Magnetism: from Stoner to Hubbard

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In collaboration with
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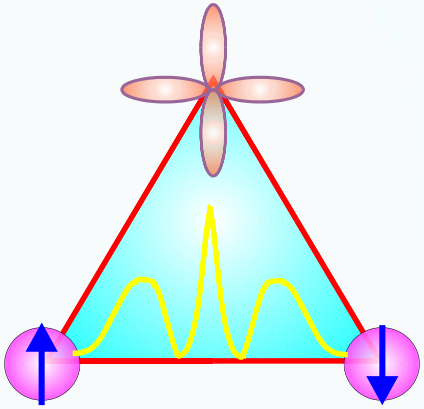
Outline

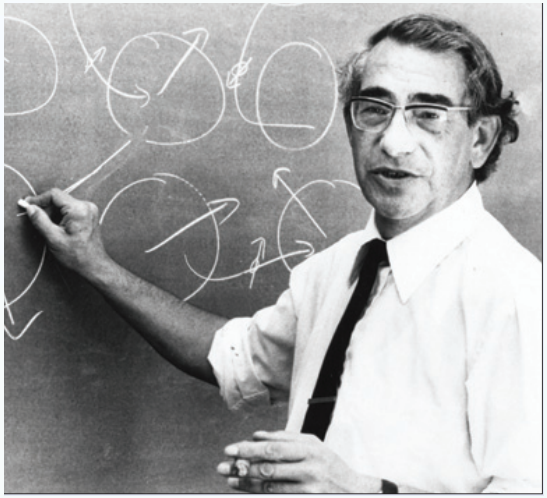


- Heisenberg, Stoner, and Hubbard
- Many-body approach: D(M)FT functionals
- Correlation effects in electronic structure
- Magnetism of correlated systems

Itinerant ferromagnetism


Stoner

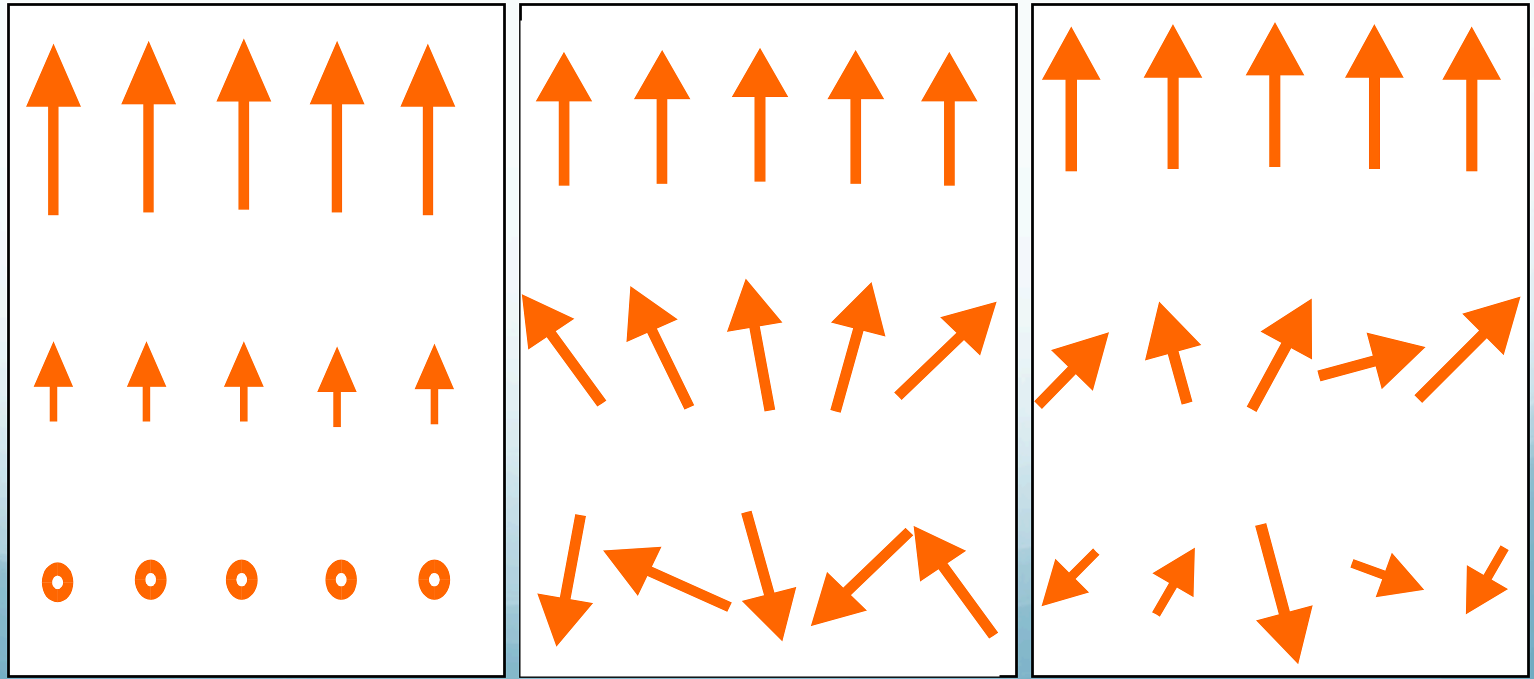

Heisenberg


Hubbard

$T=0$

$T<T_c$

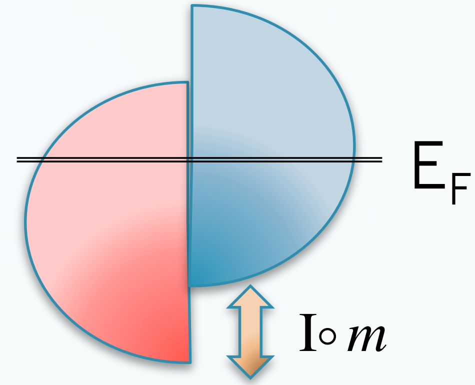
$T>T_c$



From Stoner to Hubbard

Stoner mode

$$H_s = \sum_{\mathbf{k}\sigma} (\varepsilon_{\mathbf{k}} + I < n_{-\sigma} >) c^{+}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$



Mean Field

$$\Delta h_\sigma = U < n_{-\sigma} > n_\sigma$$

Hubbard mode

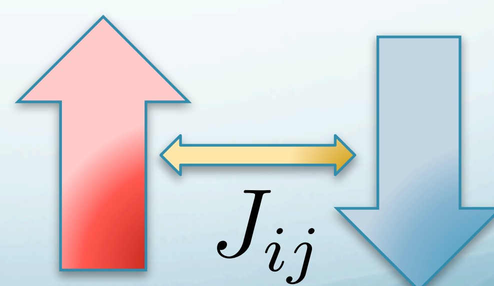
$$H_h = \sum_{ij\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + \sum_{i} U n_{i\uparrow} n_{i\downarrow}$$

$U >> t$

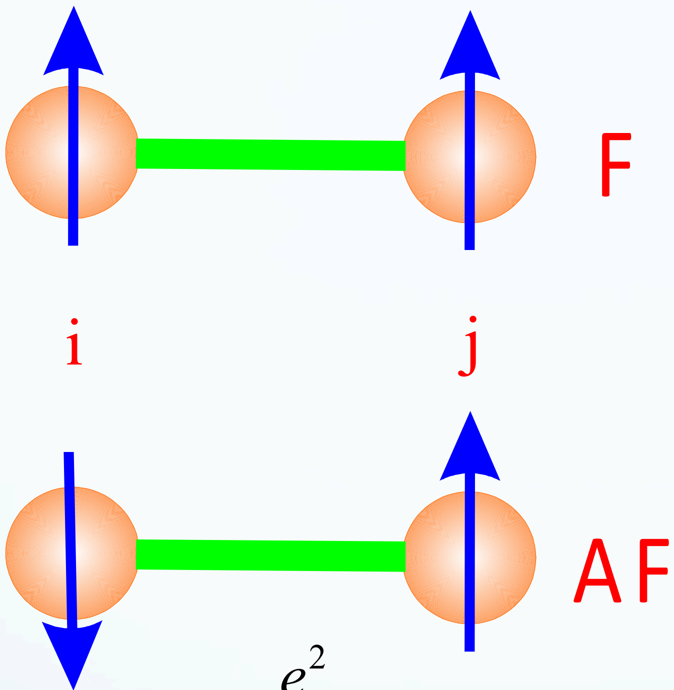
$$J = -2\frac{t^2}{U}$$

Heisenberg exchange

$$H_e = -\sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$



Magnetism of H_2: Heisenberg vs. Slater



$$J = \langle ij | \frac{e^2}{r_{12}} | ji \rangle$$

Exchange interaction:

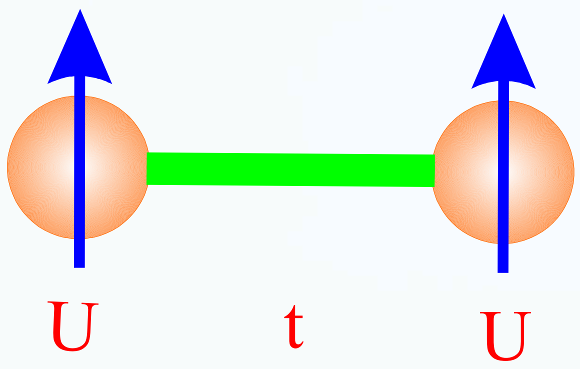
$$H_{ex} = -2J_{ij}\overrightarrow{S}_i\overrightarrow{S}_j$$

$$J = \frac{1}{2}(E_S - E_T) = E_{AF} - E_F$$

$$\begin{aligned} E_F &= |\uparrow\uparrow\rangle = E_T \\ E_{AF} &= |\uparrow\downarrow\rangle = \frac{1}{2}(E_S + E_T) \end{aligned}$$

$$\begin{aligned} \Psi_T &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle); \quad |\uparrow\uparrow\rangle; \quad |\downarrow\downarrow\rangle \\ \Psi_S &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \end{aligned}$$

Exchange interactions: Anderson



$$H = t \sum_{ij=1,2} c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i=1,2} n_{i\uparrow} n_{i\downarrow}$$

ED in subspace
$N_- = 1, N_+ = 1$

N	i	j
1	$\uparrow$	$\downarrow$
2	$\downarrow$	$\uparrow$
3	$\uparrow\downarrow$	0
4	0	$\uparrow\downarrow$

H	1	2	3	4
1	0	0	t	t
2	0	0	t	t
3	t	t	U	0
4	t	t	0	U

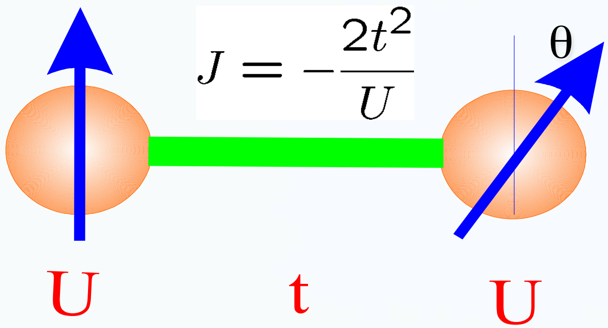
U>>t

$$E_T = 0$$

$$E_S = \frac{U}{2}\left(1 - \sqrt{1 + \frac{16t^2}{U}}\right) \approx -\frac{4t^2}{U}$$

Anderson kinetic exchange $J = -\dfrac{2t^2}{U}$

Exchange: Local force approach



Spin-polarized LSDA

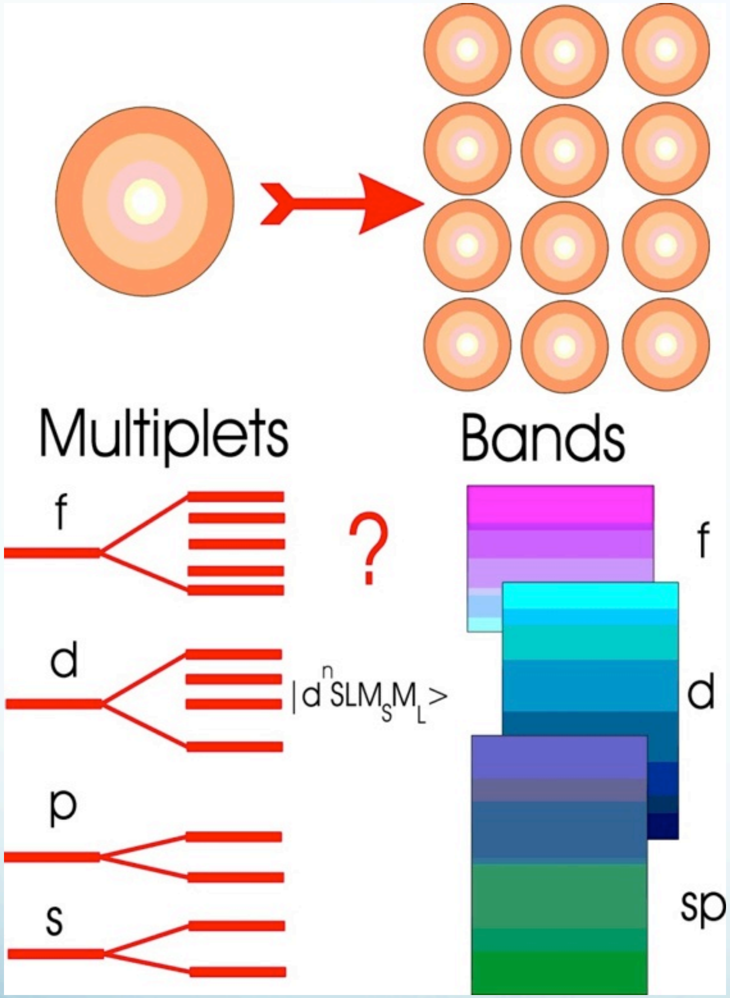
$$h_\sigma = t + \frac{1}{2} U \vec{e}\,\vec{\sigma}$$

H	$1\uparrow$	$2\uparrow$	$1\downarrow$	$2\downarrow$
$1\uparrow$	$-\frac{U}{2}$	t	0	0
$2\uparrow$	t	$-\frac{U}{2}(1-\cos\theta)$	0	$\frac{U}{2}\sin\theta$
$1\downarrow$	0	0	$\frac{U}{2}$	t
$2\downarrow$	0	$\frac{U}{2}\sin\theta$	t	$\frac{U}{2}(1-\cos\theta)$

Spectrum: $\epsilon_i = \pm\frac{1}{2}\sqrt{4t^2 + U^2 \pm Ut\sqrt{2(1 \mp \cos\theta)}}$

Exchange energy: $E_x(\theta) \approx \frac{t^2}{U}\cos\theta = -2JS^2 \vec{e}_i \vec{e}_j = -\frac{1}{2} J \cos$

From Atom to Solids



Electrons in solids:

- Effective potential
- Bloch states
- Pauli principle

Density Functional Theory (DFT)
Effective one-particle states
Local Density Approximation (LDA)

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:

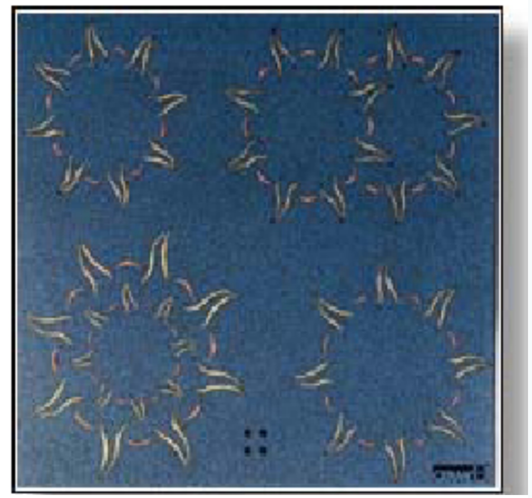
$$V_H[n] = \frac{e^2}{2}\int d\vec{r}\int d\vec{r}'\frac{n(\vec{r})n(\vec{r}')}{|\vec{r}-\vec{r}'|}$$

Effective potential:

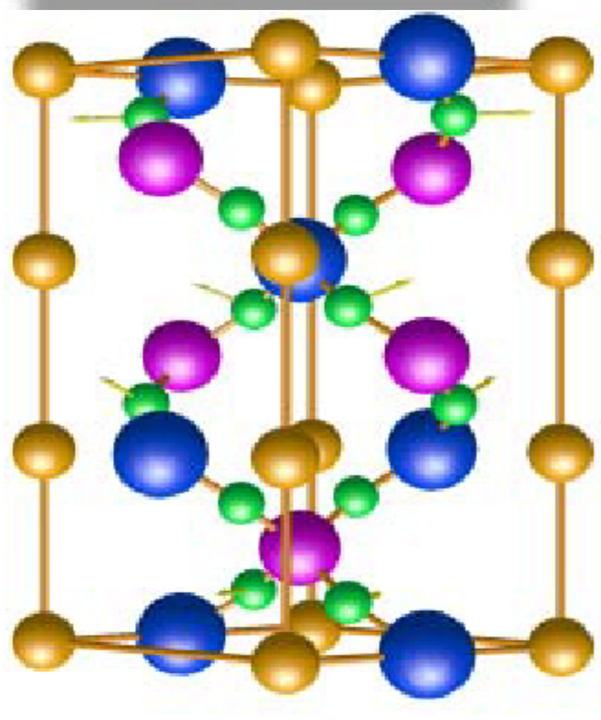
$$V_{eff}(\vec{r}) = V_{ext}(\vec{r}) + e^2\int d\vec{r}'\frac{n(\vec{r}')}{|\vec{r}-\vec{r}'|} + \frac{\delta E_{xc}[n]}{\delta n(\vec{r})}$$

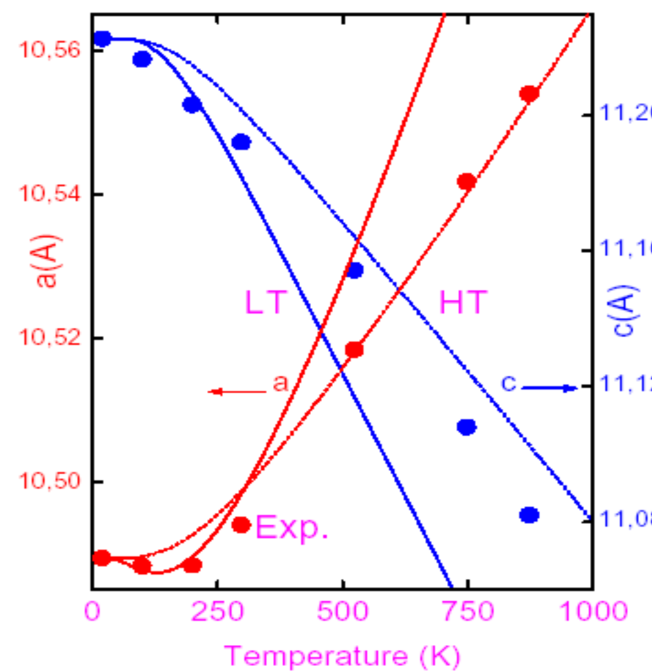
Computational Material Science: DFT

SCHOTT
Total Customer Care



CERAN-plate



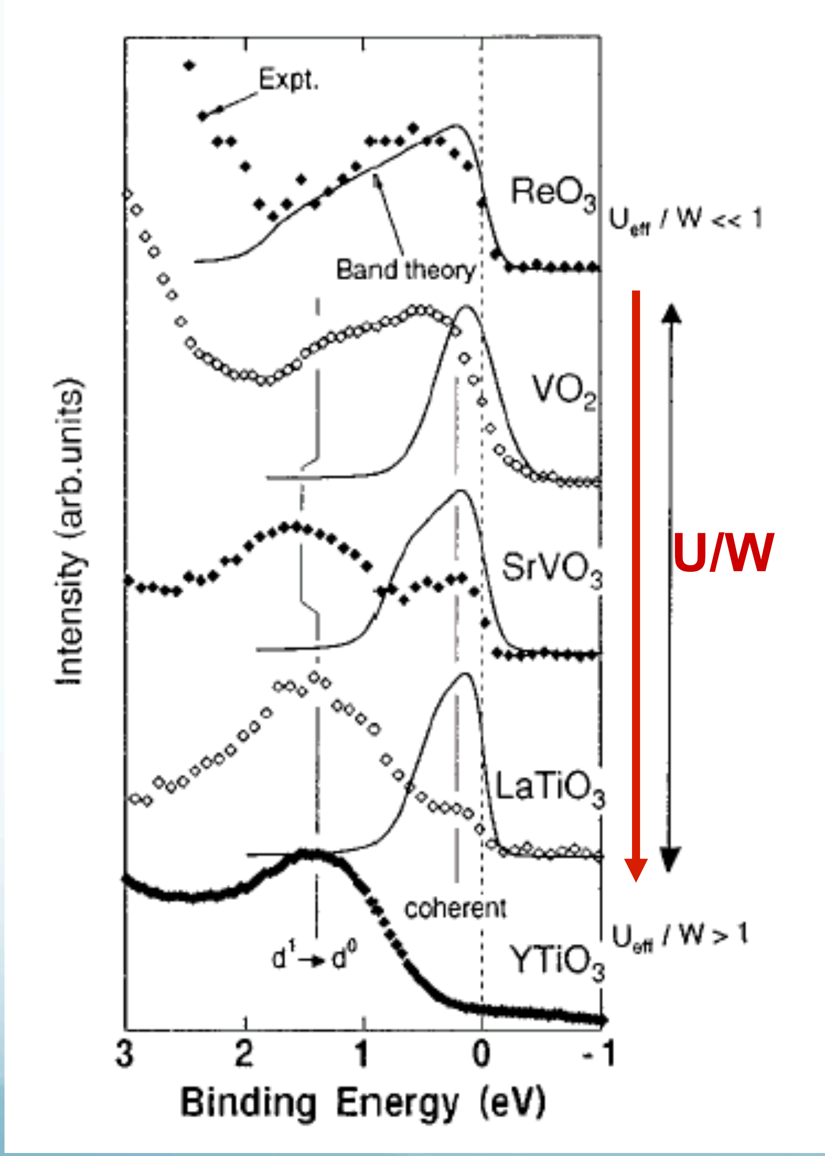


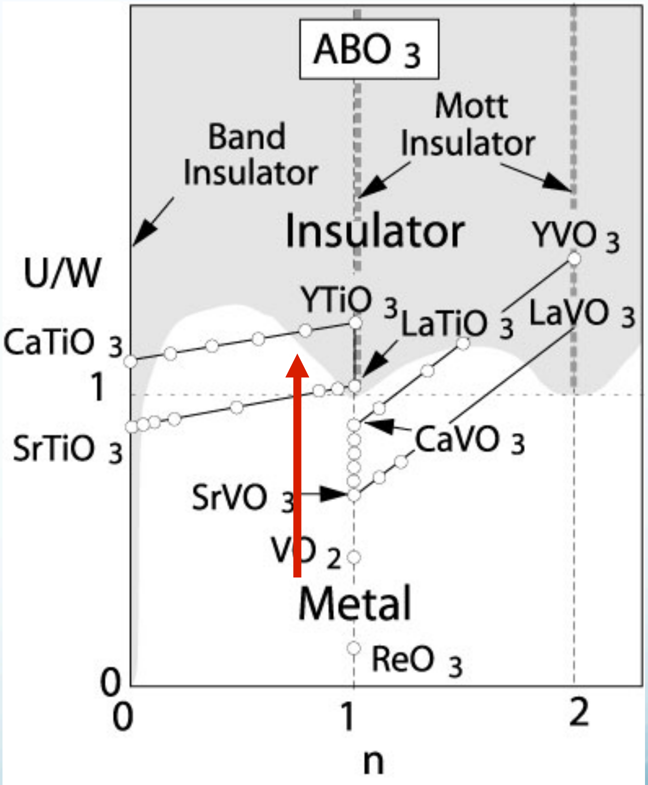
DFT-theory:
$LiAlSiO_4$

A.L, R. O. Jones,
H. Xu,P. J. Heaney,
Phys. Rev. B **58**, 6219 (1998

Correlation driven MIT

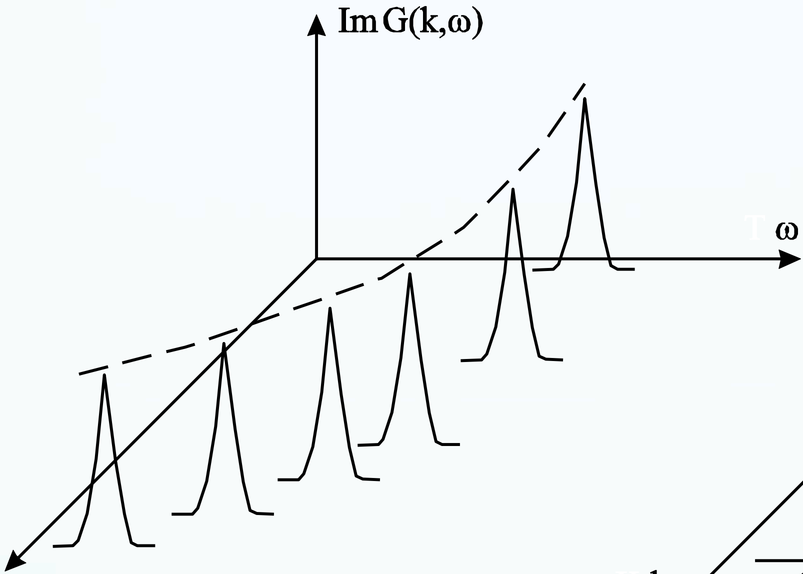
photoemission spectra (DOS)
A. Fujimori et al.



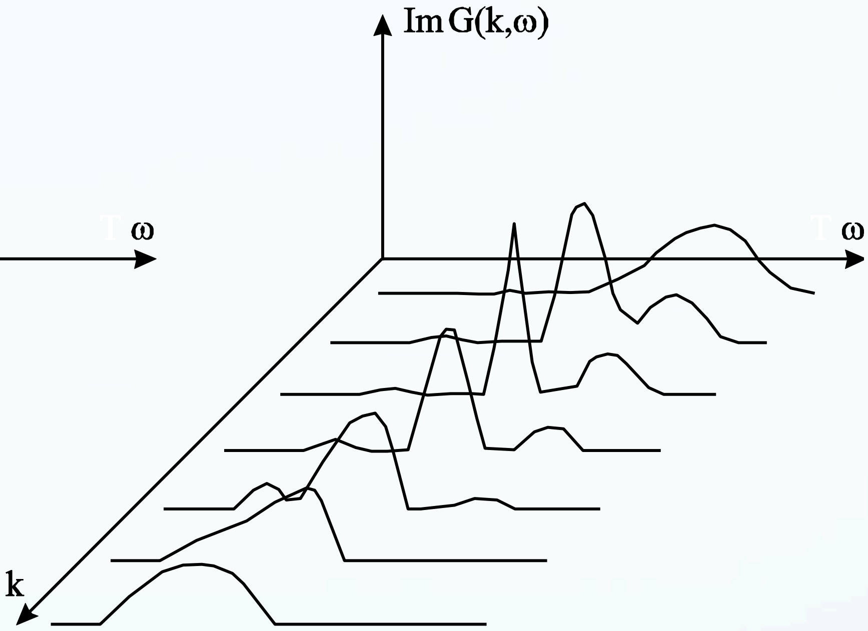


Spectral function: Correlations effects

ARPES



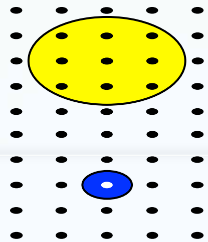
Free electrons



Correlated electrons

Strongly Correlated Electron Systems

3d - 4f
open shells materials



U<<W
Charge fluct.

U>>W
Spin fluct.

- Kondo
- Mott-Hubbard
- Heavy Fermions
- High-Tc SC
- Spin-charge order
- Colossal MR

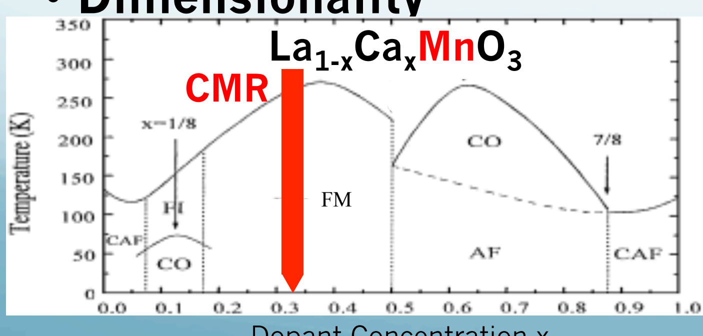
I	II	IIIb	IVb	Vb	VIb	VIIb	VIIIb			Ib	IIb	III	IV	V	VI	VII	0
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac**	Rf	Db	Sg	Bh	Hs	Mt									
Lanthanides *			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
Actinides **			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

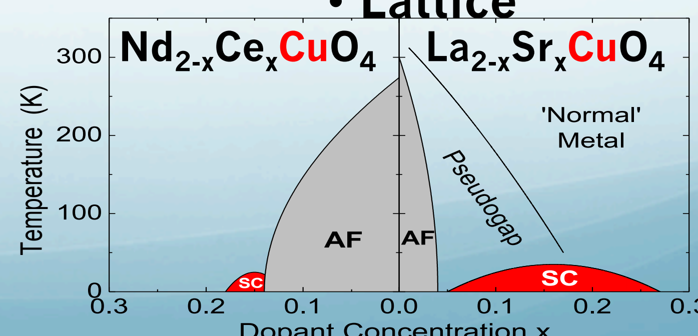
Control parameters

- Bandwidth (U/W)
- Band filling
- Dimensionality

Degrees of freedom

- Charge / Spin
- Orbital
- Lattice

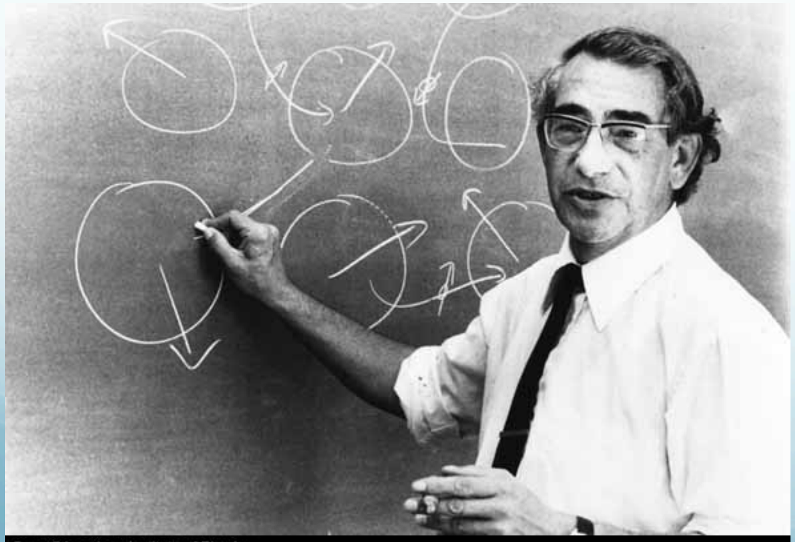




Hubbard model for correlated electrons

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

- **U/t**
- **Chemical potential**



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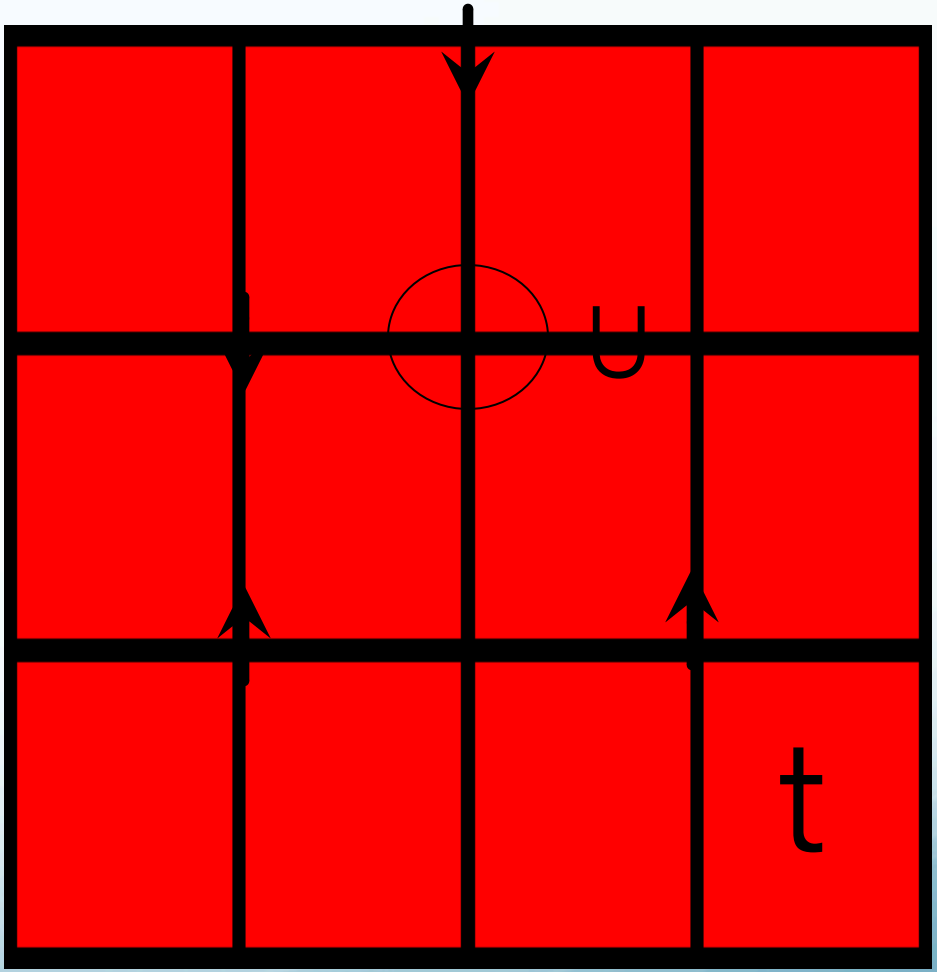

The Theory of Everything

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

Hoehnberg and Kohn: DFT

PHYSICAL REVIEW VOLUME 136, NUMBER 3B 9 NOVEMEBR 1964

Inhomogeneous Electron Gas*

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AND
W. KOHN‡
École Normale Superieure, Paris, France and Faculté des Sciences, Orsay, France

Hamiltonian in

Field Operators:

$$H = T + V + U$$

$$T \equiv \frac{1}{2}\int \nabla\psi^*(\mathbf{r})\nabla\psi(\mathbf{r})d\mathbf{r},$$

$$V \equiv \int v(\mathbf{r})\psi^*(\mathbf{r})\psi(\mathbf{r})d\mathbf{r},$$

$$U = \frac{1}{2}\int \frac{1}{|\mathbf{r}-\mathbf{r}'|}\psi^*(\mathbf{r})\psi^*(\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r})d\mathbf{r}d\mathbf{r}'$$

$$n(\mathbf{r}) \equiv (\Psi, \psi^*(\mathbf{r})\psi(\mathbf{r})\Psi)$$

$$E_v[n] \equiv \int v(\mathbf{r})n(\mathbf{r})d\mathbf{r} + F[n]$$

Path Integrals for Fermions

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

Fermions second-quantization operators (Pauli principle)

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

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)

$$\begin{aligned} \int 1 dc &= 0 \\ \int c dc &= 1 \end{aligned}$$

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

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^* 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

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

$$= \int\int dc^* dc e^{-c^* c} \sum_{n=0,1} \langle -c| \hat{O} |n\rangle \langle n| c\rangle = \int\int dc^* dc e^{-c^* c} \langle -c| \hat{O} |c\rangle$$

"Minus" due to commutation Left and Right coherent state

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

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

Gaussian Path Integrals

Only one analytical path integral:

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

Short notation

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

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

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

N=2

$$\begin{aligned}
\int D[c^* c]\, e^{-c_1^* M_{11} c_1 - c_1^* M_{12} c_1 - c_2^* M_{21} c_1 - c_2^* M_{22} c_2} &= \\
\frac{1}{2!}\int D[c^* c]\, (-c_1^* M_{11} c_1 - c_1^* M_{12} c_1 - c_2^* M_{21} c_1 - c_2^* M_{22} c_2)^2 &= \\
M_{11} M_{22} - M_{12} M_{21} &= \det M
\end{aligned}$$

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:

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

Two-particle correlation function:

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

Path Integral for Everything

Euclidean action

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

$$S = \sum_{12} c_1^* \left(\partial_\tau + t_{12}\right) c_2 + \frac{1}{4} \sum_{1234} c_1^* c_2^* U_{1234}\, c_4 c_3$$

One- and two-electron matrix elements:

$$t_{12} = \int d\mathbf{r}\, \phi_1^*(\mathbf{r}) \left(-\frac{1}{2}\nabla^2 + V(\mathbf{r}) - \mu\right) \phi_2(\mathbf{r})$$

$$U_{1234} = \int d\mathbf{r} \int d\mathbf{r}'\, \phi_1^*(\mathbf{r}) \phi_2^*(\mathbf{r}')\, U(\mathbf{r}-\mathbf{r}')\, \phi_3(\mathbf{r}) \phi_4(\mathbf{r}')$$

Shot notation:

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

One- and Two-particle Green Functions

One-particle Green function

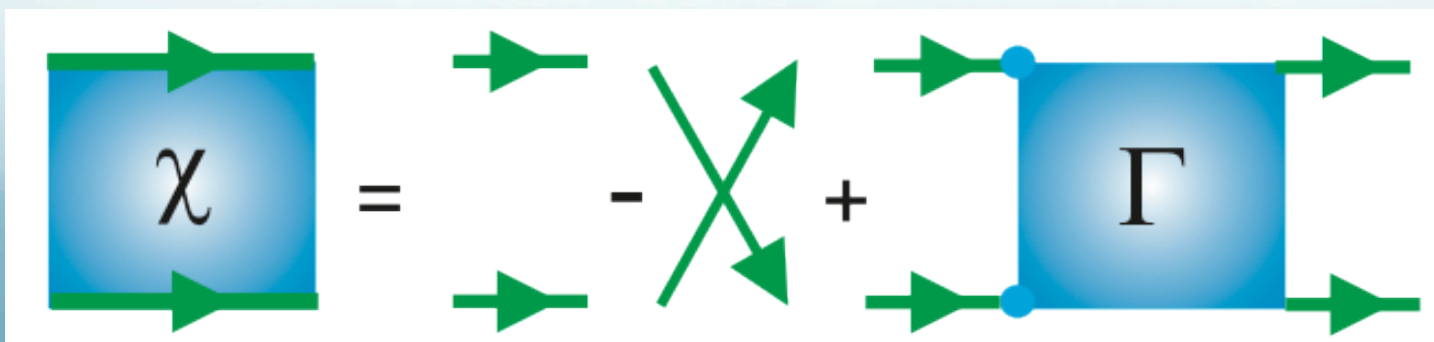
$$G_{12} = -\langle c_1 c_2^* \rangle_S = -\frac{1}{Z} \int \mathcal{D}[c^*, c]\, c_1 c_2^*\, e^{-S}$$

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:

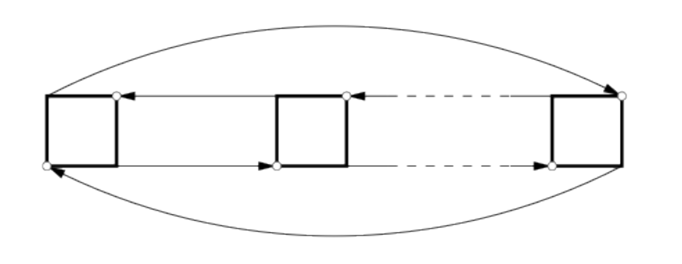
$$F[G] = F[J] - \mathrm{Tr}(JG)$$

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

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: $V^{\alpha}_{ee}=\alpha\, V_{ee}$

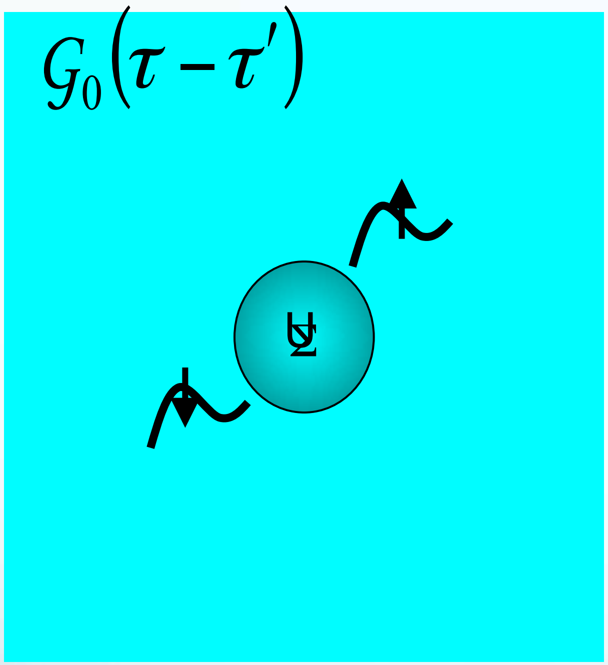
$$\Phi = \frac{1}{2}\int_0^1 d\alpha Tr[V_{ee}^{\alpha} < \psi^{+}\psi^{+}\psi\psi >]$$

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++

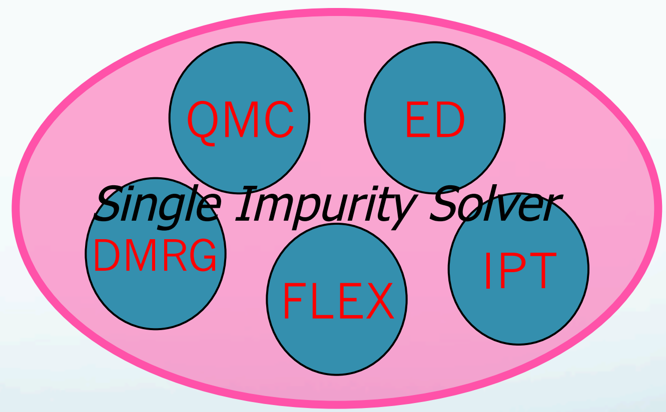
G. Kotliar et. al. RMP (2006)

Dynamical Mean Field Theory



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

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

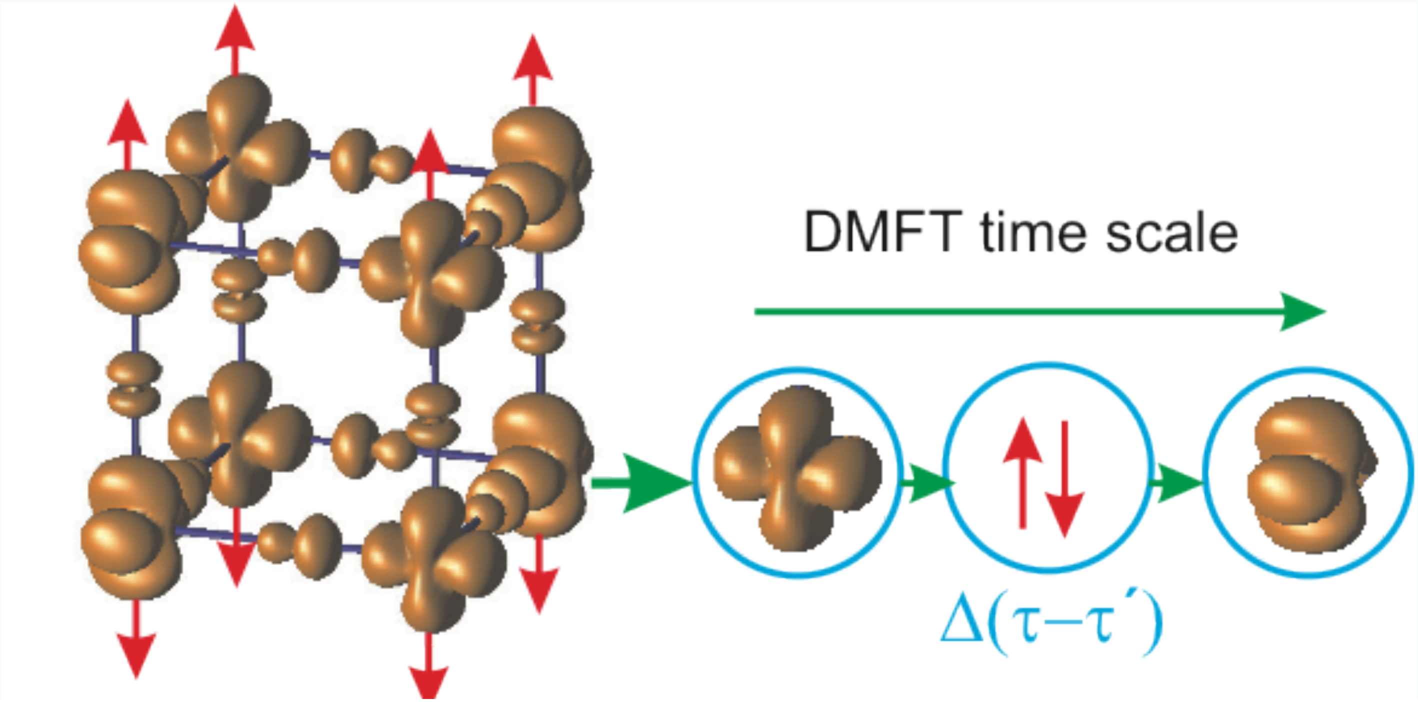


$$\hat{\Sigma}_{new}(i\omega_n)=\hat{\mathcal{G}}_0^{-1}(i\omega_n)-\hat{G}^{-1}(i\omega_n)$$

W. Metzner and D. Vollhardt (1987)

A. Georges and G. Kotliar (1992)

DMFT: Charge+Spin+Orbital Fluctuations



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

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

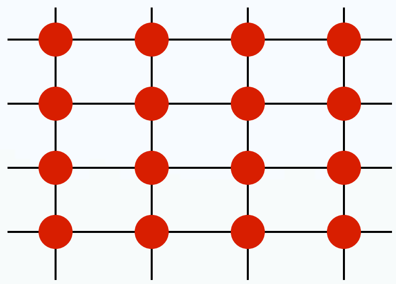
$$g_{12} = -\langle c_1 c_2^* \rangle_{\mathrm{loc}}$$

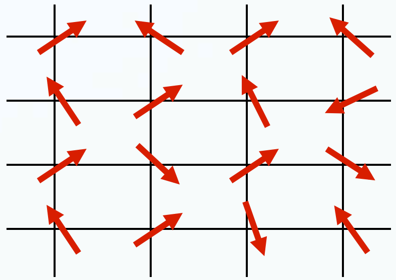
$$\sum_{\mathbf{k}} \left[g_\omega^{-1} + \Delta_\omega - t_{\mathbf{k}}\right]^{-1} = g_\omega$$

DMFT
self-consistensy

DMFT
Impurity solver

Analogy with conventional MFT





$$H = -\sum_{ij\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$$S_{eff}[G_0] = -\int\int d\tau d\tau \; c^{+}_{0\sigma} \; \underline{G_0^{-1}} \; c_{0\sigma} + U \int d\tau' \; n_{0\uparrow} n_{0\downarrow}$$

$$\underline{G_0^{-1}} = i\omega_n + \mu - t^2 G(i\omega_n)$$

$$t_{ij} \sim 1/\sqrt{z}$$

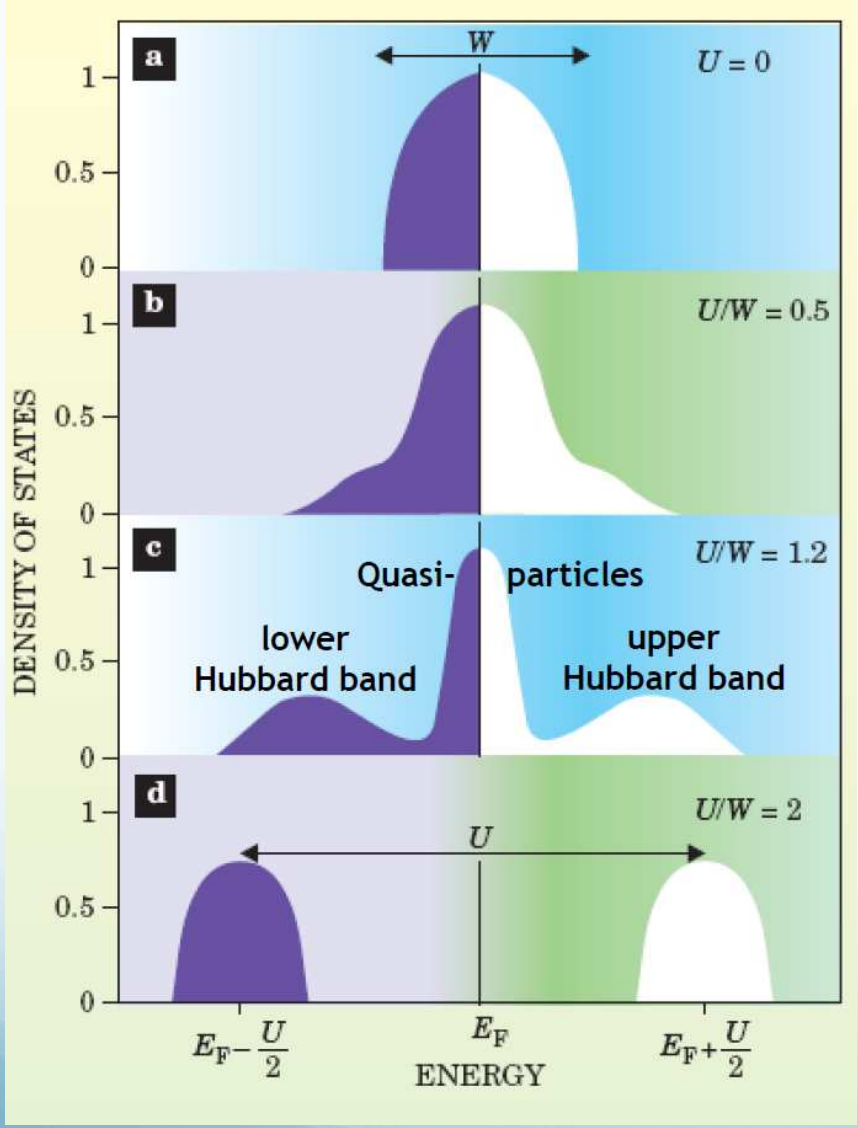
$$H = \sum_{ij} J_{ij} S_i S_j$$

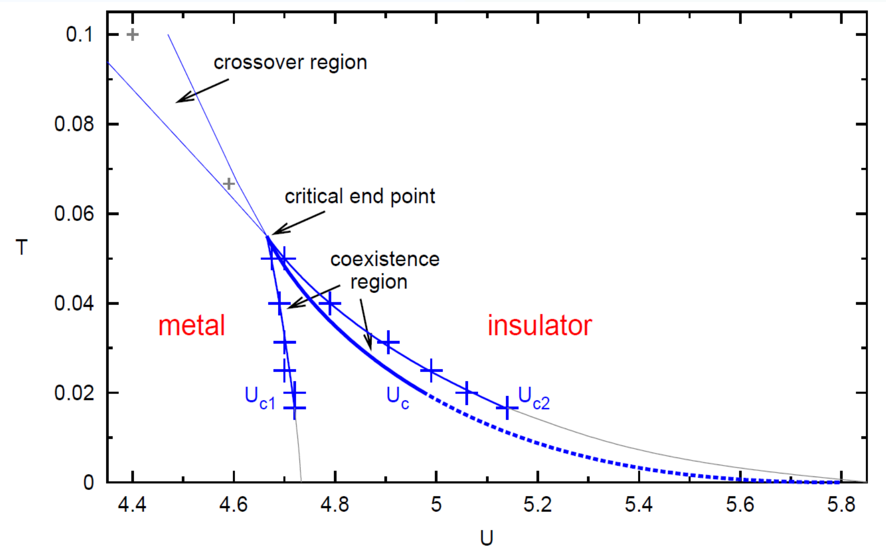
$$H_{eff} = (\sum_{i} J_{0i} S_i) S_0 = zJ\underline{m}S_0 = \underline{h_{eff}} S_0$$

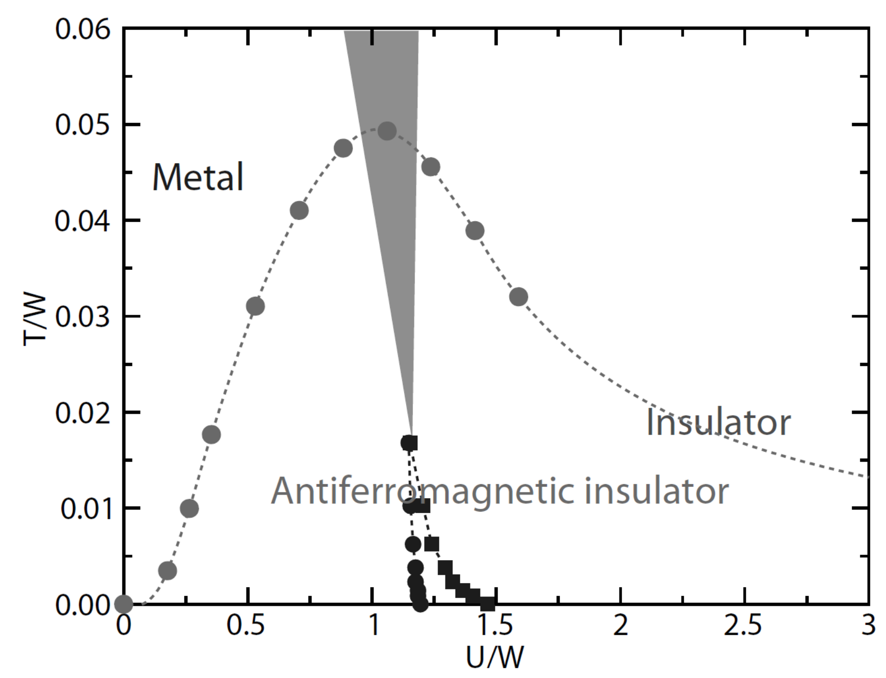
$$\underline{m} = \langle S_0 \rangle = tanh(\beta z J \underline{m})$$

$$J_{ij} \sim 1/z$$

Metal-Insulator Transition

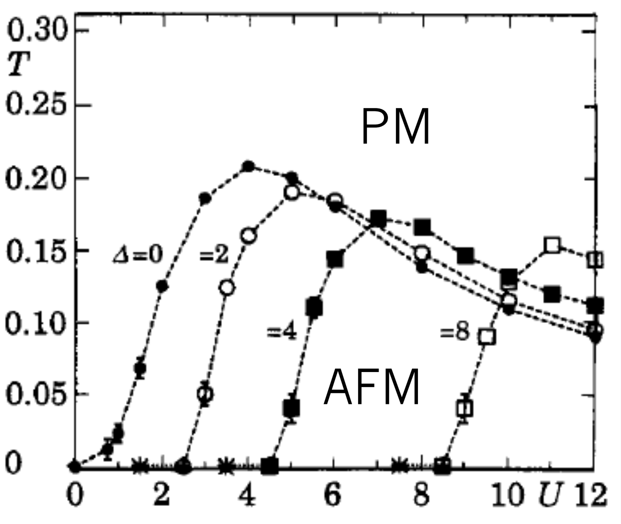




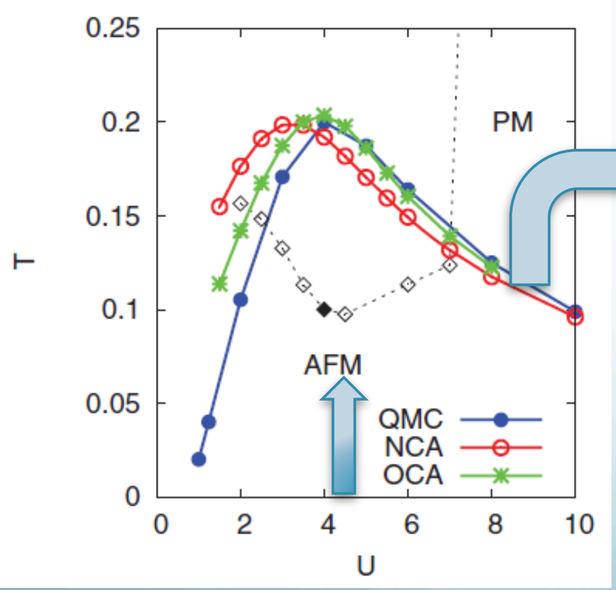


G. Kotliar and D. Vollhardt, Physics Today **3,** 53 (2004)

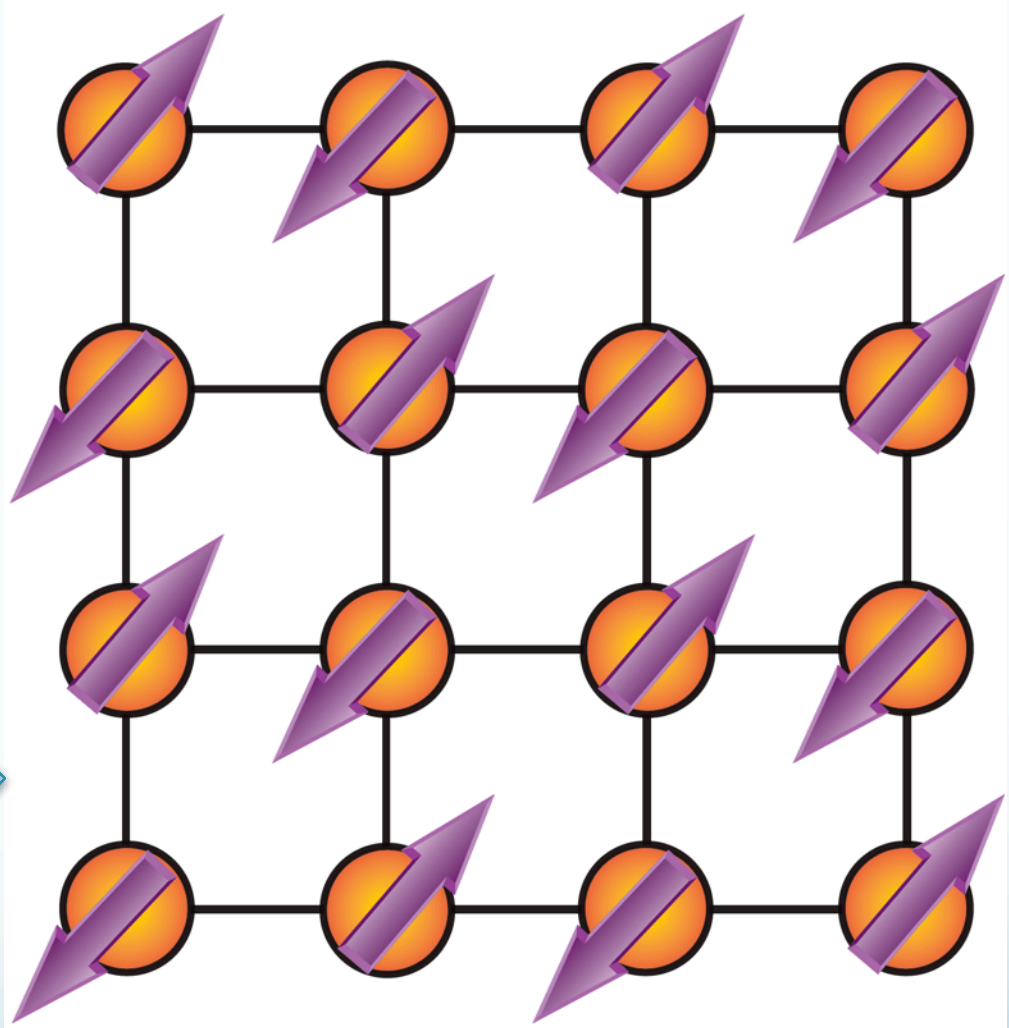
Strong correlation limit and Magnetism



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



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



U>W/2=4

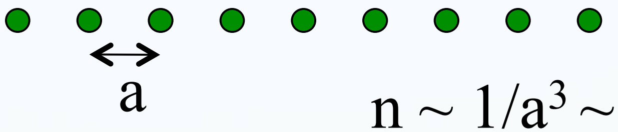
$$J_{\tau\tau'}\vec{S}_{\tau}\cdot\vec{S}_{\tau'}$$

Formation of Local Moments and AFM correlations

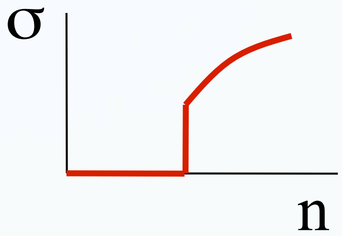
What is the Mott transition?

a correlation driven metal-insulator transition

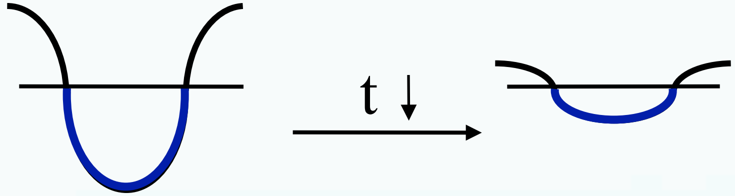
Mott ’49



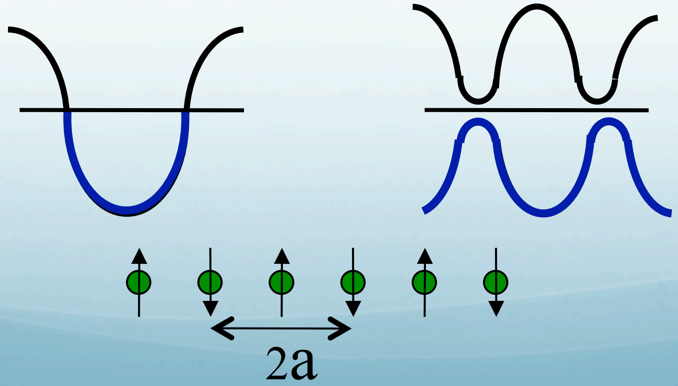
$$n \sim 1/a^3 \sim t$$

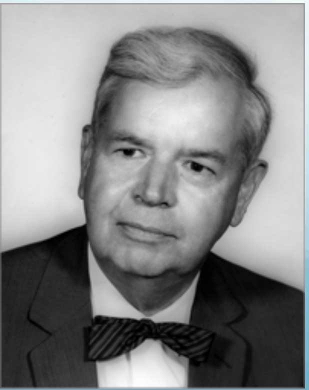


cannot be obtained in band theory:



not due to AF (weak coupling effect):



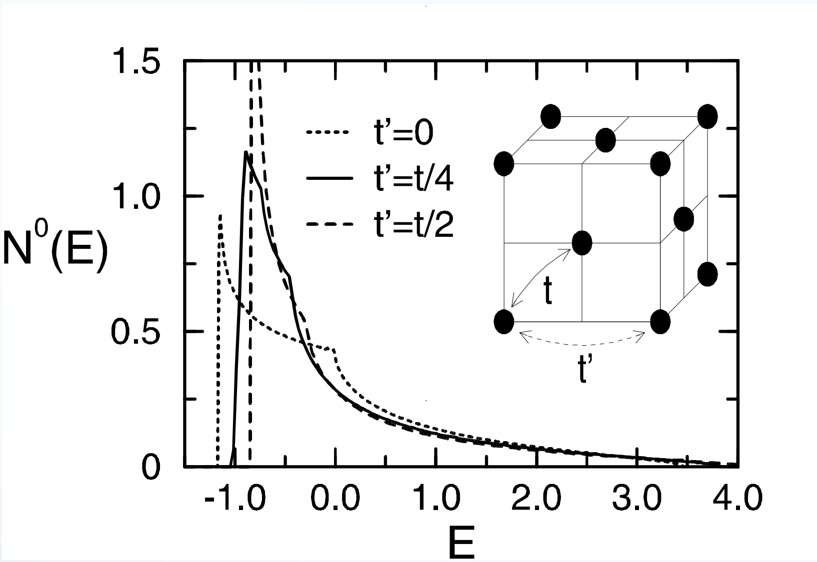


Comparison of LDA and realistic DMFT

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 $\Sigma_i(\omega)$
$E_{tot} = E_{sp} - E_{dc}$	$\Omega = \Omega_{sp} - \Omega_{dc}$
$E_{sp} = \sum_{k<k_F} \varepsilon_k$	$\Omega_{sp} = -Tr\ln[-G^{-1}]$
$E_{dc} = E_H + \int \rho V_{xc} d\mathbf{r} - E_{xc}$	$\Omega_{dc} = Tr\Sigma G - \Phi_{LW}$

DMFT model of ferromagnetism

DOS-peaks

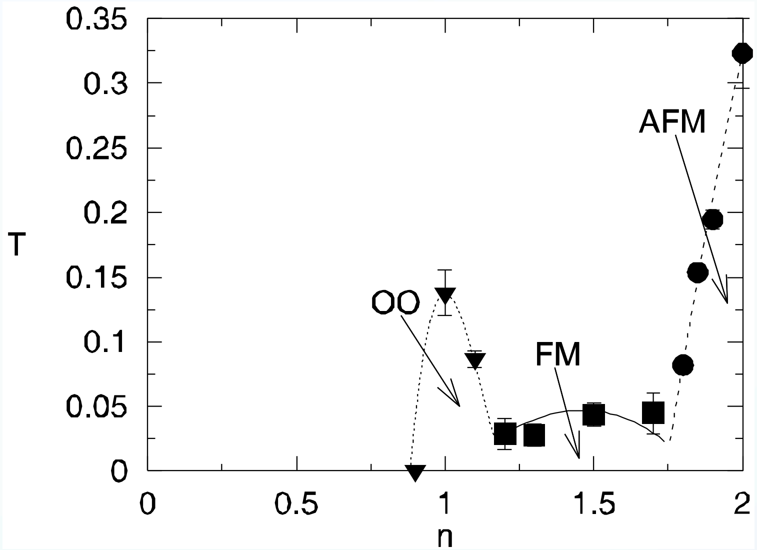


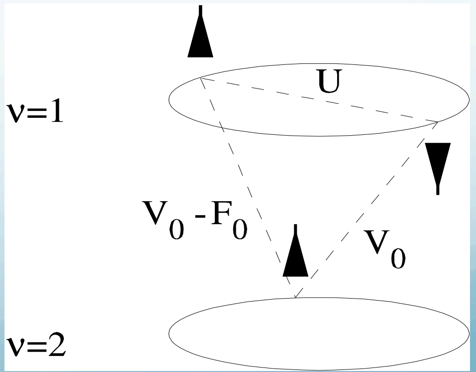
D. Vollhardt, et. al.,

In:Bandferromagnetism,

Springer, 2000

Band degeneracy





W=4

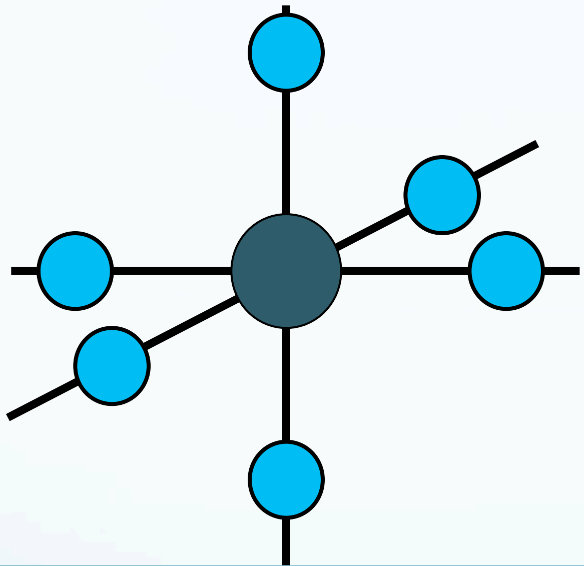
U =6

V_0=4

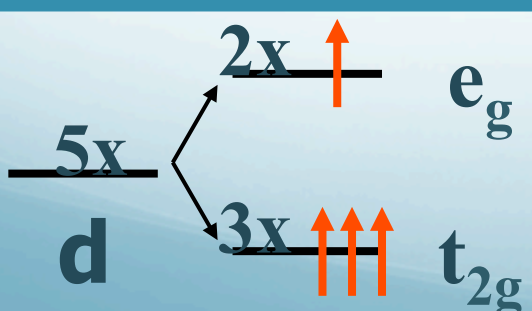
F_0=2

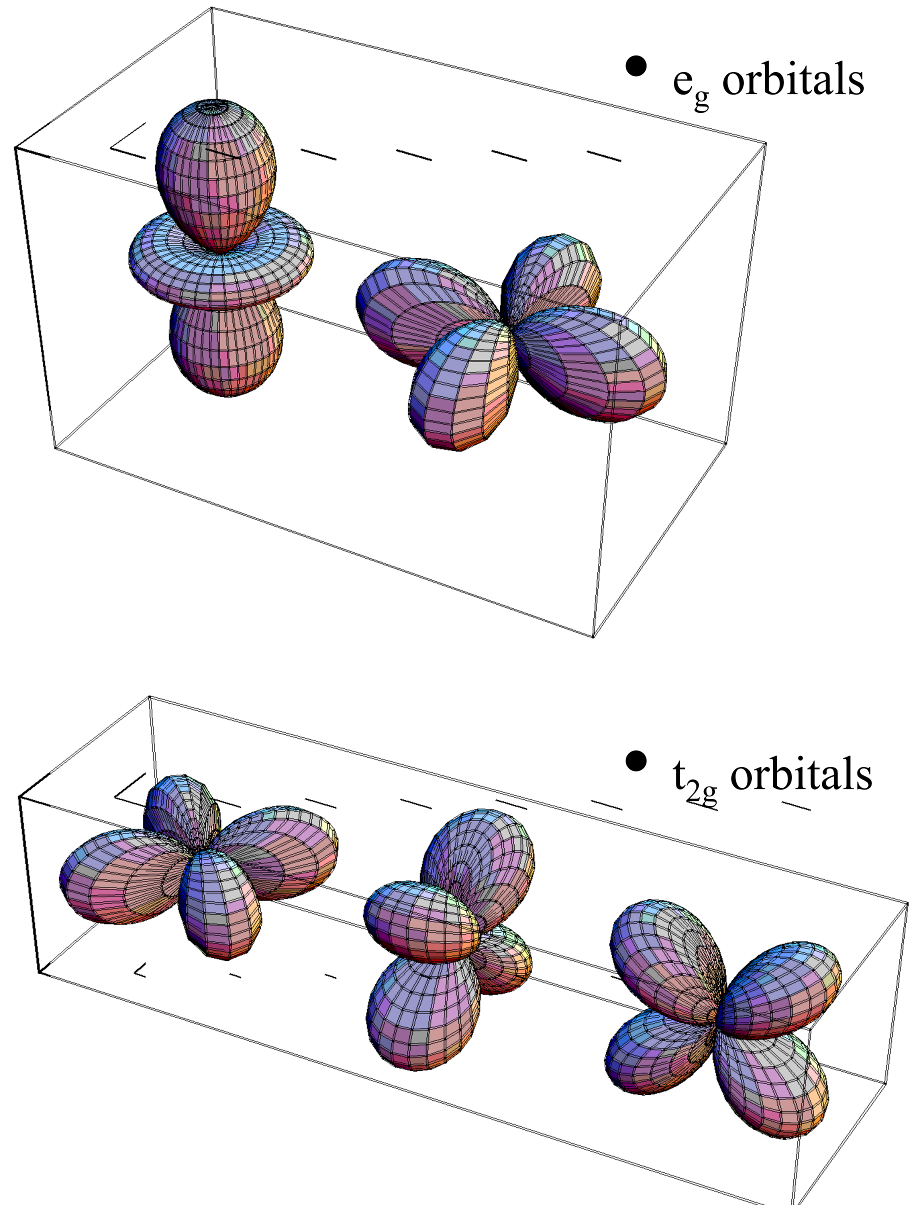
Orbital degrees of freedom

Mn (3+) = 3d^4



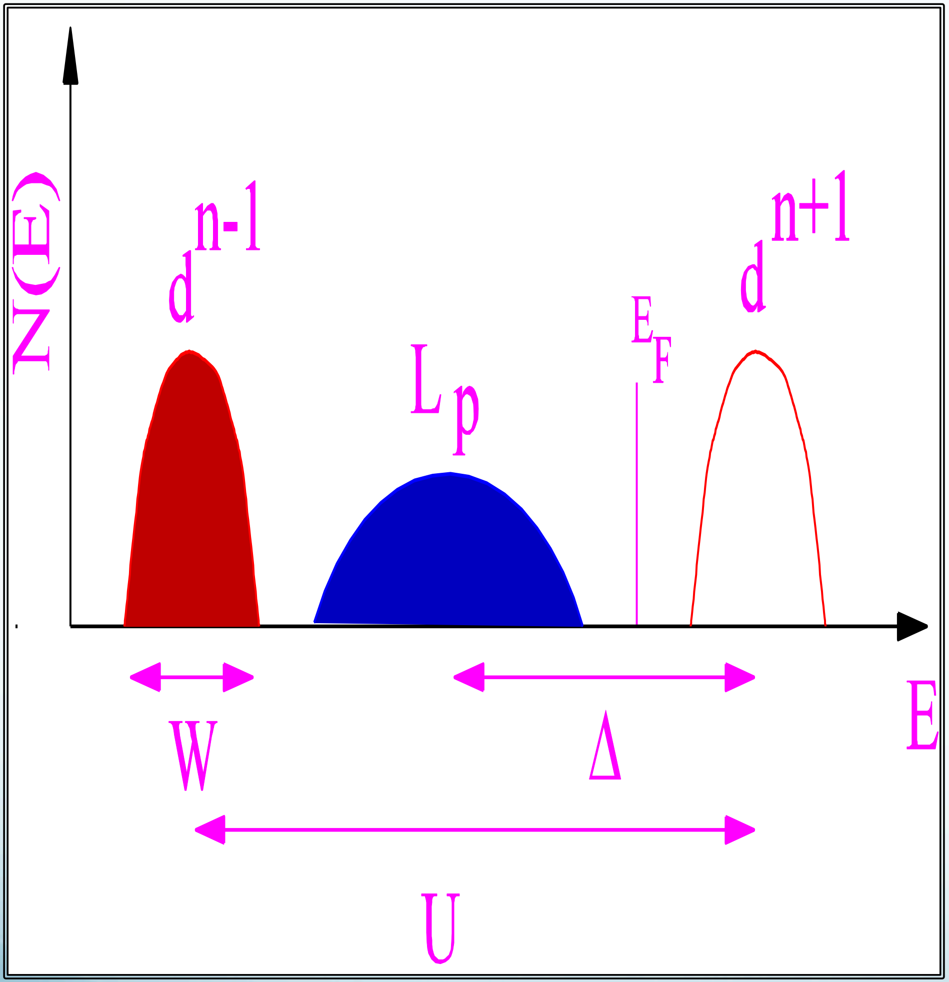
3d-ion in cubic crystal field

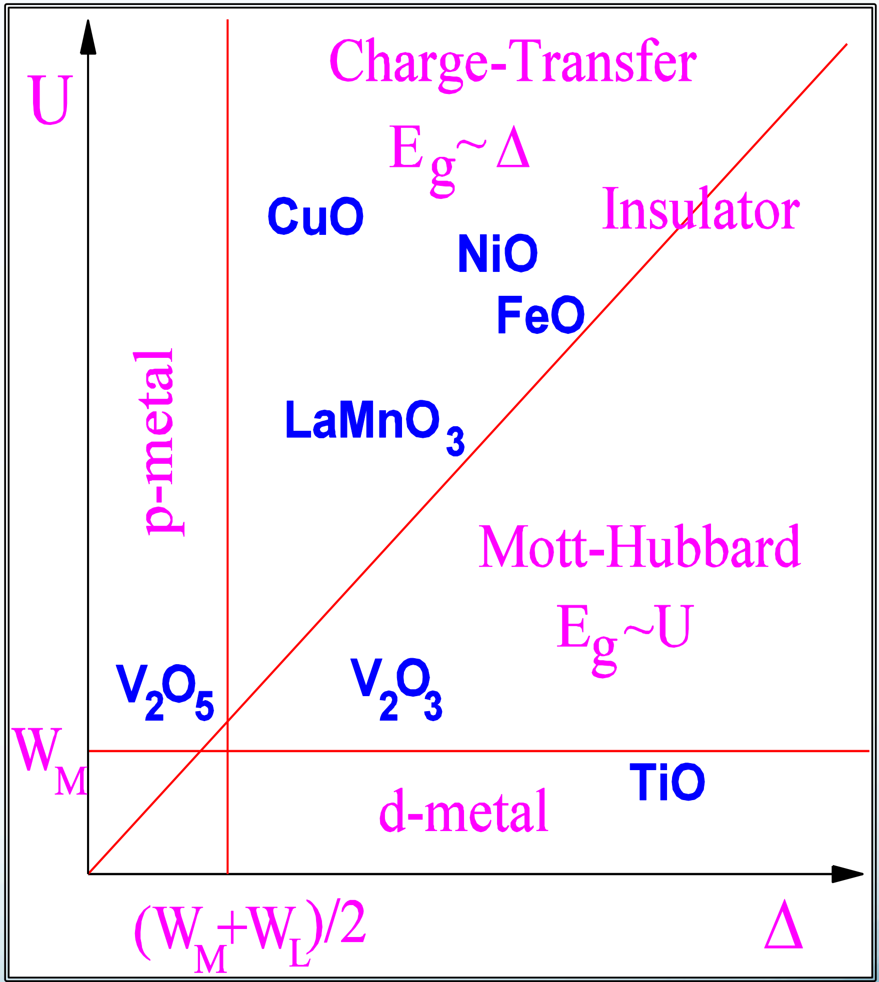




J. van der Brink, D. Khomskii

Charge transfer TMO insulators





Zaanen-Sawatzky-Allen (ZSA) phase diagram

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

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:

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

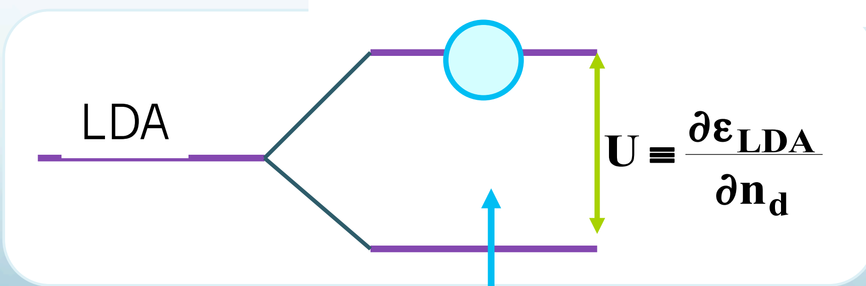
Occupied states:

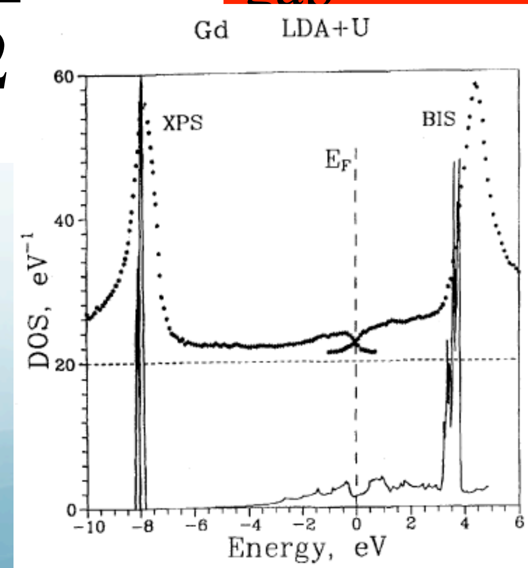
$$n_i = 1 \quad \Rightarrow \quad \varepsilon_i = \varepsilon_{LDA} - \frac{U}{2}$$

Empty states:

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

Mott-Hubbard gap





V. Anisimov et al, PRB, 44, 943 (1991)
review: J. Phys. Cond. Mat. 9, 767 (1997)

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 screened Coulomb correlations (Orbital Polarization!)

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

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

LDA-double counting term ($n^\sigma = Tr(n_{mm0}{}^\sigma)$ and $n = n^- + n^+$):

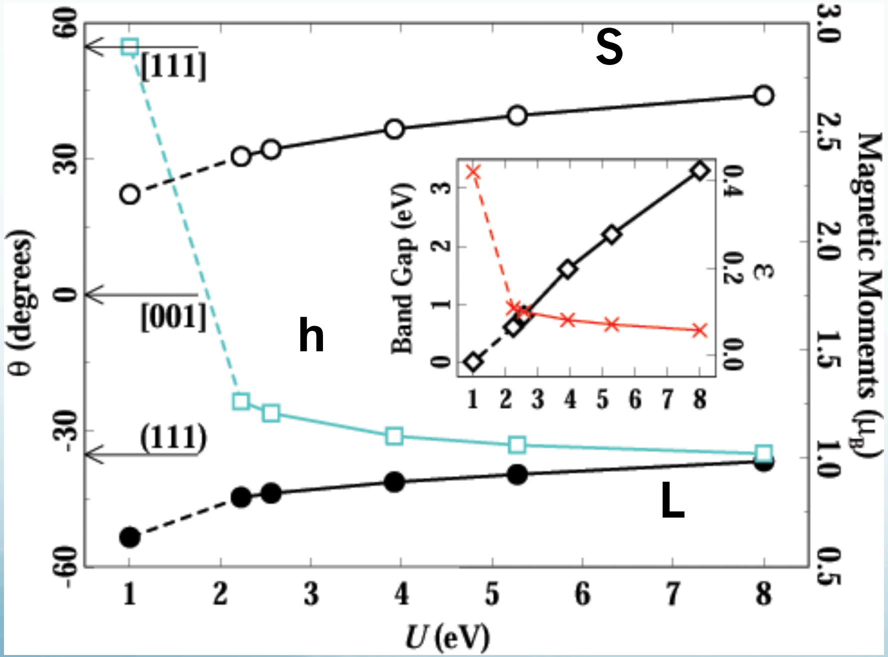
$$E_{dc}[\{n^\sigma\}] = \frac{1}{2}Un(n-1) - \frac{1}{2}J[n^\uparrow(n^\uparrow-1) + n^\downarrow(n^\downarrow-1)],$$

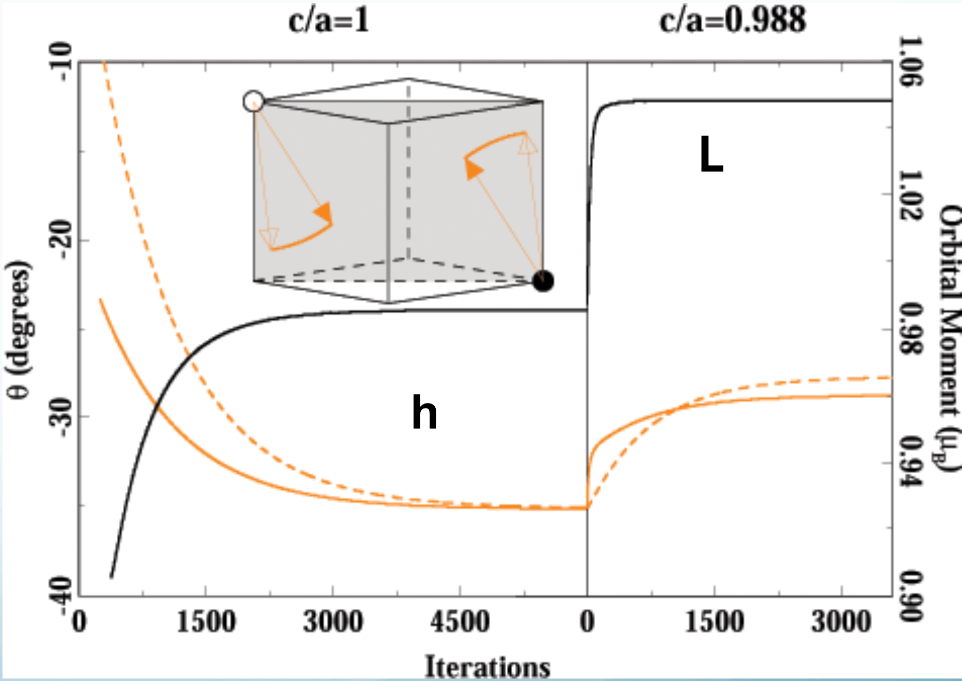
Occupation matrix for correlated electrons:

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

Spin and Orbital moments in CoO

- LDA+U+SO+non-collinear



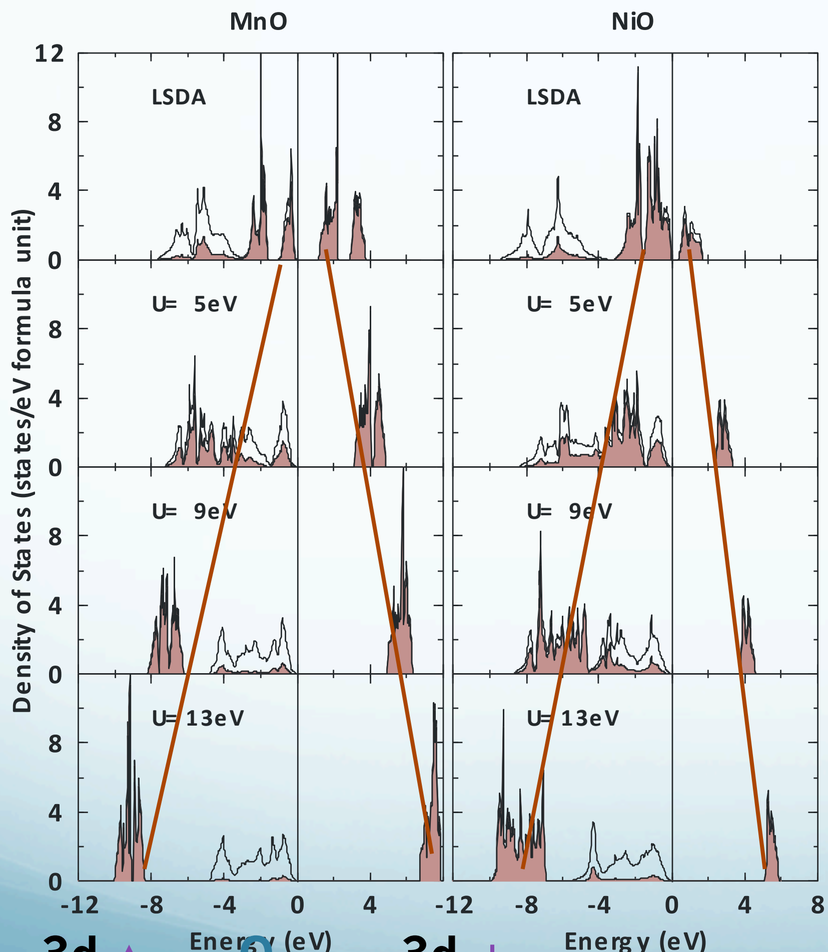


I. Solovyev, A. L., and K. Terakura, PRL 80, 5758 (1998)

Electronic structure of TMO: LDA+U

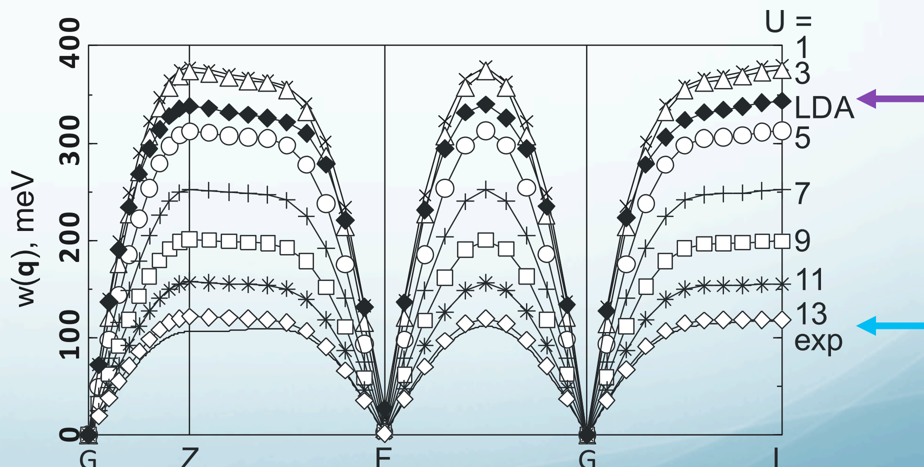
DOS

MnO **NiO**



3d ↑ O_{2p} **3d** ↓

Spin-wave Spectrum NiO
I. Solovyev



Slater: Magnetic Transition State

DFT: Janak theorem

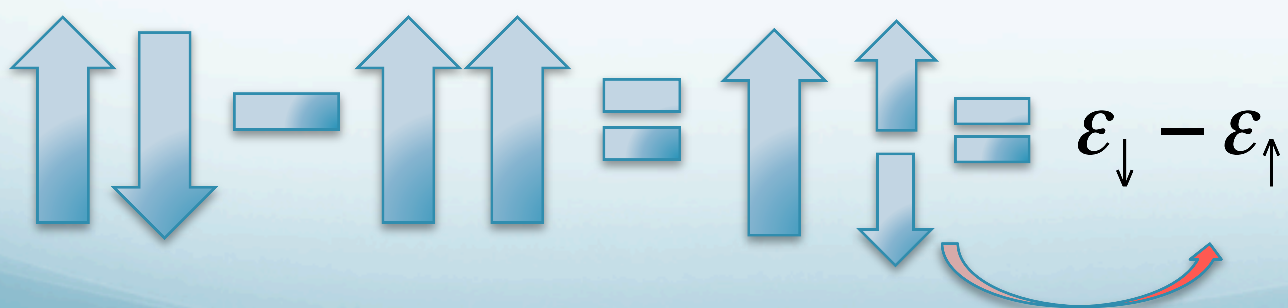
$$\varepsilon_i = \frac{\partial E[n]}{\partial n_i}$$

DFT: Transition State

$$\Delta E = E[n_i = 1] - E[n_i = 0] = \Delta n_i \left.\frac{\partial E[n]}{\partial n_i}\right|_{n_i = 1/2} = \varepsilon(n_i = 1/2)$$

Exchange interaction:

$$J = E[AF] - E[F] = \Delta\varepsilon(n_\uparrow = n_\downarrow = 1/2)$$



Local Force Theorem: Functionals

$$\begin{aligned}\Omega^d &= \Omega^d_{sp} - \Omega^d_{dc} \\ \Omega^d_{sp} &= -Tr\left\{\ln\left[\Sigma - G_0^{-1}\right]\right\} \\ \Omega^d_{dc} &= Tr\Sigma G - \Phi\end{aligned}$$

$$G^{-1} = G_0^{-1} - \Sigma$$

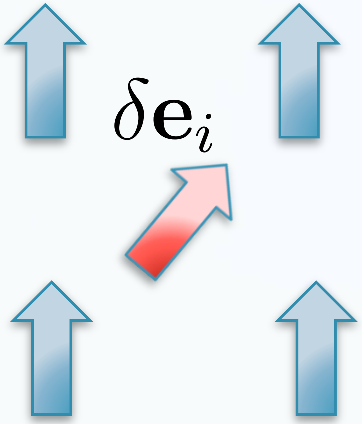
$$\Sigma = \frac{\delta\Phi}{\delta G}.$$

$$\delta\Omega = \delta^*\Omega_{sp} + \delta_1\Omega_{sp} - \delta\Omega_{dc}$$

$$\delta_1\Omega_{sp} = \delta\Omega_{dc} = TrG\delta\Sigma$$

$$\delta\Omega = \delta^*\Omega_{sp} = -\delta^*Tr\ln\left[\Sigma - G_0^{-1}\right]$$

Magnetic Torque



$$\delta\mathbf{e}_i = \delta\boldsymbol{\varphi}_i \times \mathbf{e}_i$$

$$\varSigma_i = \varSigma_i^c + \boldsymbol{\varSigma}_i^s\boldsymbol{\sigma}$$

$$\varSigma_i^{(c,s)} = \frac{1}{2}\left(\varSigma_i^{\uparrow} \pm \varSigma_i^{\downarrow}\right)$$

$$G_{ij} = G_{ij}^c + \mathbf{G}_{ij}^s\boldsymbol{\sigma}$$

$$\boldsymbol{\Sigma}_i^s = \varSigma_i^s\mathbf{e}_i$$

Magnetic Force Theorem: $$\delta\Omega = \delta^*\Omega_{sp} = \mathbf{V}_i\delta\boldsymbol{\varphi}_i$$

Magnetic Torque:

$$\mathbf{V}_i = 2Tr_{\omega L}\left[\boldsymbol{\varSigma}_i^s \times \mathbf{G}_{ii}^s\right]$$

Exchange interactions from Functional

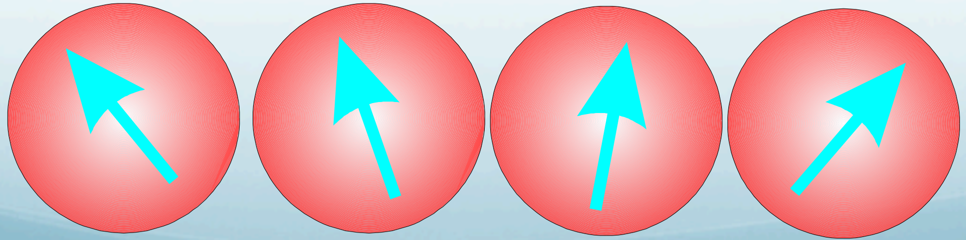
Heisenberg exchagne: $$\Omega_{spin} = -\sum_{ij} J_{ij}\mathbf{e}_i \cdot \mathbf{e}_j$$

Exchange interactions: $$J_{ij} = -Tr_{\omega L}\left(\Sigma_i^s G_{ij}^{\uparrow} \Sigma_j^s G_{ji}^{\downarrow}\right)$$

Spin wave spectrum:

$$\omega_{\mathbf{q}} = \frac{4}{M}\sum_j J_{0j}\left(1 - \cos\mathbf{q}\mathbf{R}_j\right) \equiv \frac{4}{M}[J(0) - J(\mathbf{q})]$$

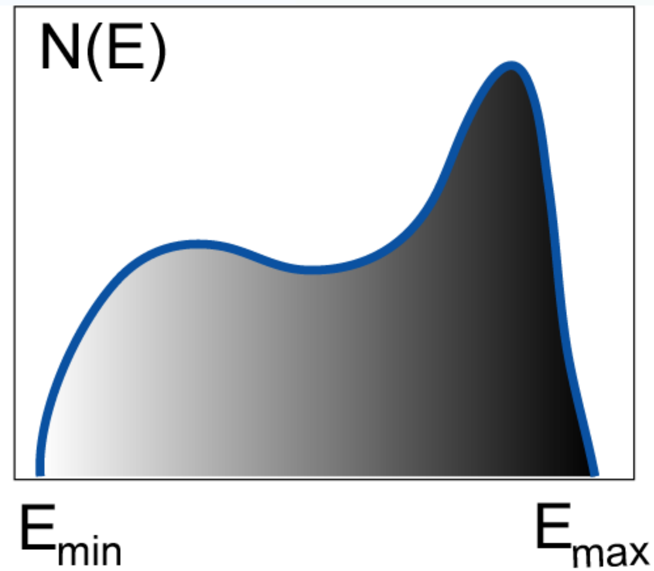
Non-collinear excitation:



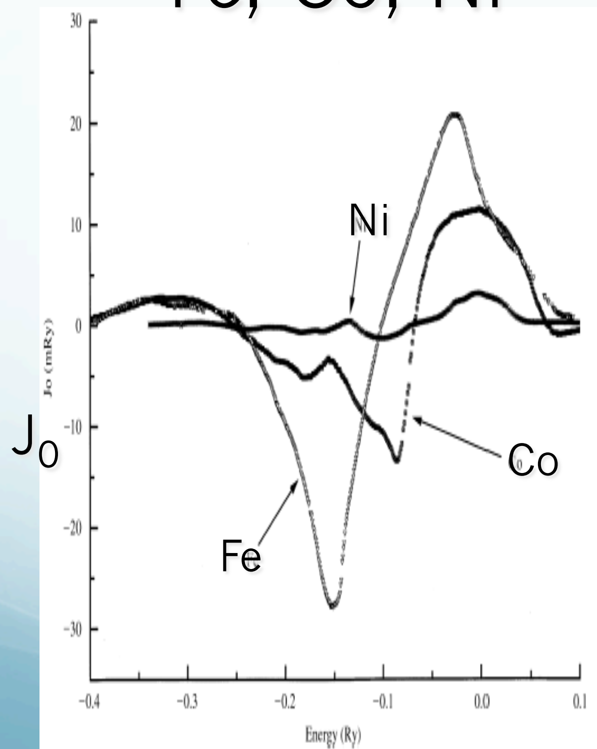
M. Katsnelson and A. L. , Phys. Rev. 61, 8906 (2000)

Exchange interactions and Band structure

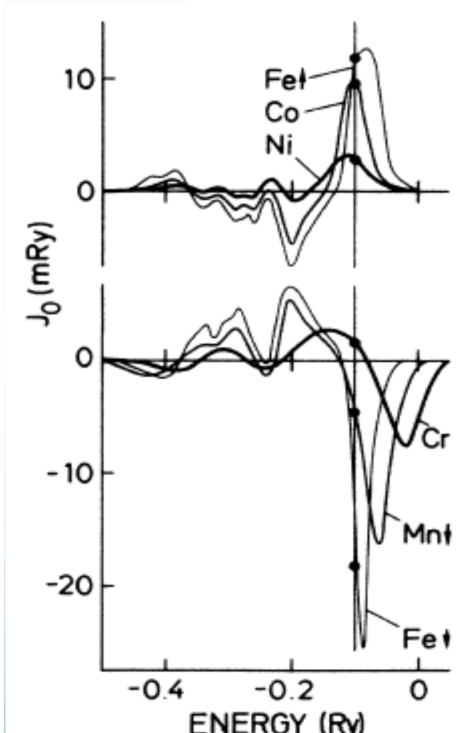
$$J_{ij} = \frac{\delta^2 E_{LDA}}{\delta \vec{e_i} \delta \vec{e_j}} = \frac{1}{\pi} Im \int_{-\infty}^{\varepsilon_F} \Delta_i T_{ij}^{\uparrow} \Delta_j T_{ji}^{\downarrow}$$

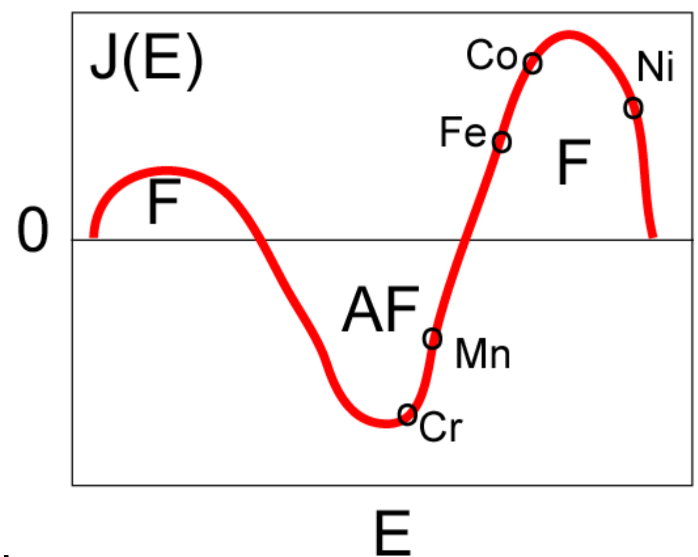


Fe, Co, Ni



3d in Ni





Green Function calculations : $J_0 = \Sigma J_{ij}$ V. Antropov, et. Al. PRB (1988)

LDA+Exchange Interactions

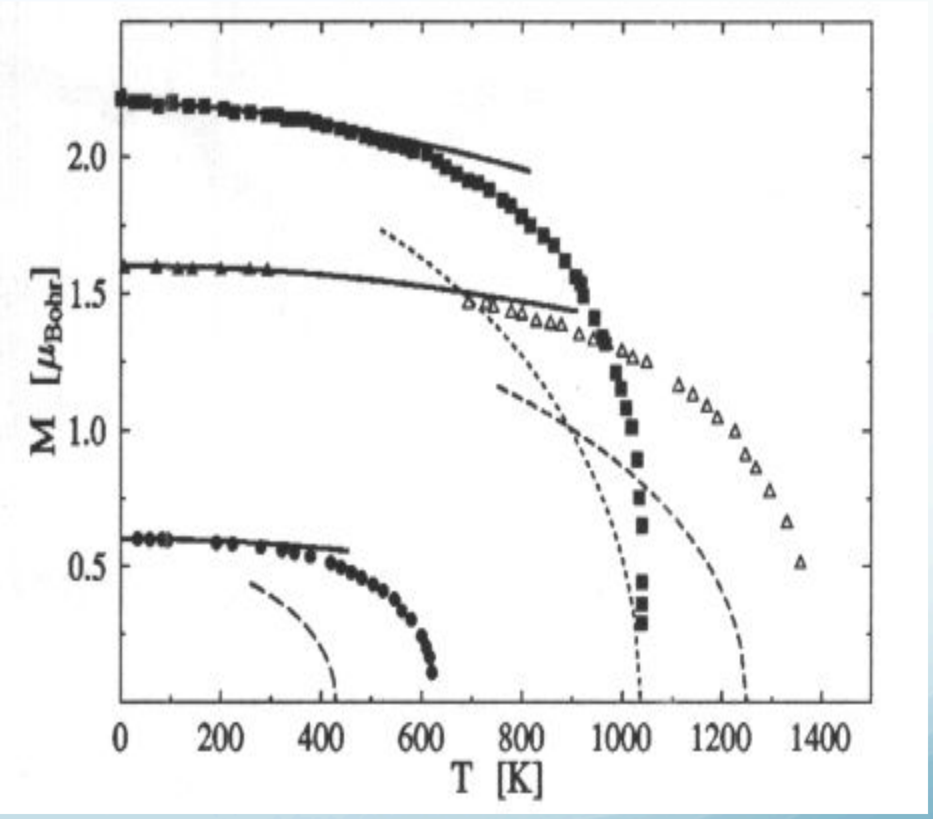
Spin-waves $T<T_c$

$$J_{ij} = \frac{1}{\pi}\int_{-\infty}^{\varepsilon_F} (V_\uparrow^i - V_\downarrow^i) G_\uparrow^{ij} (V_\uparrow^j - V_\downarrow^j) G_\uparrow^{ji} \, d\varepsilon$$

Curie temperature

$$T_c = \frac{2}{3}\sum_j J_{0j}$$

S. Halilov, et. al.,
PRB 58, 293 (1998)

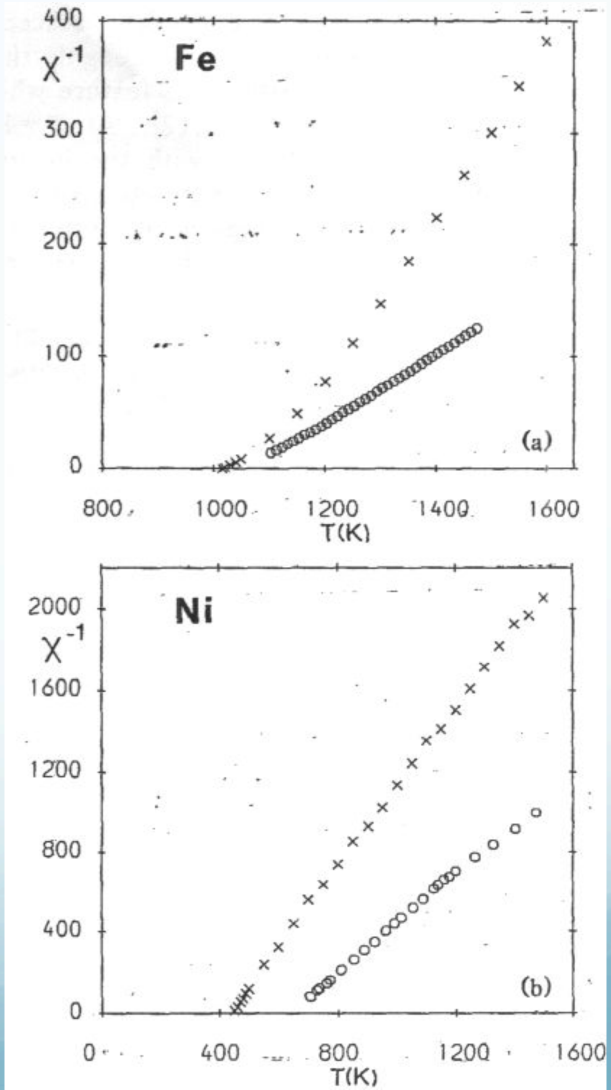


Ni Fe Co

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

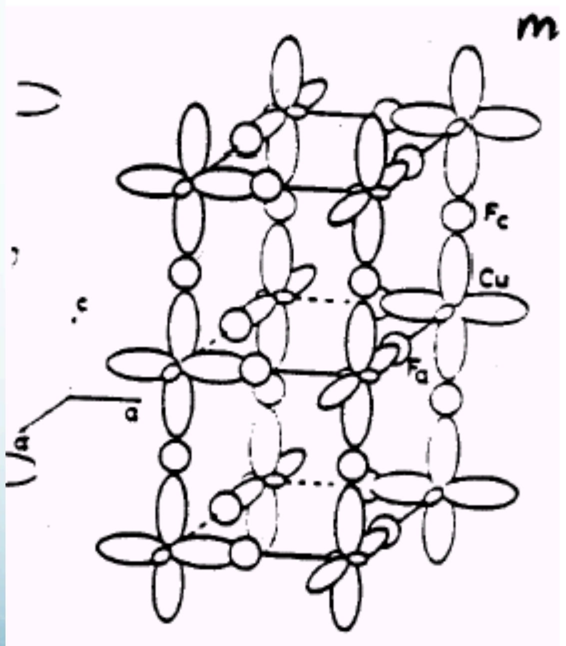
Orbital order: $KCuF_3$

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

with a single hole in e_g doubly degenerate subshell.

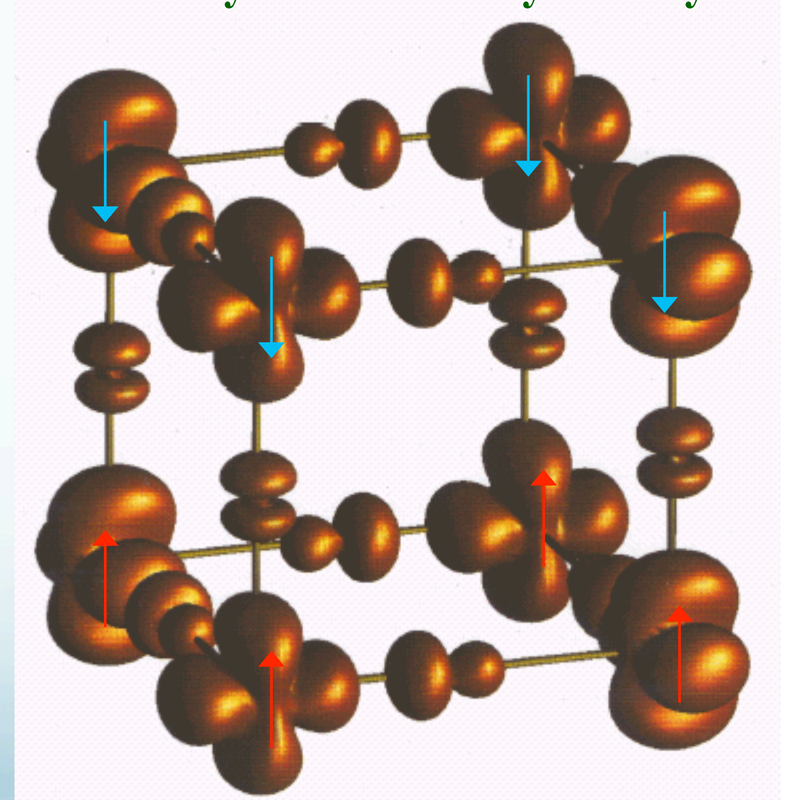
Experimental crystal structure

antiferro-orbital order



LDA+U calculations for undistorted perovskite structure

hole density of the same symmetry



A.L. V. Anisimov and J. Zaanen, Phys. Rev.B 52, R5467 (1995)

1d-AFM in KCuF3

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

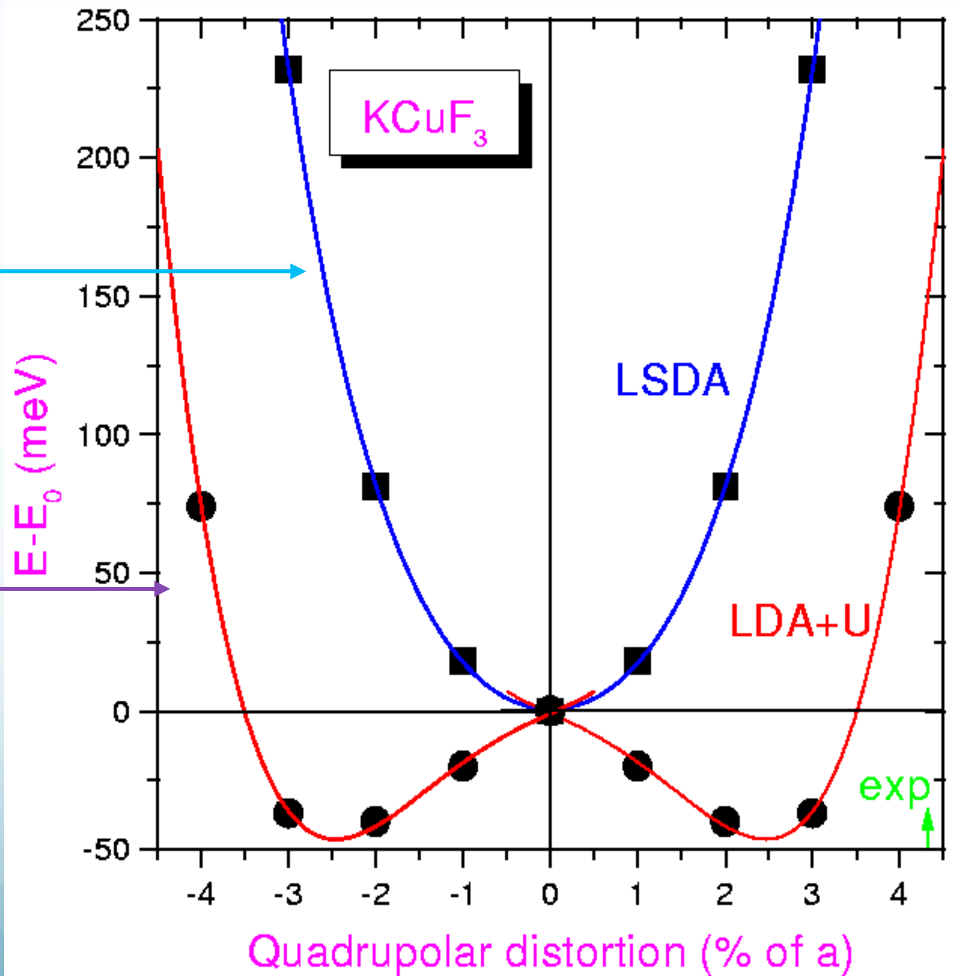
Superexchange interaction

$KCuF_3$

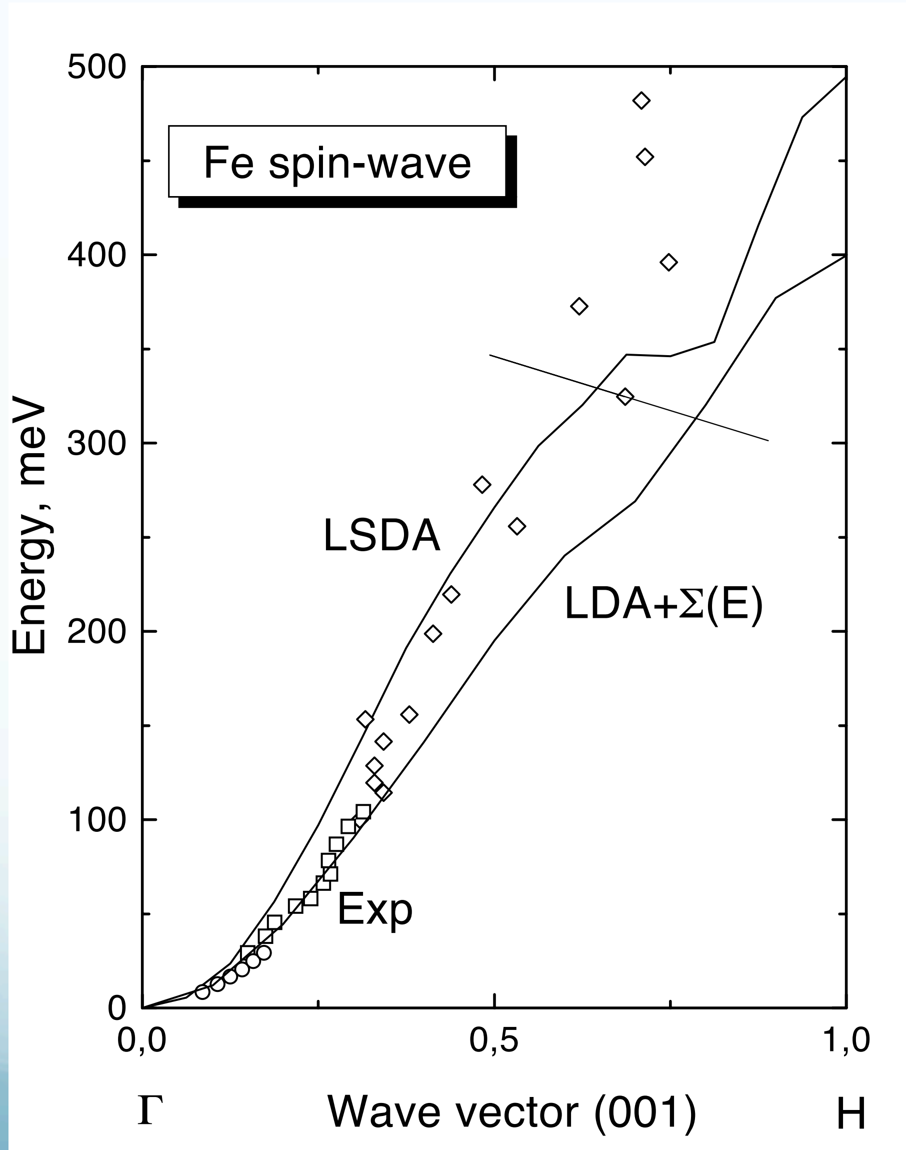
Quadrupolar distortion in $KCuF_3$

LSDA gave cubic perovskite crystal structure stable in respect to Jahn-Teller distortion of CuF_6 octahedra

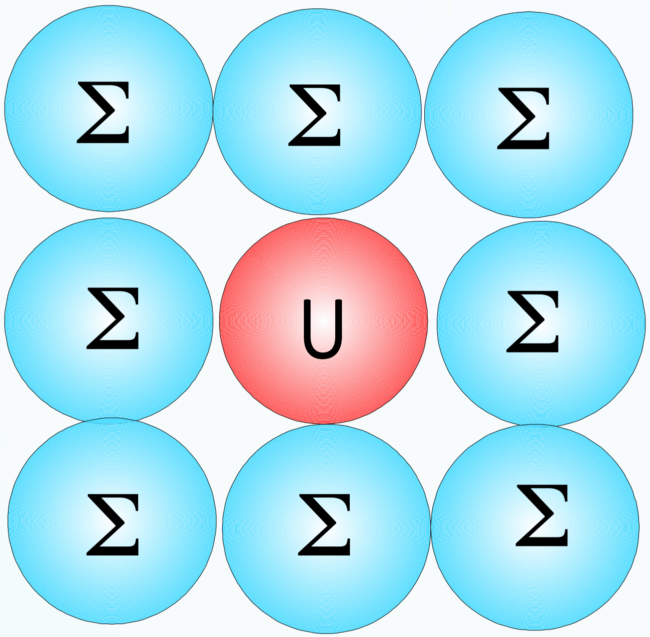
LDA+U produces total energy minimum for distorted structure



Exchange in Iron: LSDA++

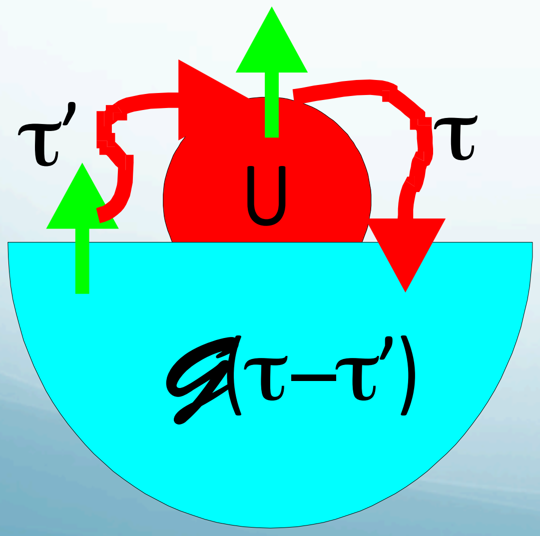


Quantum Impurity Solver



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

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



What is a best scheme?
Quantum Monte Carlo !

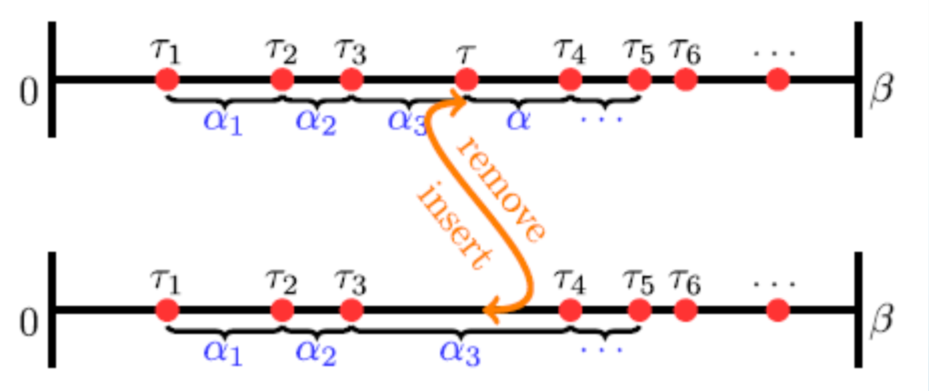
Continuous Time Quantum Monte Carlo

Partition function: $H = H_0 + V$

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

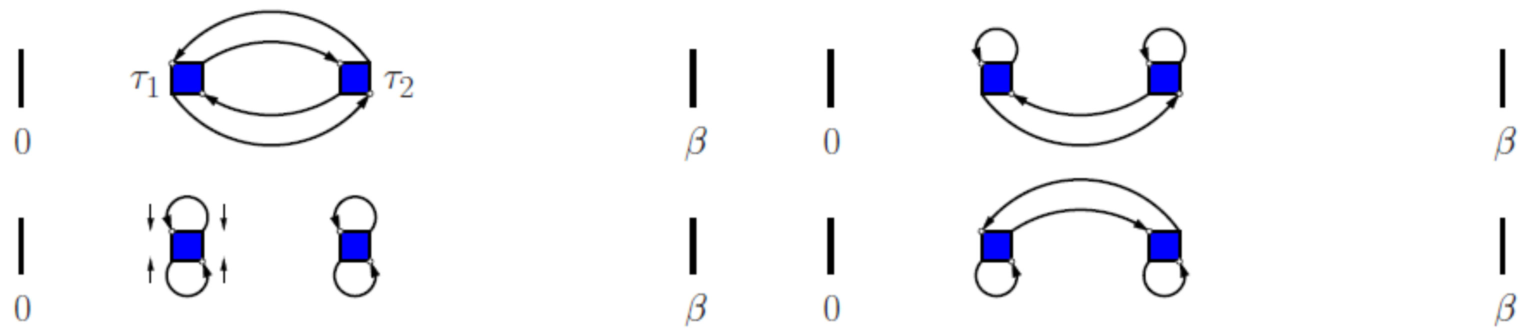
Continuous Time Quantum Monte Carlo (CT-QMC)

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



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

Weak coupling QMC: CT-INT



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

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

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

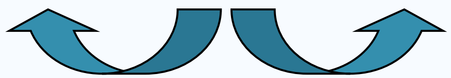
$$= \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} U^k \int d\tau_1 \ldots \int d\tau_k \text{sgn}(\det \hat{G}) \underbrace{|\det \hat{G}|}_{P(k)}$$

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

A. Rubtsov, 2004

Random walks in the *k*-space

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

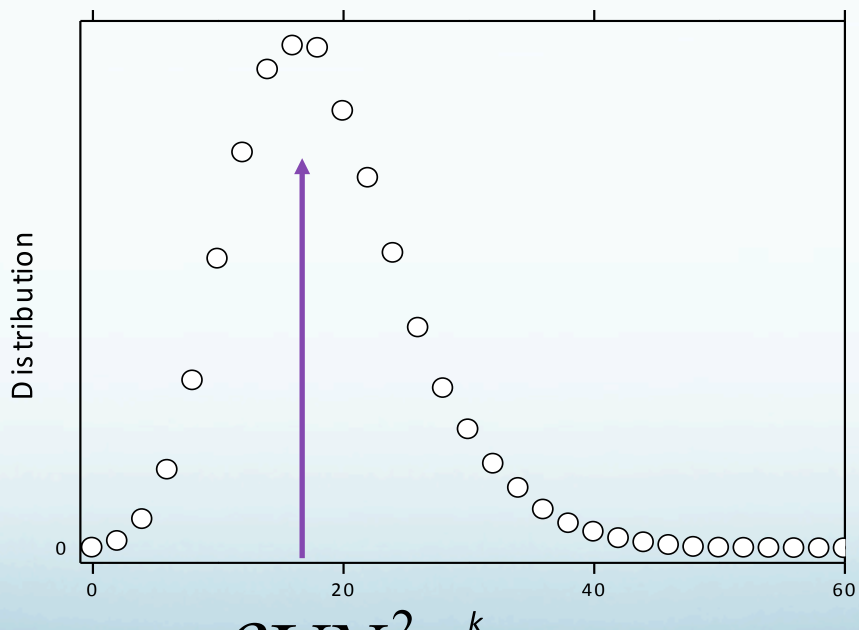


Acceptance ratio

decrease

Step *k*-1

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



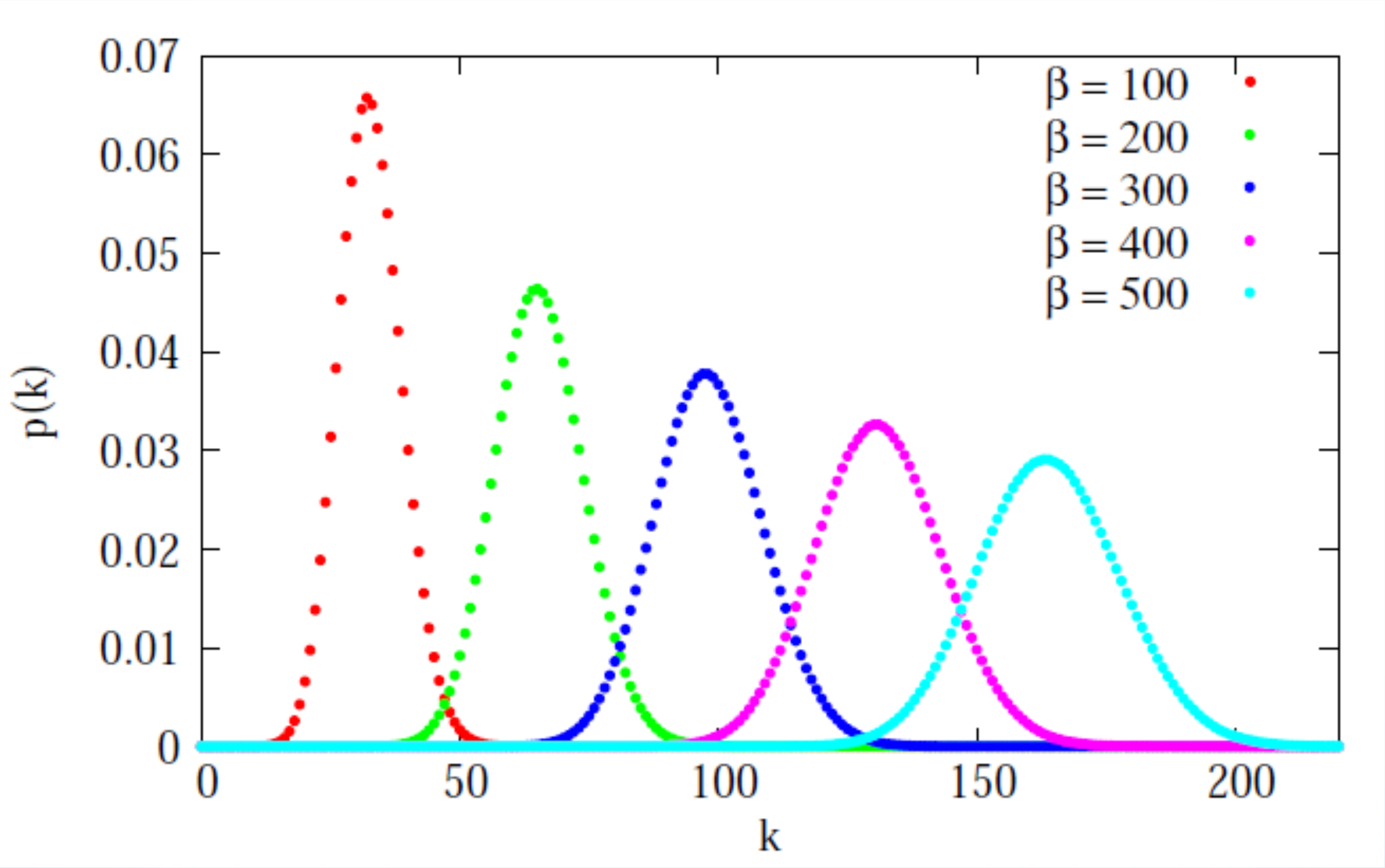
increase

Step *k*+1

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

Maximum at $\beta U N^2$

Convergence with Temperature: CT-INT



Maximum: $\beta U N^2$

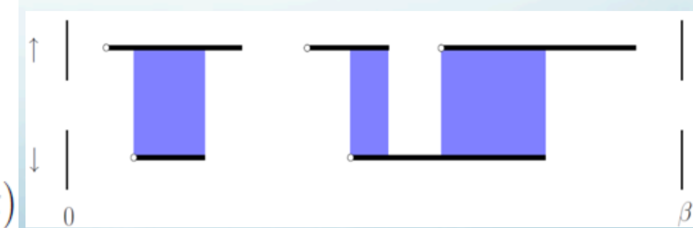
Strong-Coupling Expansion CT-HYB

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

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

$$\mathscr{Z} = \int \mathscr{D}[c^*,c]e^{-S_{\text{at}}} \sum_k \frac{1}{k!}\int_0^\beta d\tau'_1 \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau'_k \int_0^\beta d\tau_k \times$$
$$\times c(\tau_k)c^*(\tau'_k)\ldots c(\tau_1)c^*(\tau'_1)\Delta(\tau_1-\tau'_1)\ldots\Delta(\tau_k-\tau'_k)$$

$$\mathscr{Z} = \mathscr{Z}_{\text{at}} \sum_k \int_0^\beta d\tau'_1 \int_{\tau'_1}^\beta d\tau_1 \ldots \int_{\tau_{k-1}}^\beta d\tau'_k \int_{\tau'_k}^{\circ\tau'_k} d\tau_k \times$$
$$\times \langle c(\tau_k)c^*(\tau'_k)\ldots c(\tau_1)c^*(\tau'_1)\rangle_{\text{at}} \det\hat{\Delta}^{(k)}$$



P. Werner, 2006

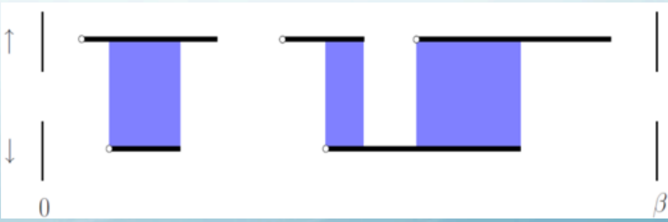
Strong-Coupling Expansion CT-HYB

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

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

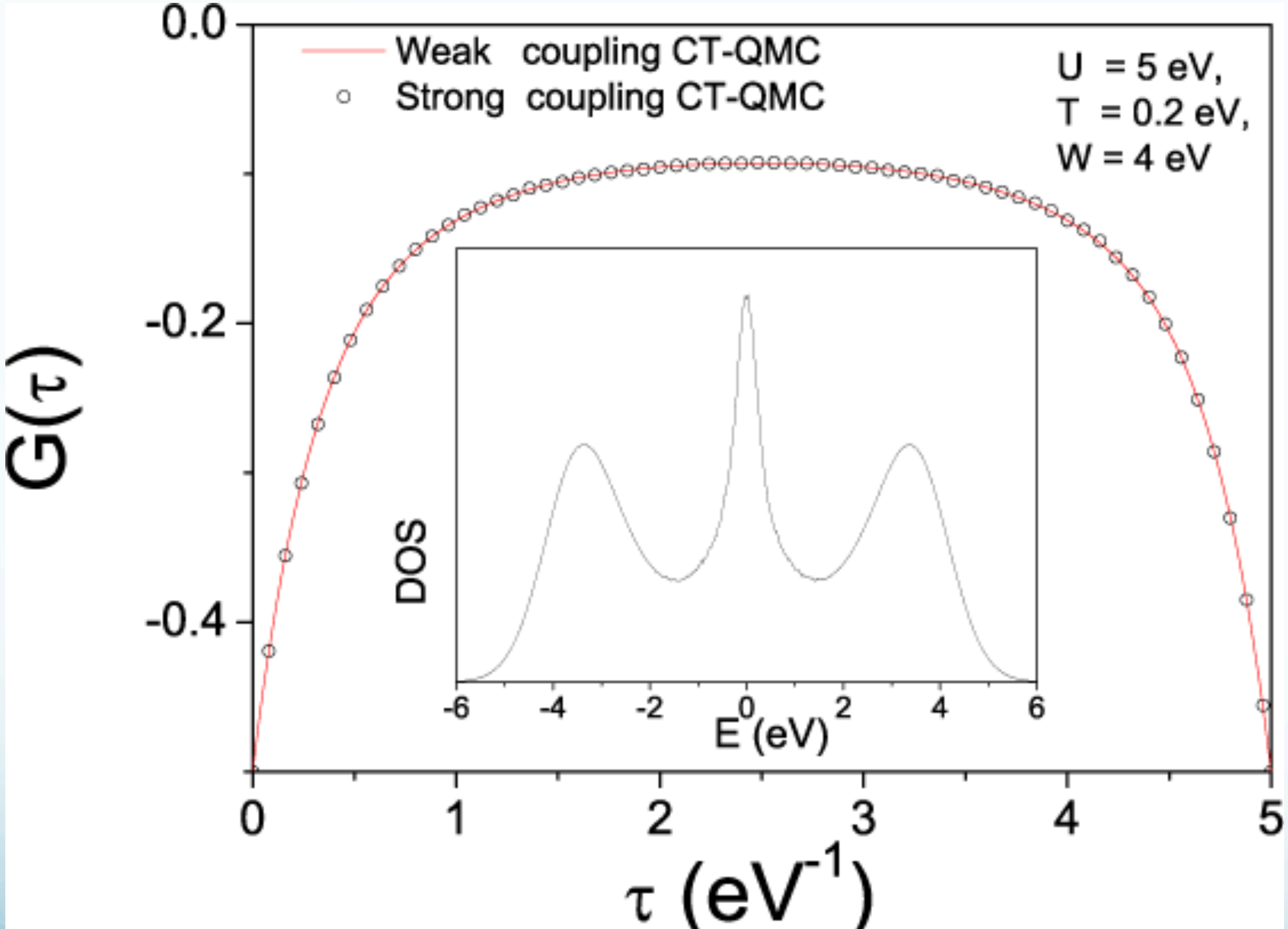
$$\mathscr{Z} = \int \mathscr{D}[c^*, c]e^{-S_{\text{at}}} \sum_k \frac{1}{k!}\int_0^\beta d\tau_1' \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_k' \int_0^\beta d\tau_k \times$$
$$\times\, c(\tau_k)c^*(\tau_k')\ldots c(\tau_1)c^*(\tau_1')\Delta(\tau_1-\tau_1')\ldots\Delta(\tau_k-\tau_k')$$

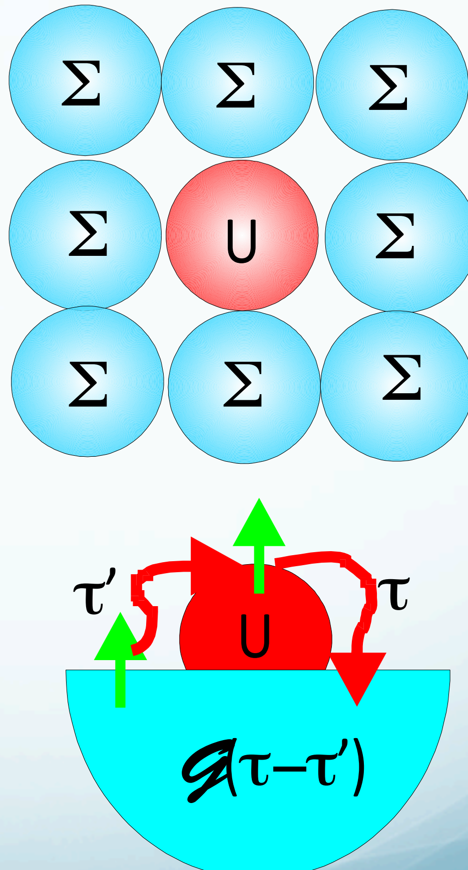
$$\mathscr{Z} = \mathscr{Z}_{\text{at}} \sum_k \int_0^\beta d\tau_1' \int_{\tau_1'}^\beta d\tau_1 \ldots \int_{\tau_{k-1}}^\beta d\tau_k' \int_{\tau_k'}^{\circ\tau_k'} d\tau_k \times$$
$$\times \langle c(\tau_k)c^*(\tau_k')\ldots c(\tau_1)c^*(\tau_1')\rangle_{\text{at}} \det \hat{\Delta}^{(k)}$$



P. Werner, 2006

Comparison of different CT-QMC

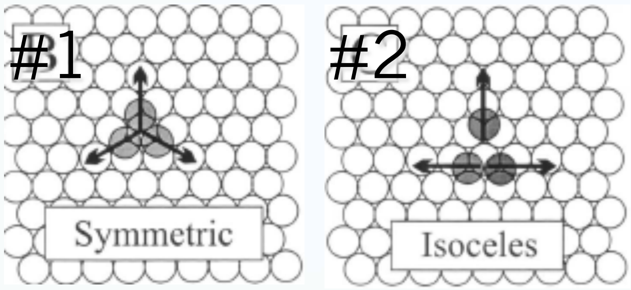




Ch. Jung, unpublished

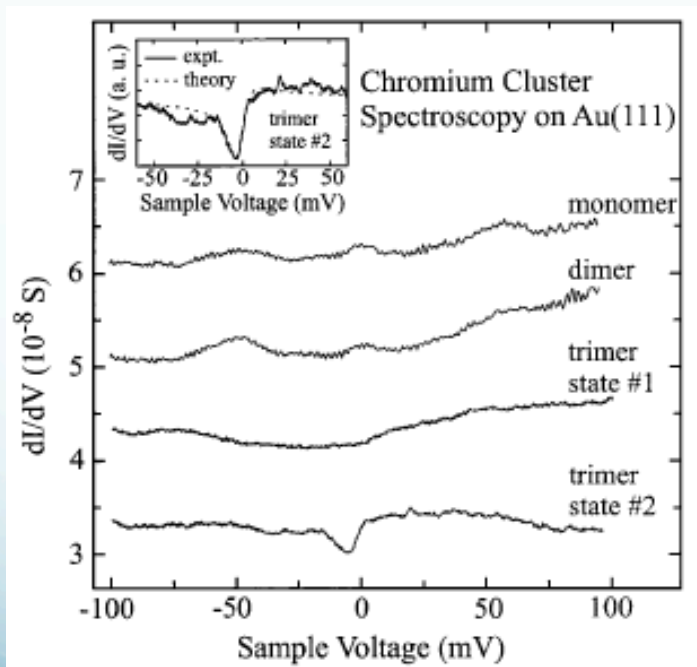
CT-QMC review:E. Gull et al. RMP (2011)

Magnetism vs. Kondo resonance

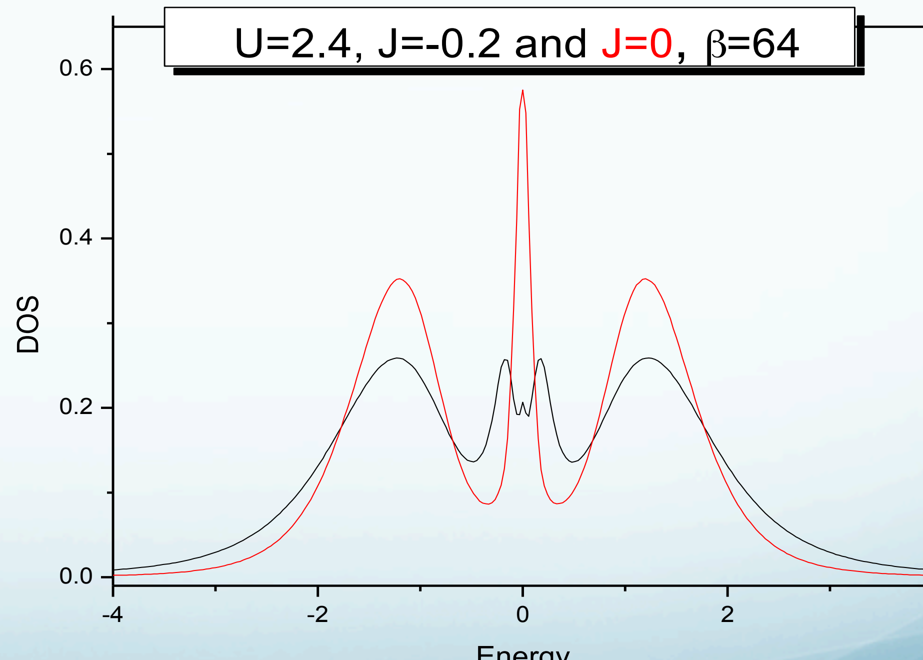


Three impurity atoms with Hubbard repulsion and exchange interaction

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



M. Crommie, PRL(2001)



CT-QMC: single vs. trimer

V. Savkin, et al, PRL 94, 026402 (2005)

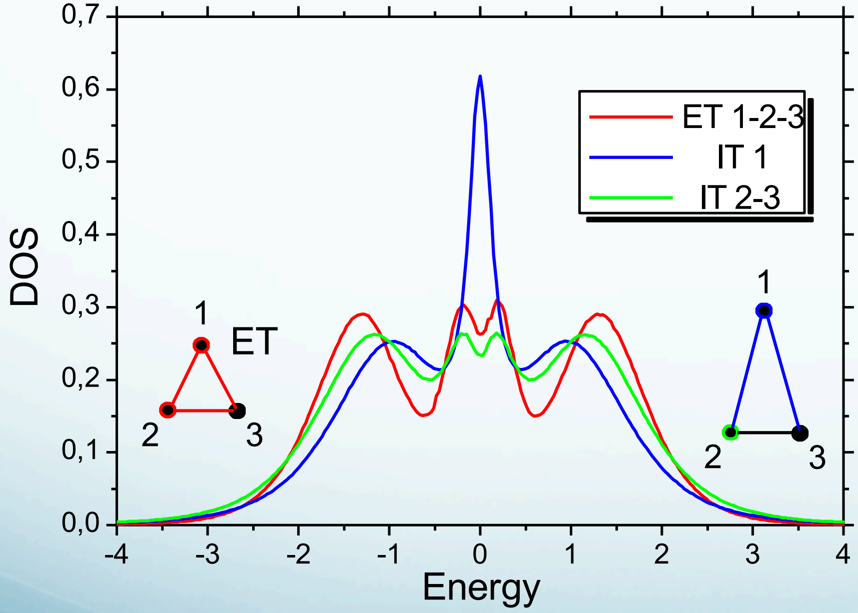
Equilateral and Isosceles Trimers

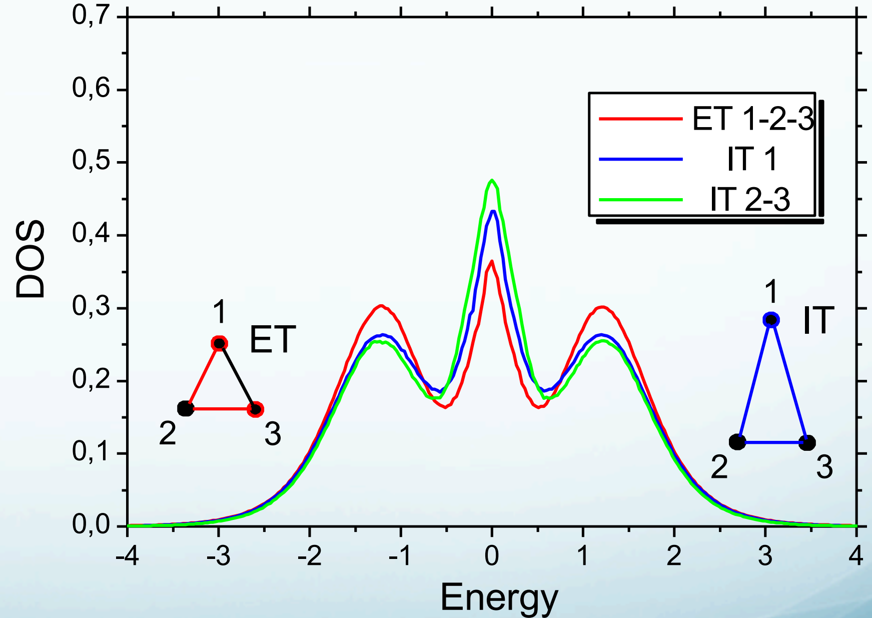
Density of states at geometry modification of the trimer

Equilateral (ET) and isosceles (IT) trimers

AFM $J_{23}=J,\ J_{12}=J_{13}=J/3$ **FM**

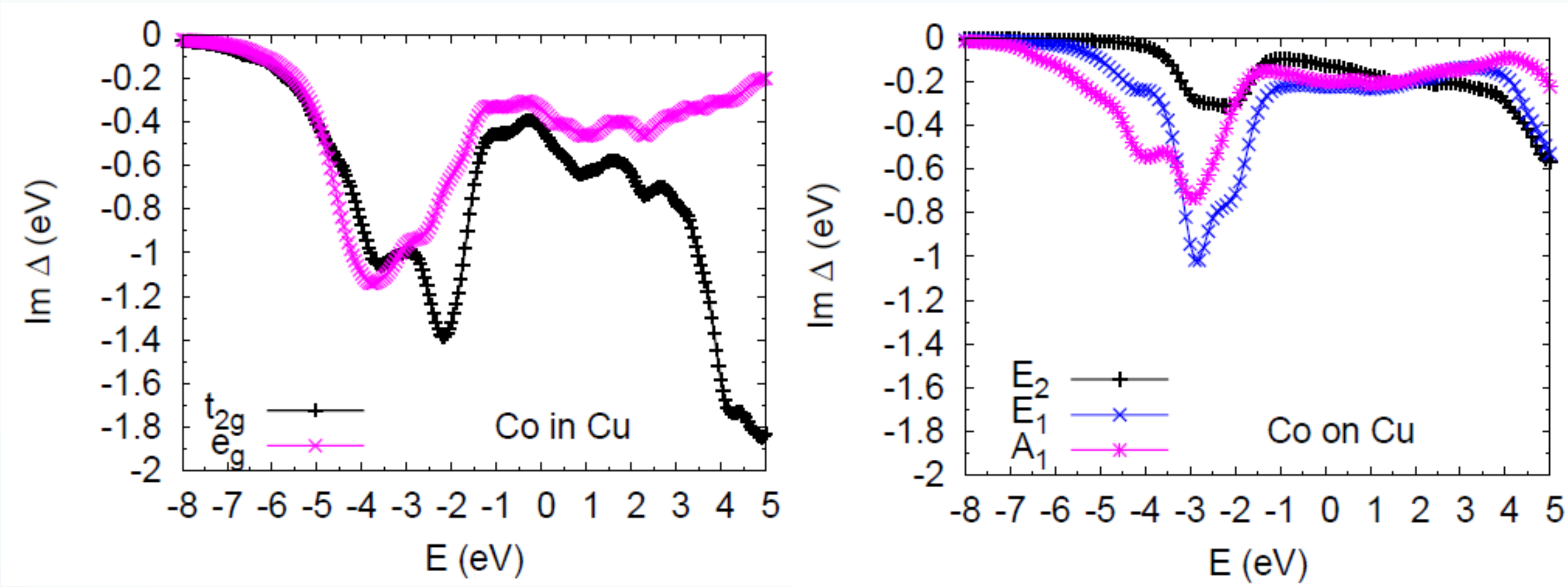
V. Savkin et al, PRL **94**, 026402 (2005)





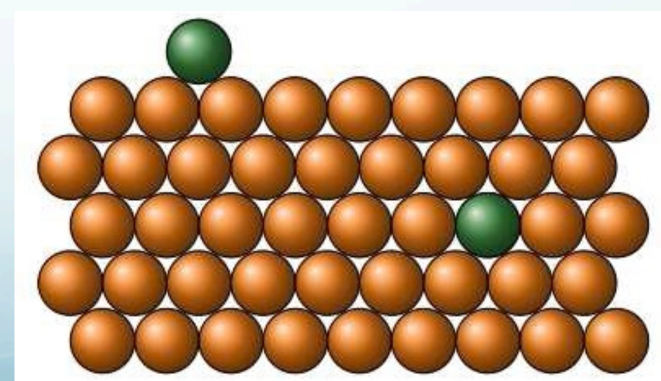
One can see a reconstruction of the Kondo resonance for isosceles trimer at antiferromagnetic exchange interaction

Hybridization function Co on/in Cu(111)

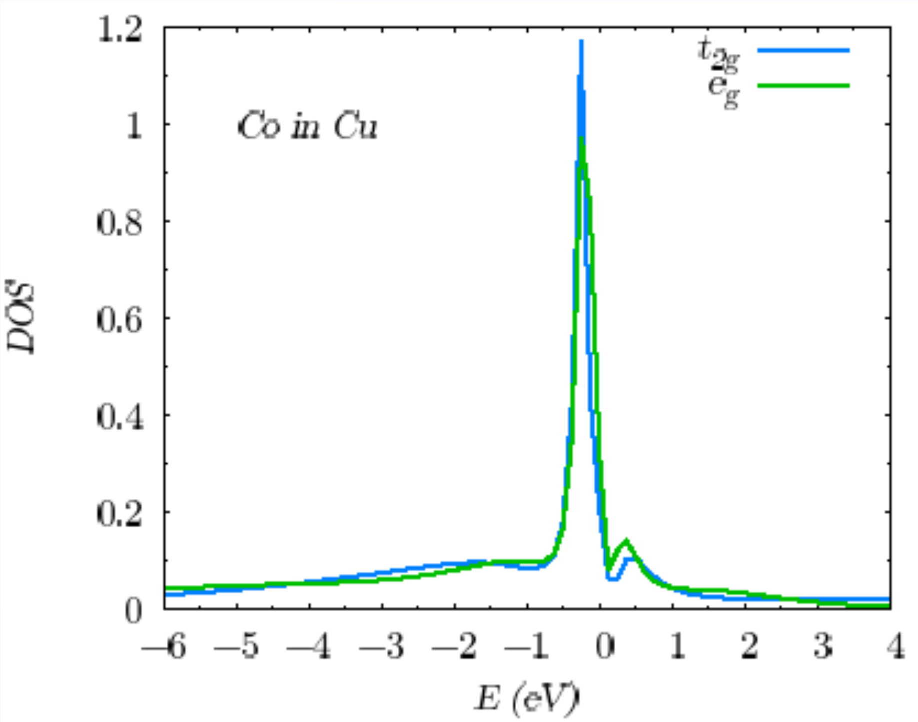


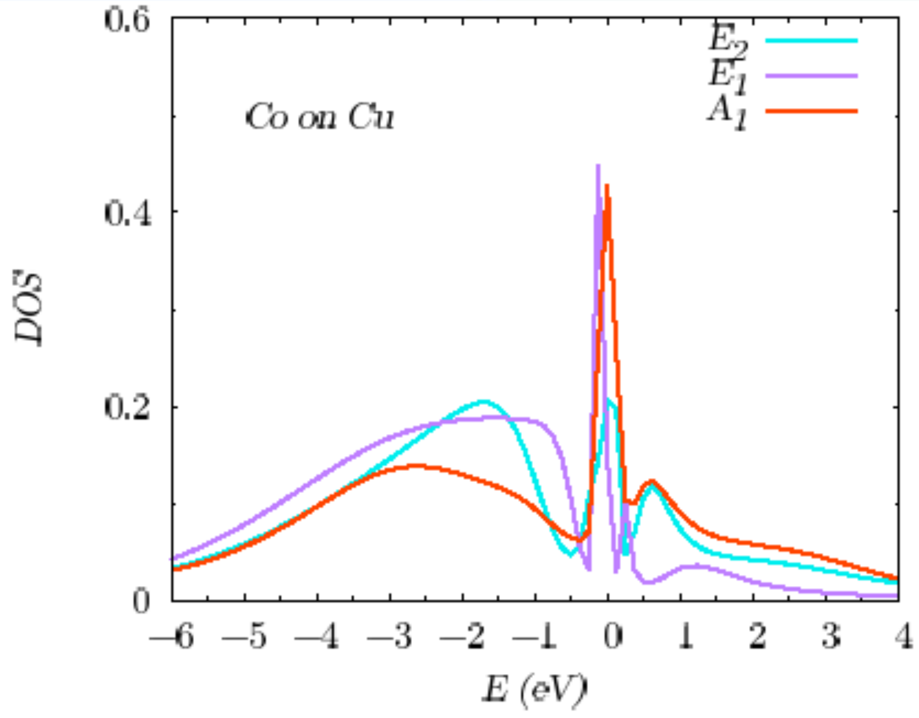
- Hybridization of Co in bulk twice stronger than on surface
- Hybridization in energy range of Cu-d orbitals more anisotropic on surface
- Co-d occupancy: *n*= 7-8

B. Surer, et al PRB (2012)



Orbitally resolved Co DOS from QMC





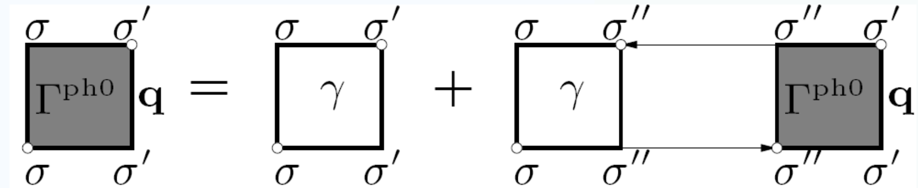
Orbitally resolved DOS of the Co impurities in bulk Cu and on Co (111) obtained from QMC simulations at temperature. $T = 0.025$ eV and chemical potential $\mu = 27$ eV and $\mu = 28$ eV, respectively.

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

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

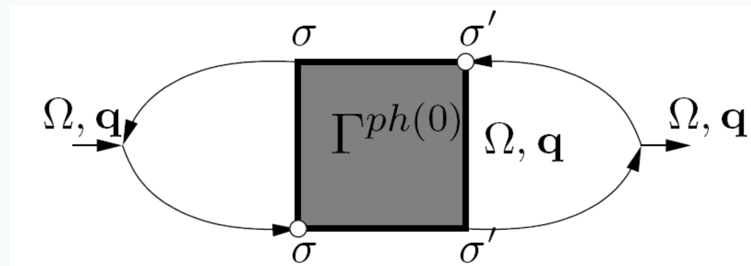
Magnetic susceptibility: nanosystems

Bethe-Salpeter Equation:

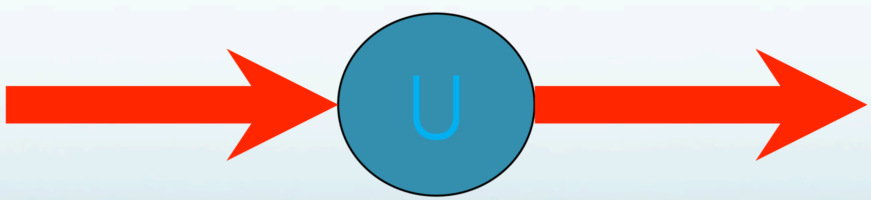


Susceptibility:

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

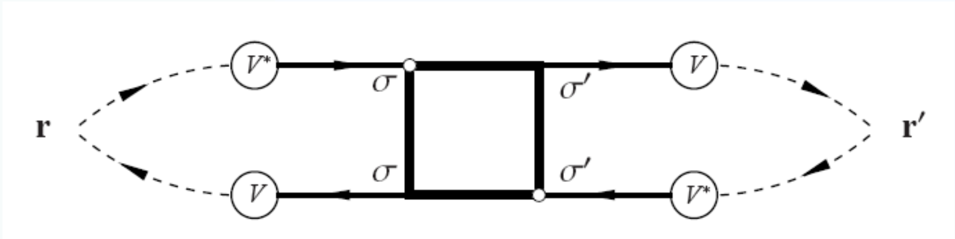


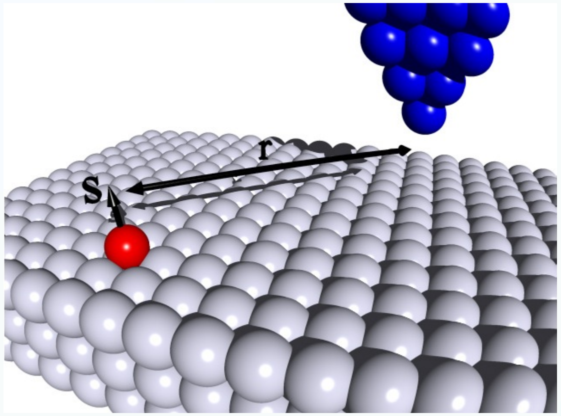
Local correlated nano-system:

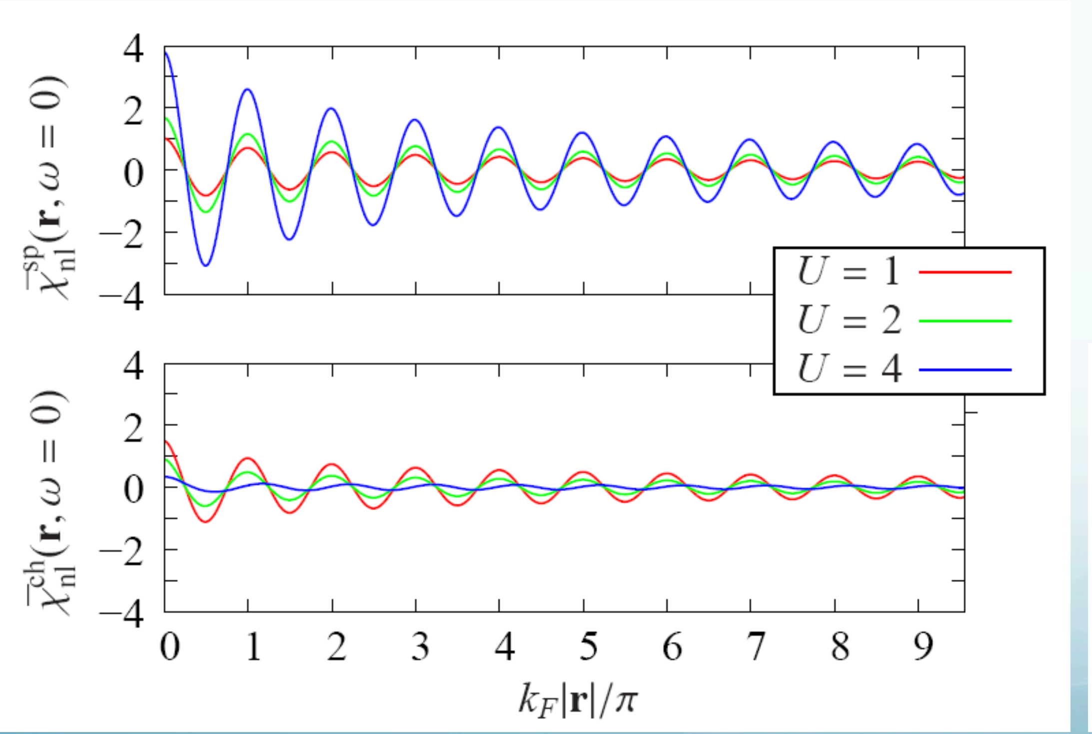


$$\chi^{-1}_{\nu,\nu'}(\vec{q},\omega) = \chi^{-1}_{0,\nu,\nu'}(\vec{q},\omega) - \gamma_{\nu,\nu'}(\omega)$$

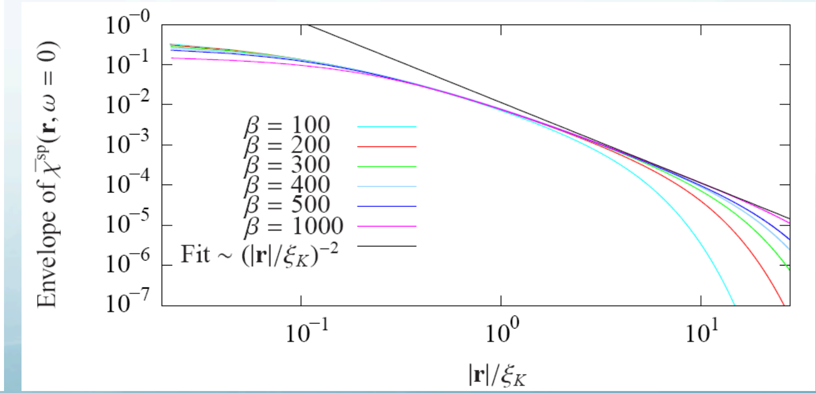
Spin and Charge susceptibility near impurity





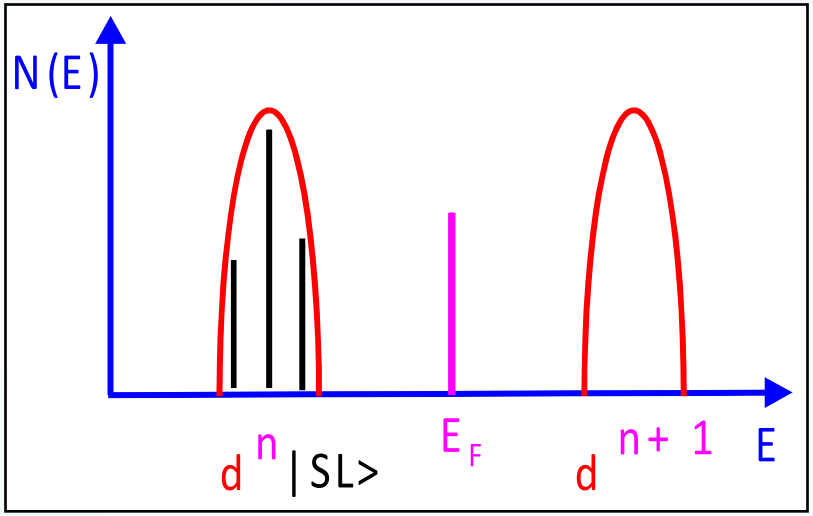


K. Patton, H. Hafermann,et.al PRB (2009)

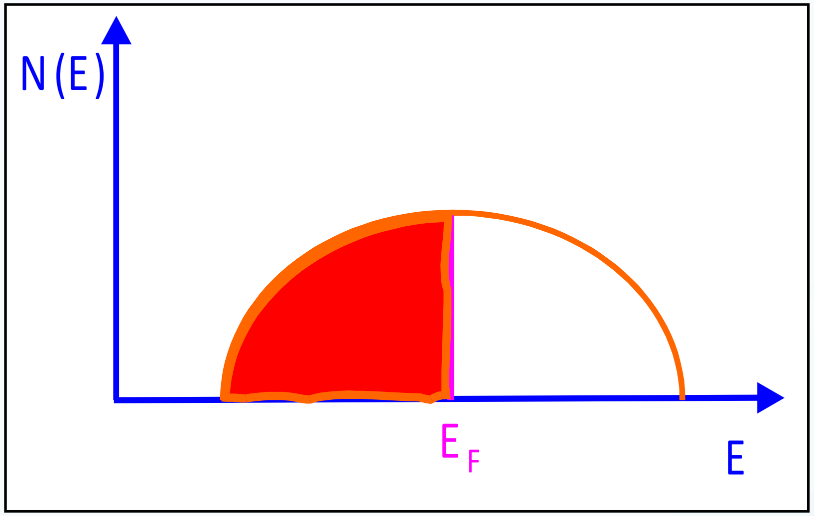


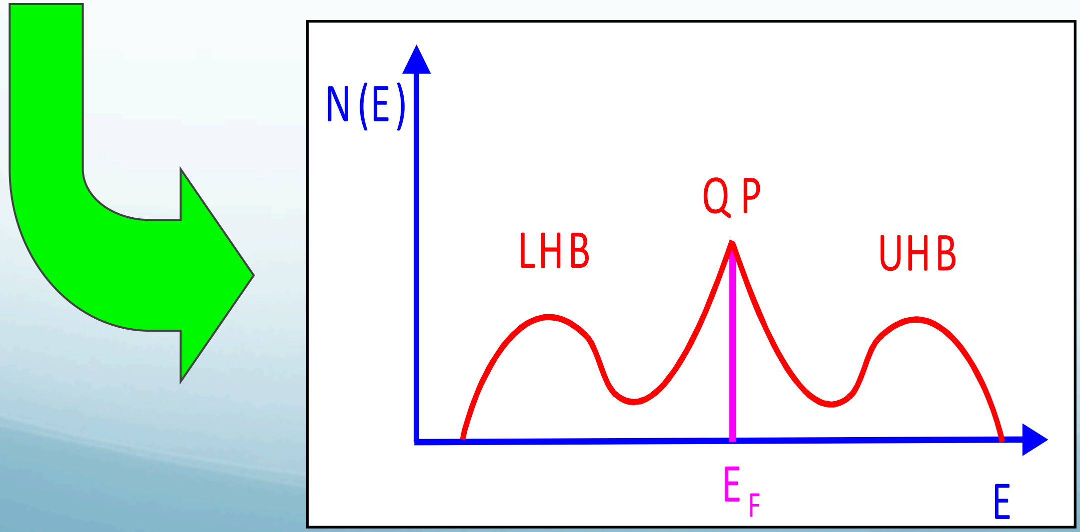
From Atom to Solid

Atomic physics



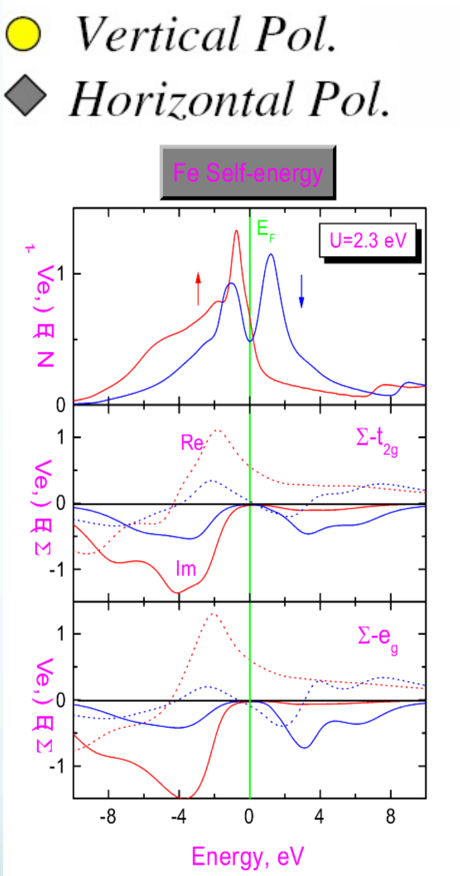
Bands effects (LDA)

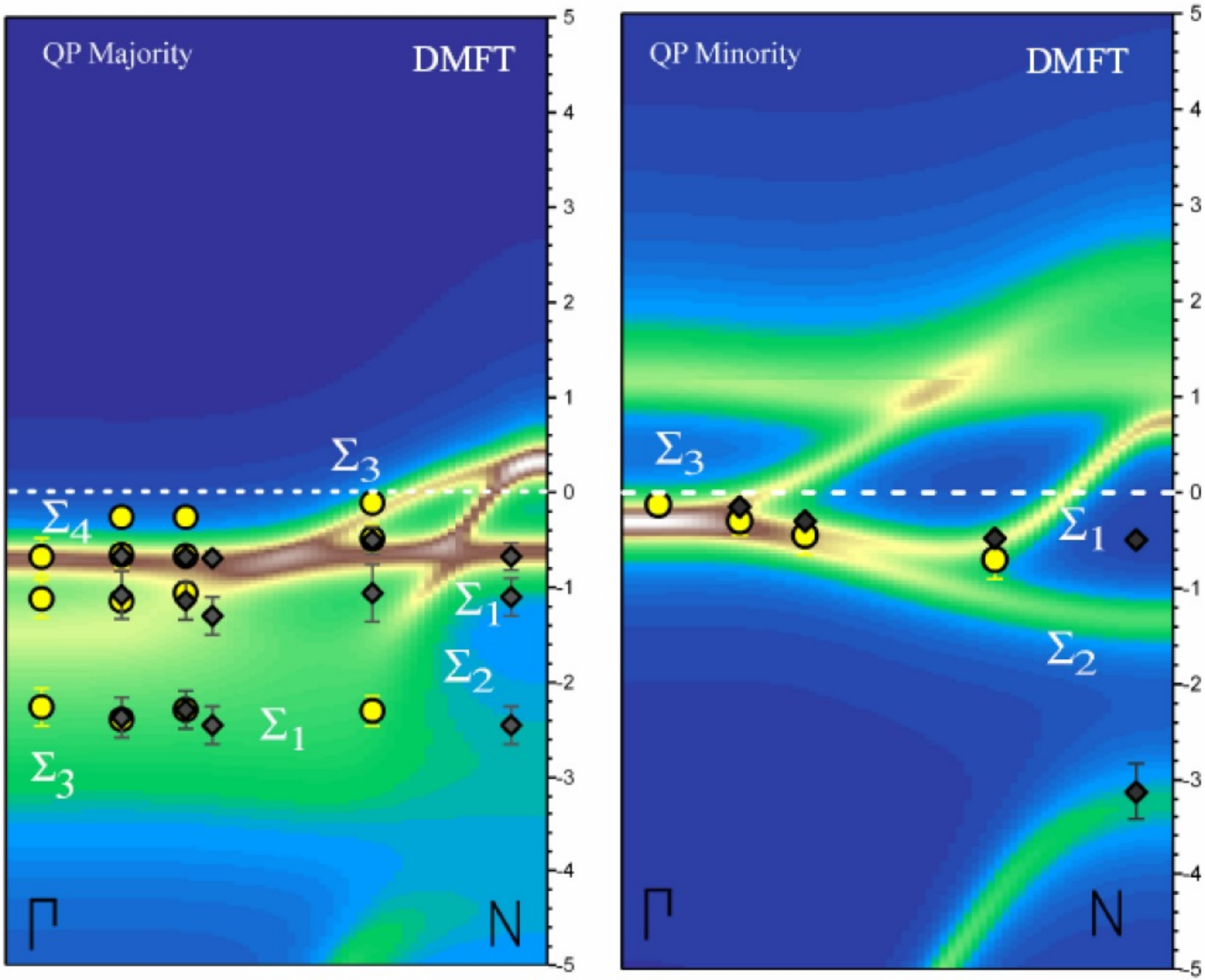




LDA+DMFT

Spectral Function Fe: ARPES vs. DMFT





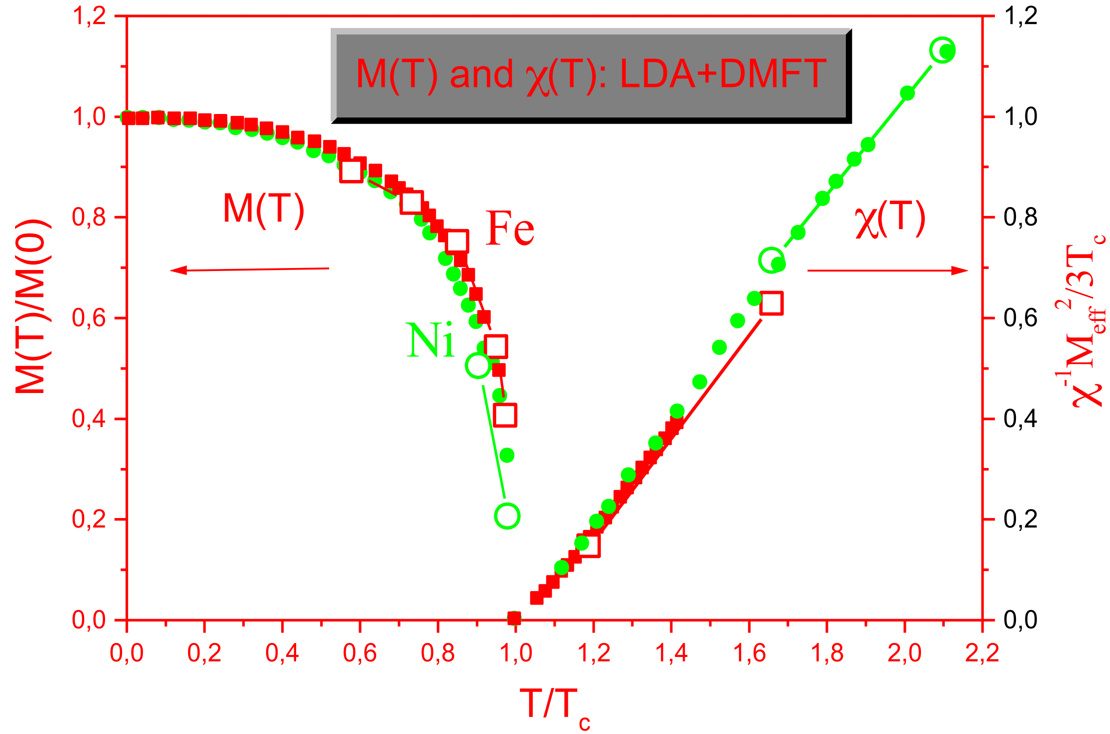
SP-ARPES (BESY)
J. Sánchez-Barriga, et al, PRL (2010)

Magnetism of metals: LDA+DMFT

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

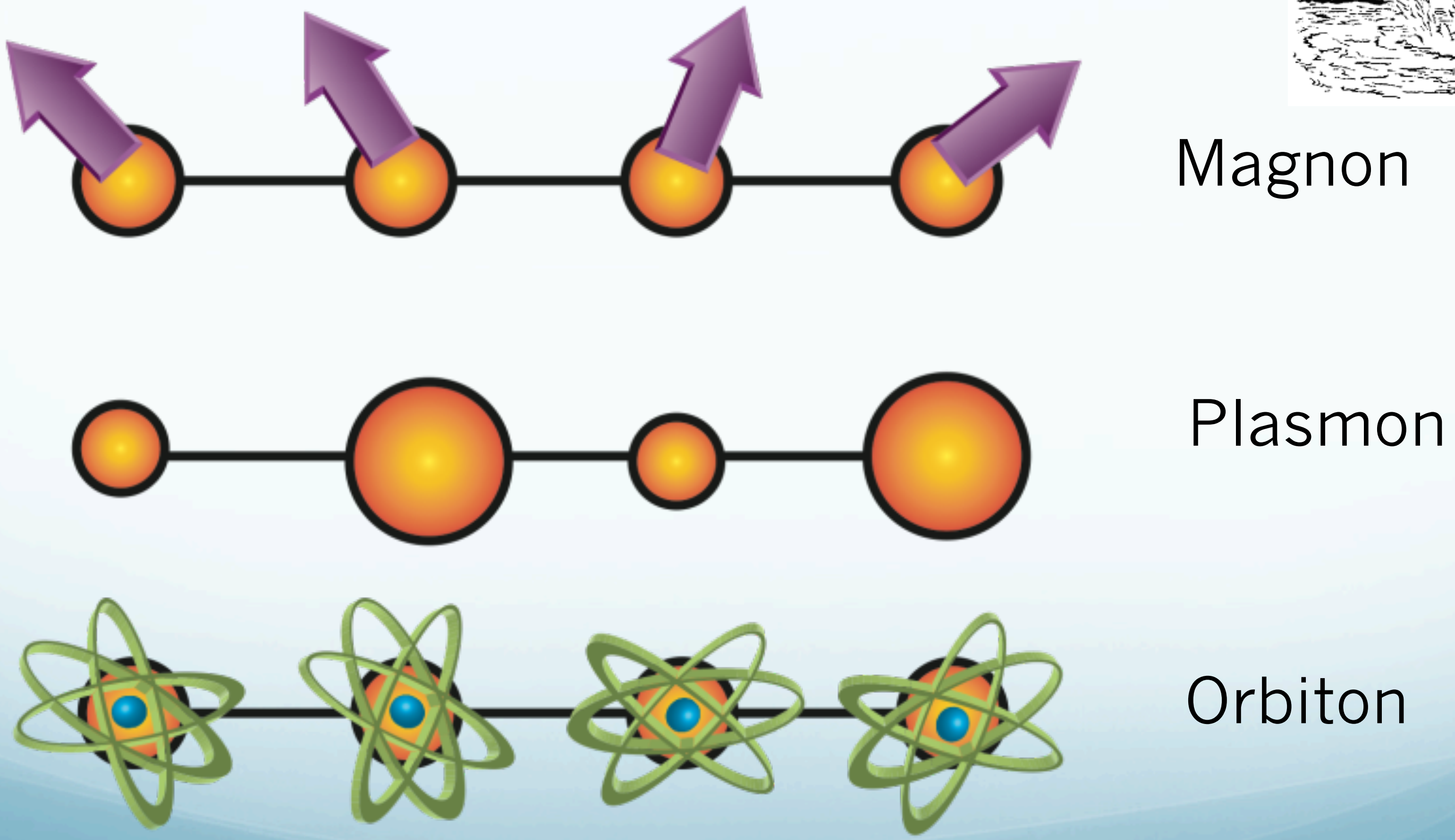
$$[S_{mm'}^{\sigma\sigma'}] \rightarrow [-S_{mm'}^{-\sigma-\sigma'}]$$

Global spin flip



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

Interaction of electrons with collective excitations



Non-local Coulomb interactions

General non-local action for solids:

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

Atomic action with local Hubbard-like interaction

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

Bosonic charge and spin variables:

$$\rho_j \equiv \sum_{\sigma\sigma'} c^\dagger_\sigma s^j_{\sigma\sigma'} c_{\sigma'} - \bar{\rho}$$

$$s^j = (1, \sigma_x, \sigma_y, \sigma_z)$$
$$j = \{0, x, y, z\}$$

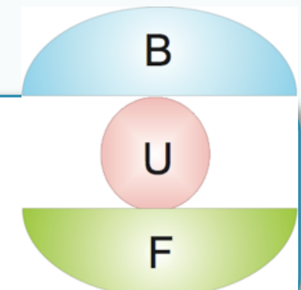
A. Rubtsov et al, Annals of Physics 327, 1320 (2012)

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)



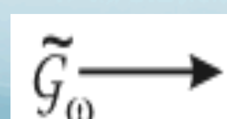
$$S_{imp} = S_{at} + \underbrace{\sum_{\nu} \Delta_\nu c_\nu^{\dagger} c_\nu}_{F} + \underbrace{\sum_{\omega} \Lambda_\omega \rho_\omega^{*} \rho_\omega}_{B}$$

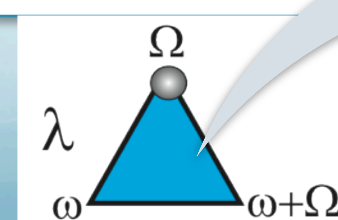
Dual boson-fermion transformation: $c^{\dagger} \rightarrow f^{\dagger}$ $\rho^{*} \rightarrow \eta^{*}$

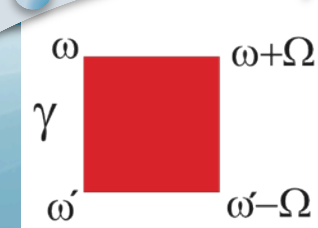
$$\tilde{S} = -\sum_{k\nu} \tilde{\mathcal{G}}_{k\nu}^{-1} f_{k\nu}^{\dagger} f_{k\nu} - \sum_{q\omega} \tilde{\mathcal{X}}_{q\omega}^{-1} \eta_{q\omega}^{*} \eta_{q\omega} + \sum_i \tilde{U}[\eta_i, f_i, f_i^{\dagger}]$$

EDMFT

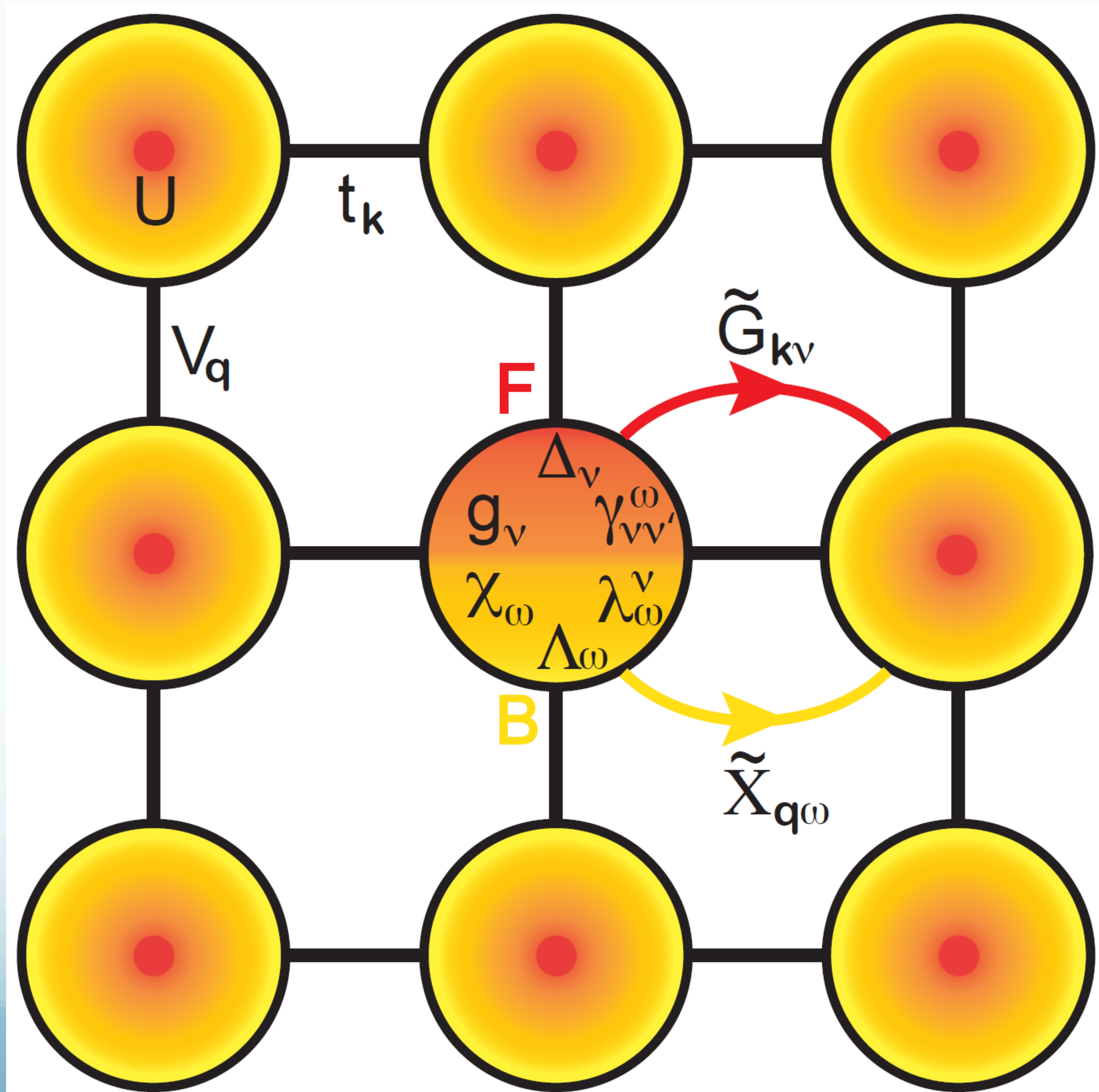
Diagrams:







Dual Boson: General Idea

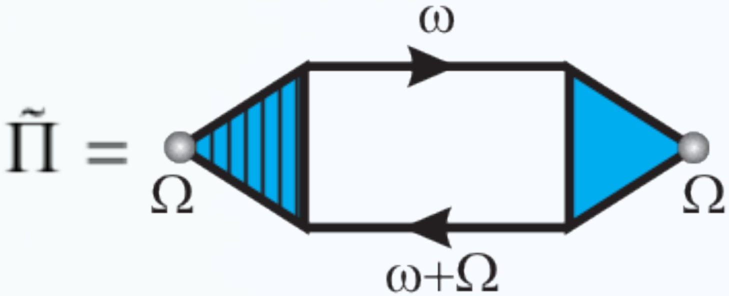


HTSC

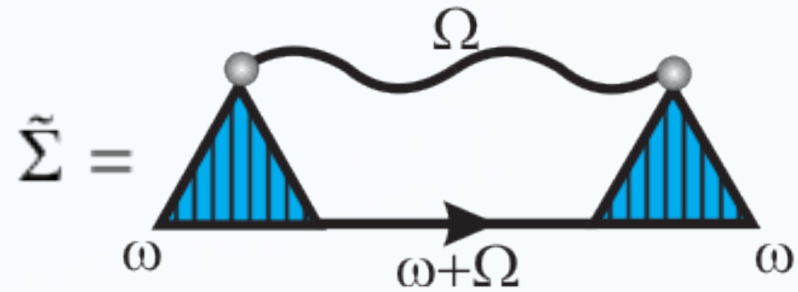
$\Lambda_\omega \sim J_{\tau\tau'} \vec{S}_\tau \cdot \vec{S}_{\tau'}$

DB-diagrammatic scheme

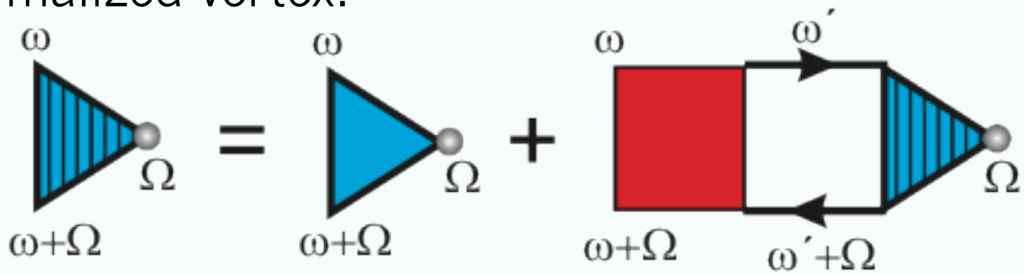
Bosonic Selfenergy



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

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

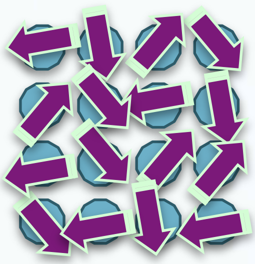
$$\sum_q X_{q\omega} = \chi_\omega$$

Δ_ν

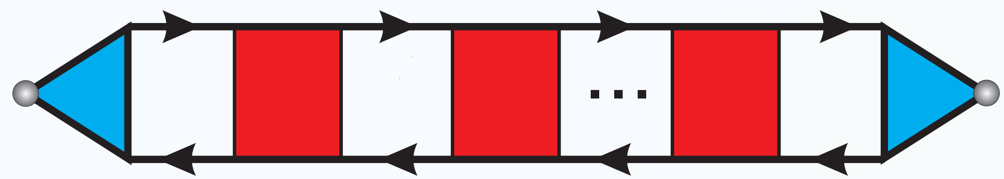
Λ_ω

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

Simple Test: Hubbard lattice



U>>t



$$\lambda_{\Omega\omega} = \chi_{\Omega}^{-1}\left(1 - \sum_{\omega'} \gamma_{\omega,\omega',\Omega}\, g_{\omega'}\, g_{\omega'-\Omega}\, s_{\sigma\sigma'}\right)$$

Fermionic Selfenergy

$$\Pi'_{\Omega K} = \left[\left(\lambda \frac{\tilde{X}^{(0)}_{\Omega K}}{1 - \gamma_{\Omega}\tilde{X}^{(0)}_{\Omega K}} \lambda\right)^{-1} + \chi_{\Omega}\right]^{-1} = \lambda_{\Omega}\tilde{X}^{(0)}_{\Omega K}\lambda_{\Omega}$$

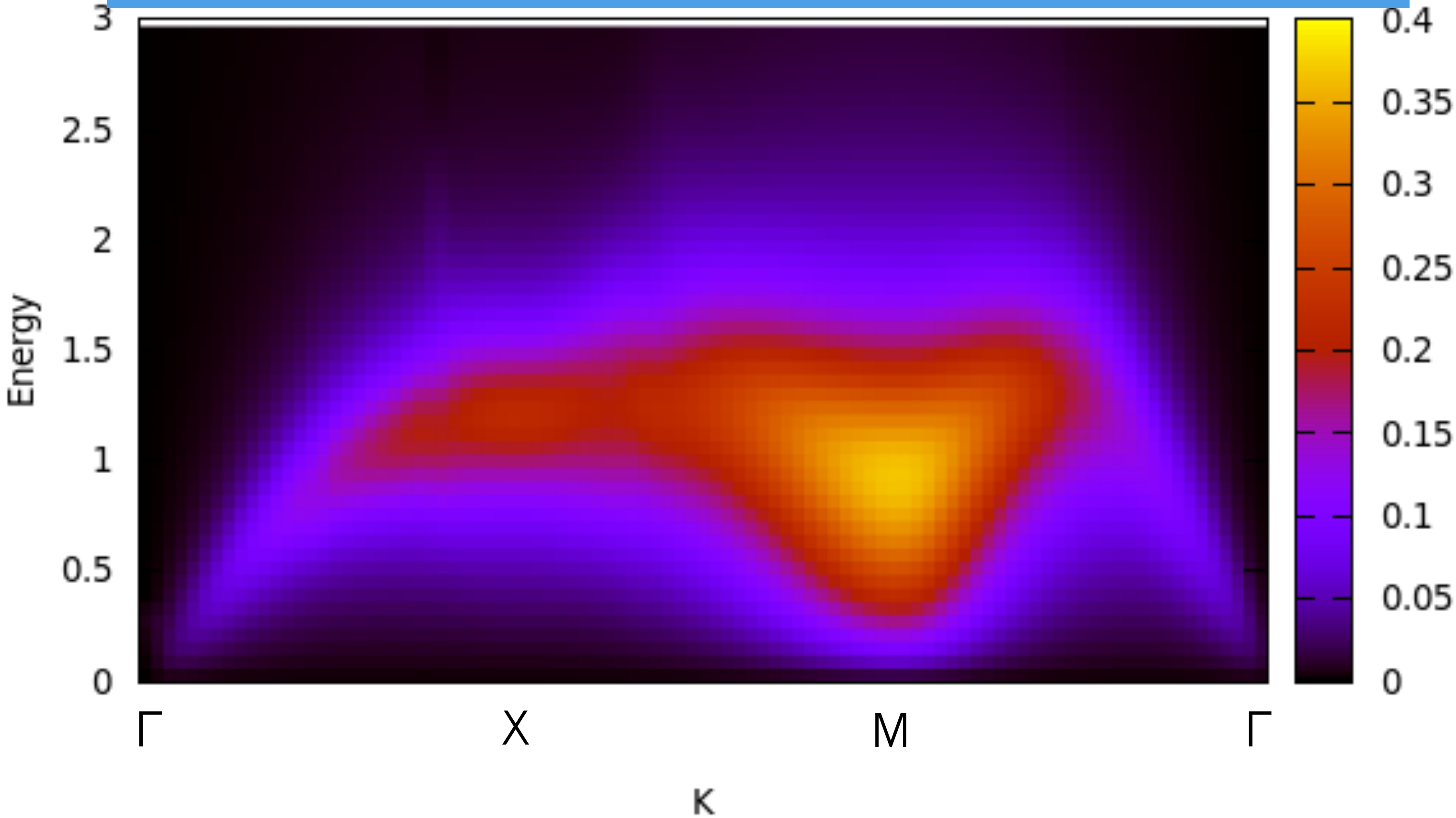
Generalization of Anderson superexchange to frequency-dependent case $J_{ij} = \frac{t^2}{U}$

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

Plasmon mode in ladder DB

How Mott transition affect plasmon mode?

U=1.5 V=0.4 t=0.25 Beta=10 Square 64x64 lattice



Susceptibility using Dual Fermion: $\langle \rho\rho \rangle_{K\to 0} \neq 0$

Summary

- Magnetism of correlation systems can be well described in the LDA+DMFT scheme
- Local correlations efficiently included in CT-QMC impurity solver

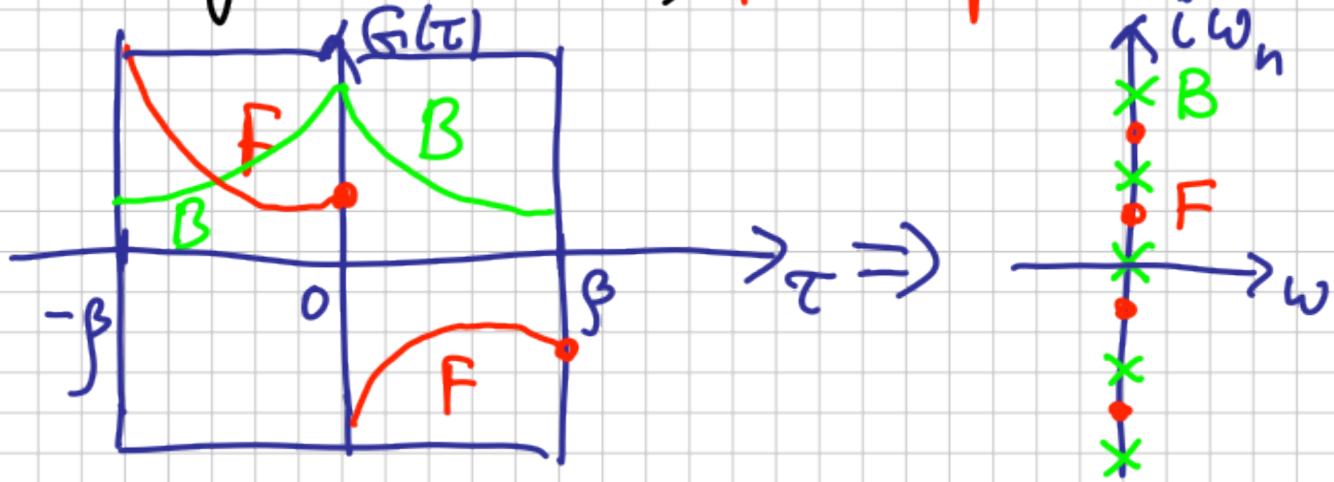
Imaginary Time and Matsubara space

Since: $[0,\beta)$

$$C(\tau+\beta)=\{C(\tau)$$

B: periodic

F: antiperiodic



then:

Matsubara frequencies:

$$\omega_n=\begin{cases}2n\frac{\pi}{\beta} & \text{- Boson}\\ (2n+1)\frac{\pi}{\beta} & \text{- Fermion}\end{cases}$$

$n=-\infty\ldots -1,0,1\ldots\infty$ integer numbers

Using:

$$\int_0^\beta d\tau\, e^{-i(\omega_n-\omega_m)\tau}=\beta\,\delta_{n,m}$$

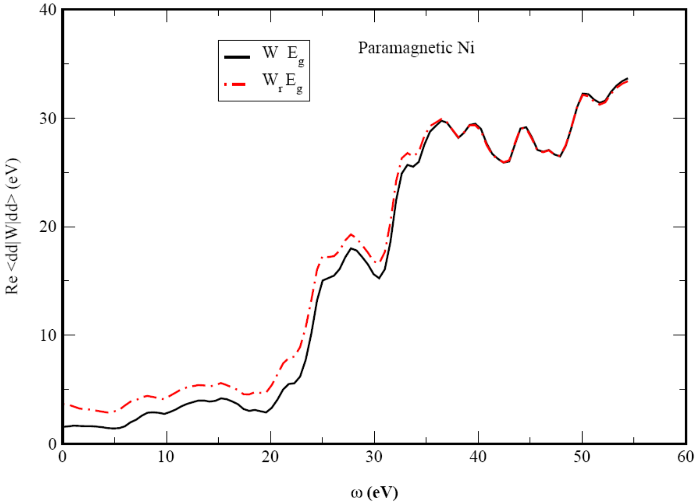
Constrain GW calculations of U

Polarisation

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

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

F. Aryasetiawanan et al PRB(2004)

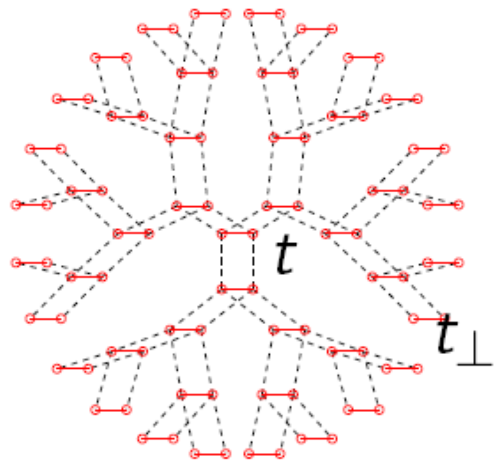


$$\begin{aligned} W &= [1 - vP]^{-1} v \\ &= [1 - vP_r - vP_d]^{-1} v \\ &= [(1 - vP_r)\{1 - (1 - vP_r)^{-1} vP_d\}]^{-1} v \\ &= \{1 - (1 - vP_r)^{-1} vP_d\}^{-1} (1 - vP_r)^{-1} v \\ &= [1 - W_r P_d]^{-1} W_r \end{aligned}$$

Double-Bethe Lattice: exact C-DMFT

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

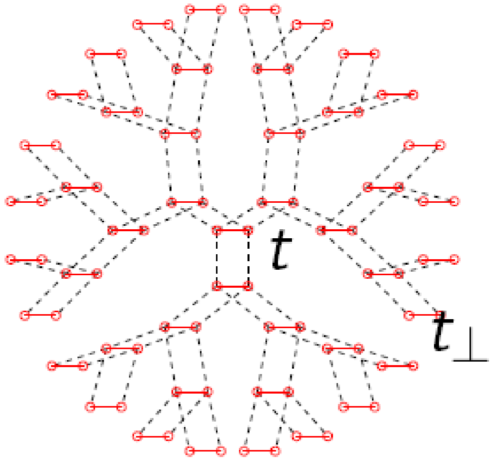
A. Ruckenstein
PRB (1999)



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

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

Self-consistent condition: C-DMFT

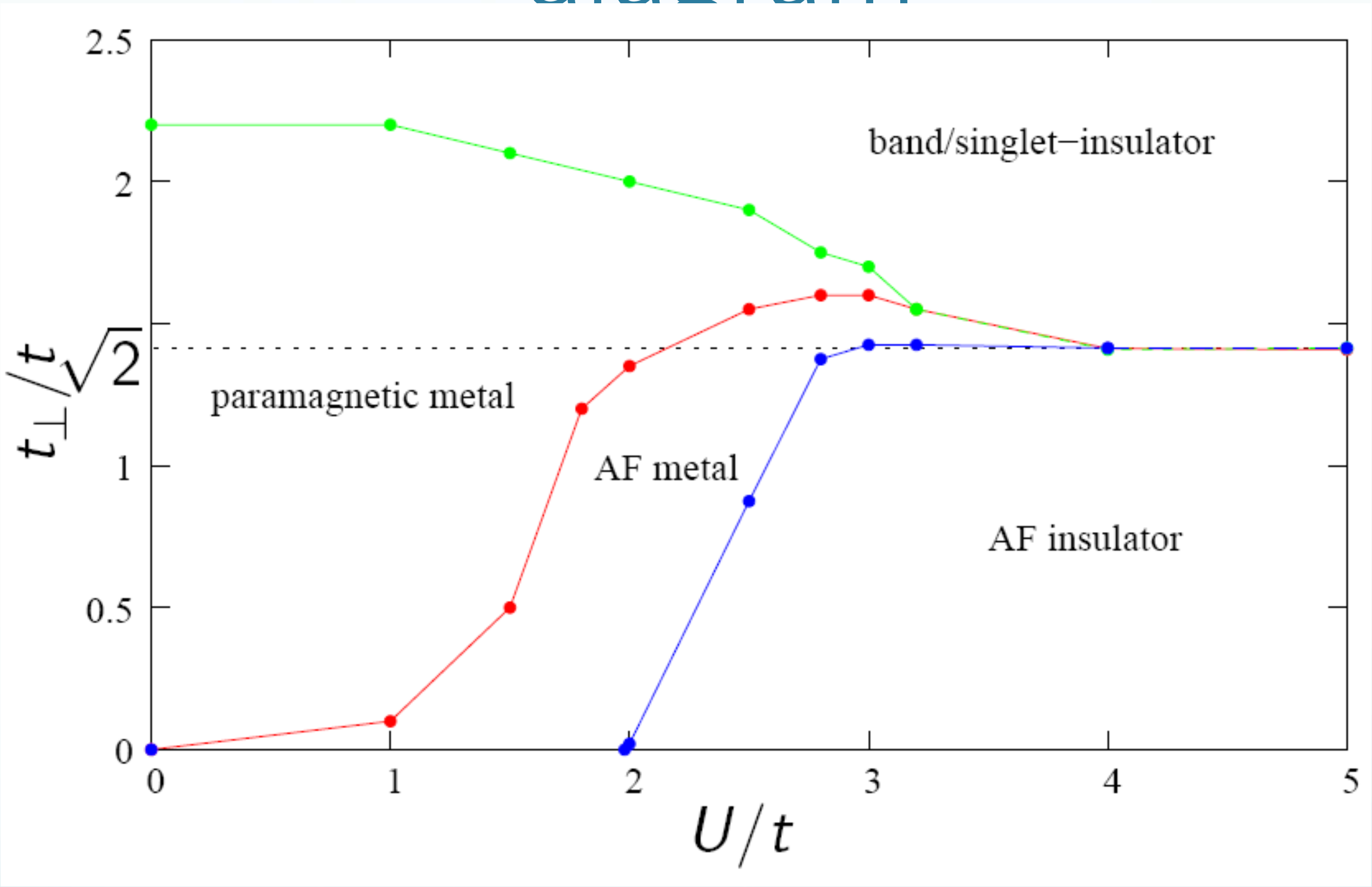


$$\mathcal{G}_\sigma^{-1}(i\omega_n) = \begin{pmatrix} i\omega_n + \mu - h\sigma & -t_\perp \\ -t_\perp & i\omega_n + \mu + h\sigma \end{pmatrix} - t^2 \mathbf{G}_{-\sigma}(i\omega_n) \ ,$$

AF-between plane

AF-plane

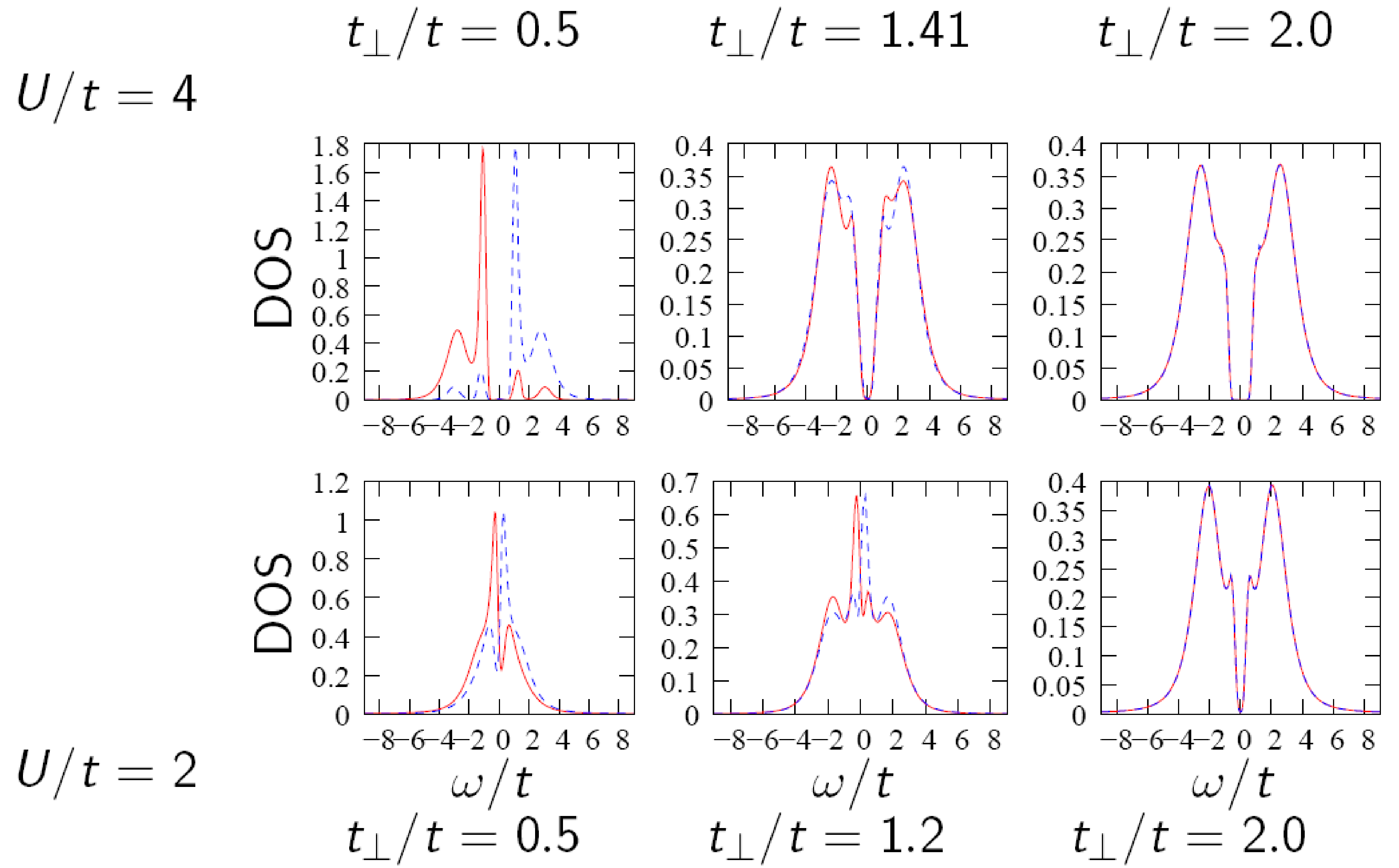
Finite temperature phase diagram



- order-disorder transition at t? / t=p2 for large U
- MIT for intermediate U

H. Hafermann, et al. EPL, **85,** 37006 (2009)

Density of States: large U



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

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

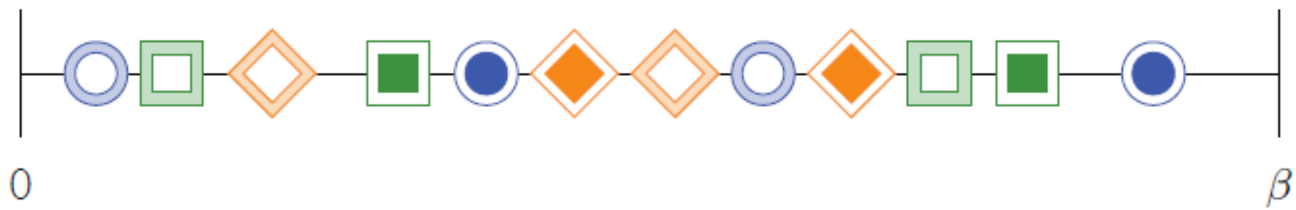
Slater integrals:

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

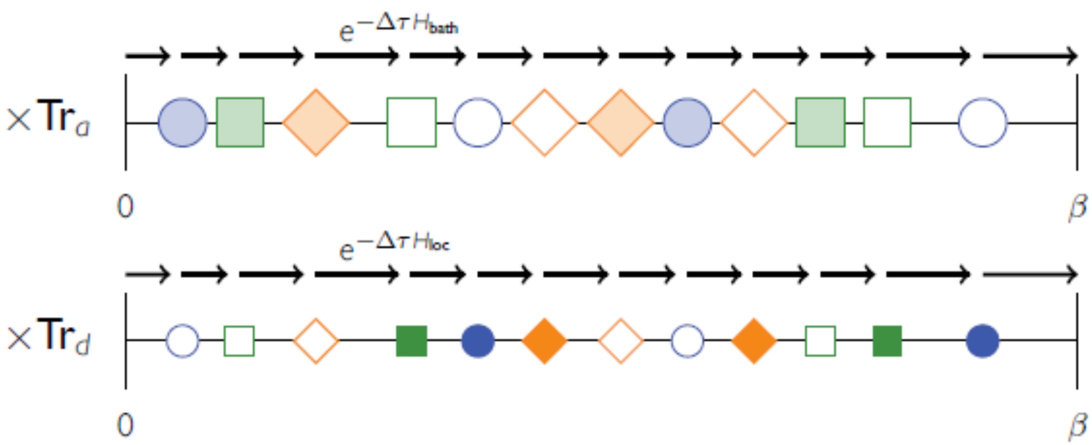
CT-HYB: General Interaction

P. Werner and A.J. Millis, PRB 74, 155107 (2006)

creation and annihilation operators for different orbitals



$$Z = \sum_{k=0}^{\infty} \int_0^{\beta} d\tau_1 \dots \int_{\tau_{k-1}}^{\beta} d\tau_k \int_0^{\beta} d\tau'_1 \dots \int_{\tau'_{k-1}}^{\beta} d\tau'_k \sum_{\substack{j_1,\dots,j_k \\ j'_1,\dots,j'_k}} \sum_{\substack{p_1,\dots,p_k \\ p'_1,\dots,p'_k}} V_{p_1}^{j_1} V_{p'_1}^{j'_1 *} \dots V_{p_k}^{j_k} V_{p'_k}^{j'_k *}$$



tracing out bath degrees of freedom gives rise to determinant weight as before

⋮

CT-HYB: Krylov code

A. M. Läuchli and P. Werner, PRB 80, 235117 (2009)

$e^{-\Delta\tau H_{\text{loc}}}$ $\quad O_k(\tau_k)$ sparse in the occupation number basis

Krylov time evolution

$$\mathbf{Tr}_d\,[\ldots] = \sum_{|\psi\rangle} \langle\psi| e^{-(\beta-\tau_k)H_{\text{loc}}} O_k(\tau_k) e^{-(\tau_k-\tau_{k-1})H_{\text{loc}}} \ldots O_1(\tau_1) e^{-\tau_1 H_{\text{loc}}} |\psi\rangle$$

Idea: compute $e^{-\tau H_{\text{loc}}}|\psi\rangle$ using Lanczos recursion

Park and Light, J. Chem. Phys (1986)

$$\begin{pmatrix} & \star & & \star & \\ & & \star & & \\ \star & & & & \star \end{pmatrix}\begin{pmatrix} \\ \\ \\ \end{pmatrix}$$

sparse matrix-vector multiplication

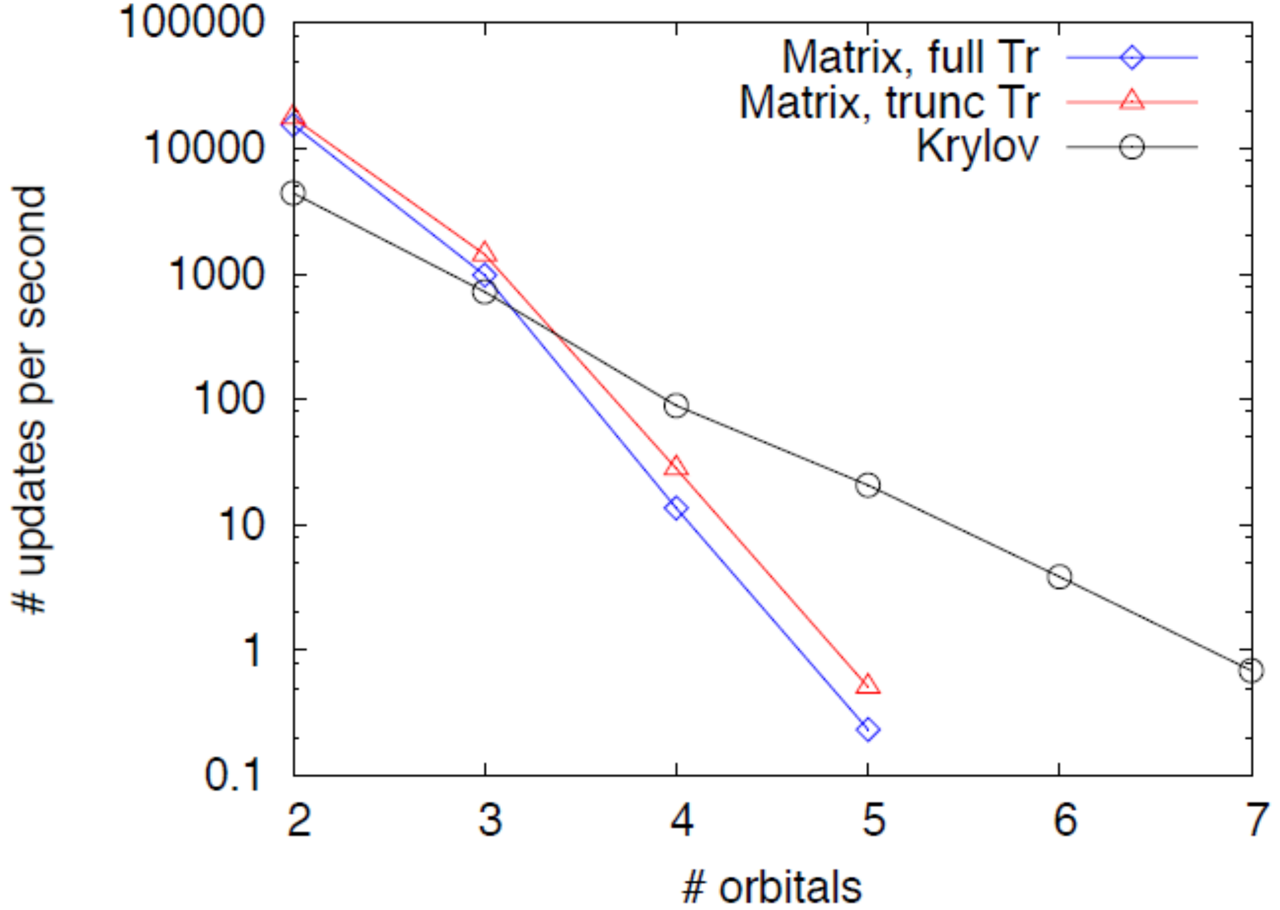
construct Krylov subspace $\mathcal{K} = \left\{ |\psi\rangle, H_{\text{loc}}|\psi\rangle, H_{\text{loc}}^2|\psi\rangle, \ldots, H_{\text{loc}}^p|\psi\rangle \right\}$

efficiently represents $e^{-\tau H_{\text{loc}}}|\psi\rangle$ for a small number p $\qquad \tau$ small $\longrightarrow$ p small

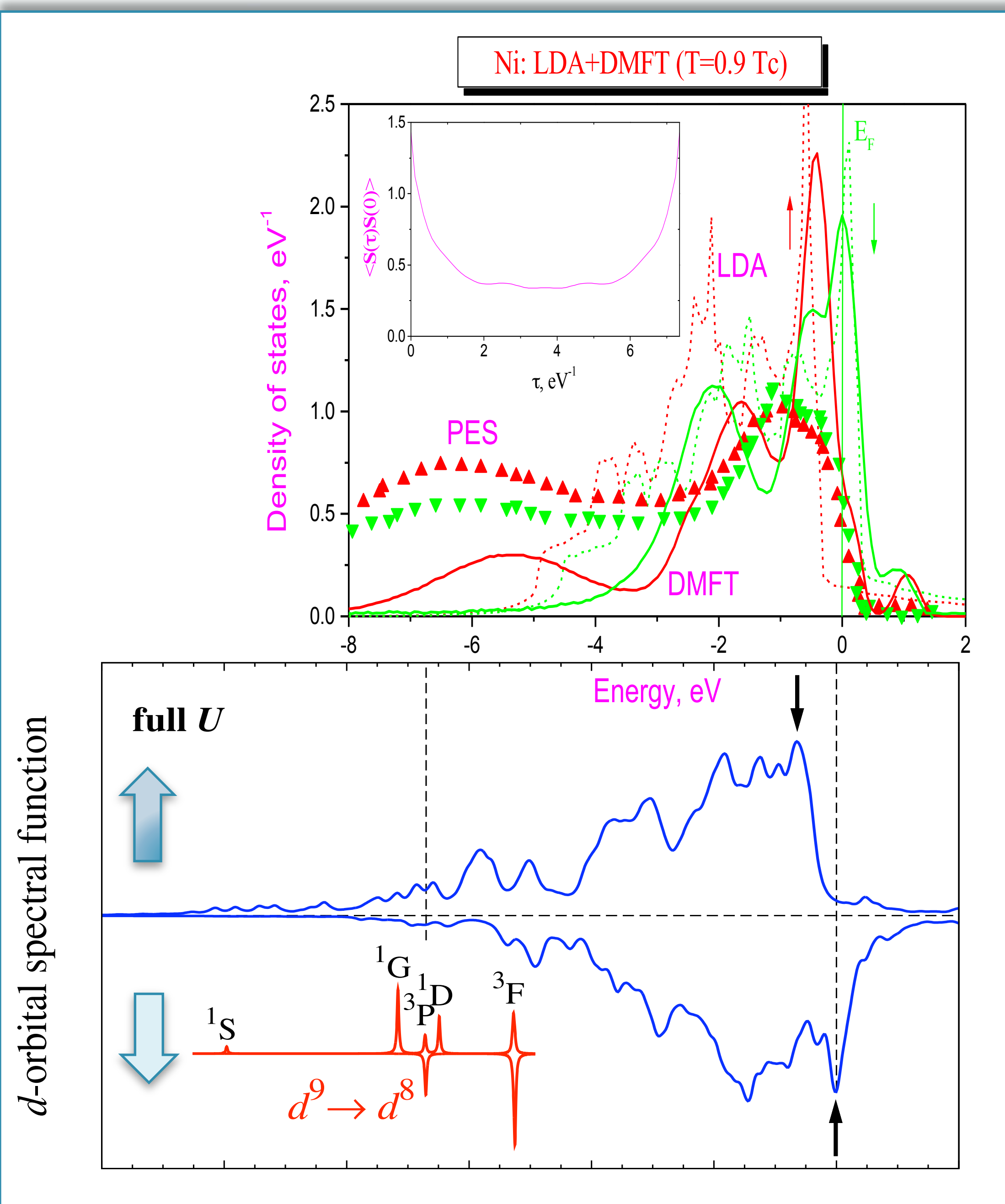
Hochbruck & Lubich, SIAM J. Numer. Anal. (1997)

CT-QMC-Krylov: performance

A. M. Läuchli and P. Werner, PRB 80, 235117 (2009)



Satellite structure in Ni



PES (LDA)

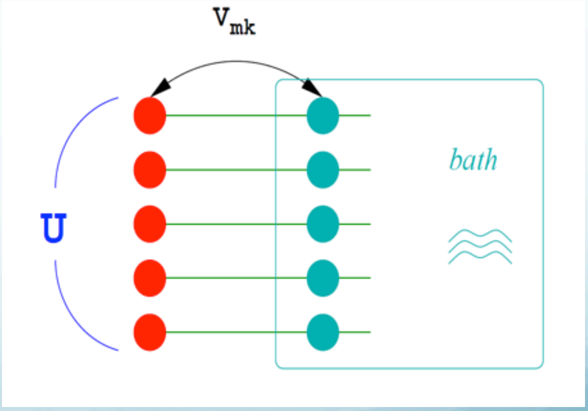
$$W_{band} = 3(4)\ \mathrm{eV}$$

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

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

LDA+DMFT+QMC

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



T-Lanczos (5d+10k)

J. Kolorenc et al PRB (2012)