Development of the LDA+DMFT Approach

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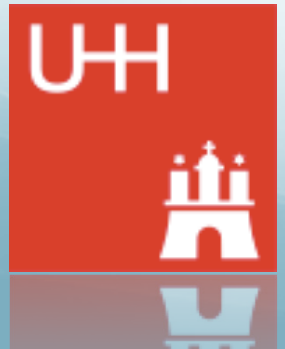

In collaboration with
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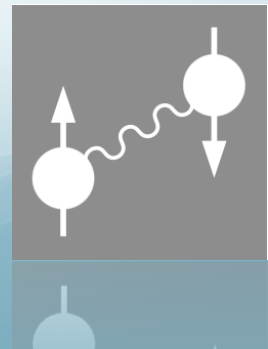
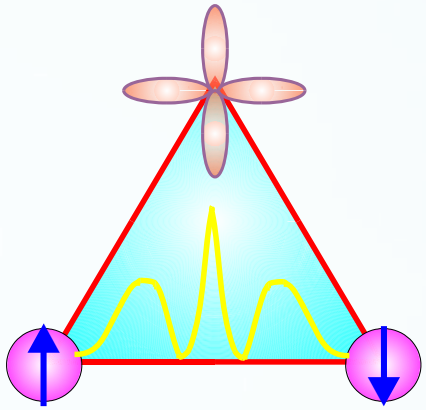
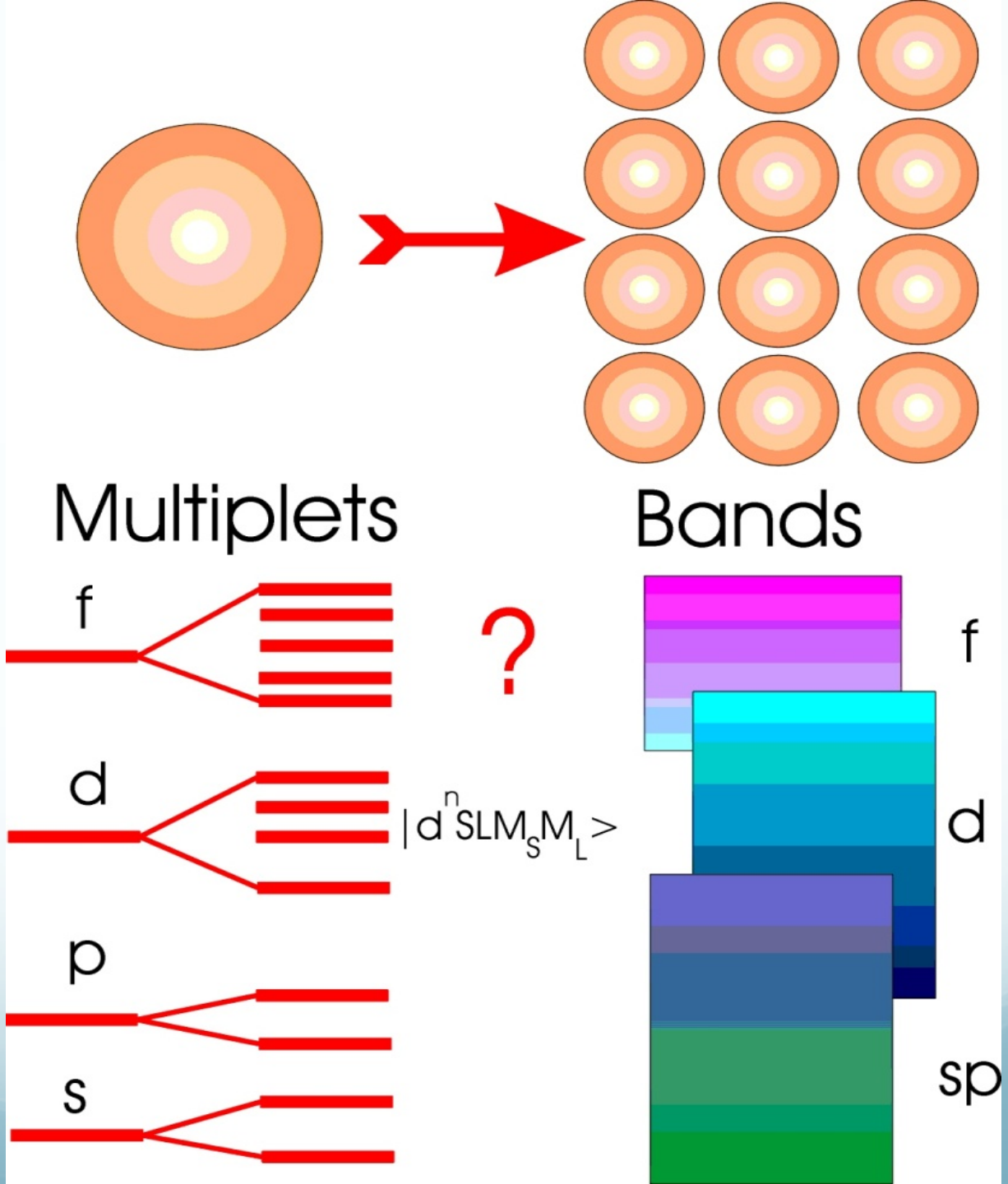


Outline



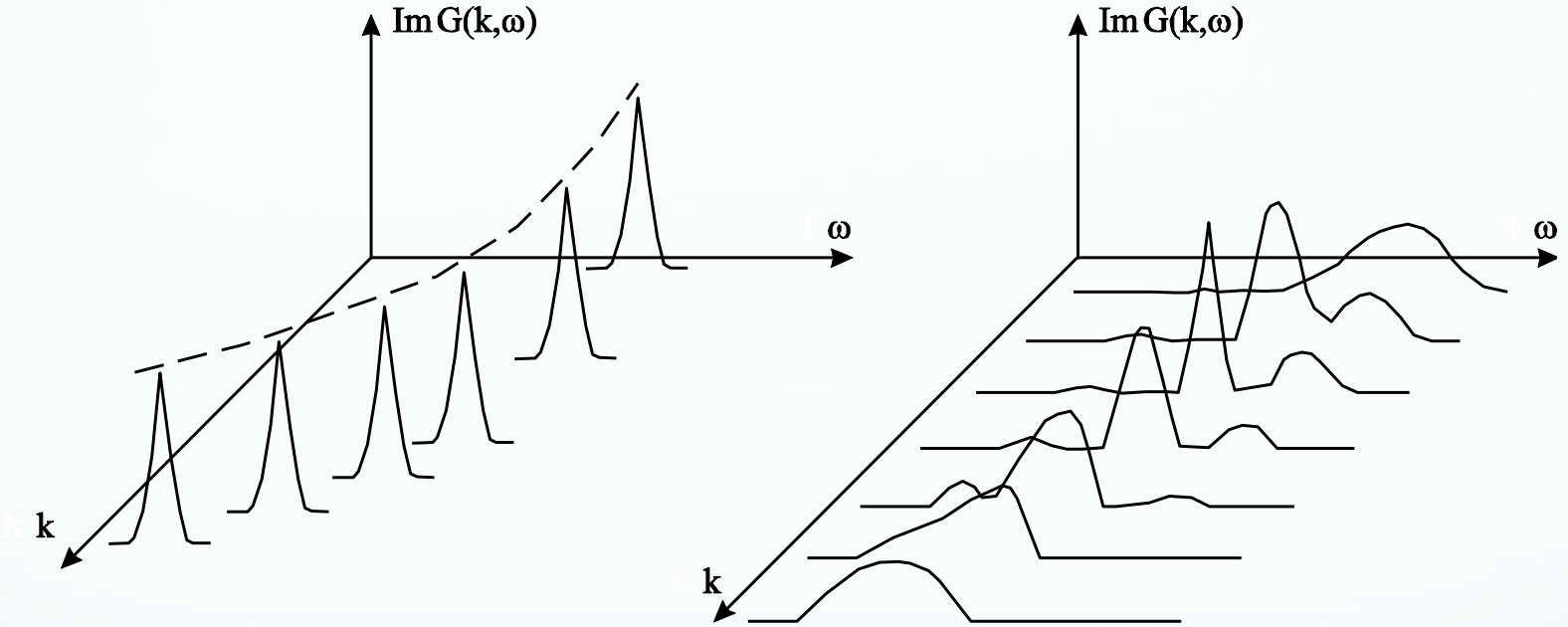
- Functional approach: from DFT to DMFT
- Local correlations: DMFT and beyond
- LDA+DMFT scheme for real materials
- Problem of double counting

From Atom to Solids



Spectral function: Correlations effects

ARPES

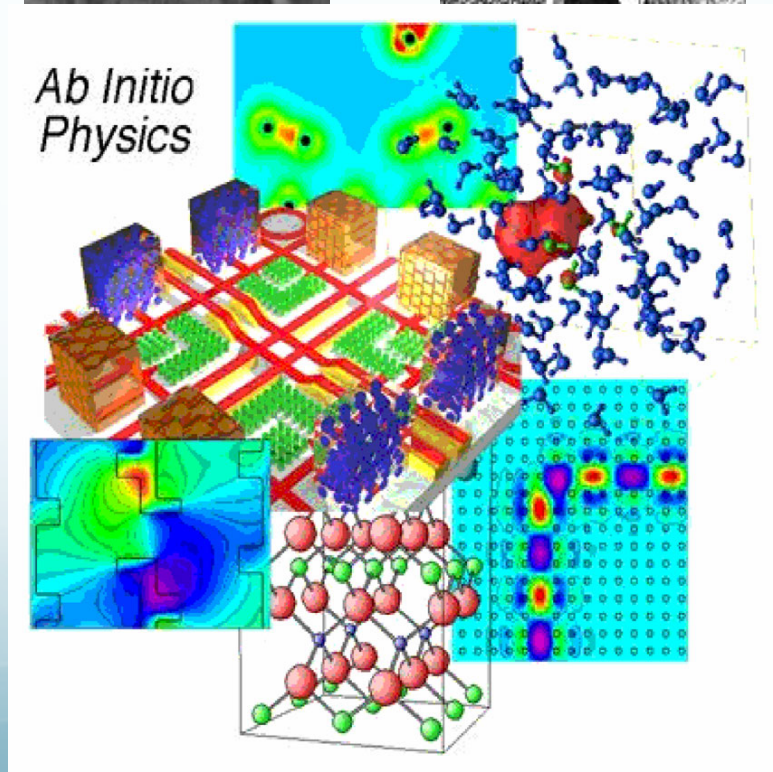


Free electrons

Correlated electrons

Computational Material Science

- Starting from Schrödinger?
- Kohn Density Functional Theory (DFT) of inhomogeneous electron gas in solids
- Strongly correlated electron systems ? Dynamical Mean-Field Theory (DMFT)



The Theory of Everything

Hamiltonian for multi-fermionic system in field-operators:

$$H = \sum_{\sigma} \int d\mathbf{r}\, \hat{\psi}^{\dagger}_{\sigma}(\mathbf{r}) \left(-\frac{1}{2}\nabla^2 + V(\mathbf{r}) - \mu \right) \hat{\psi}_{\sigma}(\mathbf{r})$$
$$+\frac{1}{2} \sum_{\sigma\sigma'} \int d\mathbf{r} \int d\mathbf{r}'\, \hat{\psi}^{\dagger}_{\sigma}(\mathbf{r}) \hat{\psi}^{\dagger}_{\sigma'}(\mathbf{r}')\, U(\mathbf{r}-\mathbf{r}')\, \hat{\psi}_{\sigma'}(\mathbf{r}') \hat{\psi}_{\sigma}(\mathbf{r})$$

Atomic Units: $\hbar = m = e = 1$

Coilomb interaction: $U(\mathbf{r}-\mathbf{r}') = 1/|\mathbf{r}-\mathbf{r}'|$

Second quantisation operators in orthonormal basis:

$$\hat{\psi}(\mathbf{r}) = \sum_{n} \phi_n(\mathbf{r}) \hat{c}_n$$
$$\hat{\psi}^{\dagger}(\mathbf{r}) = \sum_{n} \phi^{*}_n(\mathbf{r}) \hat{c}^{\dagger}_n$$

$n = (im\sigma)$

Wannier Basis: $\phi_n(\mathbf{r})$ with site, orbital andspins quantum numbers

QM-Alphabet

1-Q

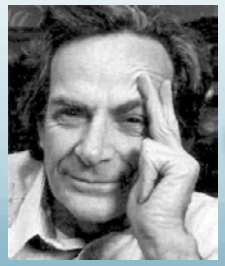
$$\left(-\frac{1}{2}\Delta + V_{eff}(\vec{r})\right)\psi(\vec{r}) = \varepsilon\psi(\vec{r})$$

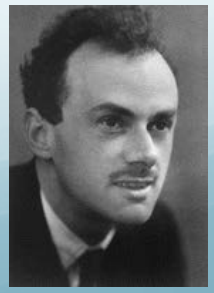
2-Q

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

3-PI

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





Path Integrals for Fermions

Short introduction from Alexei Kamenev
"Field Theory of Non-Equilibrium Systems" (Cambridge, 2011)

Fermions second-quantization operators (Pauli principle)

$$\begin{aligned} \hat{c}_i|0\rangle &= 0 \\ \hat{c}_i|1\rangle &= |0\rangle \\ \hat{c}_i^+|0\rangle &= |1\rangle \\ \hat{c}_i^+|1\rangle &= 0 \end{aligned}$$

$$\begin{aligned} \hat{c}^+\hat{c}|n\rangle &= n|n\rangle \\ \hat{c}^2 &= 0 \\ (\hat{c}^+)^2 &= 0 \\ \{\hat{c},\hat{c}^+\} &= \hat{1} \end{aligned}$$

Algebra of Grassmann anti-commuting numbers: $(\hat{c}_i^+, \hat{c}_i) \to (c_i^*, c_i)$

$$\begin{aligned} c_i c_j &= -c_j c_i \\ c_i^2 &= 0 \\ f(c) &= f_0 + f_1 c \\ f(c^*, c) &= f_{00} + f_{10}c^* + f_{01}c + f_{11}c^* c \end{aligned}$$

Grassmann numbers anticommute with fermionic operators

$$\{c, \hat{c}\} = \{c, \hat{c}^+\} = 0$$

Grassmann calculus

Differentiation: $\frac{\partial c_i}{\partial c_j} = \delta_{ij}$

N.B. order: $\frac{\partial}{\partial c_2} c_1 c_2 = -c_1$

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

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

Integration: (equivalent to differetition)

$$\int 1 dc = 0$$

$$\int c dc = 1$$

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

Coherent State

Eigenstate of annihilation operator

$$\hat{c}\,|c\rangle \;=\; c\,|c\rangle$$

Diefinition of coherent states

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

Proof

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

Left Coherent State: c^{*} is just another Grassman number

(NOT a complex conjugate)

$$\begin{aligned}
\langle c|\,\hat{c}^{+} &= \langle c|\,c^{*} \\
\langle c| &= \langle 0|\,e^{-\hat{c}c^{*}} = \langle 0|\,(1 - \hat{c}c^{*}) = \langle 0| - \langle 1|\,c^{*} \\
\langle c|\,\hat{c}^{+} &= (\langle 0| - \langle 1|\,c^{*})\,\hat{c}^{+} = -\langle 1|\,c^{*}\hat{c}^{+} = \langle 0|\,c^{*} = \langle c|\,c^{*}
\end{aligned}$$

Unity operator in coherent states

Overlap of Coherent States (non-orthogonal)

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

Resolution of Unity

$$\hat{1} = \int\int dc^* dc e^{-c^* c} |c\rangle \langle c|$$

Proof

$$\begin{aligned} \int\int dc^* dc e^{-c^* c} |c\rangle \langle c| &= \int\int dc^* dc (1 - c^* c)(|0\rangle - c|1\rangle)(\langle 0| - \langle 1| c^*) \\ &= -\int\int dc^* dc c^* c (|0\rangle \langle 0| + |1\rangle \langle 1|) = \hat{1} \end{aligned}$$

Trace of Fermionic Operators

Matrix elements of normally ordered operators

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

Trace-formula

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

"Minus" due to commutation Left and Right coherent state

$$c^* c = -c c^*$$

$$|-c\rangle = |0\rangle + c\,|1\rangle$$

Partition Function in Path Integral

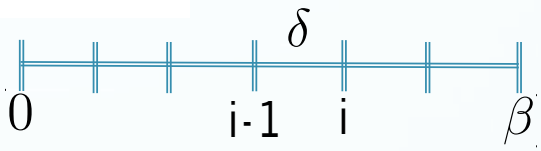
Partition Function

$$Z = Tr e^{-\beta(\hat{H}-\mu\hat{N})}$$

Using Trace Formula

$$Z = \int\int \prod_{i=1}^{N} [dc_i^* dc_i]\, e^{-\sum_{i=1}^{N} c_i^* c_i} \langle \xi c |\, e^{-\beta(\hat{H}-\mu\hat{N})}\, | c \rangle$$

Discretize $[0, \beta]$ interval with N-points $\delta = \beta/N$



$$Z = \int_{(0=\xi N)} \prod_{i=1}^{N} [dc_i^* dc_i]\, e^{-\delta \sum_{i=1}^{N} c_i^*(c_i - c_{i-1})/\delta + H(c_i^*, c_{i-1}) - \mu N(c_i^*, c_{i-1})}$$

Continuous time limit with BC: $c(0) = \xi c(\beta)$ $\xi = -1$ for fermions

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

$$S[c^*, c] = \int_0^\beta d\tau [c^* \partial_\tau c + H(c^*, c) - \mu N(c^*, c)]$$

Gaussian Path Integrals

Only one analytical path integral:

$$Z\left[J^*, J\right] = \int\int \prod_{i=1}^{N} \left[dc_i^* dc_i\right] e^{-\sum_{i,j=1}^{N} c_i^* M_{ij} c_j + \sum_{i=1}^{N}\left[c_i^* J_i + J_i^* c_i\right]} = \det\left[M\right] e^{-\sum_{i,j=1}^{N} J_i^* M_{ij}^{-1} J_j}$$

Short notation

$$\int D\left[c^* c\right] e^{-c^* M c} = \det M$$

Proof - "det": expand the exponent only N-th oder is non-zero

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

Permutations of c_i^* and c_j gives $\det M$

Examples:

N=1

$$\int D\left[c^* c\right] e^{-c_1^* M_{11} c_1} = \int D\left[c^* c\right] \left(-c_1^* M_{11} c_1\right) = M_{11} = \det M$$

N=2

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

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

$$M_{11} M_{22} - M_{12} M_{21} = \det M$$

Correlation Function: U=0

Change of variables

$$c \to c - M^{-1} j$$

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

Single-particle correlation function:

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

Two-particle correlation function:

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

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

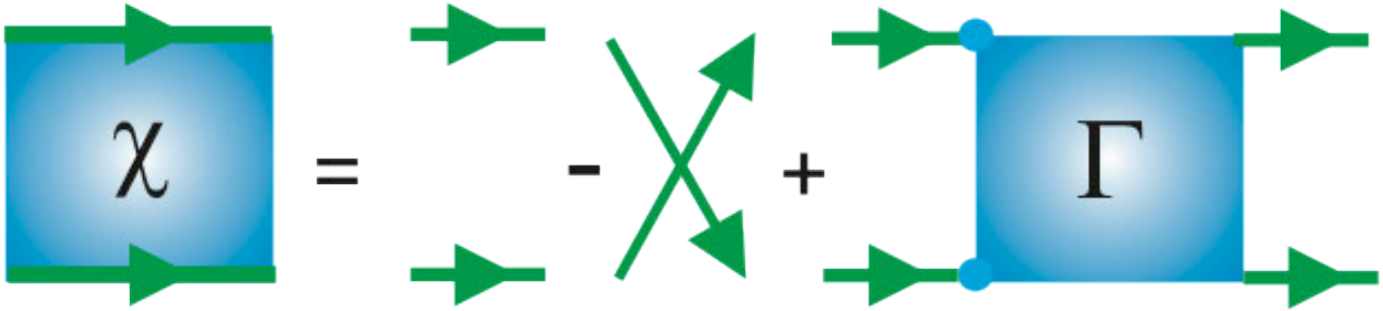
$$G_{12} = -\langle c_1 c_2^* \rangle_S = -\frac{1}{Z} \int \mathcal{D}[c^*, c]\, c_1 c_2^*\, e^{-S}$$

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:

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



Baym-Kadanoff functional

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

Partition function and Free-energy:

$$Z[J] = e^{-F[J]} = \int \mathcal{D}[c^*, c]\, e^{-S[J]}$$

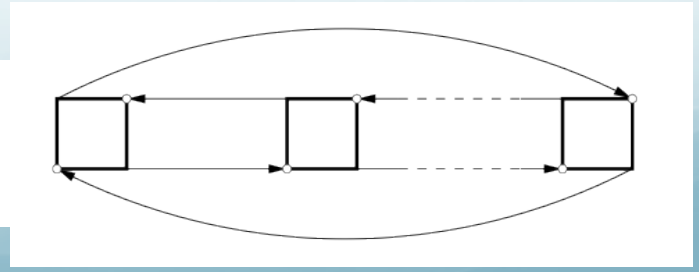
Legendre transforming from J to G:

$$F[G] = F[J] - \mathrm{Tr}(JG)$$

$$G_{12} = \frac{1}{Z[J]} \frac{\delta Z[J]}{\delta J_{12}}\bigg|_{J=0} = \frac{\delta F[J]}{\delta J_{12}}\bigg|_{J=0}$$

Decomposition into the single particle part and correlated part

$$F[G] = \mathrm{Tr} \ln G - \mathrm{Tr}\,(\Sigma G) + \Phi[G]$$

$\Phi[G] = \sum_i$ 

Functional Family

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

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 constrained field J:

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

G. Kotliar et. al. RMP (2006), A. Georges (2004) arXiv:0403123

DFT: KS-equation (1965)

Effective one-electron Schrödinger-like equation:

$$(-\frac{\hbar^2}{2m}\nabla^2 - V_{eff}(\vec{r}))\psi_i(\vec{r}) = \varepsilon_i\psi_i(\vec{r})$$

Charge density:

$$n(\vec{r}) = \sum_i^N |\psi_i(\vec{r})|^2$$

Energy Functional:

$$E[n] = T_s[n] + V_H[n] + \int n(\vec{r})V_{ext}(\vec{r})d\vec{r} + E_{xc}[n]$$

KS-kinetic energy:

$$T_s[n] = \sum_i^N \int d\vec{r}\psi_i^*(\vec{r})(-\frac{\hbar^2}{2m}\nabla^2)\psi_i(\vec{r})$$

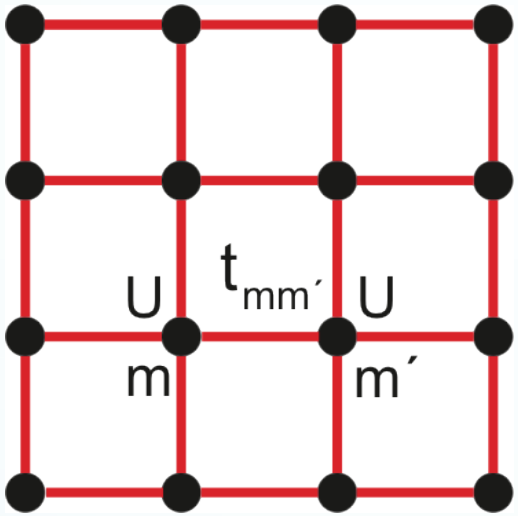
Hartree potential:

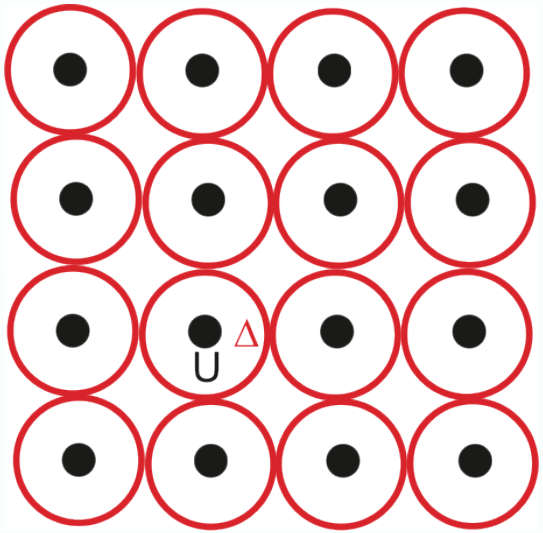
$$V_H[n] = \frac{e^2}{2}\int d\vec{r}\int d\vec{r}'\frac{n(\vec{r})n(\vec{r}')}{|\vec{r}-\vec{r}'|}$$

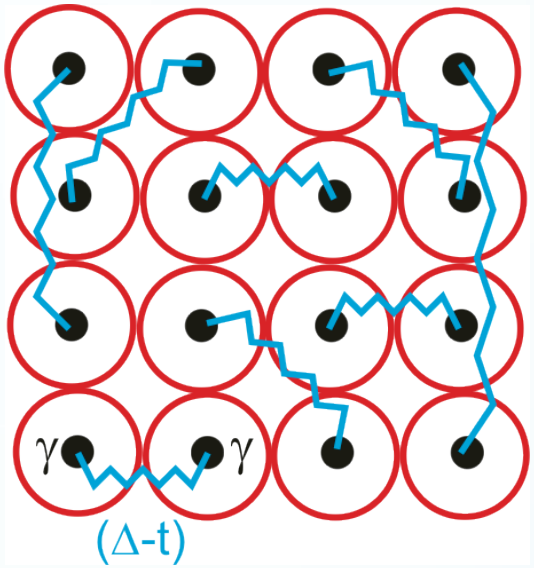
Effective potential:

$$V_{eff}(\vec{r}) = V_{ext}(\vec{r}) + e^2\int d\vec{r}'\frac{n(\vec{r}')}{|\vec{r}-\vec{r}'|} + \frac{\delta E_{xc}[n]}{\delta n(\vec{r})}$$

DMFT-functional and beyond







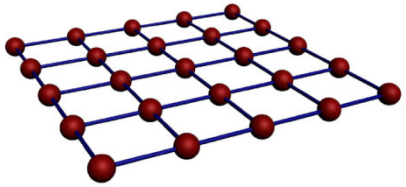
Start from
Correlated Lattice

Find the optimal
Reference System
Bath hybridization

Expand around
DMFT solution

Dual Fermion scheme

General Lattice Action $H = h + U$

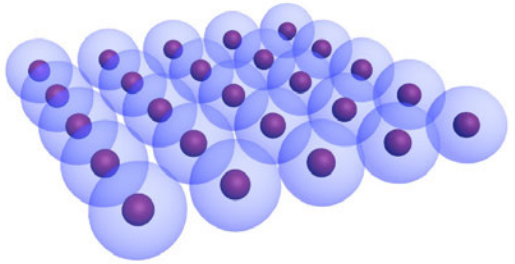


$$S[c^*,c] = \sum_{\omega k m m' \sigma} \left[h_k^{mm'} - (i\omega+\mu)1\right] c^*_{\omega k m \sigma} c_{\omega k m' \sigma} + \frac{1}{4} \sum_{i\{m,\sigma\}} \int_0^\beta U_{1234} c_1^* c_2^* c_3 c_4 d\tau$$

Reference system: Local Action with hybridization Δ_ω

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

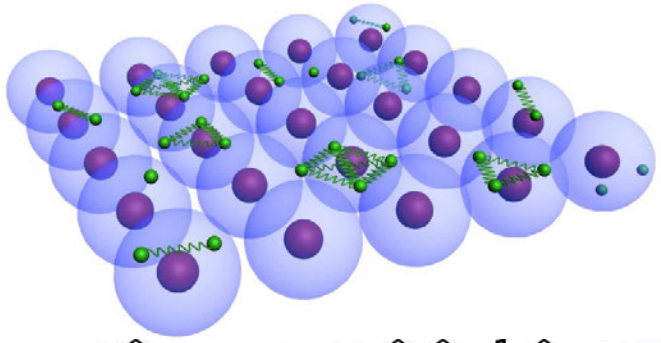
Lattice-Impurity connection:



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

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:

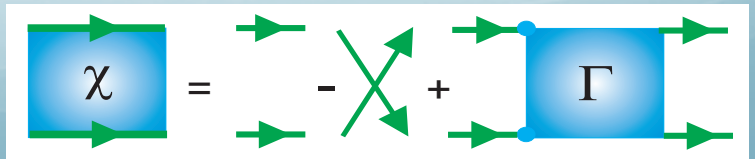
$$S_d[f^*,f]=-\sum_{k\omega}\mathcal{G}^{-1}_{k\omega}f^*_{k\omega}f_{k\omega}+\frac{1}{4}\sum_{1234}\gamma^{(4)}_{1234}f^*_1f^*_2f_4f_3+\ldots$$

Diagrammatic:

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

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

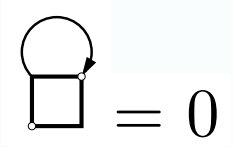
g_ν and $\chi_{\omega,\nu,\nu'}$ from CT-QMC impurity solver

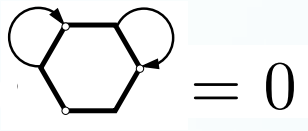


Condition for Δ and relation to DMFT

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

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

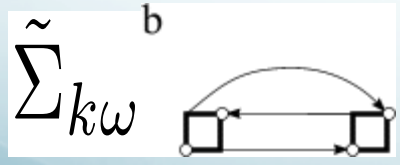




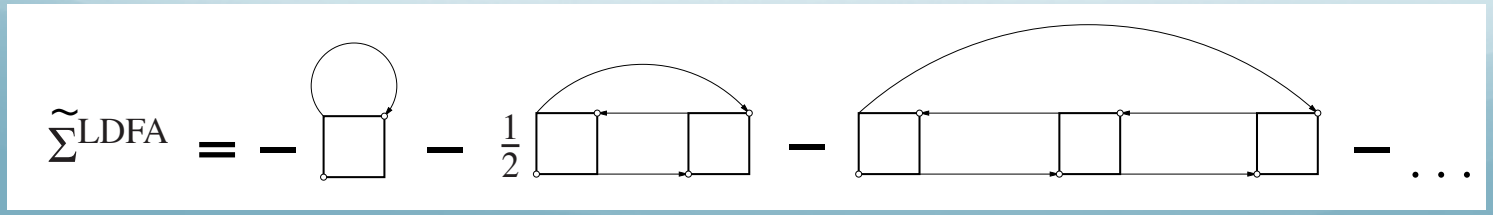
$$\frac{1}{N}\sum_{\mathbf{k}} \tilde{G}^0_\omega(\mathbf{k}) = 0 \quad \Longleftrightarrow \quad \frac{1}{N}\sum_{\mathbf{k}} G^{\mathrm{DMFT}}_\omega(\mathbf{k}) = g_\omega$$

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

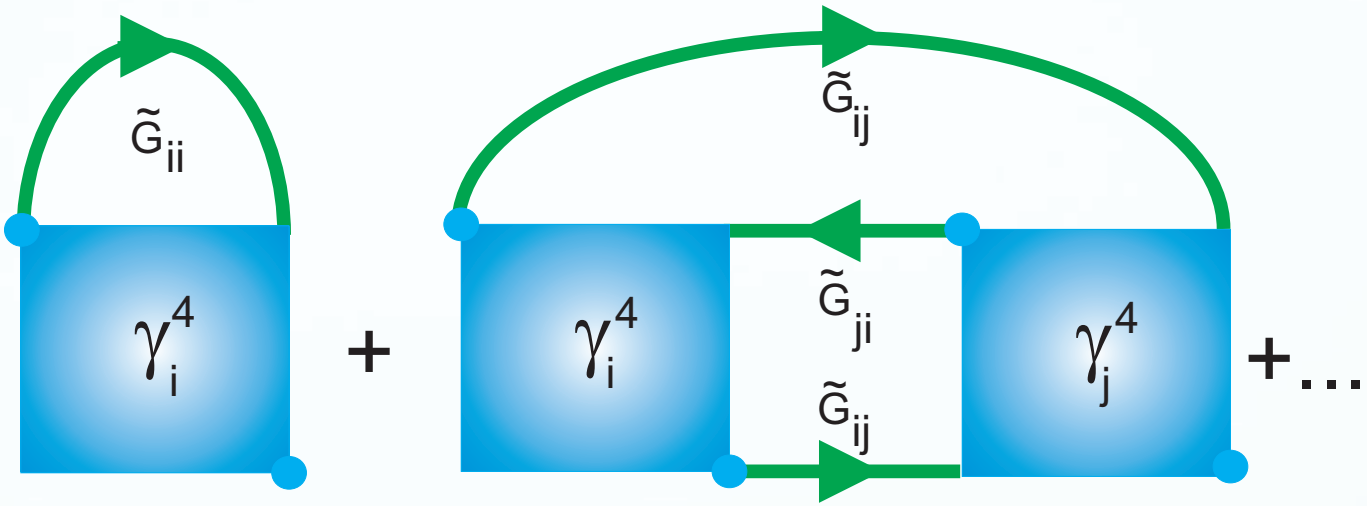
$\Sigma(k,\omega) = \Sigma_{DMFT}(\omega) + \tilde{\Sigma}(k,\omega)/[1+g\tilde{\Sigma}(k,\omega)]$ à la impurity T-matrix



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



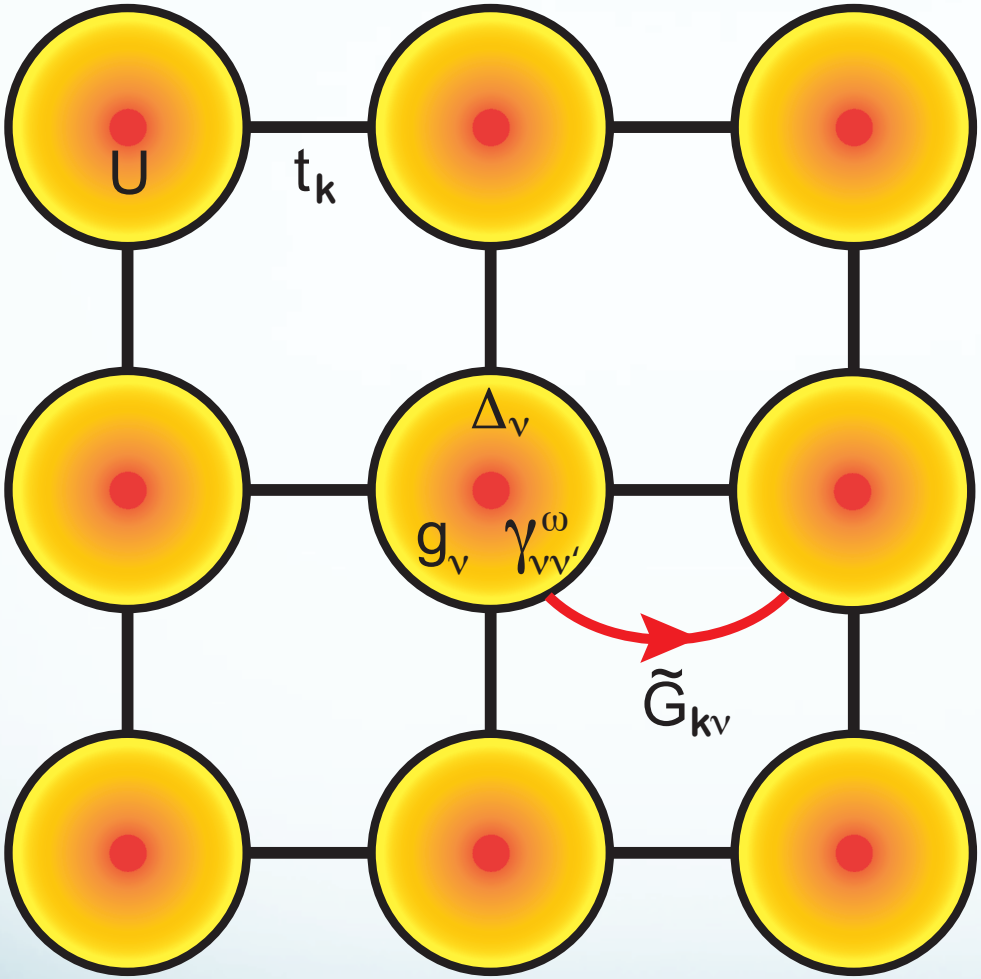
Dual Fermions: Diagrams

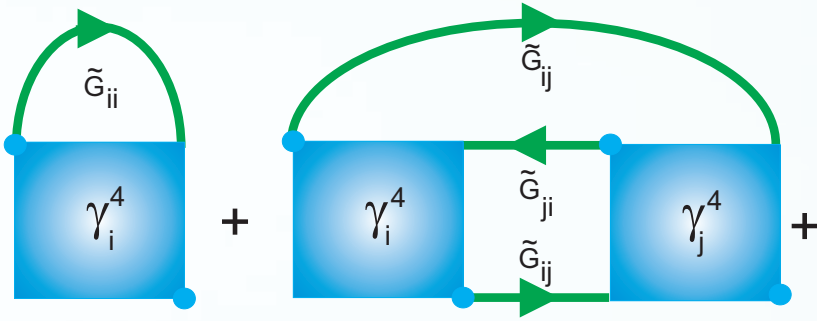


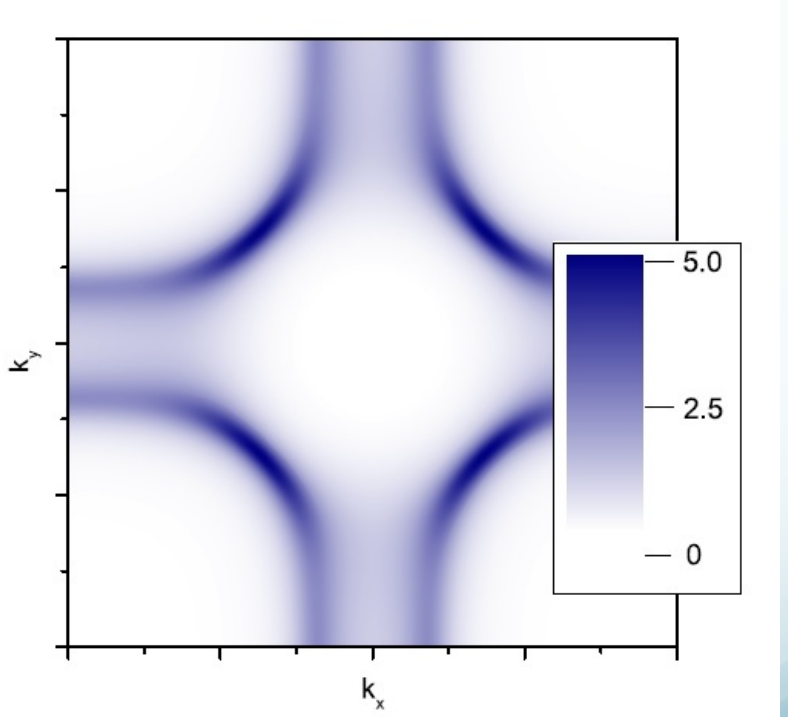
$$\tilde{\Sigma}^{(1)}_{12} = -T \sum_{34} \gamma_{1324}\, \tilde{G}^{\mathrm{loc}}_{43}$$

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

Dual Fermion: non-local correlations







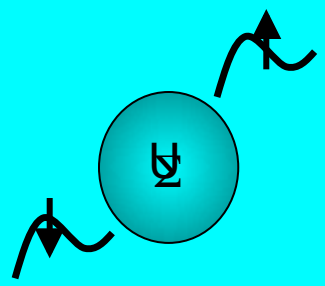
$$G_{k\omega} = [(g_\omega + g_\omega \tilde{\Sigma}_{k\omega} g_\omega)^{-1} + \Delta_\omega - t_k]^{-1}$$

FS of HTSC: cold and hot spots

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

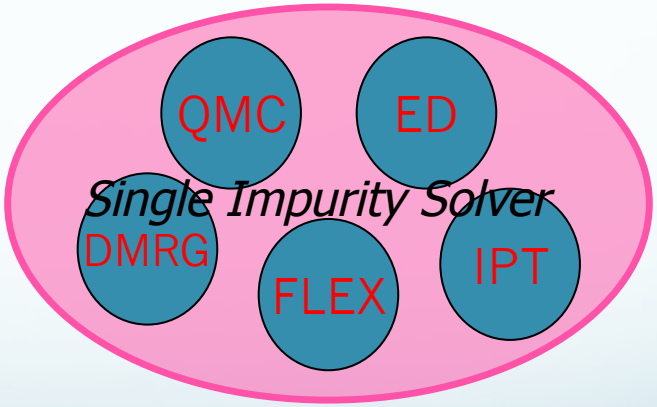
Dynamical Mean Field Theory: 25

$$\mathcal{G}_0(\tau-\tau')$$



$$\hat{G}(i\omega_n)=\frac{1}{\Omega}\sum_{k}^{BZ}\hat{G}(\vec{k},i\omega_n)$$

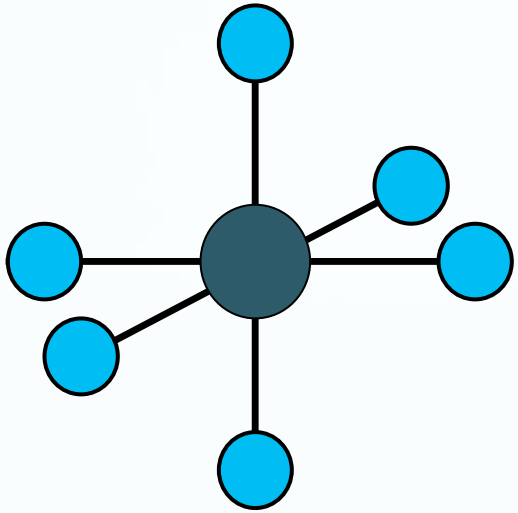
$$\hat{\mathcal{G}}_0^{-1}(i\omega_n)=\hat{G}^{-1}(i\omega_n)+\hat{\Sigma}(i\omega_n)$$



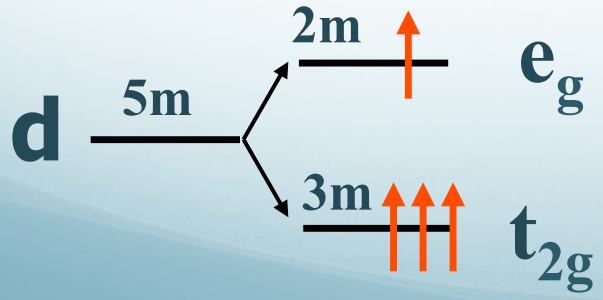
$$\hat{\Sigma}_{new}(i\omega_n)=\hat{\mathcal{G}}_0^{-1}(i\omega_n)-\hat{G}^{-1}(i\omega_n)$$

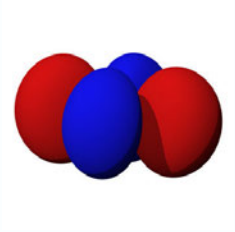
W. Metzner and D. Vollhardt (1987)
A. Georges and G. Kotliar (1992)

Orbital degrees of freedom

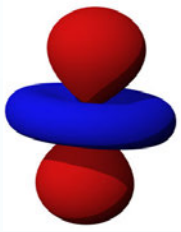


3d-ion in cubic crystal field



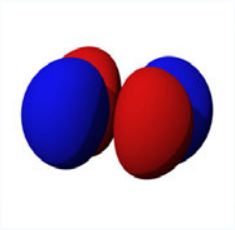


$3d_{x^2-y^2}$

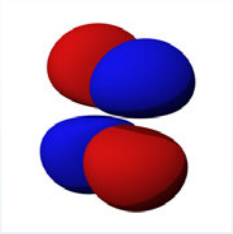


$3d_{z^2}$

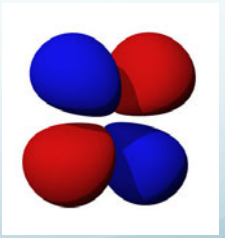
- e_g orbitals



$3d_{xy}$



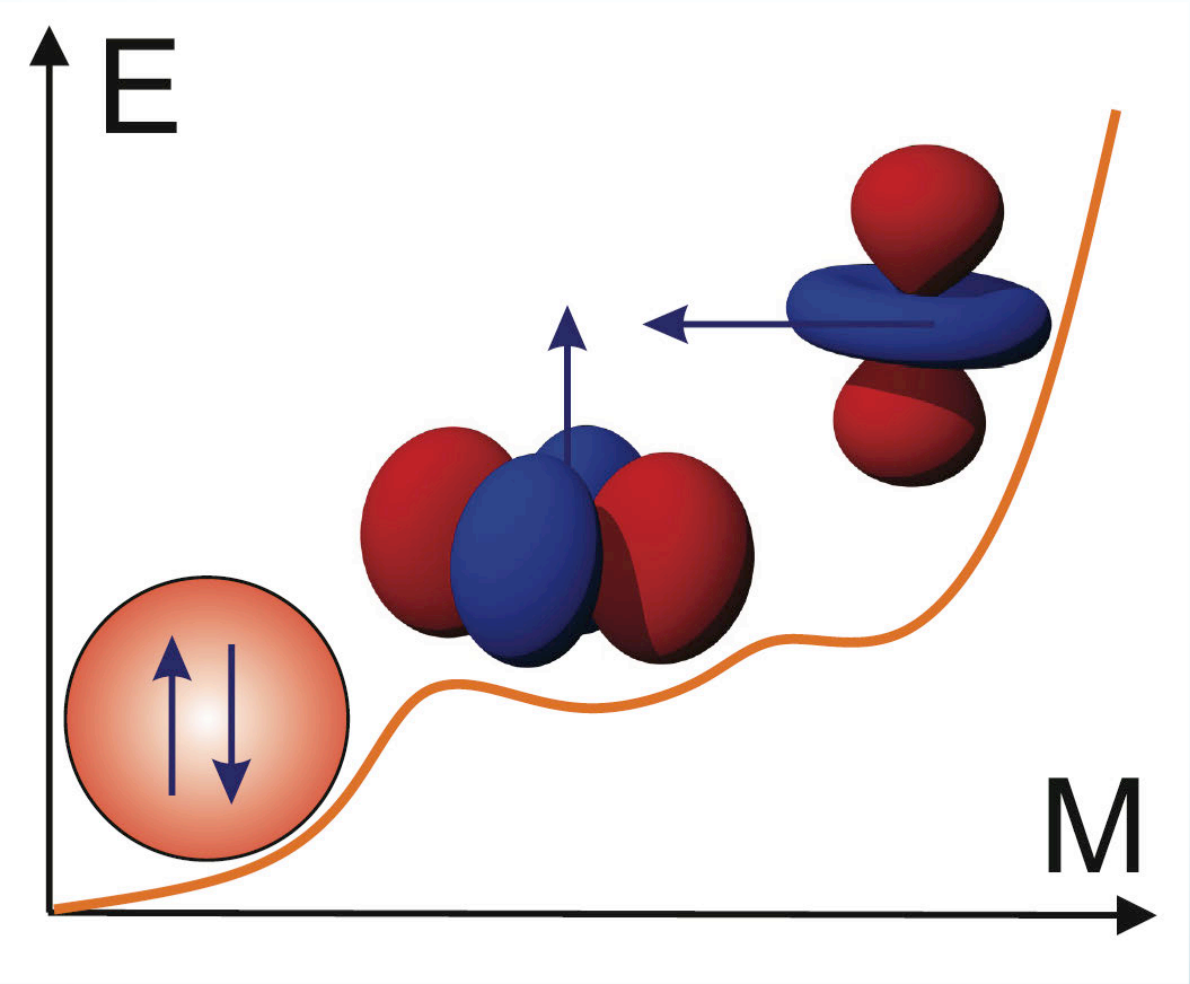
$3d_{yz}$



$3d_{xz}$

- t_{2g} orbitals

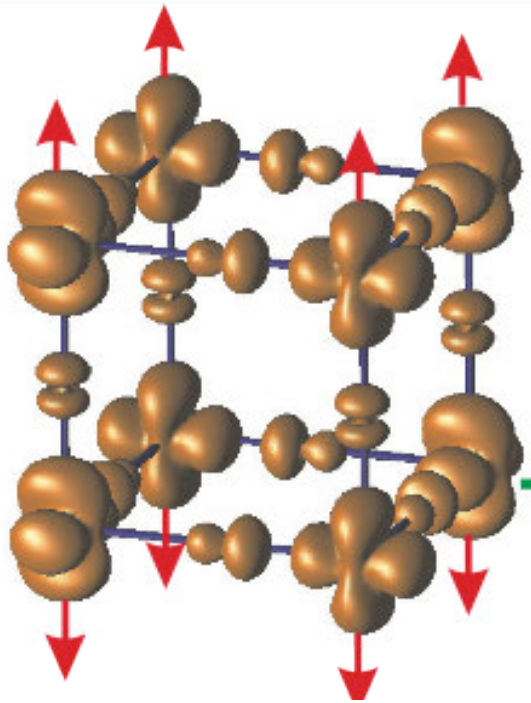
Correlated Electrons: Fluctuations

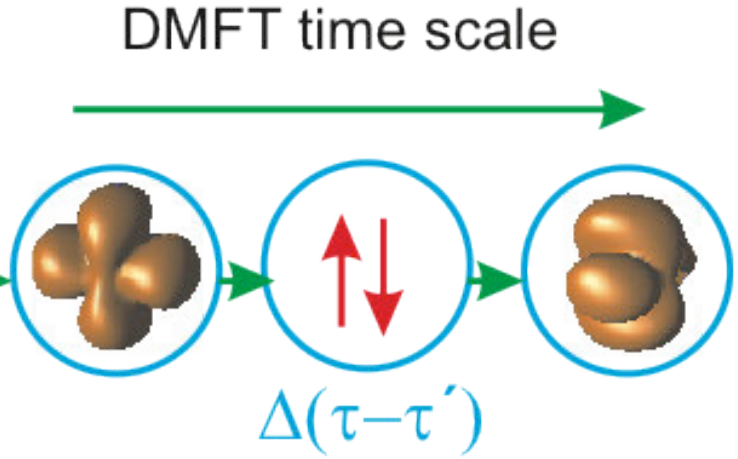


Fluctuation of charge, spin and orbital degrees of freedom related with complex behavior of correlated electronic systems

DMFT: Charge+Spin+Orbital Fluctuations

Lattice:





Local Quantum Impurity

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

$$S_{\mathrm{loc}}[c^*,c] = -\sum_{\omega\,\alpha\beta} c^*_{\omega\alpha}\left[(i\omega+\mu)\mathbf{1} - \Delta^{\alpha\beta}_{\omega}\right] c_{\omega\beta} + S_{\mathrm{U}}[c^*,c] \quad \Rightarrow \quad g_{12} = -\langle c_1 c^*_2\rangle_{\mathrm{loc}}$$

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

DMFT self-consistensy

DMFT Impurity solver

Realistic theory of correlated electron systems

DFT

- (+) Material specific
- (+) Structure specific
- (+) Fast code packages
- (±) Complex structures
- (−) Fails for strong correlations

Model based approaches

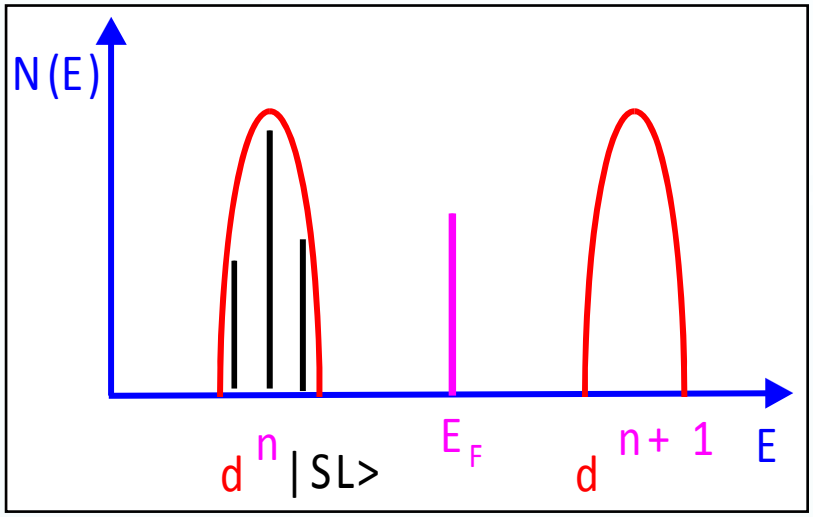
- (−) Input parameters unknown
- (+) Versatile
- (+) Systematic many body schemes

Comparison of LDA and realistic DMFT

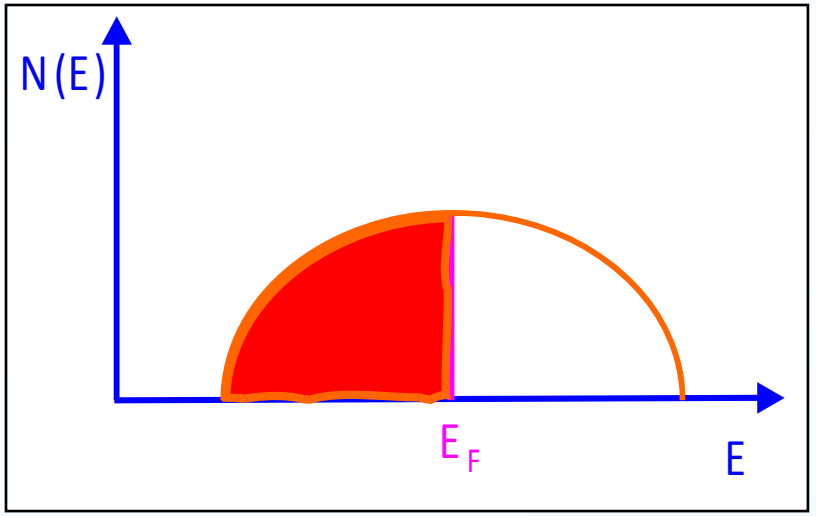
LDA	LDA+DMFT
Density functional	Baym-Kadanoff functional
Density $\rho(\mathbf{r})$	Green-Function $G(\mathbf{r}, \mathbf{r}', \omega)$
Potential $V_{xc}(\mathbf{r})$	Self-energy $\Sigma_i(\omega)$
$E_{tot} = E_{sp} - E_{dc}$	$\Omega = \Omega_{sp} - \Omega_{dc}$
$E_{sp} = \sum_{k<k_F} \varepsilon_k$	$\Omega_{sp} = -Tr \ln[-G^{-1}]$
$E_{dc} = E_H + \int \rho V_{xc} d\mathbf{r} - E_{xc}$	$\Omega_{dc} = Tr \Sigma G - \Phi_{LW}$

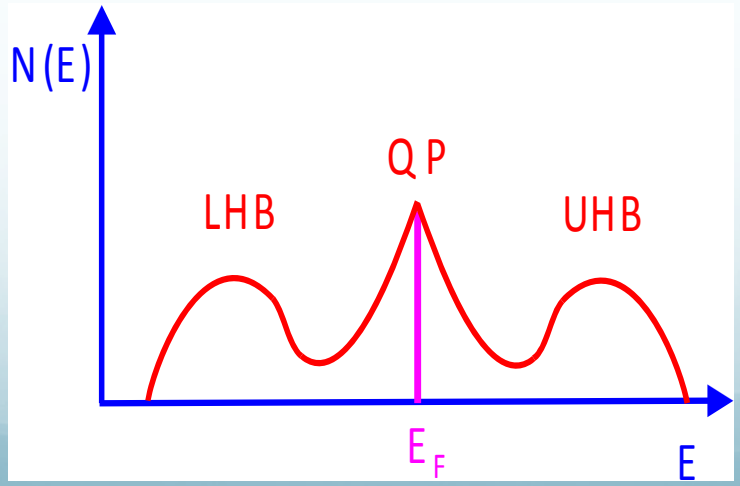
From Atom to Solid

Atomic physics (U)



Bands effects (LDA)

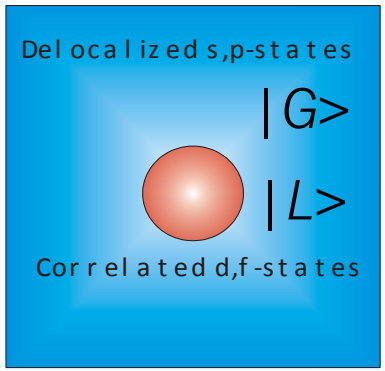




LDA+DMFT

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)

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

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

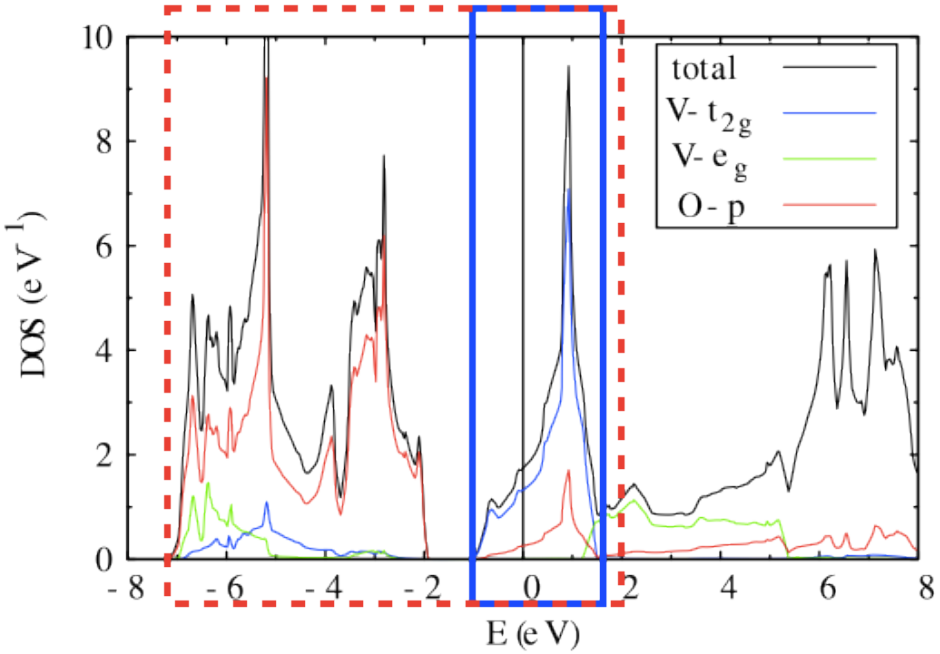
$$\Sigma_{mm'}(i\omega) = \left(G_0^{-1} - G^{-1}\right)_{mm'}$$
$$\Delta\Sigma_{mm'}(i\omega) = \Sigma_{mm'}(i\omega) - \Sigma_{dc}$$

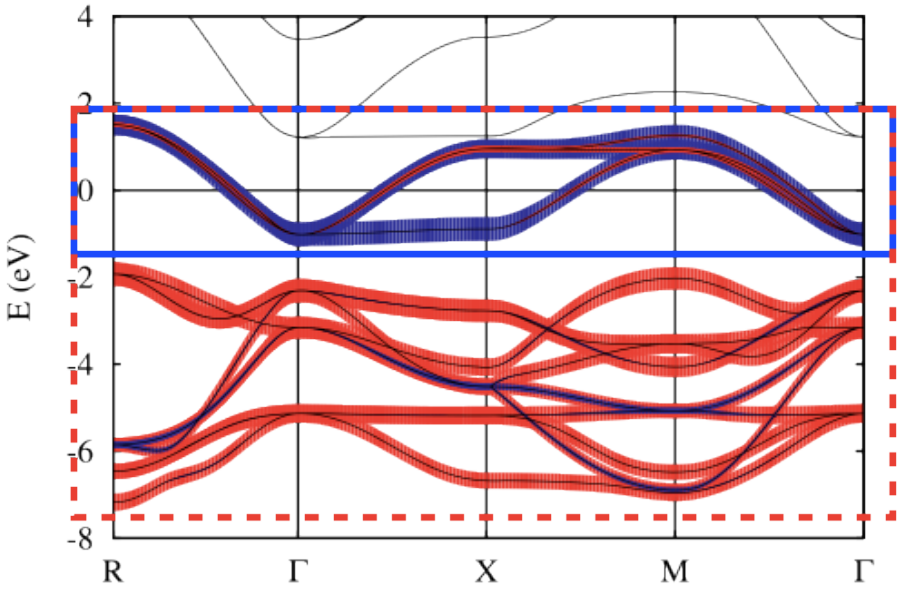
G. Trimarchi, *et al*. JPCM **20**,135227 (2008)
B. Amadon, *et al*. PRB **77**, 205112 (2008)

PAW: Projection windows

Example: $SrVO_3$

Two different choices: 1.**Vanadium t_{2g} only** 2.**Vanadium t_{2g} + Oxygen 2p**





One has to take great care, because different projection windows will lead to different descriptions of the system!

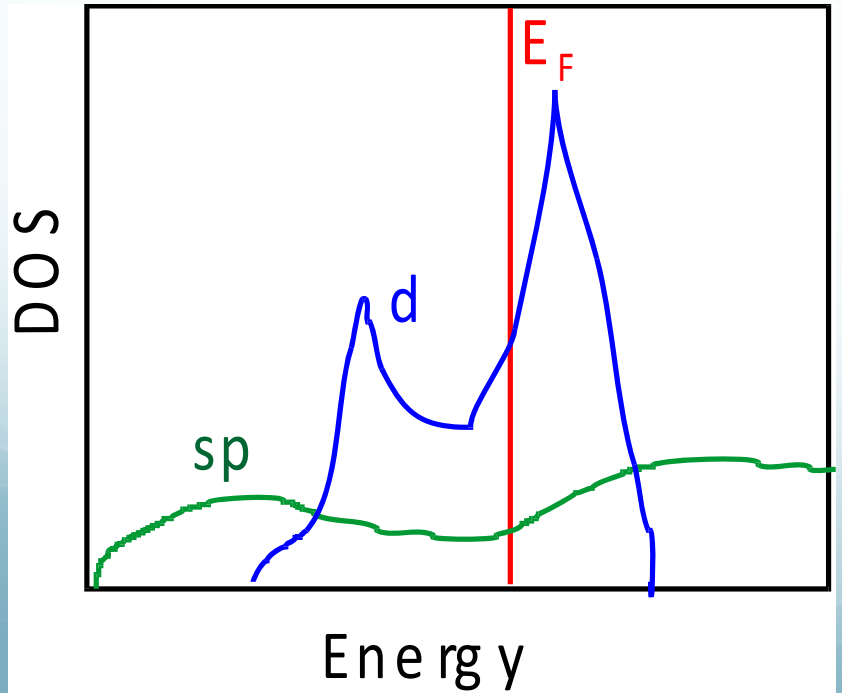
DMFT in local LMTO basis

LDA+DMFT (orthogonal |L> basis):

$$G^{-1}_{LL'}(\vec{k}, i\omega_n) = i\omega_n + \mu - H^{LDA}_{LL'}(\vec{k}) - \Sigma^{DMFT}_{LL'}(i\omega_n)$$

$$G_{LL'}(i\omega_n) = \sum_{\vec{k}\in BZ} G^{-1}_{LL'}(\vec{k}, i\omega_n)$$

$$\hat{G}(i\omega_n) = \sum_{\alpha\in O_h} \hat{U}(\alpha) \sum_{\vec{k}\in IBZ} \hat{G}(\vec{k}, i\omega_n) \hat{U}^{+}(\alpha)$$



Correlated d-states:

$$\hat{H}(\vec{k}) + \hat{\Sigma}(\omega) = \begin{pmatrix} H_{ss} & H_{ps} & H_{ds} \\ H_{sp} & H_{pp} & H_{dp} \\ H_{sd} & H_{pd} & H_{dd} + \Sigma_{dd} \end{pmatrix}$$

V. Anisimov, A. Poteryaev et al, JPCM **9**, 7359 (1997)
A.L. and M.Katsnelson, PRB **57**, 688 (1998)

Slater parametrization of U

Multipole expansion:

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

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:

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

Constrain GW calculations of U

Polarisation

$$P(\mathbf{r},\mathbf{r}';\omega) = \sum_{i}^{occ}\sum_{j}^{unocc} \psi_i(\mathbf{r})\psi_i^*(\mathbf{r}')\psi_j^*(\mathbf{r})\psi_j(\mathbf{r}') \times \left\{ \frac{1}{\omega - \varepsilon_j + \varepsilon_i + i0^+} - \frac{1}{\omega + \varepsilon_j - \varepsilon_i - i0^+} \right\}$$

F. Aryasetiawanan et al
PRB(2004)

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

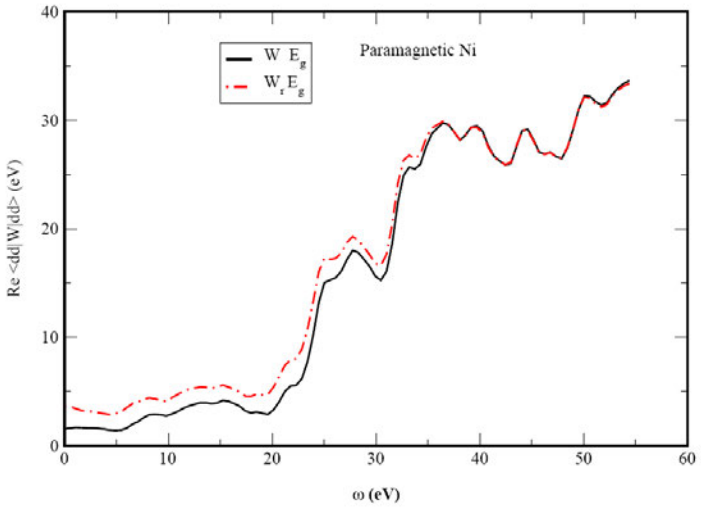
$$W = [1 - vP]^{-1} v$$

$$= [1 - vP_r - vP_d]^{-1} v$$

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

$$= \{1 - (1 - vP_r)^{-1} vP_d\}^{-1} (1 - vP_r)^{-1} v$$

$$= [1 - W_r P_d]^{-1} W_r$$

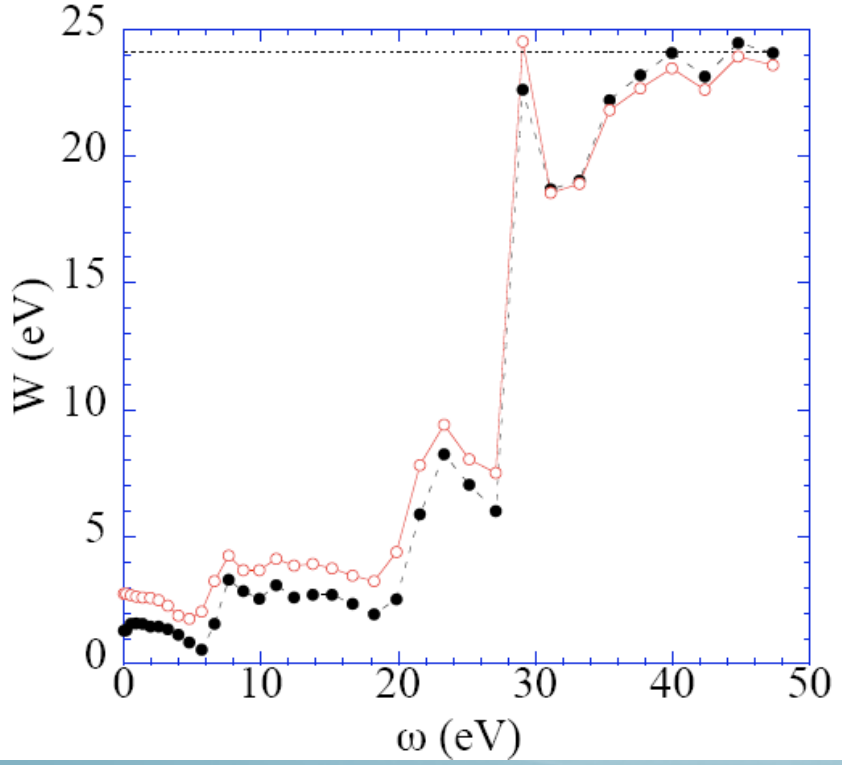


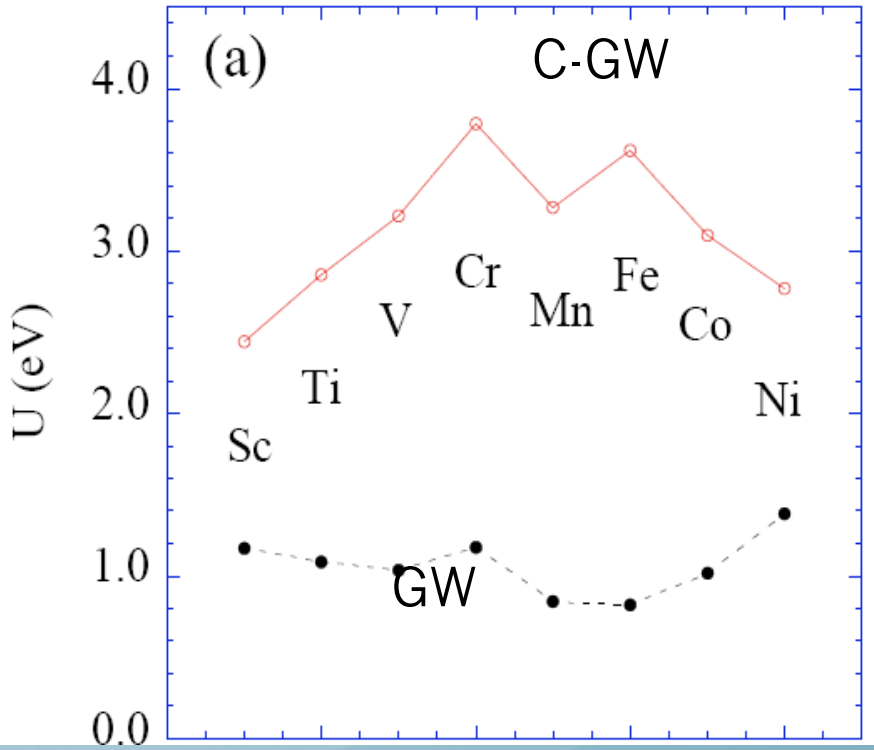
Wannier - GW and effective U(ω)

$$|\varphi_{n\mathbf{R}}\rangle = \frac{V}{(2\pi)^3}\int e^{-i\mathbf{k}\cdot\mathbf{R}}|\psi^{(\mathrm{w})}_{n\mathbf{k}}\rangle d^3k$$

$$|\psi^{(\mathrm{w})}_{n\mathbf{k}}\rangle = \sum_m \mathcal{U}_{mn}(\mathbf{k})|\psi_{m\mathbf{k}}\rangle$$

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





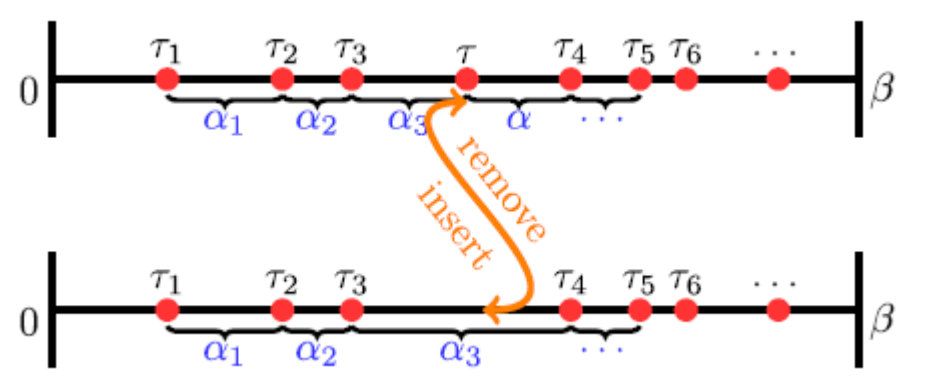
Continuous Time Quantum Monte Carlo

Partition function: $H = H_0 + V$

$$Z = \mathbf{Tr}\left[e^{-\beta H_0}\mathbf{T}_\tau e^{-\int_0^\beta d\tau V(\tau)}\right]$$

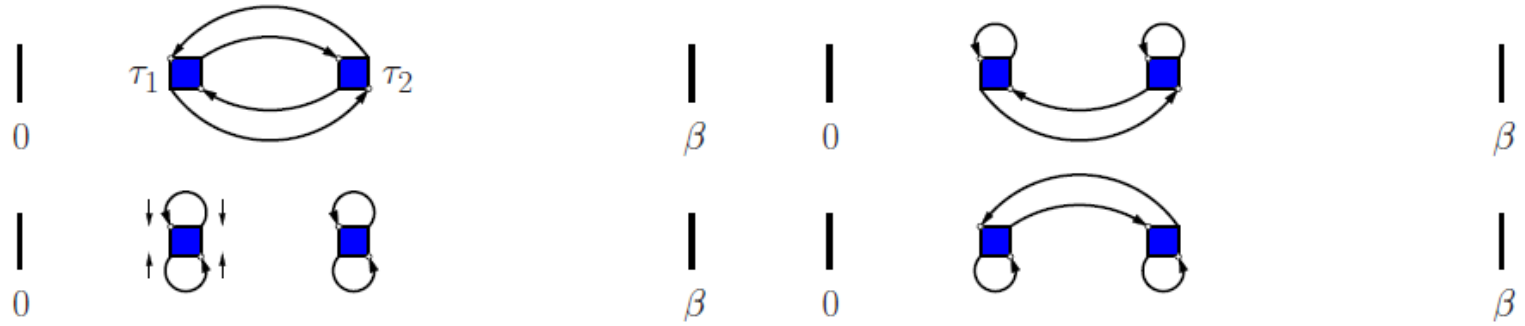
Continuous Time Quantum Monte Carlo (CT-QMC)

$$Z = \sum_{k=0}^{\infty}\int_0^\beta d\tau_1 \int_{\tau_1}^\beta d\tau_2 \ldots \int_{\tau_{k-1}}^\beta d\tau_k \mathbf{Tr}\left[e^{-\beta H_0}e^{-\tau_k H_0}(-V)\ldots e^{-(\tau_2-\tau_1)H_0}(-V)e^{-\tau_1 H_0}\right]$$



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

Weak coupling QMC: CT-INT



$$\mathcal{Z}_{\text{imp}} = \int e^{-S_0[c^*,c]+U\int_0^\beta n_\uparrow(\tau)n_\downarrow(\tau)}\mathcal{D}[c^*,c]$$

$$= \int e^{-S_0[c^*,c]} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} U^k \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_k \, c_\uparrow^*(\tau_1)c_\uparrow(\tau_1)$$

$$\times c_\downarrow^*(\tau_1)c_\downarrow(\tau_1)\ldots c_\uparrow^*(\tau_k)c_\uparrow(\tau_k)c_\downarrow^*(\tau_k)c_\downarrow(\tau_k)\,\mathcal{D}[c^*,c]$$

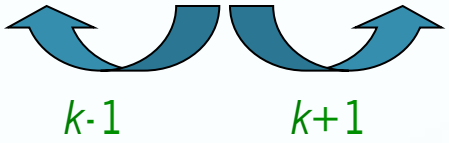
$$= \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} U^k \int d\tau_1 \ldots \int d\tau_k \text{sgn}(\det \hat{G}) \underbrace{|\det \hat{G}|}_{P(k)}$$

$$\hat{G}_{ij} = g_0(\tau_i - \tau_j)$$

A. Rubtsov, 2004

Random walks in the *k*-space

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

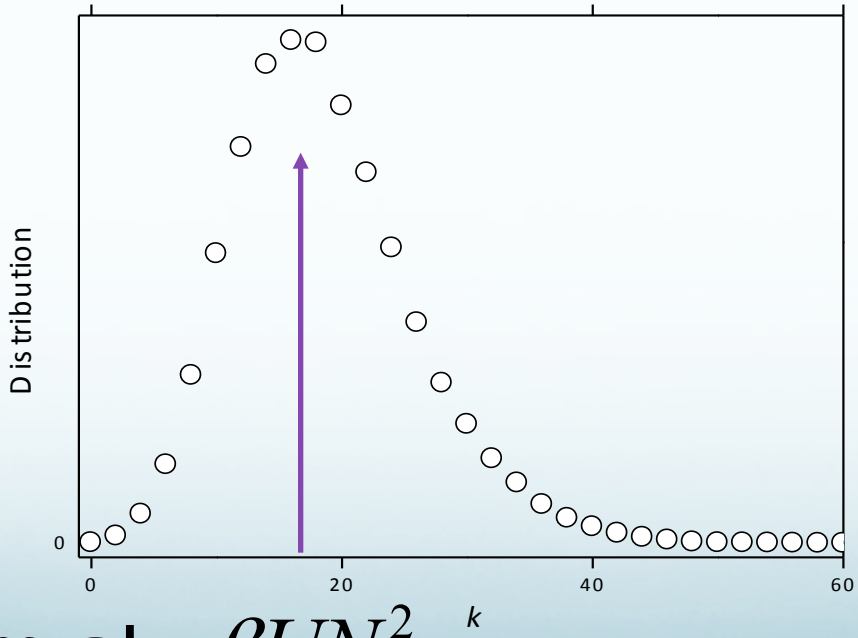


Acceptance ratio

decrease

Step *k*-1

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



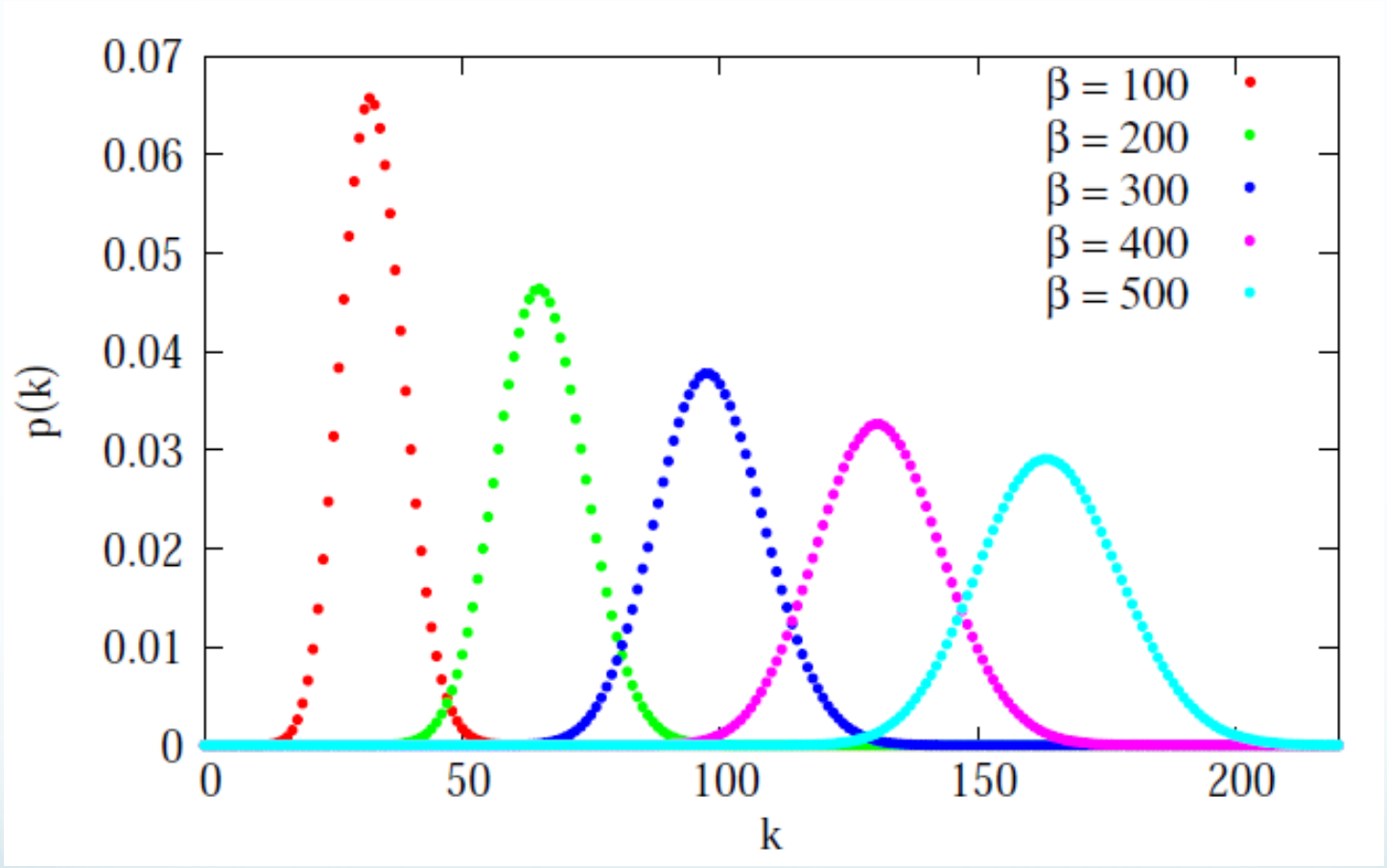
increase

Step *k*+1

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

Maximum at βUN^2

Convergence with Temperature: CT-INT



Maximum: $\beta U N^2$

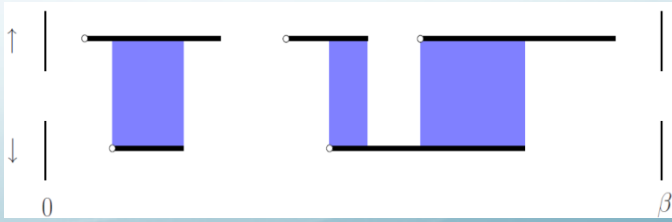
Strong-Coupling Expansion CT-HYB

$$S_{\mathrm{at}} = \int_0^\beta d\tau \sum_\sigma c_\sigma^*(\tau)[\partial_\tau - \mu]c_\sigma(\tau) + U\int_0^\beta d\tau c_\uparrow^*(\tau)c_\uparrow(\tau)c_\downarrow^*(\tau)c_\downarrow(\tau)$$

$$S_\Delta = -\int_0^\beta d\tau' \int_0^\beta d\tau \sum_\sigma c_\sigma(\tau)\Delta(\tau-\tau')c_\sigma^*(\tau')$$

$$\mathscr{Z} = \int \mathscr{D}[c^*,c]e^{-S_{\mathrm{at}}} \sum_k \frac{1}{k!}\int_0^\beta d\tau_1' \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_k' \int_0^\beta d\tau_k \times$$
$$\times c(\tau_k)c^*(\tau_k')\ldots c(\tau_1)c^*(\tau_1')\Delta(\tau_1-\tau_1')\ldots\Delta(\tau_k-\tau_k')$$

$$\mathscr{Z} = \mathscr{Z}_{\mathrm{at}} \sum_k \int_0^\beta d\tau_1' \int_{\tau_1'}^\beta d\tau_1 \ldots \int_{\tau_{k-1}}^\beta d\tau_k' \int_{\tau_k'}^{\circ\tau_k'} d\tau_k \times$$
$$\times \langle c(\tau_k)c^*(\tau_k')\ldots c(\tau_1)c^*(\tau_1')\rangle_{\mathrm{at}} \det \hat{\Delta}^{(k)}$$



P. Werner, 2006

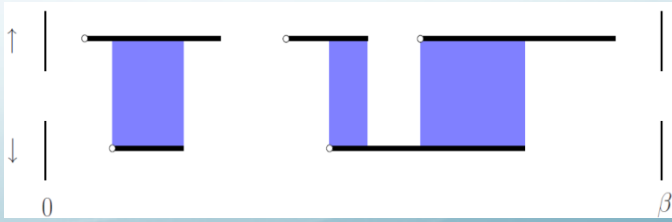
Strong-Coupling Expansion CT-HYB

$$S_{\mathrm{at}} = \int_0^\beta d\tau \sum_\sigma c_\sigma^*(\tau)[\partial_\tau - \mu]c_\sigma(\tau) + U\int_0^\beta d\tau c_\uparrow^*(\tau)c_\uparrow(\tau)c_\downarrow^*(\tau)c_\downarrow(\tau)$$

$$S_\Delta = -\int_0^\beta d\tau' \int_0^\beta d\tau \sum_\sigma c_\sigma(\tau)\Delta(\tau-\tau')c_\sigma^*(\tau')$$

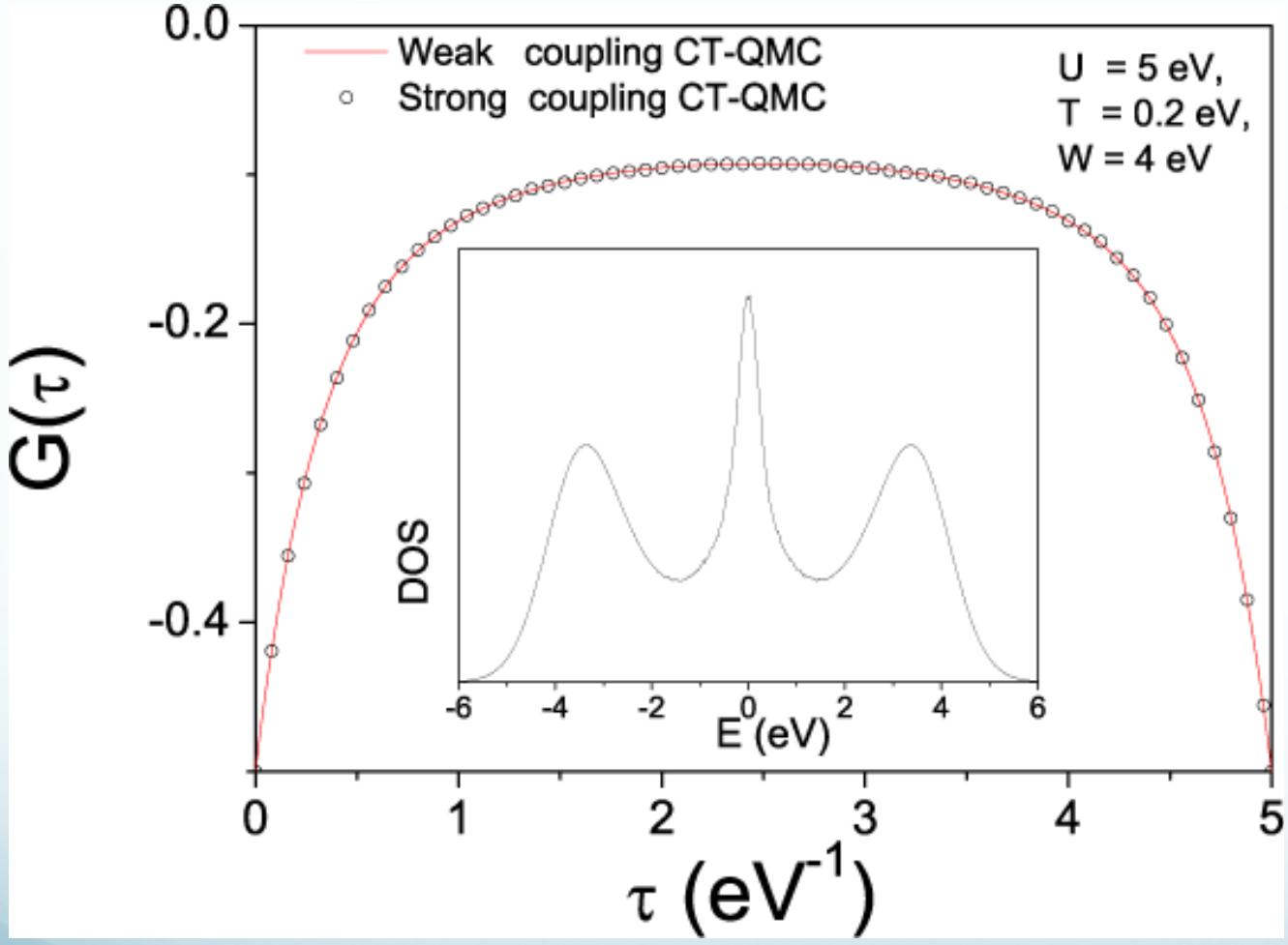
$$\mathscr{Z} = \int \mathscr{D}[c^*,c]e^{-S_{\mathrm{at}}} \sum_k \frac{1}{k!}\int_0^\beta d\tau_1' \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_k' \int_0^\beta d\tau_k \times$$
$$\times c(\tau_k)c^*(\tau_k')\ldots c(\tau_1)c^*(\tau_1')\Delta(\tau_1-\tau_1')\ldots\Delta(\tau_k-\tau_k')$$

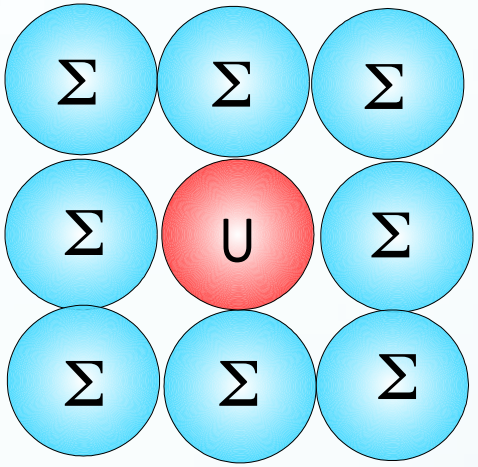
$$\mathscr{Z} = \mathscr{Z}_{\mathrm{at}} \sum_k \int_0^\beta d\tau_1' \int_{\tau_1'}^\beta d\tau_1 \ldots \int_{\tau_{k-1}}^\beta d\tau_k' \int_{\tau_k'}^{\circ\tau_k'} d\tau_k \times$$
$$\times \langle c(\tau_k)c^*(\tau_k')\ldots c(\tau_1)c^*(\tau_1')\rangle_{\mathrm{at}} \det \hat{\Delta}^{(k)}$$

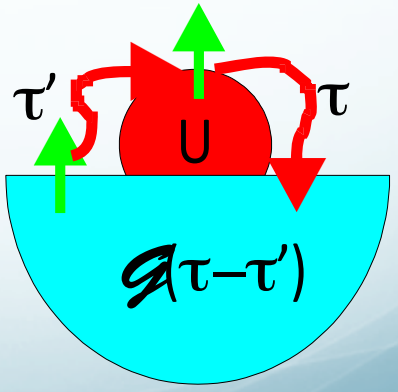


P. Werner, 2006

Comparison of different CT-QMC



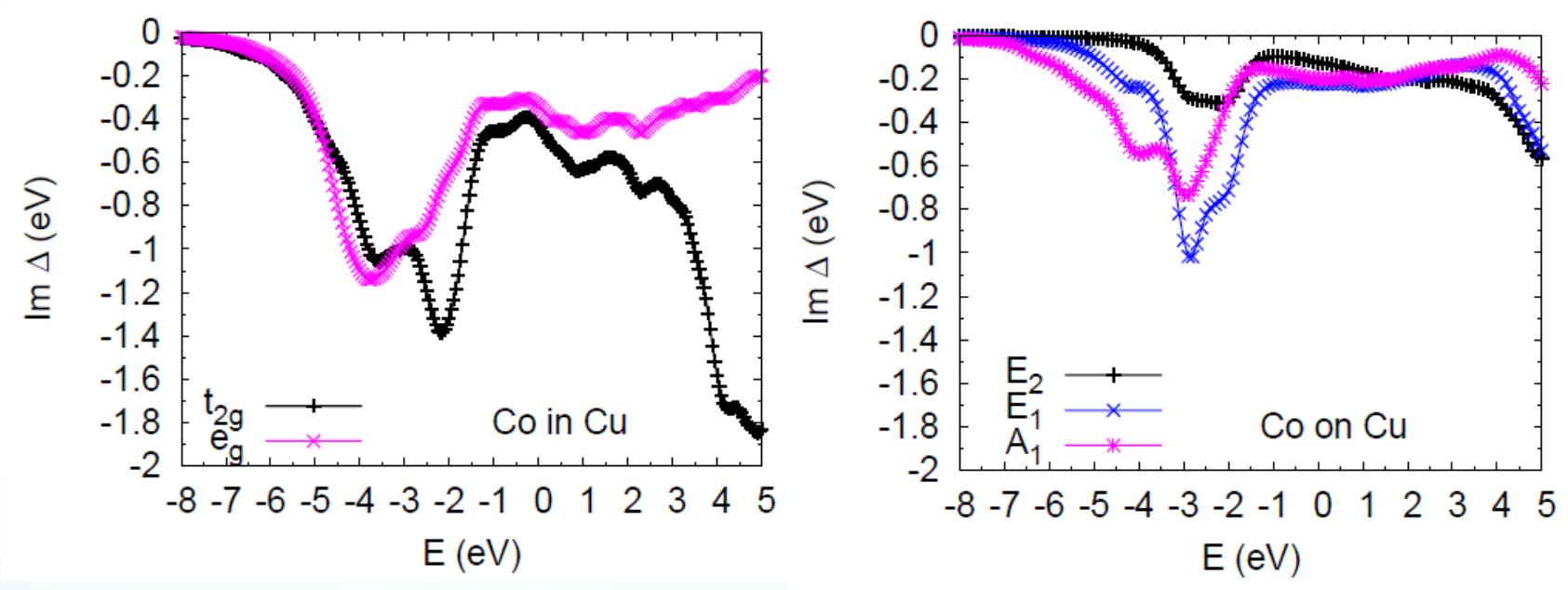




Ch. Jung, unpublished

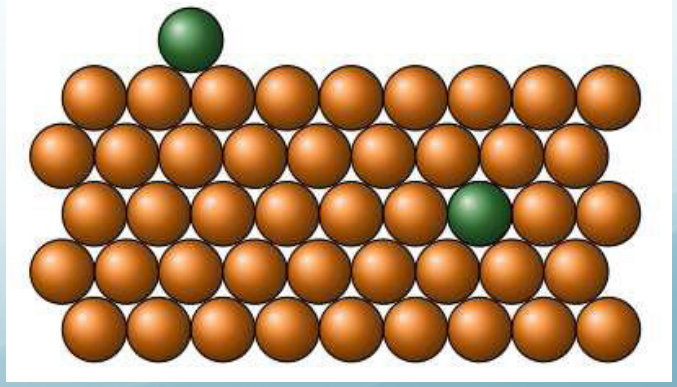
CT-QMC review: E. Gull et al. RMP (2011)

Hybridization function Co on/in Cu(111)

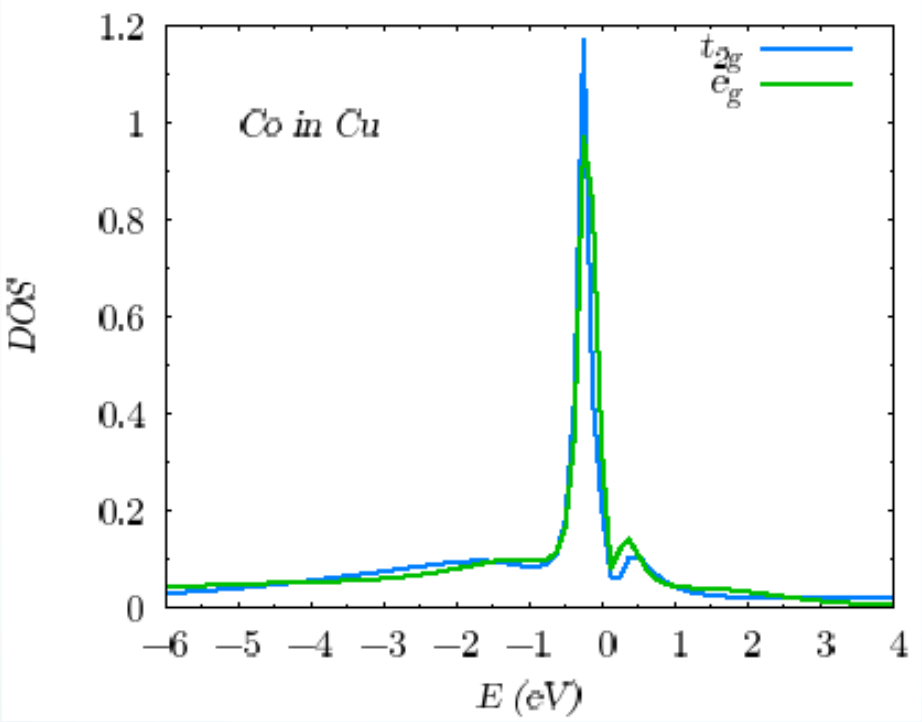


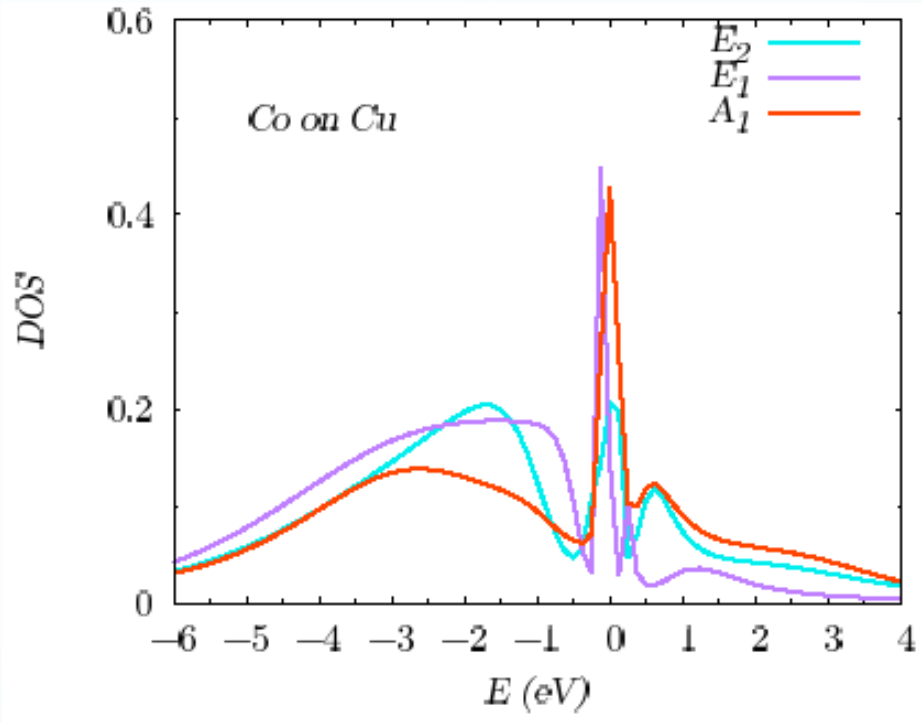
- Hybridization of Co in bulk twice stronger than on surface
- Hybridization in energy range of Cu-d orbitals more anisotropic on surface
- Co-d occupancy: *n*= 7-8

B. Surer, et al PRB (2012)



Orbitally resolved Co DOS from QMC





Orbitally resolved DOS of the Co impurities in bulk Cu and on Co (111) obtained from QMC simulations at temperature. T = 0.025 eV and chemical potential μ = 27 eV and μ = 28 eV, respectively.

All Co *d*-orbitals contribute to LDOS peak near E_F=0

B. Surer, et al, PRB (2012).

Double counting in LDA+DMFT

- Analytic models
  - Around mean field
  - Fully localized limit
- Constraint on particle number

$$\mathrm{Tr}\, G \stackrel{!}{=} \mathrm{Tr}\, G^{0}$$

$$\mathrm{Tr}\, G \stackrel{!}{=} \mathrm{Tr}\, G^{\mathrm{LDA}}$$

- Constraint on self-energy

$$\mathrm{Tr}\, \mathrm{Re}\, \Sigma(0) \stackrel{!}{=} 0$$

$$\mathrm{Tr}\, \mathrm{Re}\, \Sigma(\infty) \stackrel{!}{=} 0$$

Choice of double counting in LDA+DMFT

Shift of chemical potential for correlated state

$$G^{-1}(\vec{k},\omega) = (i\omega + \mu) - H_{LDA}(\vec{k}) + [E_{dc} - \delta\mu_c] - [\Sigma(\omega) - \delta\mu_c]$$

Natural choice $E_{dc} = \delta\mu_c$:

$$G^{-1}(\vec{k},\omega) = (i\omega + \mu) - H_{LDA}(\vec{k}) - \Sigma_c(\omega)$$

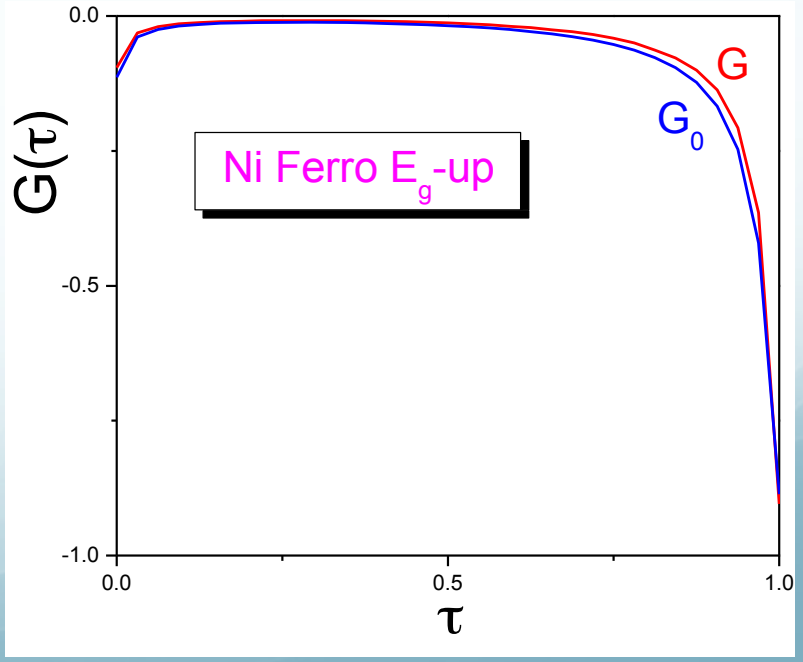
Transformations:

$$G_{c0}^{-1} = G_0^{-1} - \delta\mu_c$$

$$\Sigma_c(\omega) = G_{c0}^{-1} - G^{-1} = \Sigma_c(\omega) - \delta\mu_c$$

Condition for $\delta\mu_c$ (Friedel SR)

$$Tr[G\ ] = Tr[G_0]$$



Friedel Sum Rule

$$S_{imp} = \sum_{i,j=0}^{N} \int_0^\beta d\tau \int_0^\beta d\tau' \; c^*_{i\sigma}(\tau) \Big[-\mathcal{G}^{-1}_{\sigma}(\tau,\tau') \Big]_{ii} c_{i\sigma}(\tau') + \int_0^\beta d\tau n_{i,\uparrow}(\tau) U_{i,j} n_{i,\downarrow}(\tau)$$

One can always find find the generalized double-countings:

$$\mu_i^{dc}$$

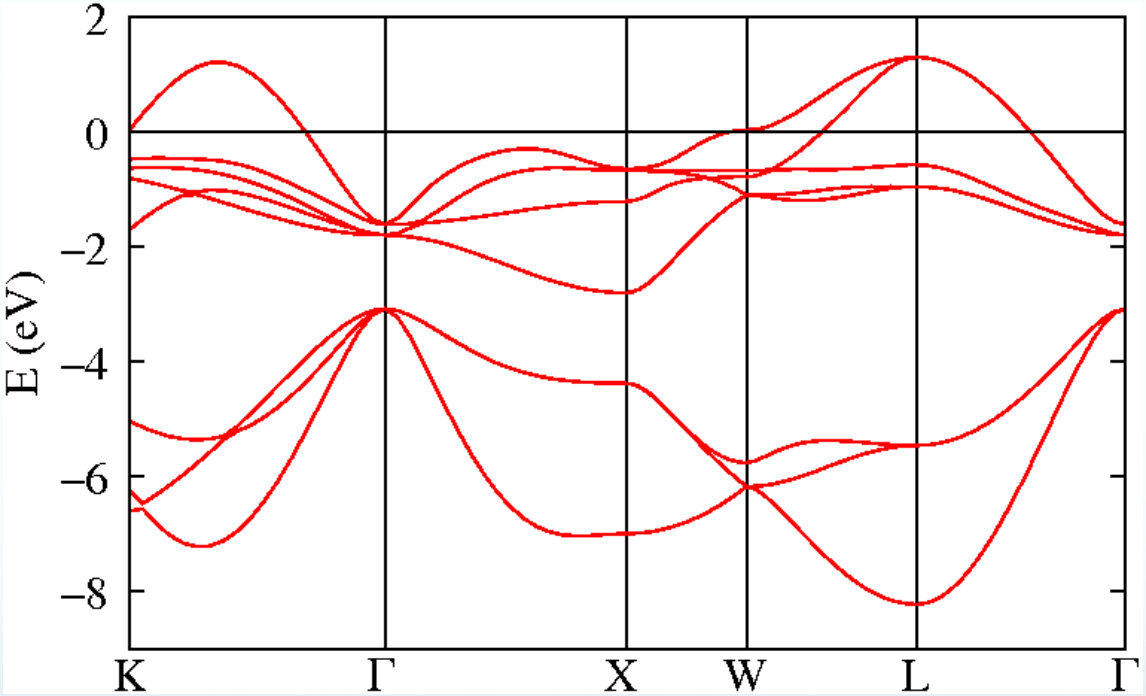
$$\widetilde{\mathcal{G}}^{-1} = \mathcal{G}^{-1} - \mu_i^{dc}$$

With LDA partial charges:

$$Tr(\widetilde{\mathcal{G}}) = TrG$$

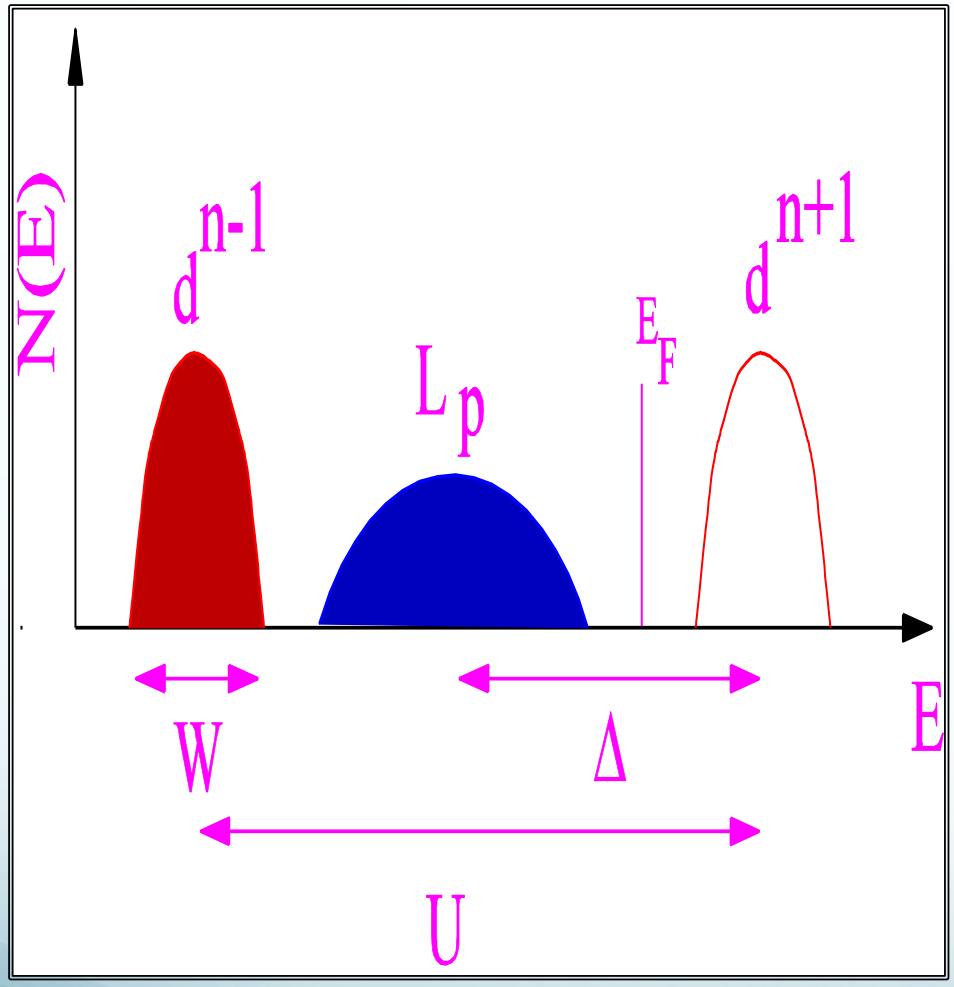
NiO – a charge transfer system

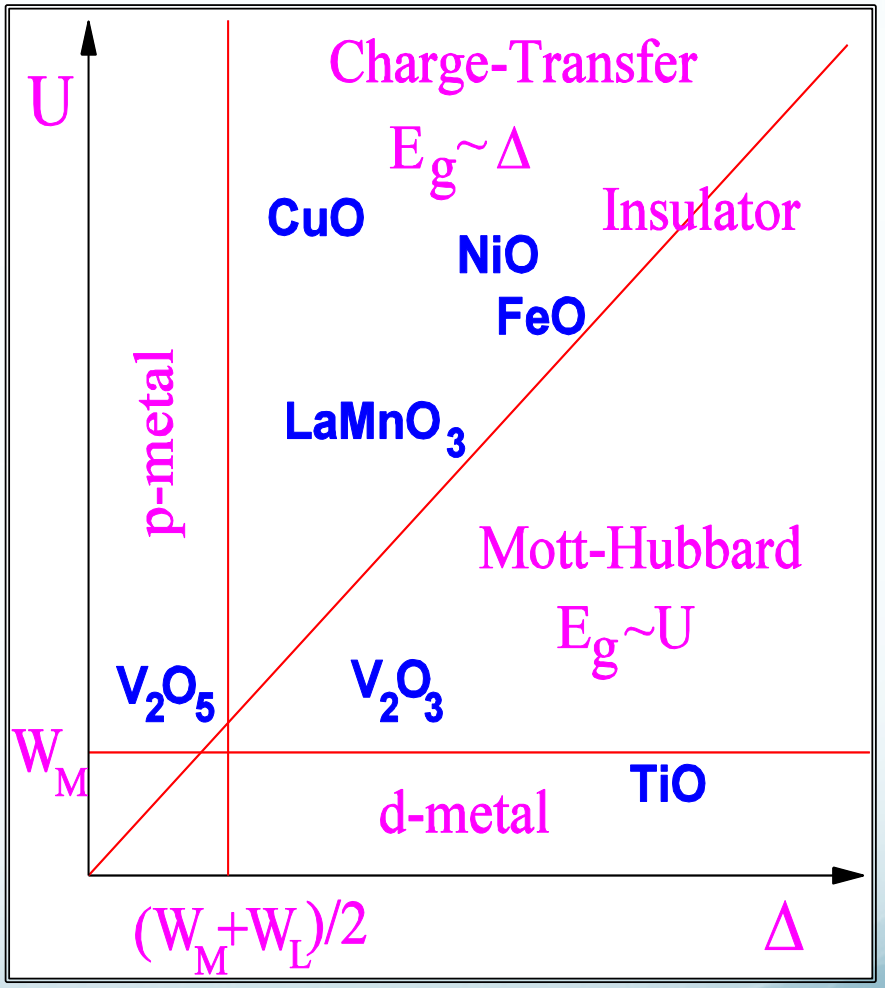
- LDA band structure (paramagnetic)



- Ni-3d orbitals as correlated subspace
- O-2d orbitals as uncorrelated subspace

Charge transfer TMO insulators

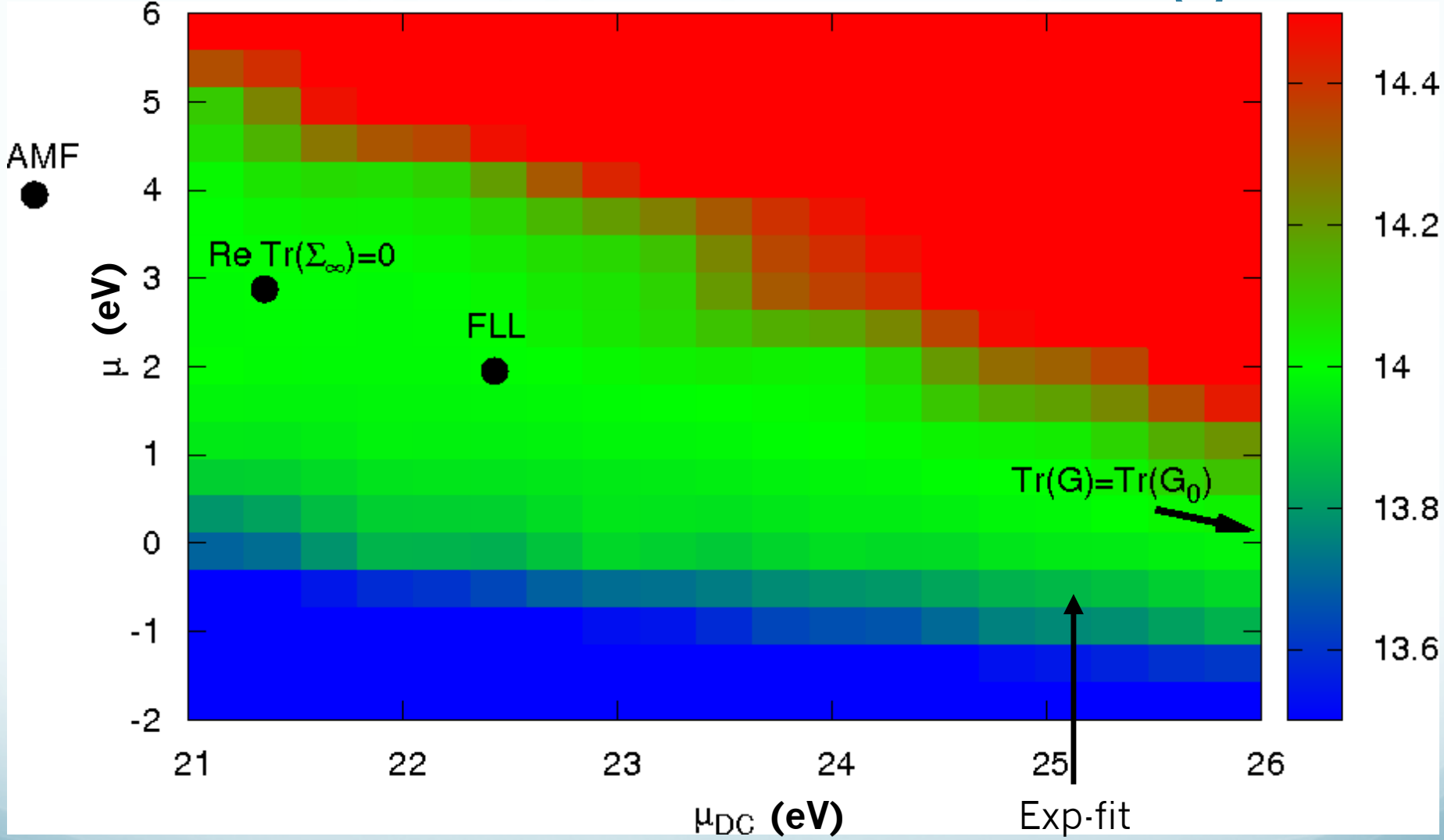




Zaanen-Sawatzky-Allen (ZSA) phase diagram

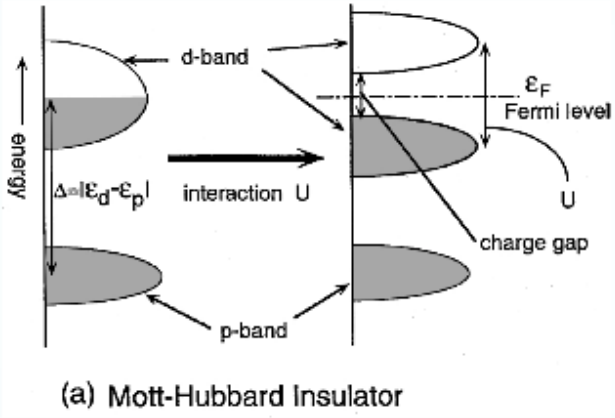
Phys. Rev. Lett. 55, 418 (1985)

NiO – double counting



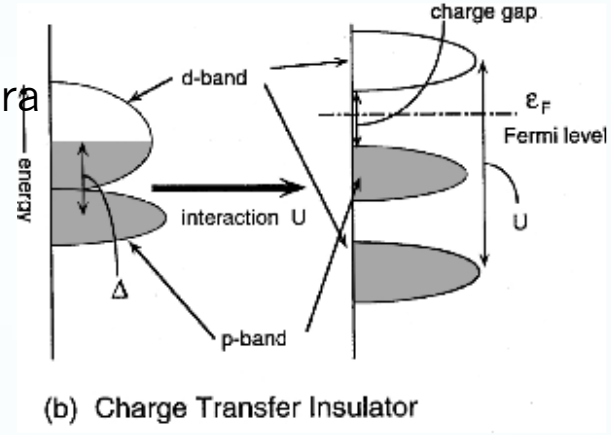
Total particle number (color encoded) as function of chemical potential μ and double counting μ_{DC}

NiO: peak positions and spectral weights



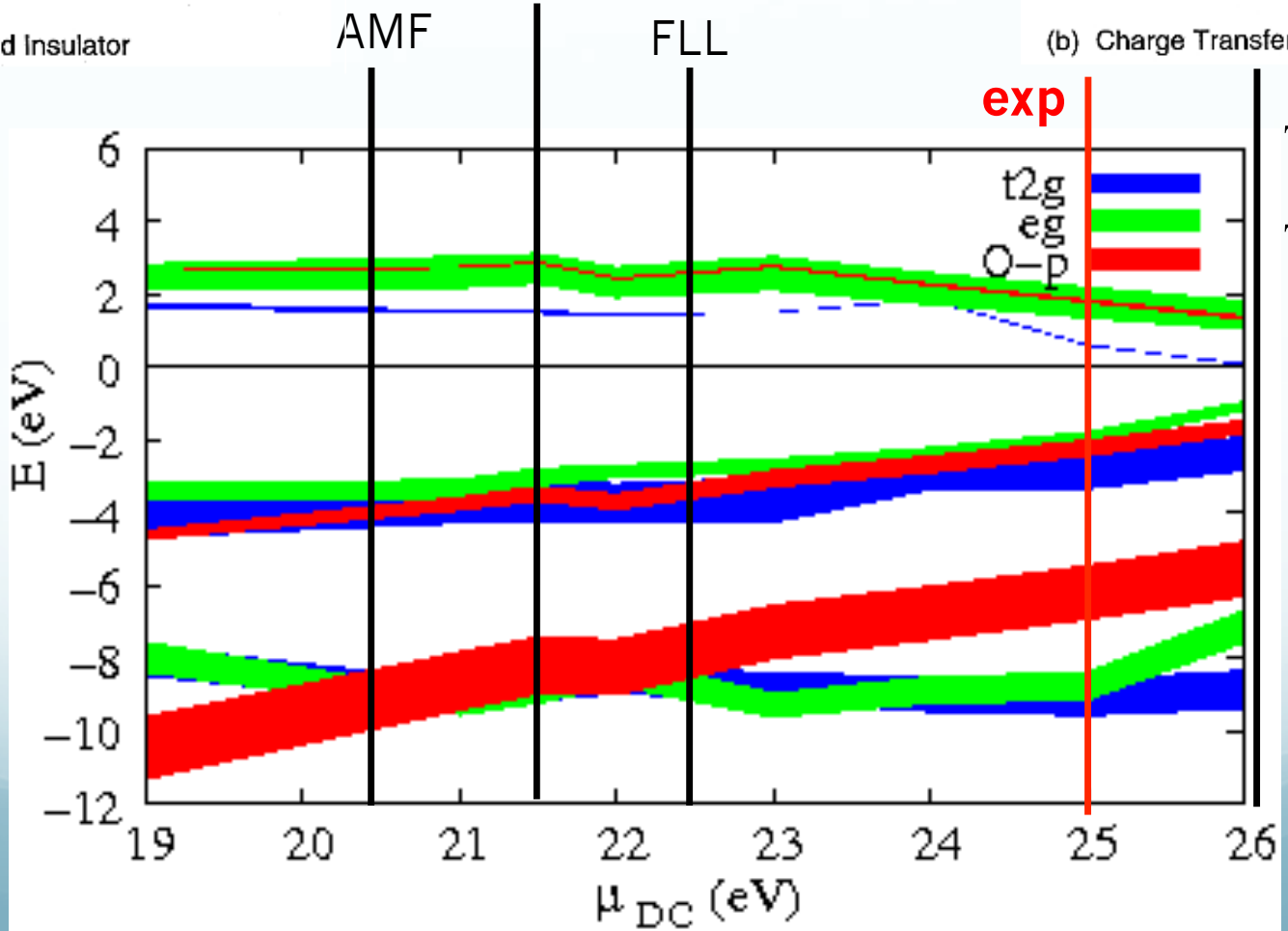
(a) Mott-Hubbard Insulator

M. Imada, A. Fujimori, and Y. Tokura
Rev. Mod. Phys. 70, 1039 (1998).



(b) Charge Transfer Insulator

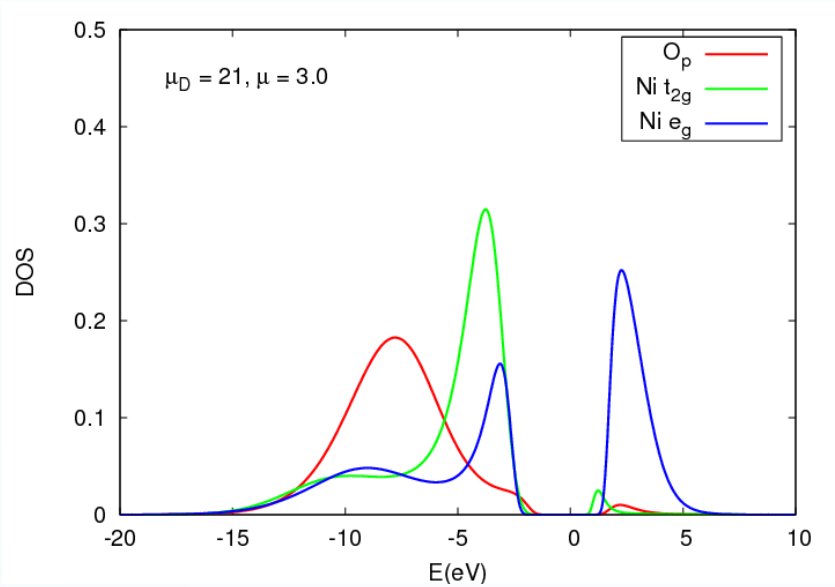
$$\mathrm{Tr}\ \mathrm{Re}\ \Sigma(\infty) \overset{!}{=} 0$$

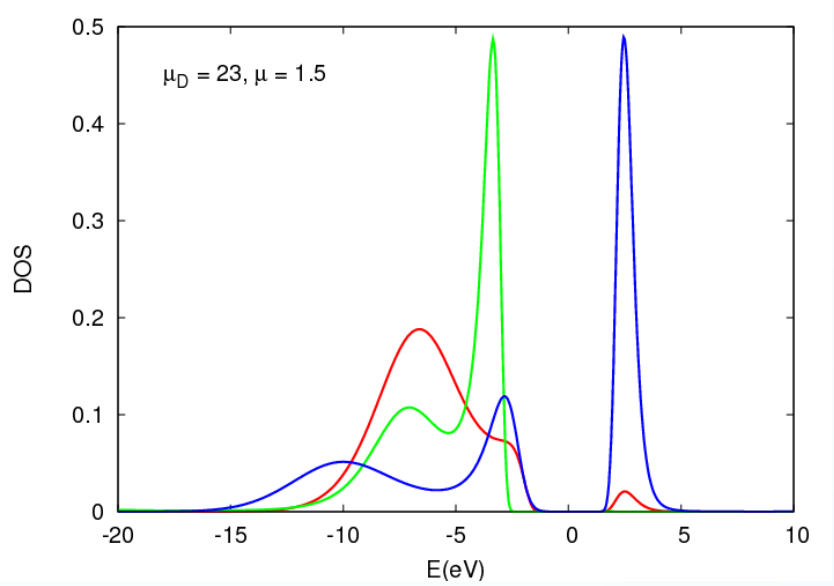


$$\mathrm{Tr}\ G \overset{!}{=} \mathrm{Tr}\ G^0$$

$$\mathrm{Tr}\ G \overset{!}{=} \mathrm{Tr}\ G^{\mathrm{LDA}}$$

Spectral functions and double counting





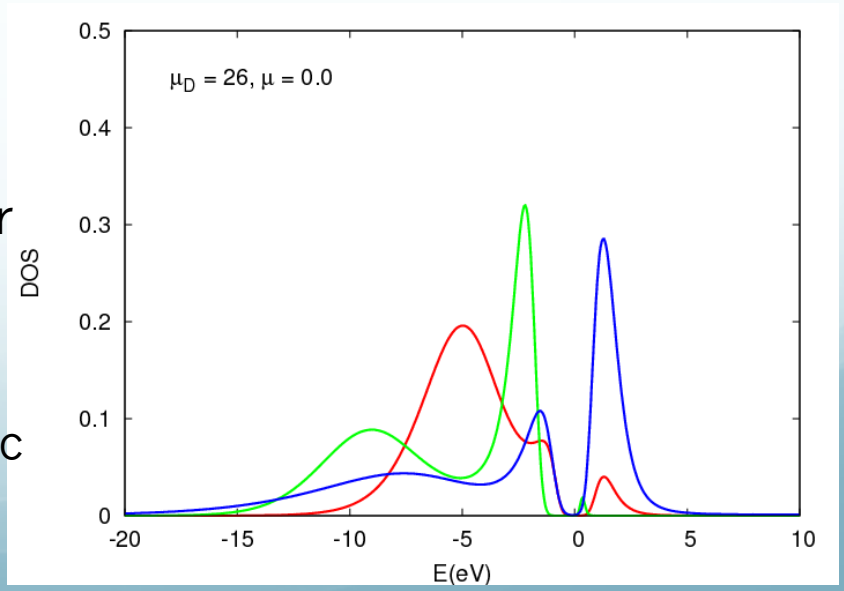
Mott insulator

$\mu_{DC} = 21\text{eV}$

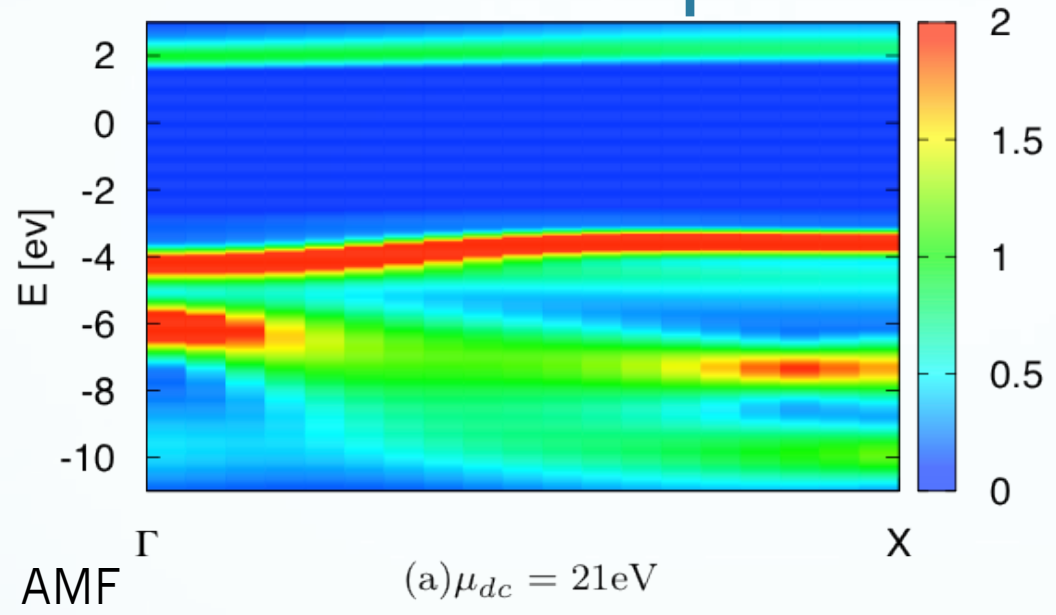
Charge transfer insulator

Almost metallic

$\mu_{DC} \geq 26\text{eV}$

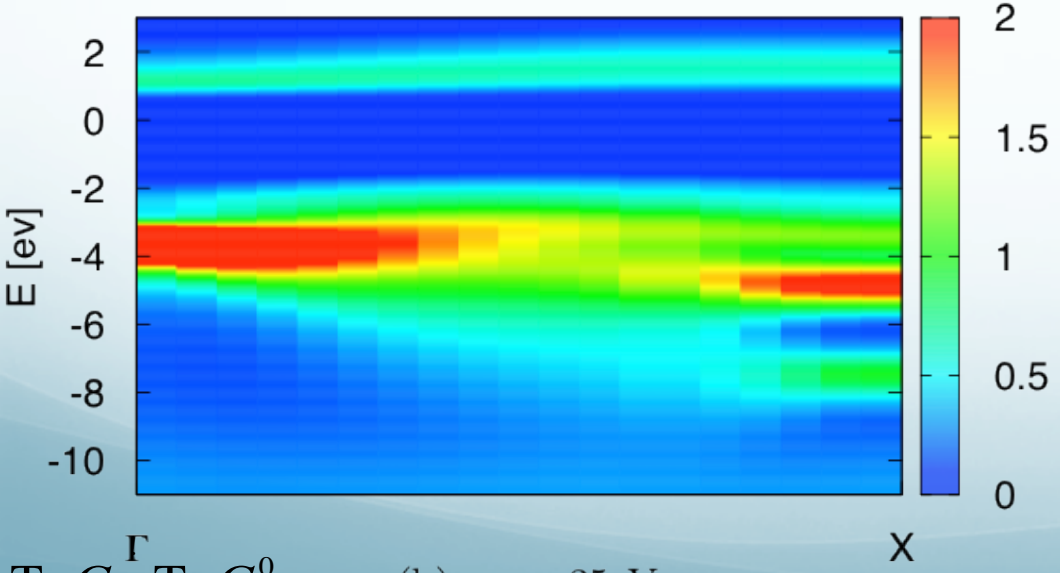


NiO: Spectral Function



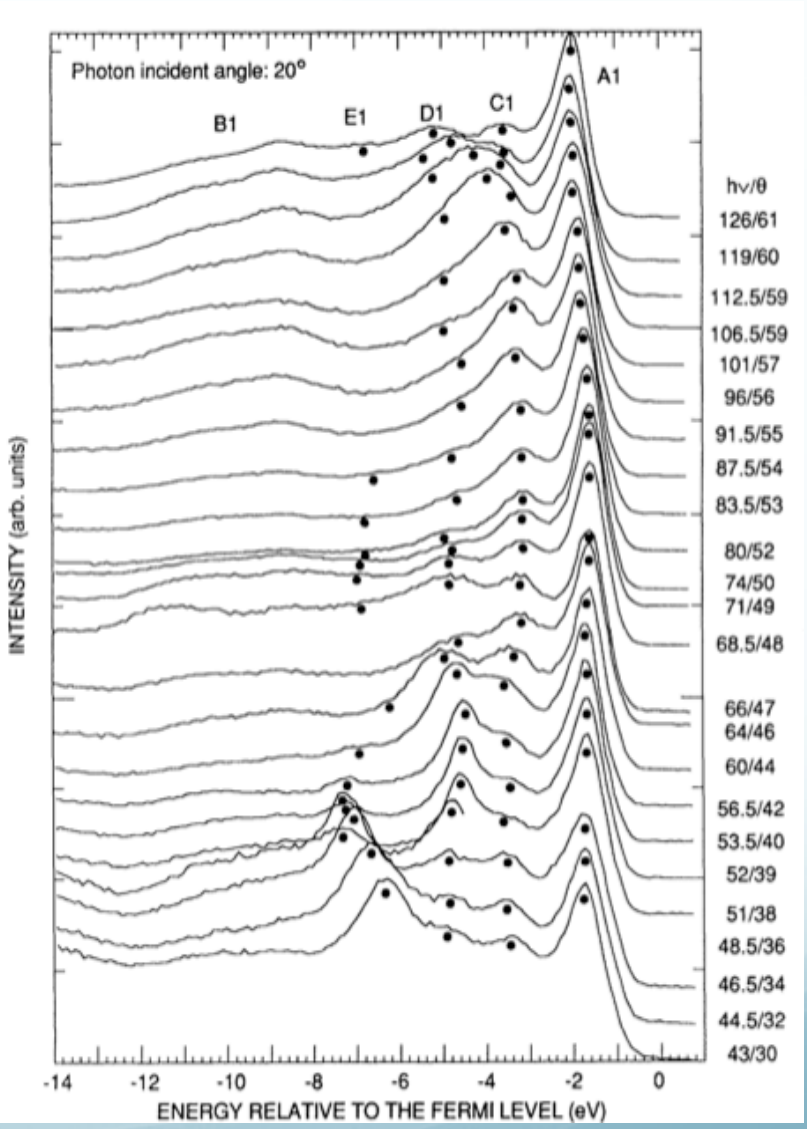
AMF

$(a)\mu_{dc} = 21\text{eV}$



$\text{Tr}\, G = \text{Tr}\, G^0$

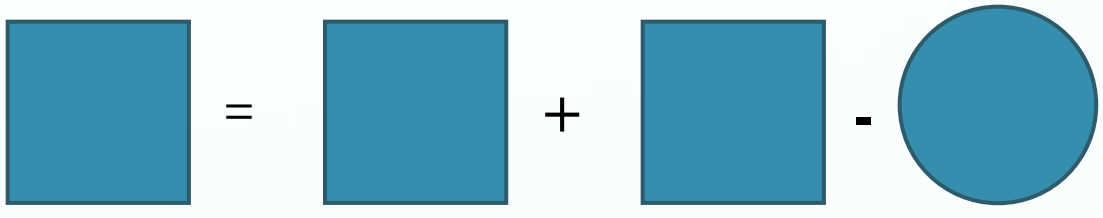
$(b)\mu_{dc} = 25\text{eV}$



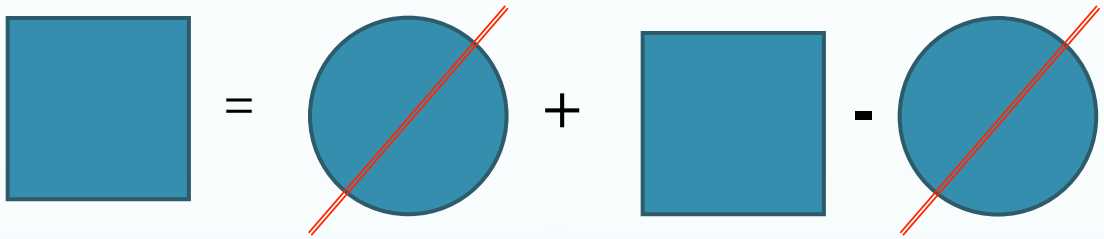
Z.X. Shen,et al PRB (1991)

Full-potential LDA+DMFT: DC problem

$F_{LDA+DMFT} = LDA + DMFT - DC$



No



Yes

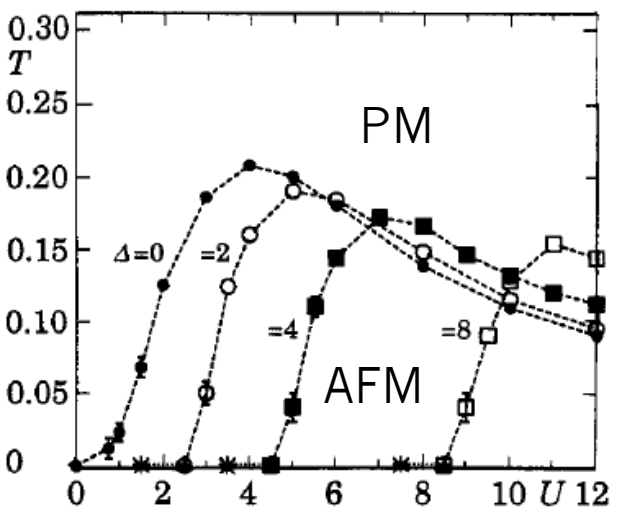
Interchange –possible!

Spherical RI-LDA+U

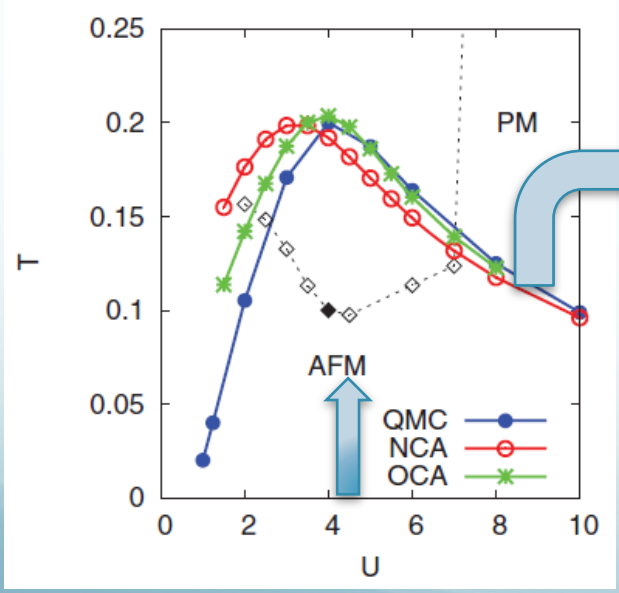
$$V_{\sigma jl}^{\mathrm{LSDA+U}} = V^{\mathrm{LSDA}} + (U - J)[\frac{1}{2}\delta_{jl} - \rho_{jl}^{\sigma}]$$

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

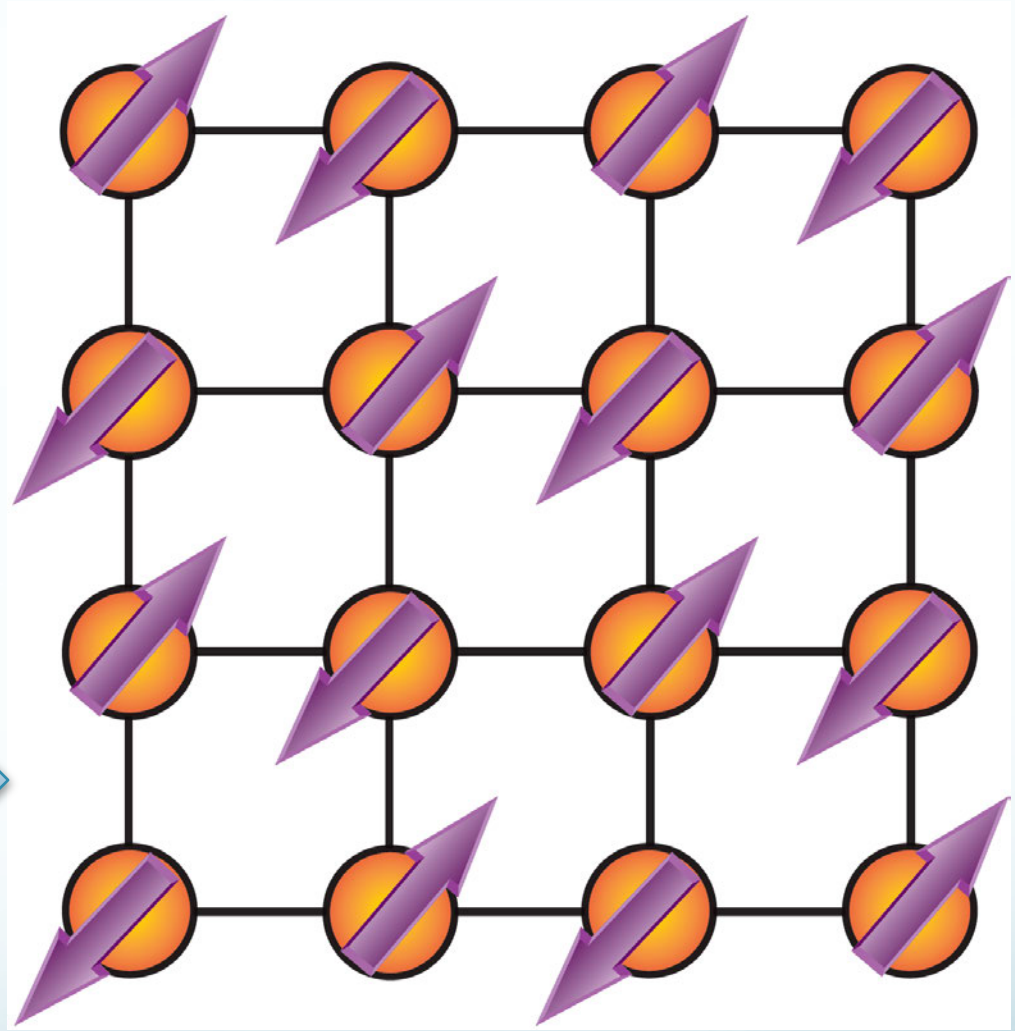
Strong correlations and Magnetism



V. Janis, et al, EPL 24, 287 (1993)



P. Werner, et al, PRB 86, 205101 (2012)



U>W/2=4

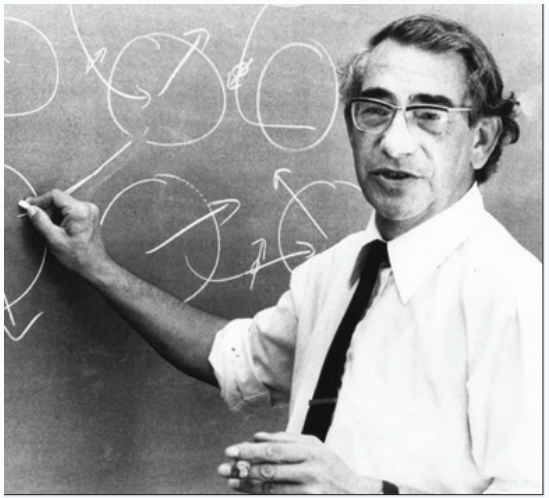
$$J_{\tau\tau'}\vec{S}_{\tau}\cdot\vec{S}_{\tau'}$$

Formation of Local Moments and AFM correlations

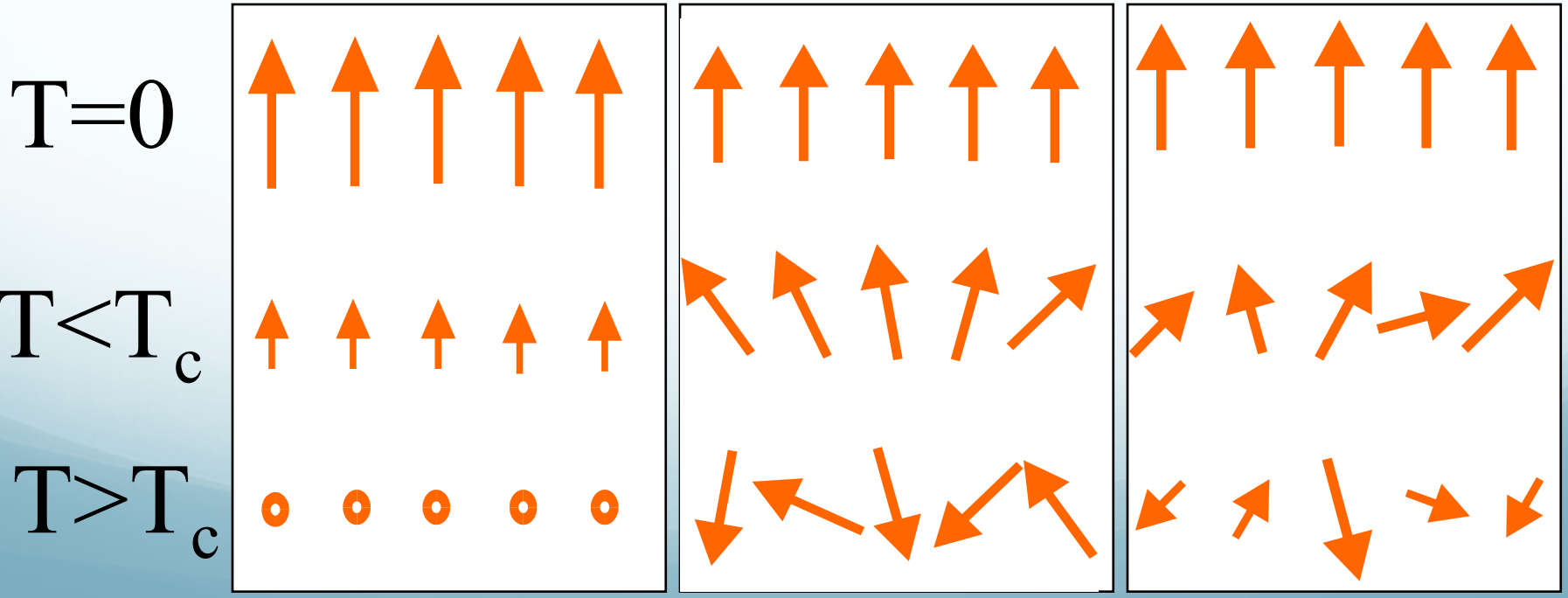
Itinerant ferromagnetism

Stoner

Heisenberg

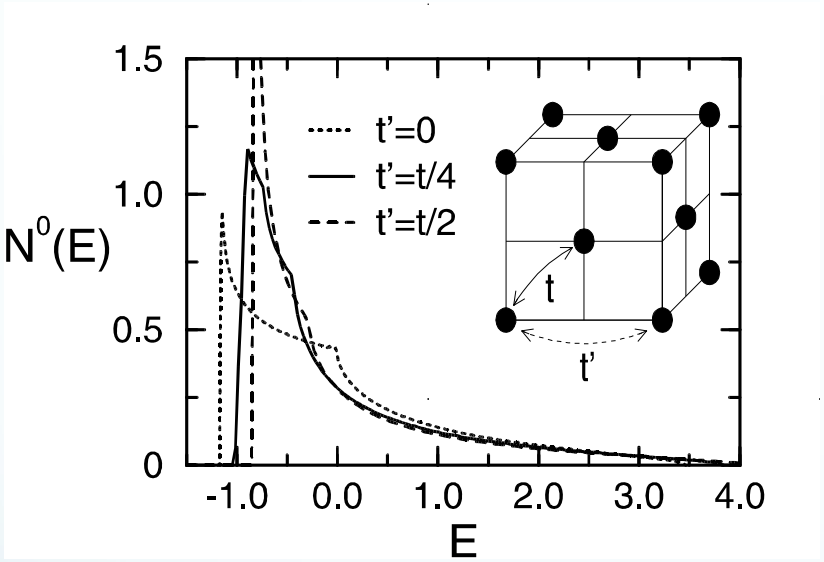


Hubbard

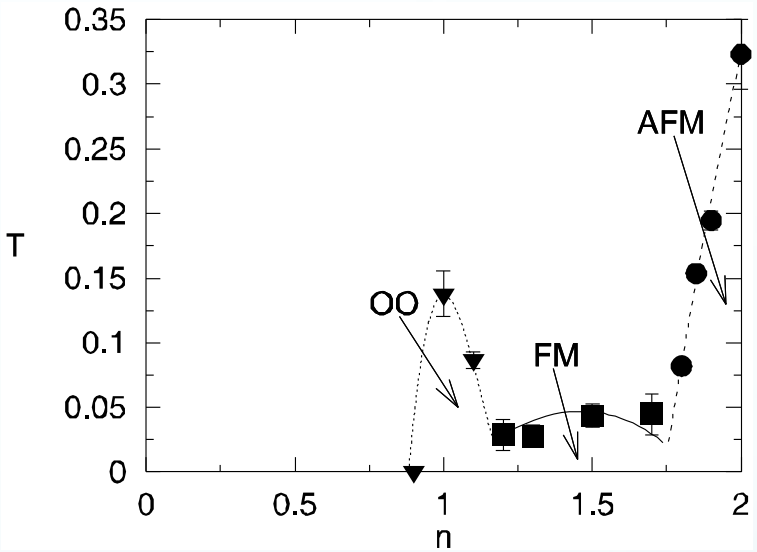


DMFT model of ferromagnetism

DOS-peaks



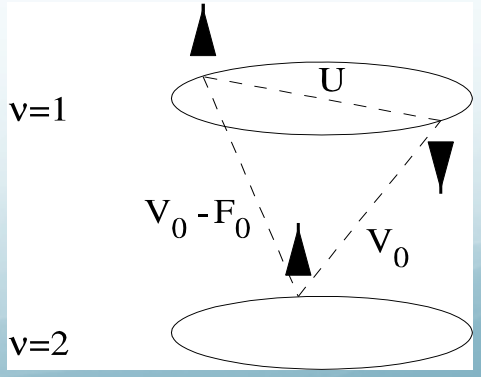
Band degeneracy



D. Vollhardt, et. al.,

In:Bandferromagnetism,

Springer, 2000

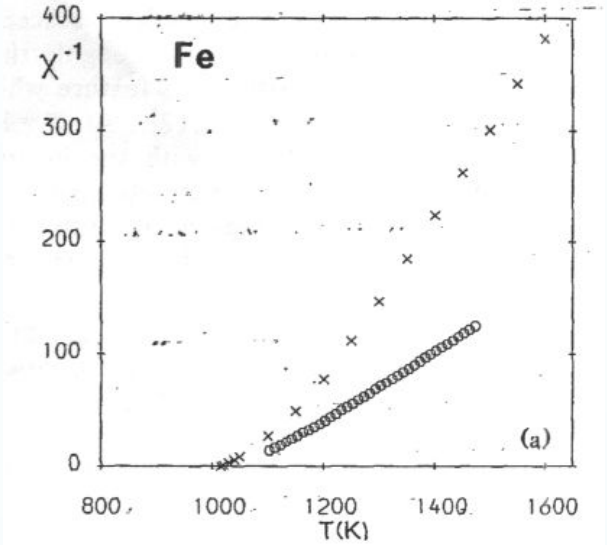


W=4
U =6
V_0=4
F_0=2

LDA+Disordered Local Moments

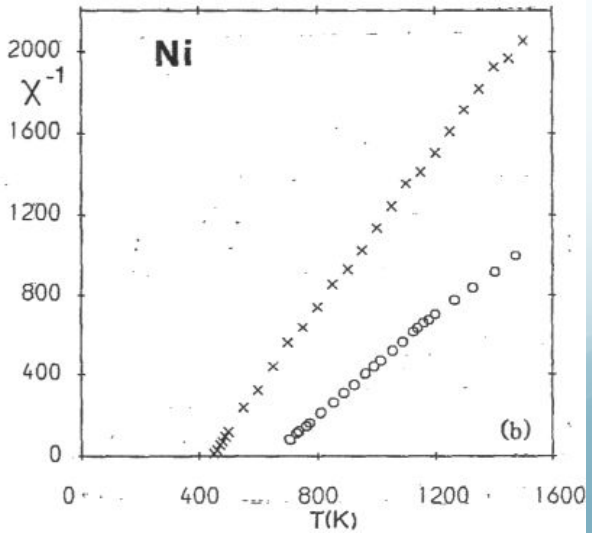
The best first-principle
Spin-fluctuation model
with classical moments

J. Staunton and B. Gyorffy
PRL69, 371 (1992)



DLM

EXP



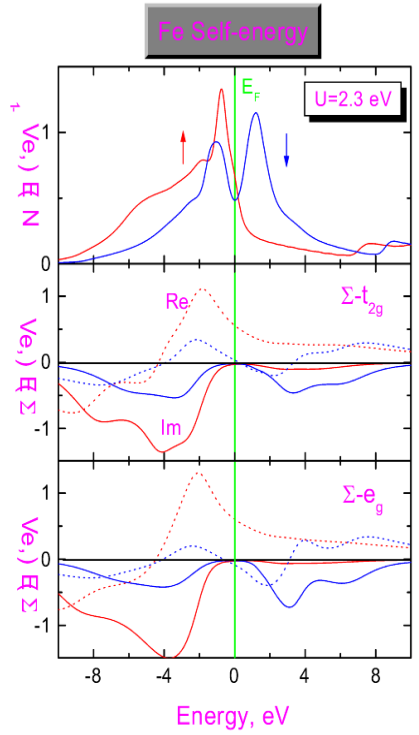
DLM

EXP

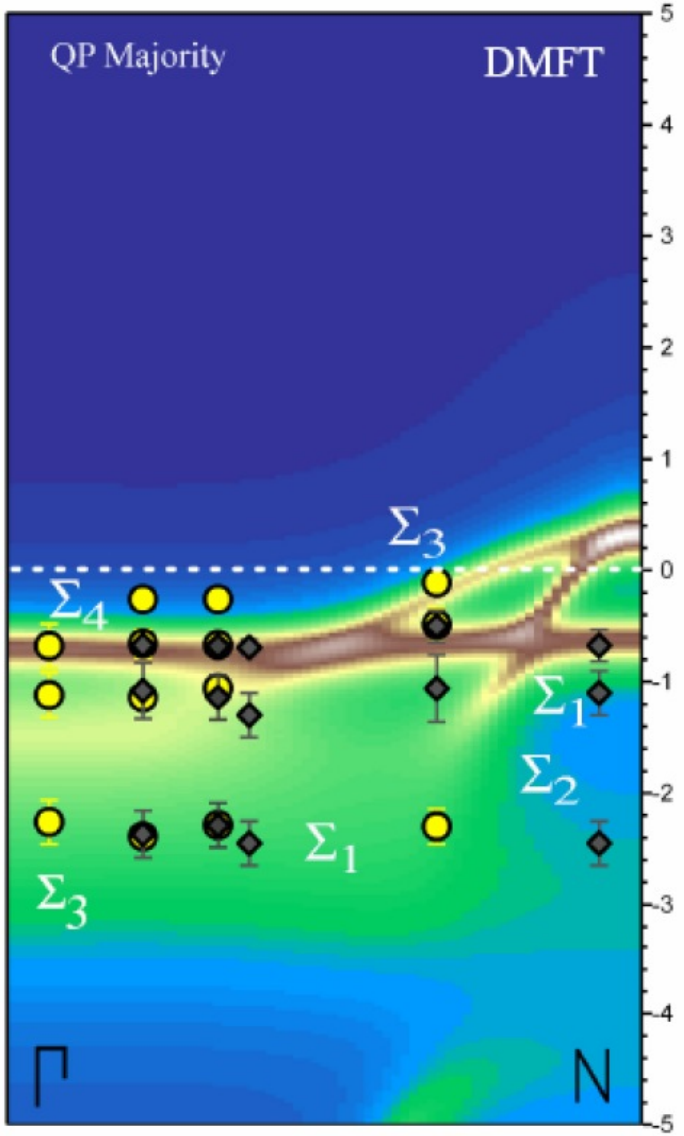
Spectral Function Fe: ARPES vs. DMFT

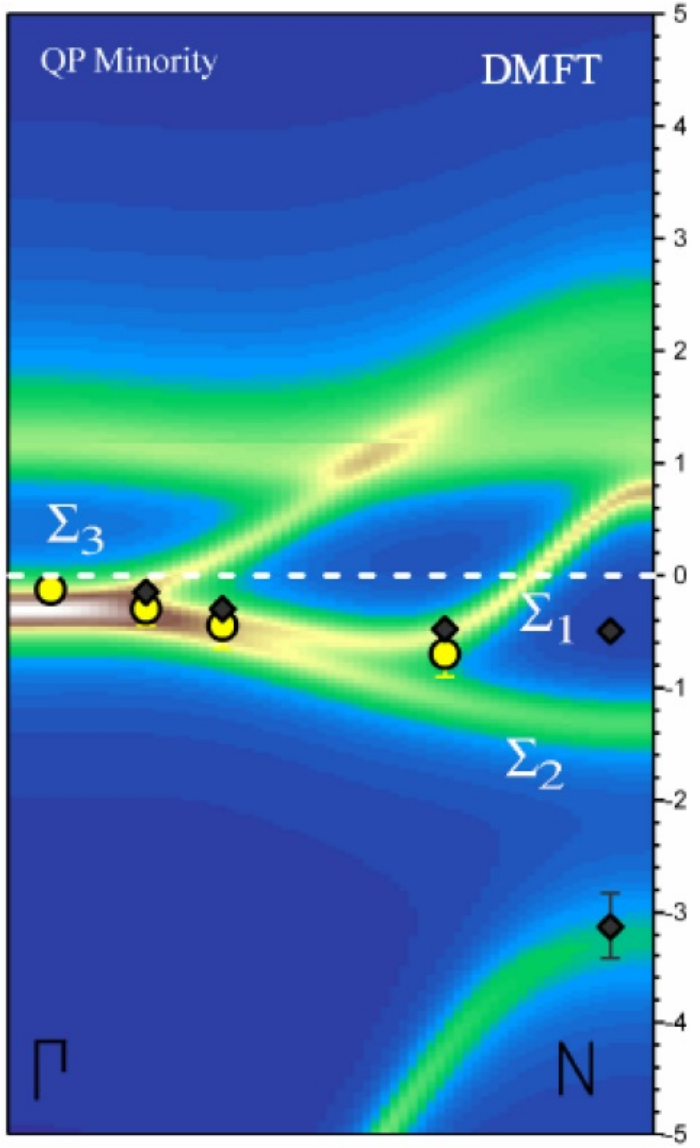
Vertical Pol.

Horizontal Pol.



SP-ARPES (BESY)
J. Sánchez-Barriga, et al, PRL (2010)



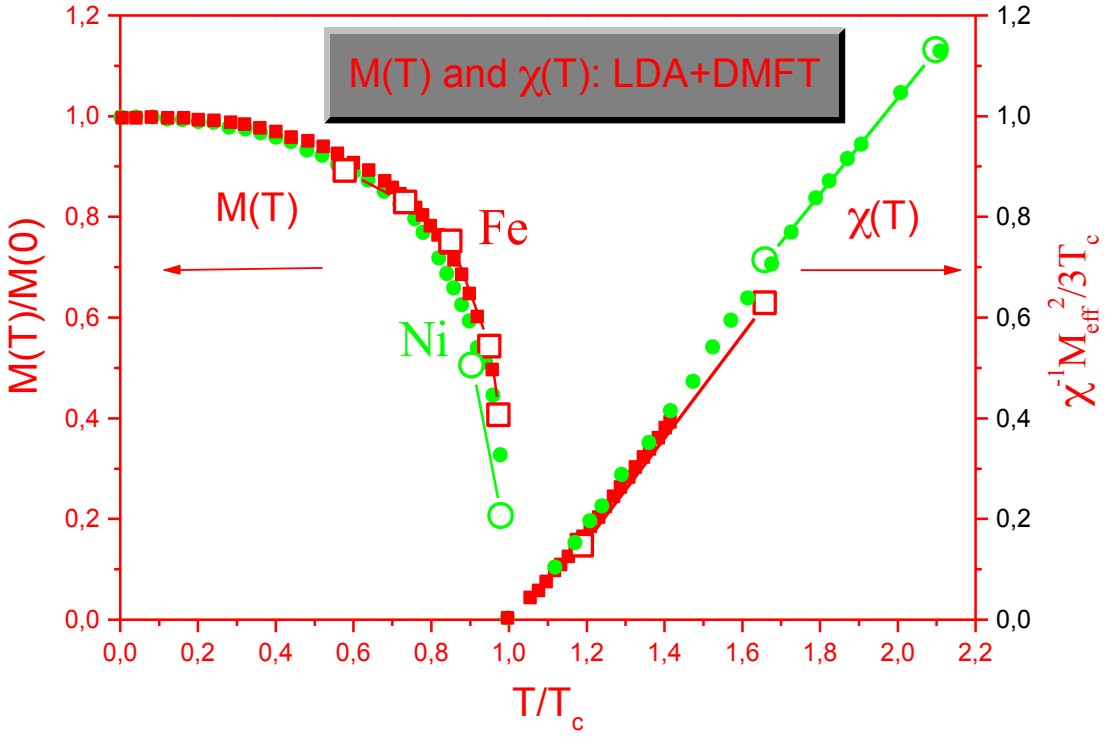


Magnetism of metals: LDA+DMFT

- **Exchange interactions in metals**
- **Finite temperature 3d-metal magnetism**

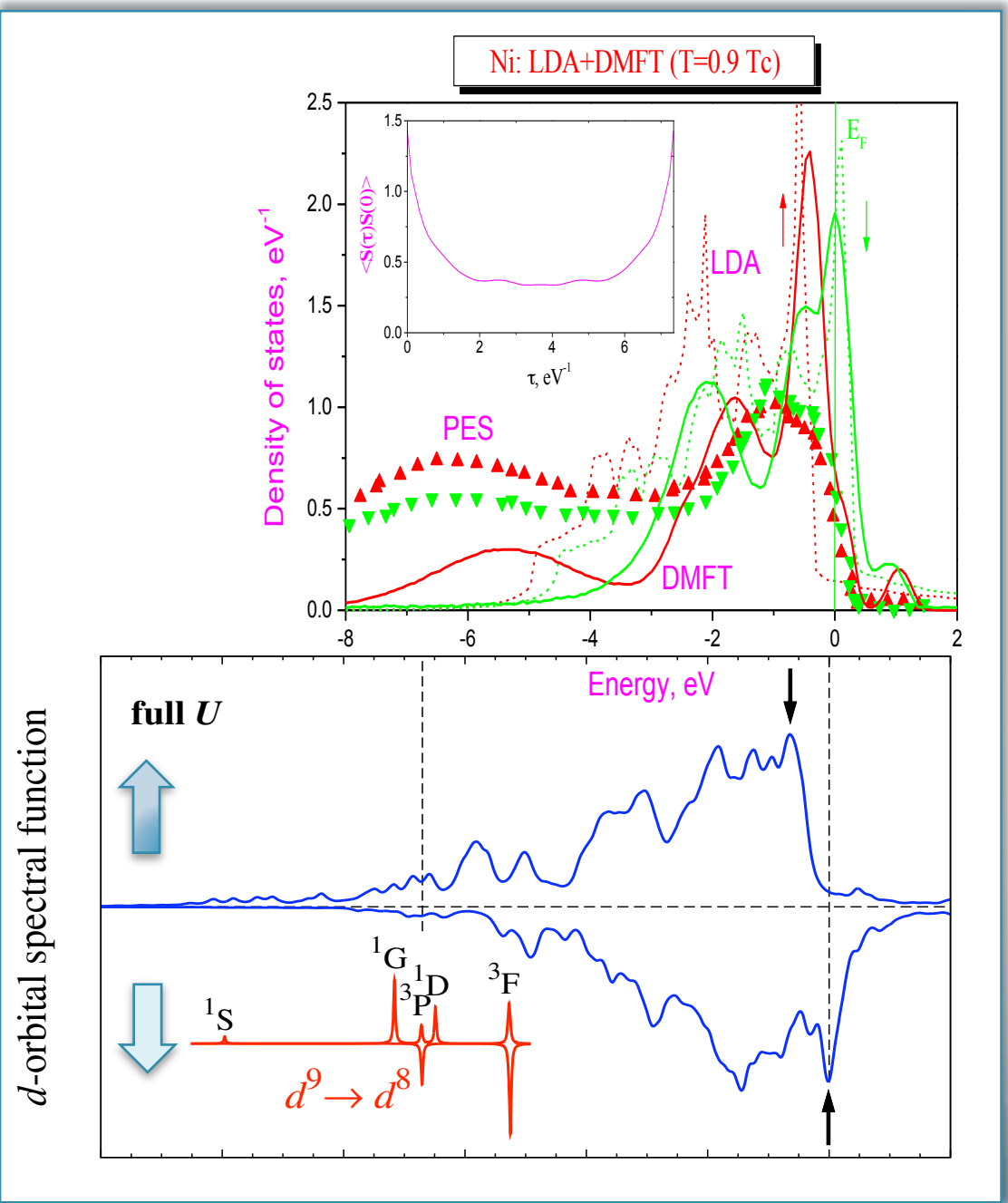
$$[S^{\sigma\sigma'}_{mm'}] \rightarrow [-S^{-\sigma-\sigma'}_{mm'}]$$

Global spin flip



A. L., M. Katsnelson and G. Kotliar, PRL87, 067205 (2001)

Satellite structure in Ni



PES (LDA)

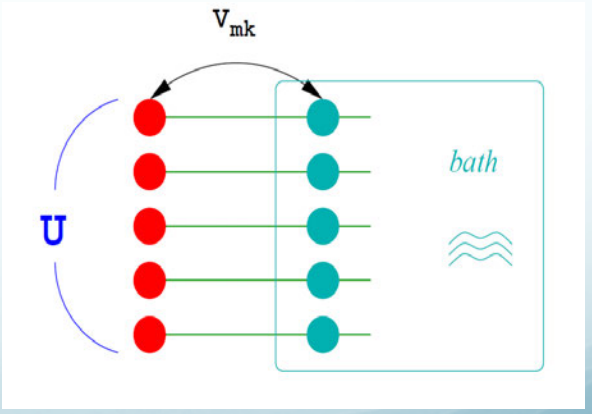
$$W_{band} = 3(4)\ \text{eV}$$

$$\Delta E_{ex} = 0.3(0.6)\ \text{eV}$$

$$E_{sat} = -6(?)\ \text{eV}$$

LDA+DMFT+QMC

A. L., M. Katsnelson and G. Kotliar, PRL (2001)



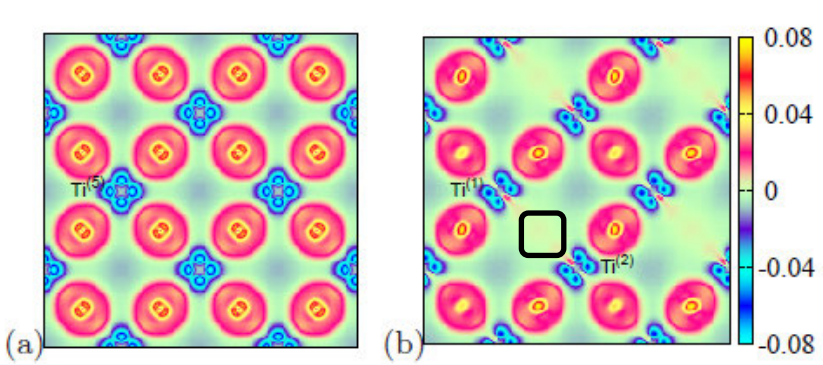
T-Lanczos (5d+10k)

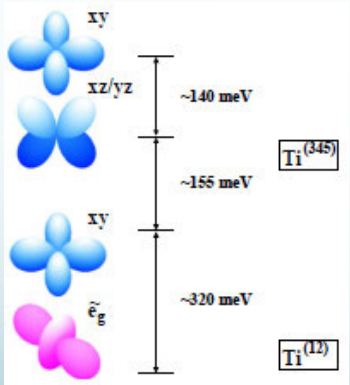
J. Kolorenc et al PRB (2012)

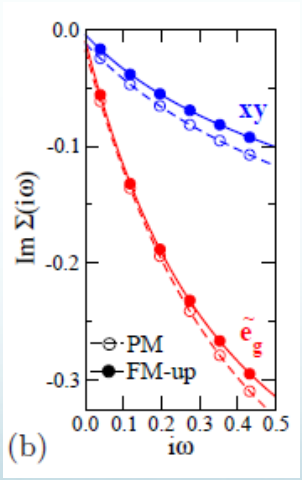
Correlated Magnetism in heterostructures

DFT + real-space DMFT for heterostructures: $LaAlO_3/SrTiO_3$

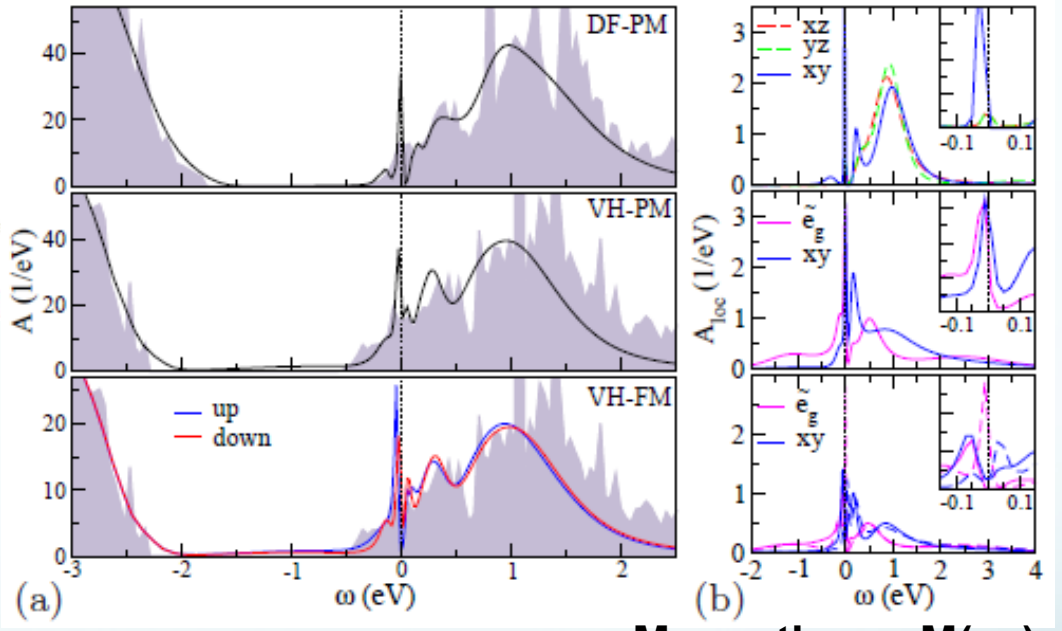
Oxygen vacancy at interface







Formation of interface resonance and FM state

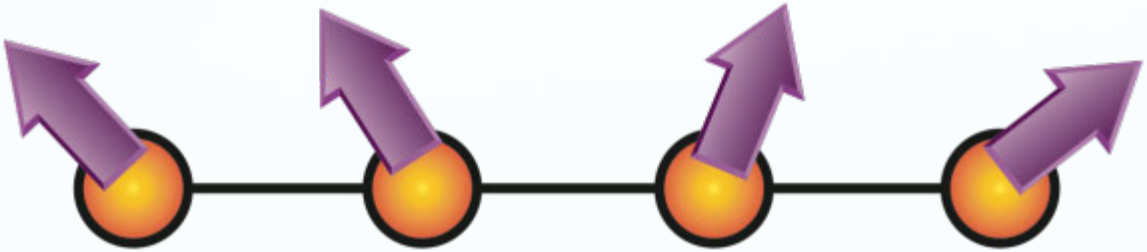


Correlation Effects:
e_g > xy
PM > FM

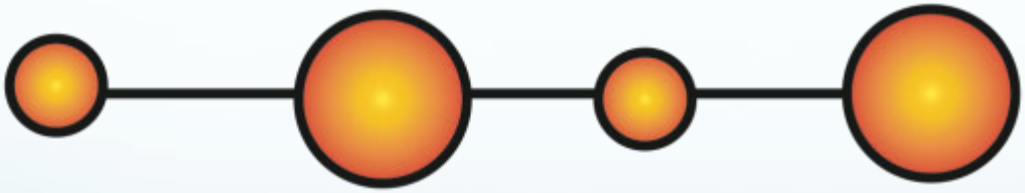
Magnetism – M(μ_B)
LSDA = 0.0
LDA+U = 0.5
DMFT = 0.1
Exp = 0.1
Double-exchange

F. Lechermann, L. Boehnke, and D. Grieger, Ch. Piefke, Phys. Rev. B 90, 085125 (2014)

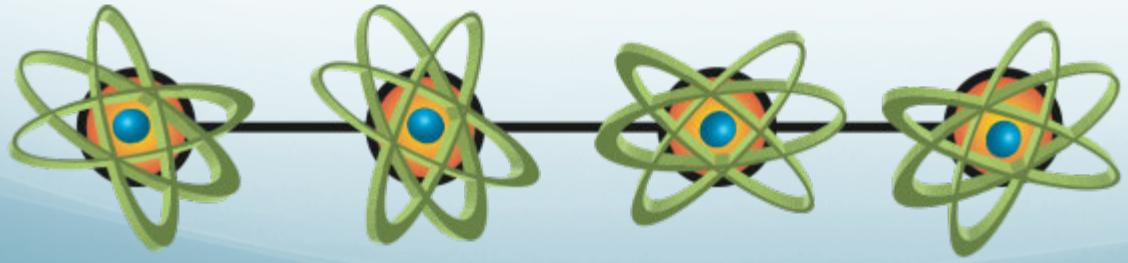
Interaction of electrons with collective excitations



Magnon



Plasmon



Orbiton

Non-local Coulomb interactions

General non-local action for solids:

$$S = \sum_i S_{at}[c_i^\dagger, c_i] + \sum_{i \neq j,\nu,\sigma} t_{ij} c_{i\nu\sigma}^\dagger c_{j\nu\sigma} + \sum_{i \neq j,\omega} V_{ij} \rho_{i\omega}^* \rho_{j\omega}$$

Atomic action with local Hubbard-like interaction

$$S_{at} = -\sum_{\nu\sigma} (i\nu + \mu) c_{\nu\sigma}^\dagger c_{\nu\sigma} + \int_0^\beta U c_\uparrow^\dagger c_\uparrow c_\downarrow^\dagger c_\downarrow d\tau$$

Bosonic charge and spin variables:

$$\rho_j \equiv \sum_{\sigma\sigma'} c_\sigma^\dagger s_{\sigma\sigma'}^j c_{\sigma'} - \bar{\rho}_j$$

$$s^j = (1, \sigma_x, \sigma_y, \sigma_z)$$

$$j = \{0, x, y, z\}$$

A. Rubtsov et al, Annals of Physics 327, 1320 (2012)

Efficient DB-perturbation theory

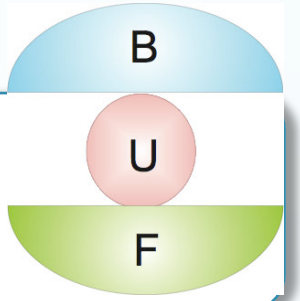
Separate local and non-local effective actions:

$$S = \sum_i S_{imp}[c_i^\dagger, c_i] + \sum_{k\nu\sigma} (t_k - \Delta_{\nu\sigma})\, c_{k\nu\sigma}^\dagger c_{k\nu\sigma} + \sum_{q\omega} (V_q - \Lambda_\omega)\, \rho_{q\omega}^* \rho_{q\omega}$$

Imuprity action with fermionic and bosonic bathes (CT-QMC)

$$S_{imp} = S_{at} + \sum_\nu \Delta_\nu c_\nu^\dagger c_\nu + \sum_\omega \Lambda_\omega \rho_\omega^* \rho_\omega$$

F B

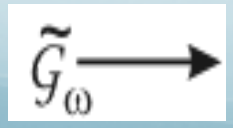


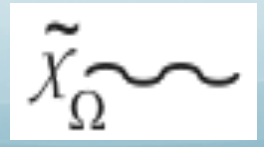
Dual boson-fermion transformation: $c^\dagger \Rightarrow f^\dagger$ $\rho^* \Rightarrow \eta^*$

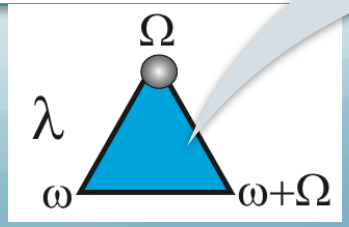
$$\tilde{S} = -\sum_{k\nu} \tilde{\mathcal{G}}_{k\nu}^{-1} f_{k\nu}^\dagger f_{k\nu} - \sum_{q\omega} \tilde{\chi}_{q\omega}^{-1} \eta_{q\omega}^* \eta_{q\omega} + \sum_i \tilde{U}[\eta_i, f_i, f_i^\dagger]$$

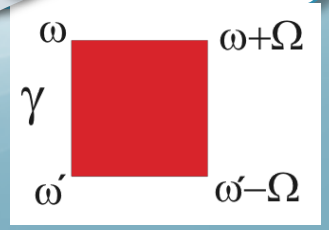
EDMFT

Diagrams:

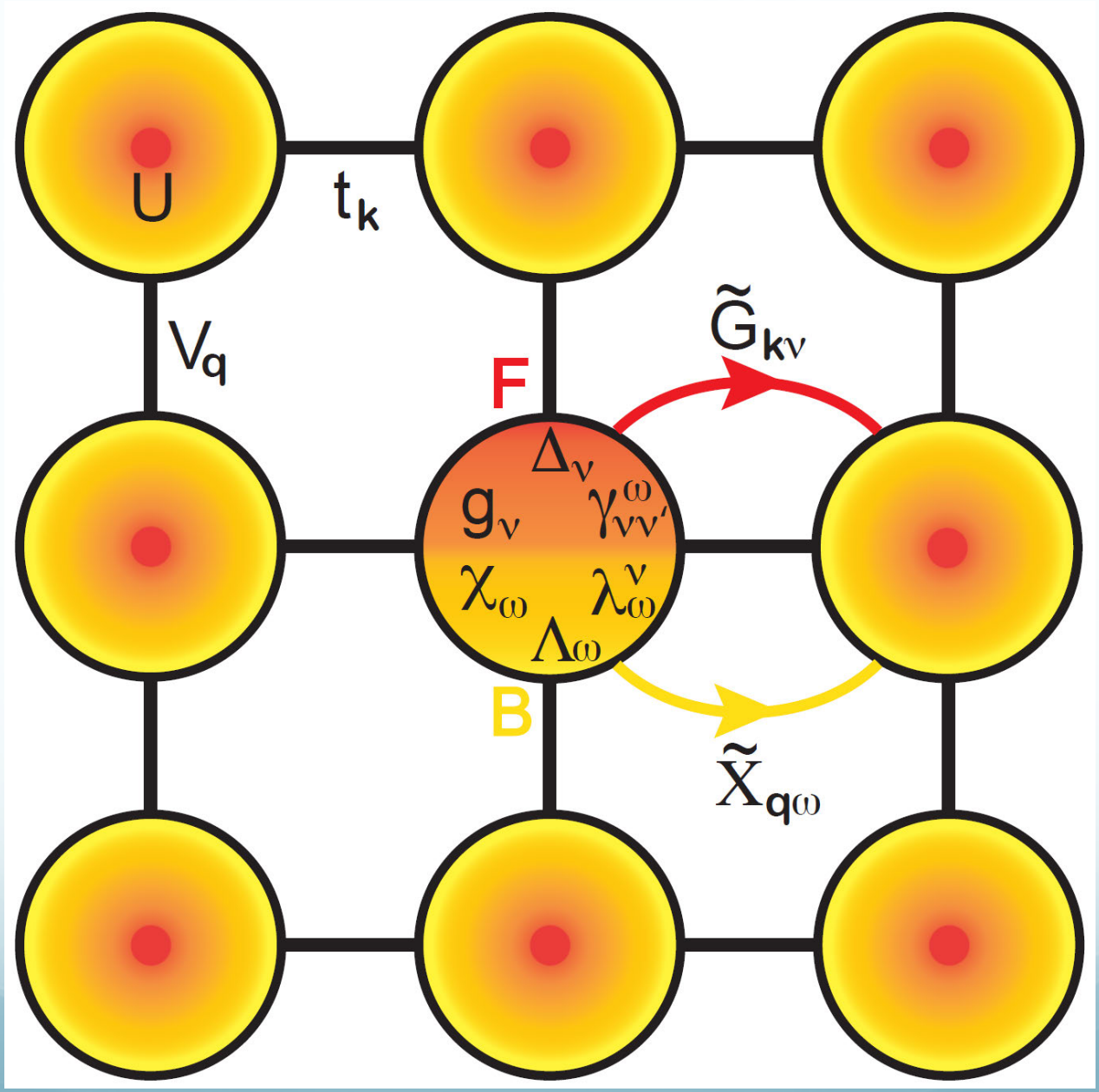








Dual Boson: General Idea

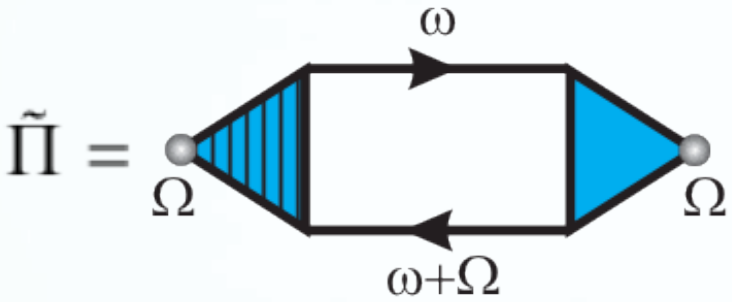


HTSC

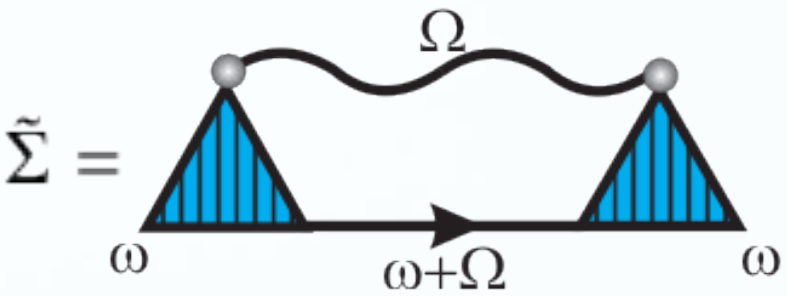
$$\Lambda_\omega \sim J_{\tau\tau'}\vec{S}_\tau \cdot \vec{S}_{\tau'}$$

DB-diagrammatic scheme

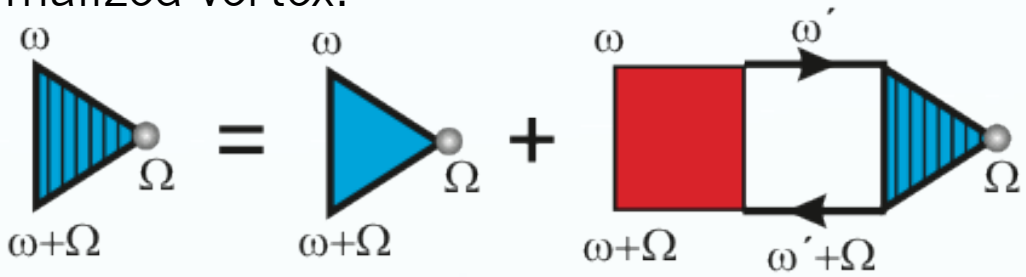
Bosonic Selfenergy



Fermionic Selfenergy



Renormalized vertex:



Fermionic and Bosonic Green Functions

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

$$X_{q\omega} = [(\chi_\omega + \chi_\omega \tilde{\Pi}_{q\omega} \chi_\omega)^{-1} + \Lambda_\omega - V_k]^{-1}$$

SCF-condition

$$\sum_k G_{k\nu} = g_\nu$$

$$\sum_q X_{q\omega} = \chi_\omega$$

Δ_ν

Λ_ω

A. Rubtsov, M.I. Katsnelson, A. L., Annals of Phys. 327, 1320 (2012)

Plasmon in correlated system: Poster of Erik van Loon

Summary

- Electronic structure of correlation systems can be well described in LDA+DMFT scheme
- Local correlations efficiently included in CT-QMC impurity solver
- The problem of Double-Counting in LDA+DMFT can be efficiently solved within GW+EDMFT (Lectuer 2)