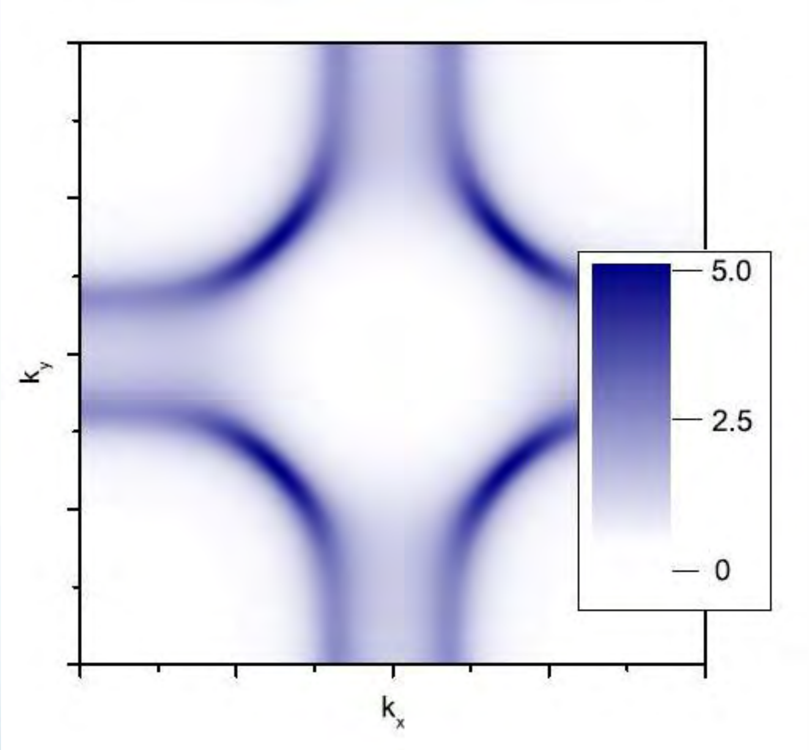
- Strong modifications through AF short-range correlations

Pseudogap in HTSC: dual fermions

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



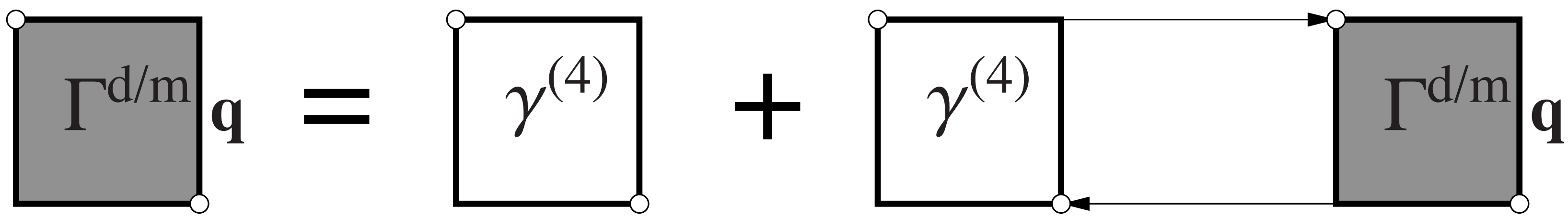
n=1



FS, n=0.85

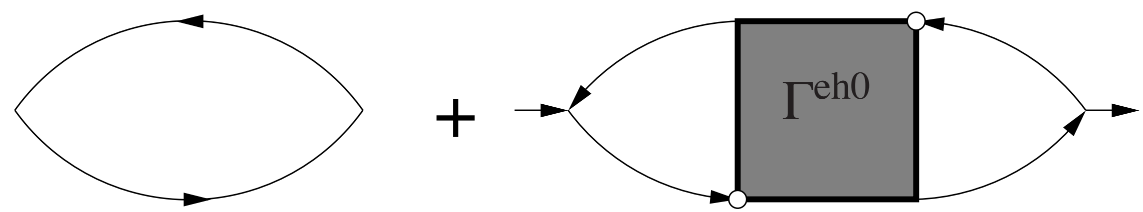
2d:

TPGF: Bethe-Salpeter Equations

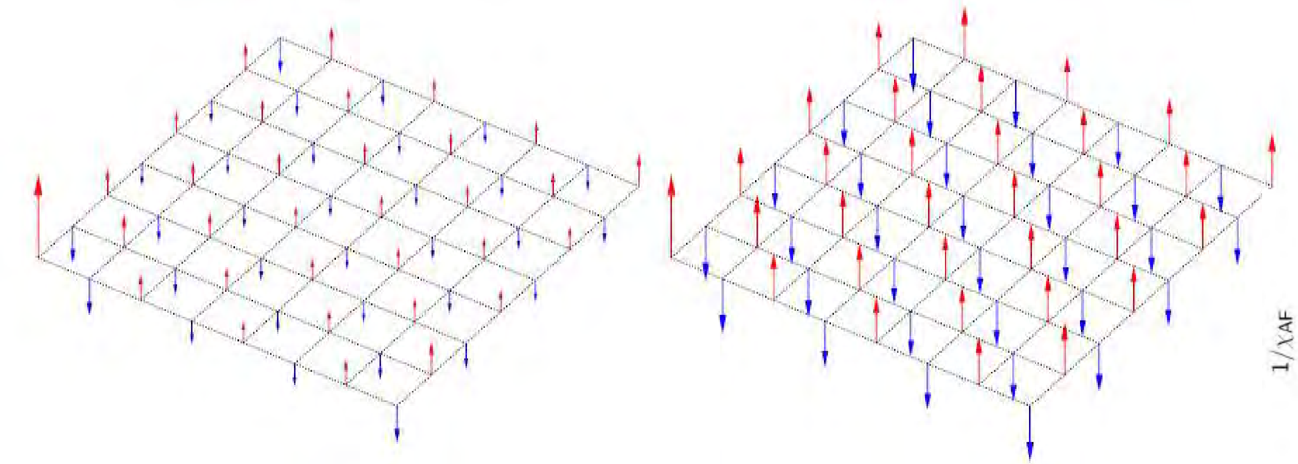


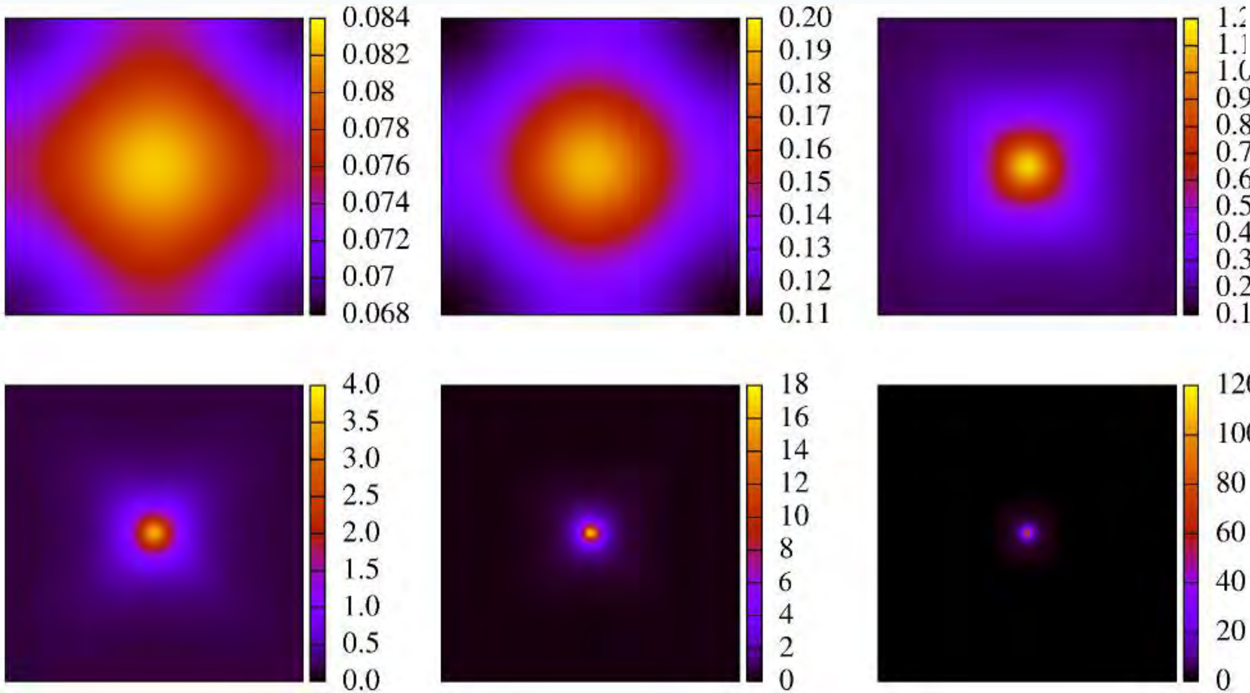
Non-local susceptibility with vertex corrections

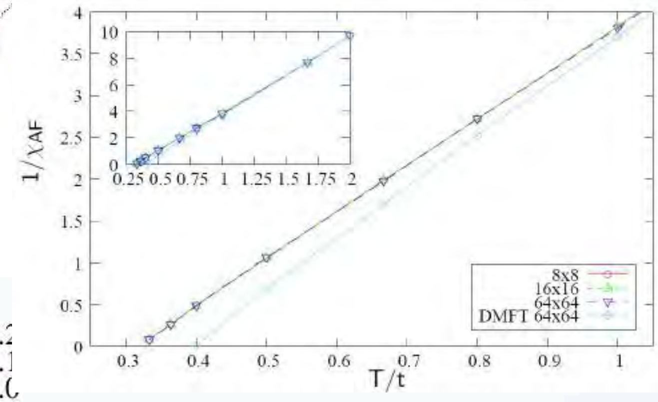
$\chi_0(\mathbf{q},\Omega) + \tilde{\chi}(\mathbf{q},\Omega) =$

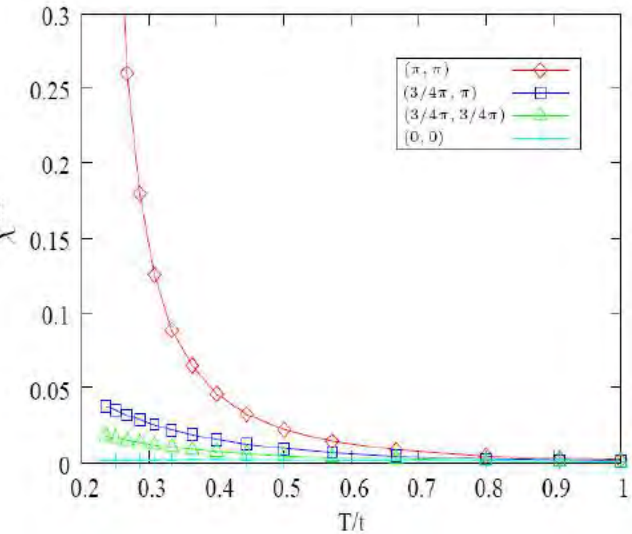


Susceptibility: 2d – Hubbard model

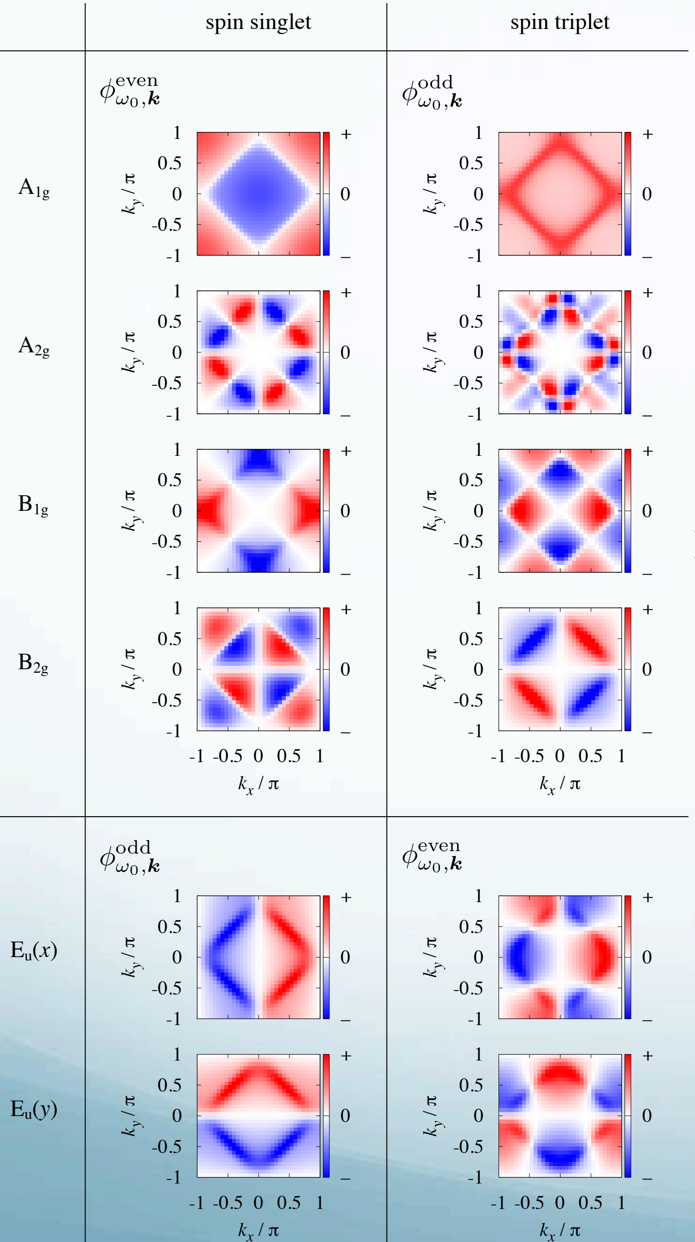




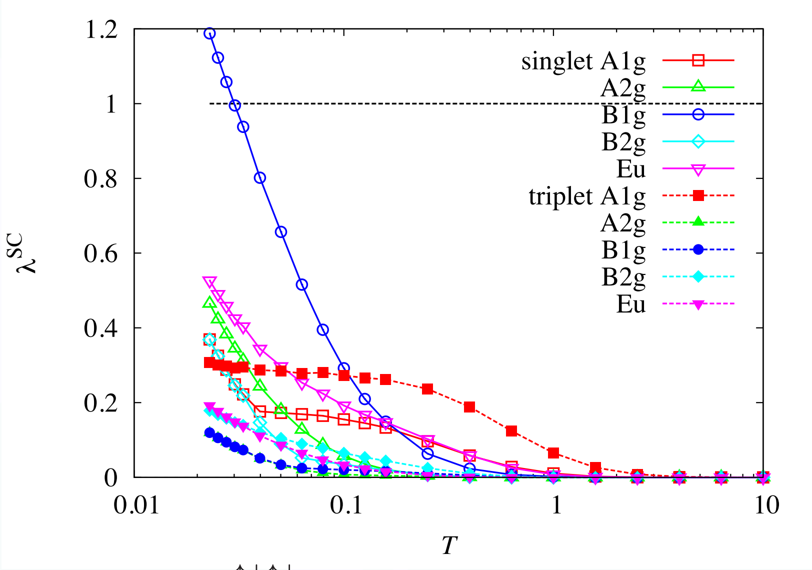




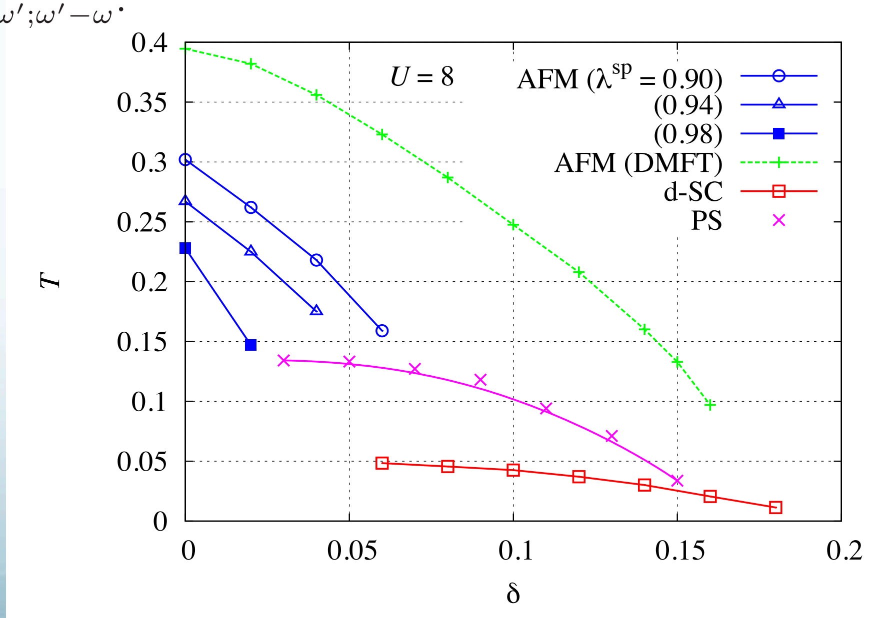
DF: AFM and SC instabilities



U=8
δ =0.15



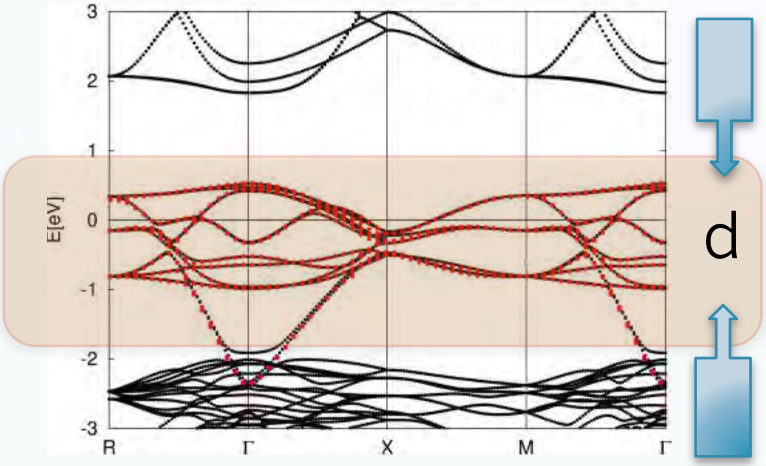
$$\Gamma^{\rm pp}_{kk'} = -\Gamma^{\uparrow\downarrow\downarrow\uparrow}_{\omega,-\omega';\omega'-\omega,\boldsymbol{k}'-\boldsymbol{k}} + \Gamma^{\uparrow\downarrow\uparrow\downarrow}_{\omega,\omega';-\omega-\omega',-\boldsymbol{k}-\boldsymbol{k}'} + \gamma^{\uparrow\downarrow\downarrow\uparrow}_{\omega,-\omega';\omega'-\omega}.$$



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

Non-local screened interactions

F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S. Biermann, A. L. PRB 70, 195104 (2004).



c-RPA screening

χ_0^t

χ_0^r V. Mazurenko, et al, PRB 94, 214411 (2016)

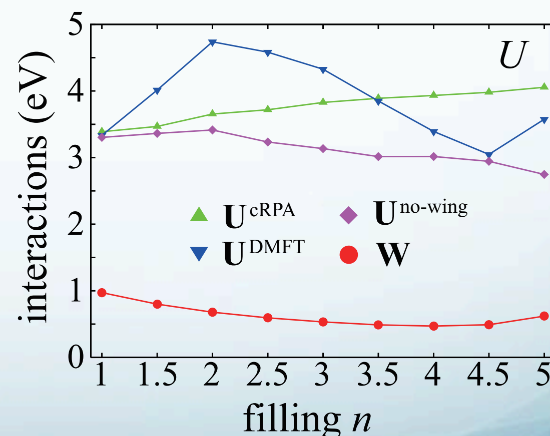
Interaction	C_2F	C_2H
U_{00}	5.16	4.69
U_{01}	2.46	2.19
U_{02}	1.66	1.11
U_{03}	1.46	0.85
J_{01}^F (screened)	0.018	0.034
J_{01}^F (bare)	0.044	0.099

$$\bar{W} = (1 - v\chi_0^r)^{-1} v \qquad W = (1 - \bar{W}\chi_0^t)^{-1}\bar{W}$$

$$U_{ij} = \left\langle ij \middle| \bar{W} \middle| ij \right\rangle$$

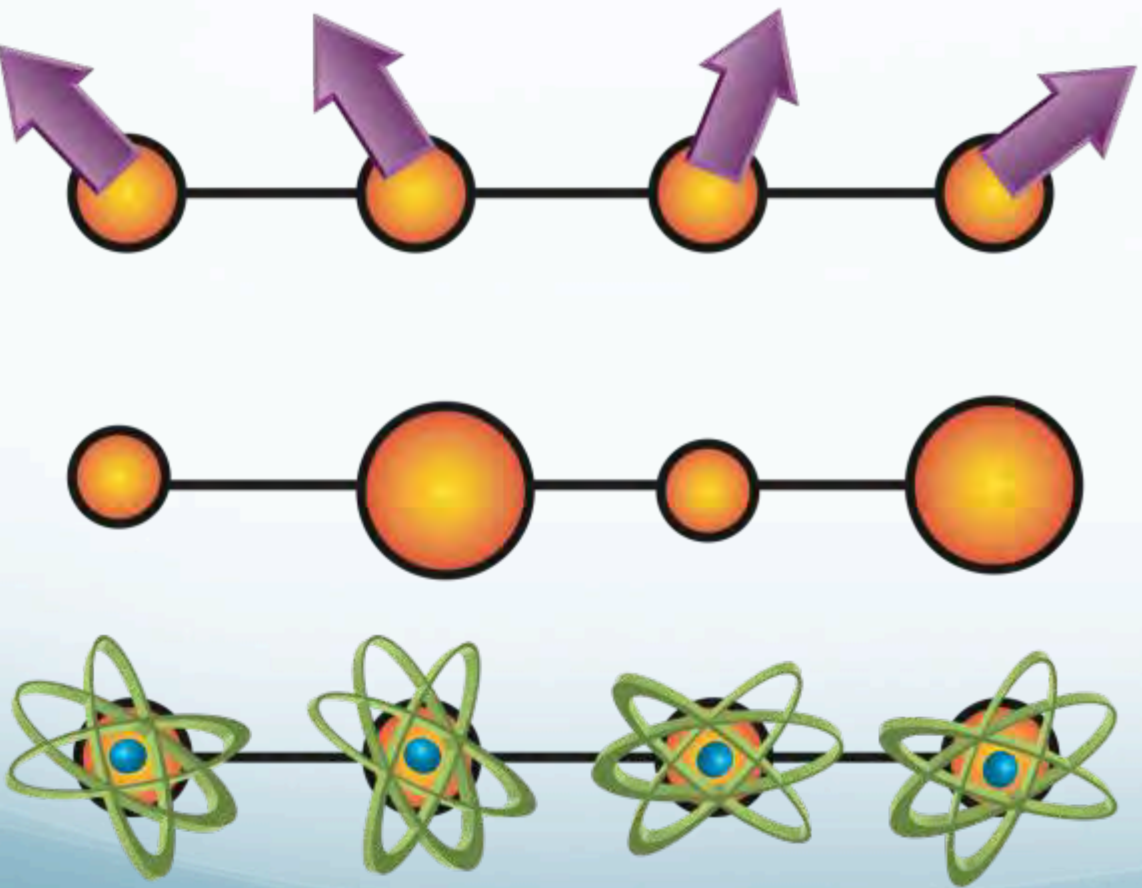
$$J_{ij} = \left\langle ij \middle| \bar{W} \middle| ji \right\rangle$$

Non-local Coulomb and Exchange



C-RPA in Wannier basis:
Y. Nomura, M. Kaltak, K. Nakamura, C. Taranto, S. Sakai, A. Toschi, R. Arita, K. Held, G. Kresse, M. Imada, PRB **86**, 085117 (2012)

Interaction of electrons with collective excitations

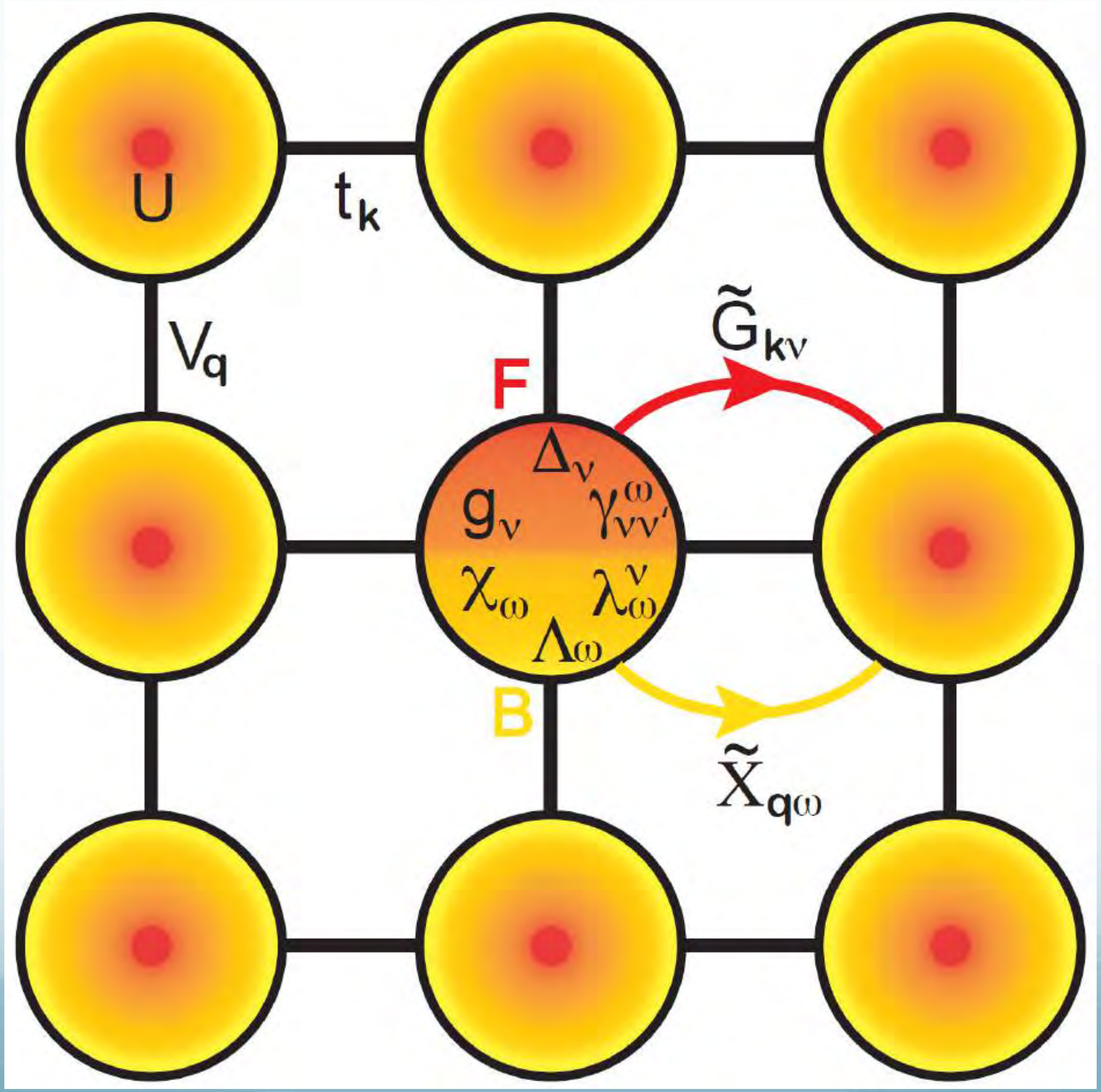


Magnons

Plasmons

Orbitons

Dual Boson: General Idea

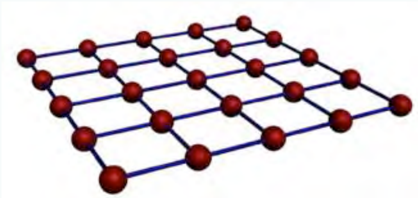


HTSC

Λ_ω ~

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

Beyond DMFT: Dual DB/DF scheme



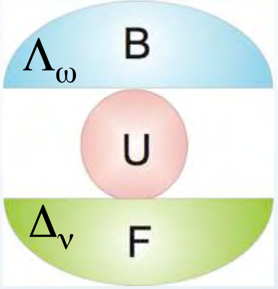
General Lattice Action: $U_{\mathbf{q}} = U + V_{\mathbf{q}}$

$$S = -\sum_{\mathbf{k}\nu\sigma} c^{+}_{\mathbf{k}\nu\sigma}[i\nu + \mu - \varepsilon_{\mathbf{k}}]c_{\mathbf{k}\nu\sigma} + \frac{1}{2}\sum_{\mathbf{q}\omega} U_{\mathbf{q}}\, n^{*}_{\mathbf{q}\omega} n_{\mathbf{q}\omega}$$

$$n_{\mathbf{q}\omega} = \sum_{\mathbf{k}\nu\sigma}(c^{*}_{\mathbf{k}\nu}c_{\mathbf{k}+\mathbf{q},\nu+\omega} - \langle c^{*}_{\mathbf{k}\nu}c_{\mathbf{k}\nu}\rangle \delta_{\mathbf{q}\omega})$$

Reference system: Local Action with hybridization Δ_ν and Λ_ω

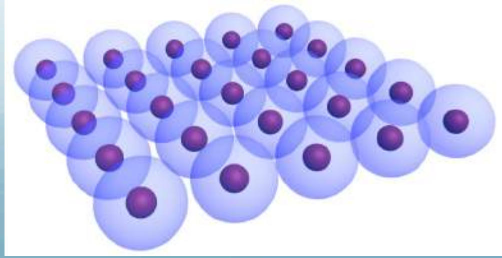
$$S_{\text{ref}} = -\sum_{\nu\sigma} c^{+}_{\nu\sigma}[i\nu + \mu - \Delta_{\nu}]c_{\nu\sigma} + \frac{1}{2}\sum_{\omega} \mathcal{U}_{\omega}\, n^{*}_{\omega} n_{\omega}$$



Lattice-Impurity connection: $S = \sum S^{(i)}_{\text{ref}} + \Delta S$

$$\Delta S = \sum_{\nu\mathbf{k}\sigma} c^{+}_{\nu\mathbf{k}\sigma}[\varepsilon_{\mathbf{k}} - \Delta_{\nu}]c_{\nu\mathbf{k}\sigma} + \frac{1}{2}\sum_{\mathbf{q}\omega}(U_{\mathbf{q}} - \mathcal{U}_{\omega})\, n^{*}_{\mathbf{q}\omega} n_{\mathbf{q}\omega}$$

$\mathcal{U}_{\omega} = U + \Lambda_{\omega}$ $\qquad$ $U_{\mathbf{q}} - \mathcal{U}_{\omega} = V_{\mathbf{q}} - \Lambda_{\omega}$



A. Rubtsov, M. Katsnelson, A.L., Ann. Phys. 327, 1320 (2012)

Dual Transformation

$$\Sigma_{k\nu} = \Sigma_{\nu}^{ref} + \bar{\Sigma}_{k\nu}$$

$$\bar{\Sigma}_{k\nu}^{-1} = \tilde{\Sigma}_{k\nu}^{-1} + G_{\nu}^{ref}$$

Fermionic Hubbard-Stratanovich transformation

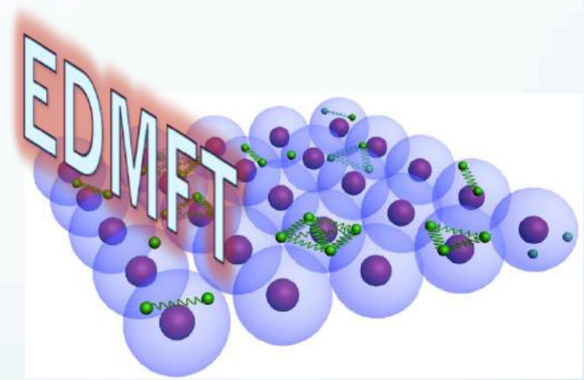
$$e^{\sum\limits_{\mathbf{k}\nu\sigma} c^*_{\mathbf{k}\nu\sigma}[\Delta_{\nu\sigma}-\varepsilon_{\mathbf{k}}]c_{\mathbf{k}\nu\sigma}} = \det[\Delta_{\nu\sigma} - \varepsilon_{\mathbf{k}}] \int D[f^*, f]\, e^{-\sum\limits_{\mathbf{k}\nu\sigma}\{f^*_{\mathbf{k}\nu\sigma}[\Delta_{\nu\sigma}-\varepsilon_{\mathbf{k}}]^{-1} f_{\mathbf{k}\nu\sigma} + c^*_{\nu\sigma} f_{\nu\sigma} + f^*_{\nu\sigma} c_{\nu\sigma}\}}$$

Bosonic Hubbard-Stratanovich transformation

$$\sqrt{\det[\Lambda_{\omega} - V_{\mathbf{q}}]}\, e^{\frac{1}{2}\sum\limits_{\mathbf{q}\omega} n^*_{\mathbf{q}\omega}[\Lambda_{\omega}-V_{\mathbf{q}}] n_{\mathbf{q}\omega}} = \int D[\phi]\, e^{-\frac{1}{2}\sum\limits_{\mathbf{q}\omega}\{\phi^*_{\mathbf{q}\omega}[\Lambda_{\omega}-V_{\mathbf{q}}]^{-1}\phi_{\mathbf{q}\omega} + n^*_{\omega}\phi_{\omega} + \phi^*_{\omega} n_{\omega}\}}$$

Dual action

$$\tilde{S} = -\sum_{\mathbf{k}\nu} f^*_{\mathbf{k}\nu} \tilde{G}_0^{-1} f_{\mathbf{k}\nu} - \frac{1}{2}\sum_{\mathbf{q}\omega} \phi^*_{\mathbf{q}\omega} \tilde{W}_0^{-1} \phi_{\mathbf{q}\omega} + \cdots$$



$$\tilde{G}_0 = [G^{-1}_{\mathrm{ref},\nu} + \Delta_{\nu} - \varepsilon_{\mathbf{k}}]^{-1} - G^{\mathrm{ref}}_{\nu} = G_{\mathrm{E}} - G^{\mathrm{ref}}_{\nu}$$

$$\tilde{W}_0 = \alpha_{\omega}^{-1}\left[[U_{\mathbf{q}} - \mathcal{U}_{\omega}]^{-1} - \chi_{\omega}\right]^{-1}\alpha_{\omega}^{-1} = W_{\mathrm{E}} - \mathcal{W}^{\mathrm{ref}}_{\omega}$$

Augmentation:

$$\alpha_{\omega} = \mathcal{W}_{\omega}/\mathcal{U}_{\omega} = (1 + \mathcal{U}_{\omega}\chi_{\omega})$$

$$\mathcal{U}_{\omega} \leftrightarrow \mathcal{W}_{\omega} \leftarrow \tilde{W}_{\mathbf{q}\omega}$$

Dual Potential

Effective Interactions:

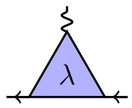
$$\tilde{V} = \frac{1}{4}\sum_{\nu\nu'\omega} \gamma_{\nu\nu'\omega}\, f^*_\nu f^*_{\nu'} f_{\nu+\omega} f_{\nu'-\omega} + \sum_{\nu\omega} (\lambda_{\nu\omega}\, f^*_\nu f_{\nu+\omega} \phi^*_\omega + h.c.)$$

Definition of correlation functions

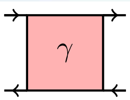
$$G_{\mathbf{k}\nu}/G^{\mathrm{ref}}_\nu = -\langle c \;\; c^+ \rangle_{\mathbf{k}\nu/\nu\,\mathrm{ref}},$$

$$X_{\mathbf{q}\omega}/\chi_\omega = -\langle n \;\; n^* \rangle_{\mathbf{q}\omega/\omega\,\mathrm{ref}},$$

$$\mathcal{W}_\omega = \mathcal{U}_\omega + \mathcal{U}_\omega \chi_\omega \mathcal{U}_\omega,$$



$$\lambda_{\nu\omega} = g_\nu^{-1} g_{\nu+\omega}^{-1} \alpha_\omega^{-1} \langle c_\nu c^*_{\nu+\omega} n_\omega \rangle_{\mathrm{loc}}$$



$$\gamma_{\nu\nu'\omega} = g_\nu^{-1} g_{\nu'}^{-1} g_{\nu'-\omega}^{-1} g_{\nu+\omega}^{-1} \left[\langle c_\nu c_{\nu'} c^*_{\nu'-\omega} c^*_{\nu+\omega} \rangle - g_\nu g_{\nu'} (\delta_\omega - \delta_{\nu',\nu+\omega}) \right]$$

DB: Full impurity vertex $\gamma_{\nu\nu'\omega}$ with $\tilde{G}_{\mathbf{k}\nu}$

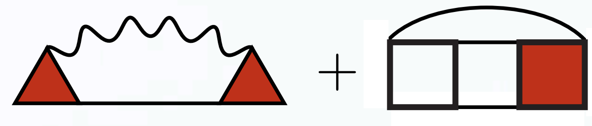
is equivalent to Bare irreducible vertex $\overline{\gamma}^{2\mathrm{PI}\,\varsigma}_{\nu\nu''\omega}$ and $G_\nu(\mathbf{k})$

in normal Ladder-perturbation theory

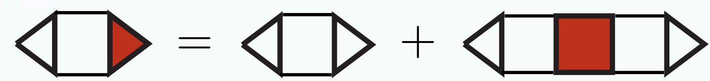
Lattice GF and SCF-condition

Lattice two-point correlation functions

$$G^{-1}_{\mathbf{k}\nu} = G^{-1}_{\mathrm{E}} - \tilde{\Sigma}_{\mathbf{k}\nu}(1 + G^{\mathrm{ref}}_{\nu}\tilde{\Sigma}_{\mathbf{k}\nu})^{-1}$$

$\tilde{\Sigma}_{\mathbf{k}\nu} =$ 

$$W^{-1}_{\mathbf{q}\omega} = W^{-1}_{\mathrm{E}} - \tilde{\Pi}_{\mathbf{q}\omega}(1 + \mathcal{W}^{\mathrm{ref}}_{\omega}\tilde{\Pi}_{\mathbf{q}\omega})^{-1}$$

$\tilde{\Pi}_{\mathbf{q}\omega} =$ 

Self-consistent conditions:

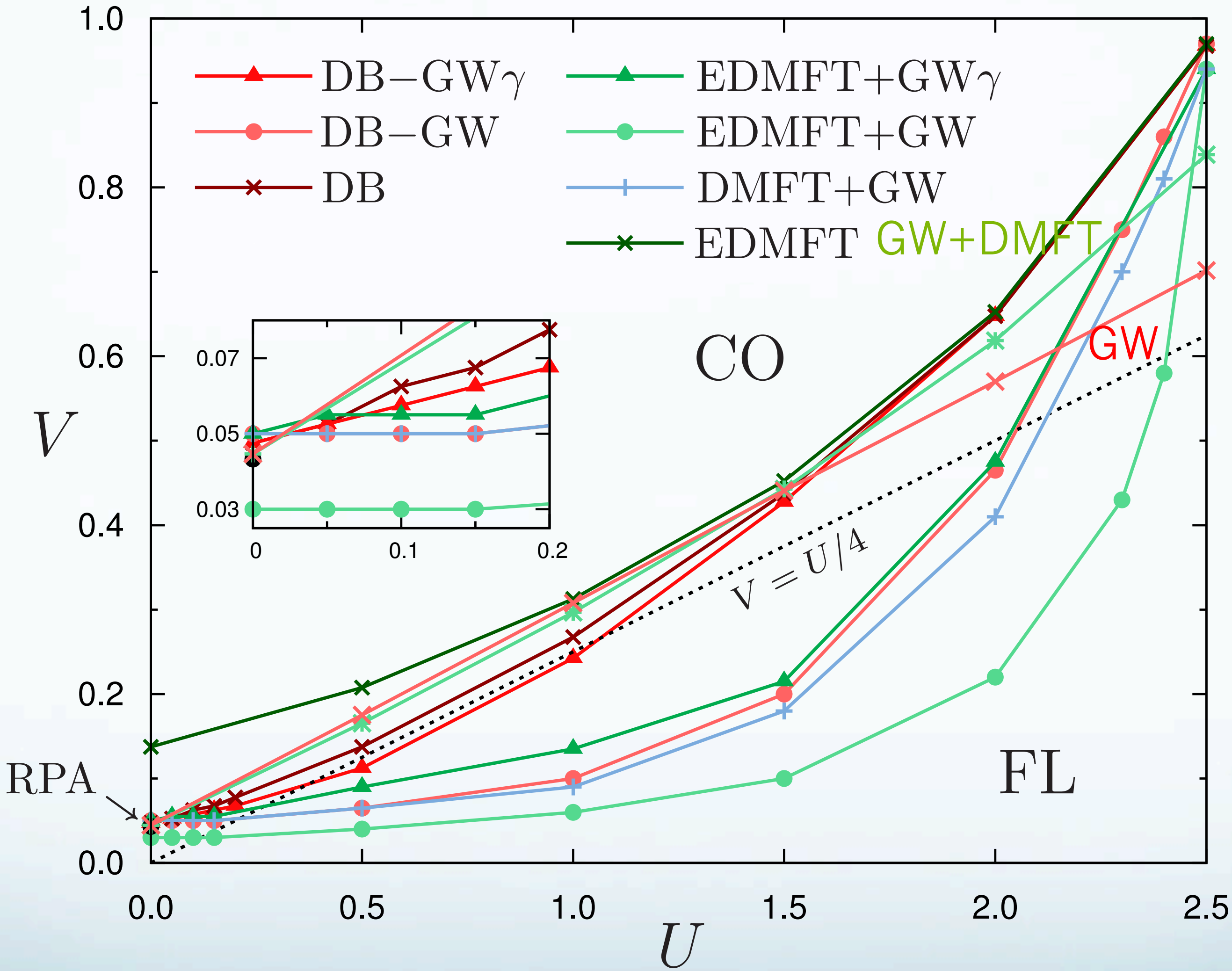
$$\sum_{\mathbf{k}} G_{\mathbf{k}\nu} = G^{\mathrm{ref}}_{\nu},$$

$$\sum_{\mathbf{q}} W_{\mathbf{q}\omega} = \mathcal{W}^{\mathrm{ref}}_{\omega}. \qquad \text{vs.} \qquad \sum_{\mathbf{q}} X_{\mathbf{q}\omega} = \chi_{\omega}$$

Lattice susceptibility

$$X_{\mathbf{q}\omega} = \tilde{U}^{-1}_{\mathbf{q}\omega}\alpha^{-1}_{\omega}\tilde{W}_{\mathbf{q}\omega}\alpha^{-1}_{\omega}\tilde{U}^{-1}_{\mathbf{q}\omega} - \tilde{U}^{-1}_{\mathbf{q}\omega}$$

Comparisson GW+DMFT

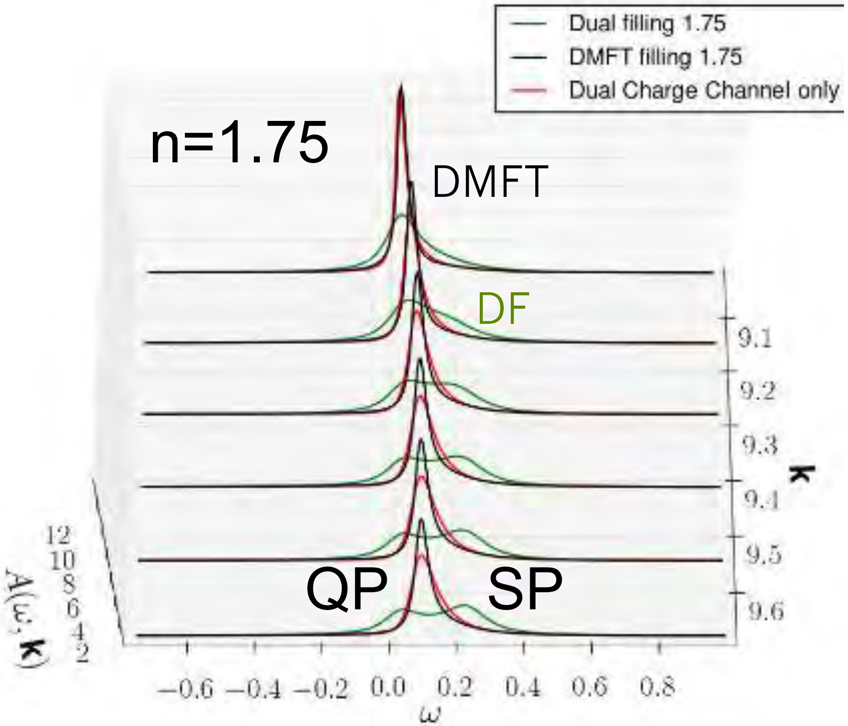


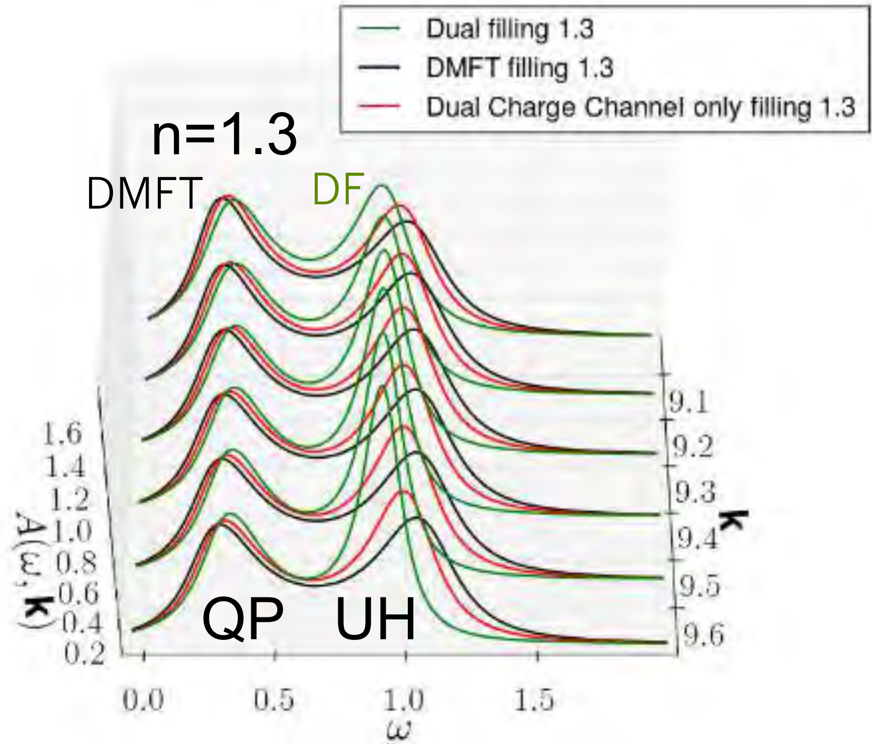
DB+GW: E. Stepanov, A. Huber, E. van Loon, A. L., M. Katsnelson PRB **94**, 205110 (2016)

GW+DMFT: Th. Ayral, S. Biermann, Ph. Werner, L. BoehnkePRB **95**, 245130 (2017)

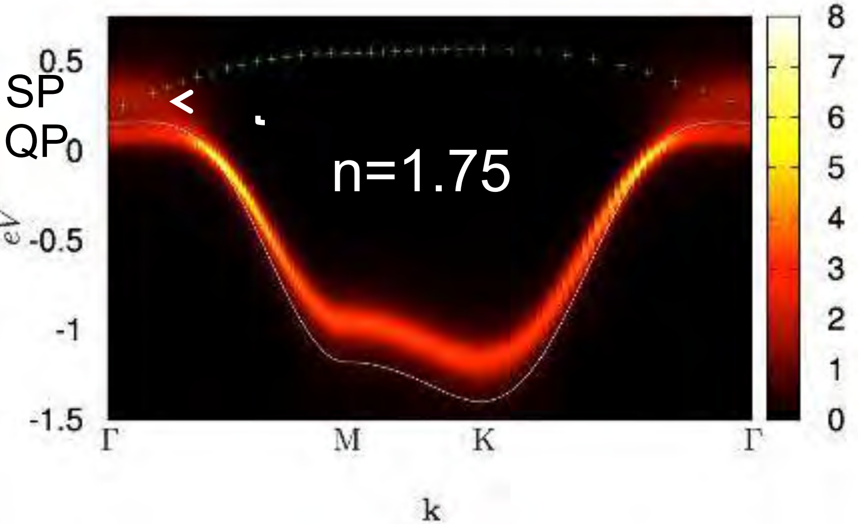
GW+DMFT: S. Biermann, F. Aryasetiawan, and A. Georges, PRL **90**, 086402 (2003)

Spin-Polaron near van Hove singularity in real Material: Na_xCoO_2





DF-spectral function Na_xCoO_2



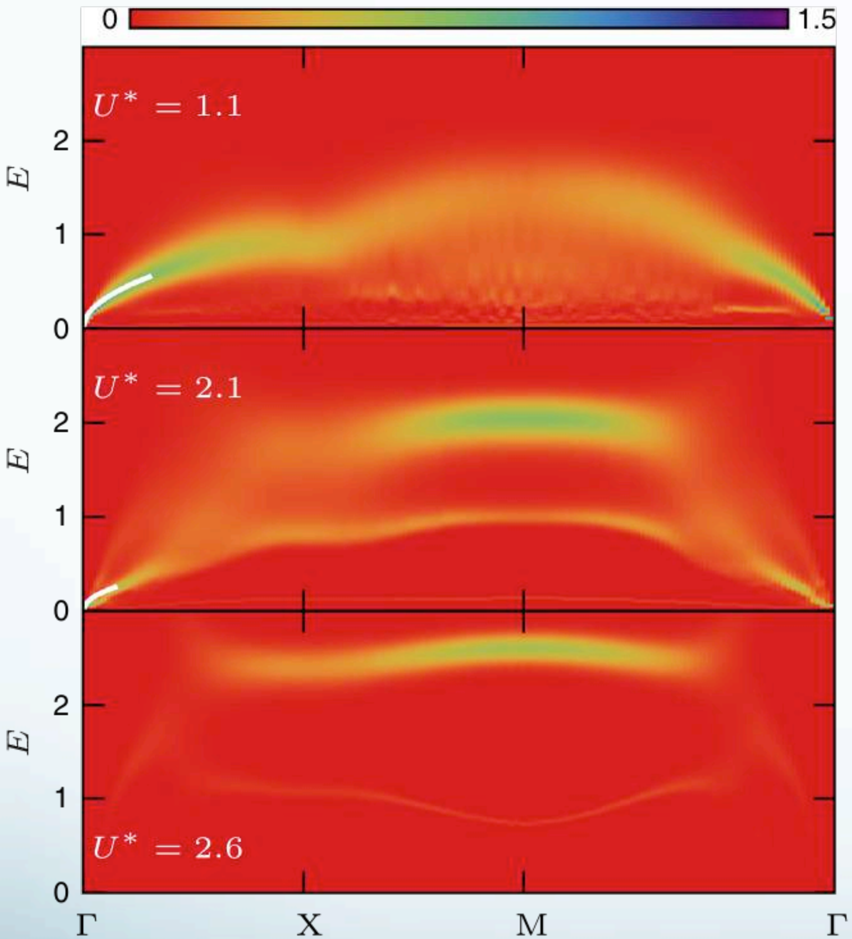
A. Wilhelm, F. Lechermann, H. Hafermann, M. Katsnelson, A. L. Phys. Rev. B 91, 155114 (2015)

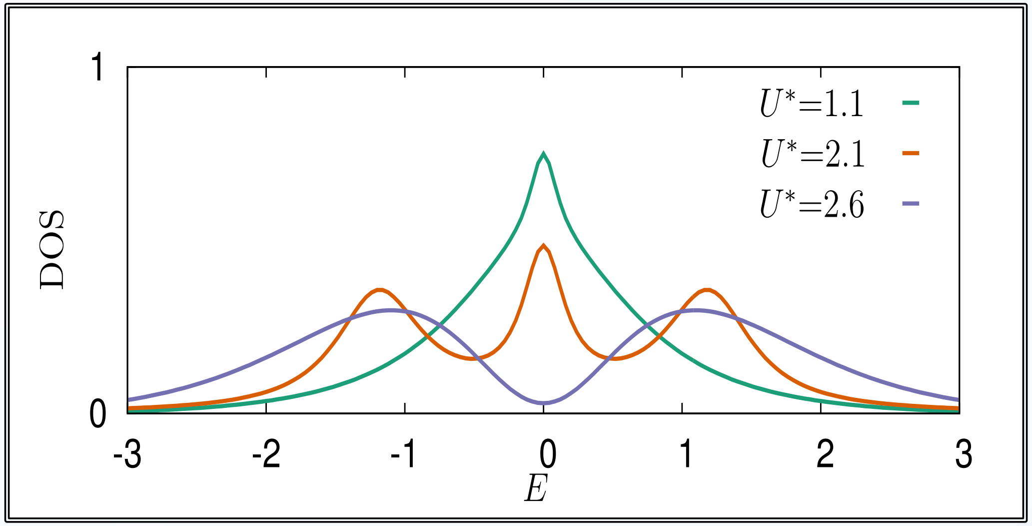
Spin-Polaron physics for n=1.75

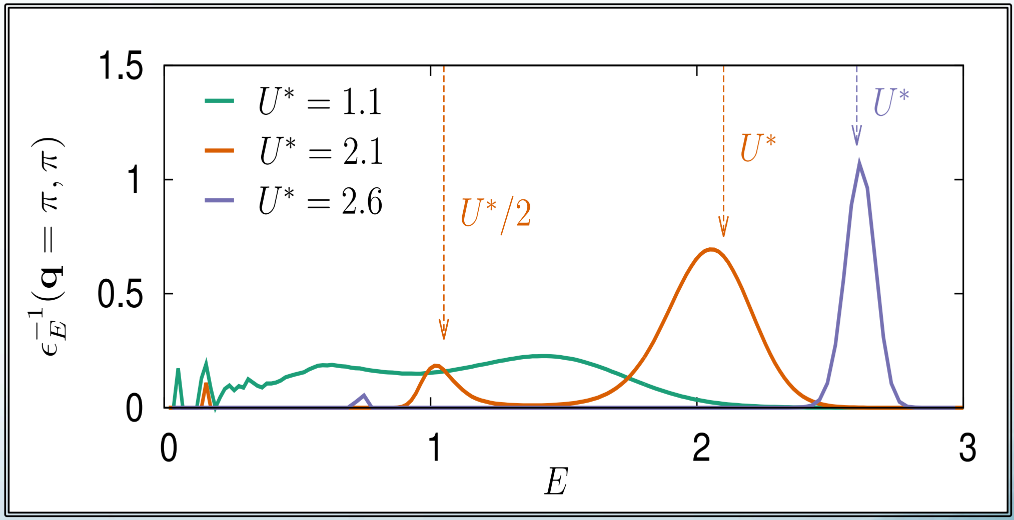
$$E(k) = -\frac{2t\left(t - J\cos k\right)}{|t| + J}$$

1d t-J model, M. Katsnelson (1982)

Plasmon in strongly correlated materials







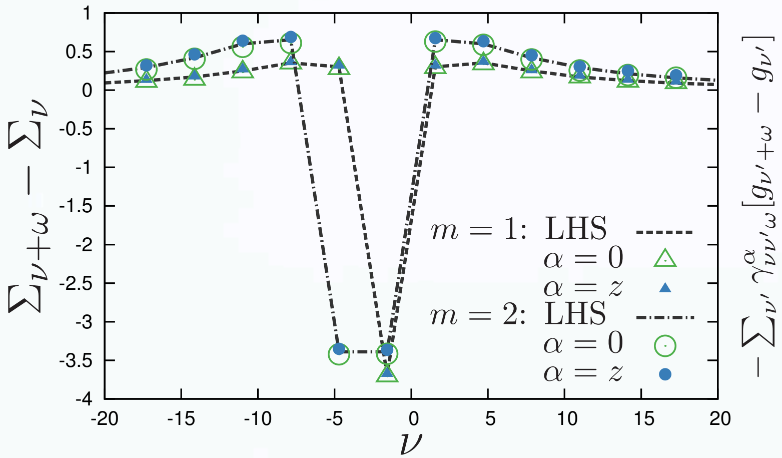
Single plasmon mode for q->0

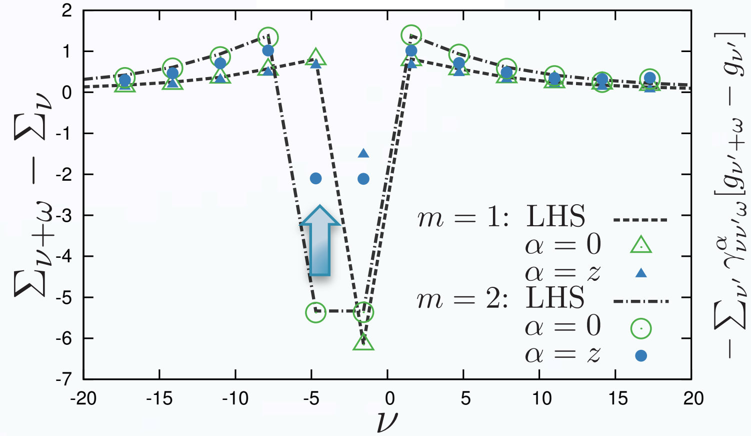
Erik van Loon, et all, PRL **113**, 246407 (2014)

Conservation in DMFT and DB

F. Krien, et al, PRB **96**, 075155 (2017)

$\frac{1}{2}\sum_{\omega} \mathbf{s}_\omega \Lambda^{sp}_\omega \mathbf{s}_\omega$ Vectror boson





Lattice Ward identity

$k \equiv (\mathbf{k}, \nu) \quad q \equiv (\mathbf{q}, \omega)$

$$\Sigma_{k+q} - \Sigma_k = \sum_{k'} \Gamma^{\text{irr},\alpha}_{kk'q}[G_{k'+q} - G_{k'}],$$

	DMFT	DB
2P self-consistent	✗	✓
charge conservation	✓	✓
spin conservation	✓	✗ ✓ S_z

Imuprity Ward identity

$$\Sigma_{\nu+\omega} - \Sigma_\nu = \sum_{\mathbf{k}'\nu'} \Gamma^{\text{irr},\alpha}_{\nu\nu'\omega}[G_{\mathbf{k}'+\mathbf{q},\nu'+\omega} - G_{\mathbf{k}'\nu'}]$$

$$= \sum_{\nu'} \Gamma^{\text{irr},\alpha}_{\nu\nu'\omega}[G_{\text{loc},\nu'+\omega} - G_{\text{loc},\nu'}].$$

DB/DF-scheme: interpretation

Hamiltonian action with local in time,
but large (tall and beatiful) U

(troubles,troubles)

Non-Hamiltonian action with retarded V, formally including all ordres of interaction (but negligible!)

(can be hidden in your pocket,
not much food required)

Summary

- Strong-coupling DB/DF-theory based on a ladder approximation is a conserving theory of electron-“anyon“ interaction