Band structure calculations for strongly correlated materials using LDA+DMFT

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Outline

Band structures and effects of strong electronic correlations

Approaches for correlated electron systems $\rightsquigarrow$ DMFT

The LDA+DMFT method: setup and applications

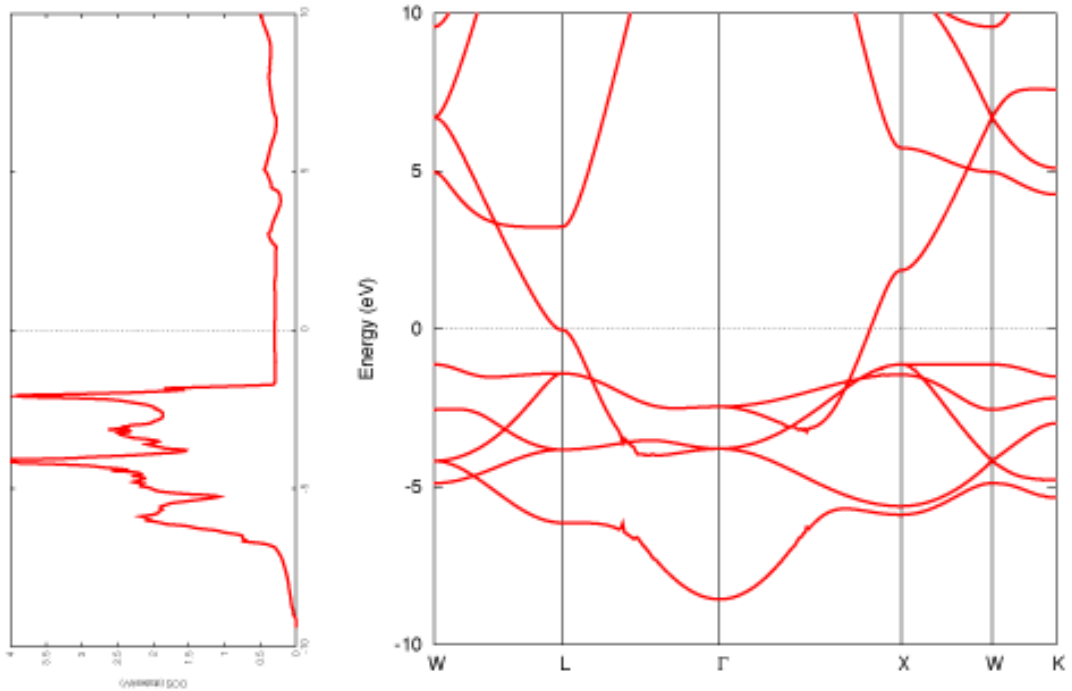
Auxiliary-field quantum Monte Carlo algorithm

QMC DMFT solvers: recent developments

Summary and outlook

Motivation: band structures and effects of strong electronic correlations

Conventional band structure results (here for fcc Au)



Density functional theory (DFT) $\rightsquigarrow$ bands with dispersion $\varepsilon_{n,\boldsymbol{k}}$

$\boldsymbol{k}$ integration $\rightsquigarrow$ spectra $A(\varepsilon)$

How? Use $\boldsymbol{k}$-resolved spectral function $A(\boldsymbol{k},\varepsilon) = \sum_n \delta(\varepsilon - \varepsilon_{n,\boldsymbol{k}})$

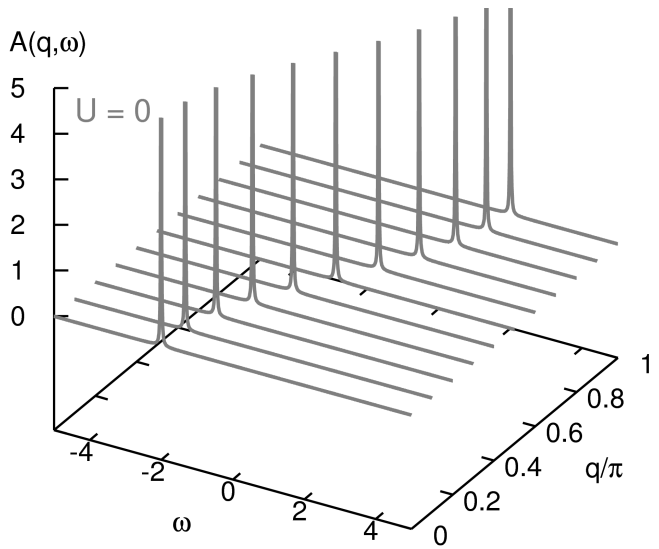
$\rightsquigarrow A(\varepsilon) = \frac{1}{V_B}\int d^3k\, A(\boldsymbol{k},\varepsilon)$

Note: all contributions to $A(\boldsymbol{k},\varepsilon)$ are singular!

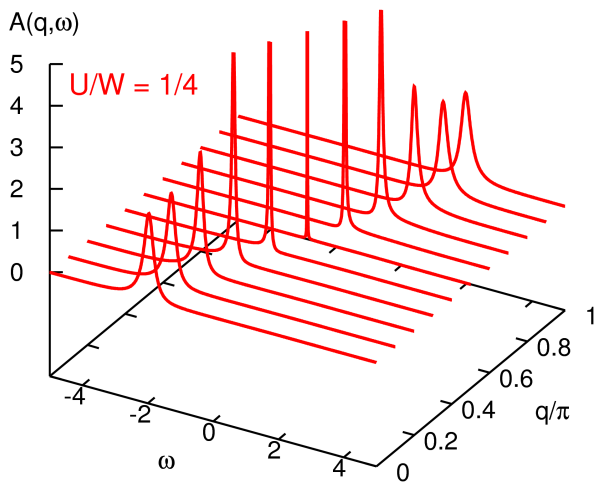
Is this physical? No: correlations lead to finite lifetimes $\sim$ broadening of $A(\boldsymbol{k},\varepsilon)$!

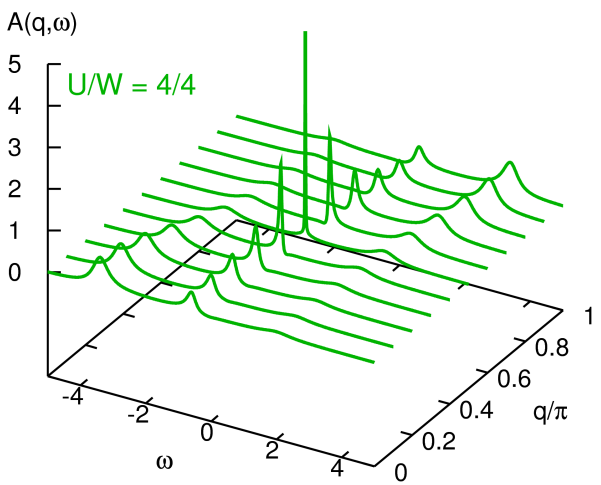
Illustration: single-band model

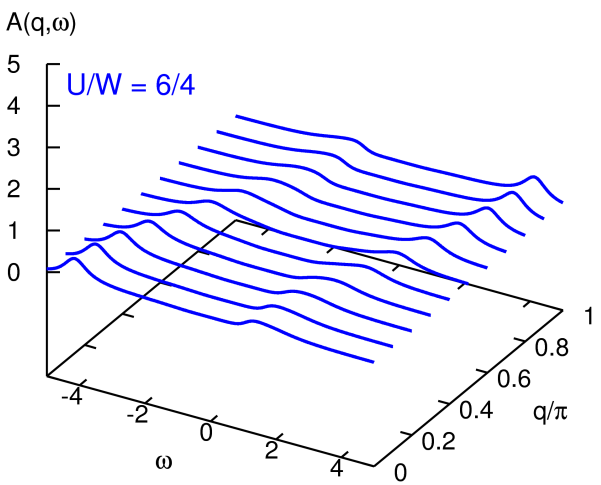
(i) tight-binding model of independent electrons
($q \sim k_x$, $\omega \sim \varepsilon$)



(ii) Hubbard model with local electron-electron interaction U (at half filling)







Better italian cuisine: lasagne, not spaghetti!

Goals of LDA+DMFT

Capture strong-correlation effects, e.g., Mott transition: beyond $\circ$ LDA $\circ$ DFT?

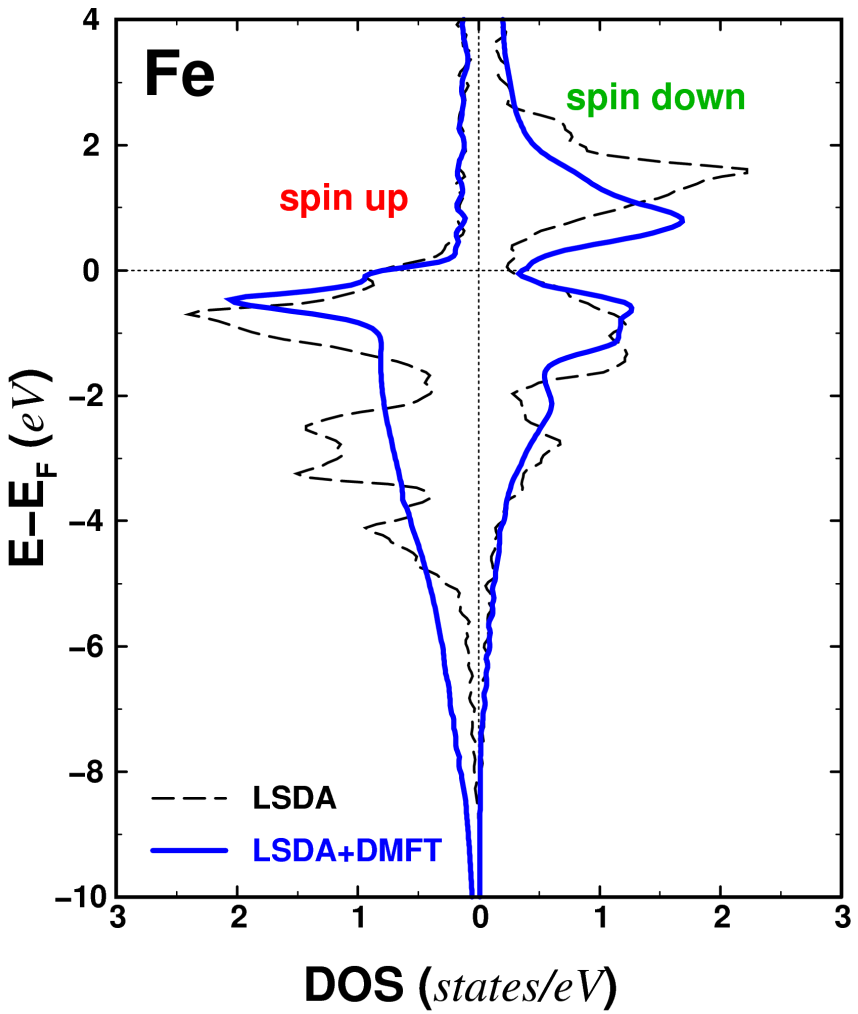
But also weak-correlation effects:

beyond DFT: "spaghetti" $\xrightarrow{\Sigma(\omega)}$ "lasagne"

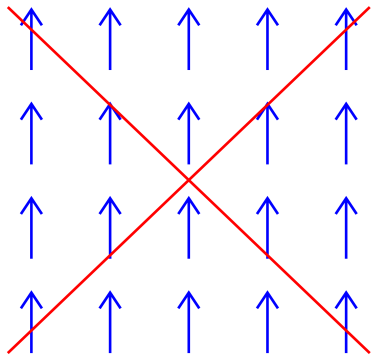
beyond DFT: calculate transition temperatures, e.g., Curie temperature

beyond LDA: correct gaps, moments, equilibrium volume. . .

Effects of strong correlations: Itinerant ferromagnetism and half-metallicity

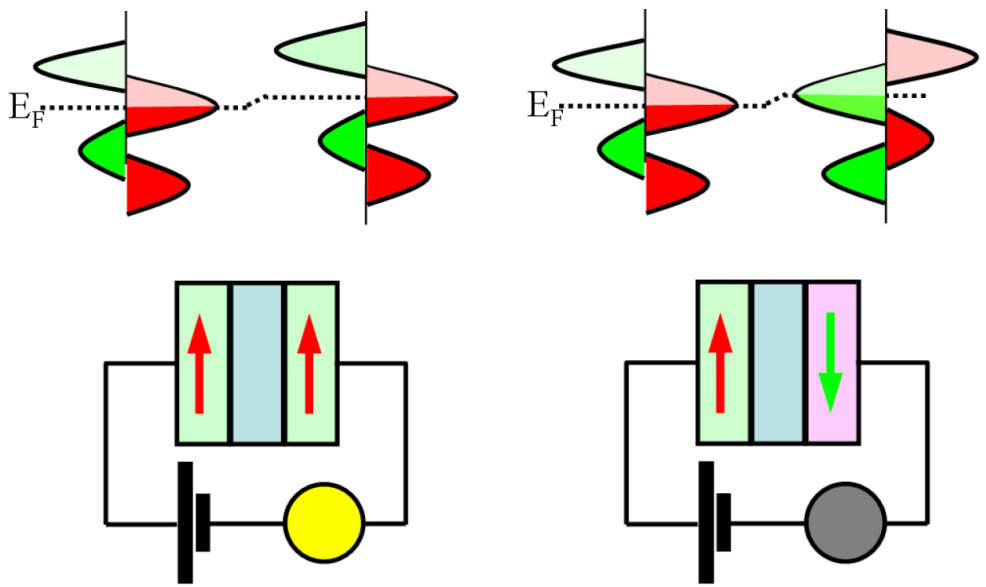


[Chioncel et. al, PRB (2003)]



Spin models insufficient

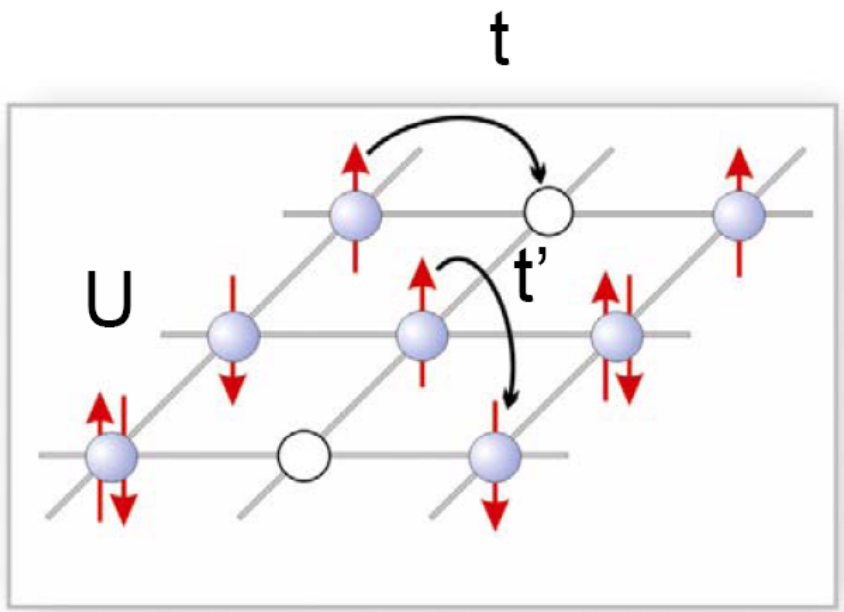
Technological goal: TMR with half metals



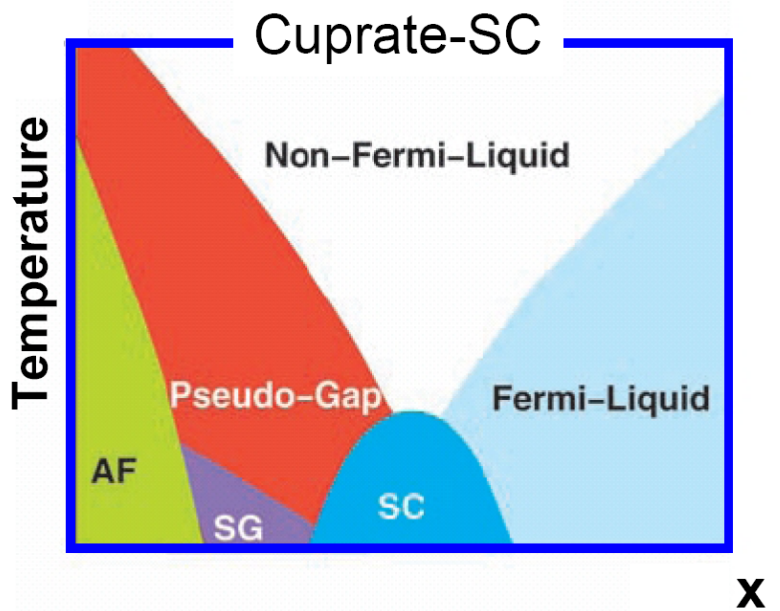
Qualitatively captured by LDA, modifications in LDA+DMFT

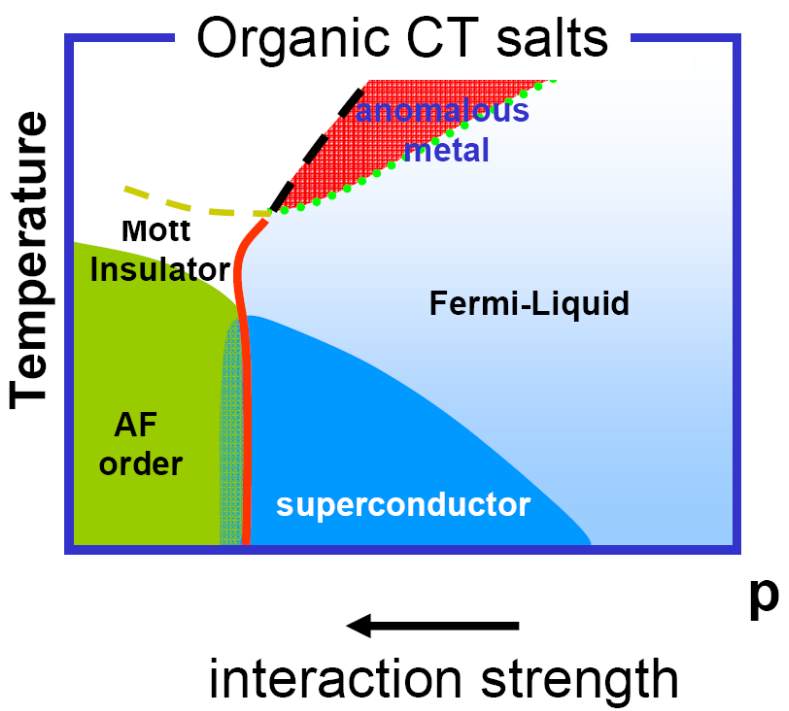
Complex phases of cuprate and organic superconductors

High-T_c physics contained in 2D Hubbard model?



Are antiferromagnetic (AF) and Mott insulating phases essential for superconductivity?

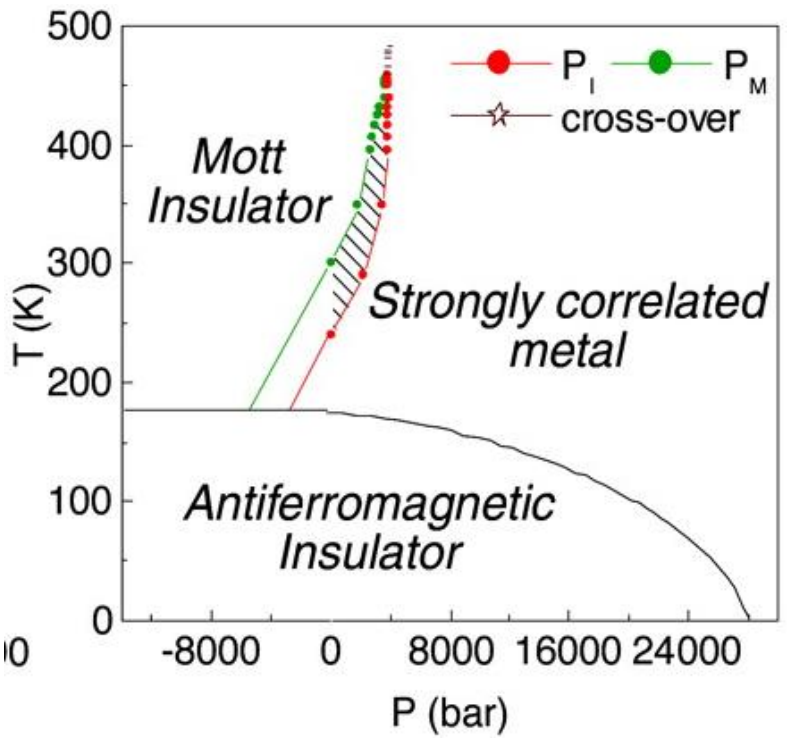




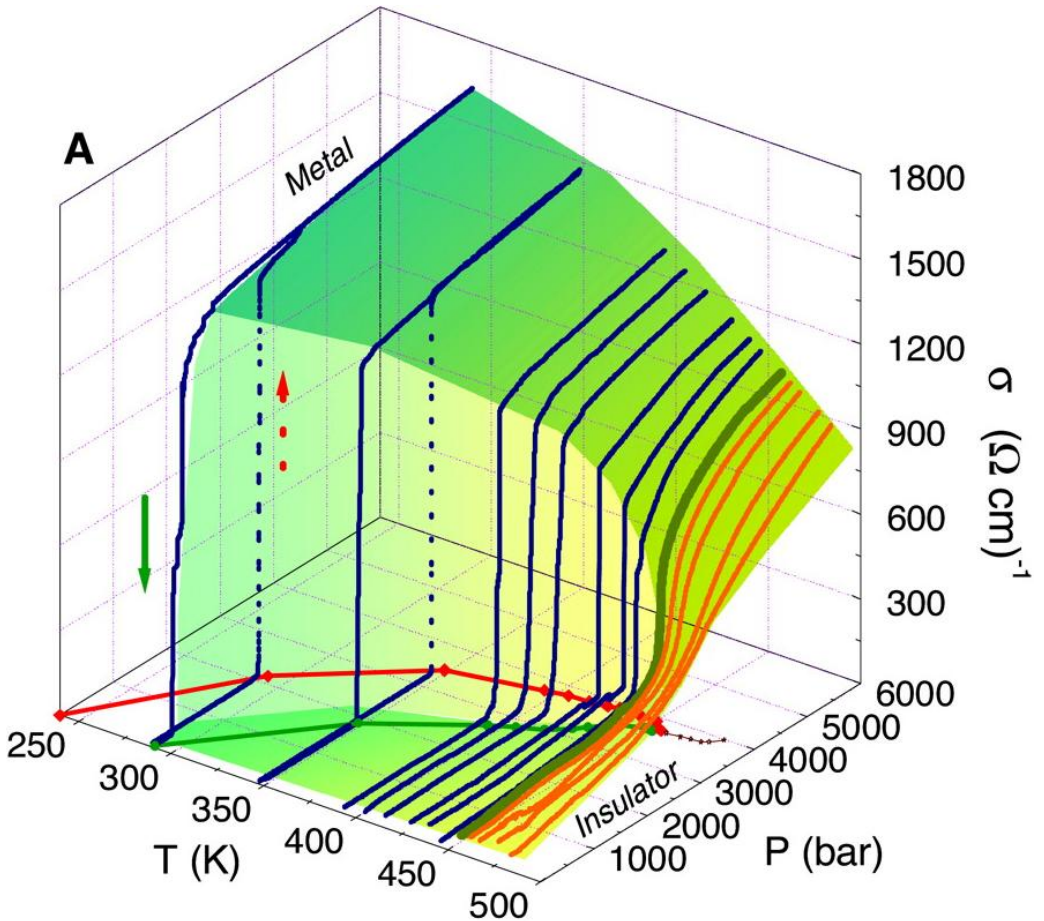
Mott metal-insulator transition

Prototype example: V_2O_3 doped with Cr/Ti and/or under pressure

Phase diagram



Electrical conductivity



[Limelette et al., Science 302, 89 (2003)]

No paramagnetic Mott insulator (spin degeneracy, no doubling of unit cell) in DFT!

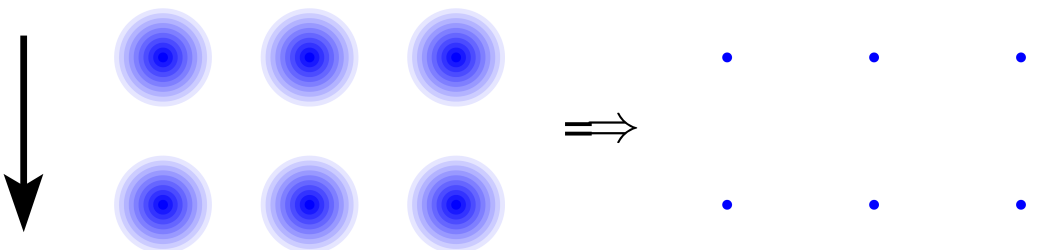
Approaches for correlated electron systems

Microscopic modeling I

General Hamiltonian for nuclei and electrons

$$H = \sum_{i=1}^{N_e} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{k=1}^{L} \frac{\boldsymbol{P}_k^2}{2M_k} + \sum_{k<l} \frac{Z_k Z_l\, e^2}{|\boldsymbol{R}_k - \boldsymbol{R}_l|} - \sum_{i,k} \frac{Z_k\, e^2}{|\boldsymbol{r}_i - \boldsymbol{R}_k|} + \sum_{i<j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

Born-Oppenheimer approximation (0^{th}order)



$$H = \sum_{i=1}^{N_e} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{i} V(\boldsymbol{r}_i) + \sum_{i<j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

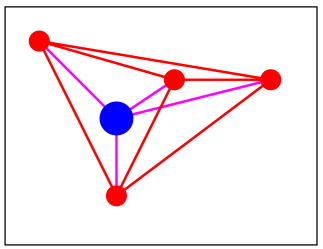
Classes of theoretical approaches for electronic problem

- continuum methods: density functional theory (DFT), variational+diffusion QMC, . .
- methods for lattice electrons

Density functional theory in LDA

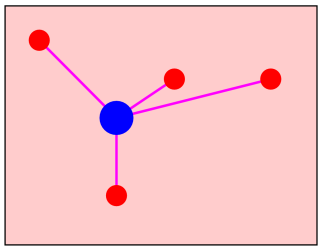
Density functional theory (DFT)

- exact ground state approach
- based on electron density $\rho(\boldsymbol{r})$
- Kohn-Sham equations solve effective single-particle problem
- result: ground state energy + $\rho(\boldsymbol{r})$
- heuristics: band structure
- problem: exchange-correlation potential unknown

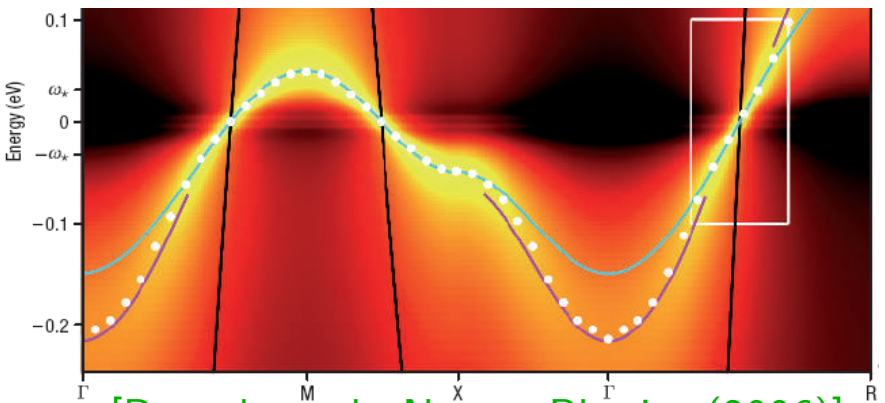


many-body

DFT $\Longrightarrow$



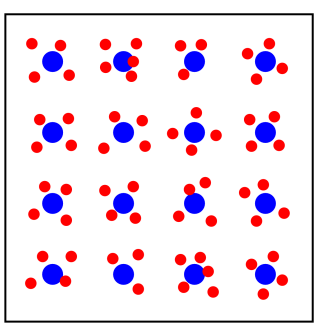
single-particle



[Byzcuk et al., Nature Physics (2006)]

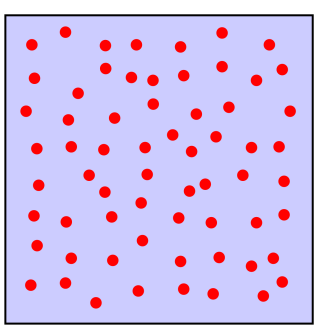
Local density approximation (LDA)

- exchange-correlation potential from jellium model (parametrized QMC)
- not reliable for correlated systems
- often good results
- basis for LDA+U and LDA+DMFT



e^- in solid

LDA $\Longrightarrow$

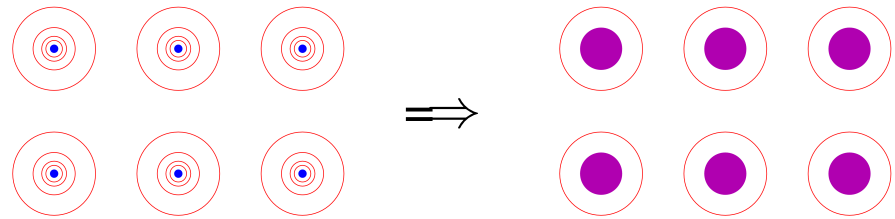


jellium model

Microscopic modeling II

$$H = \sum_{i=1}^{N_e} \frac{\boldsymbol{p}_i^2}{2m} + \sum_i V(\boldsymbol{r}_i) + \sum_{i<j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

reduction to valence electrons ↓



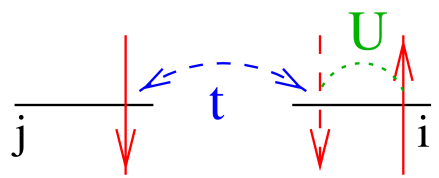
$$H = \sum_{i=1}^{N_v} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{i=1}^{N_v} V^{\text{ion}}(\boldsymbol{r}_i) + \sum_{i=1}^{N_v-1} \sum_{j=i+1}^{N_v} V^{ee}(\boldsymbol{r}_i, \boldsymbol{r}_j)$$

occupation number formalism ↓ Wannier orbitals

$$\hat{H} = \sum_{i\nu j\sigma} t_{ij}^{\nu} \, \hat{c}_{i\nu\sigma}^{\dagger} \, \hat{c}_{j\nu\sigma} + \frac{1}{2} \sum_{\nu\nu'\mu\mu'} \sum_{ijmn} \sum_{\sigma\sigma'} \mathcal{V}_{ijmn}^{\nu\nu'\mu\mu'} \, \hat{c}_{i\nu\sigma}^{\dagger} \, \hat{c}_{j\nu'\sigma'}^{\dagger} \, \hat{c}_{n\mu'\sigma'} \, \hat{c}_{m\mu\sigma}$$

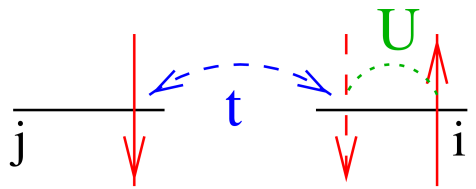
Hubbard model

$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} \, (\hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



Approaches for Hubbard-type models

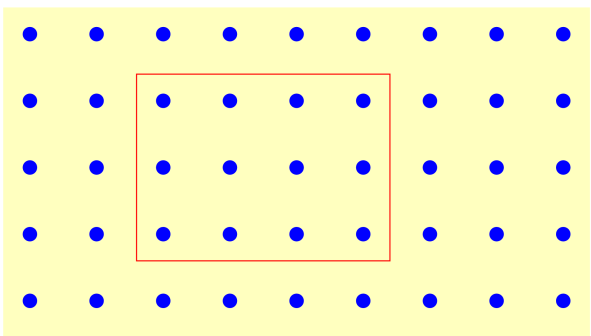
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}\right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



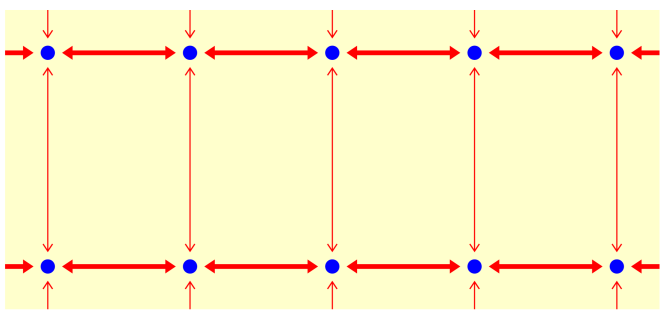
Perturbation theory

- $U \to 0$: Hartree-Fock
  2^{nd} order PT, . . .
- $t/U \to 0$ (for $n = 1$)
  $\rightsquigarrow$ Heisenberg model

finite clusters: ED, QMC



$d \to 1$: Bethe ansatz, DMRG



Dynamical mean-field theory (DMFT): local self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$

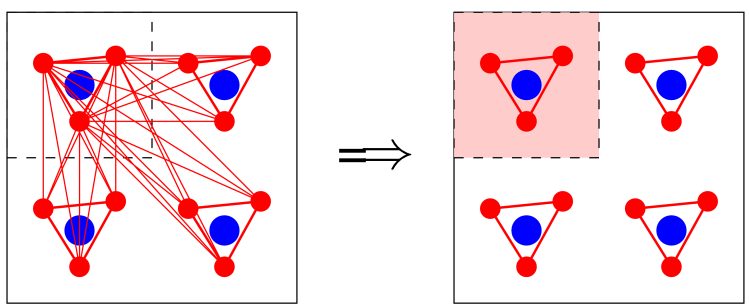
[Metzner, Vollhardt, PRL (1989), Georges, Kotliar, PRL (1992), Jarrell, PRL (1992)]

\+ non-perturbative $\rightsquigarrow$ valid at MIT

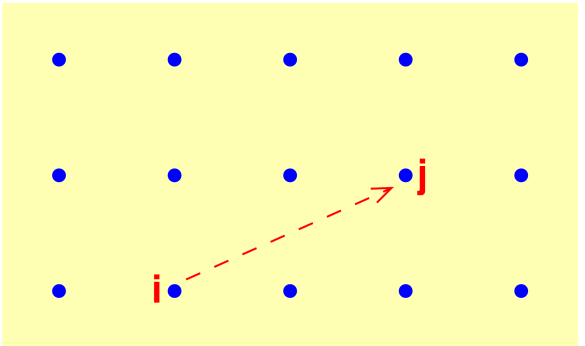
\+ dynamical on-site correlations preserved

\+ in thermodynamic limit

+/− exact for coordination $Z \to \infty$



Excursus: Green function and self-energy

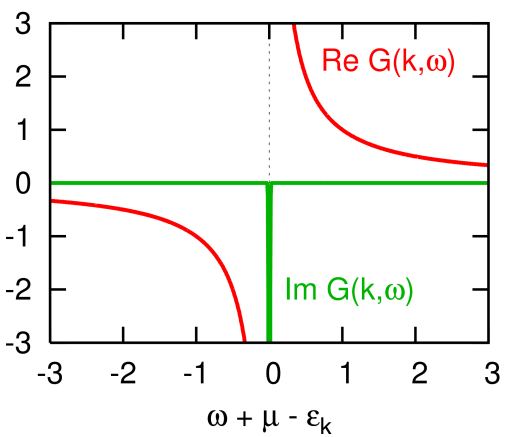


Single-particle Green function (lattice sites i, j):

$$G_{ij}(t_1, t_2) = -\langle c_j(t_2)\, c_i^\dagger(t_1)\rangle$$

Translation invariance in space and time: $G_{ij}(t_1, t_2) \equiv G_{j-i}(t_2 - t_1) \overset{\text{Fourier}}{\longrightarrow} G(\boldsymbol{k}, \omega)$

Noninteracting limit (dispersion $\varepsilon_{\boldsymbol{k}}$): $G^0(\boldsymbol{k}, \omega) = \dfrac{1}{\omega + \mu - \varepsilon_{\boldsymbol{k}}}$



Self-energy Σ quantifies impact of interactions:

$$G(\boldsymbol{k}, \omega) = \frac{1}{\omega + \mu - \varepsilon_{\boldsymbol{k}} - \Sigma(\boldsymbol{k}, \omega)}$$

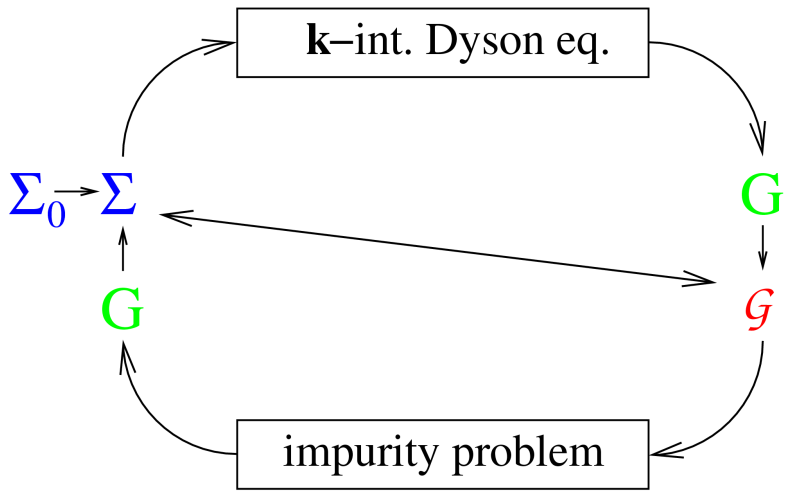
Locality of self-energy $\Sigma(\boldsymbol{k}, \omega) \equiv \Sigma(\omega)$ within DMFT simplifies local Green function:

$$G(\omega) \equiv G_{ii}(\omega) = \int d\varepsilon \frac{N^0(\varepsilon)}{\omega + \mu - \varepsilon - \Sigma(\omega)}; \qquad N^0(\varepsilon) = \frac{1}{N}\sum_{\boldsymbol{k}} \delta(\varepsilon - \varepsilon_{\boldsymbol{k}})$$

$\boldsymbol{k}$ integrated Dyson equation — noninteracting DOS

Iterative solution of DMFT equations

0. Initialize self-energy
1. Solve Dyson equation
2. Solve single impurity Anderson model (SIAM)

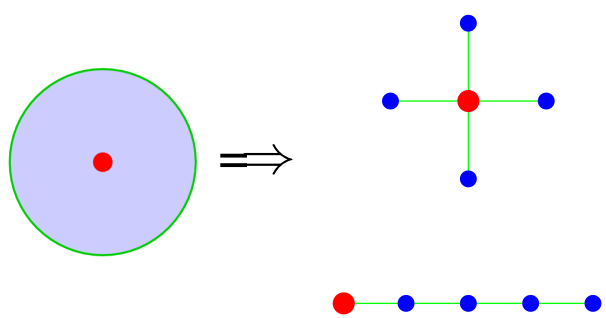


← DOS / t_{ij} / $\varepsilon_{\nu \boldsymbol{k}}$

← local interactions

Impurity solver:

- Iterative perturbation theory (IPT; not controlled)
- Quantum Monte-Carlo (QMC)
- Exact diagonalization (ED; large finite-size errors)
- Numerical renormalization group (NRG; 1-2 bands)
- Density matrix renormalization group (DMRG)
- Self-energy functional theory (SFT) + ED



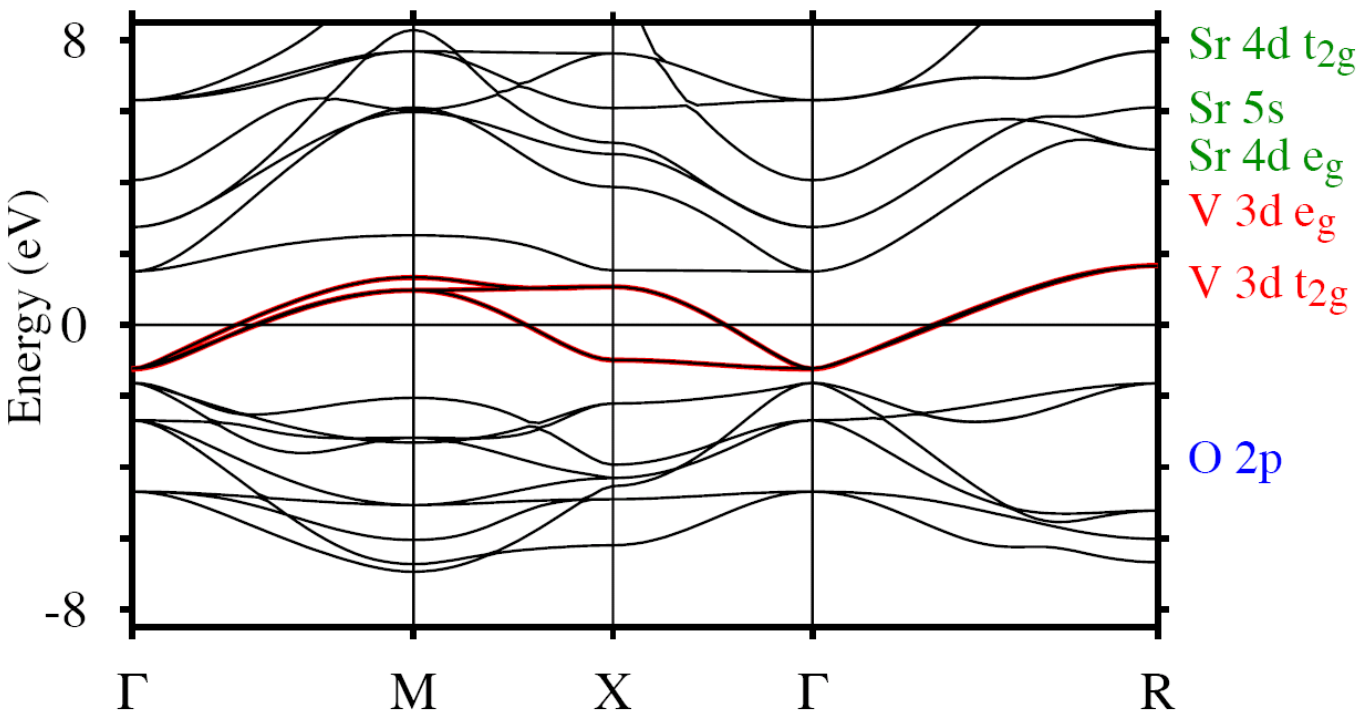
LDA+DMFT method: setup and applications

LDA+DMFT philosophy:

Interactions among extended orbitals well screened; should be captured by LDA.

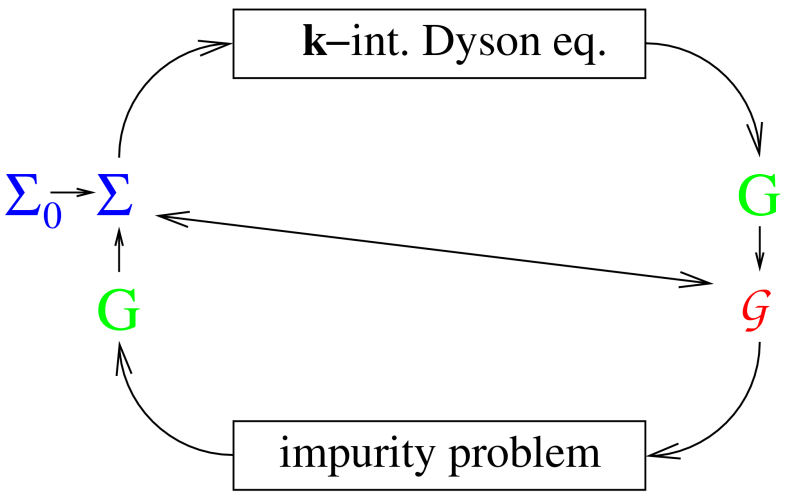
Many-body treatment (only) for narrow bands near Fermi energy (typically 3d, 4f)

Example: $SrVO_3$ (cubic perovskite) – NMTO bands with downfolding to V 3d t_{2g} bands

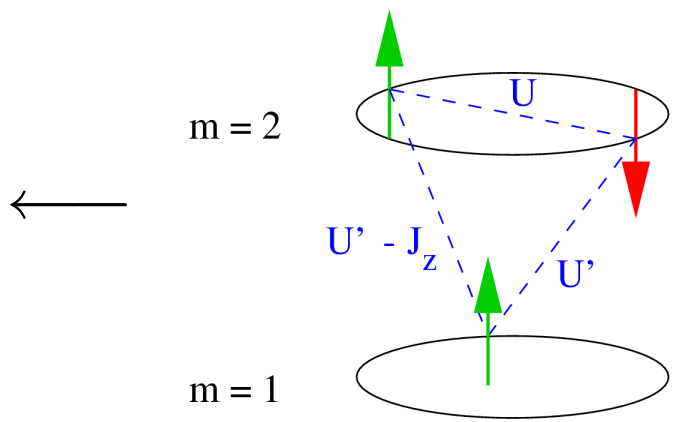


Here: simplest case – all correlated bands are equivalent

LDA+DMFT for M equivalent bands ($m = 1 \ldots M$)



$$G^{m,\sigma}(\omega) \equiv G^{m,\sigma}_{ii}(\omega) = \int d\varepsilon \, \frac{N^{\mathrm{LDA}}(\varepsilon)}{\omega + \mu - \varepsilon - \Sigma(\omega)}$$

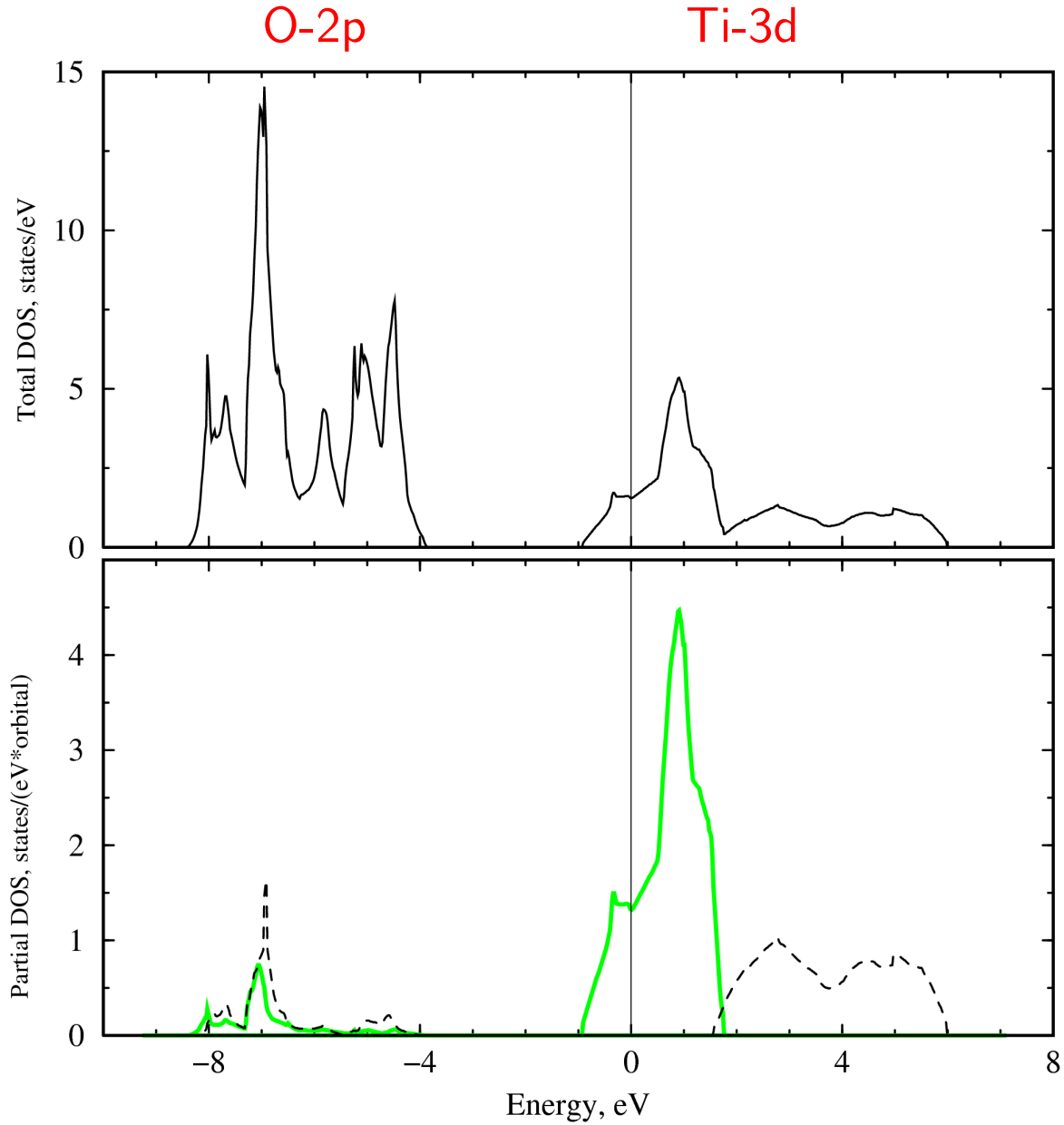


Interaction parameters U, U', J: e.g. from constrained LDA

Early example: perovskite $La_{1-x}Sr_xTiO_3$ ($x = 0.06$)

TB-LMTO-ASA calculation (for $x = 0$, cubic unit cell)

Spectral weight near Fermi energy: nearly pure 3d t_{2g} character



[I.A. Nekrasov, K. Held, NB, A.I. Poteryaev, V.I. Anisimov, and D. Vollhardt, EPJP 18, 55 (2000)]

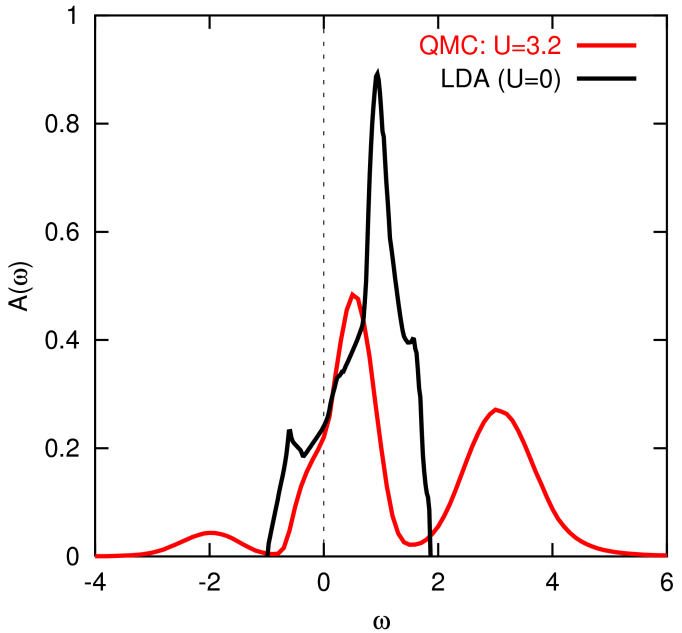
Impact of correlations?

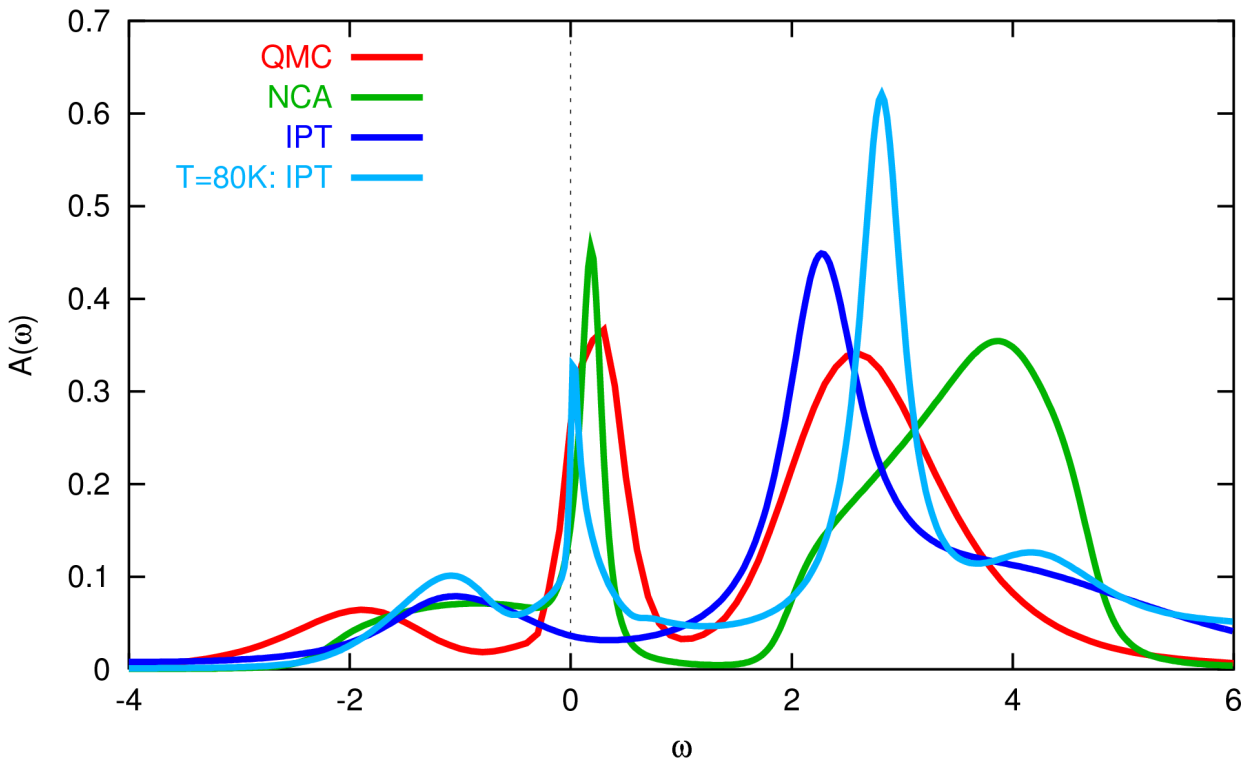
$U = U' = 3.2$ eV, $J = 0$

LDA+DMFT(QMC):

Reduction of quasiparticle peak,

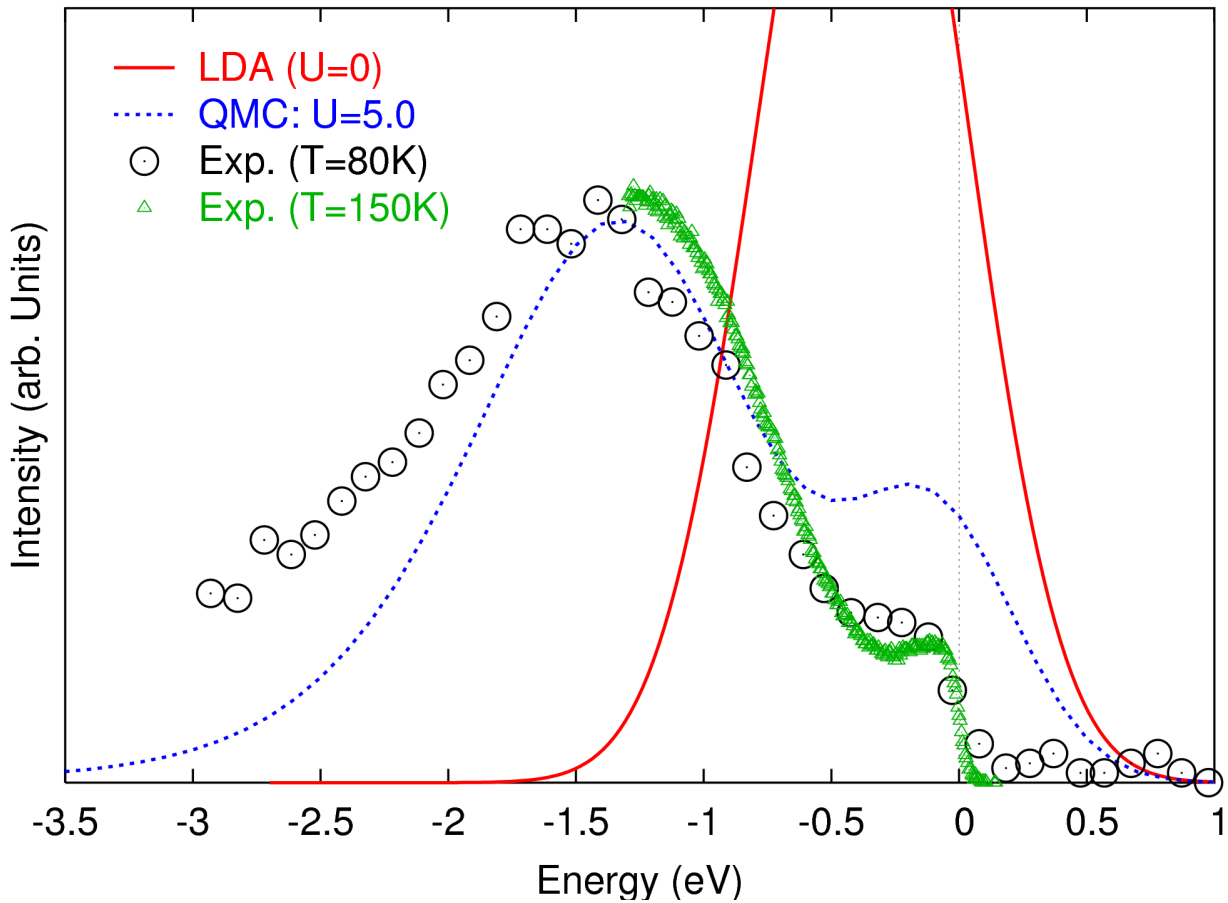
appearance of Hubbard bands





Method for solving DMFT matters!

Photoemission spectra for $La_{1-x}Sr_xTiO_3$



[Nekrasov, Held, NB, Poteryaev, Anisimov, Vollhardt, (2000)]

Reasonable accuracy, drastic improvement over LDA

But: old QMC code not accurate near MIT $\rightsquigarrow$ eliminate $\Delta\tau$ discretization error!

LDA+DMFT for general case: multiple inequivalent bands

Now: LDA density of states not enough, need Hamiltonian in localized basis
(e.g.: Wannier functions)

For any (orthogonal) $\boldsymbol{k}$ space basis:

DFT band structure can be Fourier transformed to real space

$\rightsquigarrow$ single-particle Hamiltonian

$$\hat{H}_{\mathrm{LDA}} = \sum_{ilm,jl'm',\sigma} (\delta_{ilm,jl'm'}\ \varepsilon_{ilm}\ \hat{n}^{\sigma}_{ilm} + t_{ilm,jl'm'}\ \hat{c}^{\sigma\dagger}_{ilm}\hat{c}^{\sigma}_{jl'm'}).$$

Here:

	i, j	indices of unit cells
	l, l'	indices of atoms in unit cell
	m, m'	orbital indices (ranges depend on l, l')
	σ	spin

and orbital occupation $\hat{n}^{\sigma}_{ilm} = \hat{c}^{\sigma\dagger}_{ilm}\hat{c}^{\sigma}_{ilm}$,

For LDA+DMFT: choose basis which includes localized orbitals, i.e. 3d states.

Now add interactions between the localized electrons ($i = i_d$ and $l = l_d$):

$$\hat{H} = \hat{H}_{\mathrm{LDA}} + \frac{1}{2} \sum_{i=i_d, l=l_d} {\sum_{m\sigma, m'\sigma'}}' U^{\sigma\sigma'}_{mm'} \, \hat{n}_{ilm\sigma} \, \hat{n}_{ilm'\sigma'} + \text{spin-flip terms} - \hat{H}^{U}_{\mathrm{LDA}}$$

Double counting correction $\hat{H}^{U}_{\mathrm{LDA}}$ $\rightsquigarrow$ shift in chemical potential (Anisimov, 1991)

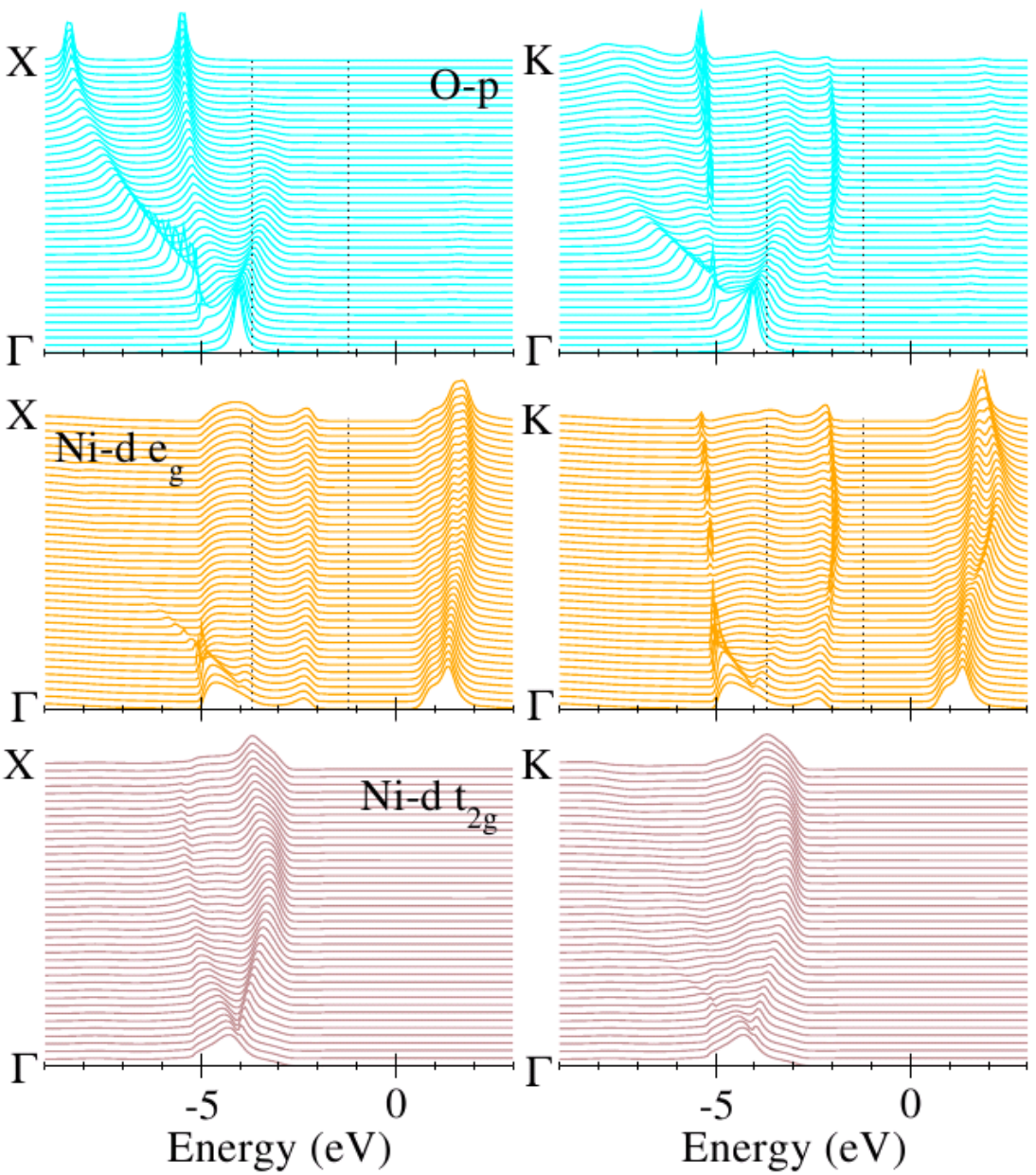
$$\varepsilon^{0}_{il_dm} = \varepsilon_{il_dm} - \bar{U}(n_d - \frac{1}{2}) + \frac{J}{2}(n_d - 1) \qquad \text{(paramagnetic case)}$$

$\rightsquigarrow$ $\boldsymbol{k}$-integrated Dyson equation (DMFT self-consistency equation):

$$G_{qlm,q'l'm'}(\omega) = \frac{1}{V_B} \int d^3k \left(\left[\, \omega \mathbb{1} + \mu \mathbb{1} - H^{0}_{\mathrm{LDA}}(\boldsymbol{k}) - \Sigma(\omega) \right]^{-1} \right)_{qlm,q'l'm'} .$$

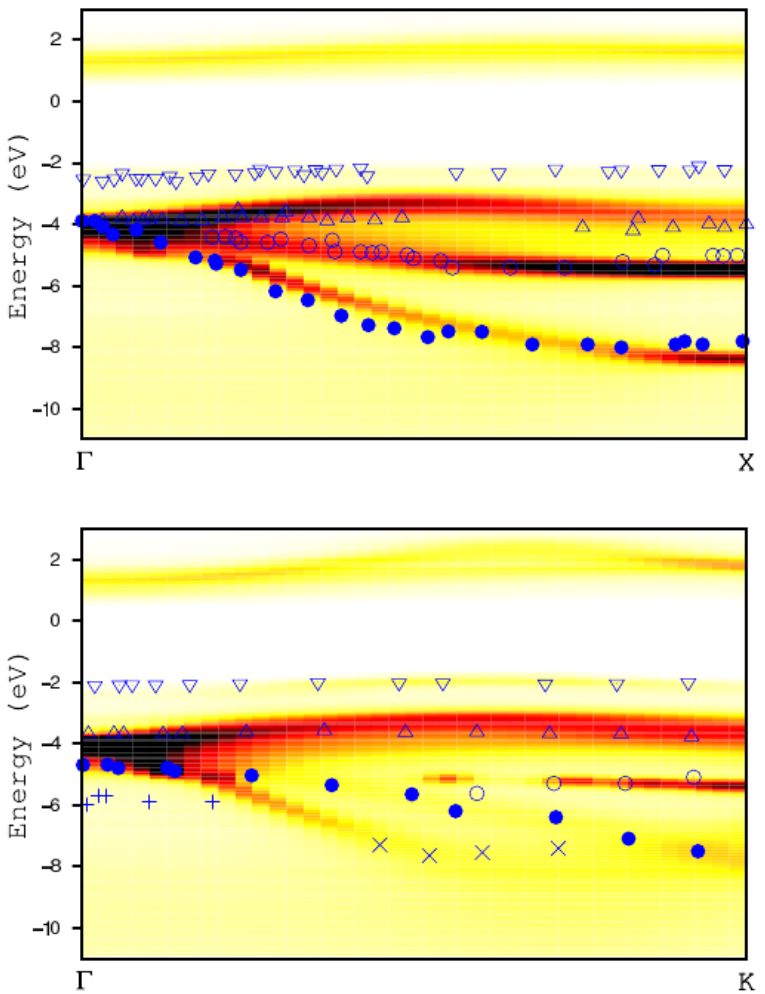
Matrix equation!

Recent example: NiO



all Ni 3d states + O 2p

$\rightsquigarrow 8 \times 8$ matrices



[Kunes, Anisimov, Skornyakov, Lukoyanov, Vollhardt, arXiv:0705.1692]

Flow diagram for DFT

First principles information:
atomic numbers, crystal structure (lattice, atomic positions)

Choose initial electronic density $\rho(\mathbf{r})$

Calculate effective potential using the LDA

$$V_{\text{eff}}(\mathbf{r}) = V_{\text{ion}}(\mathbf{r}) + \int d^3\mathbf{r}'\; V_{ee}(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}') + \frac{\delta E_{\text{xc}}[\rho]}{\delta\rho(\mathbf{r})}$$

Solve Kohn-Sham equations

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{eff}}(\mathbf{r}) - \varepsilon_i\right]\varphi_i(\mathbf{r}) = 0$$

Calculate electronic density $\rho(\mathbf{r}) = \sum_i^N |\varphi_i(\mathbf{r})|^2$

Iterate to self-consistency

Calculate band structure $\varepsilon_i(\mathbf{k})$, partial and total DOS,
total energy $E[\rho]$, Hamiltonian in localized basis ...

Flow diagram for DMFT

Choose an initial self-energy Σ

Calculate G from Σ via the k-integrated Dyson equation:

$$G_{qlm,q'l'm'}(\omega) = \frac{1}{V_B} \int d^3k \left(\left[\omega \mathbb{1} + \mu \mathbb{1} - H^0_{\mathrm{LDA}}(\mathbf{k}) - \Sigma(\omega) \right]^{-1} \right)_{qlm,q'l'm'}$$

$$\mathcal{G}(\omega) = (G^{-1}(\omega) + \Sigma(\omega))^{-1}$$

Calculate G from $\mathcal{G}$ via the DMFT single-site problem

$$G^{\sigma}_{\nu m}(\tau) = -\frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi]\mathcal{D}[\psi^*] \psi^{\sigma}_m \, \psi^{\sigma *}_m e^{\mathcal{A}[\psi,\psi^*,\mathcal{G}^{-1}(\tau)]}$$

$$\Sigma_{\mathrm{new}}(\omega) = \mathcal{G}^{-1}(\omega) - G^{-1}(\omega)$$

Iterate with $\Sigma = \Sigma_{\mathrm{new}}$ until convergence, i.e. $||\Sigma - \Sigma_{\mathrm{new}}|| < \epsilon$

Problem: occupation of LDA orbitals may have changed $\rightsquigarrow$ charge inconsistency!

Auxiliary-field QMC algorithm [Hirsch, Fye (1986)]

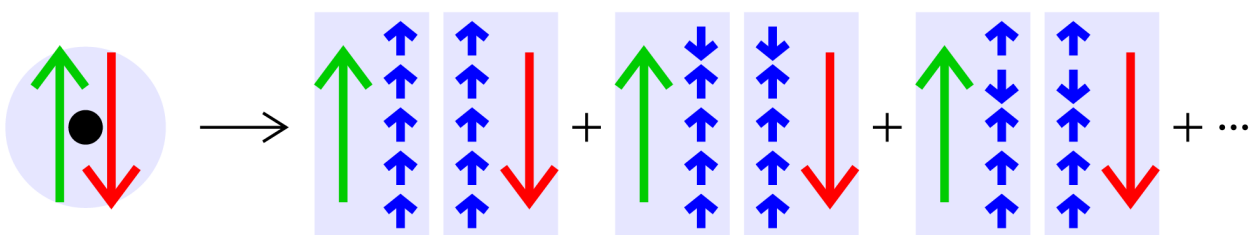
Green-Funktion G in imaginary time (fermionic Grassmann variables ψ, ψ^*):

$$G_\sigma(\tau_2-\tau_1) = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi]\,\mathcal{D}[\psi^*]\ \psi_\sigma(\tau_1)\psi^*_\sigma(\tau_2)\ \exp\Big[\mathcal{A}_0 - U\sum_{\sigma\sigma'}\int_0^\beta d\tau\,\psi^*_\sigma\psi_\sigma\psi^*_{\sigma'}\psi_{\sigma'}\Big]$$

Discretization $\beta = \Lambda\,\Delta\tau$, Trotter decoupling $e^{-\beta(\hat{T}+\hat{V})} = \lim_{\Lambda\to\infty}\left[e^{-\Delta\tau\hat{T}}e^{-\Delta\tau\hat{V}}\right]^\Lambda$

Use $\hat{n}_\uparrow\hat{n}_\downarrow = \frac{1}{2}\left[\hat{n}_\uparrow + \hat{n}_\downarrow - \left(\hat{n}_\uparrow - \hat{n}_\downarrow\right)^2\right]$; discrete Hubbard-Stratonovich transformation

$$\exp\left[\Delta\tau U\left(\hat{n}_\uparrow - \hat{n}_\downarrow\right)^2/2\right] = \frac{1}{2}\sum_{s=\pm1}\exp\left[\lambda s\left(\hat{n}_\uparrow - \hat{n}_\downarrow\right)\right]; \qquad \cosh(\lambda) = \exp(\Delta\tau U/2)$$



Wick theorem:

$$G = \frac{\sum M \det\{M\}}{\sum \det\{M\}}$$

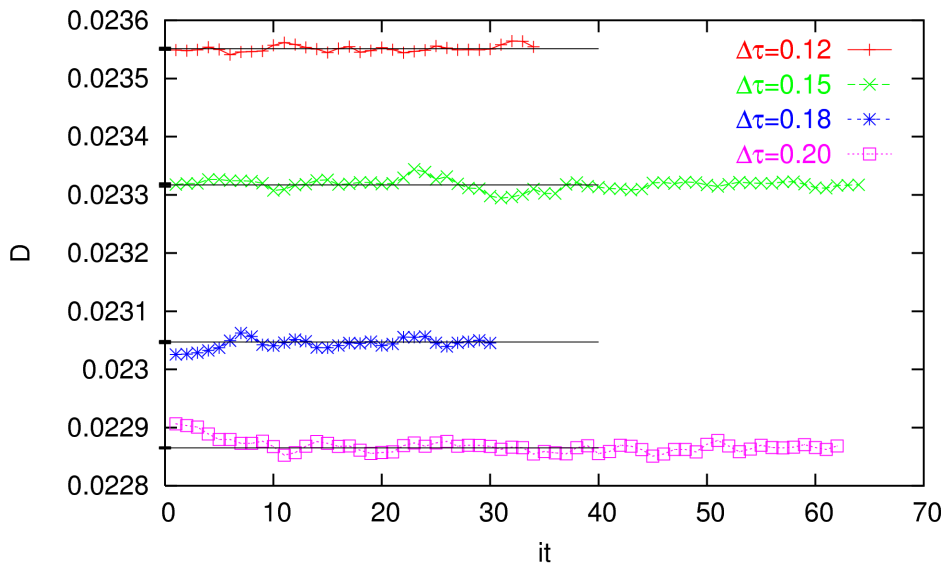
Metropolis MC importance sampling over auxiliary Ising field $\{s\}$: 2^Λ configurations

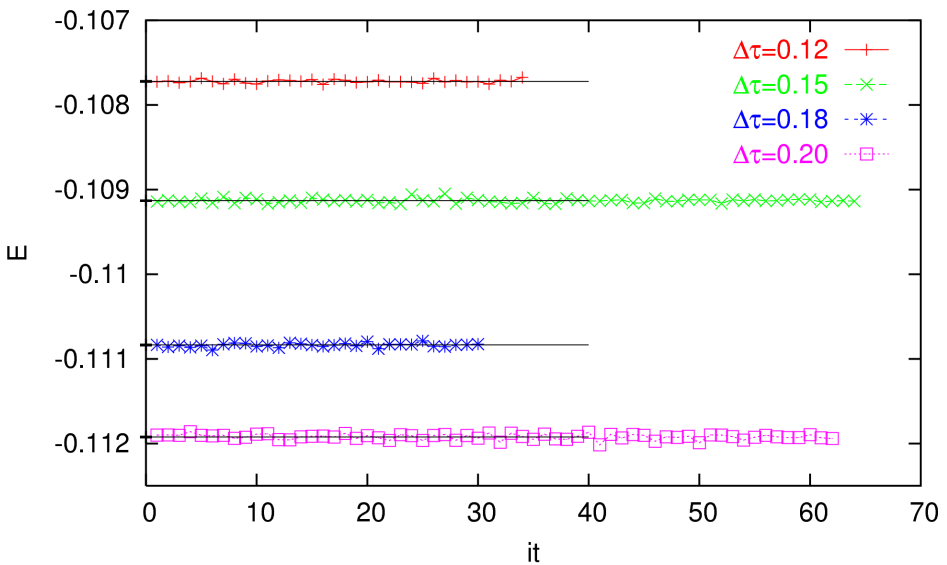
\+ numerically exact, + no sign problem, − effort scales as T^{-3}

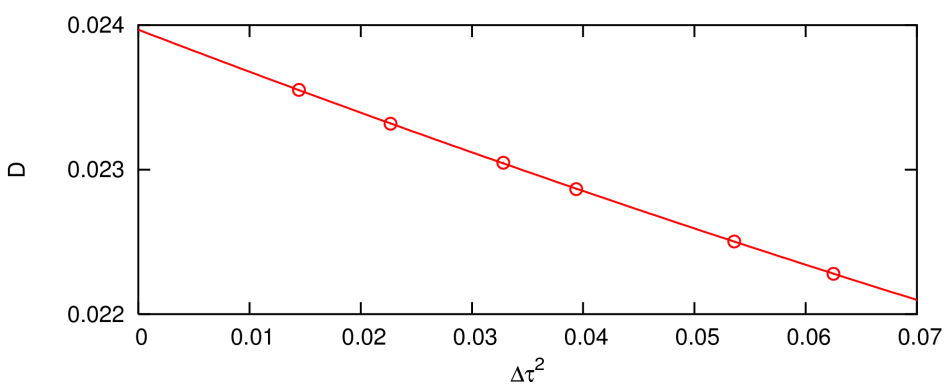
Contributions to DMFT-QMC error bars:

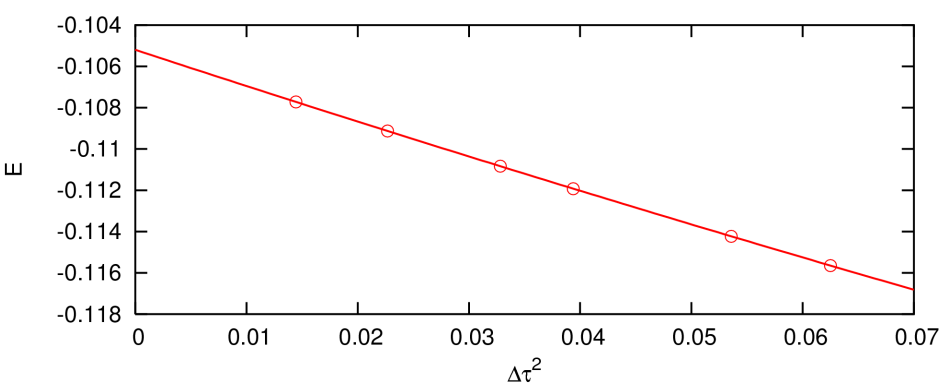
- statistical fluctuations + warm-up
- convergency (of self-consistency cycle)
- discretization (Trotter error and Fourier transform)

Example: half-filled Hubbard model, $U = 5$, $W = 4$, $T = 0.04$ (Mott insulator)



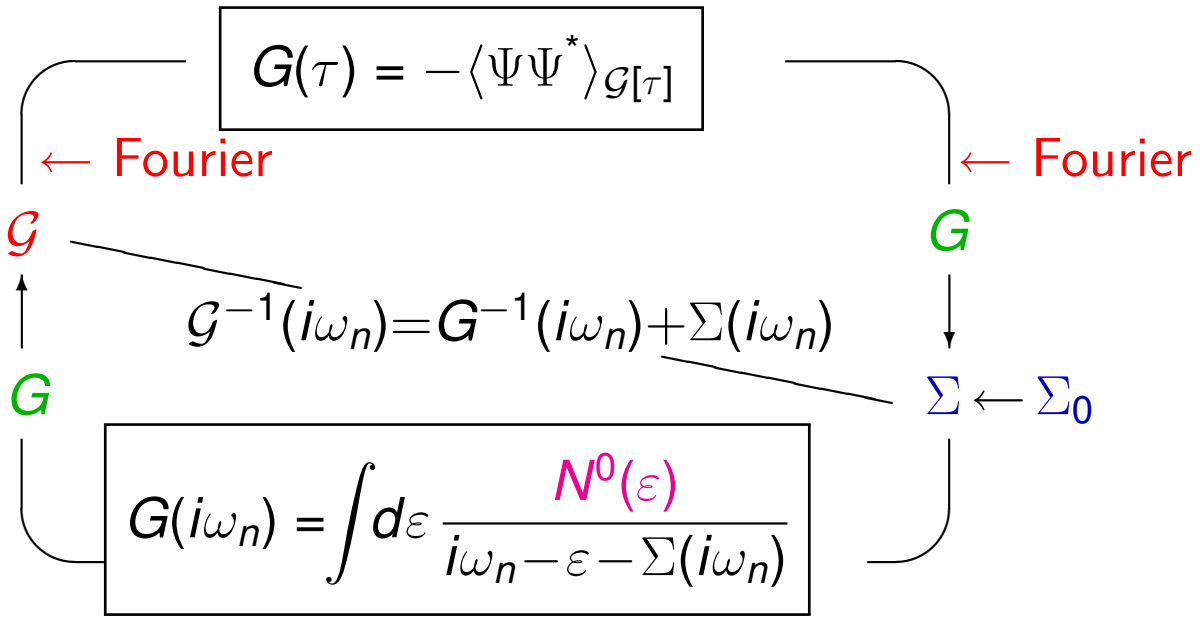




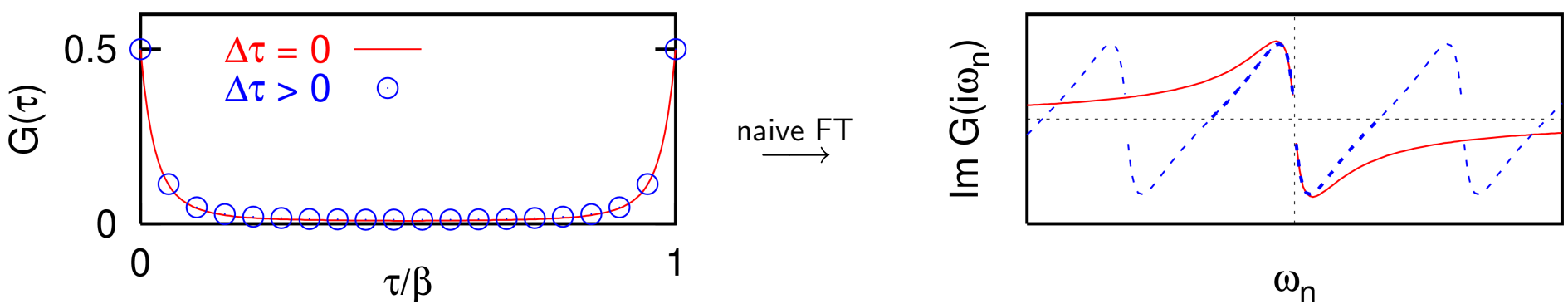


Problems with Fourier transformations in DMFT-QMC cycle

Iterative solution of DMFT equations (for imaginary-time impurity solver)



Naive discrete Fourier transformation $\rightsquigarrow$ oscillations (instead of $G(\omega) \overset{\omega\to\infty}{\longrightarrow} 1/\omega$)

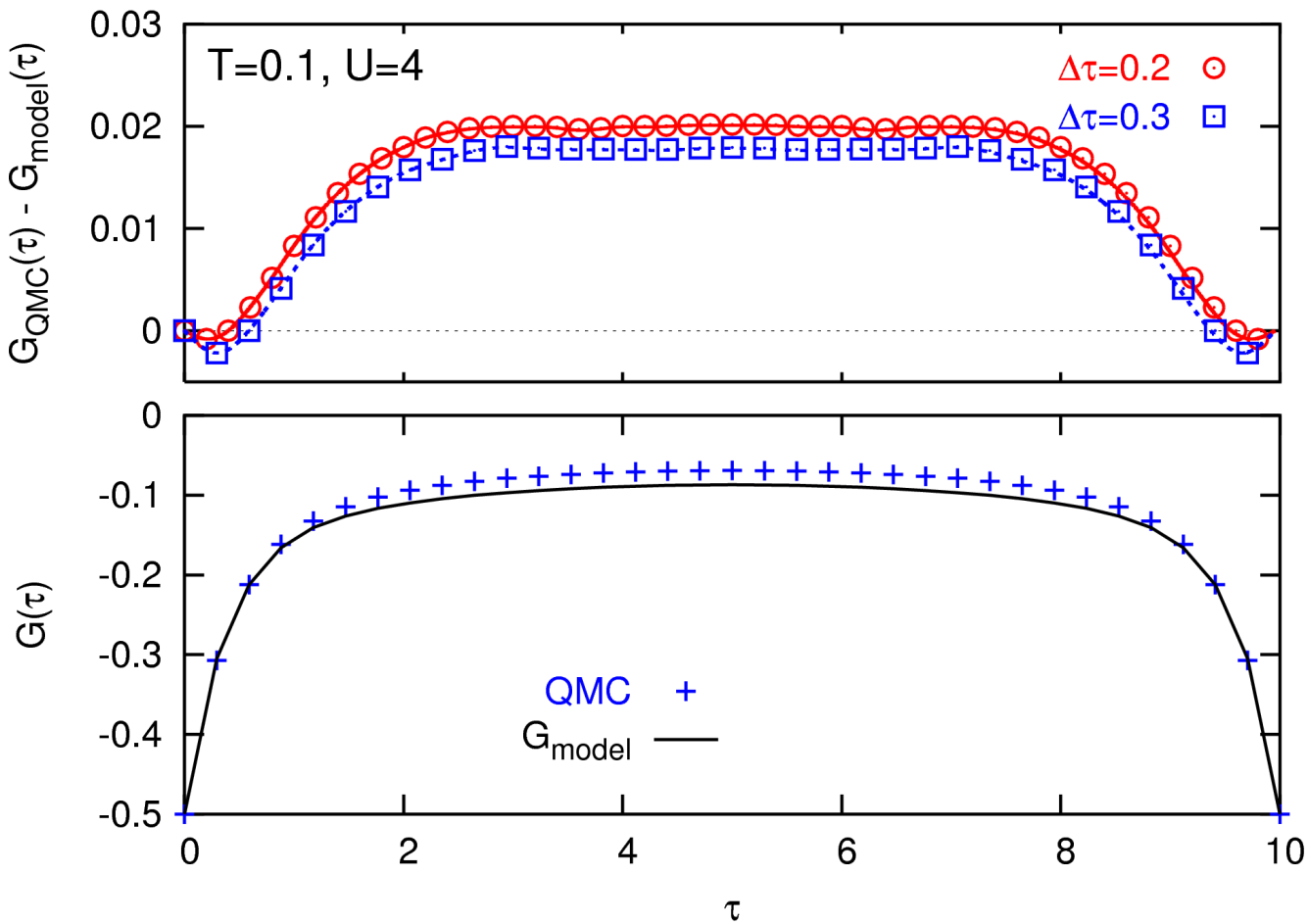


1st solution: correct unphysical behavior for $|\omega| \lesssim \omega_{\text{Nyquist}}$ by transformation [Ulmke]

2nd solution: interpolate $G_{\mathrm{QMC}}(\tau)$ by cubic splines [Jarrell, Krauth, Gull, . . .]

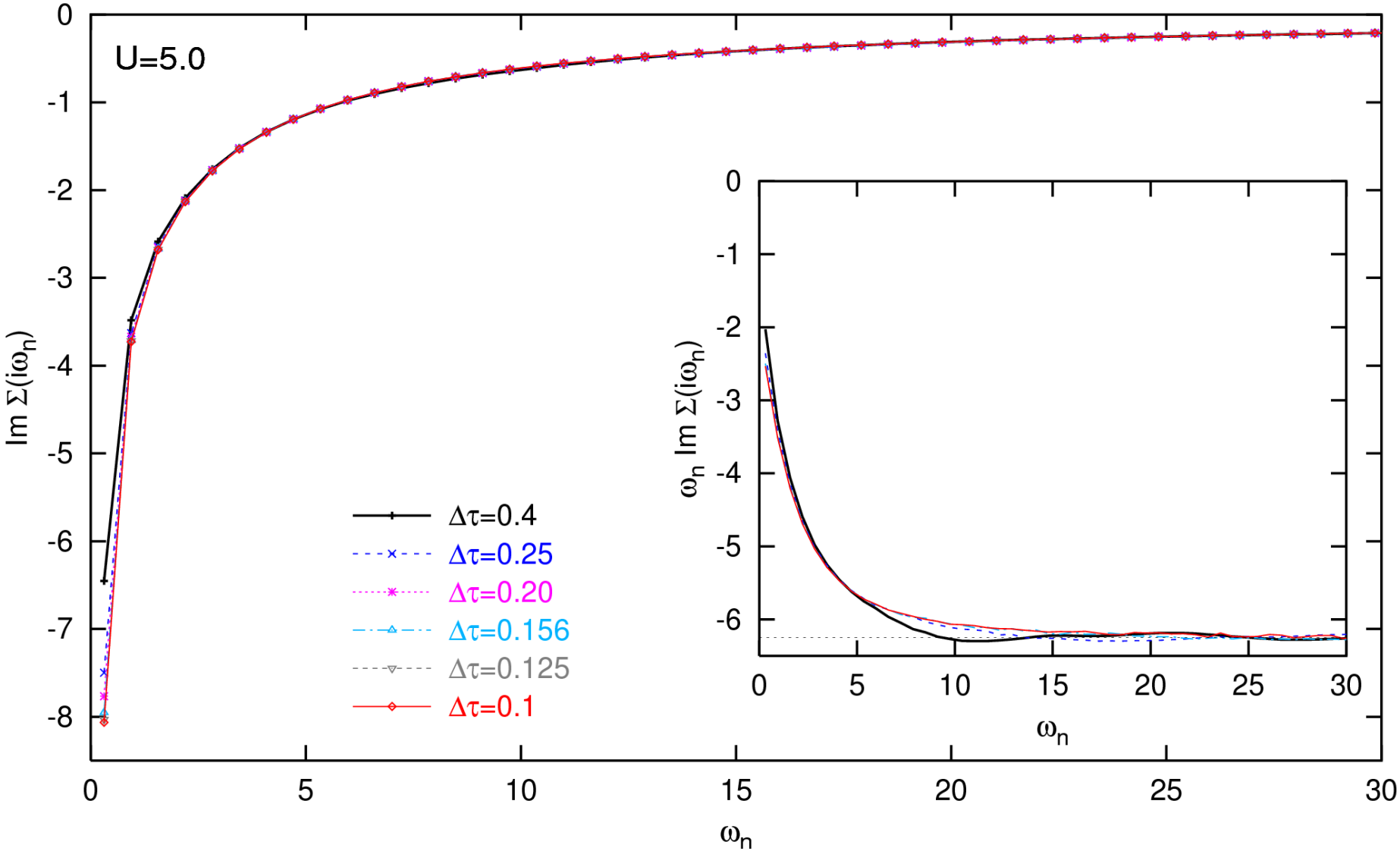
But: $\dfrac{d^2G(\tau)}{d\tau^2}$ maximal for $\tau \to 0, \beta$ $\rightsquigarrow$ natural boundary conditions inappropriate

- adjust boundary cond. [Oudovenko]
- spline-fit only difference w.r.t. reference problem:
  - IPT [Jarrell]
  - high-frequency expansion for $\Sigma(\omega)$ + param. [Knecht, NB]



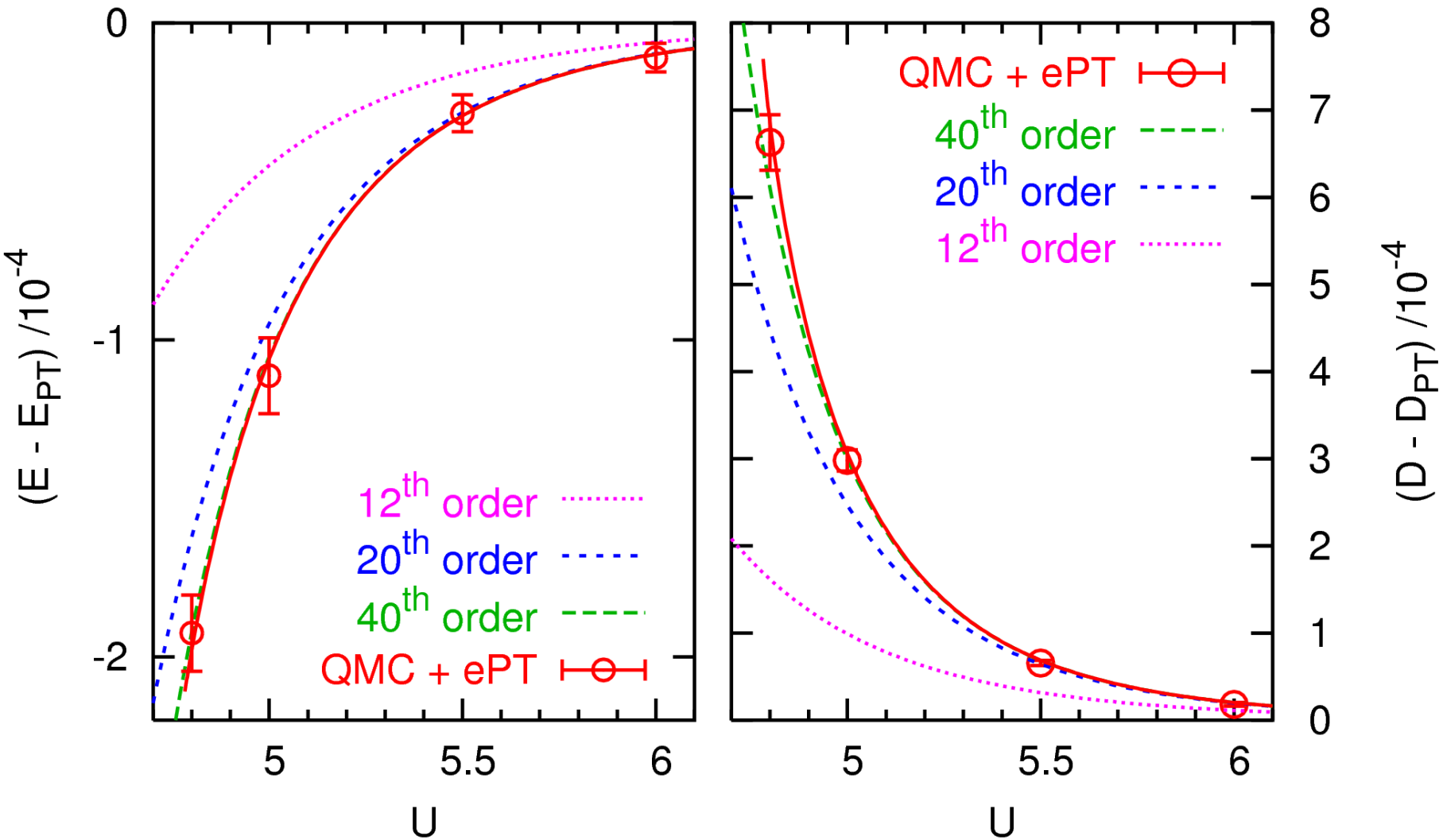
$$\Sigma_\sigma(\omega) = U\left(\langle \hat{n}_{-\sigma}\rangle - \tfrac{1}{2}\right)\omega^0 + U^2\langle \hat{n}_{-\sigma}\rangle\left(1 - \langle \hat{n}_{-\sigma}\rangle\right)\omega^{-1} + \mathcal{O}(\omega^{-2})$$

Sensitive test: self-energy $\Sigma(i\omega_n)$ for insulating phase ($T = 0.1$, $U = 5.0$)



Rapid convergence at all frequencies for "QMC + $1/\omega$" DMFT solver

Extreme QMC precision for Mott insulator



[N. Blümer and E. Kalinowski, Phys. Rev. B 71, 195102 (2005)]

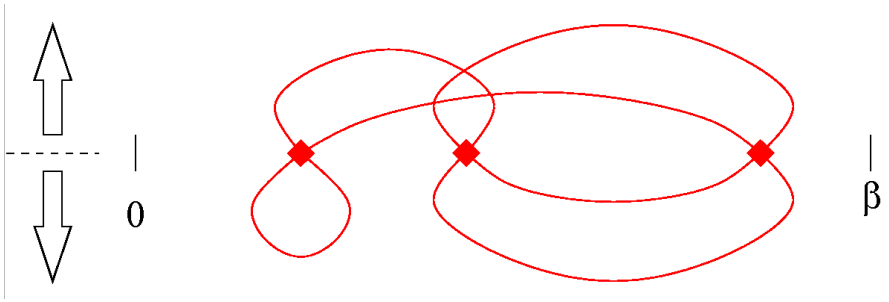
HF-QMC accuracy only challenged by self-energy functional theory (SFT)

QMC DMFT solvers: recent developments

New development: continuous-time QMC algorithms

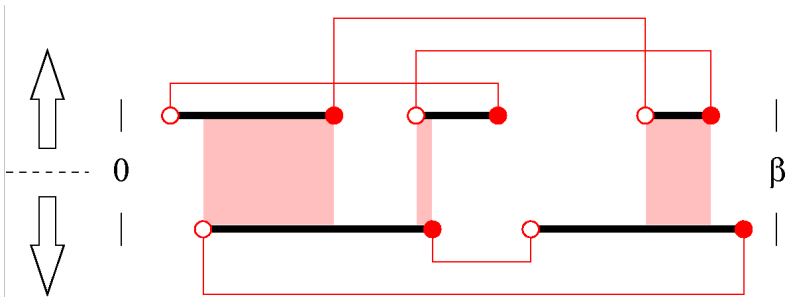
1. weak-coupling expansion

[Rubtsov, Savkin, Lichtenstein, PRB (2005)]



2. hybridization expansion

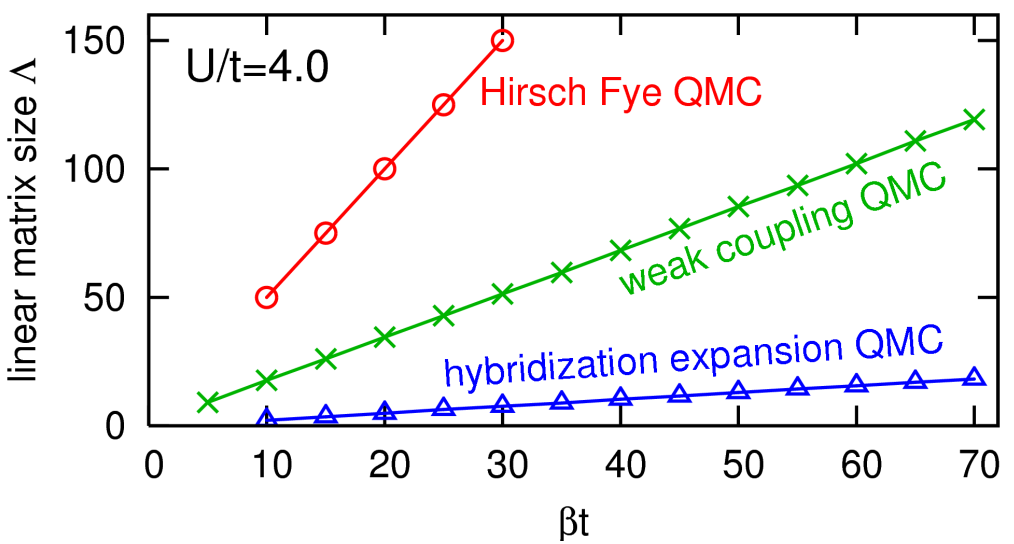
[Werner et al., PRL (2006)]



CT-QMC methods: smaller matrices

All QMC methods: effort $\propto \Lambda^3$

Claim [Troyer (2006)]:
CT-QMC more efficient than
HF-QMC by orders of magnitude



Performance analysis: CT-QMC methods versus HF-QMC

Performance analysis of continuous-time solvers for quantum impurity models

Emanuel Gull,[1] Philipp Werner,[2] Andrew Millis,[2] and Matthias Troyer[1]

[1] *Institut für theoretische Physik, ETH Zürich, CH-8093 Zürich, Switzerland*
[2] *Columbia University, 538 West, 120th Street, New York, NY 10027, USA*

Impurity solvers play an essential role in the numerical investigation of strongly correlated electrons systems within the "dynamical mean field" approximation. Recently, a new class of continuous-time solvers has been developed, based on a diagrammatic expansion of the partition function in either the interactions or the impurity-bath hybridization. We investigate the performance of these two complimentary approaches and compare them to the well-established Hirsch-Fye method. The results show that the continuous-time methods, and in particular the version which expands in the hybridization, provide substantial gains in computational efficiency.

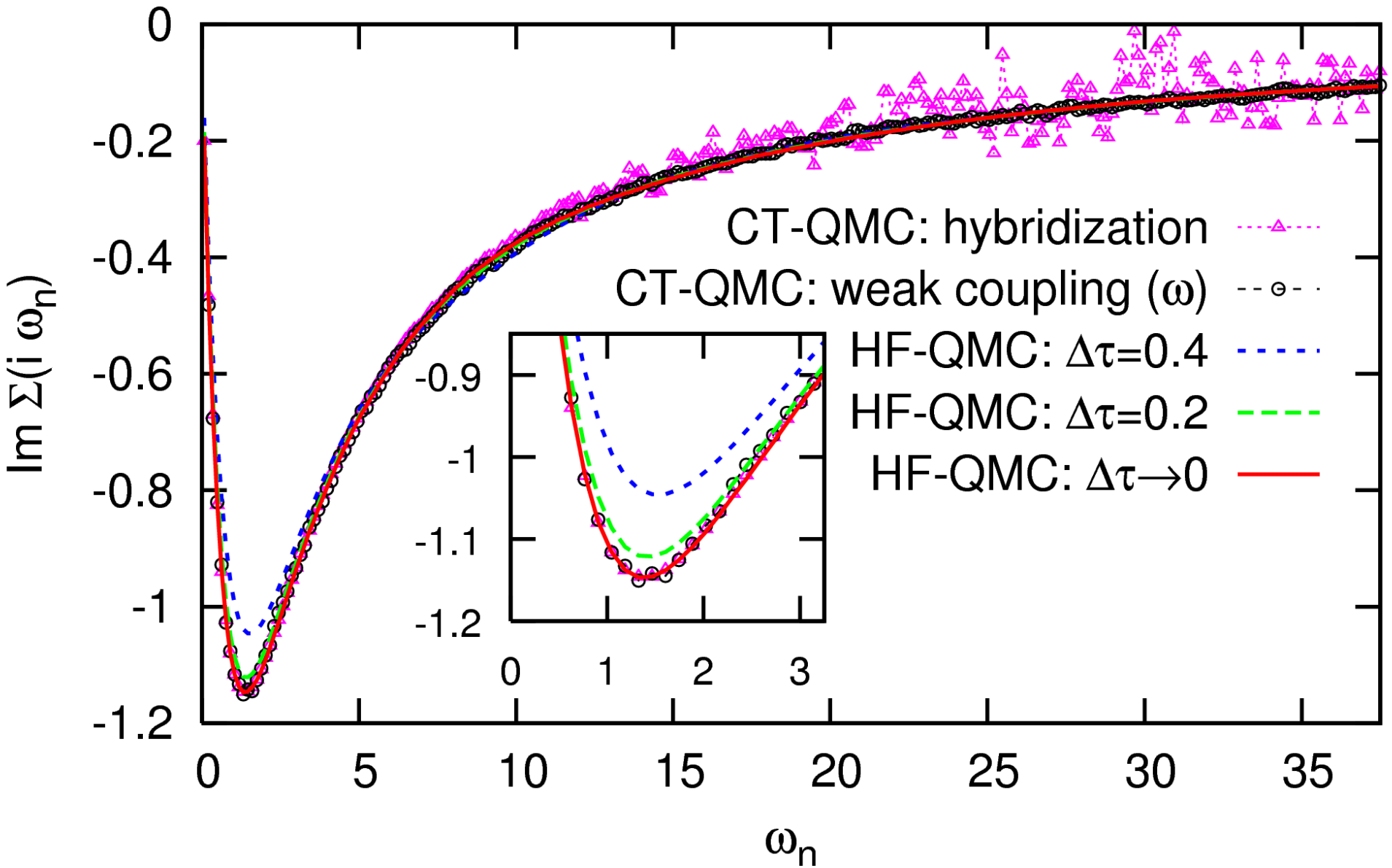
PACS numbers: 71.10.-w, 71.10.Fd, 71.28.+d, 71.30.+h

[cond-mat/0609438]

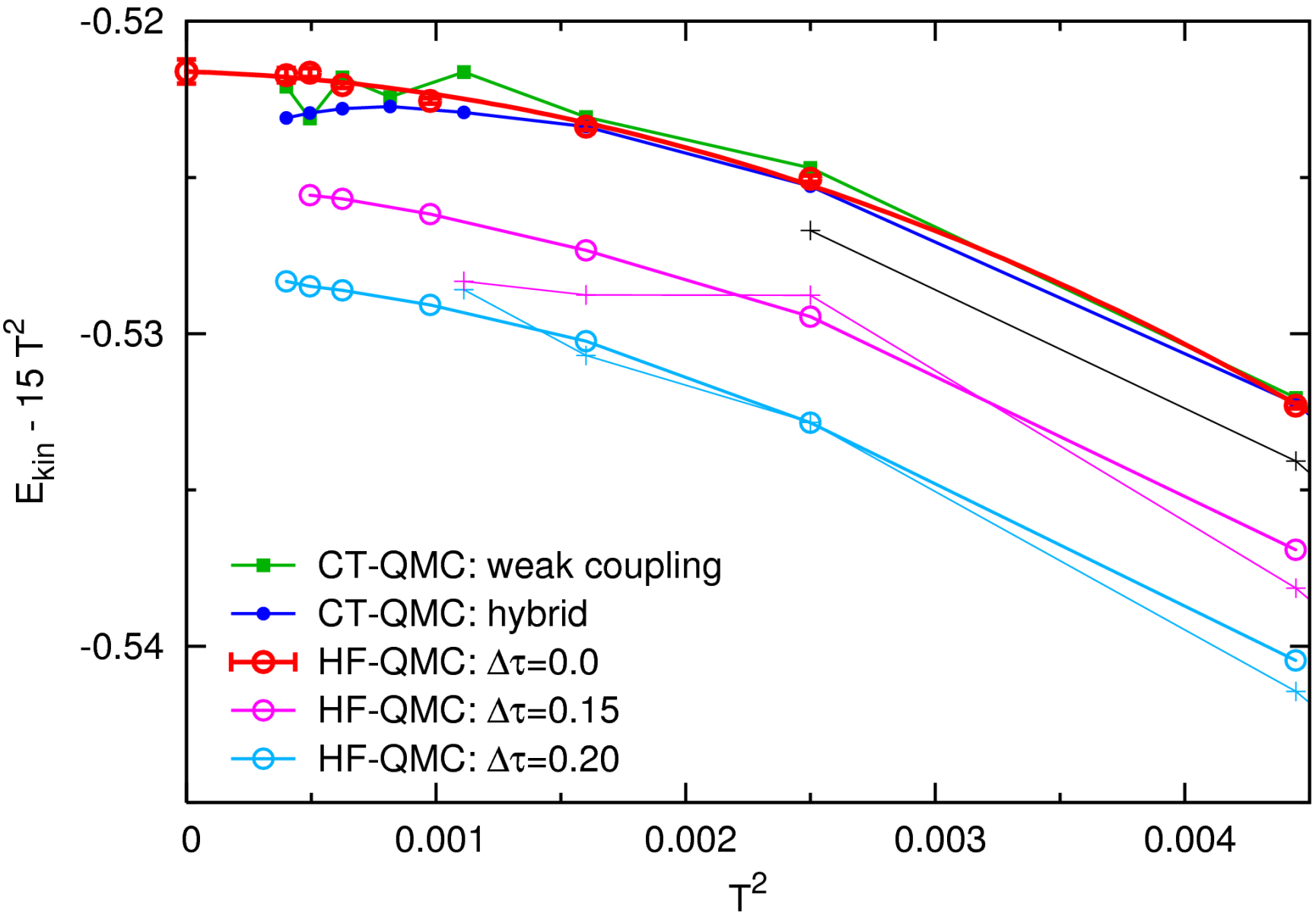
- Test case: 1-band Hubbard model (semi-elliptic DOS, $n = 1$, $W = 4$) for $U = 4$
- Constant computer time: 140 hours on Opteron 244 per data point
- Focus on low temperatures: $T = 1/45$
- Additional results for doped model (also different U)

Good Hirsch-Fye implementation? Fair comparison? Precision of results?

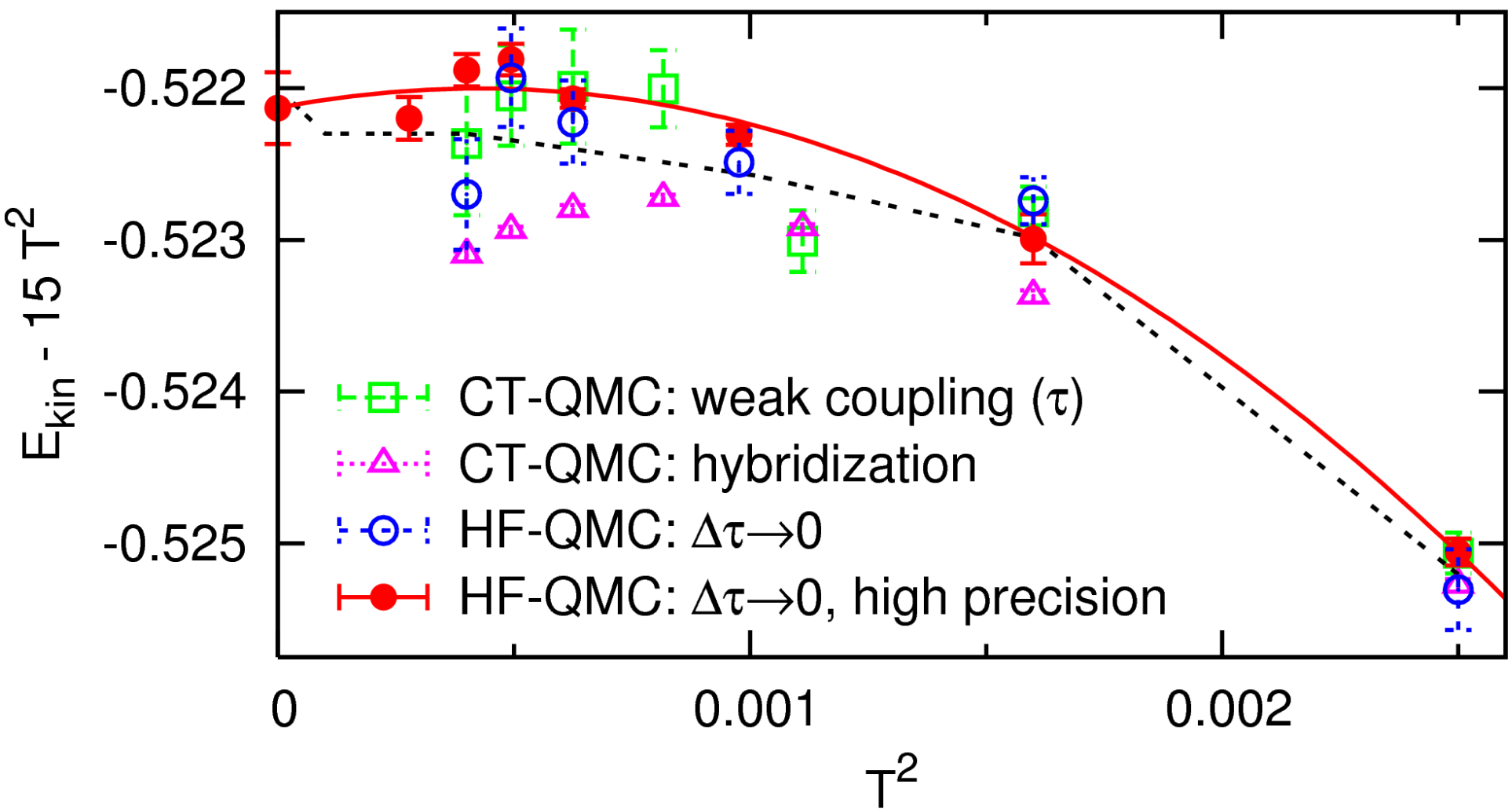
Self-energy on imaginary axis ($T = 1/45$, $U = 4$



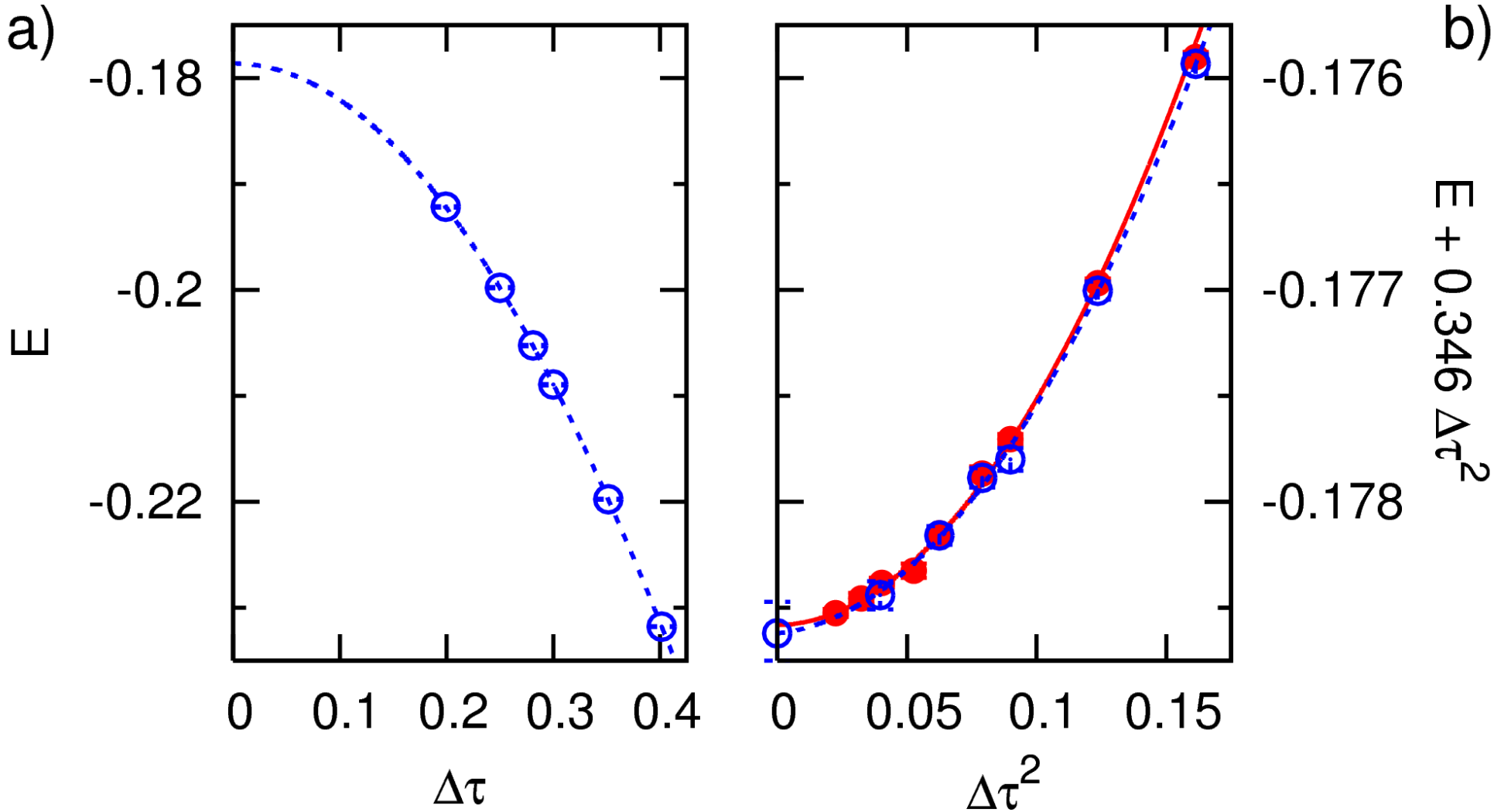
Energetics: kinetic energy for $U = 4$ (first: higher effort for HF-QMC)



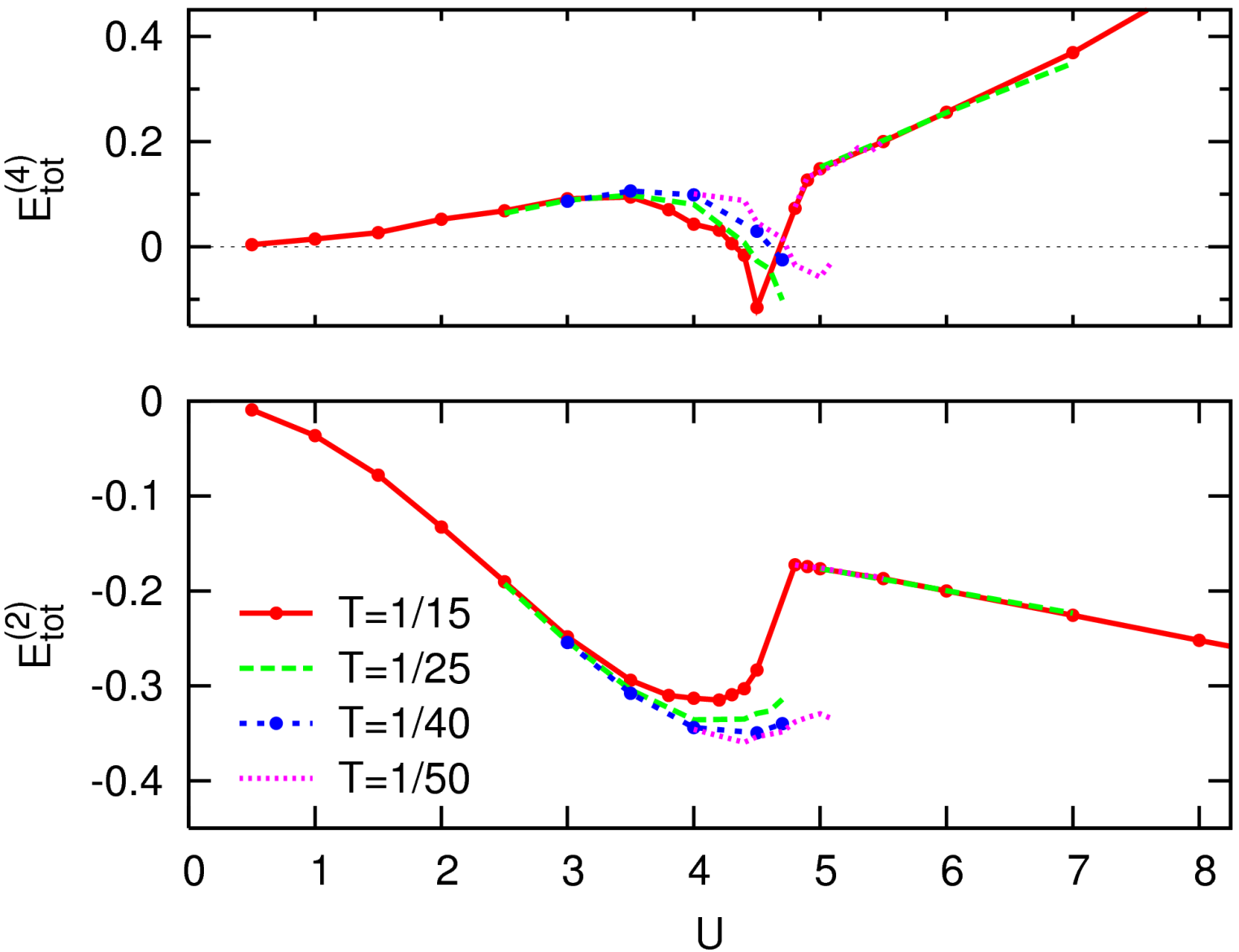
Energetics: kinetic energy for $U = 4$ (same effort for HF-QMC)



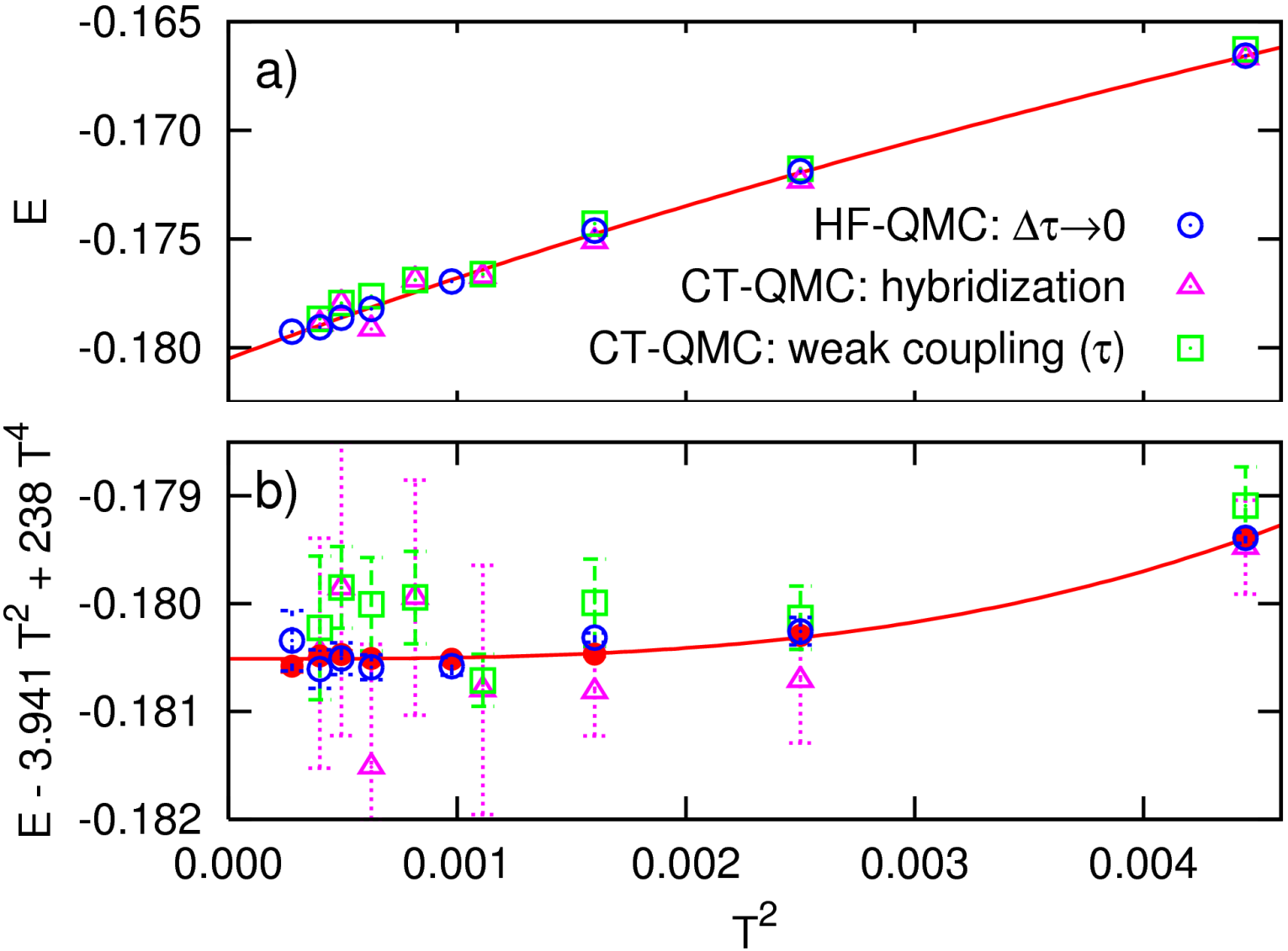
Essential step in HF-QMC: extrapolation $\Delta\tau \to 0$



$\Delta\tau$ dependence very regular (except at phase transition)

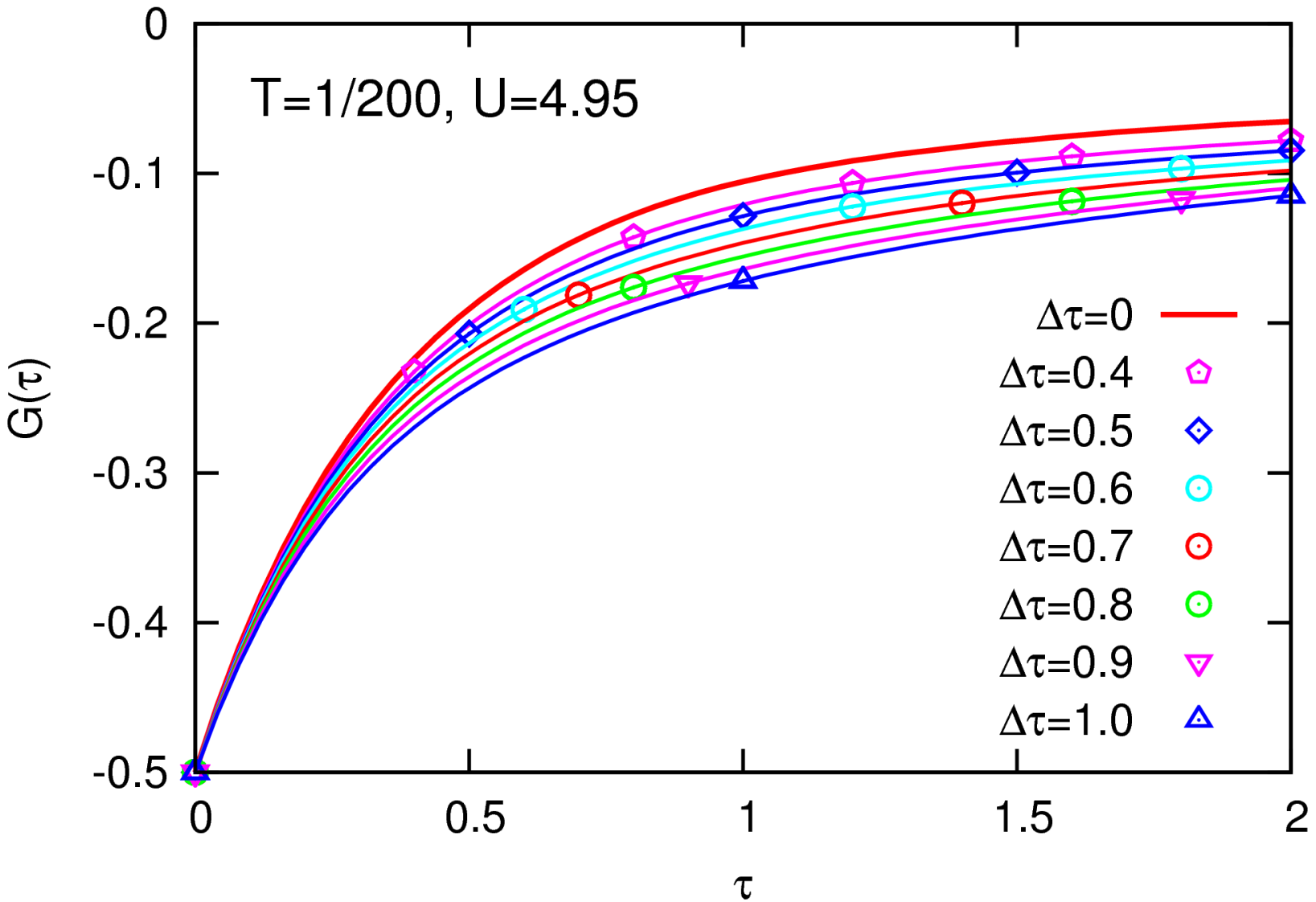


Comparison for total energy



HF-QMC more efficient (much higher precision at same cost) [NB, arXiv:0708.1749]

New: numerically exact Green functions at low T from HF-QMC



Also: first densities of states without discretization error from HF-QMC . . .

Summary

Band structures and effects of (strong) electronic correlations

Theory: DFT, (multi-band) Hubbard models, DMFT, LDA+DMFT

High-precision Hirsch-Fye quantum Monte-Carlo algorithm

Efficiency: HF-QMC competitive with continuous-time QMC

Not covered: Theory of half-metallic double perovskites
Flavor-selective Mott transitions in ultracold quantum gases

Outlook

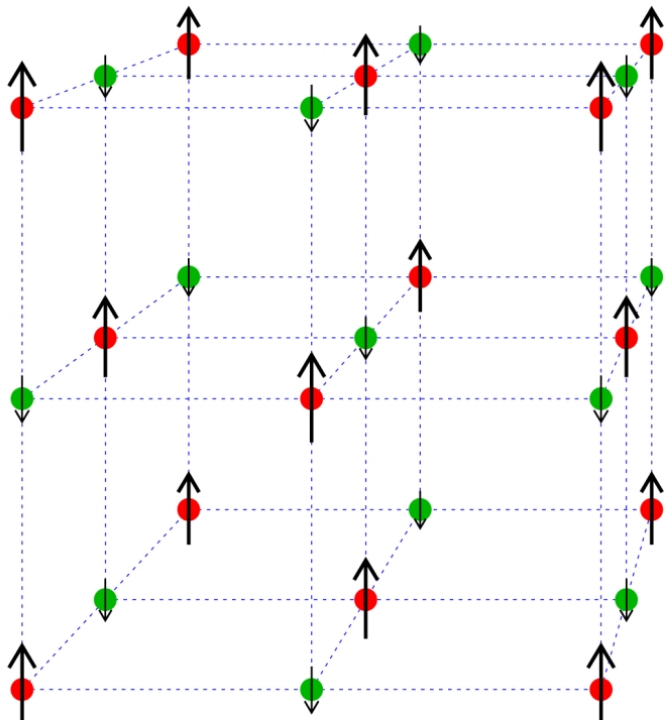
Further improved (better/faster) DMFT solvers

Cluster extensions of DMFT

More complicated systems, full self-consistency, GW+DMFT . . .

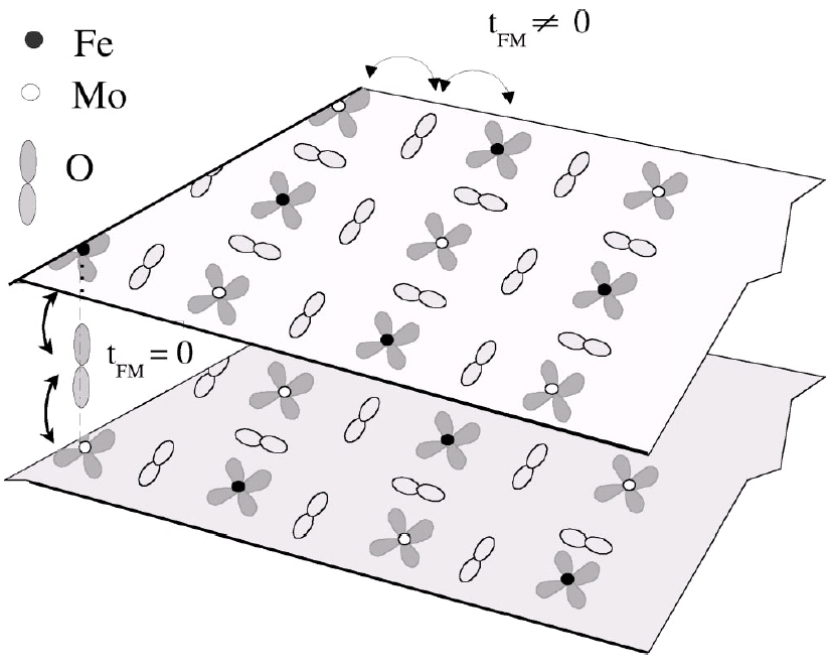
Microscopic theory of half-metallic double perovskites

Goal: correlated-electron theory for Sr_2FeMoO_6 and Sr_2FeReO_6



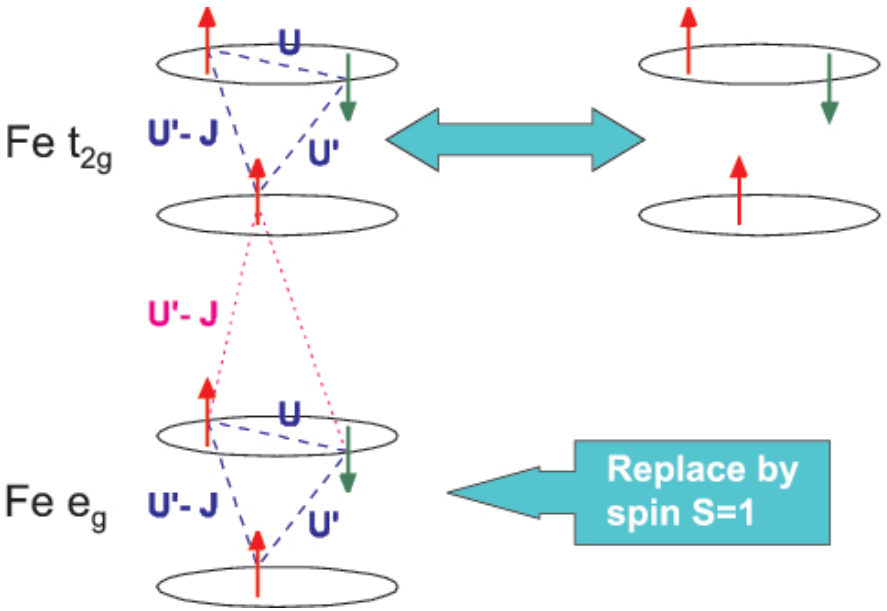
Valences (Sr_2FeMoO_6) Sr^{2+} [Kr]
Fe^{3+} [Ar] 3d5
Mo^{5+} [Kr] 4d1
O^{2-} [Ne]

Cubic symmetry $\longrightarrow$ 3 degenerate t_{2g} bands
2 degenerate e_g bands



t_{2g} hybridization
Fe - O - Mo/Re
[Petrone, Aligia (2002)]

Microscopic theory of half-metallic double perovskites



Full-Hamiltonian LDA+DMFT calculations for 2-site 3-band Hubbard model with

- Fe t_{2g} - t_{2g} interactions
- Fe t_{2g} - e_g interactions
- Fe - Mo/Re hybridization
- controlled DMFT solver: QMC

$$H = \varepsilon_F \sum_{i\alpha\sigma} n^f_{i\alpha\sigma} + \varepsilon_M \sum_{i\alpha\sigma} n^m_{i\alpha\sigma}$$

$$+ U \sum_{i\alpha} n^f_{i\alpha\uparrow} n^f_{i\alpha\downarrow} + \sum_{i\sigma\sigma'} \sum_{\alpha\neq\alpha'} (U' - J\,\delta_{\sigma\sigma'})\, n^f_{i\alpha\sigma} n^f_{i\alpha'\sigma'} - J \sum_{i\alpha} \vec{S}_i \cdot \vec{s}^f_{i\alpha}$$

$$- t_{MF} \sum_{\langle ij\rangle\alpha\sigma} (f^\dagger_{i\alpha\sigma} m_{j\alpha\sigma} + \text{h.c.}) - t_{MM} \sum_{\langle jj'\rangle\alpha\sigma} (m^\dagger_{j\alpha\sigma} m_{j'\alpha\sigma} + \text{h.c.})$$

$t_{MF} \approx 0.25\text{eV}$, $t_{MM} \approx 0.15\text{eV}$, $t_{FF} \approx 0.03\text{eV}$, [Phillips et al. (2003)]

Microscopic theory of half-metallic double perovskites

Preliminary DMFT-QMC results (moderate interactions $\sim 1\,eV$)

- t_{2g} fillings
  - $n_{\mathrm{Fe}} = 3.47$
  - $n_{\mathrm{Mo/Re}} = 1.75$
- t_{2g} moments
  - $m_{\mathrm{Fe}} = 1.5\mu_B$
  - $m_{\mathrm{Mo/Re}} = -1.0\mu_B$
- $n = 5.2$, $m = 2.5\mu_B$

todo:

◊ adjust fillings

◊ stronger interactions

◊ check QMC, MEM ...

◊ make contact with experiments