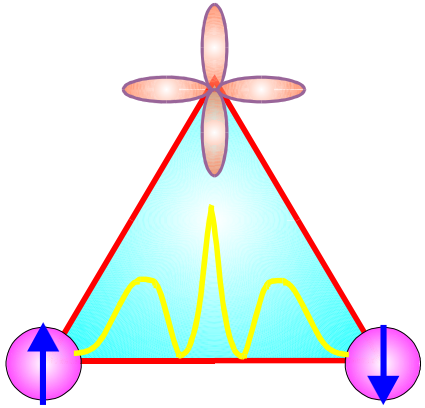


Continuous time quantum Monte Carlo method for multiorbital strongly correlated systems

Evgeny Gorelov

University of Hamburg

In collaboration with:

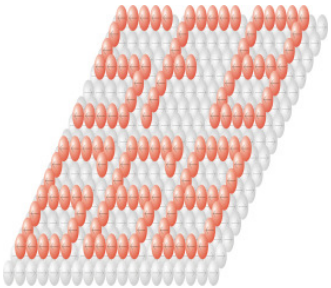
A. Lichtenstein (Hamburg)

A. Rubtsov (Moscow)

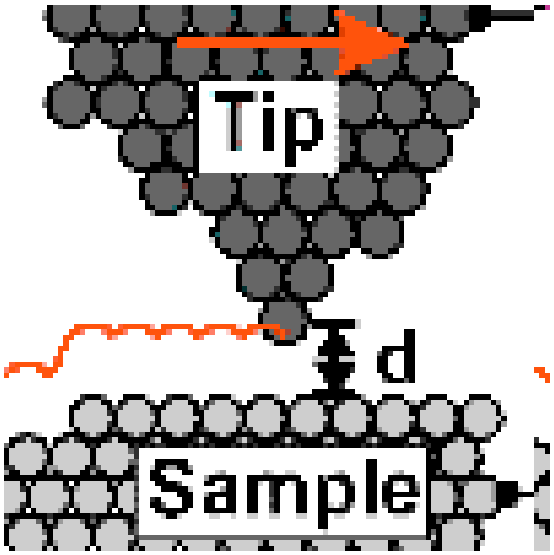
V. Anisimov (Ekaterinburg)

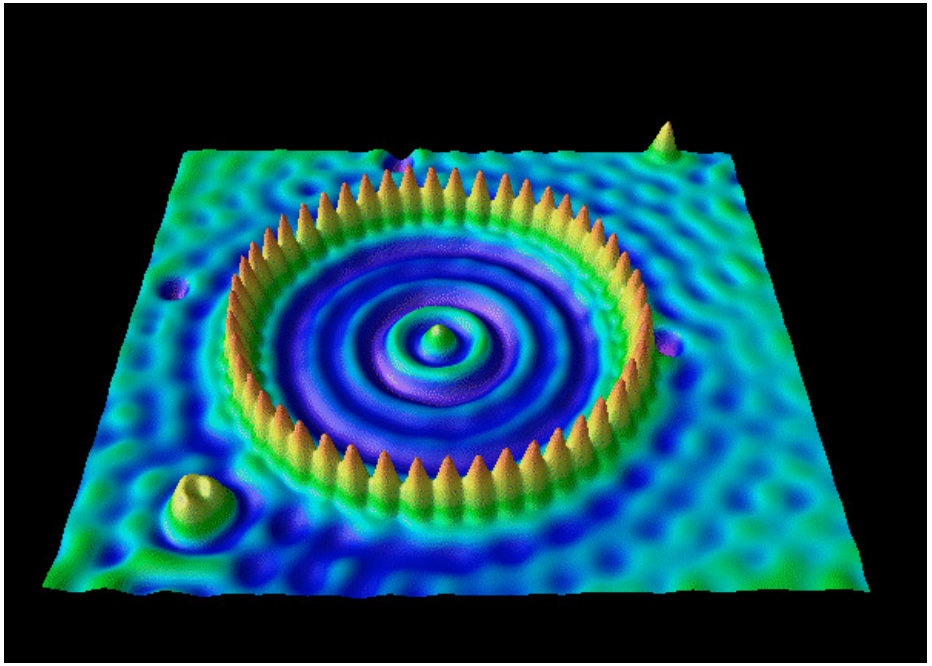
A. Shick (Prague)

Prague, 11.03.2008



Motivation: STM





www.physnet.uni-hamburg.de/home/vms/pascal/stm.htm

www.almaden.ibm.com

Theoretical problem is: how to treat realistic multiorbital systems with full atomic Coulomb interaction

Outline

- CT-QMC formalism
- Kondo model
- Multi-orbital impurity problem, Co in Cu
- Correlated solids, Sr_2RuO_4
- Conclusions

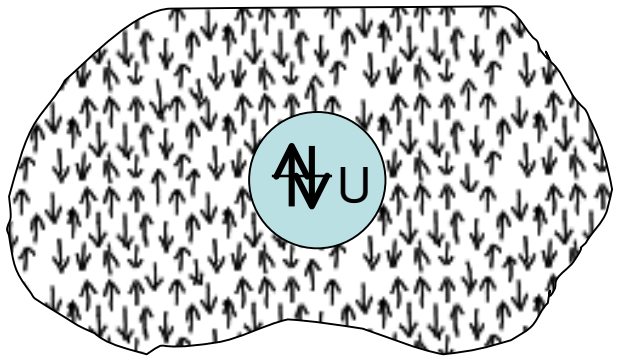
I. Theory. Impurity problem

Multiorbital Anderson impurity model:

$$H = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{\substack{ijkl \\ \sigma\sigma'}} U_{ijkl} c^\dagger_{i\sigma} c^\dagger_{j\sigma'} c_{l\sigma'} c_{k\sigma}$$

$$+ \sum_{j\mathbf{k}\sigma} [\epsilon_j(\mathbf{k}) - \mu] d^\dagger_{j\sigma} d_{j\sigma} + \sum_{i\mathbf{k}\sigma} V_{i\mathbf{k}} (d^\dagger_{\mathbf{k}\sigma} c_{i\sigma} + c^\dagger_{i\sigma} d_{\mathbf{k}\sigma})$$

On-site Coulomb repulsion: $H_{int} = U n_\uparrow n_\downarrow$



Impurity action:

$$S = S_0 + S_{int}$$

$$= -\int_0^\beta d\tau d\tau' \sum_\sigma c^\dagger_\sigma(\tau) \mathcal{G}^{-1}_\sigma(\tau - \tau') c_\sigma(\tau') + \int_0^\beta d\tau U n_\uparrow(\tau) n_\downarrow(\tau)$$

$$\mathcal{G}^{-1}_\sigma(i\omega) = i\omega + \mu - \Delta_\sigma(i\omega)$$

$$G(\tau - \tau') = \langle T_\tau c^\dagger(\tau) c(\tau') \rangle_S = \frac{Tr\left[T_\tau e^{-S} c^\dagger(\tau) c(\tau')\right]}{Tr\left[T_\tau e^{-S}\right]}$$

Perturbation expansion

Perturbation-series expansion for the partition function:

$$Z = Tr\left[T_\tau e^{-(S_0+S_{int})}\right]$$

$$= \sum_k \frac{(-1)^k}{k!}\int_0^\beta d\tau_1 \ldots d\tau_k Tr\left[T_\tau e^{-S_0}\, U^k\, n_\uparrow(\tau_1)n_\downarrow(\tau_1)...n_\uparrow(\tau_k)n_\downarrow(\tau_k)\right]$$

$$= \sum_k \frac{(-U)^k}{k!}\int_0^\beta d\tau_1 \ldots d\tau_k \left\langle T_\tau c^\dagger(\tau_1)c(\tau_1)...c^\dagger(\tau_k)c(\tau_k)\right\rangle_{S_0}$$

According to Wick's theorem:

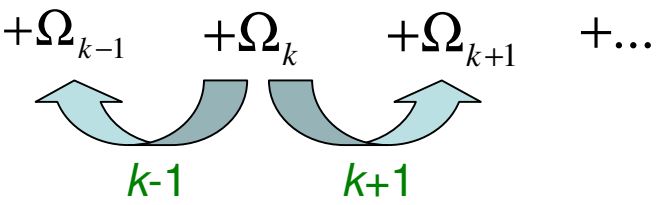
$$\left\langle T_\tau c^\dagger(\tau_1)c(\tau_1)...c^\dagger(\tau_k)c(\tau_k)\right\rangle_{S_0} = \det|\mathcal{G}(\tau_l,\tau_m)| = D^k$$

Random walks in the space of Ω_k

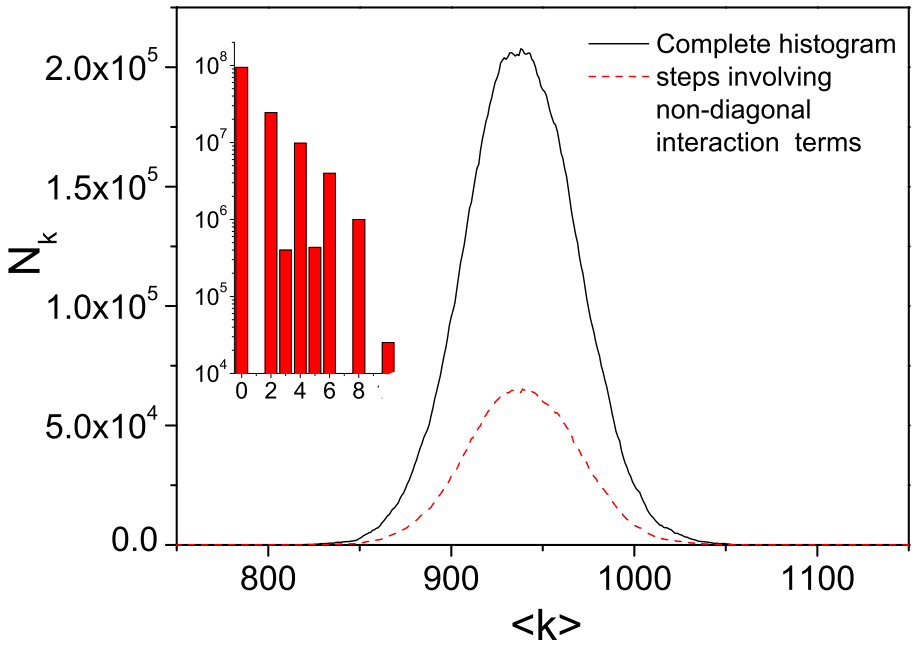
$$Z = \sum_k Z_0 \int_0^\beta d\tau_1 \dots d\tau_k \frac{(-U)^k}{k!} D^k = \sum_k \int_0^\beta d\tau_1 \dots d\tau_k \Omega_k$$

$$\Omega_k = Z_0 \frac{(-U)^k}{k!} D^k$$

random walks over expansion terms: $Z = \dots +$



An example of Ω_k distribution



Acceptance ratio

Step *k*-1

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

Step *k*+1

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

Rubtsov et al., JETP Lett **80** 61 (2004),
PRB **72** 035122 (2005)

Measuring of Green's functions

Perturbation-series expansion for the Green function:

$$G(\tau-\tau') \equiv Z^{-1} < Tc^{\dagger}(\tau)c(\tau')e^{-S_{int}} >$$

$$\Omega_k = Z_0 \frac{(-U)^k}{k!} D^k$$

$$= Z^{-1} \sum_k \int d\tau_1 \int d\tau_1' ... \int d\tau_{2k}' G^{(2k)}(\tau,\tau')\Omega_k(\tau_1,\tau_1',...,\tau_{2k}')$$

$$G^{(2k)}(\tau,\tau') = \frac{< Tc^{\dagger}(\tau)c(\tau')c^{\dagger}(\tau_1)c(\tau_1')...c^{\dagger}(\tau_{2k})c(\tau_{2k}') >}{< Tc^{\dagger}(\tau_1)c(\tau_1')...c^{\dagger}(\tau_{2k})c(\tau_{2k}') >} = \frac{D^{(2k+1)}}{D^{(2k)}}$$

Perturbation-series expansion for the four point correlator:

$$\chi(\tau,\tau',\tau'',\tau''') \equiv Z^{-1} < Tc^{\dagger}(\tau)c(\tau')c^{\dagger}(\tau'')c(\tau''')e^{-S_{int}} >$$

$$= Z^{-1} \sum_k \int d\tau_1 \int d\tau_1' ... \int d\tau_{2k}' \chi^{(2k)}(\tau,\tau',\tau'',\tau''')\Omega_k(\tau_1,\tau_1',...,\tau_{2k}')$$

$$\chi^{(2k)}(\tau,\tau',\tau'',\tau''') = \frac{< Tc^{\dagger}(\tau)c(\tau')c^{\dagger}(\tau'')c(\tau''')c^{\dagger}(\tau_1)c(\tau_1')...c^{\dagger}(\tau_{2k})c(\tau_{2k}') >}{< Tc^{\dagger}(\tau_1)c(\tau_1')...c^{\dagger}(\tau_{2k})c(\tau_{2k}') >}$$

$$= \frac{D^{(2k+2)}}{D^{(2k)}}$$

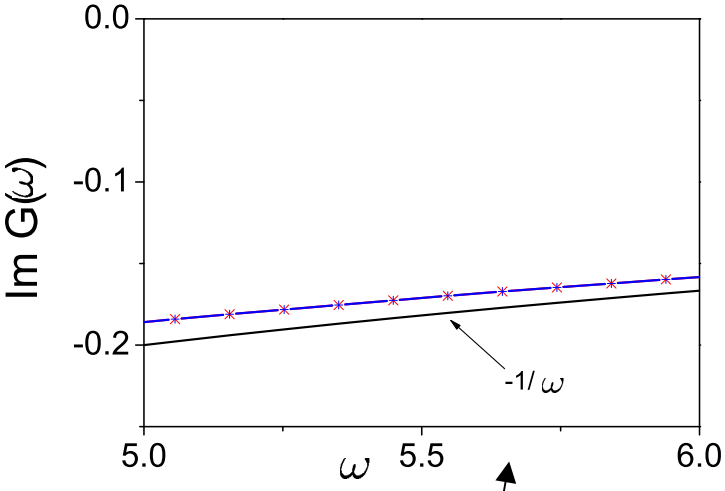
Computational details

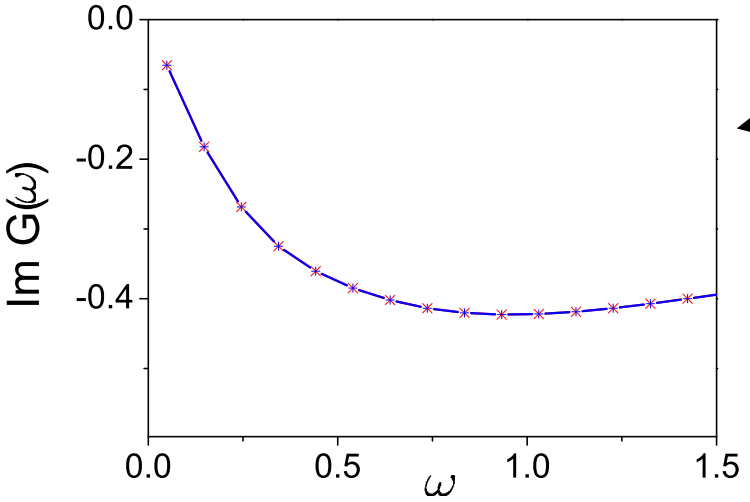
D^{-1} – matrix:

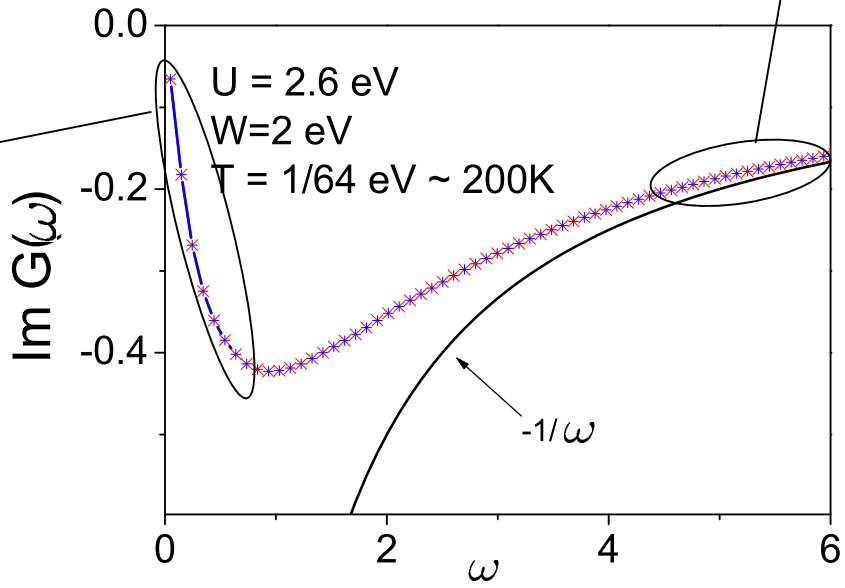
$$D = [\mathcal{G}(\tau_l, \tau_m)]$$

$$G(\tau, \tau') = \mathcal{G}(\tau, \tau') - \sum_{i,j} \mathcal{G}(\tau, \tau_i) D^{-1}_{i,j} \mathcal{G}(\tau_j, \tau')$$

$$G(\omega) = \mathcal{G}(\omega) - \mathcal{G}(\omega) \left[\frac{1}{\beta} \sum_{i,j} D^{-1}_{i,j} e^{i\omega(\tau_i - \tau_j)} \right] \mathcal{G}(\omega)$$







Computational details, multiorbital formalism

Interaction of the general form:

$$H_{int} = U n_\uparrow n_\downarrow \quad \Rightarrow \quad H_{int} = \sum_{\substack{ijkl \\ \sigma\sigma'}} U_{ijkl} c^\dagger_{i\sigma} c^\dagger_{j\sigma'} c_{l\sigma'} c_{k\sigma}$$

$$\Omega_k = Z_0 \frac{(-U)^k}{k!} D^k \quad \Rightarrow \quad \Omega_k = Z_0 \frac{(-1)^k}{k!} U^{r'_1 r'_2}_{r_1 r_2} \ldots U^{r'_{2k-1} r'_{2k}}_{r_{2k-1} r_{2k}} D^{r_1 r_2 \ldots r_{2k}}_{r'_1 r'_2 \ldots r'_{2k}}$$

$$\int_0^\beta d\tau \quad \Rightarrow \quad \int dr = \sum_{\{ijml\sigma\sigma'\}} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_{2k},$$

$$r = \{\tau, i, \sigma\}$$

$$D = [\mathcal{G}(\tau_p, \tau_q)]$$

Green's functions calculation:

$$G_{ij}(\tau, \tau') = \mathcal{G}_{ij}(\tau, \tau') - \sum_{n,m}^{K} \mathcal{G}_{ij_n}(\tau, \tau_n) D^{-1}_{n,m} \mathcal{G}_{i_m j}(\tau_m, \tau')$$

$$G_{ij}(\omega) = \mathcal{G}_{ij}(\omega) - \frac{1}{\beta} \sum_{n,m}^{K} \mathcal{G}_{ij_n}(\omega) D^{-1}_{n,m} e^{i\omega(\tau_n - \tau_m)} \mathcal{G}_{i_m j}(\omega),$$

Sign problem: introduction of α parameters

$$Z = \sum_k \sum_{\{ijml\sigma\sigma'\}} Z_0 \int_0^\beta d\tau_1 \dots d\tau_k \frac{(-1)^k}{k!} U_{i_1 j_1 m_1 l_1} \dots U_{i_k j_k m_k l_k} D^{\tau_1 \tau_2 \dots \tau_k}_{\tau'_1 \tau'_2 \dots \tau'_k}$$

$$S_0 = \sum_{ij\sigma} \int_0^\beta \int_0^\beta \left(-\mathcal{G}^{-1}_{ij}(\tau - \tau') + \frac{1}{2} \sum_{\{ml\sigma'\}} \alpha^{\sigma'}_{ml} (U_{ilmj} + U_{lijm}) \delta_{\tau\tau'} \right) c^\dagger_{i\sigma} c_{j\sigma} d\tau d\tau'$$

$$S_{int} = \frac{1}{2} \sum_{\{ijml\sigma\sigma'\}} \int_0^\beta U_{ijml} (c^\dagger_{i\sigma} c_{l\sigma} - \alpha^\sigma_{il})(c^\dagger_{j\sigma'} c_{m\sigma'} - \alpha^{\sigma'}_{jm}) d\tau.$$

$$\alpha^\sigma_{ii} + \alpha^{\sigma'}_{jj} = \bar{\alpha}$$

$$D^{\tau_1 \tau_2 \dots \tau_k}_{\tau'_1 \tau'_2 \dots \tau'_k} = \det |\mathcal{G}_{i_p l_q}(\tau_p, \tau_q) - \alpha^\sigma_{i_p l_q} \delta_{pq}|$$

$$\alpha^\sigma_{ij} + \alpha^{\sigma'}_{kl} = 0$$

Rubtsov et al., JETP Lett **80** 61 (2004),
PRB **72** 035122 (2005)

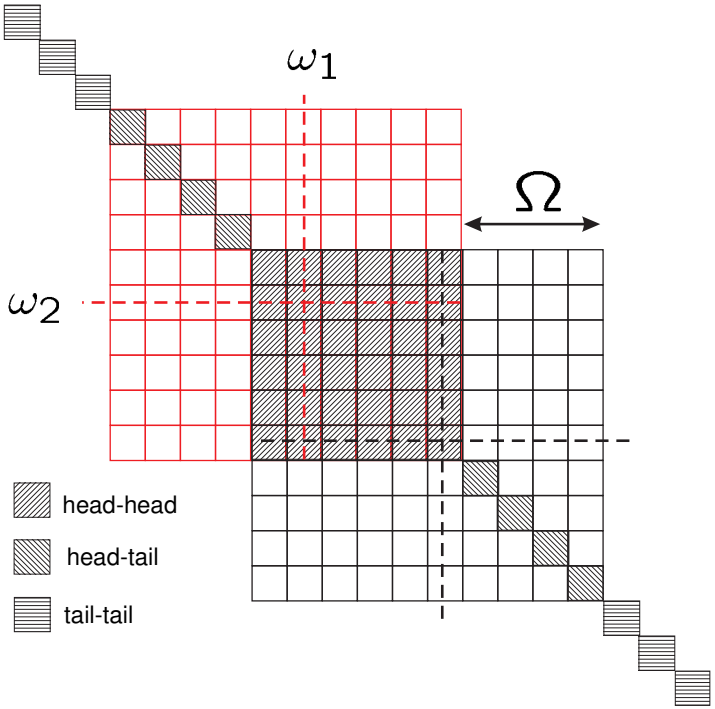
Susceptibility

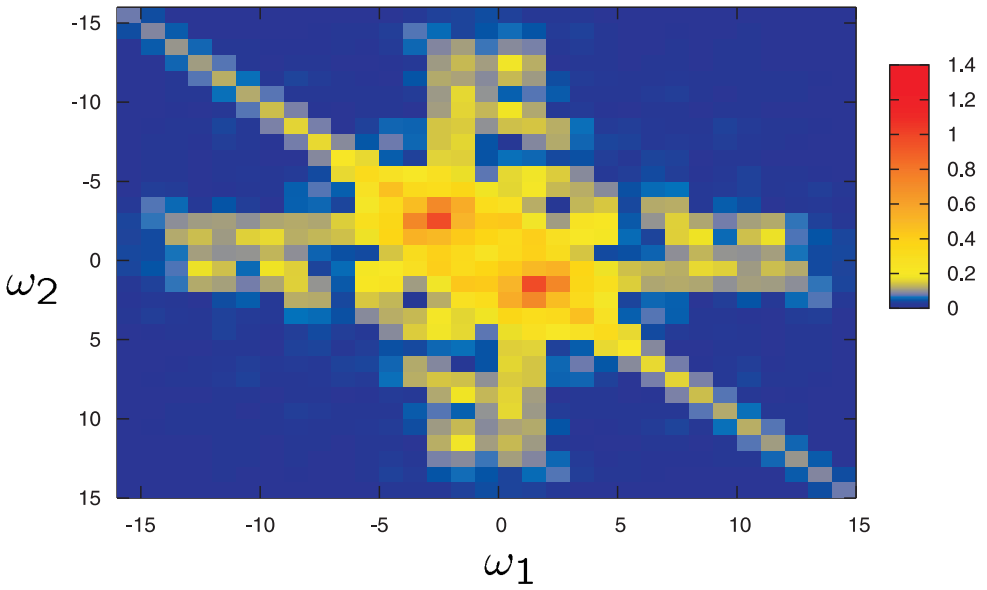
$$\chi^{+-}(\tau) = \left\langle S^{+}(\tau) S^{-}(0) \right\rangle = \left\langle c_{\uparrow}^{\dagger}(\tau) c_{\downarrow}(\tau) c_{\downarrow}^{\dagger}(0) c_{\uparrow}(0) \right\rangle$$

$$\chi^{+-}(\Omega) = \frac{1}{\beta} \sum_{\omega_1, \omega_2 = -\infty}^{\infty} G_{\uparrow}(\omega_1 + \Omega, \omega_2 + \Omega) G_{\downarrow}(\omega_2, \omega_1)$$

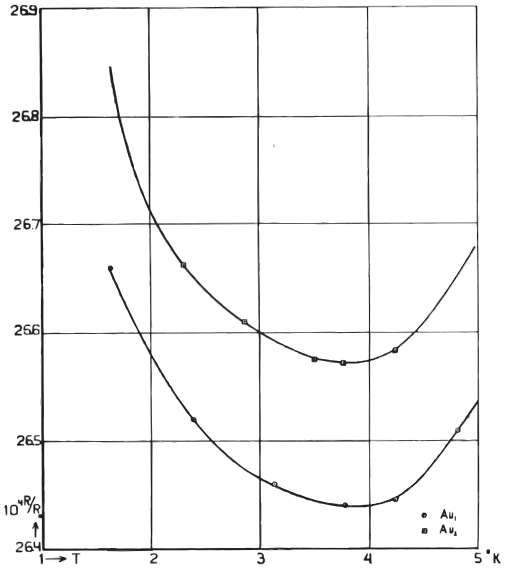
$$G(\omega, \omega') = \mathcal{G}(\omega)\delta_{\omega,\omega'} - \mathcal{G}(\omega) \left[\frac{1}{\beta} \sum_{i,j} e^{i\omega\tau_i} D^{-1}_{i,j} e^{-i\omega'\tau_j} \right] \mathcal{G}(\omega')$$

$$D = [\mathcal{G}(\tau_l, \tau_m)]$$

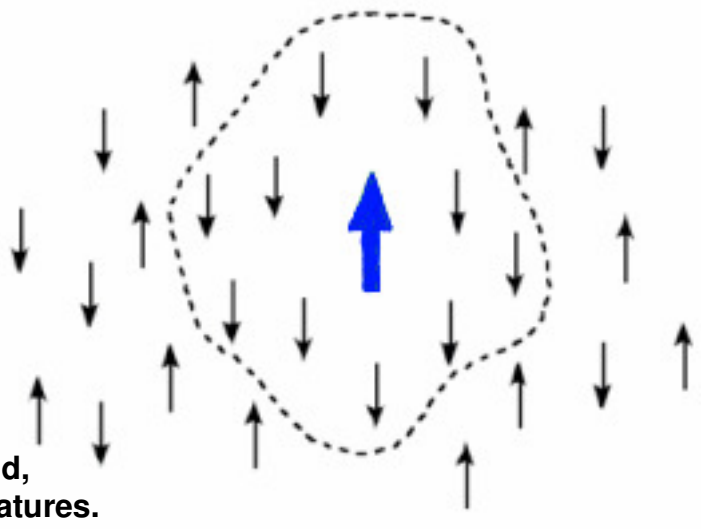


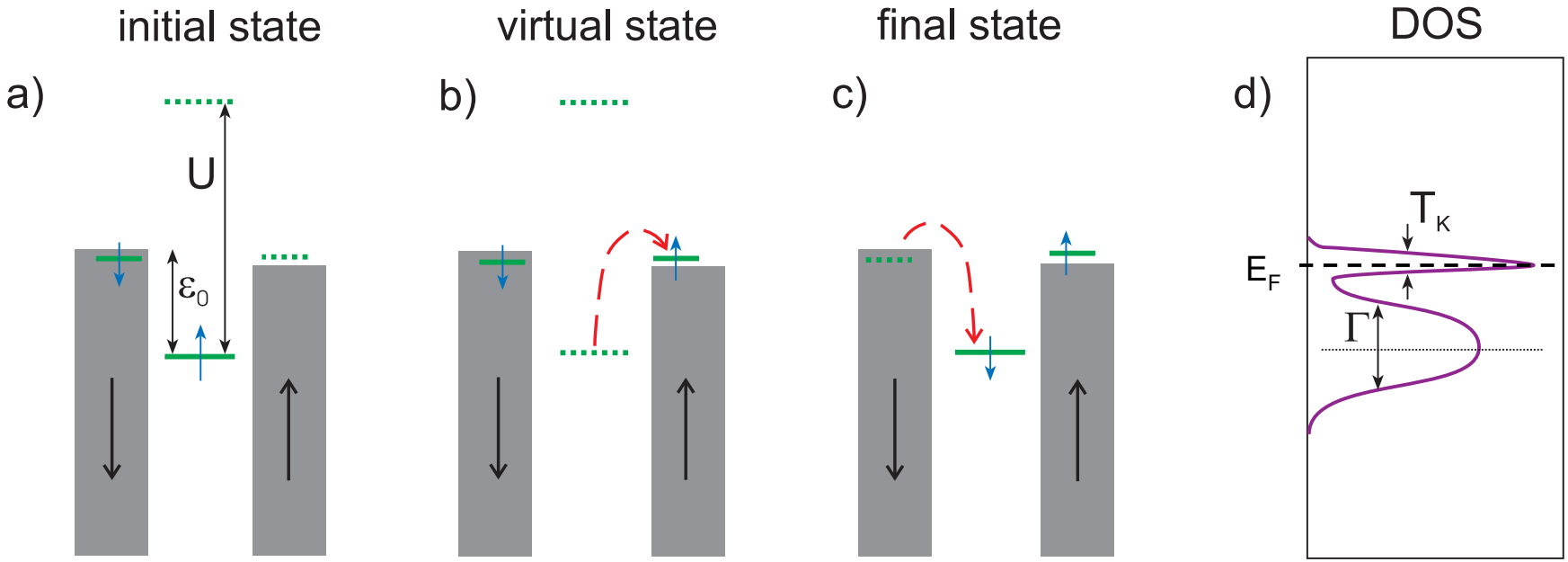


II. Kondo effect, introduction



W. J. de Haas, J. de Boer, and G. J. van den Berg. The electrical resistance of gold, copper and lead at low temperatures. *Physica*, 1:1115, 1933



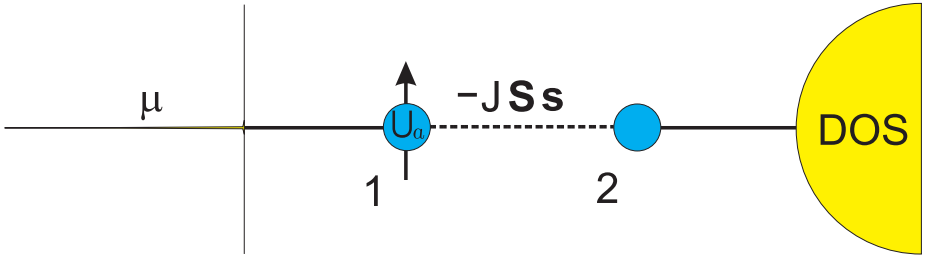


Adapted from L. Kouwenhoven and L. Glazman, *Revival of the Kondo effect*, Physics World (2001)

Abrikosov's representation

$$H_{sd} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

$$- \sum_{\mathbf{k}\mathbf{k}'} J_{kk'} \left[S^{+} c^{\dagger}_{\mathbf{k}\downarrow} c_{\mathbf{k}'\uparrow} + S^{-} c^{\dagger}_{\mathbf{k}\uparrow} c_{\mathbf{k}'\downarrow} + S_z \left(c^{\dagger}_{\mathbf{k}\uparrow} c_{\mathbf{k}'\uparrow} - c^{\dagger}_{\mathbf{k}\downarrow} c_{\mathbf{k}'\downarrow} \right) \right]$$



$$S^{+} = a^{\dagger}_{\uparrow} a_{\downarrow}, \quad S^{-} = a^{\dagger}_{\downarrow} a_{\uparrow}, \quad S_z = \frac{1}{2}(a^{\dagger}_{\uparrow} a_{\uparrow} - a^{\dagger}_{\downarrow} a_{\downarrow}), \quad n^{a}_{\sigma} = a^{\dagger}_{\sigma} a_{\sigma}, \quad n^{c}_{\sigma} = c^{\dagger}_{\sigma} c_{\sigma}$$

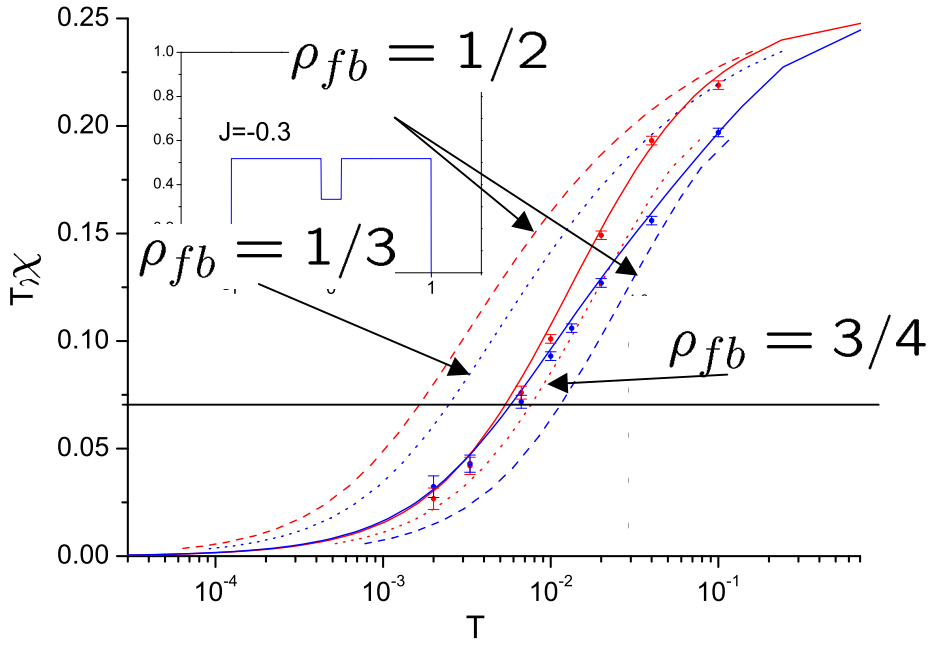
$$H_{int} = -2J(S^z s^z + 1/2(S^{+} s^{-} + S^{-} s^{+}))$$

$$= -J/2 \left[(n^{a}_{\uparrow} n^{c}_{\uparrow} + n^{a}_{\downarrow} n^{c}_{\downarrow}) + (n^{a}_{\uparrow} n^{c}_{\downarrow} + n^{a}_{\downarrow} n^{c}_{\uparrow}) \right.$$

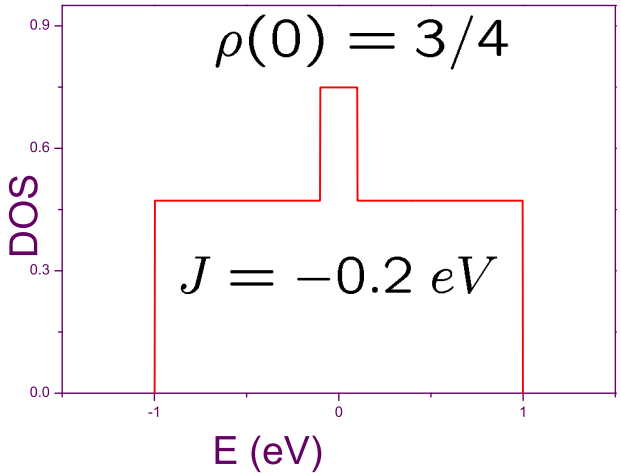
$$\left. + 2(a^{\dagger}_{\uparrow} c_{\uparrow} c^{\dagger}_{\downarrow} a_{\downarrow} + c^{\dagger}_{\uparrow} a_{\uparrow} a^{\dagger}_{\downarrow} c_{\downarrow}) \right]$$

A. A. Abrikosov. Electron scattering on magnetic impurities in metals and anomalous resistivity effects. *Physics* 2, 5 (1965)

Kondo impurity in non-uniformal bath DOS

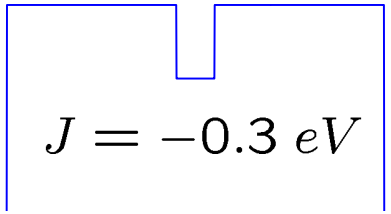


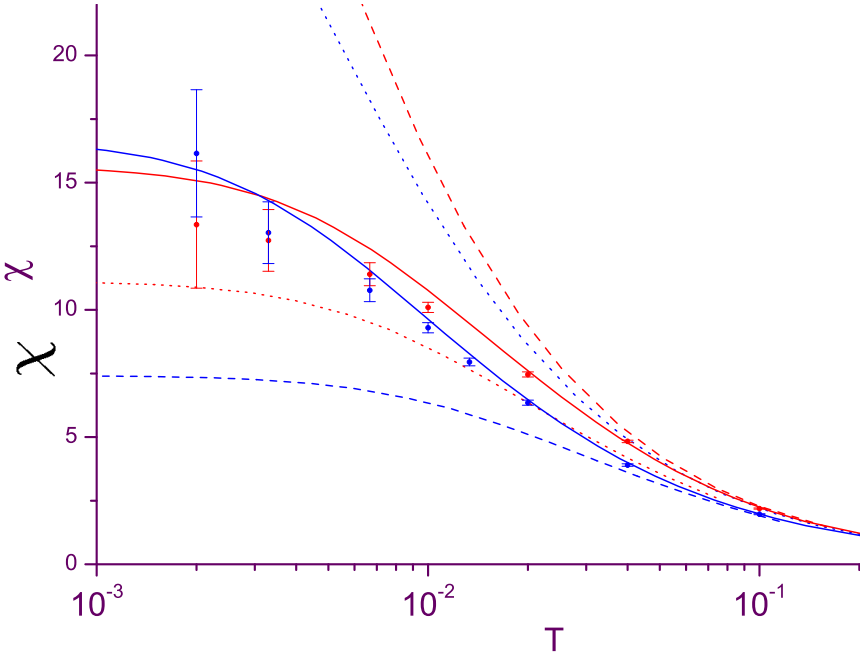
$$T_K \propto De^{-\frac{1}{2J\rho(E_F)}}$$



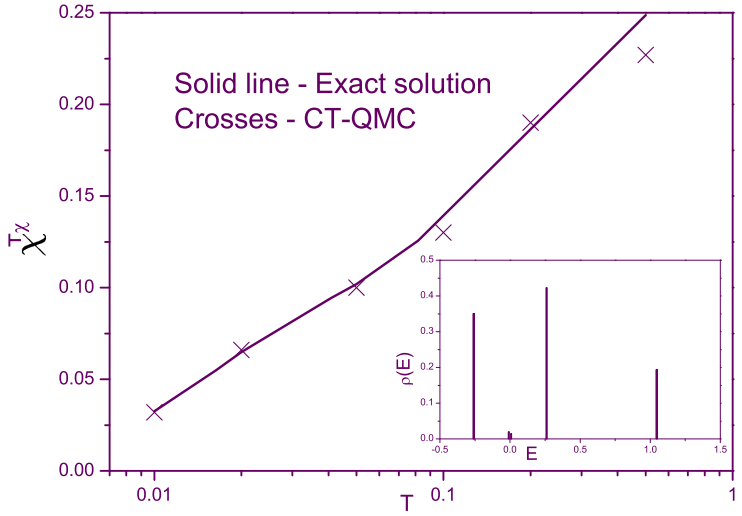
(NRG calculations by A. Zhuravlev)

$$\rho(0) = 1/3$$

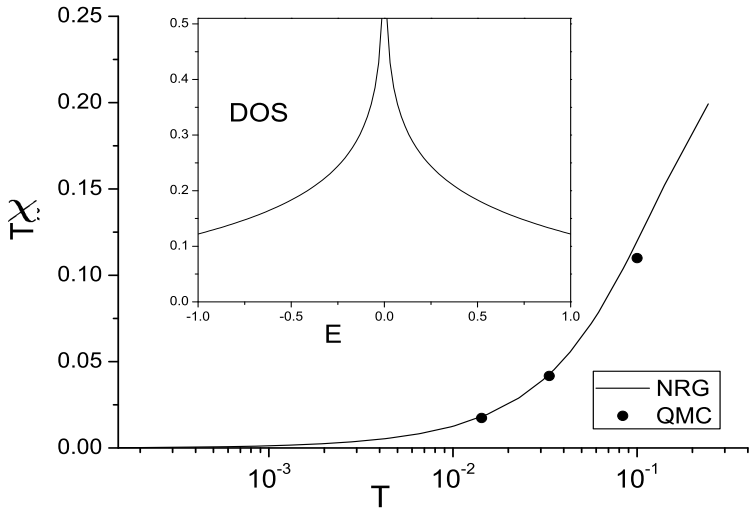


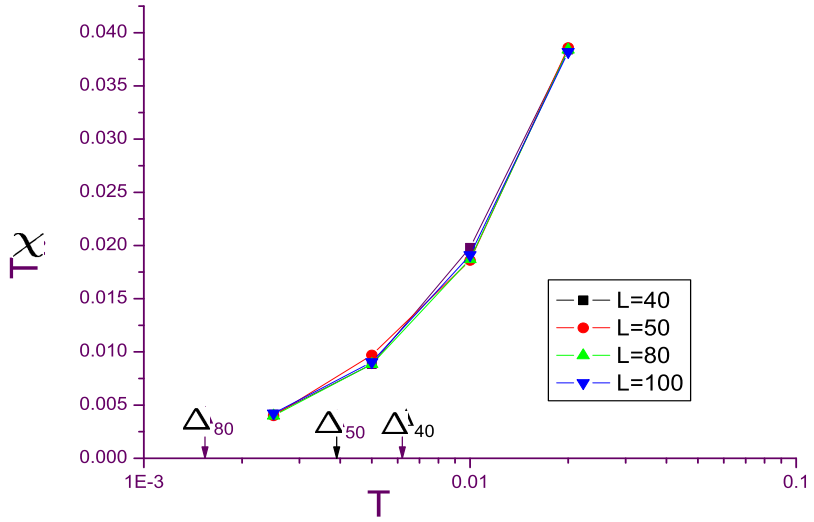


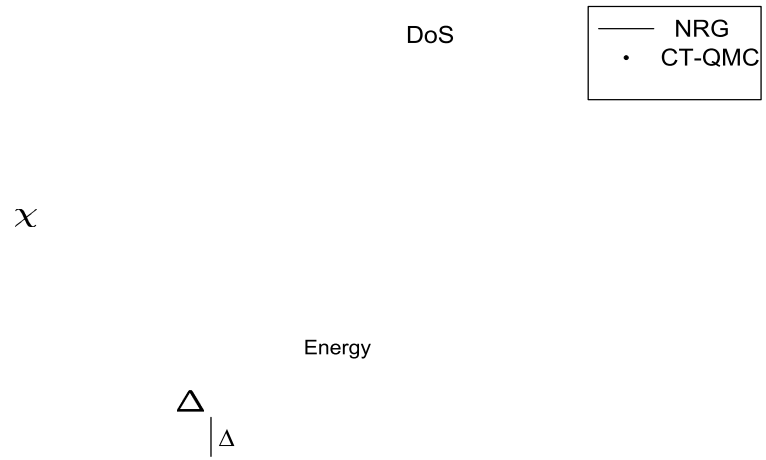
Kondo impurity in realistic bath DOS



$$T_K \propto De^{-\frac{1}{2J\rho(E_F)}}$$

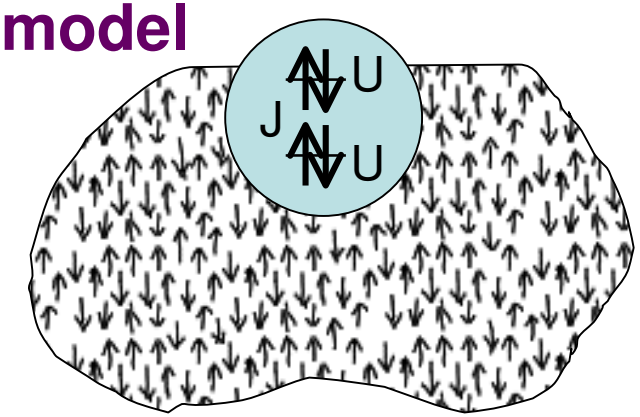






A. Zhuravlev, I. Zharekeshev, E. Gorelov, A. I. Lichtenstein, E. R.Mucciolo, S. Kettemann, "Nonperturbative Scaling Theory of FreeMagneticMoment Phases in DisorderedMetals", Phys. Rev. Lett. 99, 247202 (2007)

III. Multiorbital impurity model



Interaction of general form:

$$H_{loc} = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{\substack{ijkl \\ \sigma\sigma'}} U_{ijkl} c^{\dagger}_{i\sigma} c^{\dagger}_{j\sigma'} c_{l\sigma'} c_{k\sigma}$$

Rotationally invariant Hamiltonian:

$$H_{loc} = - \sum_{\langle ij \rangle m\sigma} t_m c^{\dagger}_{im\sigma} c_{jm\sigma} + U \sum_{im} n_{im\uparrow} n_{im\downarrow} + U' \sum_{\substack{i \\ \sigma \neq \sigma' \\ m \neq m'}} n^{\dagger}_{im\sigma} n_{im'\sigma'} +$$

$$+ (U' - J) \sum_{\substack{i\sigma \\ m \neq m'}} n_{im\sigma} n_{im'\sigma} + J \sum_{\substack{i \\ \sigma \neq \sigma' \\ m \neq m'}} \left(c^{\dagger}_{im\sigma} c^{\dagger}_{im'\sigma'} c_{im\sigma'} c_{im'\sigma} + c^{\dagger}_{im\sigma} c^{\dagger}_{im\sigma'} c_{im'\sigma} c_{im'\sigma'} \right)$$

$$U' = U - 2J$$

C. Castellani et al., *PRB*, **18**, 4945 (1978)

5-band model: general U vertex

$$H_{loc} = \sum_{ij\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{ijkl\sigma\sigma'} U_{ijkl} c^+_{i\sigma} c^+_{j\sigma'} c_{l\sigma'} c_{k\sigma}$$

Slater parametrization of U for atom

Multipole expansion:

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

Coulomb matrix elements in Y_{lm} basis:

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

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:

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

Constrain LDA: U and J

Average Coulomb parameter:

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

Average exchange parameter:

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

For d-electrons: $J = \frac{1}{14}(F^2 + F^4), \quad \frac{F^2}{F^4} = 0.625$

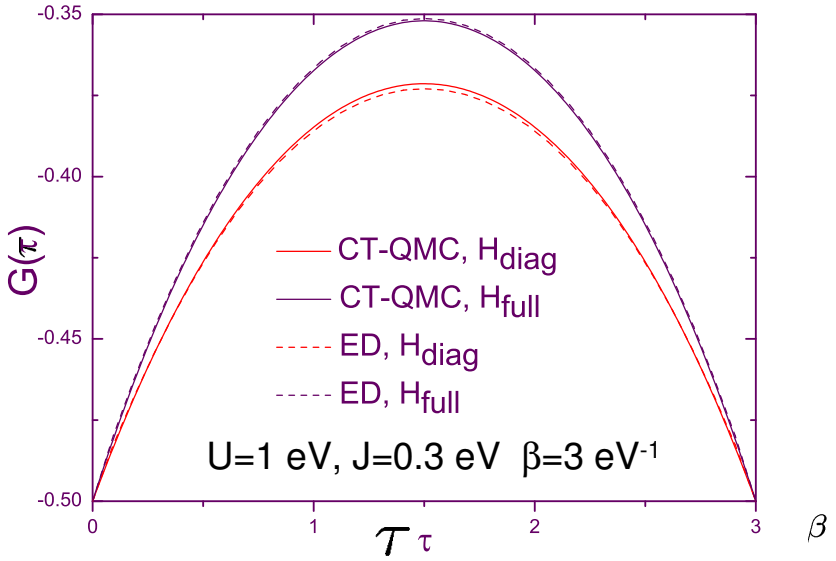
Coulomb and exchange interactions:

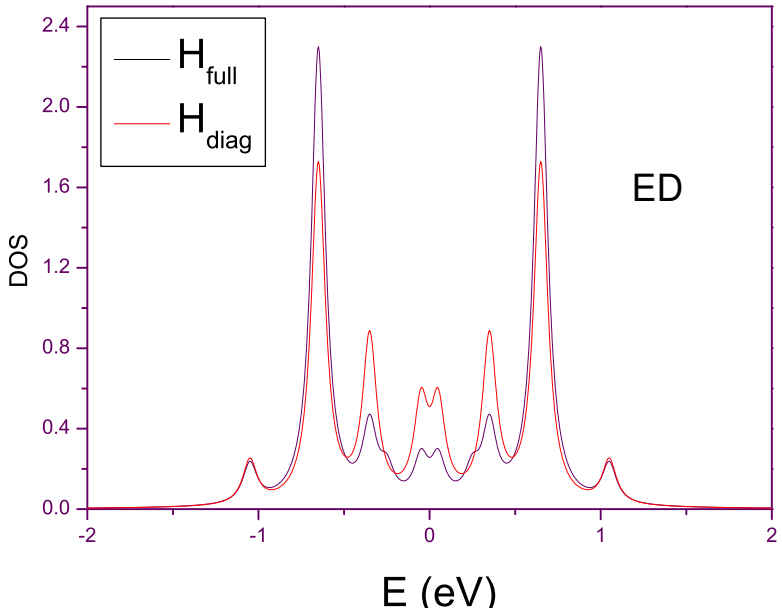
$$U_{mm'} = < mm'|U|mm' >$$
$$J_{mm'} = < mm'|U|m'm >$$

Anisimov et al., *J. Phys.: Condens. Matter* **9**, 767 (1997)

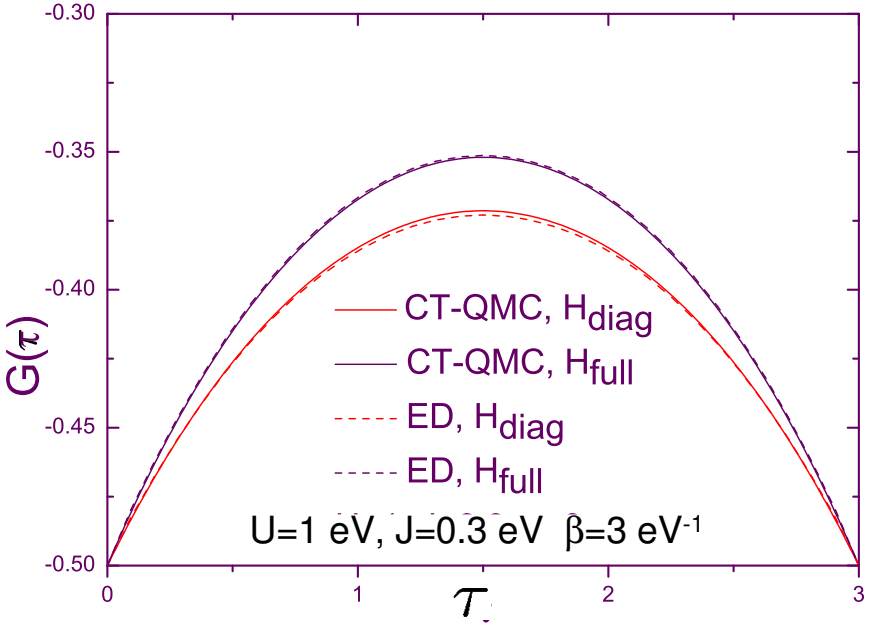
Effects of spin-flip interaction

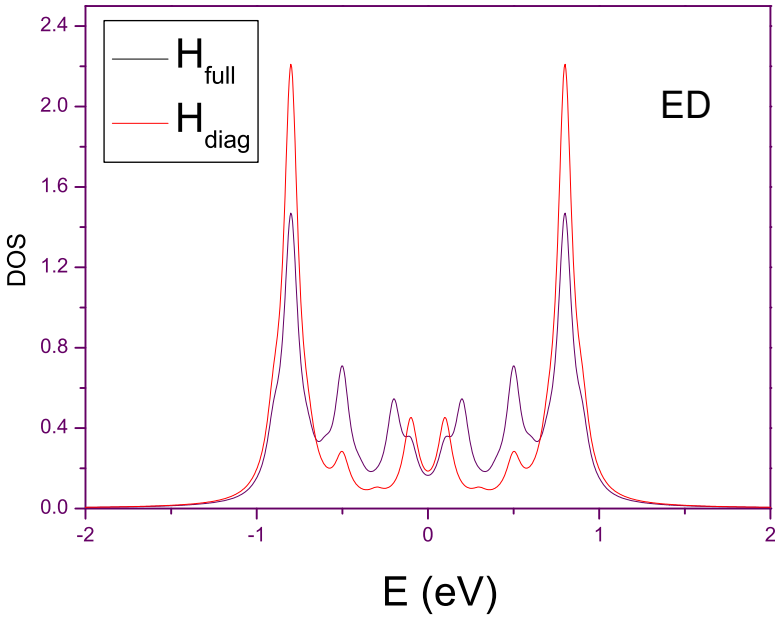
Two-orbital impurity in the atomic limit





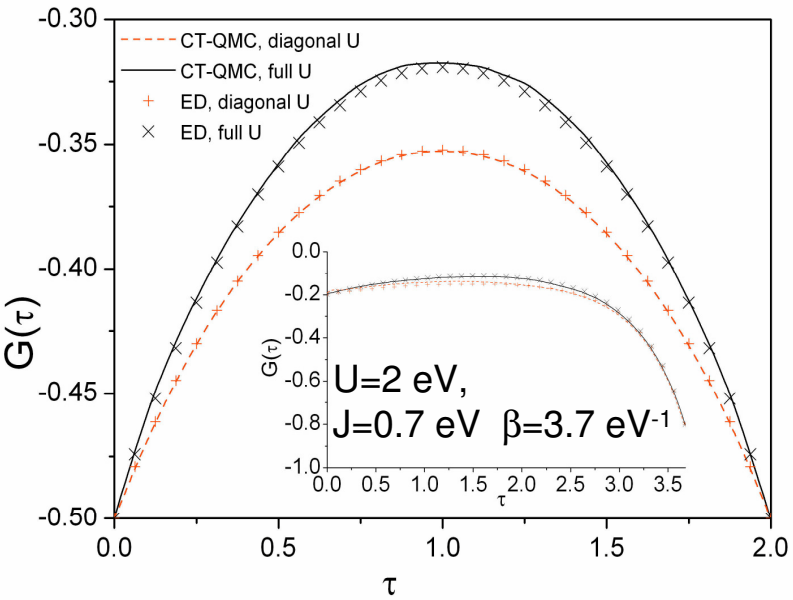
Three-orbital impurity in the atomic limit





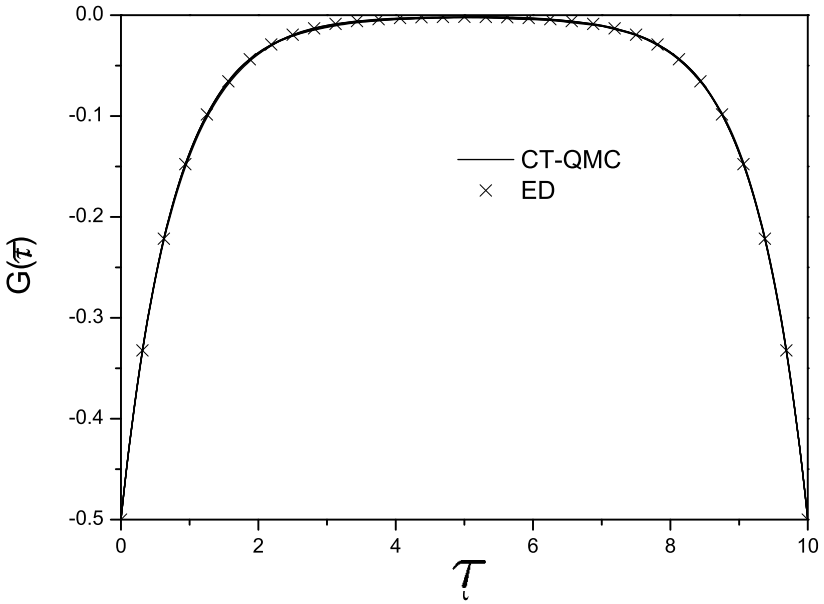
5-orbital impurity model in the atomic limit

High temperature



U=1 eV, J=0.4 eV
β=2 eV^{-1} (T~5800 K)

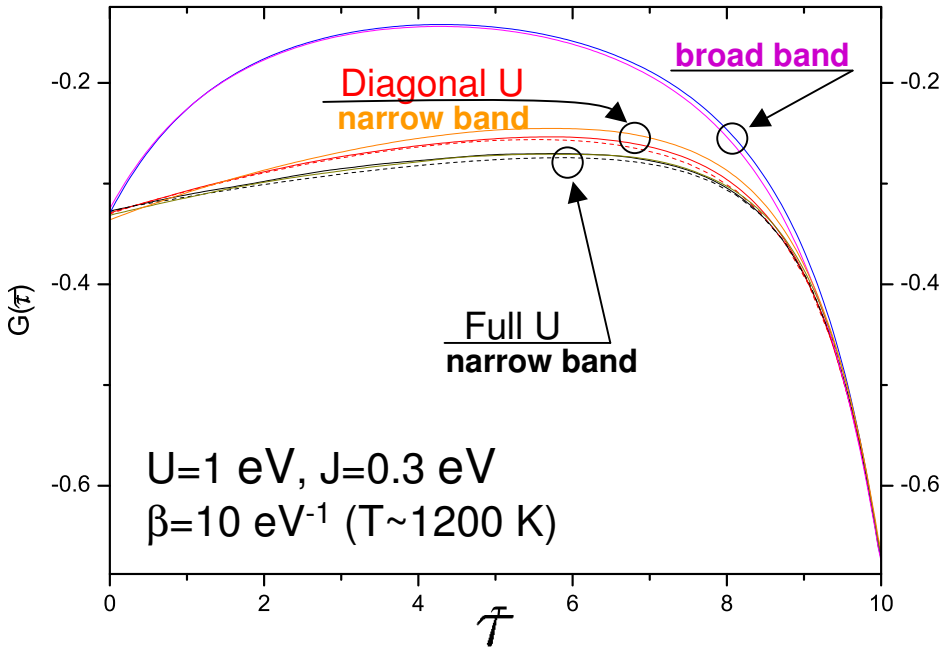
Low temperature, d^5 configuration

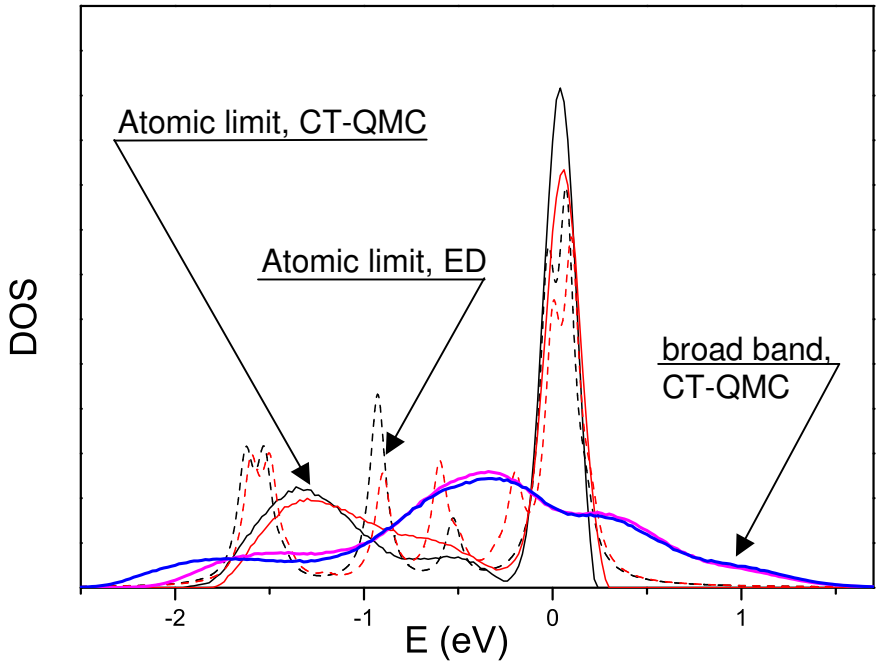


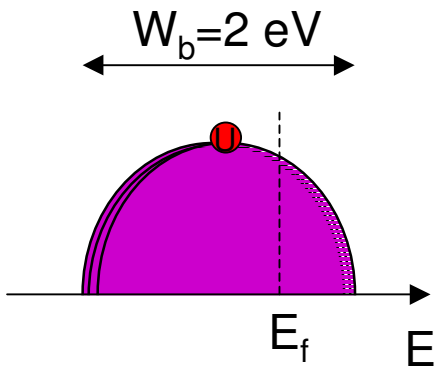
U=1 eV, J=0.4 eV
β=10 eV^{-1} (T~1200 K)

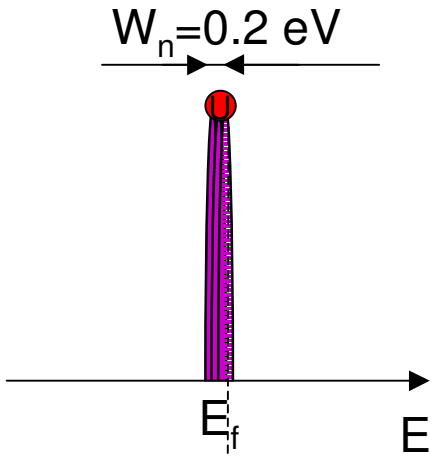
Spin-flip interaction vs. coupling to bath

Three-orbital fully degenerated impurity





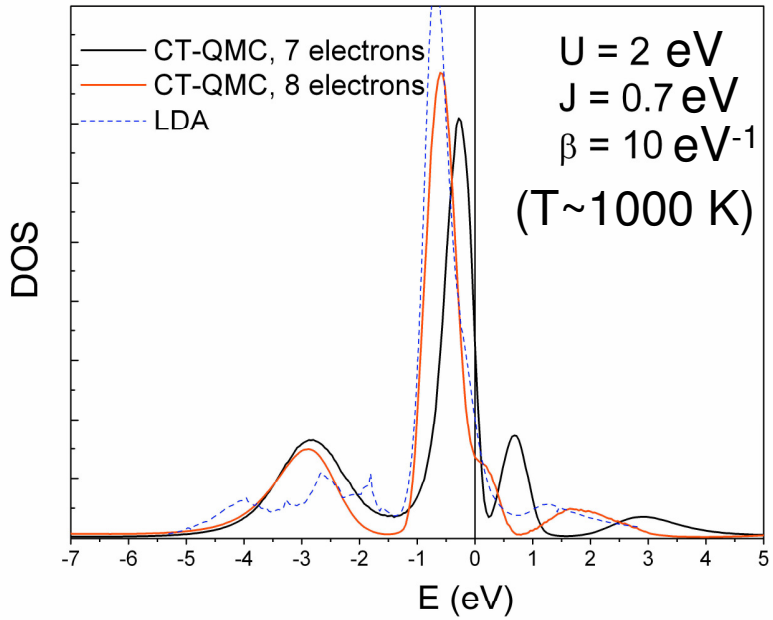




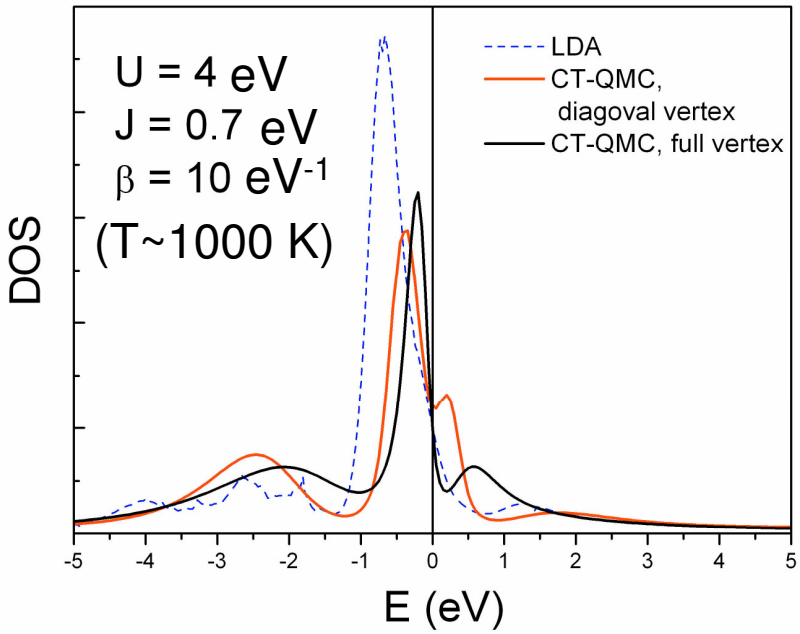
Broad band: W_b= 2 eV
Narrow band: W_n=0.2 eV

5-band realistic model, Co atom in bulk Cu

- Comparison of d^7 and d^8 configuration



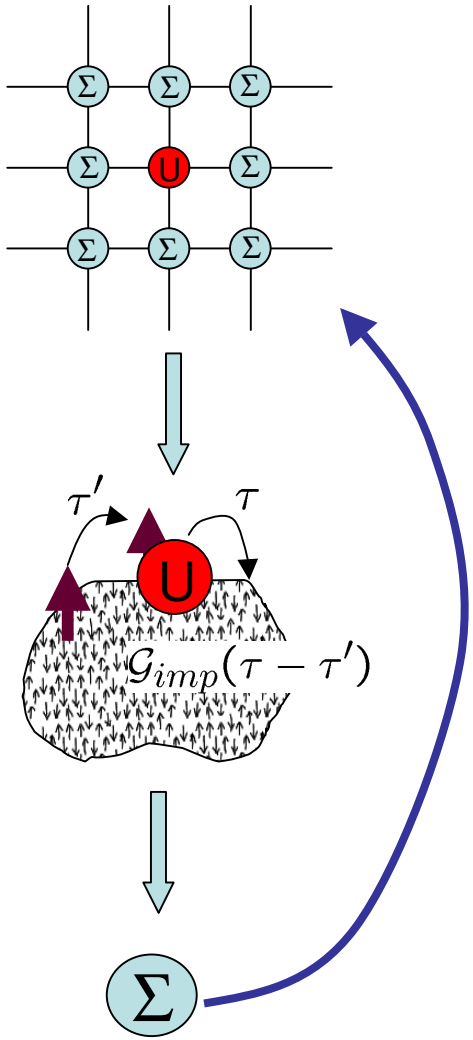
- Comparison of diagonal and full U in d^7 configuration



Quasiparticle weight:

$$Z = \left[1 - \left.\frac{\partial Im\Sigma(i\omega)}{\partial(i\omega)}\right|_{\omega=\omega_1}\right]^{-1} \approx 0.5$$

IV. Lattice model, DMFT approximation



$$G_{loc}(i\omega_n) = \sum_{\mathbf{k}} (G_0^{-1}(\mathbf{k}, i\omega_n) - \Sigma(i\omega_n))^{-1}$$

$$\mathcal{G}_{imp}^{-1}(i\omega_n) = G_{loc}^{-1}(i\omega_n) + \Sigma(i\omega_n).$$

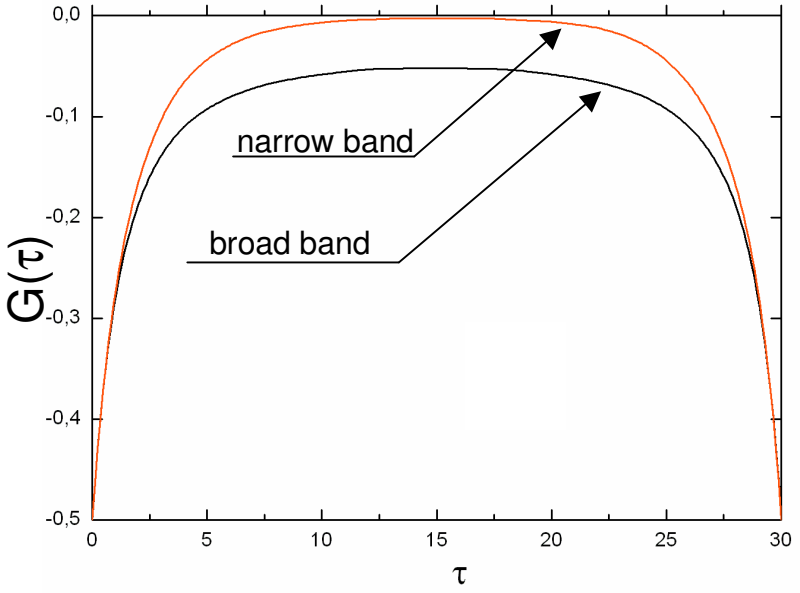
$$G_{imp}(\tau) = -\left\langle T_\tau c(\tau) c^\dagger(0) \right\rangle_{S_{imp}}$$

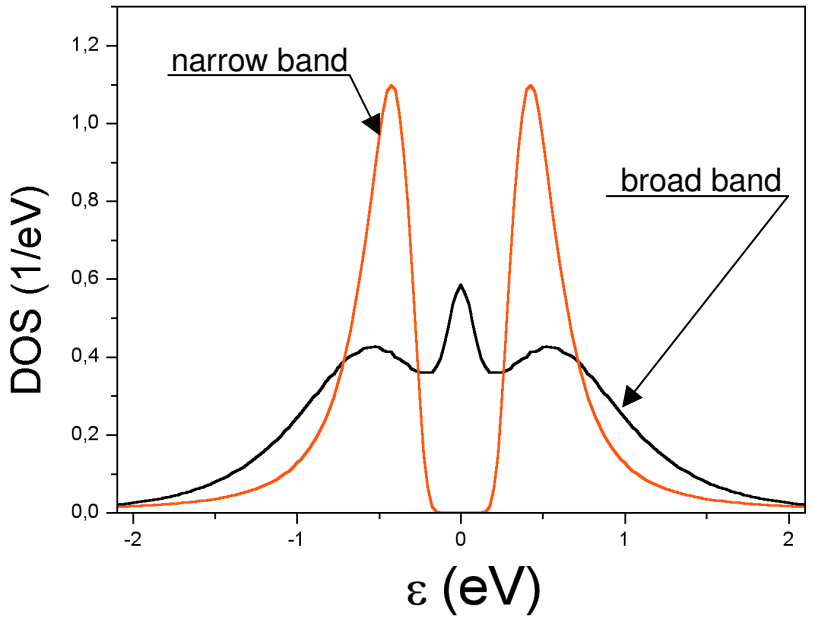
$$\Sigma(i\omega_n) = \mathcal{G}_{imp}^{-1}(i\omega_n) - G_{imp}^{-1}(i\omega_n)$$

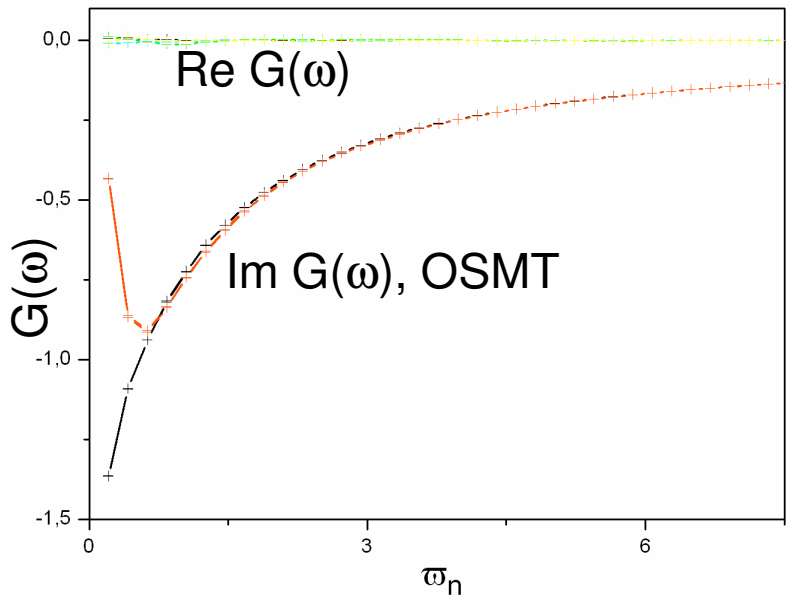
2-band lattice model

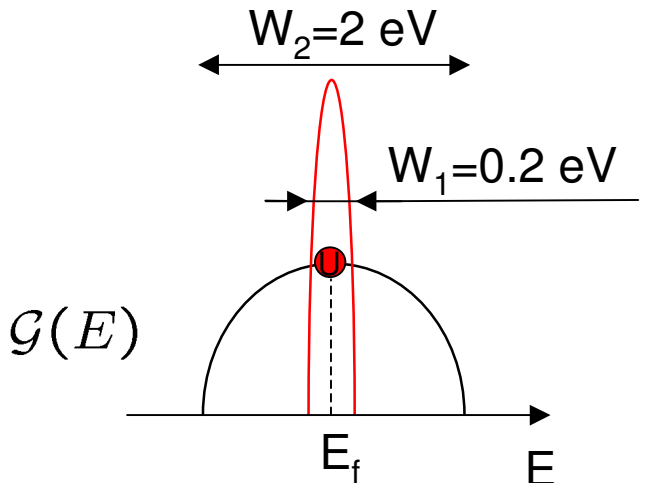
- DMFT, orbital-selective Mott transition (OSMT)

U = 1.2 eV, J = 0.2 eV,
β= 30 eV^{-1} (T~400 K),
W_1 = 2 eV, W_2 = 0.2 eV



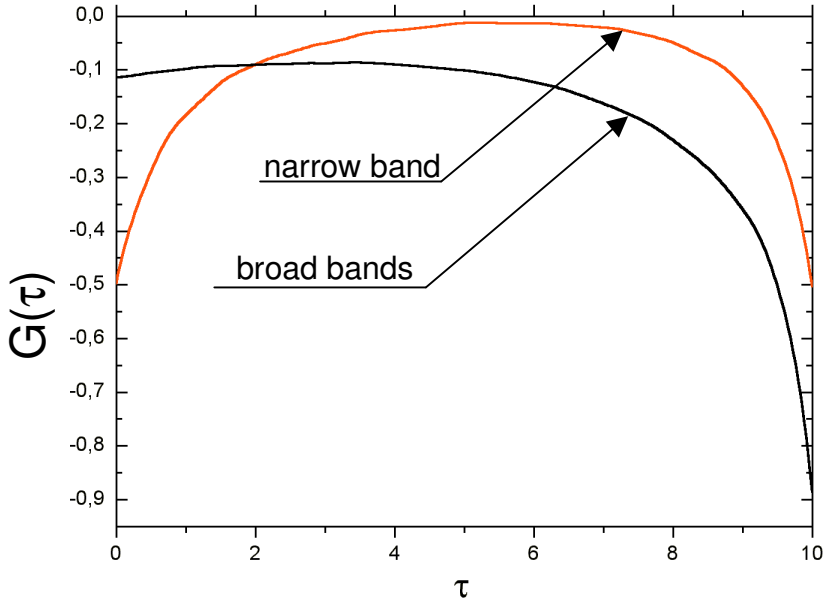






3-band lattice model, non-integer occupancy

- DMFT: orbital-selective Mott transition

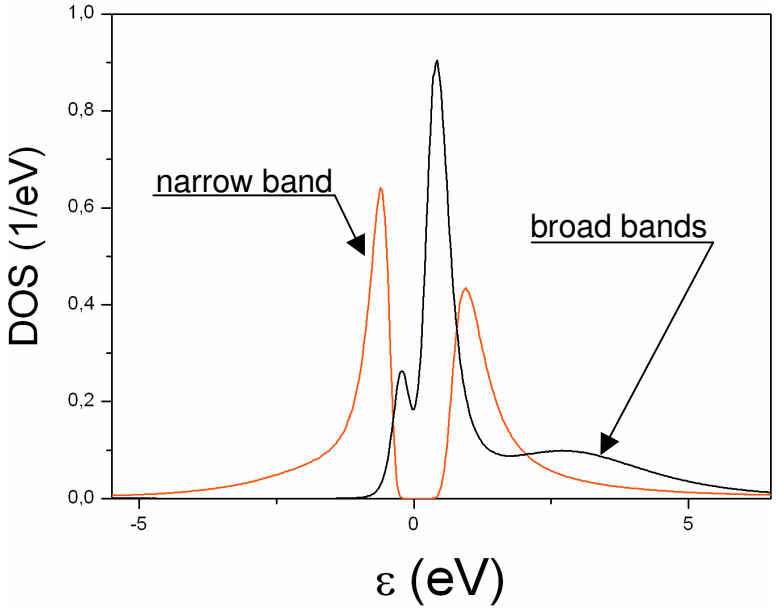


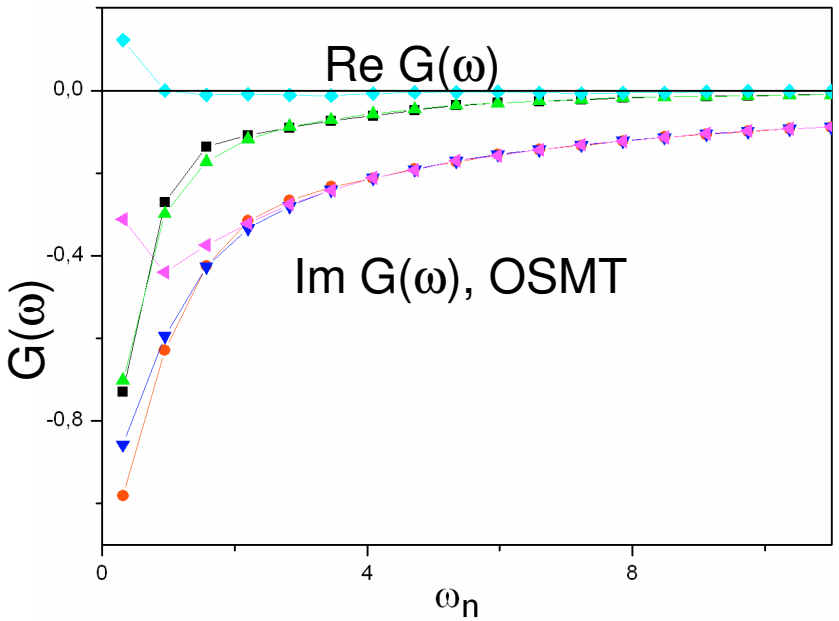
n=1.4 electrons

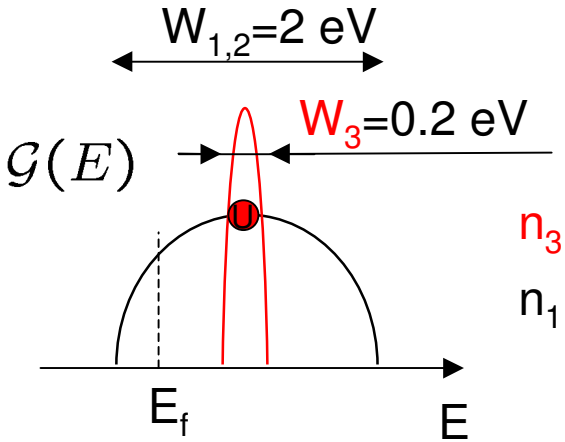
U = 2.7 eV, J = 0.7 eV,

β= 10 eV^{-1} (T~1200 K),

$W_1 = W_2 = 2$ eV, $W_3 = 0.2$ eV





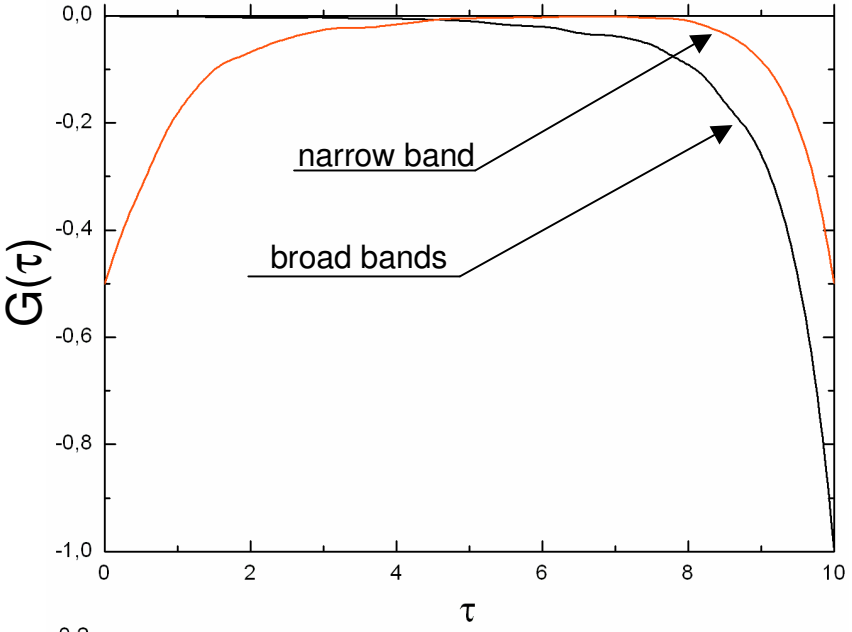


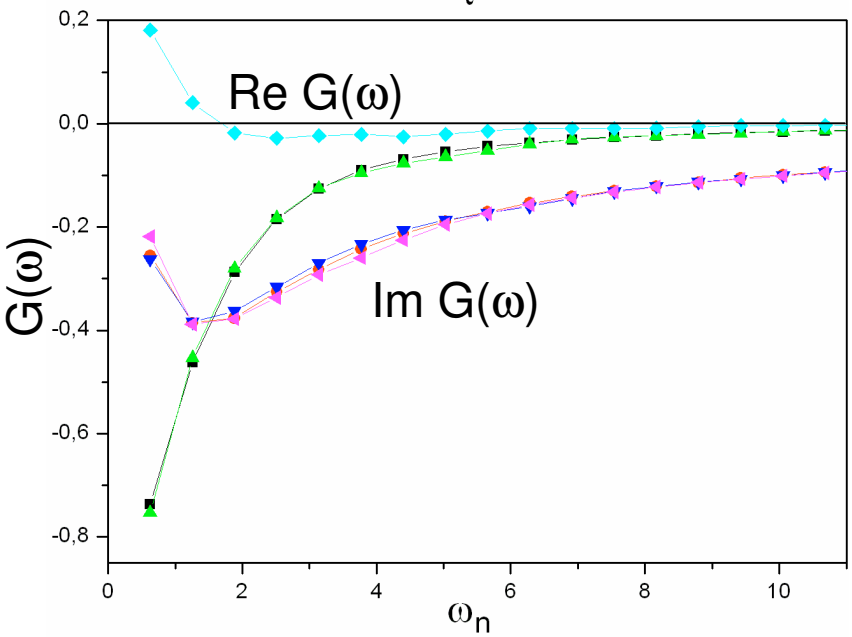
n_3 =1 electron

n_1 =n_2 =0.2 electrons

3-band lattice model, integer occupancy

- DMFT: Mott insulator + band insulator

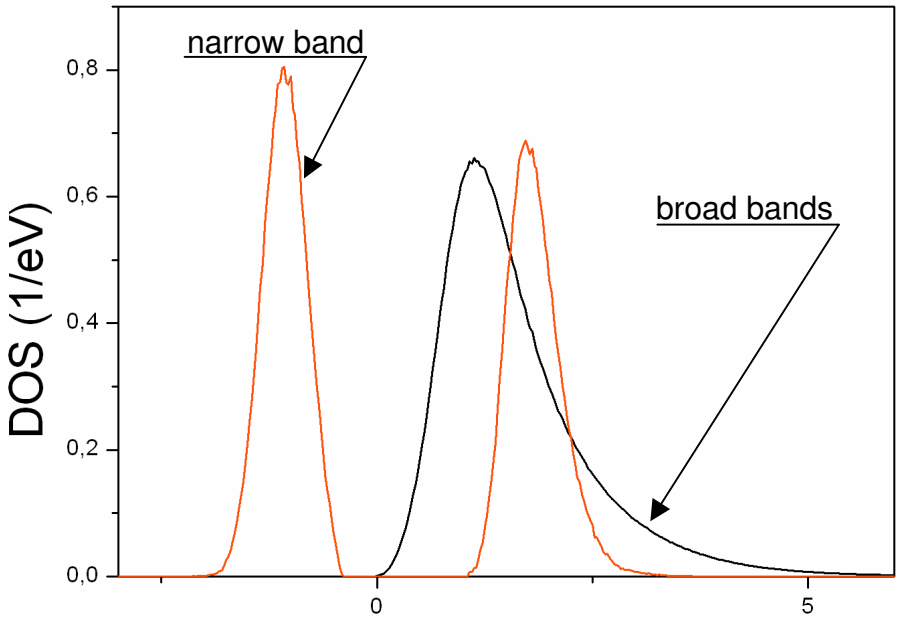


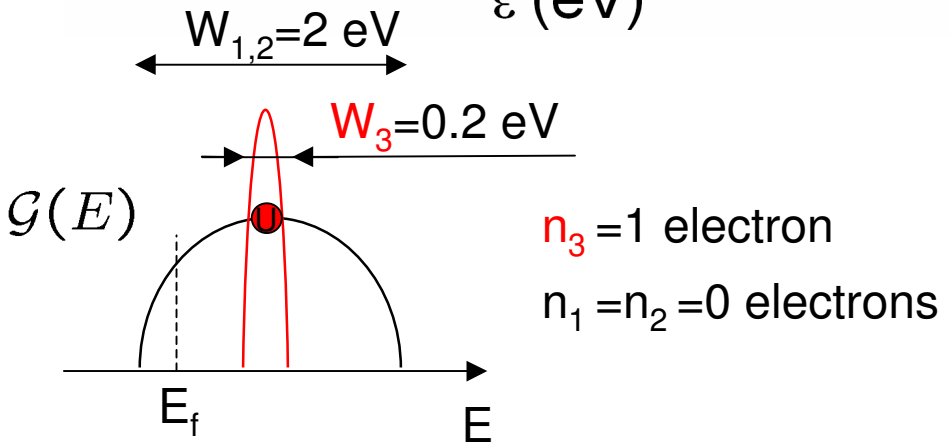


n=1 electron

U = 2.7 eV, J = 0.7 eV, = 10 eV^{-1}

(T~1200 K), $W_1 = W_2 = 2$ eV, $W_3 = 0.2$ eV



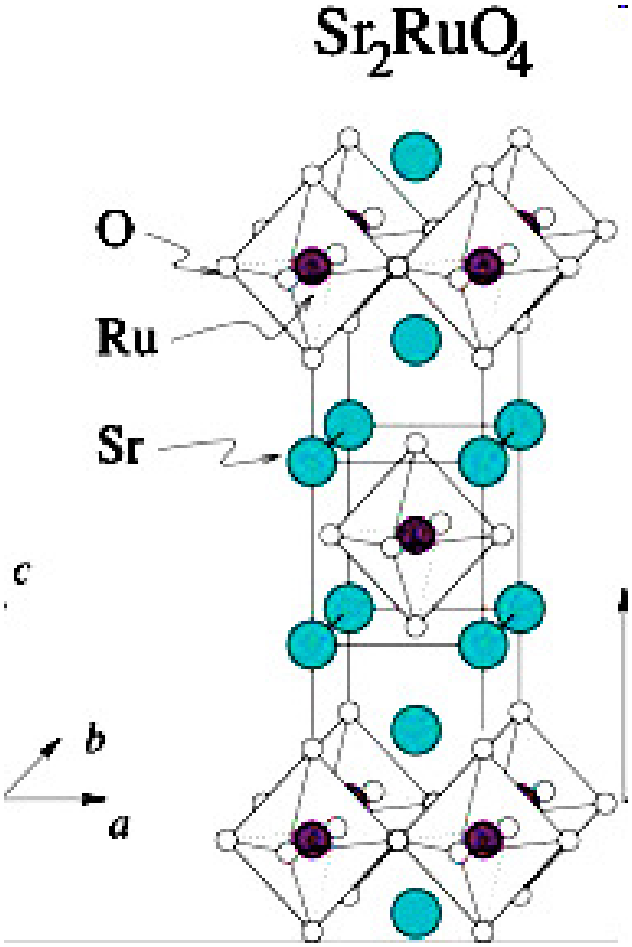


n_3 =1 electron

n_1 =n_2 =0 electrons

Sr_2RuO_4: 3-band lattice model within LDA+DMFT scheme

- 4d t_{2g} Ru orbitals



John Passaneau, Penn State

- LDA + DMFT scheme

$$G_{loc}(i\omega_n) = \int_{-\infty}^{\infty} dE \frac{N^{LDA}(E)}{i\omega_n - \Sigma(i\omega_n) - E}$$

$$\mathcal{G}^{-1}_{imp}(i\omega_n) = G^{-1}_{loc}(i\omega_n) + \Sigma(i\omega_n)$$

Impurity solver

$$G^{-1}_{imp}(i\omega_n)$$

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

V. I. Anisimov et al., J. Phys.: Condens. Matter **9**, 7359 (1997)
A. I. Lichtenstein et al., Phys. Rev. B **57**, 6884 (1998)

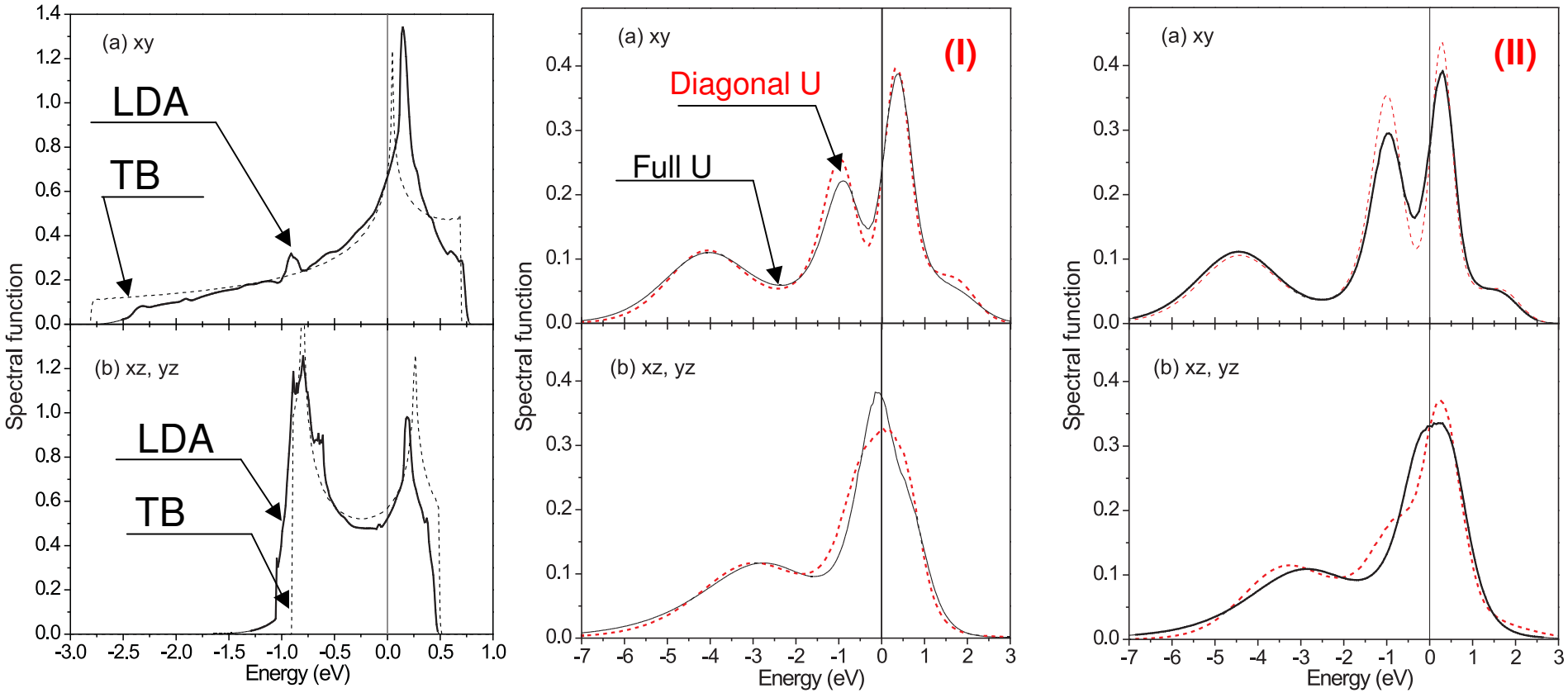
Sr_2RuO_4: 3-band lattice model within LDA+DMFT scheme

- TB and LDA results

CT-QMC DMFT results:

for LDA DOS

for TB DOS



Interaction parameters: U = 3.1 eV, J = 0.7 eV, $\beta = 5\ eV^{-1}$ (T~2300 K)

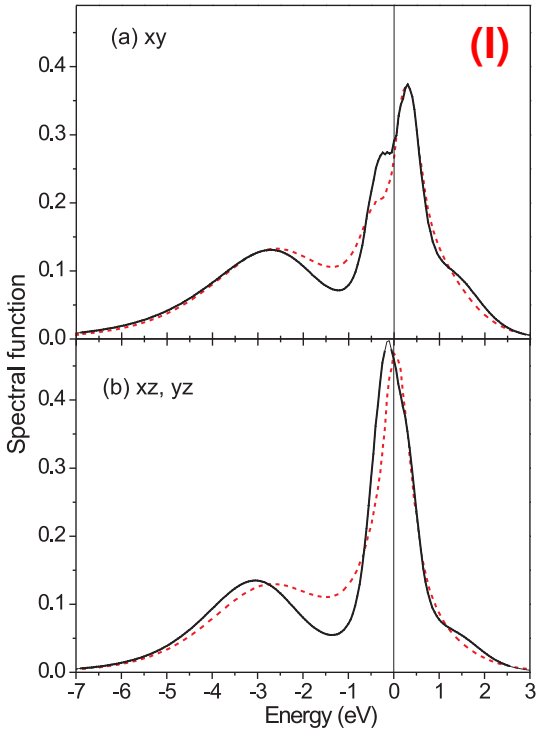
LDA results **(I)** – Z. Pchelkina et al., PRB **75**:035122 (2007)

TB results **(II)** - A. Liebsch et al., PRL **84**(7):1591 (2000)

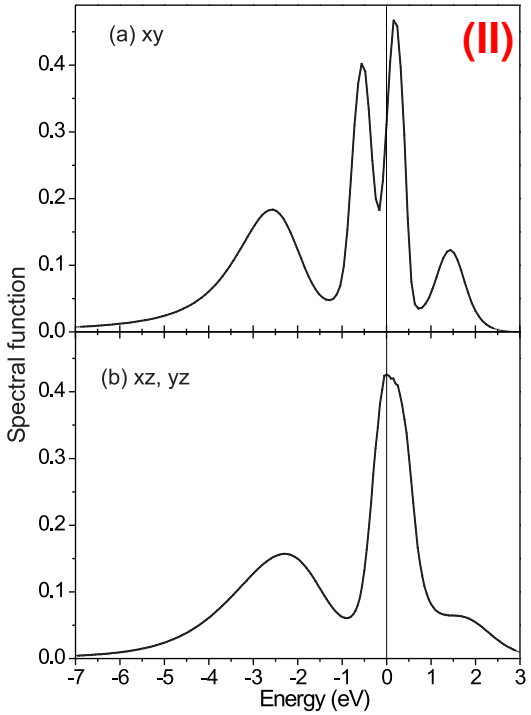
Sr_2RuO_4: 3-band lattice model within LDA+DMFT scheme

CT-QMC DMFT results:

for LDA DOS



for TB DOS



Interaction parameters:

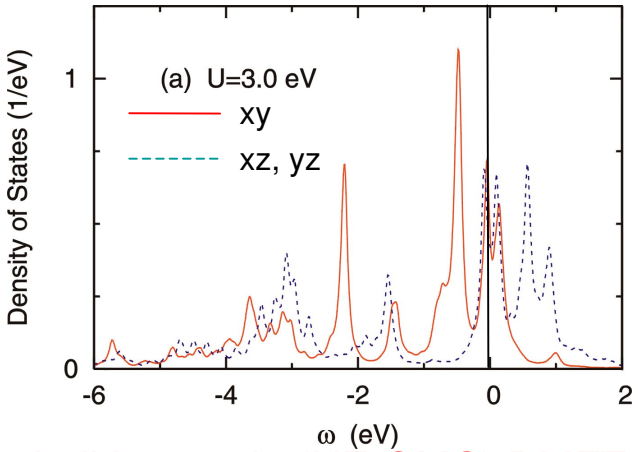
U = 3.1 eV, J = 0.7 eV, β = 10 eV^{-1} (T~1200 K)

Z. Pchelkina et al., PRB **75**:035122 (2007)

A. Liebsch et al., PRL **98,** 216403 (2007)

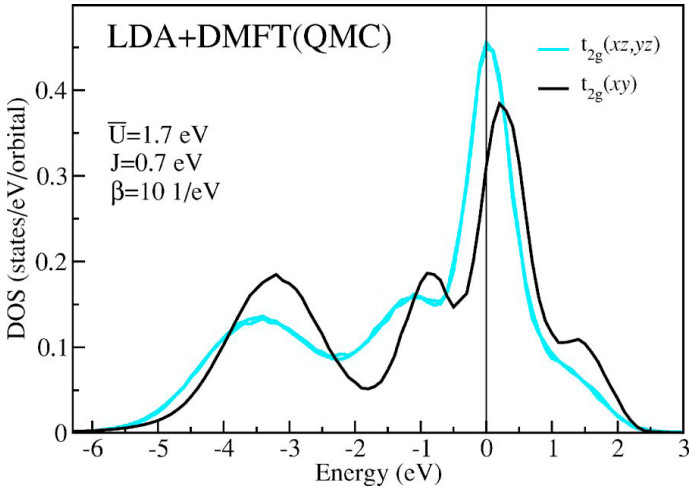
- A. Liebsch and H. Ishida. ED DMFT

  U = 3 eV, J = 0.75 eV, β = 50 eV^{-1}



- Z. Pchelkina et al. (HF-QMC) DMFT:

  U = 3.1 eV, J = 0.7 eV, β = 10 eV^{-1}



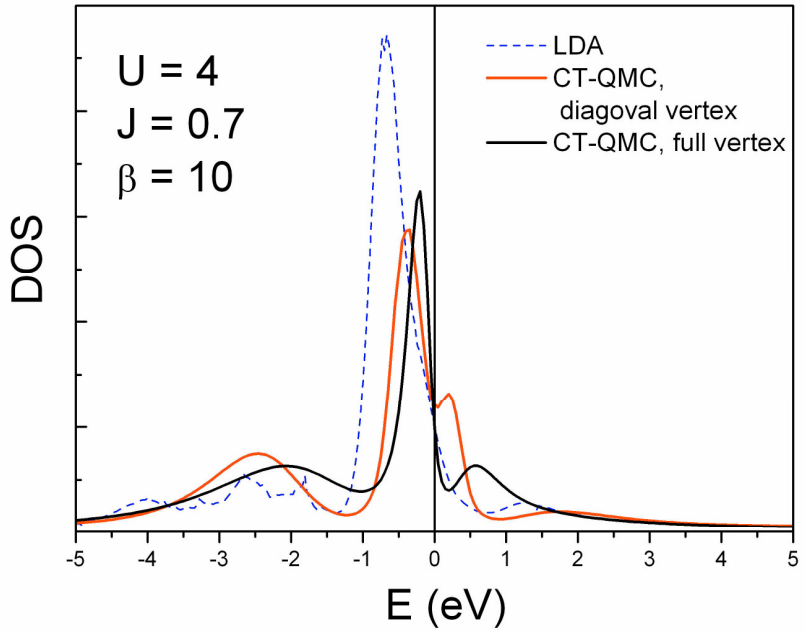
Conclusions

- We developed general and efficient CT-QMC formalism for multi-orbital problems
- A general scheme for investigation a susceptibilities of general impurity model coupled to bath with arbitrary DOS is proposed
- The 3-orbital impurity model with rotationally invariant interaction including spin-flip terms has no sign problem in CT-QMC
- For a first time realistic 5-orbital impurity model for Co in Cu have been investigated
- We show a possibility of LDA+DMFT calculation for rotationally invariant 3-band lattice problem in CT-QMC

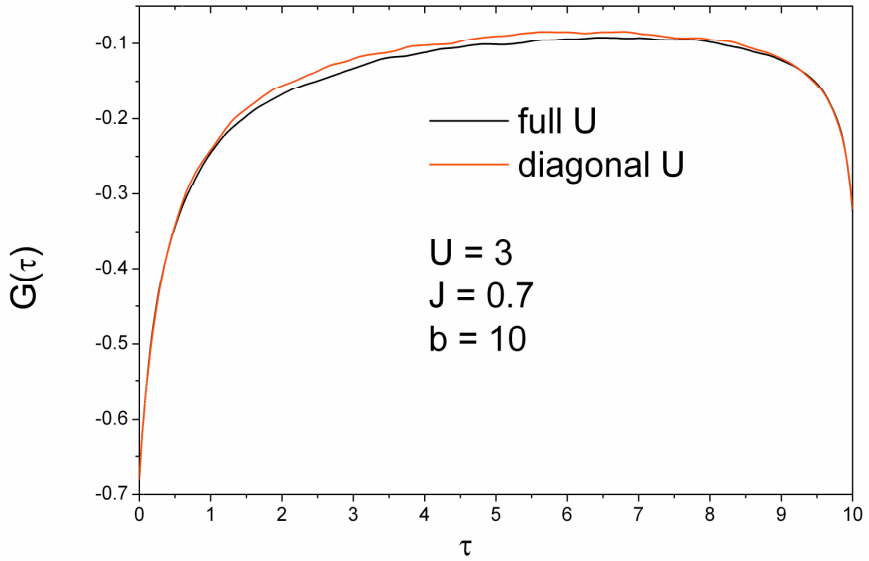
5-band realistic model, Co atom in bulk Cu

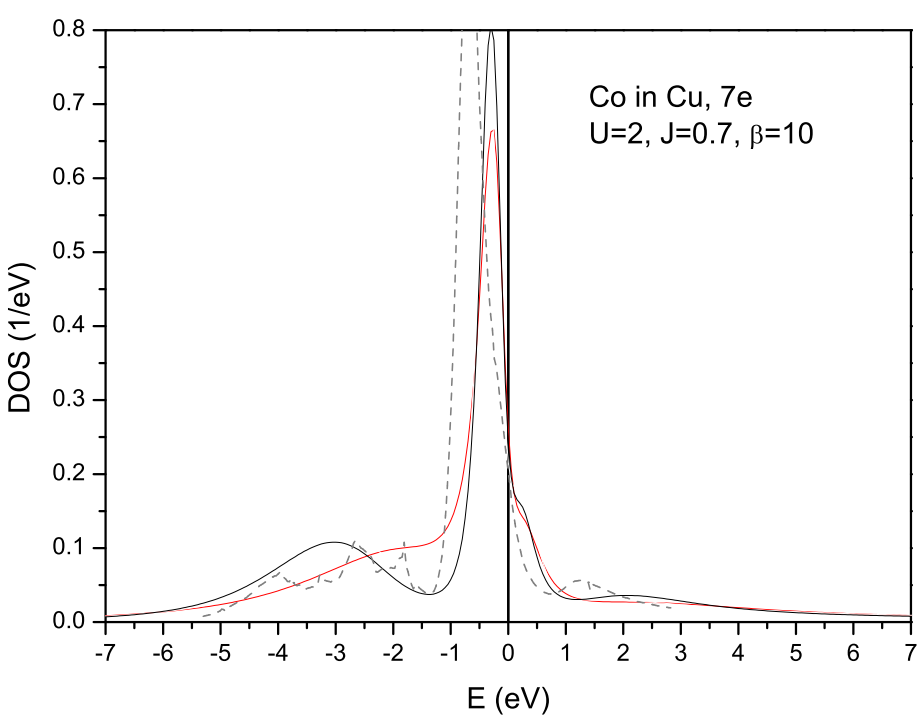
- Comparison of d^7 and d^8 configuration

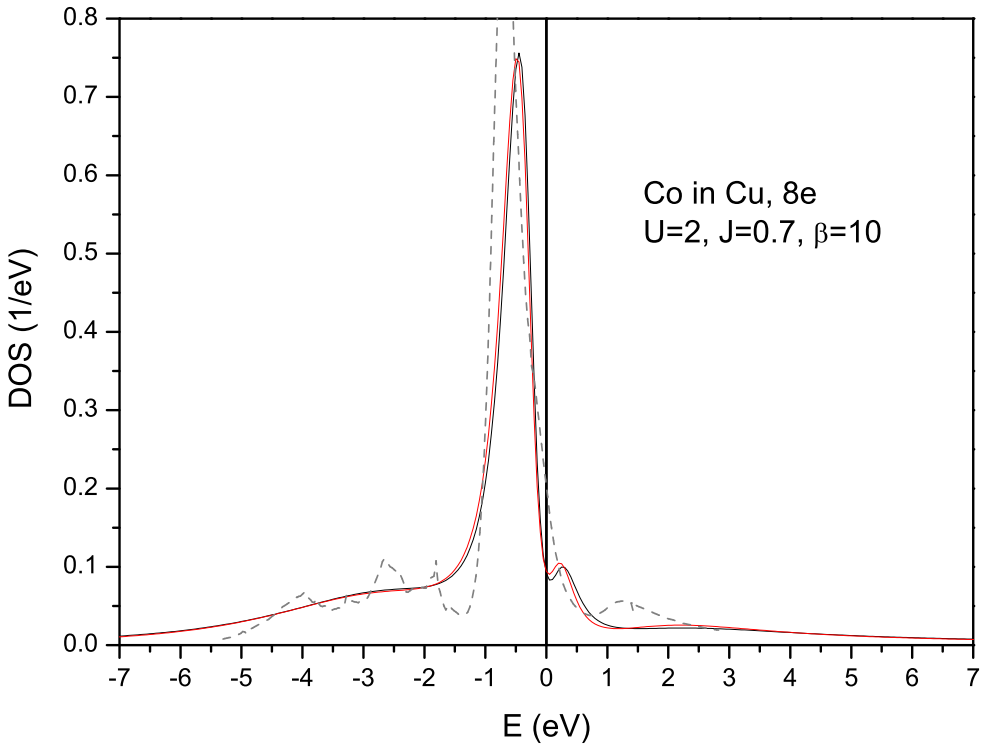
- Comparison of diagonal and full U



- d^7 configuration, U = 3



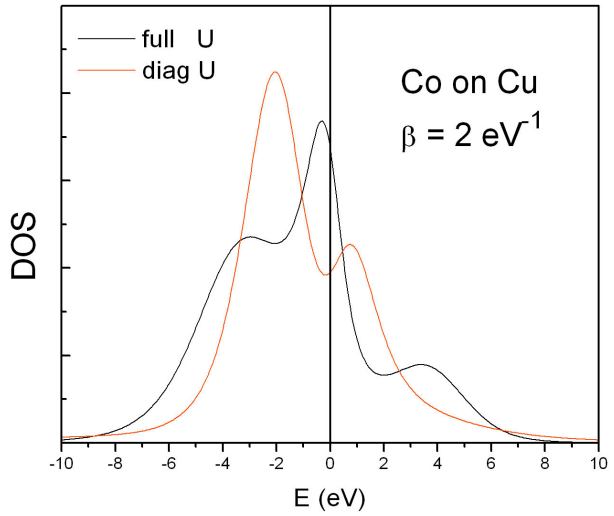

Co in Cu, 7e
U=2, J=0.7, β=10
DOS (1/eV)
E (eV)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
-7
-6
-5
-4
-3
-2
-1
0
1
2
3
4
5
6
7

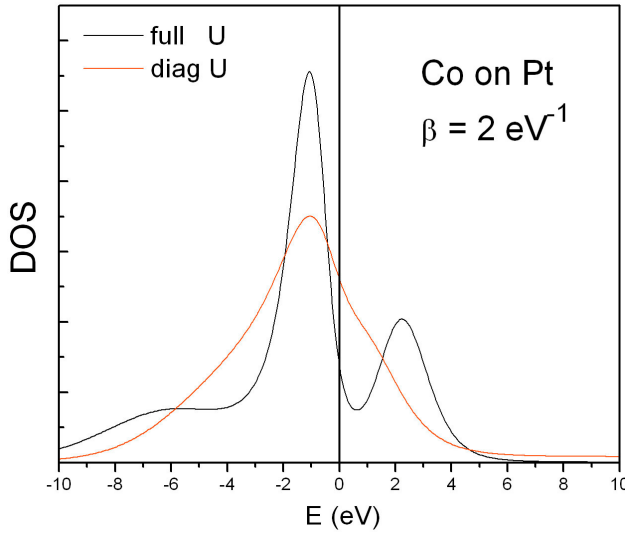

Co in Cu, 8e
U=2, J=0.7, β=10
DOS (1/eV)
E (eV)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
-7
-6
-5
-4
-3
-2
-1
0
1
2
3
4
5
6
7

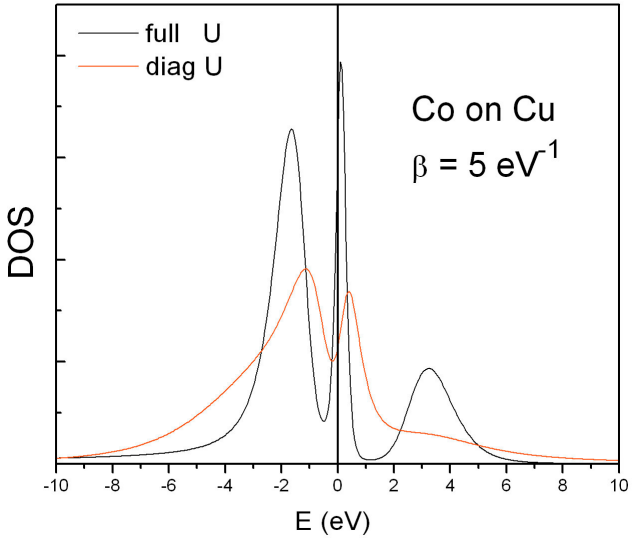
5-band realistic model, Co adatom on Cu (111) or Pt (111) surface. Spin-orbital coupling is taken into account

- CT-QMC results U = 4, J = 0.7

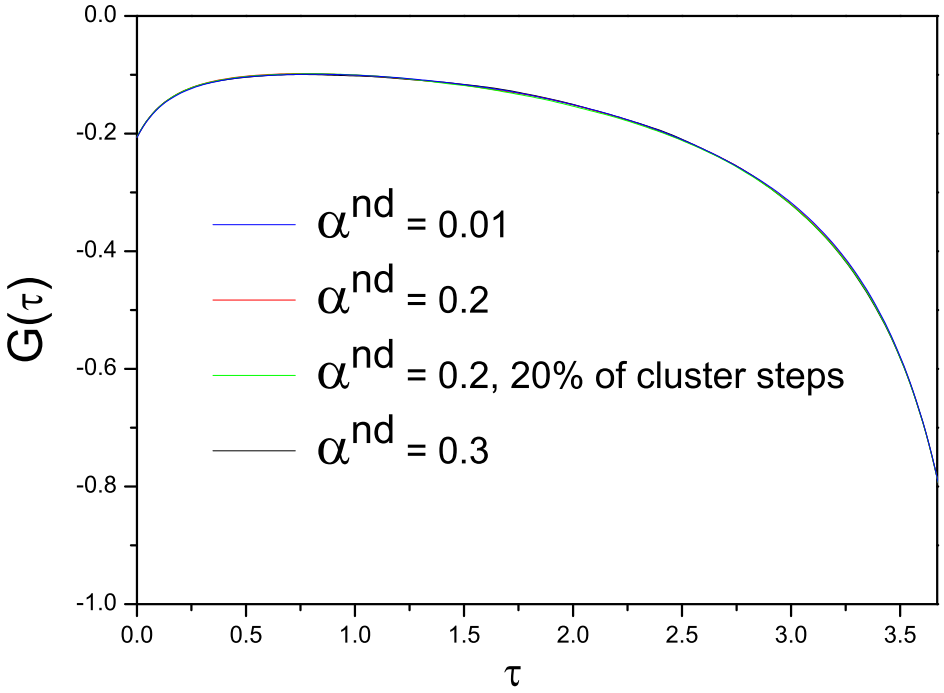
- LDA results (from A. Shick, Prague)

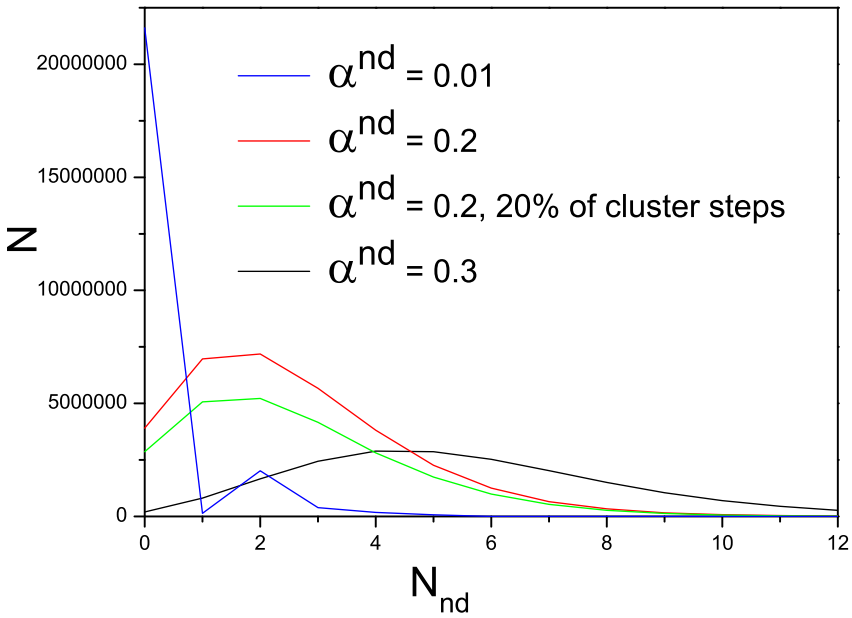


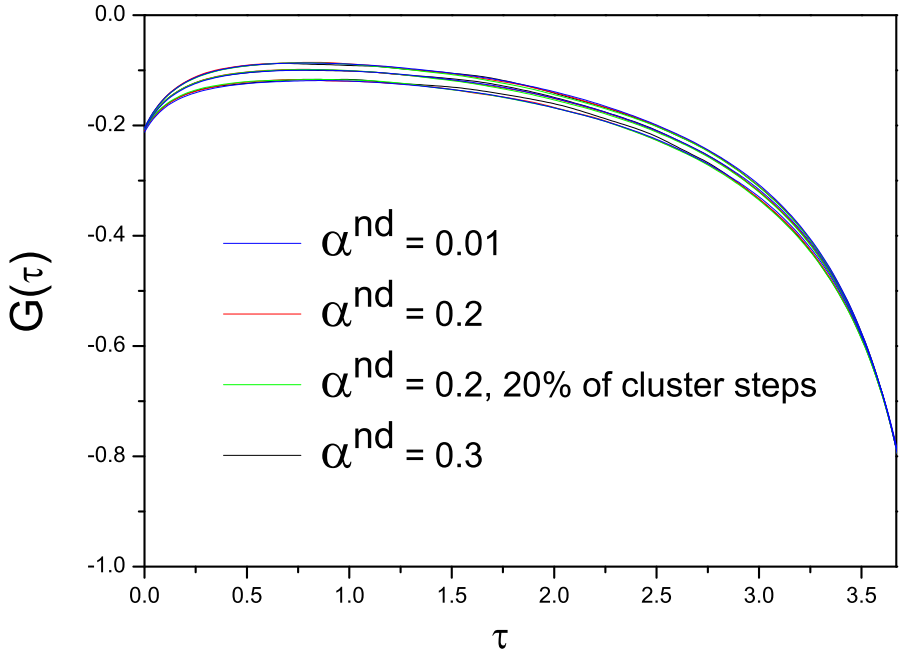


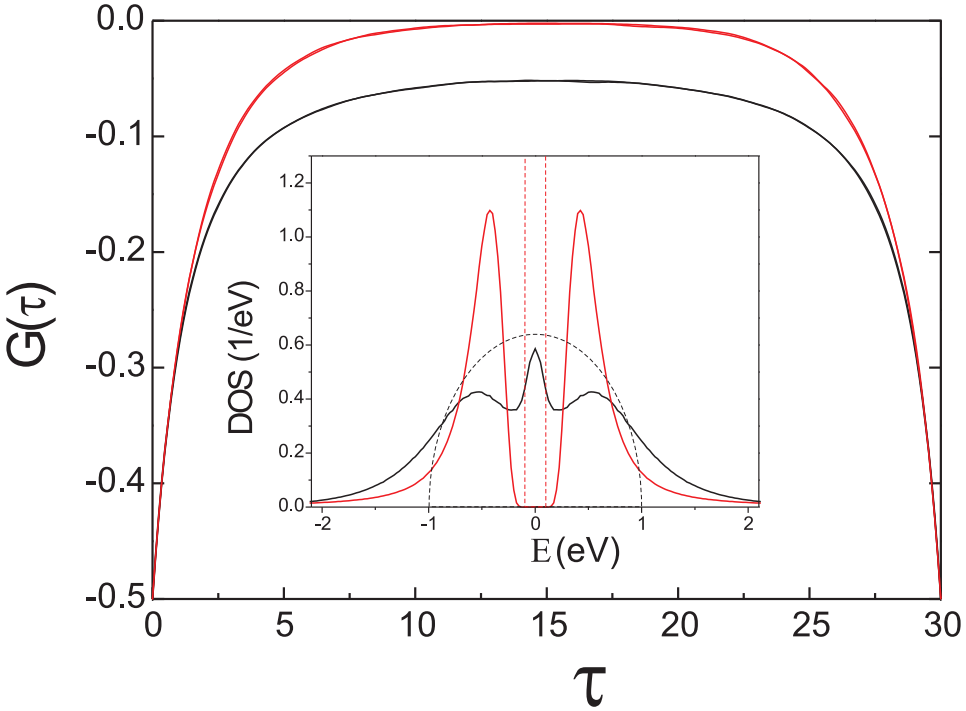


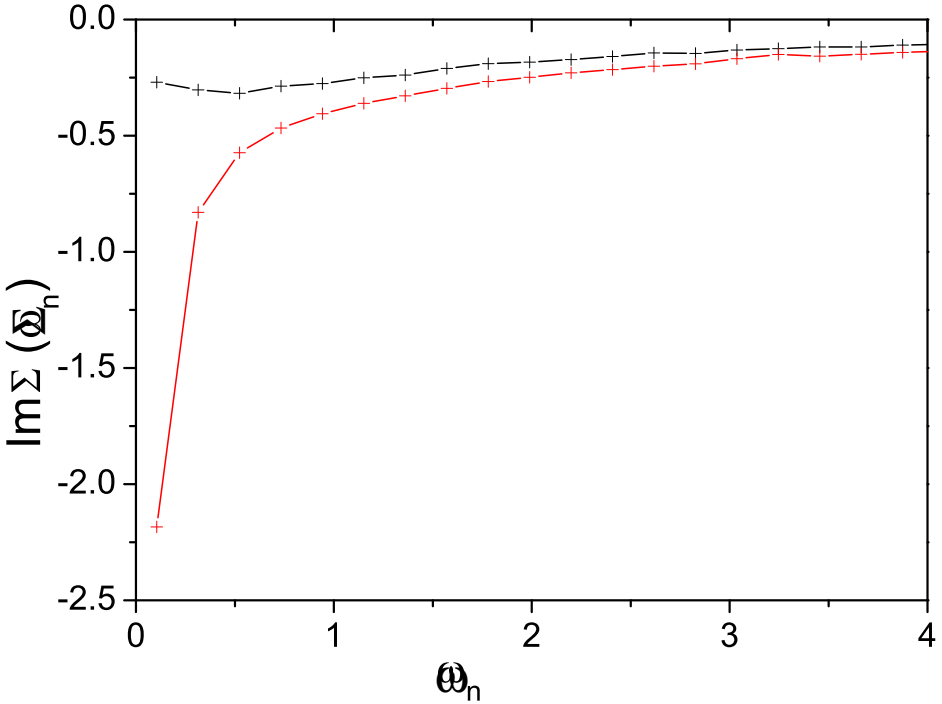
Distribution of U-fields: computational effort

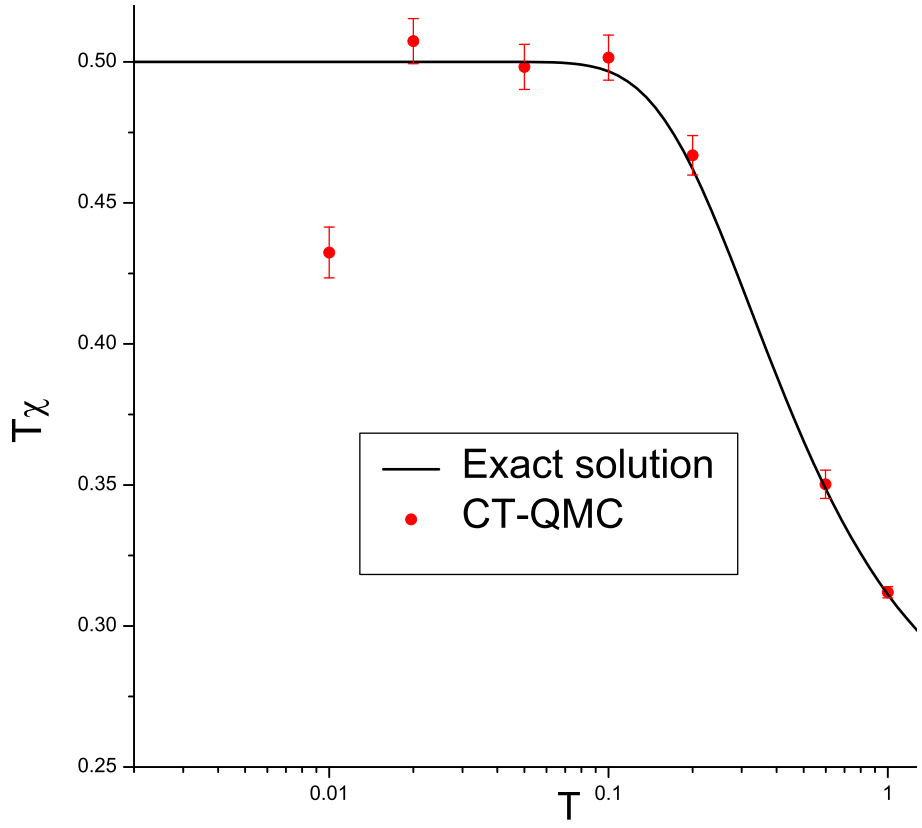

G(τ)
τ
α^nd = 0.01
α^nd = 0.2
α^nd = 0.2, 20% of cluster steps
α^nd = 0.3

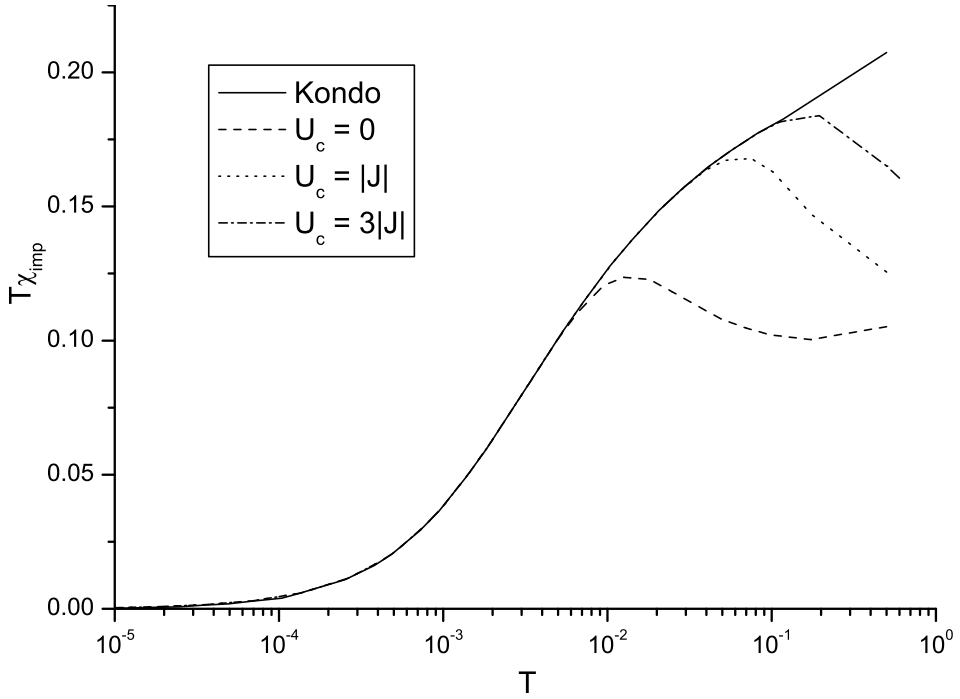

N
N_nd
α^nd = 0.01
α^nd = 0.2
α^nd = 0.2, 20% of cluster steps
α^nd = 0.3

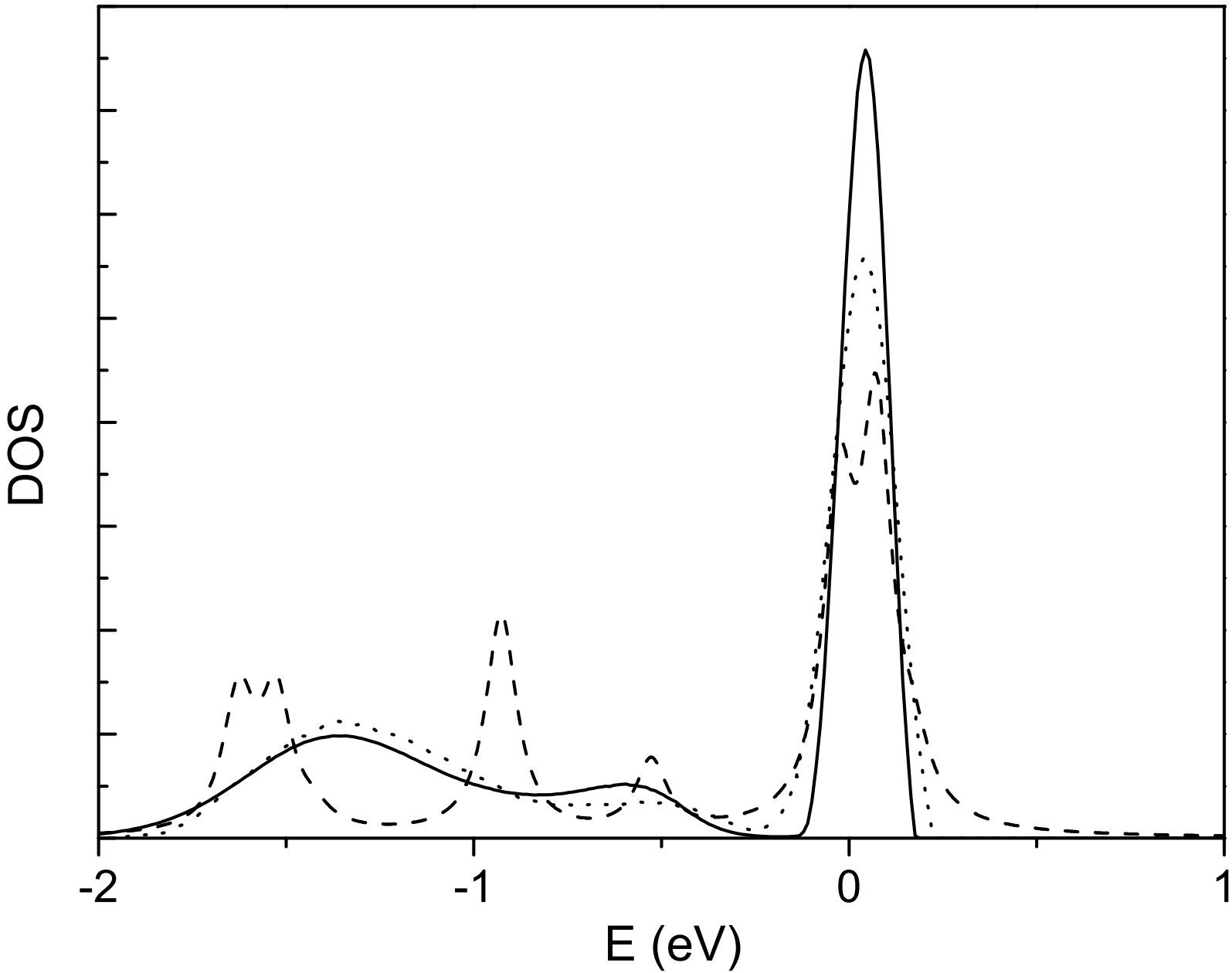

G(τ)
τ
α^nd = 0.01
α^nd = 0.2
α^nd = 0.2, 20% of cluster steps
α^nd = 0.3


G(τ)
τ
DOS (1/eV)
E (eV)


Im Σ (ω_n)
ω_n


0.50
0.45
0.40
0.35
0.30
0.25
Tχ
0.01
0.1
1
T
Exact solution
CT-QMC


0.20
0.15
0.10
0.05
0.00
Tχimp
10-5
10-4
10-3
10-2
10-1
100
T
Kondo
Uc = 0
Uc = |J|
Uc = 3|J|


DOS
-2
-1
0
1
E (eV)