From LDA+U to realistic correlated calculations

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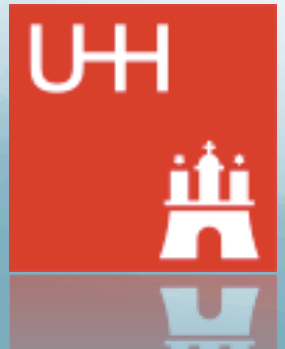

In collaboration with
E. Stepanov, E. van Loon,
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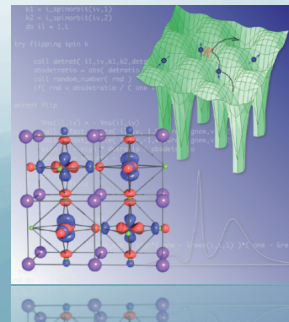


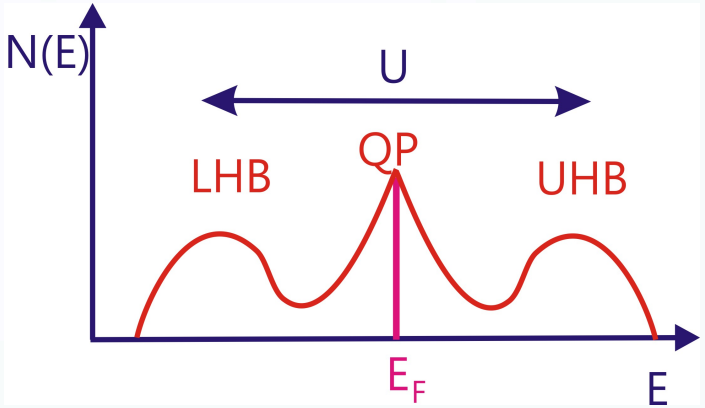
Outline

- Zoo of correlated materials
- LDA+U: spin-charge-orbital ordering
- LDA+DMFT: symplest dynamical effects
- GW+EDMFT: screened U from DB-perspective
- Conclusions

Correlated Materials

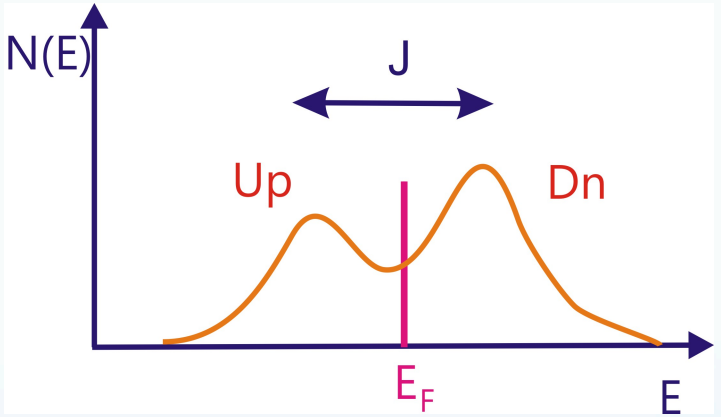
Hubbard-metal

(correlations due to U)
Single-band DMFT



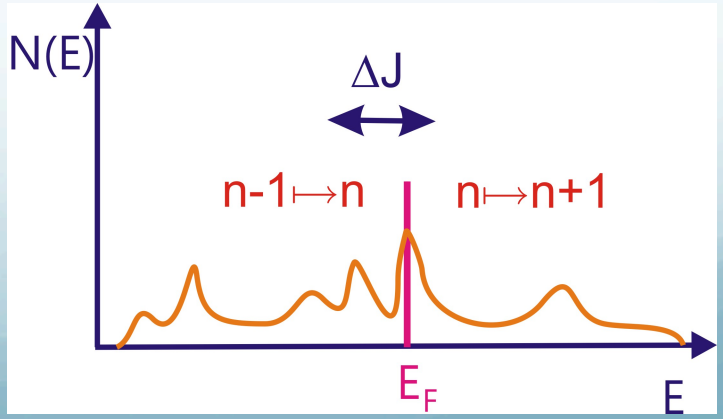
Hunds-metal

(correlations due to J)
Fe-based HTSC



Racah-metal

(correlations due to F_k)
f-compounds



LDA+U: static mean-filed approximation

LDA+U functional:

$$E = E_{LDA} + \frac{U}{2}\sum_{ij} n_i n_j - \frac{U}{2} n_d (n_d - 1)$$

One-electron energies:

$$\varepsilon_i = \frac{\partial E}{\partial n_i} = \varepsilon_{LDA} + U\left(\frac{1}{2} - n_i\right)$$

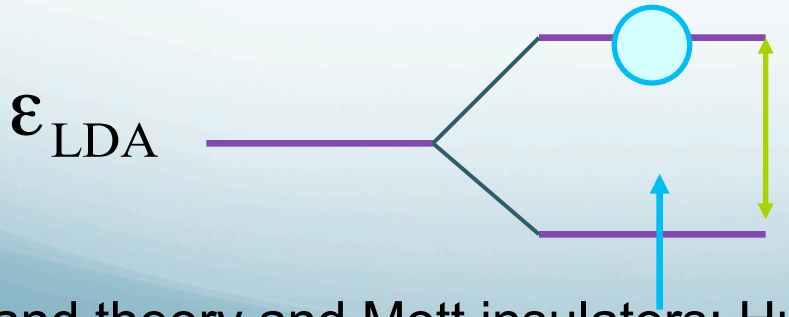
Occupied states:

$$n_i = 1 \Rightarrow \varepsilon_i = \varepsilon_{LDA} - \frac{U}{2}$$

Empty states:

$$n_i = 0 \Rightarrow \varepsilon_i = \varepsilon_{LDA} + \frac{U}{2}$$

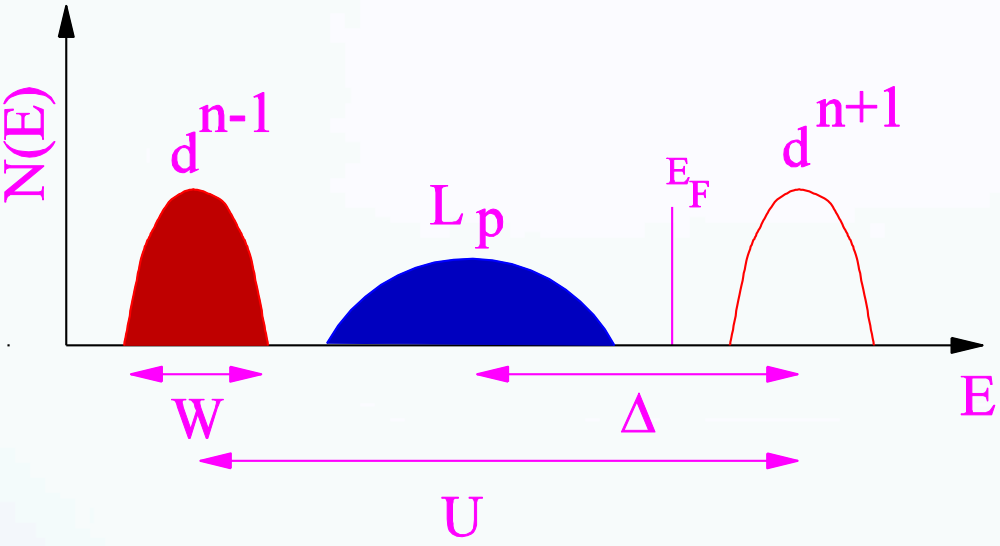
Mott-Hubbard gap



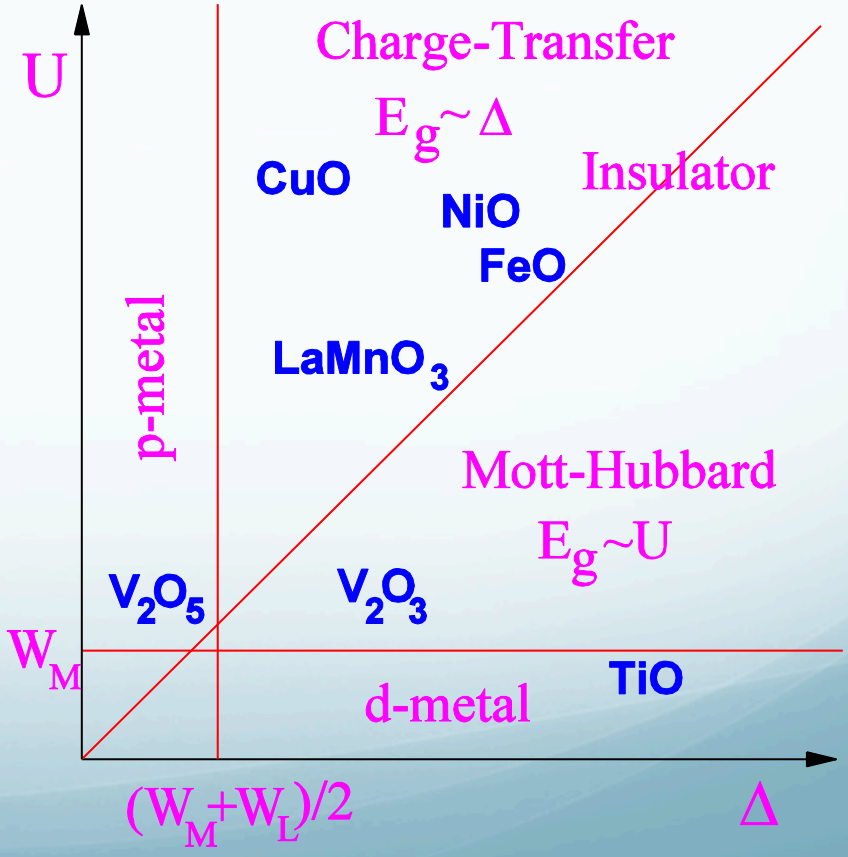
$$U \equiv \frac{\partial \varepsilon_{LDA}}{\partial n_d}$$

"Band theory and Mott insulators: Hubbard U instead of Stoner I "
V. I. Anisimov, J. Zaanen, and O. K. Andersen, PRB, 44, 943 (1991)

Charge transfer TMO insulators



Zaanen-Sawatzky-Allen (ZSA) phase diagram



Rotationally invariant LDA+U

LDA+U functional

$$E^{LSDA+U}[\rho^\sigma(\mathbf{r}),\{n^\sigma\}] = E^{LSDA}[\rho^\sigma(\mathbf{r})] + E^U[\{n^\sigma\}] - E_{dc}[\{n^\sigma\}]$$

Local screend Coulomb interaction

$$E^U[\{n^\sigma\}] = \frac{1}{2}\sum_{\{m\},\sigma}\{\langle m,m''\mid V_{ee}\mid m',m'''\rangle n^\sigma_{mm'}n^{-\sigma}_{m''m'''} +$$

$$+(\langle m,m''\mid V_{ee}\mid m',m'''\rangle - \langle m,m''\mid V_{ee}\mid m''',m'\rangle)n^\sigma_{mm'}n^\sigma_{m''m'''}\}$$

LDA-double counting term ($n^\sigma = \mathrm{Tr}(n_{mm'}{}^\sigma)$ and $n = n^\uparrow + n^\downarrow$):

$$E_{dc}[\{n^\sigma\}] = \frac{1}{2}Un(n-1) - \frac{1}{2}J[n^\uparrow(n^\uparrow-1) + n^\downarrow(n^\downarrow-1)],$$

Occupation matrix for correlated electrons:

$$n^\sigma_{mm'} = -\frac{1}{\pi}\int^{E_F} ImG^\sigma_{ilm,ilm'}(E)dE$$

A. L., J. Zaanen, and V. I. Anisimov, PRB 52, R5467 (1995)

General LDA+U formulation

$$H_U = \frac{Un^2}{2} - \sum_\sigma \frac{Jn_\sigma^2}{2} - \sum_\sigma \left[\frac{U-J}{2} (S_\sigma n_\sigma^2 + P_\sigma n_\sigma) \right]$$

AMF: $S = 1/(2l+1),\ P = 0$

SIC: $S = 0,\ P = 1/2$

FLL is the right "DFT" mean field for localized systems, $n_{m\sigma}$= 1 or 0

AMF is the right "DFT" mean field for for uniform occupancy, $n_{m\sigma} = \langle n_\sigma \rangle$

Generalization: $(2l+1)S_\sigma + P_\sigma = 1$

$$n_\sigma^2/(2l+1) \le \sum_m n_{m\sigma}^2 \le n_\sigma$$

A. Petukhov, L. Chioncel, I. Mazin, A.L., PRB 67, 153106 (2003).

Slater parametrization of U

Multipole expansion – atomic-like symmetry:

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|}=\sum_{kq}\frac{4\pi}{2k+1}\frac{r_<^k}{r_>^{k+1}}Y_{kq}^*(\hat{r})Y_{kq}(\hat{r}')$$

Coulomb matrix elements in Y_{lm} basis:

$$< mm'||m''m''' >=\sum_k a_k(m,m'',m',m''')F^k$$

Angular part – 3j symbols

$$a_k(m,m',m''',m''')=\sum_{q=-k}^{k}(2l+1)^2(-1)^{m+q+m'}\begin{pmatrix} l & k & l \\ 0 & 0 & 0\end{pmatrix}^2\begin{pmatrix} l & k & l \\ -m & -q & m'\end{pmatrix}\begin{pmatrix} l & k & l \\ -m'' & q & m'''\end{pmatrix}$$

Slater integrals:

$$F^k=e^2\int_0^\infty r^2dr|\varphi_d(r)|^2\int_0^\infty (r')^2dr'|\varphi_d(r')|^2\frac{r_<^k}{r_>^{k+1}}$$

V. Anisimov, F. Aryasetiawan and A. L., JPCM **9**, 767 (1997)

Average interaction: U and J

Average Coulomb parameter:

$$U = \frac{1}{(2l+1)^2} \sum_{mm'} U_{mm'} = F^0$$

Average Exchange parameter:

$$J = \frac{1}{(2l+1)^2} \sum_{mm'} J_{mm'} = \sum_{k \neq 0} \begin{pmatrix} l & k & l \\ 0 & 0 & 0 \end{pmatrix}^2 F^k$$

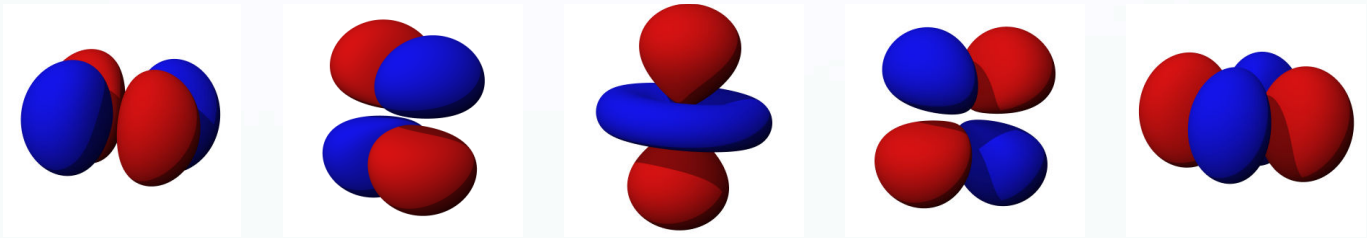
For d-electrons: $J_d = \frac{1}{14}(F^2 + F^4)$

Coulomb and exchange interactions:

$$U_{mm'} = < mm' || mm' >$$
$$J_{mm'} = < mm' || m'm >$$

Density-Density U-matrix

$$\hat{H}_{\mathrm{ee}}^{\mathrm{dens-dens}} = \frac{1}{2}\sum_{m,m',\sigma} U_{mm'}\hat{n}_{m,\sigma}\hat{n}_{m',-\sigma} + \frac{1}{2}\sum_{m\neq m',\sigma}(U_{mm'} - J_{mm'})\hat{n}_{m,\sigma}\hat{n}_{m',\sigma}$$



$3d_{xy}$ $3d_{yz}$ $3d_{z^2}$ $3d_{xz}$ $3d_{x^2-y^2}$

$$U_{mm'} = \begin{pmatrix} U_0 & U_0-2J_1 & U_0-2J_2 & U_0-2J_1 & U_0-2J_3 \\ U_0-2J_1 & U_0 & U_0-2J_4 & U_0-2J_1 & U_0-2J_1 \\ U_0-2J_2 & U_0-2J_4 & U_0 & U_0-2J_4 & U_0-2J_2 \\ U_0-2J_1 & U_0-2J_1 & U_0-2J_4 & U_0 & U_0-2J_1 \\ U_0-2J_3 & U_0-2J_1 & U_0-2J_2 & U_0-2J_1 & U_0 \end{pmatrix}$$

$$J_{mm'} = \begin{pmatrix} U_0 & J_1 & J_2 & J_1 & J_3 \\ J_1 & U_0 & J_4 & J_1 & J_1 \\ J_2 & J_4 & U_0 & J_4 & J_2 \\ J_1 & J_1 & J_4 & U_0 & J_1 \\ J_3 & J_1 & J_2 & J_1 & U_0 \end{pmatrix}$$

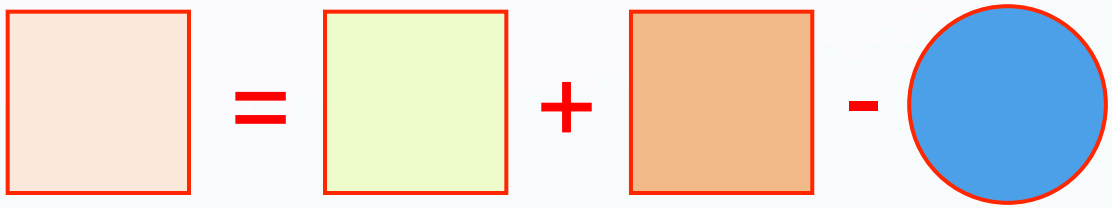
NB: different notation for U and J

Maurits Haverkort, PhD (2005)

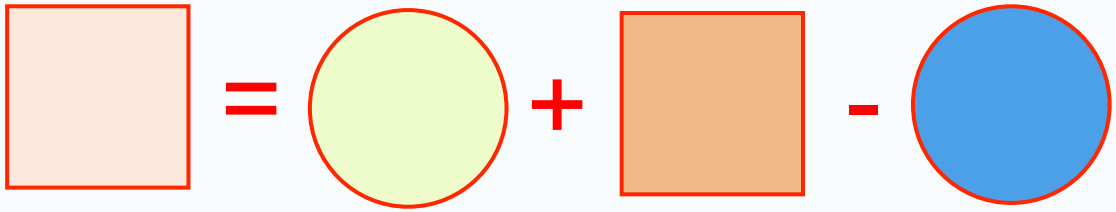
$$\begin{aligned} U_0 &= F^0 + \frac{8}{7}\frac{F^2+F^4}{14} \\ J_1 &= \frac{3}{49}F^2 + \frac{20}{9}\frac{1}{49}F^4 \\ J_2 &= -2\frac{5}{7}\frac{F^2+F^4}{14} + 3J_1 \\ J_3 &= 6\frac{5}{7}\frac{F^2+F^4}{14} - 5J_1 \\ J_4 &= 4\frac{5}{7}\frac{F^2+F^4}{14} - 3J_1. \end{aligned}$$

Full-potential LDA+U: a problem

$$E_{LDA+U} = LDA + U - DC$$



No



Yes

Spherical RI-LDA+U  Interchange is possible!

$$V_{\sigma jl}^{\mathrm{LSDA+U}} = V^{\mathrm{LSDA}} + (U - J)[\frac{1}{2}\delta_{jl} - \rho_{jl}^{\sigma}]$$

S. Dudarev et. al. PRB 57, 1505 (1998)

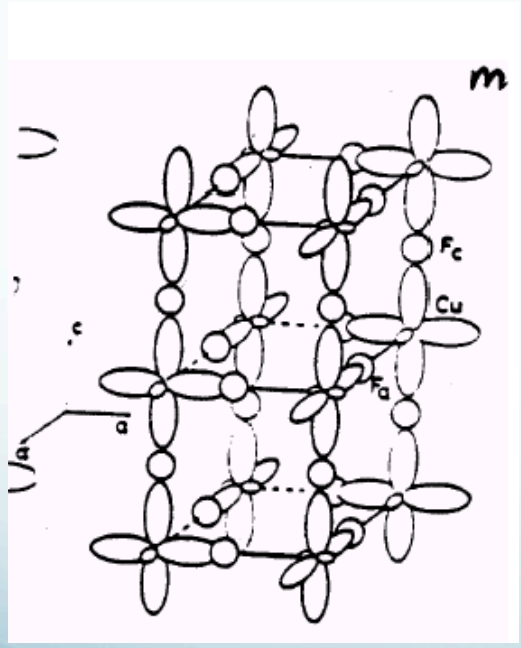
Orbital order: $KCuF_3$

In $KCuF_3$ Cu^{+2} ion has d^9 configuration

with a single hole in e_g doubly degenerate subshell.

Experimental crystal structure

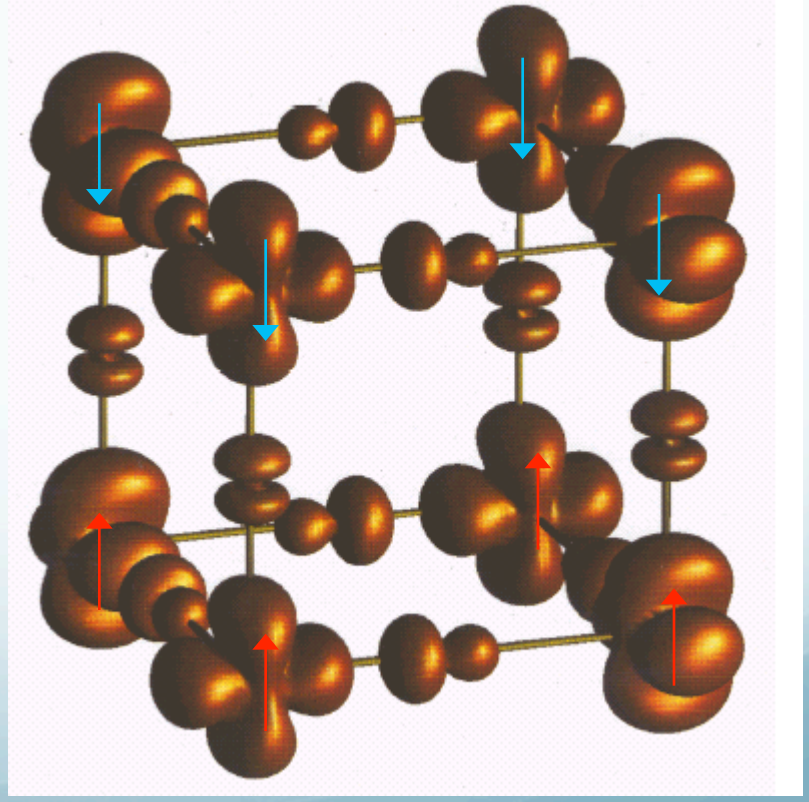
antiferro-orbital order



J(K)	Jc	Jab
Theory	-240	+6
Exp.	-202	+3

LDA+U calculations for *undistorted* perovskite structure

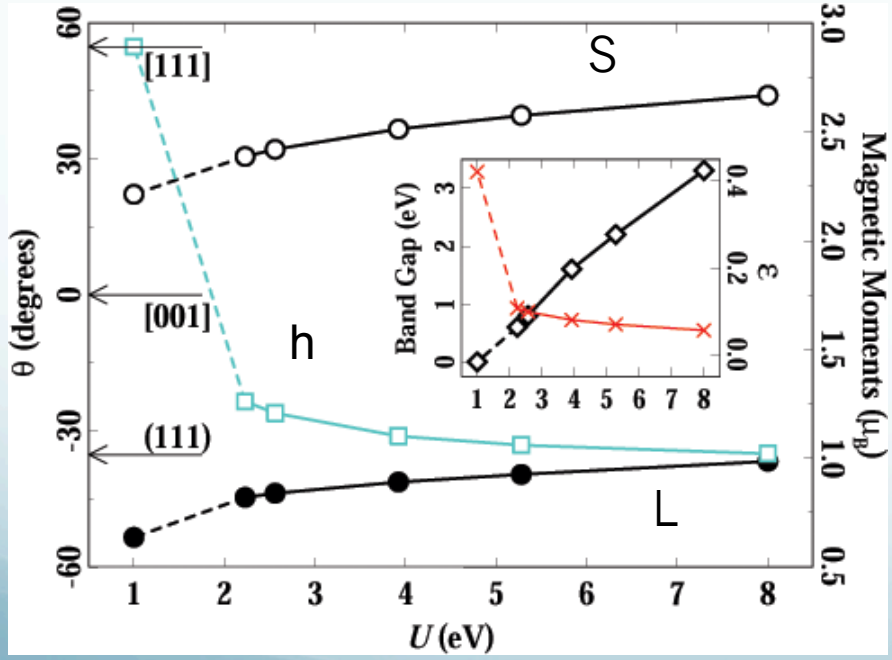
hole density of the same symmetry

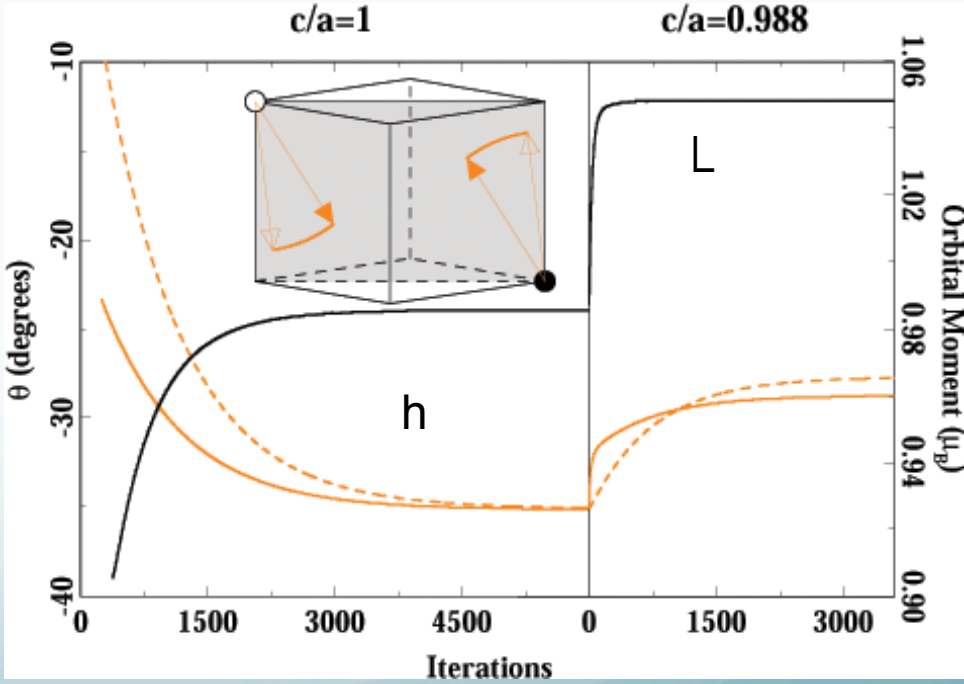


A. L., J. Zaanen, and V. I. Anisimov, PRB 52, R5467 (1995)

Spin and Orbital moments in CoO

- LDA+U+SO+non-collinear
- Useful tools for topological insulators





I. Solovyev, A. L, and K. Terakura, PRL 80, 5758 (1998)

The Best of Both Worlds: LDA+DMFT

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

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

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

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

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

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

Applications:
Paramagnetic, paraorbital strongly correlated metals

short range spin and orbital order

Cluster LDA+DMFT approximation

A. Poteryaev, A. L, and G. Kotliar, PRL **93**, 086401 (2004)
S. Biermann, A. Poteryaev, A. L, and A. Georges PRL **94**, 026404 (2005)

Baym-Kadanoff Functional

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

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

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

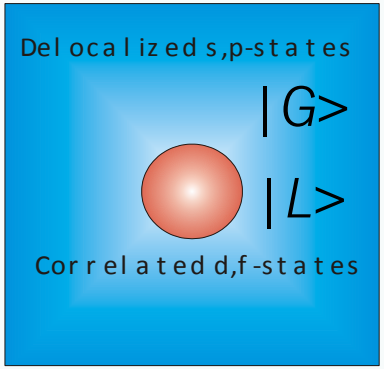
Different Functionals and "source" field J

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

G. Kotliar, et al. Rev. Mod. Phys. **78**, 865 (2006), A. Georges (2004) arXiv/0403123

General Projection formalism for LDA+DMFT

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



P. Blöchl, PRB **50,** 17953 (1994)

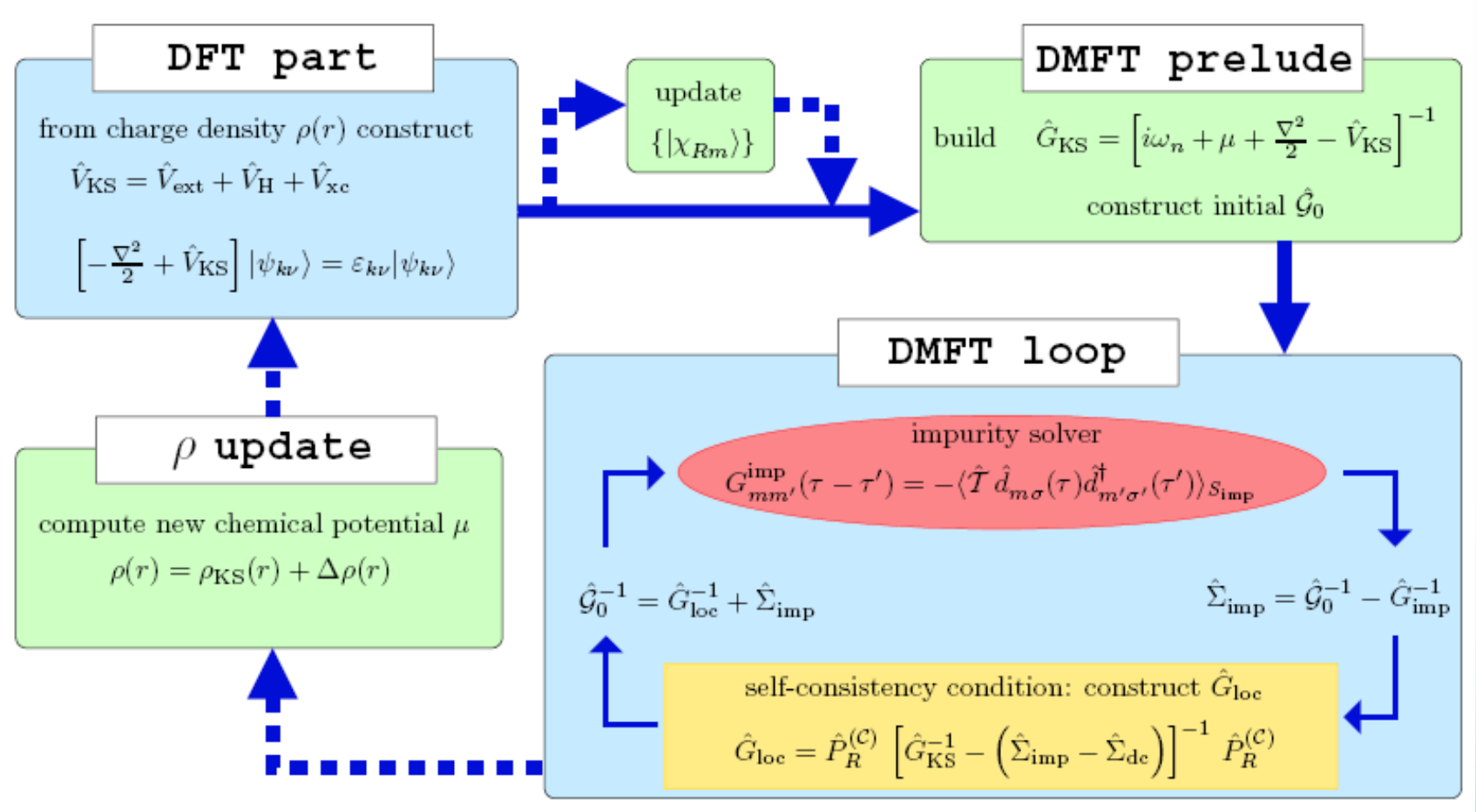
$$G^c_{mm'}(i\omega) = \sum_{\vec{k}\,nn'} \langle L_m|G_n\rangle \left[(i\omega+\mu)\,\hat{1} - \hat{H}_{KS}(\vec{k}) - \Delta\Sigma(i\omega)\right]^{-1}_{nn'} \langle G_{n'}|L_{m'}\rangle$$

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

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

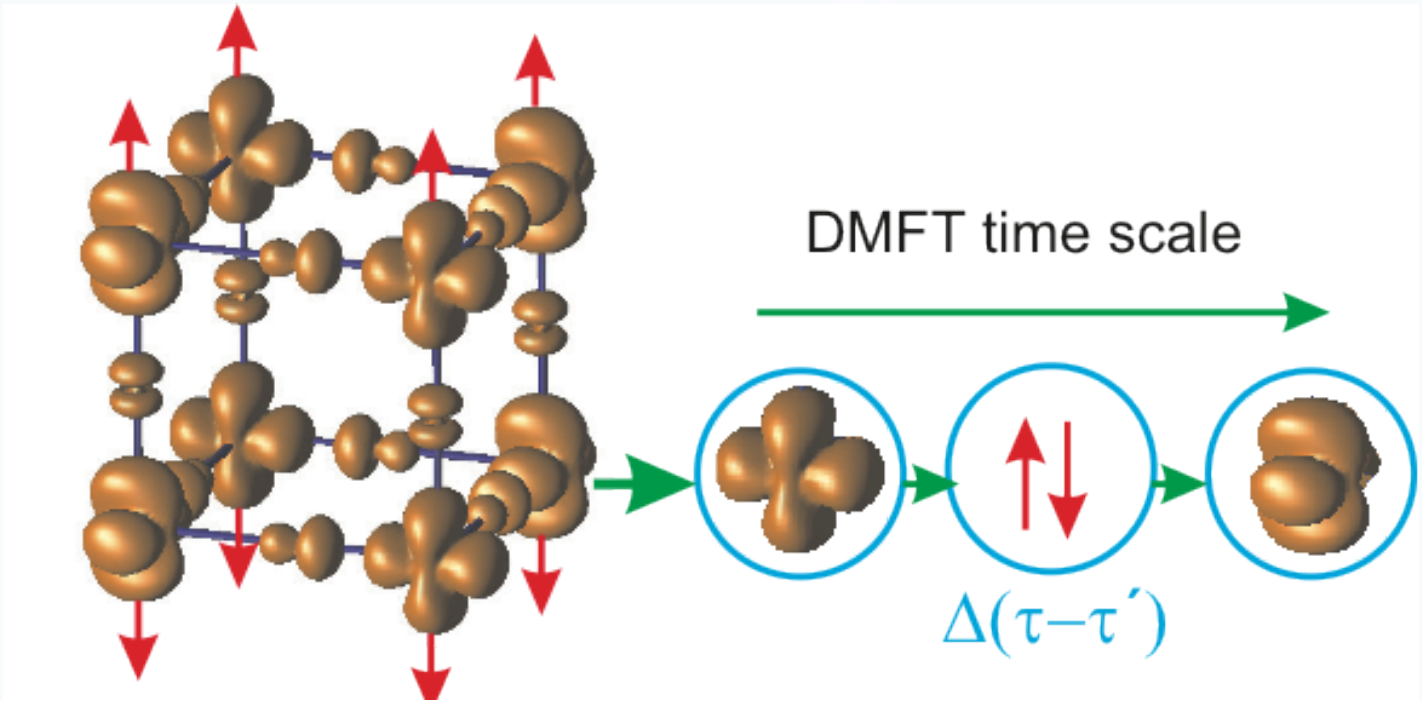
G. Trimarchi, I. Leonov, N. Binggeli, D. Korotin, V. Anisimov. JPCM **20**,135227 (2008)
B. Amadon, F. Lechermann, A. Georges, F. Jollet, T. Wehling, and A. L., PRB **77**, 205112 (2008)

Self-Consistent LDA+DMFT



F. Lechermann, et al, PRB (2007)

LDA+DMFT: Charge+Spin+Orbital Fluctuations



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

$$S_{\mathrm{loc}}[c^*,c] = -\sum_{\omega\,\alpha\beta} c^*_{\omega\alpha}\left[(i\omega+\mu)\mathbf{1} - \Delta^{\alpha\beta}_{\omega}\right] c_{\omega\beta} + S_{\mathrm{U}}[c^*,c] \quad \Rightarrow \quad g_{12} = -\langle c_1 c_2^* \rangle_{\mathrm{loc}}$$

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

DMFT self-consistensy

DMFT Impurity solver

Continuous Time Quantum Monte Carlo

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

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

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)

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

E. Gull, A. Millis, A.L., A. Rubtsov, M. Troyer, Ph. Werner, Rev. Mod. Phys. **83**, 349 (2011)

Constrained c-RPA calculations of U

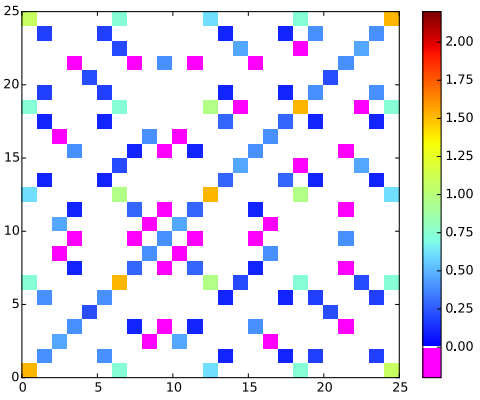
PHYSICAL REVIEW B **70**, 195104 (2004)

Frequency-dependent local interactions and low-energy effective models from electronic structure calculations

F. Aryasetiawan,[1] M. Imada,[2,3] A. Georges,[4,5] G. Kotliar,[6] S. Biermann,[4] and A. I. Lichtenstein[7]

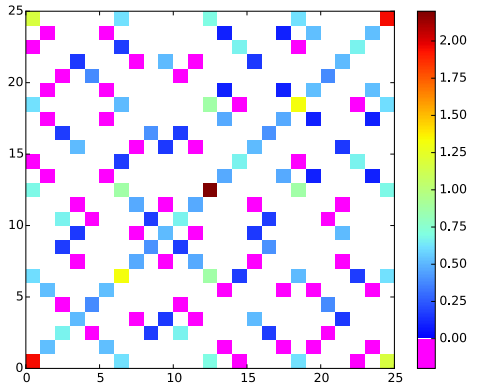
$$U_{nn',mm'}(\tau-\tau') \doteq \int d^3r d^3r' \, \phi_n^*(\mathbf{r})\phi_{n'}(\mathbf{r}) W_r(\mathbf{r},\mathbf{r}';\tau-\tau')\phi_m^*(\mathbf{r}')\phi_{m'}(\mathbf{r}')$$

3d



Slater

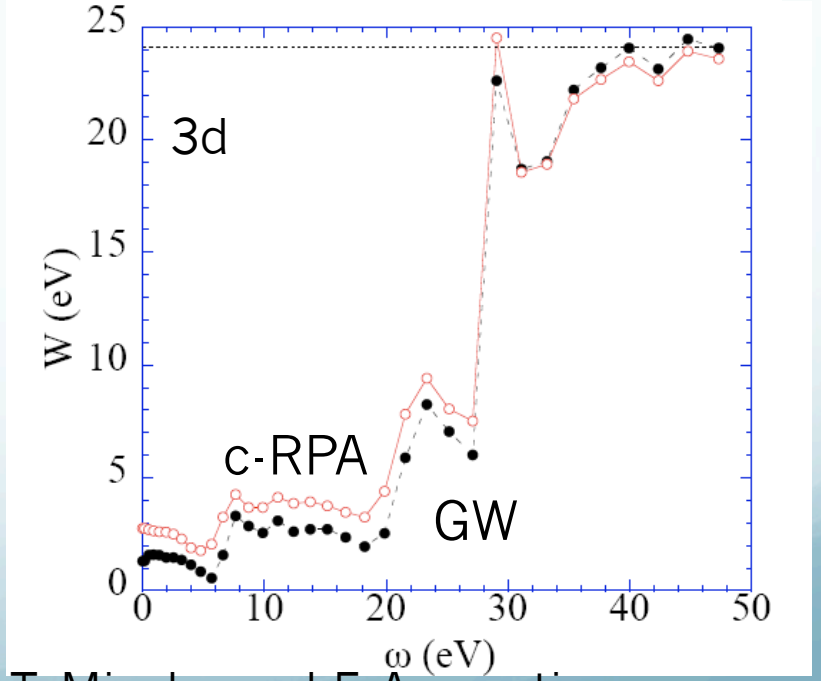
Spher. Sym.



C-RPA

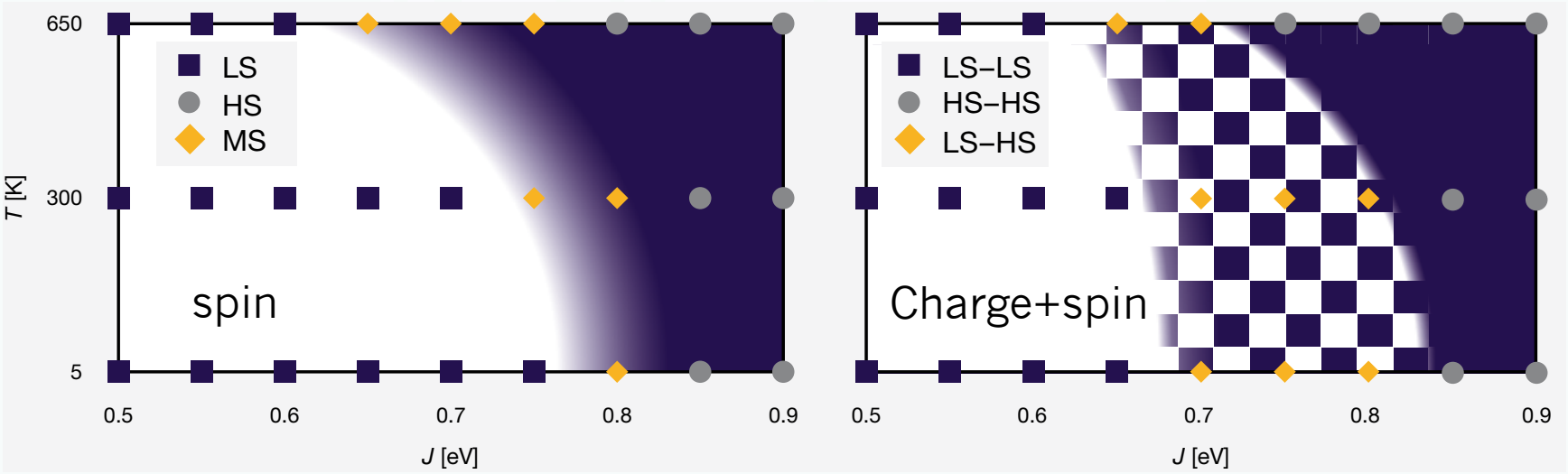
Cubic. Sym.

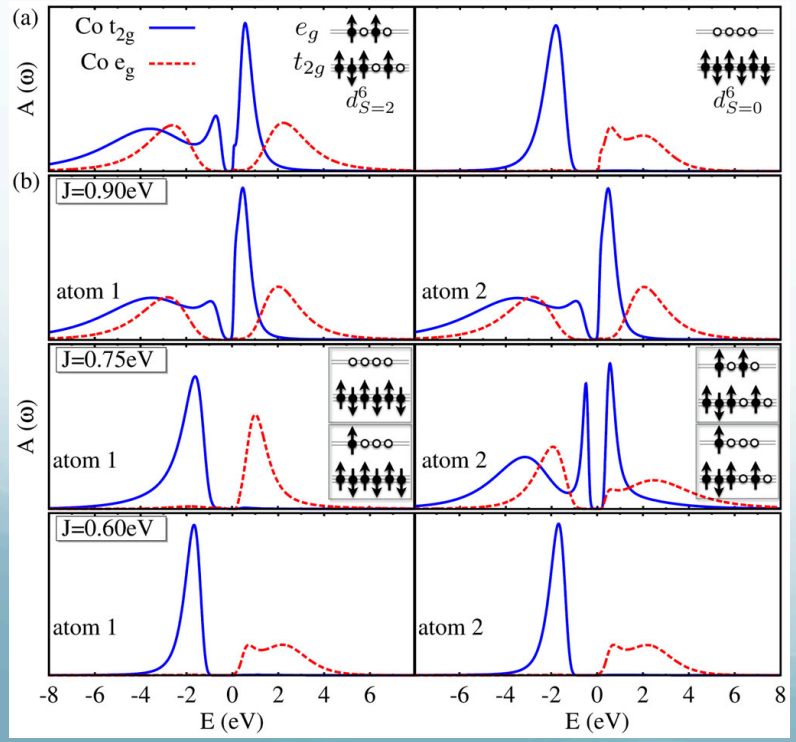
$$W_r(\omega) = [1 - vP_r(\omega)]^{-1} v$$

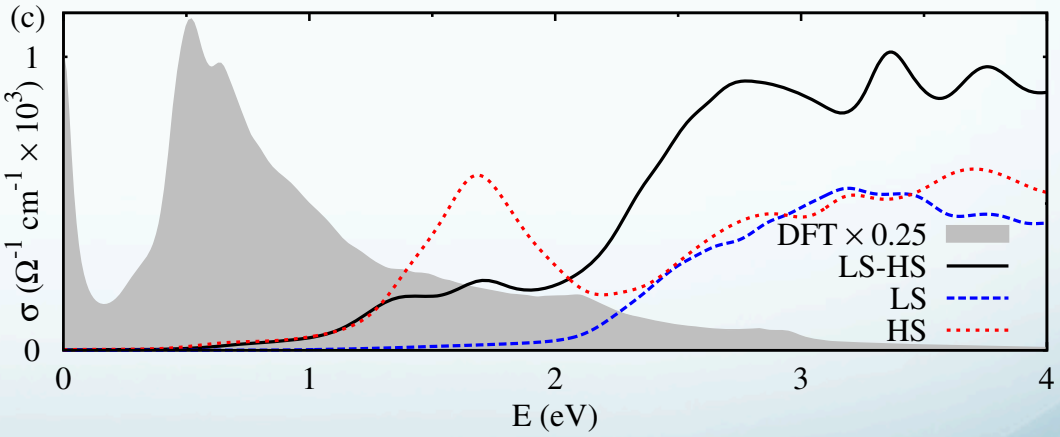


T. Miyake and F. Aryasetiawan
Phys. Rev. B 77, 085122 (2008)

Charge and Spin Fluctuations in $LaCoO_3$

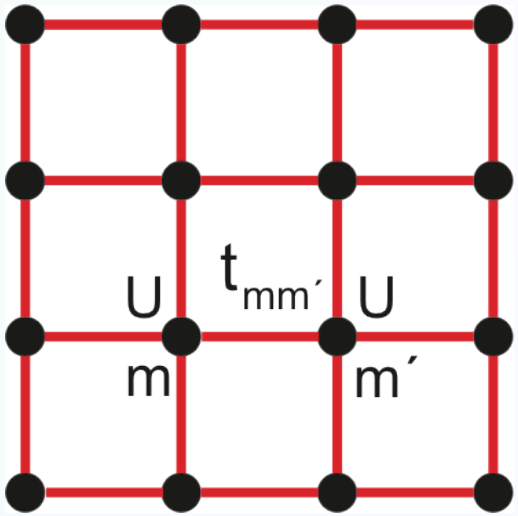


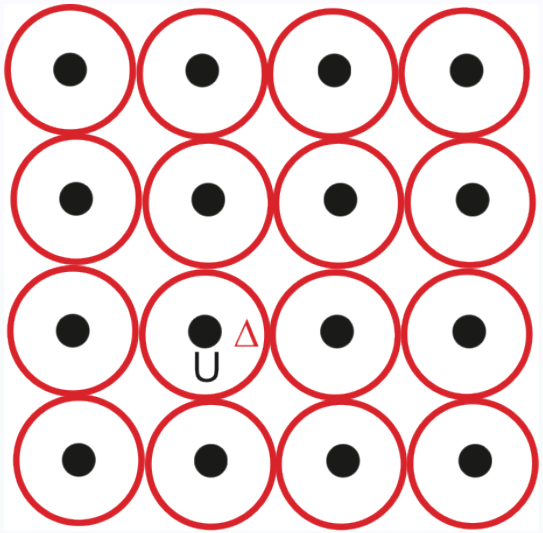


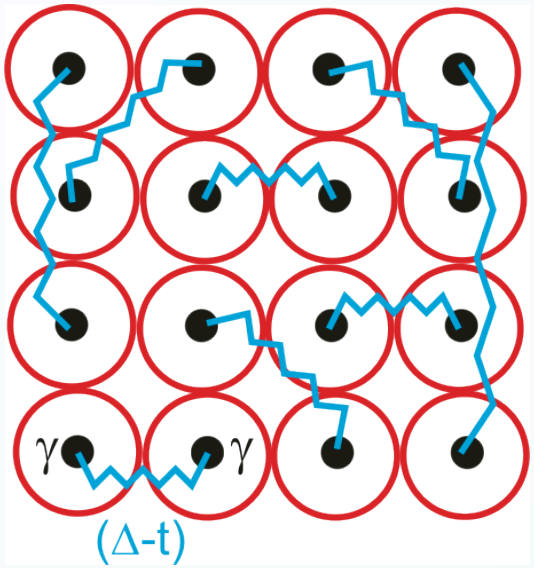


M. Karolak, M. Izquierdo, S. Molodtsov, A. L., PRL **115,** 046401 (2015)

DMFT-functional and beyond







Start from
Correlated Lattice

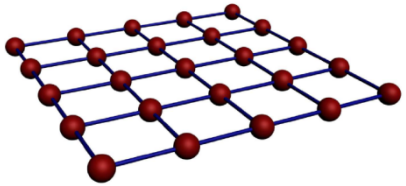
Find the optimal
Reference System
Bath hybridization

Expand around
DMFT solution

A.Georges, et al, Rev. Mod. Phys. (1996)

Beyond DMFT: Dual Fermion scheme

General Lattice Action $H = h + U$

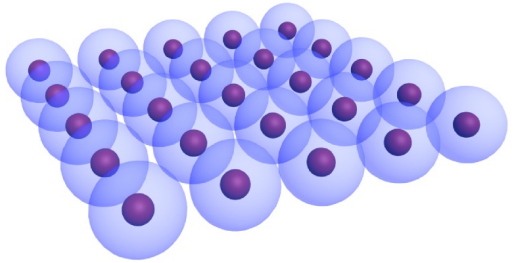


$$S[c^*,c] = \sum_{\omega k m m' \sigma} \left[h_k^{mm'} - (i\omega + \mu)1\right] c^*_{\omega k m \sigma} c_{\omega k m' \sigma} + \frac{1}{4} \sum_{i\{m,\sigma\}} \int_0^\beta U_{1234} c_1^* c_2^* c_3 c_4 d\tau$$

Reference system: Local Action with hybridization Δ_ω

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

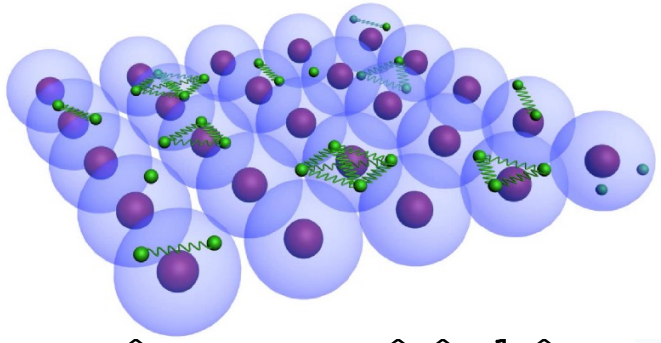
Lattice-Impurity connection:



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

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

Dual Fermions



Gaussian path-integral

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

With

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

new Action:

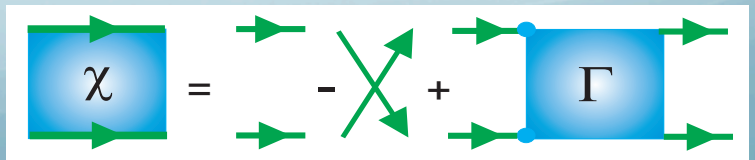
$$S_d[f^*,f]=-\sum_{k\omega}\mathcal{G}^{-1}_{k\omega}f^*_{k\omega}f_{k\omega}+\frac{1}{4}\sum_{1234}\gamma^{(4)}_{1234}f^*_1f^*_2f_4f_3+\ldots$$

Diagrammatic:

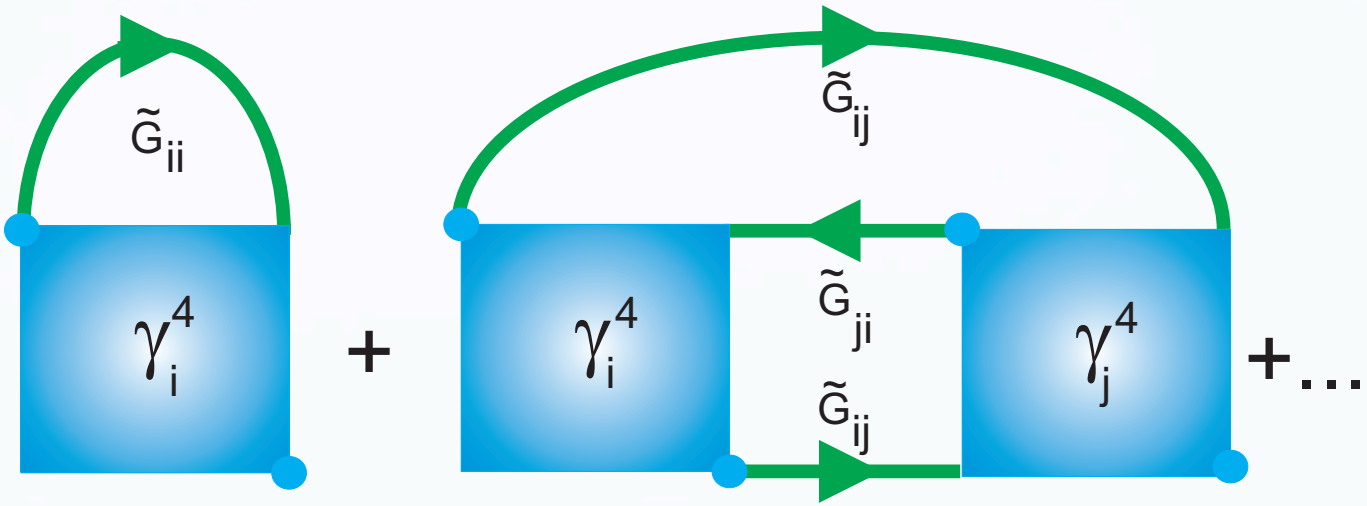
$$\tilde{\mathcal{G}}_{k\omega}=(g_\omega^{-1}+\Delta_\omega-t_k)^{-1}-g_\omega$$

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

g_ν and $\chi_{\omega,\nu,\nu'}$ from CT-QMC impurity solver



Dual Fermions: Diagrams



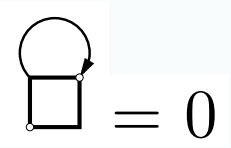
$$\tilde{\Sigma}^{(1)}_{12} = -T \sum_{34} \gamma_{1324}\, \tilde{G}^{\mathrm{loc}}_{43}$$

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

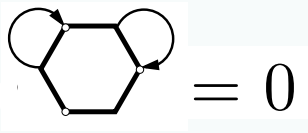
Condition for Δ and relation to DMFT

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

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



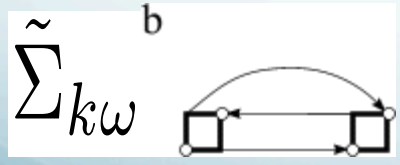
$$\frac{1}{N}\sum_{\mathbf{k}} \tilde{G}^0_\omega(\mathbf{k}) = 0 \quad \Longleftrightarrow \quad \frac{1}{N}\sum_{\mathbf{k}} G^{\mathrm{DMFT}}_\omega(\mathbf{k}) = g_\omega$$



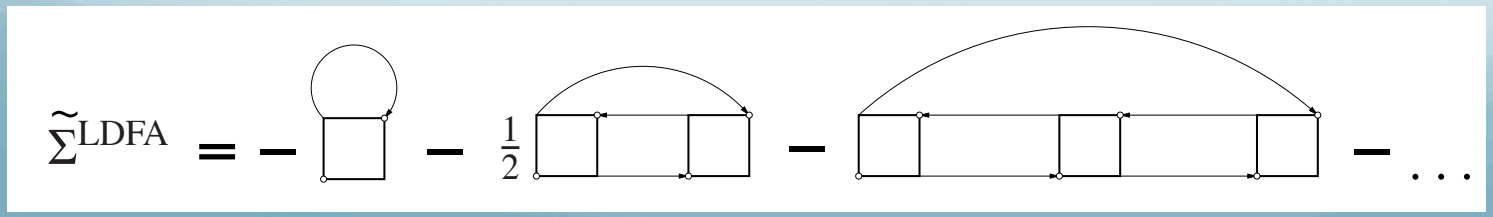
Higher-order diagrams give corrections to the DMFT self-energy,
and already the leading-order correction is nonlocal.

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

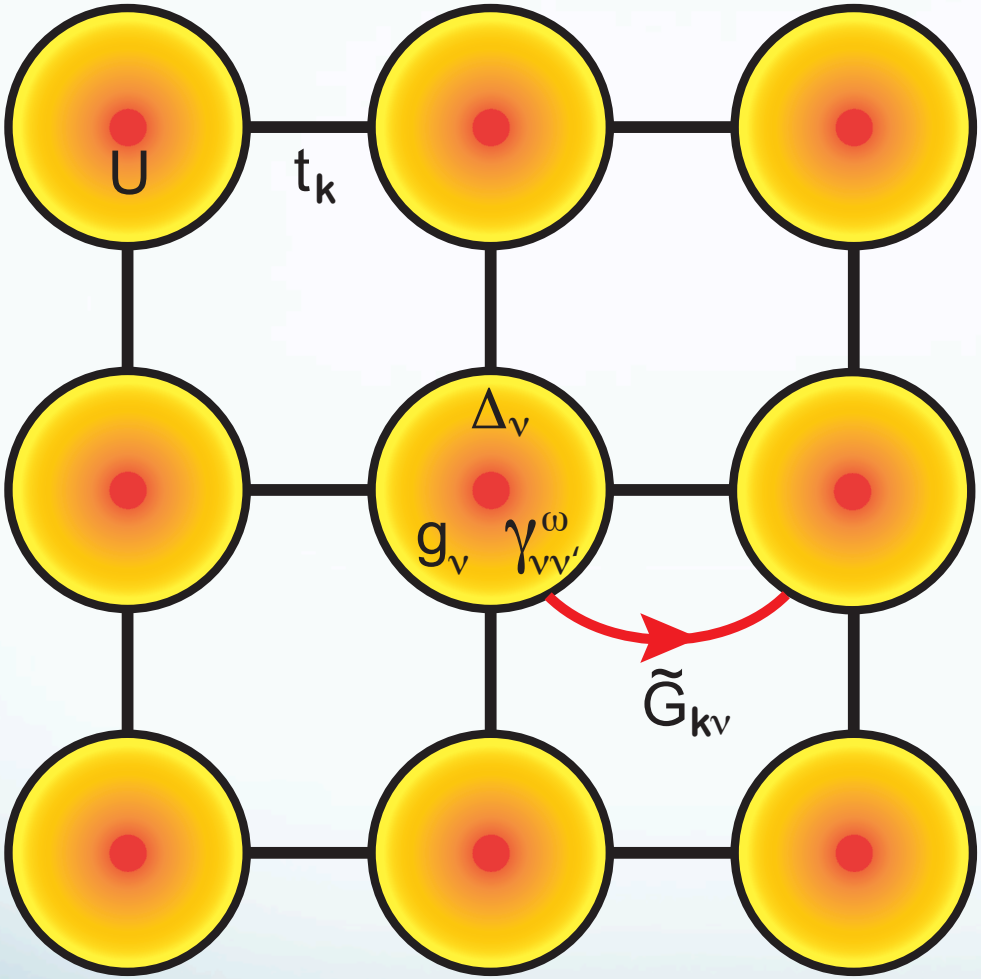
à la impurity T-matrix

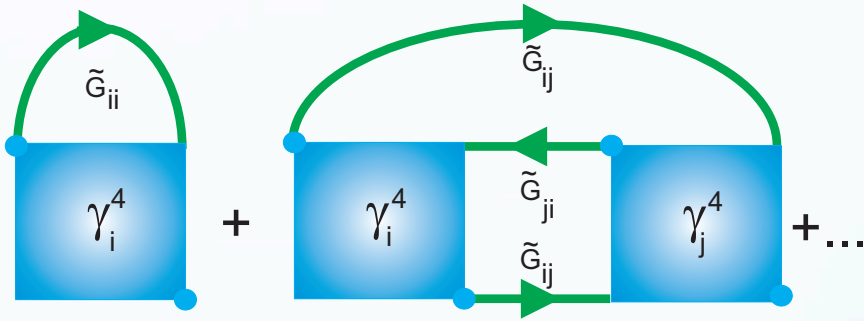


$$G_{k\omega} = [(g_\omega + g_\omega \tilde{\Sigma}_{k\omega} g_\omega)^{-1} + \Delta_\omega - t_k]^{-1}$$



Dual Fermion: Beyond DMFT

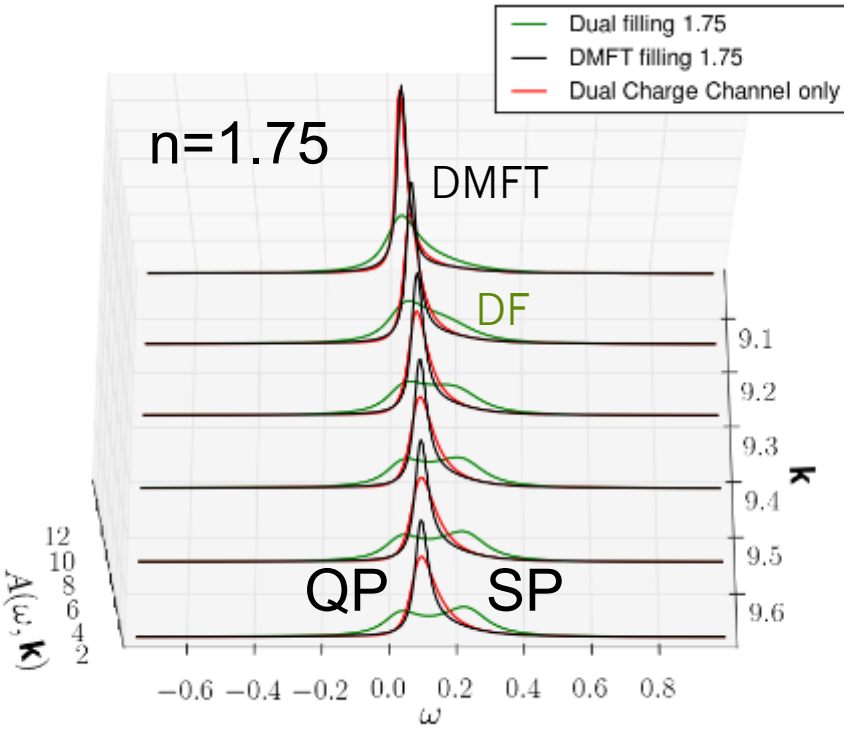


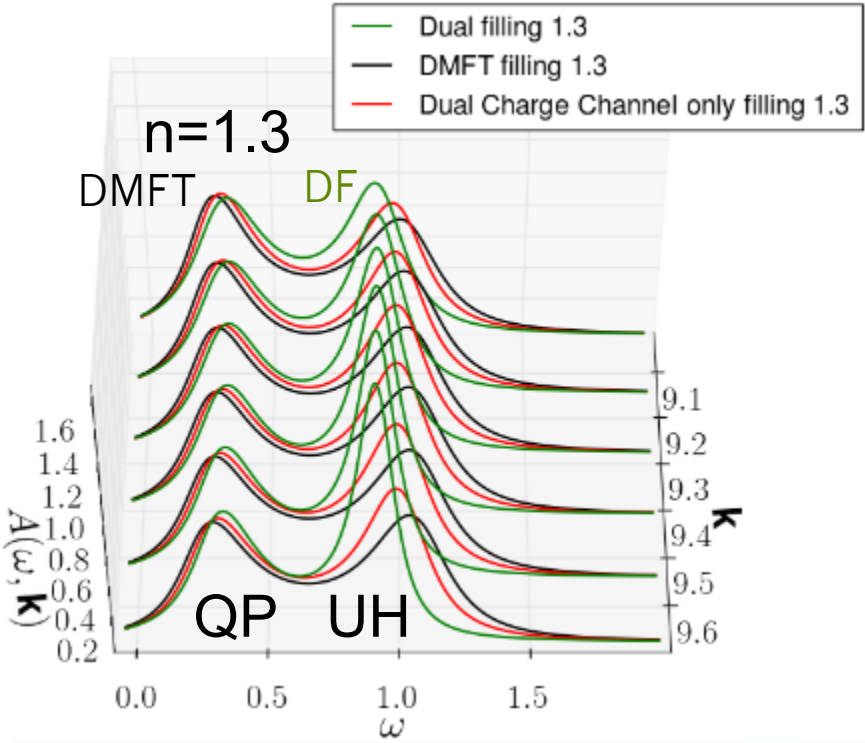


$$G_{k\omega} = [(g_\omega + g_\omega \tilde{\Sigma}_{k\omega} g_\omega)^{-1} + \Delta_\omega - t_k]^{-1}$$

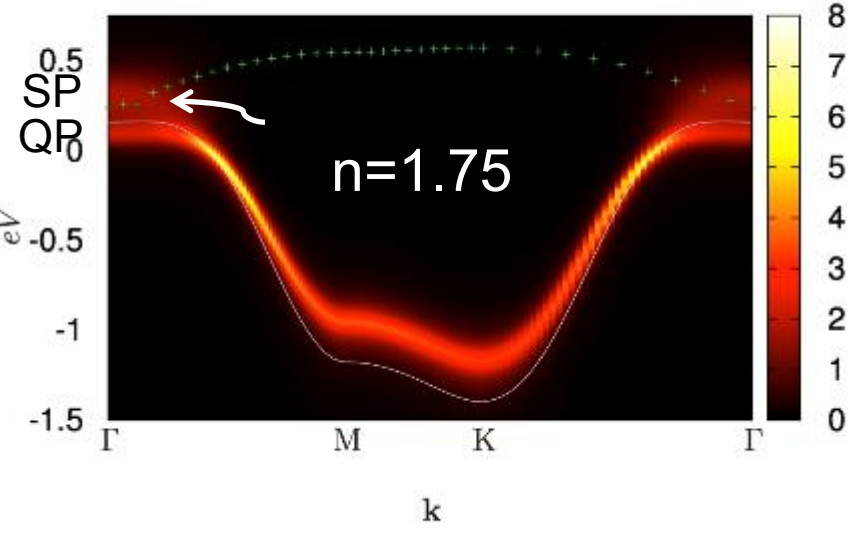
A. Rubtsov, et al, PRB **77**, 033101 (2008)

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)

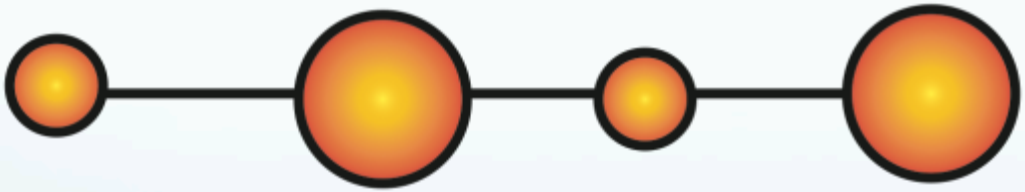
Spin-Polaron physics for n=1.75

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

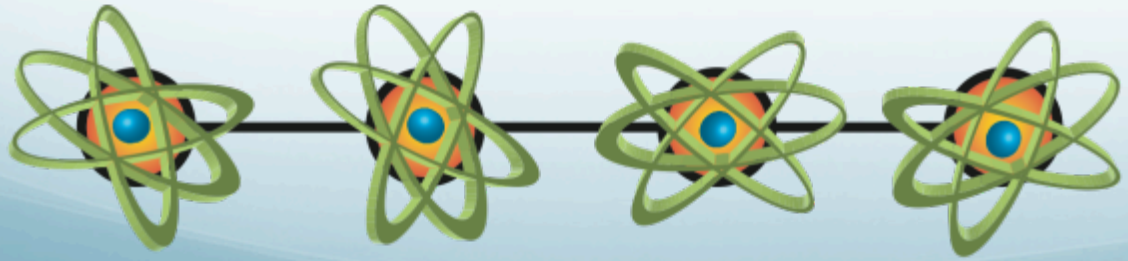
1d t-J model, M. Katsnelson (1982)

Interaction of electrons with collective excitations

Magnons

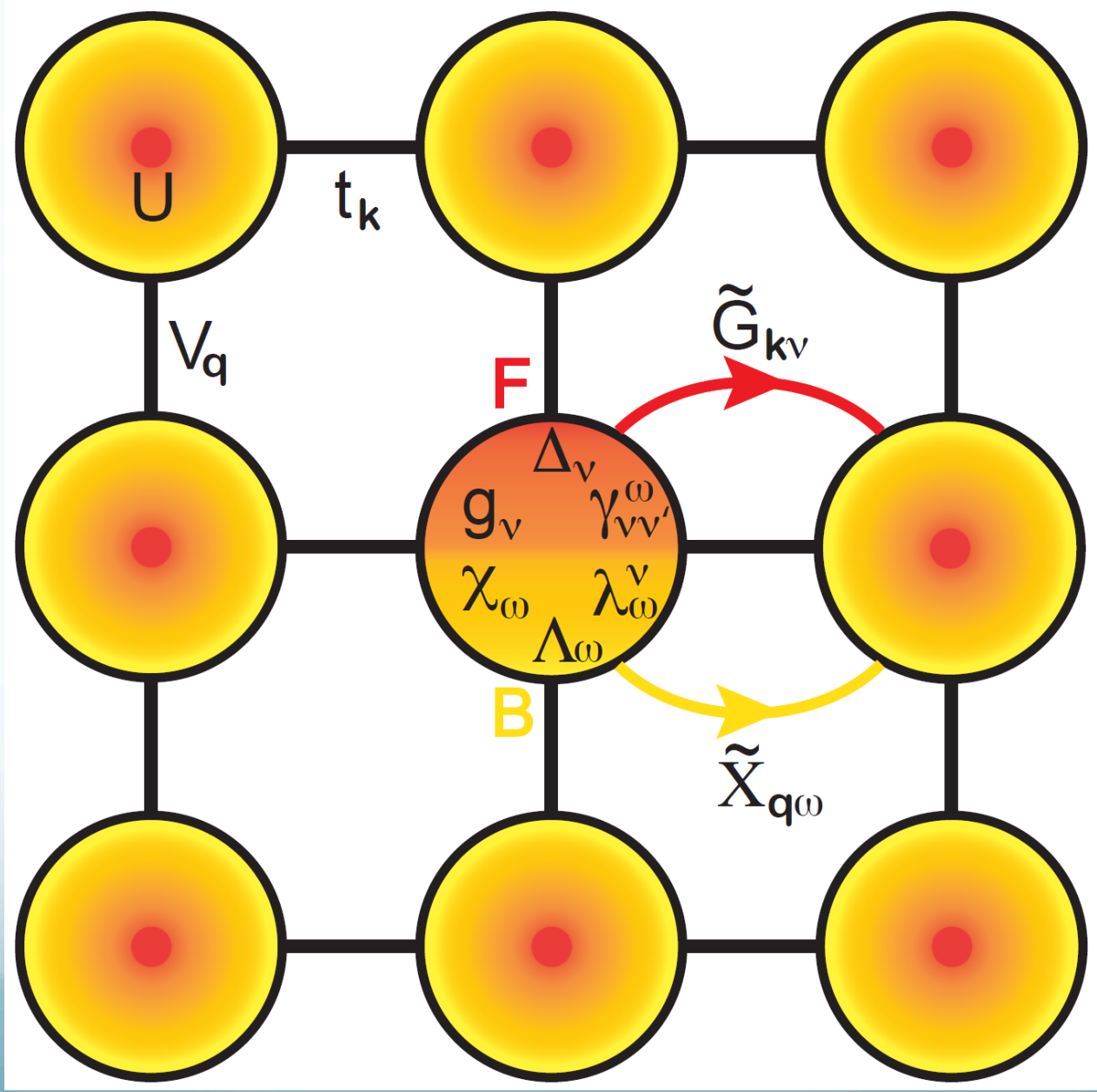


Plasmons



Orbitons

Dual Boson: General Idea

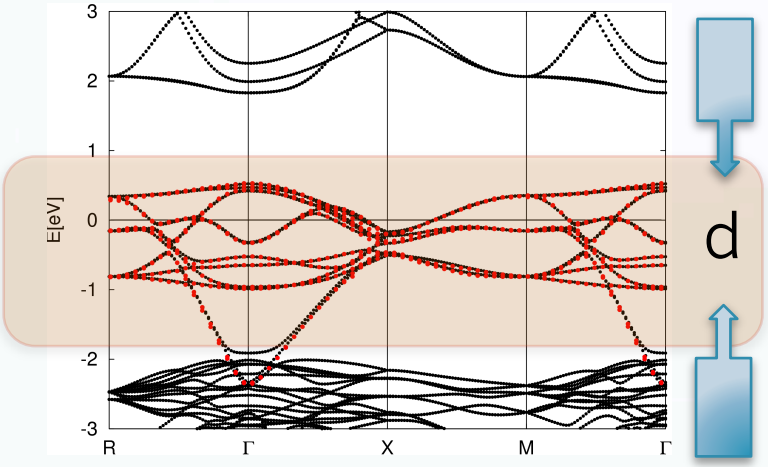


HTSC

$\Lambda_\omega \sim J_{\tau\tau'}\vec{S}_\tau \cdot \vec{S}_{\tau'}$

Non-local screened interactions

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



c-RPA screening

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

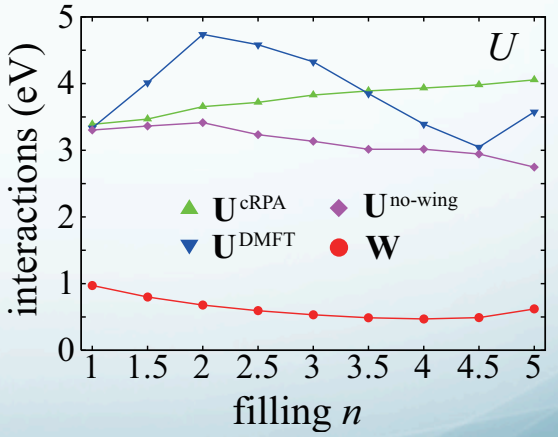
V. Mazurenko, et al, arXiv:1610.04059

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

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

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

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)

Screened Non-Local U

Starting „low-energy“ Hamiltonian with screened interactions (also Jq S*S)

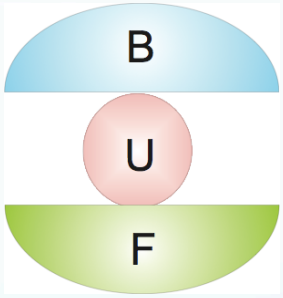
$$S = -\sum_{\mathbf{k}\nu\sigma} G^{-1}_{0\mathbf{k}\nu} c^{+}_{\mathbf{k}\nu\sigma} c_{\mathbf{k}\nu\sigma} + \frac{1}{2}\sum_{\mathbf{q}\omega} U_{\mathbf{q}\omega} n^{*}_{\mathbf{q}\omega} n_{\mathbf{q}\omega}$$

Only „d-bands“ bare Green‘s function $n_{\mathbf{q}\omega} = \sum_{\mathbf{k}\nu\sigma}(c^{+}_{\mathbf{k}\nu} c_{\mathbf{k}+\mathbf{q},\nu+\omega} - \langle c^{+}_{\mathbf{k}\nu} c_{\mathbf{k}\nu}\rangle \delta_{\mathbf{q}\omega})$

$$G_{0\mathbf{k}\nu} = [i\nu + \mu - \varepsilon_{\mathbf{k}}]^{-1}$$

Screened Coulomb interaction for „d-bands“

$$U_{\mathbf{q}\omega} = U_{\omega} + V_{\mathbf{q}\omega}$$



Reference System $S = \sum_i S^{(i)}_{\mathrm{ref}} + \Delta S$

$$S_{\mathrm{ref}} = -\sum_{\nu\sigma} \mathcal{G}_{0\,\mathbf{k}\nu} c^{+}_{\nu\sigma} c_{\nu\sigma} + \frac{1}{2}\sum_{\omega} \mathcal{U}_{\omega}\, n^{*}_{\omega} n_{\omega}$$

$$\Delta S = \sum_{\mathbf{k}\nu\sigma} \tilde{\varepsilon}_{\mathbf{k}\nu}\, c^{+}_{\mathbf{k}\nu\sigma} c_{\mathbf{k}\nu\sigma} + \frac{1}{2}\sum_{\mathbf{q}\omega} \tilde{U}_{\mathbf{q}\omega}\, n^{*}_{\mathbf{q}\omega} n_{\mathbf{q}\omega}$$

Notations:

$$\mathcal{G}_{0\,\mathbf{k}\nu} = [i\nu + \mu - \Delta_{\nu}]^{-1}$$

$$\tilde{\varepsilon}_{\mathbf{k}\nu} = \varepsilon_{\mathbf{k}} - \Delta_{\nu}$$

$$\tilde{U}_{\mathbf{q}\omega} = U_{\mathbf{q}\omega} - \mathcal{U}_{\omega}$$

Dual Boson Transformation

Effective reference interactions: $\mathcal{U}_\omega = U_\omega + \Lambda_\omega$

Effective inon-local interactions: $U_{\mathbf{q}\omega} - \mathcal{U}_\omega = V_{\mathbf{q}\omega} - \Lambda_\omega$

Definition of correlation functions

$$G_{\mathbf{k}\nu}/G^{\mathrm{ref}}_\nu = -\left\langle c \;\; c^+ \right\rangle_{\mathbf{k}\nu/\nu\,\mathrm{ref}},$$
$$X_{\mathbf{q}\omega}/\chi_\omega = -\left\langle n \;\; n^* \right\rangle_{\mathbf{q}\omega/\omega\,\mathrm{ref}},$$
$$\mathcal{W}_\omega = \mathcal{U}_\omega + \mathcal{U}_\omega \chi_\omega \mathcal{U}_\omega,$$

Bosonic Hubbard-Stratanovich transformation

$$e^{\frac{1}{2}\sum_{\mathbf{q}\omega} n^*_{\mathbf{q}\omega}\tilde{U}_{\mathbf{q}\omega} n_{\mathbf{q}\omega}} = \sqrt{\det[\tilde{U}^{-1}_{\mathbf{q}\omega}]} \int D[\tilde{n}]\, e^{\frac{1}{2}\sum_{\mathbf{q}\omega}\left\{-\tilde{n}^*_{\mathbf{q}\omega}\tilde{U}^{-1}_{\mathbf{q}\omega}\tilde{n}_{\mathbf{q}\omega} + n^*_\omega \tilde{n}_\omega + \tilde{n}^*_\omega n_\omega\right\}}$$

Dual action

$$\tilde{S} = -\sum_{\mathbf{k}\nu}\tilde{G}^{-1}_{0\mathbf{k}\nu}\tilde{c}^+_{\mathbf{k}\nu\sigma}\tilde{c}_{\mathbf{k}\nu\sigma} - \frac{1}{2}\sum_{\mathbf{q}\omega}\tilde{W}^{-1}_{0\mathbf{q}\omega}\tilde{n}^*_{\mathbf{q}\omega}\tilde{n}_{\mathbf{q}\omega} + \dots$$

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

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

EDMFT

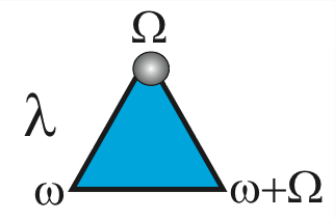
Rescale: $\tilde{n}_{\mathbf{q}\omega} \longrightarrow \tilde{n}_{\mathbf{q}\omega}\alpha^{-1}_\omega$

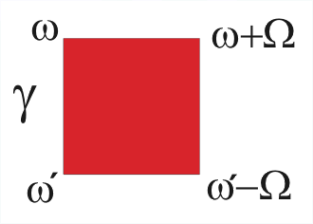
$$\alpha_\omega = \mathcal{W}_\omega/\mathcal{U}_\omega = (1 + \mathcal{U}_\omega\chi_\omega)$$

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

Effective electron boson interaction

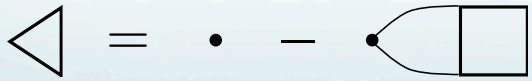
$$\tilde{V} = \gamma^3_{\nu\omega}\, \tilde{c}^+_{\nu} \tilde{c}_{\nu+\omega} \tilde{n}^*_{\omega} + \frac{1}{4}\, \gamma^4_{\nu\nu'\omega}\, \tilde{c}^+_{\nu} \tilde{c}^+_{\nu'} \tilde{c}_{\nu+\omega} \tilde{c}_{\nu'-\omega} + \ldots$$





Relation between $\gamma^3_{\nu\omega}$ and $\gamma^4_{\nu\nu'\omega}$

$$\gamma_{\nu\omega} = \alpha^{-1}_{\omega} \sum_{\nu'} \left[1 - \gamma^{4,0}_{\nu\nu'\omega} g_{\nu'} g_{\nu'-\omega}\right]$$



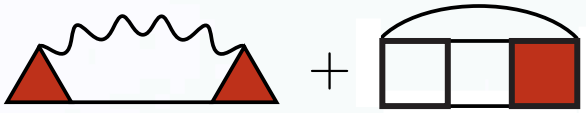
Even if $\gamma^4_{\nu\nu'\omega}$=0 there is the non-thero part of $\gamma^3_{\nu\omega} = \alpha^{-1}_{\omega}$ or

electron-boson interaction beyond EDMFT

Lattice GF and SCF-condition

Lattice two-point correlation functions

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



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

Self-consistent conditions:

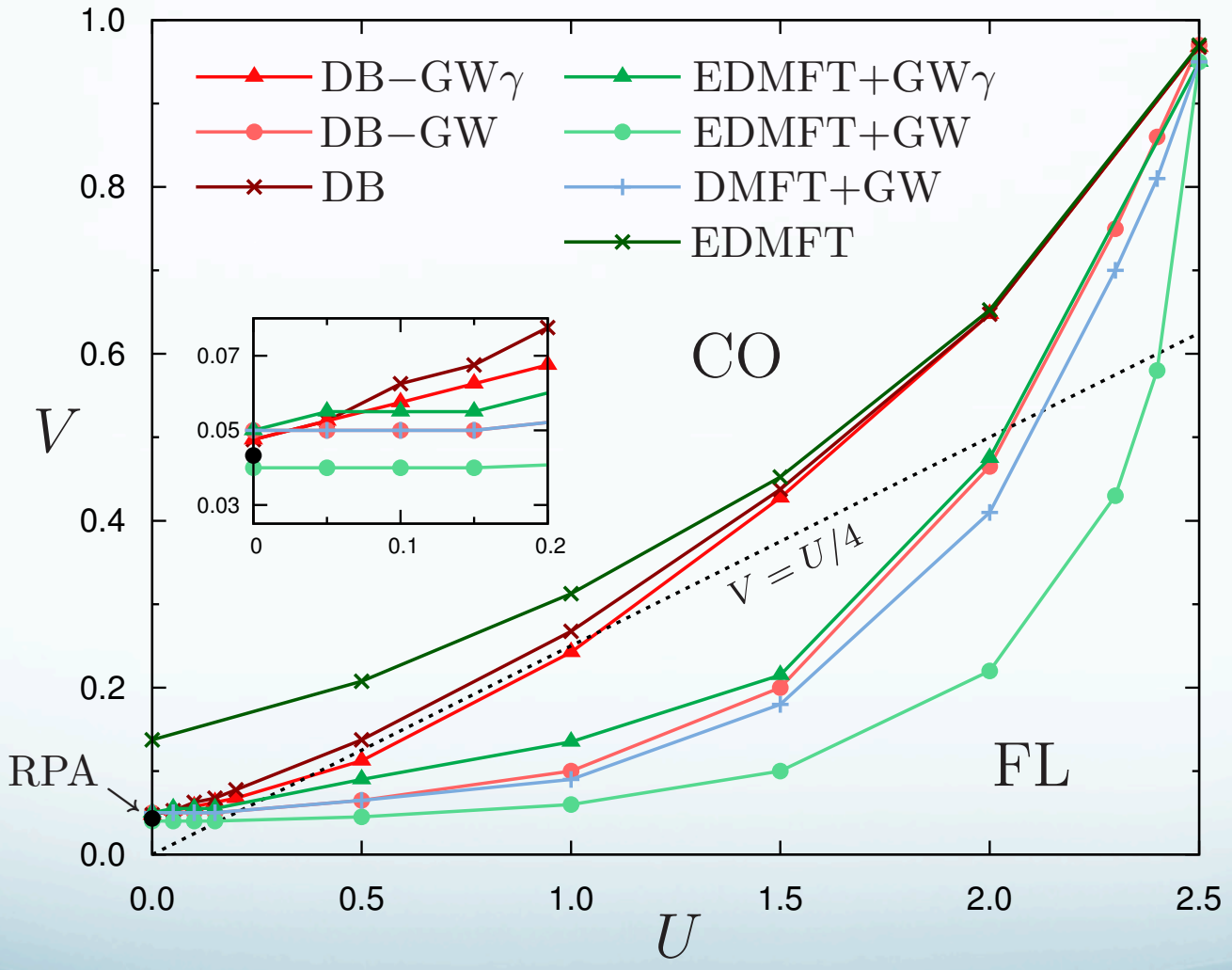
$$\sum_{\mathbf{k}} G_{\mathbf{k}\nu} = G^{\mathrm{ref}}_{\nu},$$

$$\sum_{\mathbf{q}} W_{\mathbf{q}\omega} = \mathcal{W}^{\mathrm{ref}}_{\omega}.$$

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 by E. Stepanov, A. Huber, E. van Loon, A. L., M. Katsnelson arXiv:1604.07734

Summary

- DFT+U is efficient scheme for S-O-C ordering
- DFT+DMFT is an optimal for correlated metals
- GW+DMFT is perfect for non-local screened interaction