Update on implementations in DFT+DMFT in ABINIT.

DE LA RECHERCHE À L'INDUSTRIE

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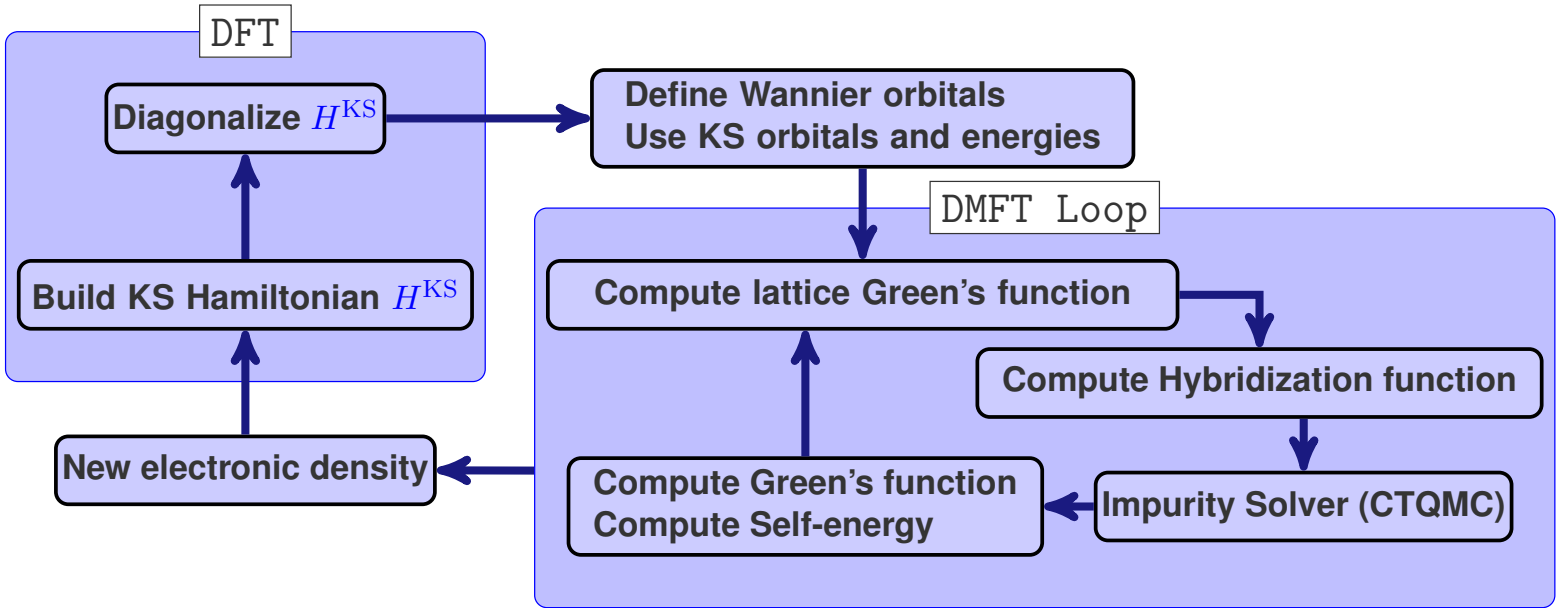
DFT+DMFT Scheme



- Scheme implemented in ABINIT

  L.V. Pourovskii, B. Amadon, S. Biermann, A. Georges Phys. Rev. B **76**, 235101 (2007)
  B. Amadon, F. Lechermann, A. Georges, F. Jollet, T. Wehling and A. I. Lichtenstein Phys. Rev. B **77**, 205112 (2008)
  B. Amadon, Journal of Physics: Condensed Matter **24**, 075604 (2012).
  J. Bieder and B. Amadon Phys. Rev. B **89** (19), 195132 (2014).

Two important points

- Definition of correlated Wannier orbitals
- Resolution of Anderson model (Continuous Time Quantum Monte Carlo)

Introduction

Three topics:

- Improved calculation of Projected Wannier functions: orthonormalization.
- Continuous Time Quantum Monte Carlo for DMFT
  - Calculation of Green's function with Legendre Polynomials.
  - Calculation of occupations of atomic configurations.

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Projected Local Orbital Wannier functions

- We define $|\tilde{\chi}^{\mathbf{R}}_{\mathbf{k}m}\rangle$ as a sum over a limited number of KS states in the window energy $\mathcal{W}$ of projection of KS states over atomic orbitals.

$$|\tilde{\chi}^{\mathbf{R}}_{\mathbf{k}m}\rangle \equiv \sum_{\nu\in\mathcal{W}} \langle\Psi_{\mathbf{k}\nu}|\chi^{\mathbf{R}}_{\mathbf{k}m}\rangle|\Psi_{\mathbf{k}\nu}\rangle = P^{\mathbf{R}}_{m\nu}(\mathbf{k})^*|\Psi_{\mathbf{k}\nu}\rangle$$

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- $|\tilde{\chi}^{\mathbf{R}}_{\mathbf{k}m}\rangle$ need to be orthonormalized to give true Wannier functions $|w^{\mathbf{R}}_{\mathbf{k}m}\rangle$.

$$O^{\mathbf{R},\mathbf{R}'}_{m,m'}(\mathbf{k}) = \langle\tilde{\chi}^{\mathbf{R}}_{\mathbf{k}m}|\tilde{\chi}^{\mathbf{R}'}_{\mathbf{k}m'}\rangle = \sum_{\nu} P^{\mathbf{R}}_{m\nu}(\mathbf{k})P^{\mathbf{R}'}_{m'\nu}(\mathbf{k})^* \qquad (1)$$

or $$O^{\mathbf{R},\mathbf{R}'}_{m,m'} = \langle\tilde{\chi}^{\mathbf{R}}_{\mathbf{T}m}|\tilde{\chi}^{\mathbf{R}'}_{\mathbf{T}m'}\rangle = \sum_{\nu\mathbf{k}} P^{\mathbf{R}}_{m\nu}(\mathbf{k})P^{\mathbf{R}'}_{m'\nu}(\mathbf{k})^* \qquad (2)$$

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- $|w^{\mathbf{R}}_{\mathbf{k}m}\rangle$ is thus obtained though:

$$|w^{\mathbf{R}}_{\mathbf{k}m}\rangle = \sum_{\mathbf{R}',m'} \left\{[O]^{-1/2}\right\}^{\mathbf{R},\mathbf{R}'}_{m,m'} |\tilde{\chi}^{\mathbf{R}'}_{\mathbf{k}m'}\rangle$$

For several atoms, default choice is now choice (1) (variable `dmft_wanorthnorm=2`)

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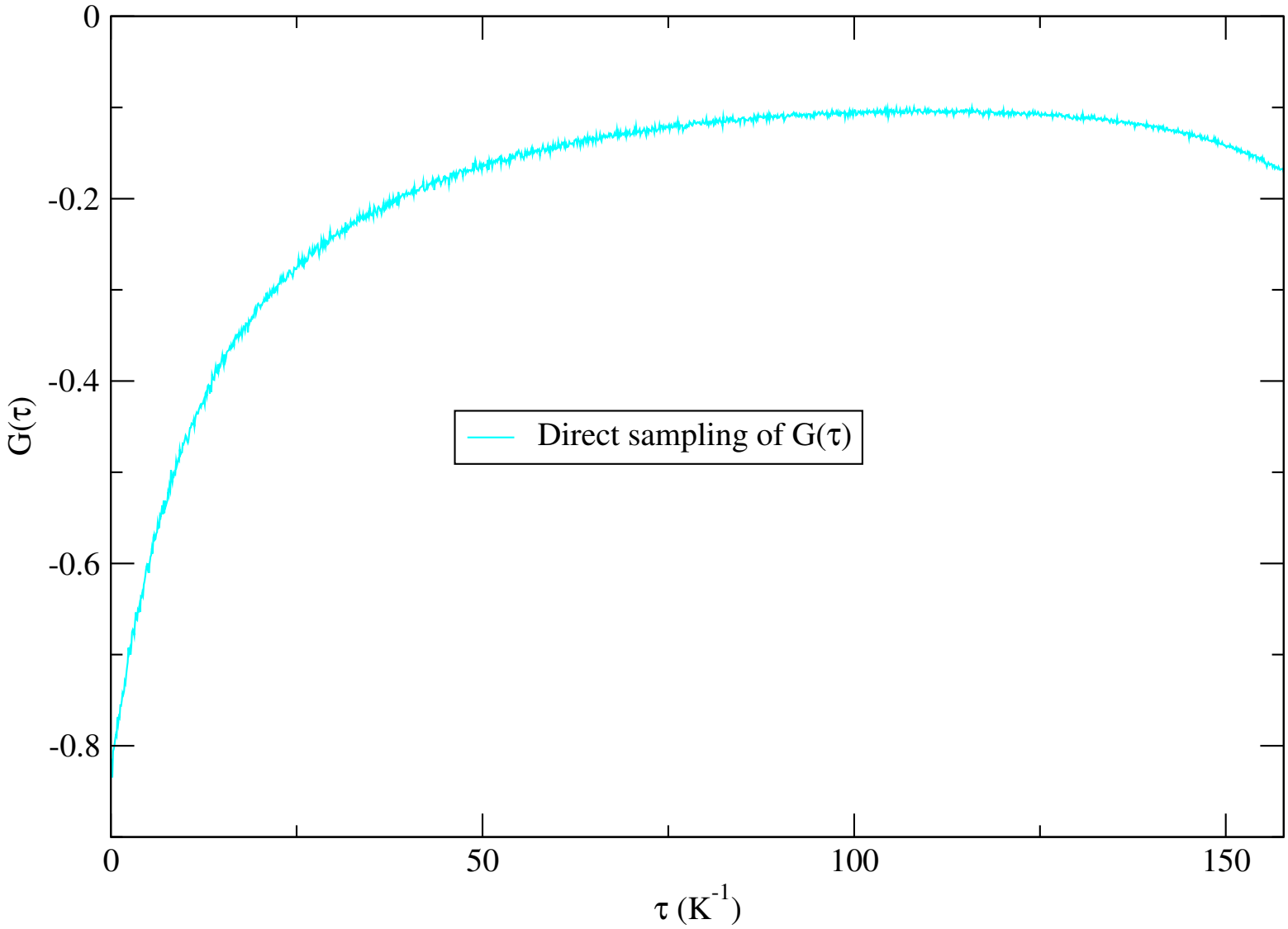
CTQMC calculation: role of noise

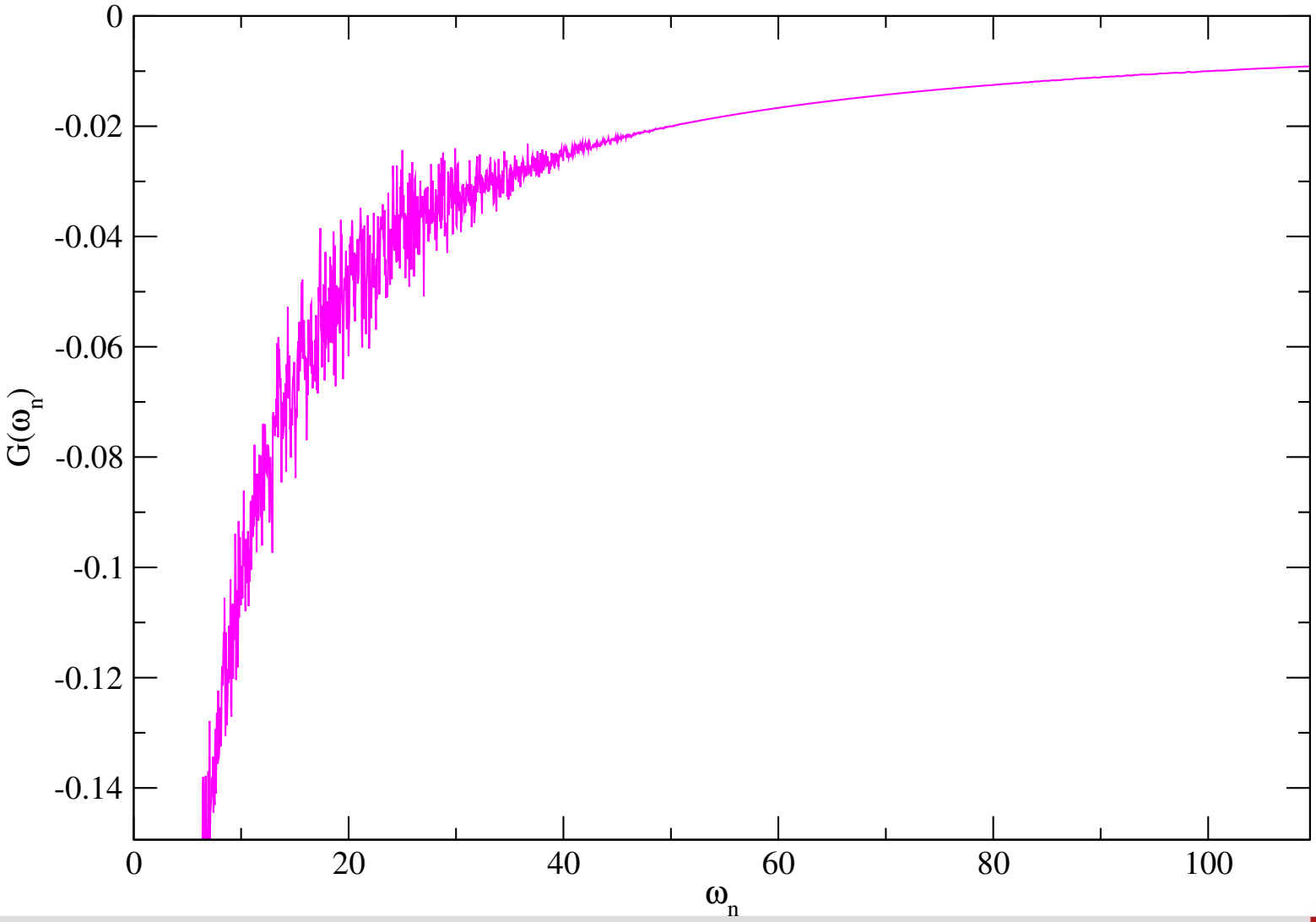
- The output of the CTQMC calculation is the Green's function $G(\tau)$.

Green function in imaginary time



Green function in imaginary frequency

Fourier transformation gives :



CTQMC calculation: role of noise

- It is a quantity that can be noisy
- Legendre polynomial expansion is a possible solution proposed by L. Boehnke *et al* Phys. Rev. B 84, 075145 (2011).
  - Based upon a filtering of large component of the expansion.

Legendre expansion of Green's function

Legendre Polynomials expansion:

$$G(\tau) = \sum_{l \geq 0} \frac{\sqrt{2l+1}}{\beta} P_l(x(\tau))\, G_l,$$

$$G_l = \sqrt{2l+1} \int_0^\beta d\tau\, P_l(x(\tau))\, G(\tau).$$

where $x(\tau) = 2\tau/\beta - 1$ and G_l denote the coefficients of $G(\tau)$ in the Legendre basis.

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The G_l can be computed directly in the Monte Carlo simulation.

Legendre expansion of Green's function

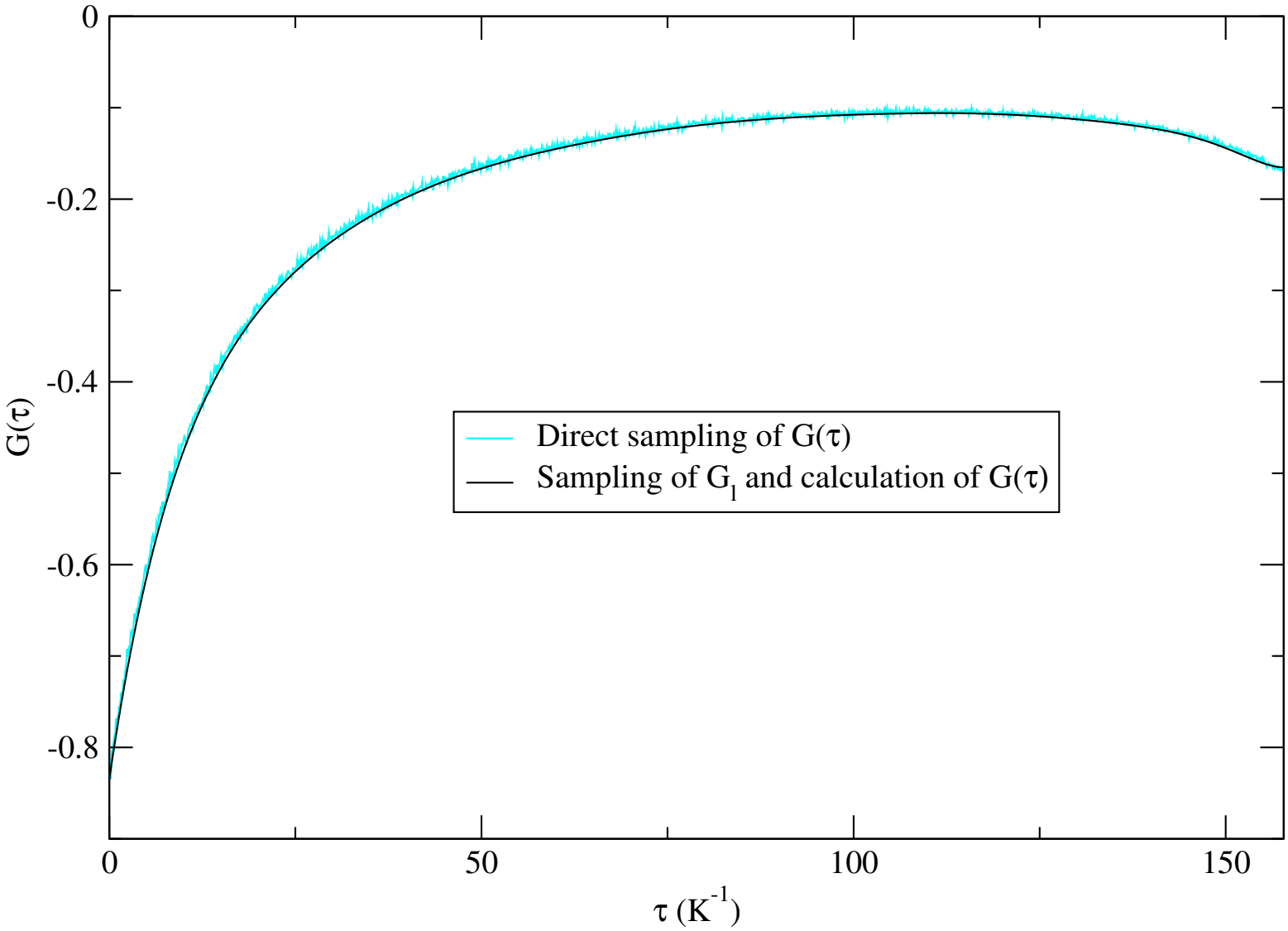
The Green's function in imaginary frequency can be computed directly by taking analytically the Fourier transform:

$$G(i\omega_n) = \sum_{l\geq 0} G_l \frac{\sqrt{2l+1}}{\beta} \int_0^\beta d\tau \; \mathrm{e}^{i\omega_n \tau} \; P_l(x(\tau))$$
$$= \sum_{l\geq 0} T_{nl} G_l .$$

where the unitary transformation T_{nl} can be shown to be

$$T_{nl} = (-1)^n \, i^{l+1} \sqrt{2l+1} \; j_l\left(\frac{(2n+1)\pi}{2}\right)$$

Green function in imaginary time



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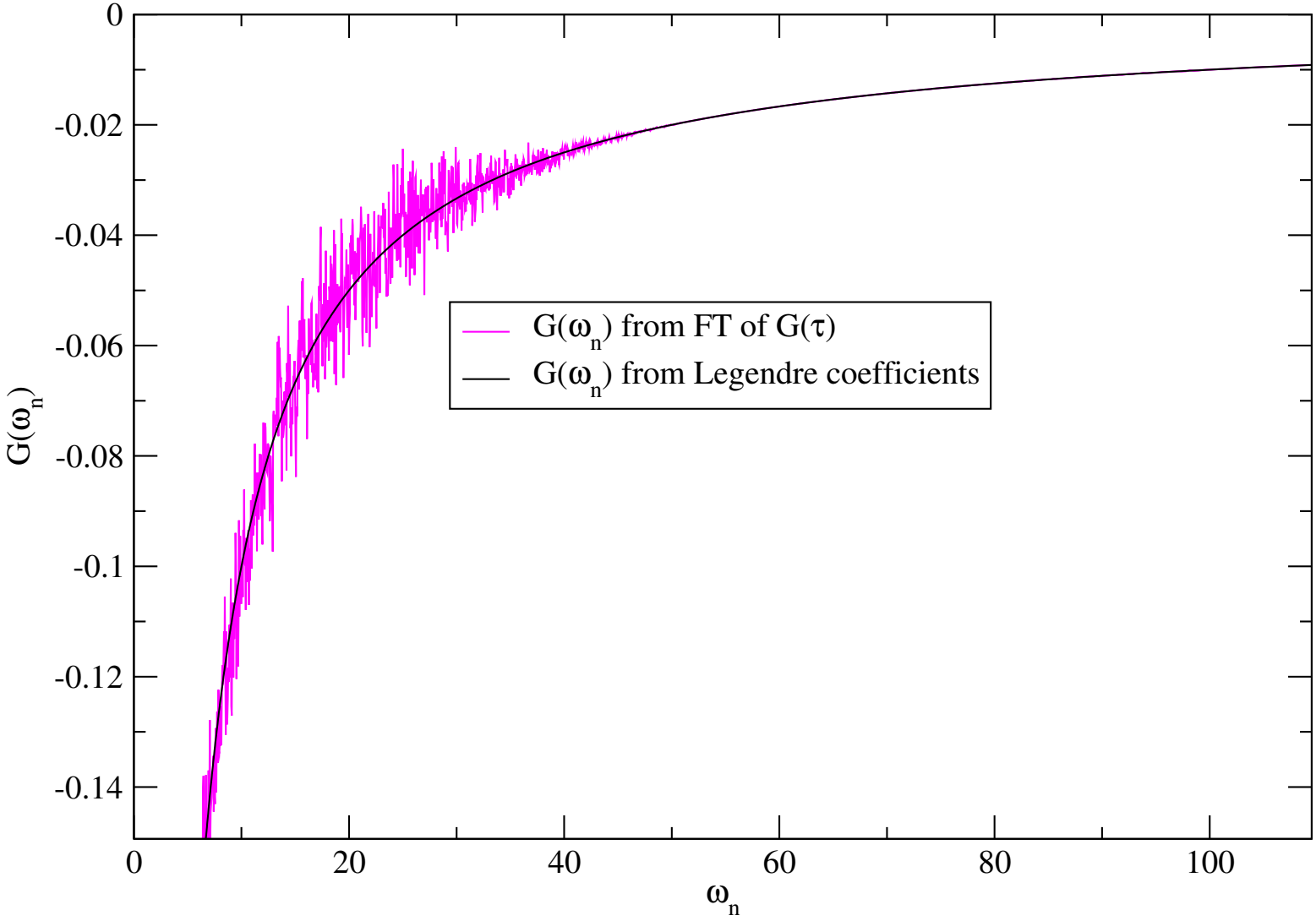

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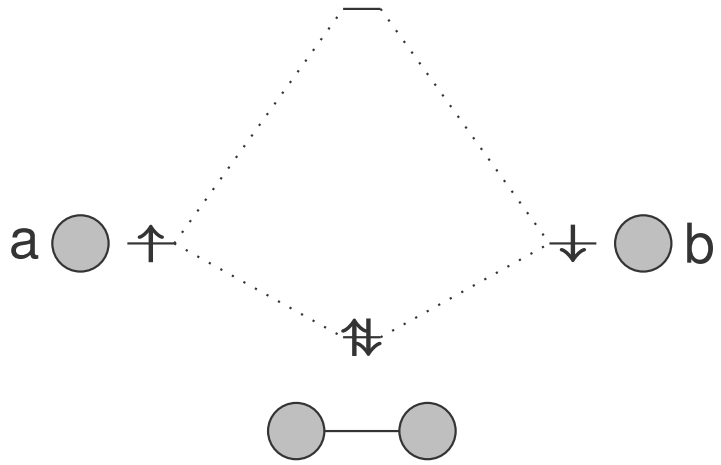
Occupations of atomic configurations

H_2 molecule



bonding state $|\sigma_g\rangle = \frac{1}{\sqrt{2}}|a\rangle + \frac{1}{\sqrt{2}}|b\rangle$

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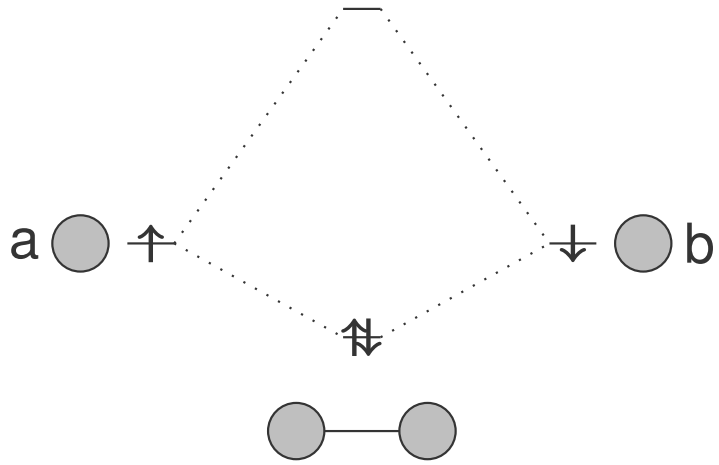

bonding state $|\sigma_g\rangle = \frac{1}{\sqrt{2}}|a\rangle + \frac{1}{\sqrt{2}}|b\rangle$

With $U = 0$, the wavefunction is :

$$|\Psi_t\rangle = |\sigma_g\sigma_g\rangle = \left(\frac{1}{\sqrt{2}}|a\rangle + \frac{1}{\sqrt{2}}|b\rangle\right)\left(\frac{1}{\sqrt{2}}|a\rangle + \frac{1}{\sqrt{2}}|b\rangle\right)$$

$$= \frac{1}{2}|aa\rangle + \frac{1}{2}|ab\rangle + \frac{1}{2}|ba\rangle + \frac{1}{2}|bb\rangle \quad \Rightarrow \text{Occup. of config } a^0\text{: } 0.25 \mid a^1\text{: } 0.50 \mid a^2\text{: } 0.25$$

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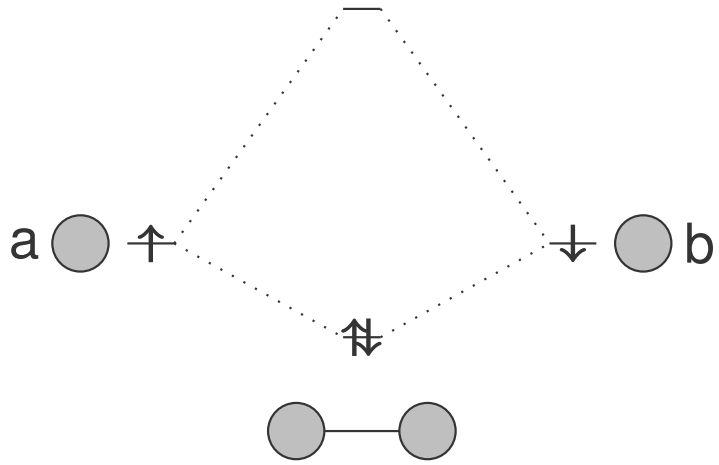

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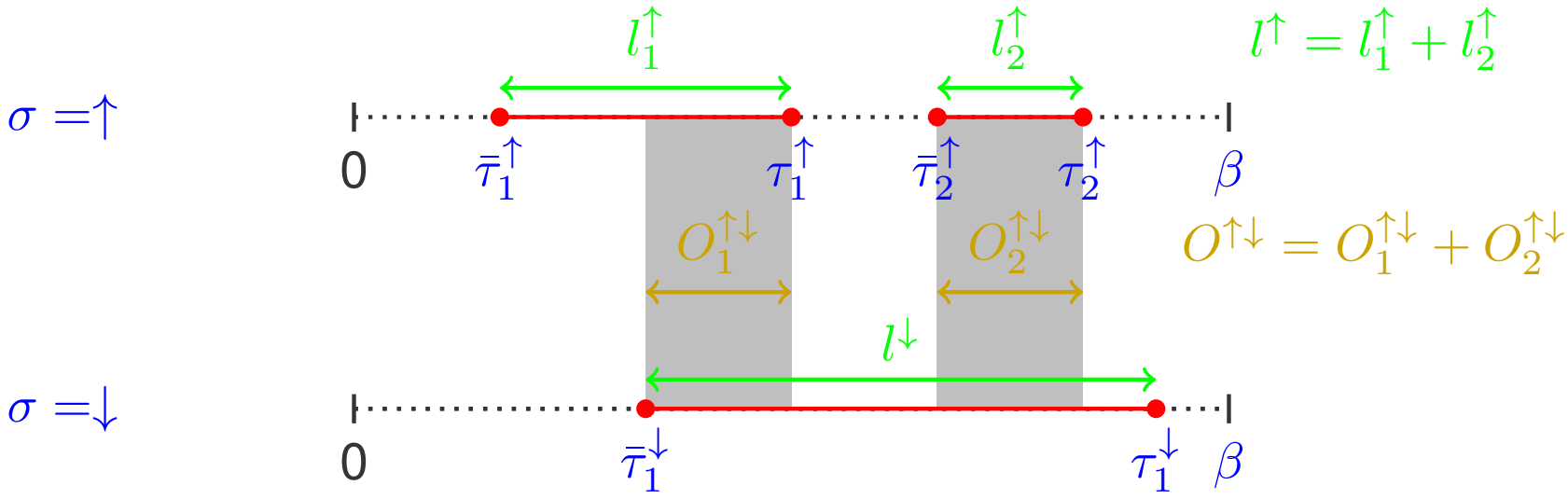
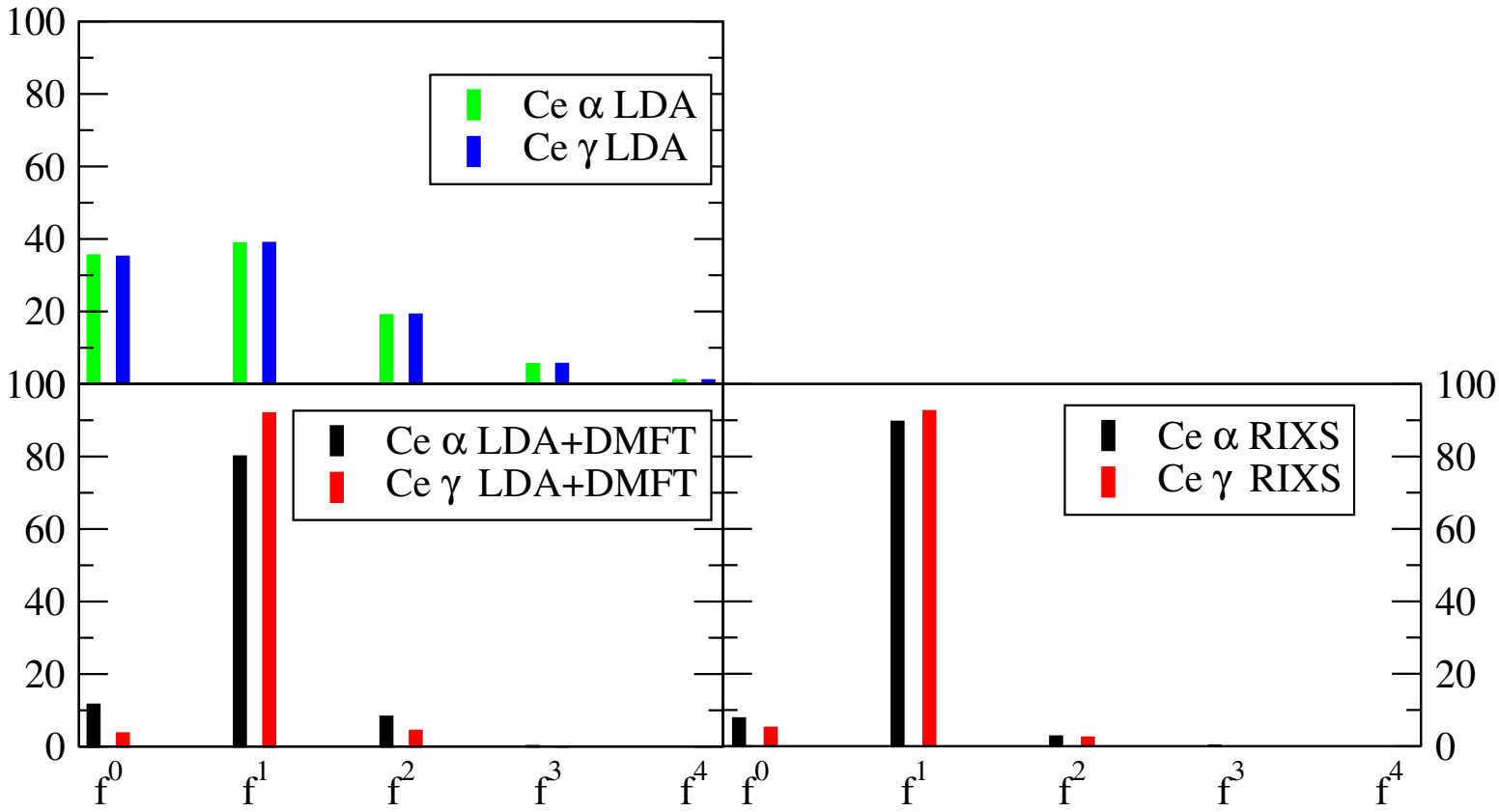
If U is non zero, and goes to infinity, the wavefunction is

$$|\Psi_t\rangle = \frac{1}{\sqrt{2}}|ab\rangle + \frac{1}{\sqrt{2}}|ba\rangle \quad \Rightarrow \text{Occup. of config } a^0\text{: } 0.00 \mid a^1\text{: } 1.00 \mid a^2\text{: } 0.00$$

Method of calculation



Exemple of cerium



RIXS data: Rueff *et al* PRL **96**, 237403 (2006)

Conclusion and perspectives

- Wannier function orthonormalization: usefull also for cRPA.
- Reduction of noise with Legendre Polynomial.
  - Also possible: direct calculation of the self-energy
- Calculation of configurations occupations
  - Might be generalized to identify configurations with different quantum numbers

Projects

- Forces in DFT+DMFT
- Extension of SOC.

Thanks to
J.B. Morée, and R. Outerovitch