Continuous-time quantum Monte Carlo algorithms for impurity models

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IP PARIS

Continuous-time quantum Monte Carlo algorithms

- **Motivation: quantum impurity problems**

  Historical importance of quantum impurity problems and algorithmic developments

- **Continuous-time quantum Monte Carlo (CT-QMC) methods**

  Introduction to the idea of CT-QMC methods and their different versions

- **The interaction-expansion algorithm (CT-INT)**

  Write a perturbation series expansion in the Coulomb interaction

- **The hybridization-expansion algorithm (CT-HYB)**

  Write a perturbation series expansion in the hybridization function

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References

- Quantum impurity problems:
  A. C. Hewson, "The Kondo Problem to Heavy Fermions", Cambridge University Press

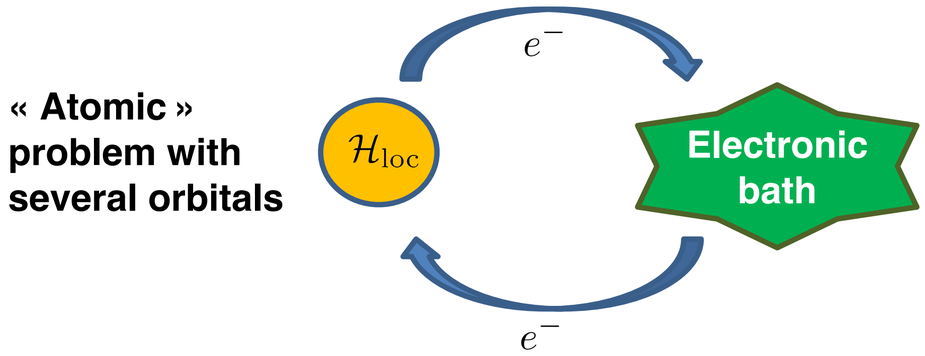
- CT-QMC solvers: *E. Gull et al., RMP (2011)*
  - The interaction-expansion algorithm
    Rubtsov et al. , PRB (2005) and Rubtsov and Lichtenstein, JETP Lett. (2004)
  - The hybridization-expansion algorithm
    Werner and Millis, PRB (2006) and Werner et al., PRL (2006)

- Dynamical mean-field theory: *A. Georges et al., RMP (1996)*

- Open source CT-QMC solver used in TRIQS tutorial:
  - CT-HYB: *https://triqs.github.io/cthyb*
  - CT-INT: *https://github.com/TRIQS/ctint_tutorial*

Quantum impurity problems

- They generically describe the behavior of a magnetic impurity embedded in an electronic host
- The impurity is a set of “orbitals” carrying local many-body interactions. It can exchange electrons with an uncorrelated fermionic bath.



- Impurity models have a long history, e.g. the Kondo problem
- Lead to the development of models and methods

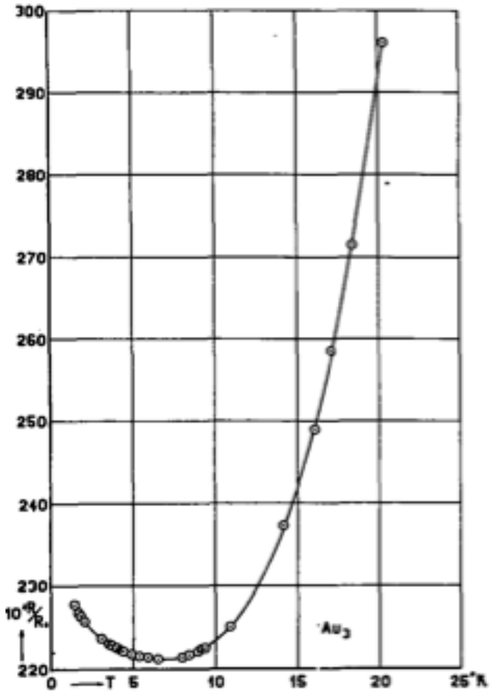
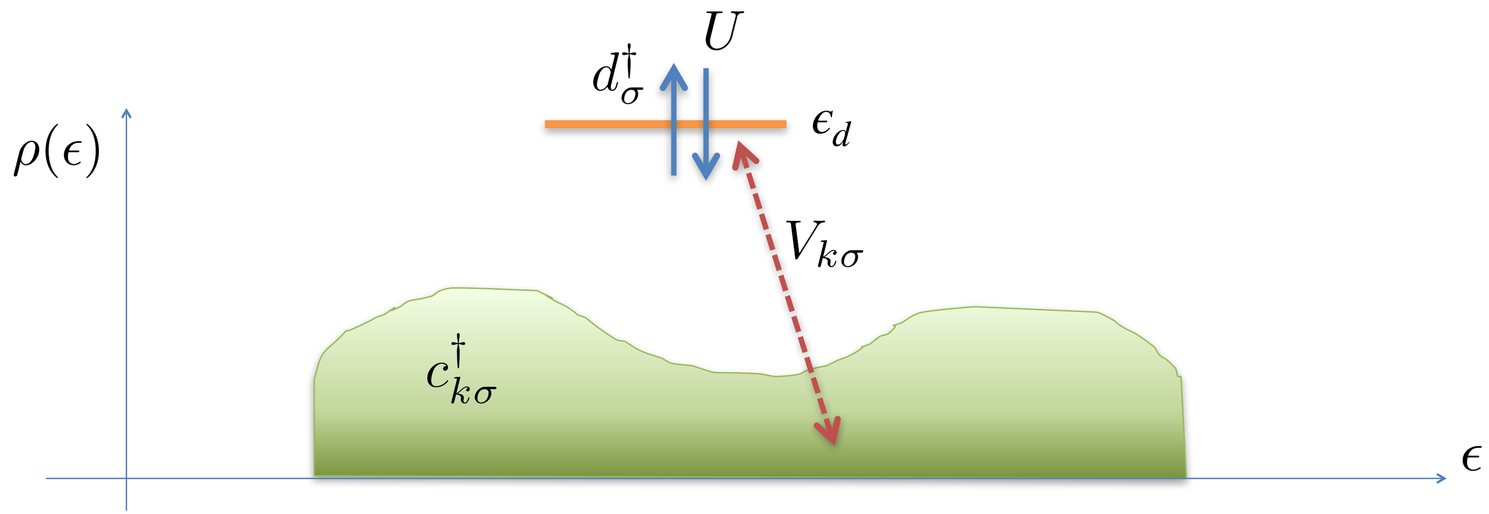


Fig. 1. Electrical resistance of Au_3.

de Haas, van den Berg, 1936

The Anderson model

- A very successful model to understand magnetic impurities in a metallic host is the Anderson model
- Hamiltonian:



$$\mathcal{H} = \sum_{\sigma=\uparrow,\downarrow} \epsilon_0 d^\dagger_\sigma d_\sigma + U n_{d\uparrow} n_{d\downarrow} + \sum_{k,\sigma} V_{k\sigma} c^\dagger_{k\sigma} d_\sigma + \text{h.c.} + \sum_{k,\sigma} \epsilon_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma}$$

local many-body interaction

hybridization to the bath

free bath states

The Anderson model

- When $U = 0$, the Anderson model can be solved
- Its non-interacting Green function is then

$$G_0(i\omega_n) = \frac{1}{i\omega_n - \epsilon_d - \Delta(i\omega_n)}$$

where

$$\Delta(i\omega_n) = \sum_k \frac{|V_k|^2}{i\omega_n - \epsilon_k}$$

hybridization function: describes the transition between the bath and the orbital

- The Anderson impurity model is completely determined by the interaction U and the hybridization function Δ
- The model can be generalized (more orbitals, sites, etc.)

A difficult problem!

- The Anderson model is a many-body (correlated) problem with an infinite number of degrees of freedom! It has attracted a lot of interest and many techniques have been developed:
- (Semi) Analytical methods
  - Bethe Ansatz, BCFT
  - Non-crossing approximation
- Numerical algorithms
  - Exact diagonalization
  - Numerical renormalization group
  - Density matrix renormalization group
  - Continuous-time quantum Monte Carlo algorithms
  - And many more…
- All have pros and cons!

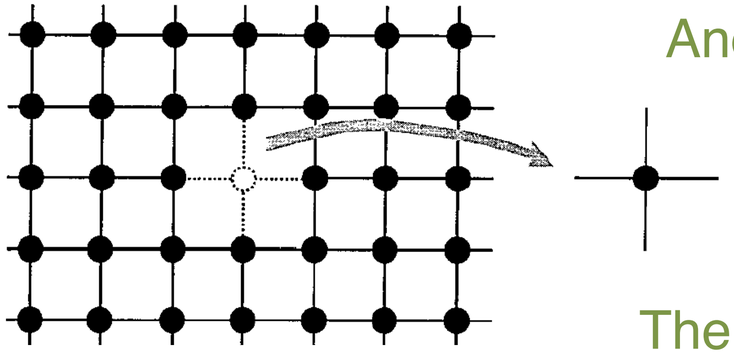
Our goal: solve the DMFT equations

A. Georges and G. Kotliar, PRB (1992)
A. Georges et al., RMP (1996)

- The dynamical mean-field theory makes an approximation of a lattice model using an auxiliary quantum impurity problem

Lattice Hubbard model

$$\mathcal{H} = \sum_k \epsilon_k c_k^\dagger c_k + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



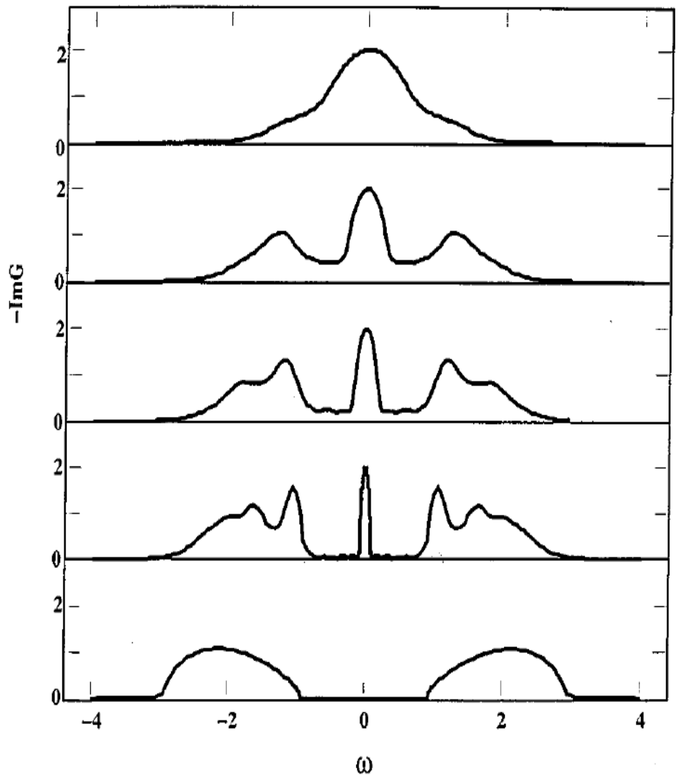
Anderson impurity model

Bath G_0

The bath has to be set self-consistently

The DMFT aficionado wish list

- The impurity solver must compute the local Green's function
- Bath can have a rich structure, be gapped (insulators, superconductors)
- Structures appear at all scales (transfer of spectral weight in the Mott transition)
- The impurity solver must be able to treat many orbitals (e.g. realistic materials)
- The interaction Hamiltonian can be generic (pair-hopping, spin flip terms)
- The model is studied in different temperature regimes
- One would like to be able to have real-frequency spectra



Continuous-time quantum Monte Carlo algorithms

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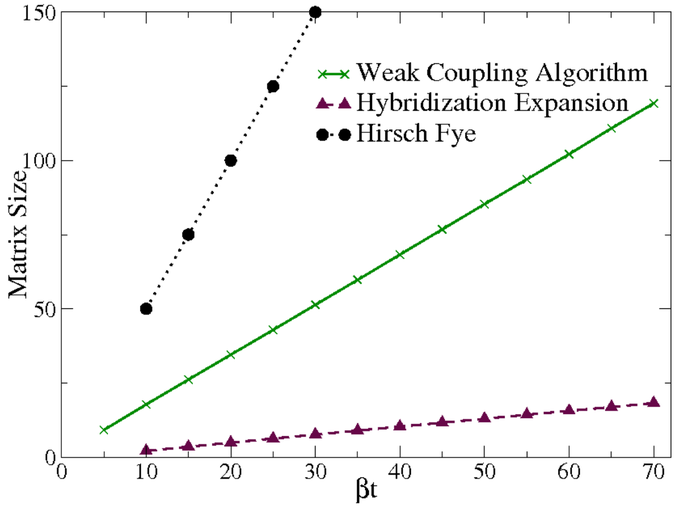
Continuous-time quantum Monte Carlo methods

- They have been a small revolution!



- They exist in different flavors:
  - CT-INT: Interaction expansion
  - CT-HYB: Hybridization expansion
  - CT-AUX: Auxiliary-field formulation

- The underlying principle is the same for all these algorithms
  - Write a series expansion of the partition function and physical observables
  - Sample the contributions stochastically (Monte Carlo)
  - Compute quantities of interest (Green's function, …)

Continuous-time quantum Monte Carlo methods

- Different version correspond to different ways to construct your perturbation series

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_I$$

- CT-INT (and also CT-AUX)
  - H_0 is the non-interacting system and H_I the Coulomb interaction

    We want to compute $Z = \sum_n a_n U^n$

    computing the a_n involves many integrals that we will compute using a Monte Carlo algorithm

- CT-HYB
  - H_0 is the “atomic limit” and H_I is the hybridization to the bath Δ

    We want to compute " $Z = \sum_n a_n \Delta^n$ "

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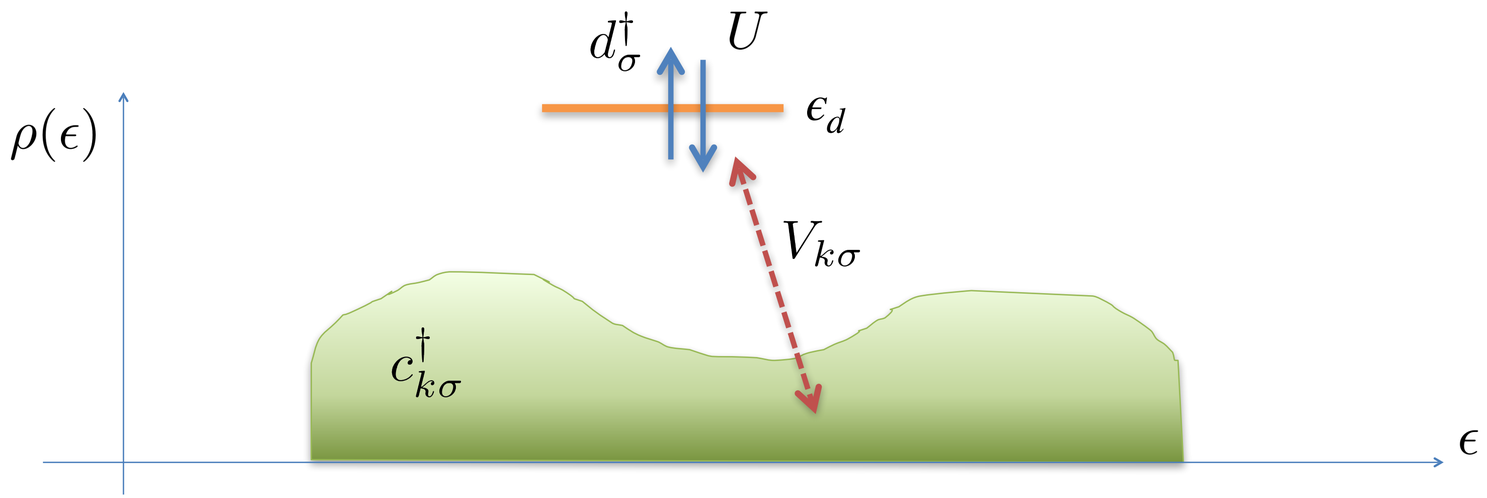
Interaction expansion CT-QMC

- We focus on the simplest Anderson model (can be generalized to multi-orbital problems)
- We want to derive an expansion around the non-interacting limit (expansion in the interaction)



$$\mathcal{H} = \sum_{\sigma=\uparrow,\downarrow} \epsilon_0 d^\dagger_\sigma d_\sigma + U n_{d\uparrow} n_{d\downarrow} + \sum_{k,\sigma} V_{k\sigma} c^\dagger_{k\sigma} d_\sigma + \text{h.c.} + \sum_{k,\sigma} \epsilon_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma}$$

Interaction expansion CT-QMC

- We want to write a series expansion in U. We have $H = H_0 + H_I$ with $H_I = U n_\uparrow n_\downarrow$

- We start from the equation of motion for the evolution operator

$$\partial_\tau \hat{U}(\tau, \tau') = -\hat{H}_I(\tau)\, \hat{U}(\tau, \tau')$$

  where we have used the interaction picture

$$\hat{A}(\tau) = e^{\tau H_0} A\, e^{-\tau H_0} \qquad\qquad \hat{U}(\tau, \tau') = e^{\tau H_0} U(\tau, \tau')\, e^{-\tau' H_0}$$

- Integration the equation above yields

$$\hat{U}(\tau, \tau') = 1 - \int_{\tau'}^{\tau} d\tau_1\, \hat{H}_I(\tau_1) \hat{U}(\tau_1, \tau')$$

Interaction expansion CT-QMC

- Repeating the procedure:

$$\hat{U}(\tau,\tau') = 1 - \int_{\tau'}^{\tau} d\tau_1\, \hat{H}_I(\tau_1) + \int_{\tau'}^{\tau} d\tau_1 \int_{\tau'}^{\tau_1} d\tau_2\, \hat{H}_I(\tau_1)\hat{H}_I(\tau_2) - \int_{\tau'}^{\tau} d\tau_1 \int_{\tau'}^{\tau_1} d\tau_2 \int_{\tau'}^{\tau_2} d\tau_3\, \hat{H}_I(\tau_1)\hat{H}_I(\tau_2)\hat{H}_I(\tau_3) + \dots$$

- Pushing the integration limits to τ and introducing the time-ordering operator T_τ

$$\hat{U}(\tau,\tau') = 1 - \int_{\tau'}^{\tau} d\tau_1\, \hat{H}_I(\tau_1) + \frac{1}{2!}\int_{\tau'}^{\tau} d\tau_1 \int_{\tau'}^{\tau} d\tau_2\, T_\tau\left[\hat{H}_I(\tau_1)\hat{H}_I(\tau_2)\right] - \frac{1}{3!}\int_{\tau'}^{\tau} d\tau_1 \int_{\tau'}^{\tau} d\tau_2 \int_{\tau'}^{\tau} d\tau_3\, T_\tau\left[\hat{H}_I(\tau_1)\hat{H}_I(\tau_2)\hat{H}_I(\tau_3)\right] + \dots$$

$$\hat{U}(\tau,\tau') = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_{\tau'}^{\tau} d\tau_1 \cdots \int_{\tau'}^{\tau} d\tau_n\, T_\tau\left[\hat{H}_I(\tau_1)\cdots\hat{H}_I(\tau_n)\right]$$

Interaction expansion CT-QMC

- We want to compute the partition function

$$Z = \mathrm{Tr}\, e^{-\beta \mathcal{H}_0}\, \hat{U}(\beta, 0)$$

- Remembering that the average value of an operator in the non-interacting system is

$$\langle A \rangle_0 = \frac{1}{Z_0} \mathrm{Tr}\, e^{-\beta H_0} A$$

we obtain

$$\frac{Z}{Z_0} = \left\langle \hat{U}(\beta, 0) \right\rangle_0 = \sum_{n=0}^{\infty} \frac{(-U)^n}{n!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \, \langle T_\tau \left[\hat{n}_\uparrow \hat{n}_\downarrow(\tau_1) \cdots \hat{n}_\uparrow \hat{n}_\downarrow(\tau_n) \right] \rangle_0$$

Interaction expansion CT-QMC

- The final step is to use Wick's theorem to compute the non-interacting averages

$$\frac{Z}{Z_0} = \left\langle \hat{U}(\beta,0) \right\rangle_0 = \sum_{n=0}^{\infty} \frac{(-U)^n}{n!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \, \left\langle T_\tau \left[\hat{n}_\uparrow \hat{n}_\downarrow(\tau_1) \cdots \hat{n}_\uparrow \hat{n}_\downarrow(\tau_n) \right] \right\rangle_0$$

$$\frac{Z}{Z_0} = \left\langle \hat{U}(\beta,0) \right\rangle_0 = \sum_{n=0}^{\infty} \frac{(-U)^n}{n!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \, \det M_\uparrow^{(n)} \, \det M_\downarrow^{(n)}$$

$$M_\sigma^{(n)} = \begin{pmatrix} G_{0\sigma}(0^-) & G_{0\sigma}(\tau_1 - \tau_2) & \dots & G_{0\sigma}(\tau_1 - \tau_n) \\ G_{0\sigma}(\tau_2 - \tau_1) & G_{0\sigma}(0^-) & \dots & G_{0\sigma}(\tau_2 - \tau_n) \\ \vdots & \vdots & \ddots & \vdots \\ G_{0\sigma}(\tau_n - \tau_1) & G_{0\sigma}(\tau_n - \tau_2) & \dots & G_{0\sigma}(0^-) \end{pmatrix}$$

$$G_0(i\omega_n) = \frac{1}{i\omega_n - \epsilon_d - \Delta(i\omega_n)}$$

Interaction expansion CT-QMC

- We have an expression for Z as a series in powers of U^n

$$\frac{Z}{Z_0} = \left\langle \hat{U}(\beta, 0) \right\rangle_0 = \sum_{n=0}^{\infty} \frac{(-U)^n}{n!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \det M_\uparrow^{(n)} \det M_\downarrow^{(n)}$$

- Similar derivations lead to the following expression for the Green function

$$G_\sigma(i\omega_n) = G_{0\sigma}(i\omega_n) - G_{0\sigma}(i\omega_n) K_\sigma(i\omega_n) G_{0\sigma}(i\omega_n)$$

$$K_\sigma(i\omega_n) = \frac{\sum_{n=0}^{\infty} \frac{(-U)^n}{n!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \det M_\uparrow^{(n)} \det M_\downarrow^{(n)} \left(\sum_{ij} e^{i\omega_n(\tau_i - \tau_j)} \left[M_\sigma^{(n)} \right]^{-1}_{ij} \right)}{\sum_{n=0}^{\infty} \frac{(-U)^n}{n!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \det M_\uparrow^{(n)} \det M_\downarrow^{(n)}}$$

We want to compute the integrals stochastically

Monte Carlo elements

$$K_\sigma(i\omega_n) = \frac{\sum_{n=0}^{\infty} \frac{(-U)^n}{n!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \, \det M_\uparrow^{(n)} \, \det M_\downarrow^{(n)} \left(\sum_{ij} e^{i\omega_n(\tau_i - \tau_j)} \left[M_\sigma^{(n)} \right]^{-1}_{ij} \right)}{\sum_{n=0}^{\infty} \frac{(-U)^n}{n!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \, \det M_\uparrow^{(n)} \, \det M_\downarrow^{(n)}}$$

- Monte Carlo sum $\displaystyle\sum_{\mathcal{C}}^{\mathrm{MC}} \equiv \sum_n \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n$
- Configuration $\mathcal{C} = \{n, \tau_1, \ldots, \tau_n\}$
- Probability distribution $\rho(\mathcal{C}) = |w(\mathcal{C})|$ with $w(\mathcal{C}) = \dfrac{(-U)^n}{n!} \det M_\uparrow^{(n)} \, \det M_\downarrow^{(n)}$

Very different from the Boltzmann weight!

- Compute

$$K_\sigma(i\omega_n) = \frac{\sum_{\mathcal{C}}^{\mathrm{MC}} \sum_{ij} e^{i\omega_n(\tau_i - \tau_j)} \left[M_\sigma^{(n)} \right]^{-1}_{ij} \, \mathrm{sign}(w(\mathcal{C}))}{\sum_{\mathcal{C}}^{\mathrm{MC}} \mathrm{sign}(w(\mathcal{C}))}$$

The fermionic sign problem

- Imagine we want to compute this average:

$$\langle f \rangle = \frac{\sum_x w(x) f(x)}{\sum_x w(x)}$$

- We use the absolute value of $w(x)$ as a probability

$$\langle f \rangle = \frac{\sum_x |w(x)| f(x) \mathrm{sign}(w(x))}{\sum_x |w(x)| \mathrm{sign}(w(x))} \sim \frac{\sum_{i=1}^N f(x_i) \mathrm{sign}(w(x_i))}{\sum_{i=1}^N \mathrm{sign}(w(x_i))}$$

- If signs alternate the denominator is very small and there is a big variance!
- The average sign typically decreases exponentially with temperature, system size, etc.
- Fermionic problems very often suffer from this sign problem!

Sign problem in interaction expansion CT-QMC

$$\frac{Z}{Z_0} = \left\langle \hat{U}(\beta, 0) \right\rangle_0 = \sum_{n=0}^{\infty} \frac{(-U)^n}{n!} \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \, \det M_\uparrow^{(n)} \, \det M_\downarrow^{(n)}$$

- The sign will alternate with n and it will lead to a terrible sign problem. But there is a trick

$$U n_\uparrow n_\downarrow = \frac{U}{2} \sum_{s=\uparrow,\downarrow} \Big(n_\uparrow - \alpha_{s\uparrow}\Big)\Big(n_\downarrow - \alpha_{s\downarrow}\Big) + \underbrace{\frac{U}{2}\Big(n_\uparrow + n_\downarrow\Big)} + \text{const} \qquad \alpha_{s\sigma} = \frac{1}{2} + (2\delta_{s\sigma} - 1)\delta$$

we absorb this term in the chemical potential

Wick's theorem still holds but the matrices change slightly $M \to D$

$$Z = Z_0 \sum_n \frac{(-U)^n}{n!} \int d\tau_i \frac{1}{2^n} \sum_{s_i} \Big\langle T_\tau (n_{d\uparrow}(\tau_1) - \alpha_{s_1\uparrow}) \cdots (n_{d\uparrow}(\tau_n) - \alpha_{s_n\uparrow}) \Big\rangle_0 \Big\langle T_\tau (n_{d\downarrow}(\tau_1) - \alpha_{s_1\downarrow}) \cdots (n_{d\downarrow}(\tau_n) - \alpha_{s_n\downarrow}) \Big\rangle_0$$

we now have an extra sum over auxiliary spins

tuning δ can help the sign problem a lot

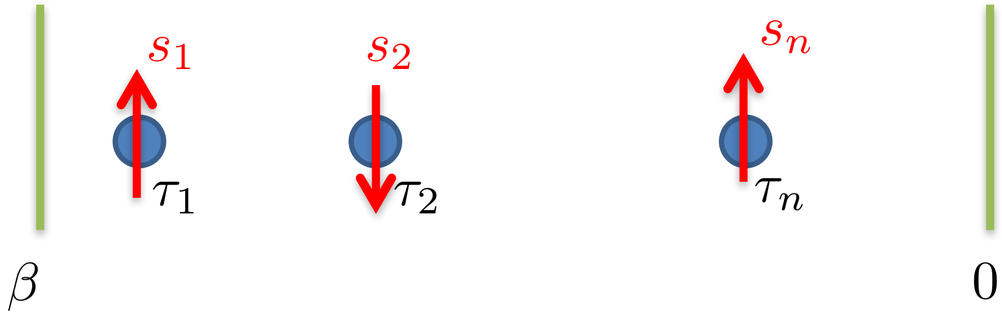
Monte Carlo elements after trick

- MC sum:

$$\sum_{\mathcal{C}}^{\mathrm{MC}} = \sum_{n} \int_{\tau_1 > \cdots > \tau_n} d\tau_1 \cdots d\tau_n \sum_{s_1} \cdots \sum_{s_n}$$

- The configurations are diagrams of the perturbation expansion. They can be seen as a set of interaction vertices at different imaginary times with an auxiliary spin s_i at every vertex.

$$\mathcal{C} = \{n, \tau_i, s_i\} =$$

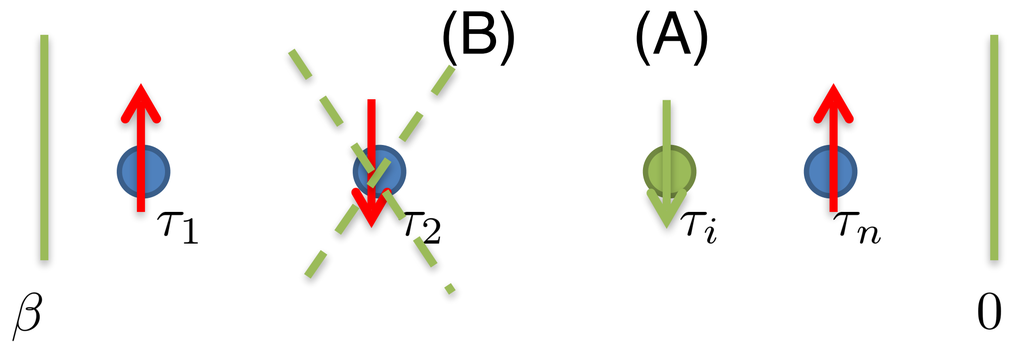


- The weight of every diagram is given by the absolute value of

$$w(\mathcal{C}) = \left(\frac{-U}{2}\right)^n \det D_n^{\uparrow} \det D_n^{\downarrow}$$

Generating diagrams

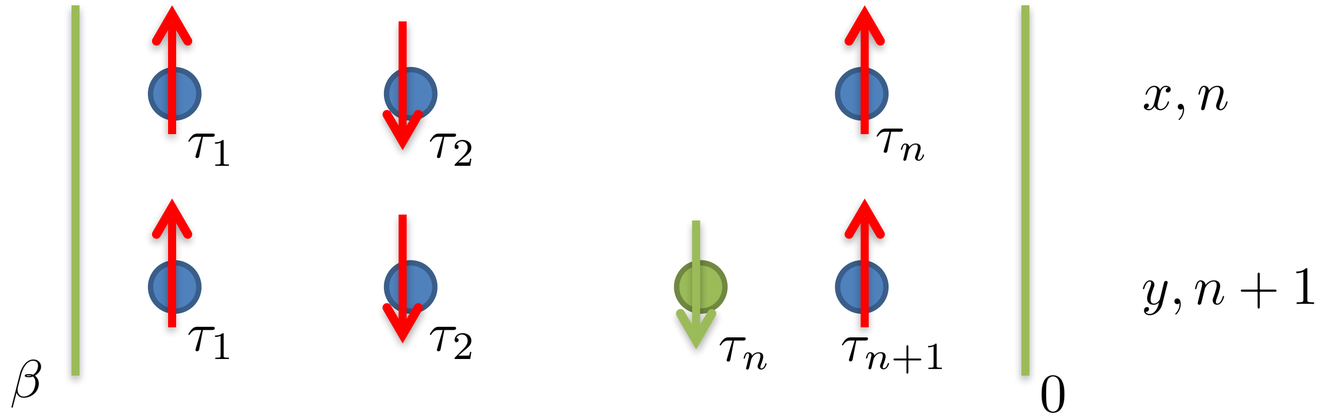
- We need to create a Markov chain of diagrams
- We can propose any changes to go from one diagram to another. A simple solution is to use two “moves”:
- An insertion of a vertex: we pick a random imaginary time and insert a vertex with a spin randomly up or down (A)
- A removal of a vertex: pick a random vertex and remove it (B)



Insertion of a vertex

- What is the acceptance rate?

$$A_{x,y} = \min\left[1, \frac{P_{y,x}\rho(y)}{P_{x,y}\rho(x)}\right]$$



$$P_{x,y}\rho(x) = \frac{1}{2} \times \frac{1}{2} \times \frac{d\tau_{n+1}}{\beta} \times \left| \left(\frac{-U}{2}\right)^n \det D_n^{\uparrow} \det D_n^{\downarrow} \prod_{i=1}^{n} d\tau_i \right|$$

$$P_{y,x}\rho(y) = \frac{1}{2} \times \frac{1}{n+1} \times \left| \left(\frac{-U}{2}\right)^{n+1} \det D_{n+1}^{\uparrow} \det D_{n+1}^{\downarrow} \prod_{i=1}^{n+1} d\tau_i \right|$$

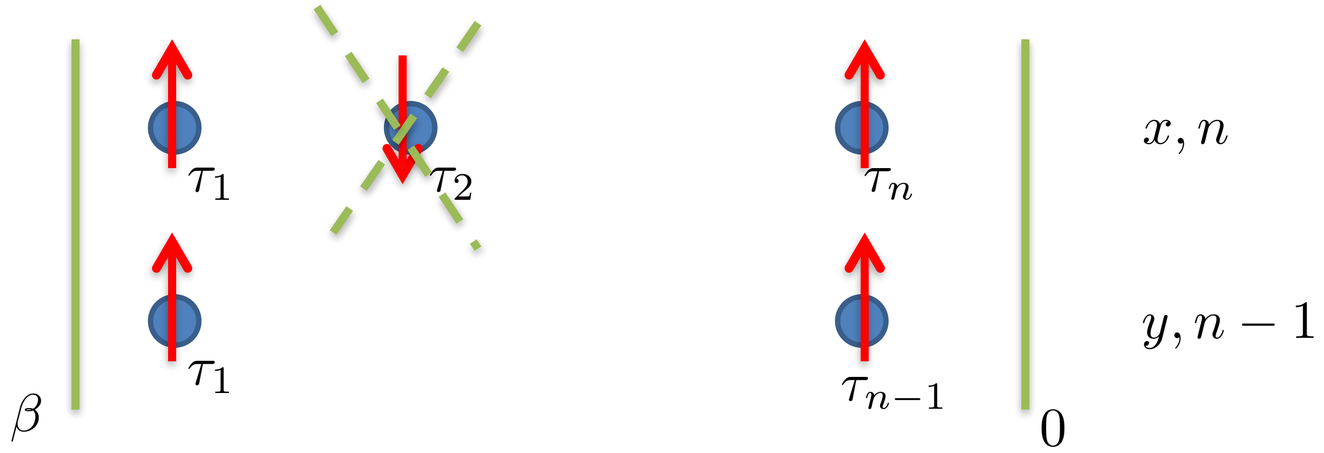
- Accept move with:

$$A_{x,y} = \min\left[1, \left| \frac{-U\beta}{n+1} \times \frac{\det D_{n+1}^{\uparrow} D_{n+1}^{\downarrow}}{\det D_n^{\uparrow} D_n^{\downarrow}} \right| \right]$$

Removal of a vertex

- What is the acceptance rate?

$$A_{x,y} = \min\left[1, \frac{P_{y,x}\rho(y)}{P_{x,y}\rho(x)}\right]$$



$$P_{x,y}\rho(x) = \frac{1}{2} \times \frac{1}{n} \times \left| \left(\frac{-U}{2}\right)^n \det D_n^{\uparrow} \det D_n^{\downarrow} \prod_{i=1}^{n} d\tau_i \right|$$

$$P_{y,x}\rho(y) = \frac{1}{2} \times \frac{1}{2} \times \frac{d\tau_n}{\beta} \times \left| \left(\frac{-U}{2}\right)^{n-1} \det D_{n-1}^{\uparrow} \det D_{n-1}^{\downarrow} \prod_{i=1}^{n-1} d\tau_i d\tau_i' \right|$$

- Accept move with:

$$A_{x,y} = \min\left[1, \left| \frac{-n}{U\beta} \times \frac{\det D_{n-1}^{\uparrow} D_{n-1}^{\downarrow}}{\det D_n^{\uparrow} D_n^{\downarrow}} \right| \right]$$

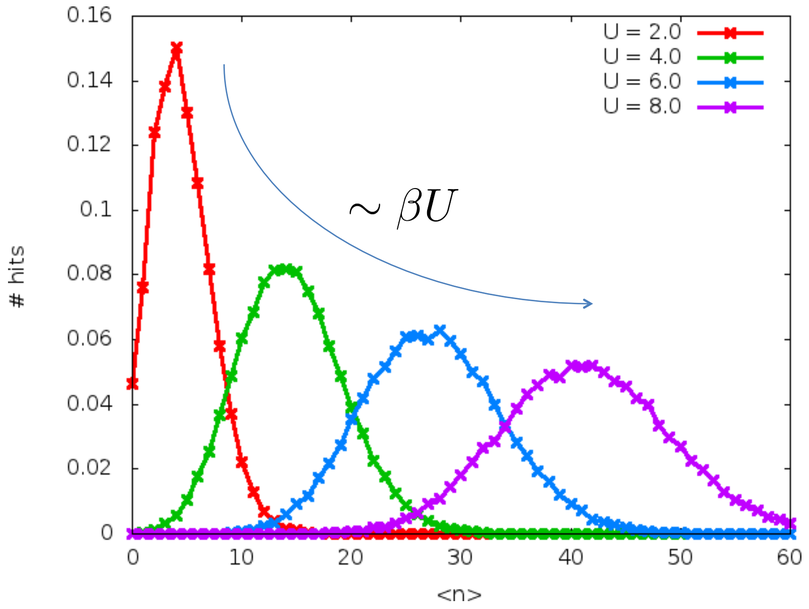
Computational effort

- The effort comes from the calculation of the determinants and of the inverse matrix (needed for the Green's function measure)

$$Z = Z_0 \int_{\mathcal{C}} \left(\frac{-U}{2}\right)^n \det D_n^{\uparrow} \det D_n^{\downarrow}$$

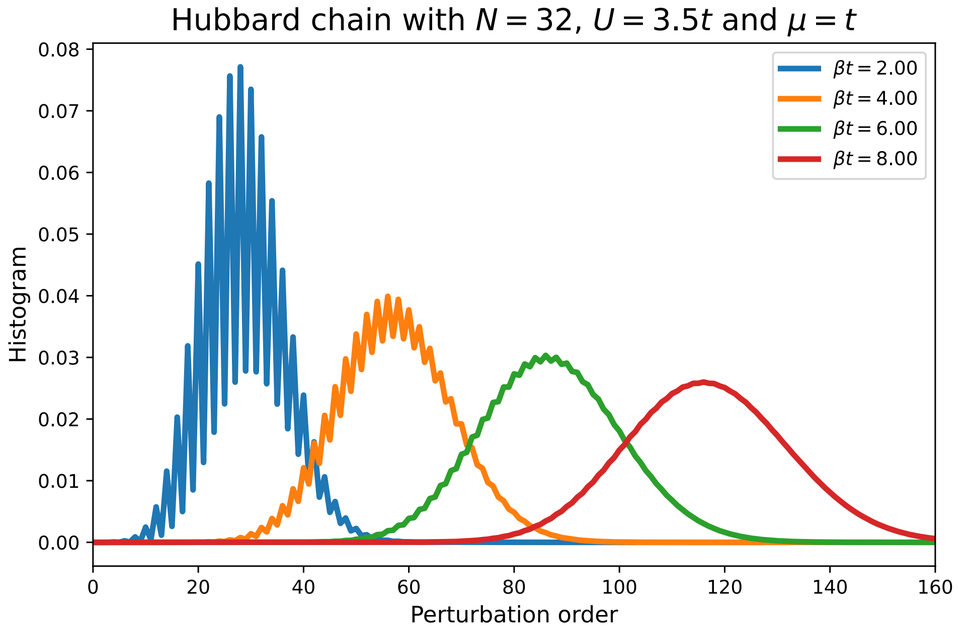
$$G_\sigma(i\omega_n) \sim G_{0\sigma}(i\omega_n) - \frac{1}{\beta Z} G_{0\sigma}^2(i\omega_n) \sum_{\mathcal{C}}^{\mathrm{MC}} \sum_{ij} [D_n^\sigma]_{ij}^{-1} e^{i\omega_n(\tau_i - \tau_j)} \times \mathrm{sign}(w(\mathcal{C}))$$

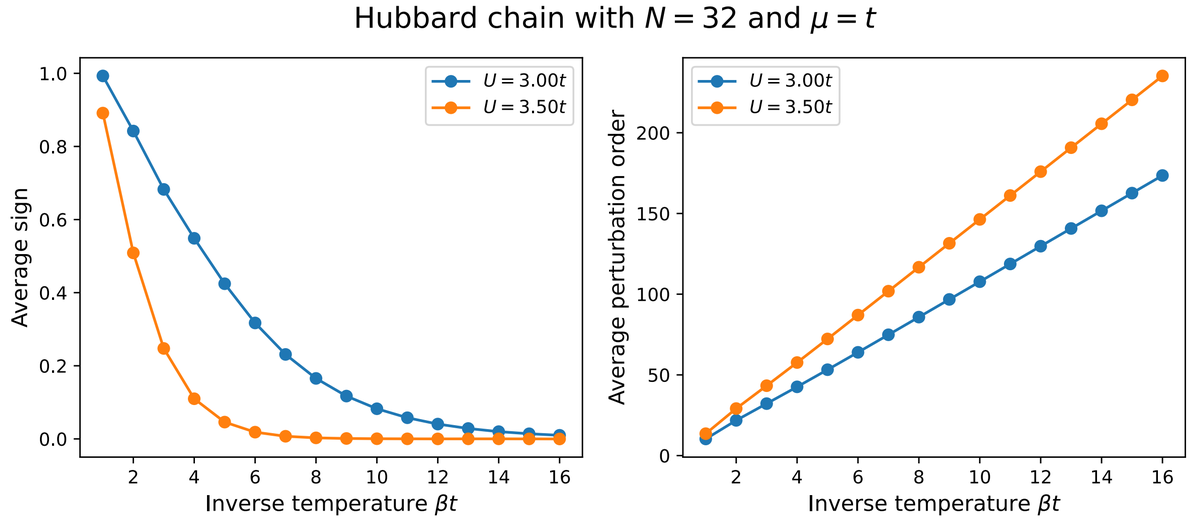
- It would be very slow to calculate them from scratch at every move
- They can be updated quickly using the Sherman-Morrison formula
- The computational effort grows in $\mathcal{O}(n^3)$

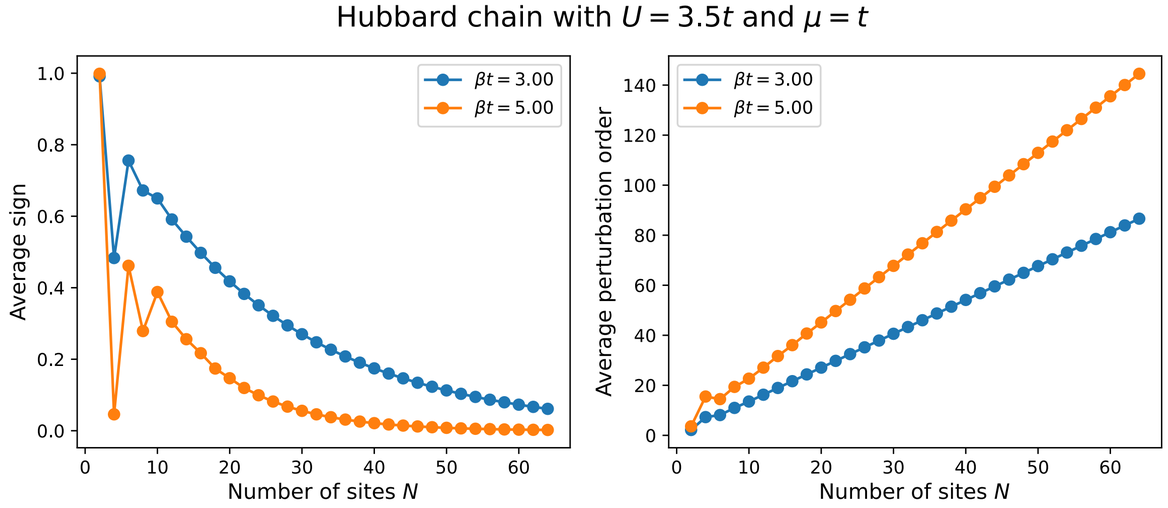


Sign problem in the generic case

- Simple investigation on Hubbard chain







Continuous-time quantum Monte Carlo algorithms

- Motivation: quantum impurity problems

  Historical importance of quantum impurity problems and algorithmic developments

- Continuous-time quantum Monte Carlo (CT-QMC) methods

  Introduction to the idea of CT-QMC methods and their different versions

- The interaction-expansion algorithm (CT-INT)

  Write a perturbation series expansion in the Coulomb interaction

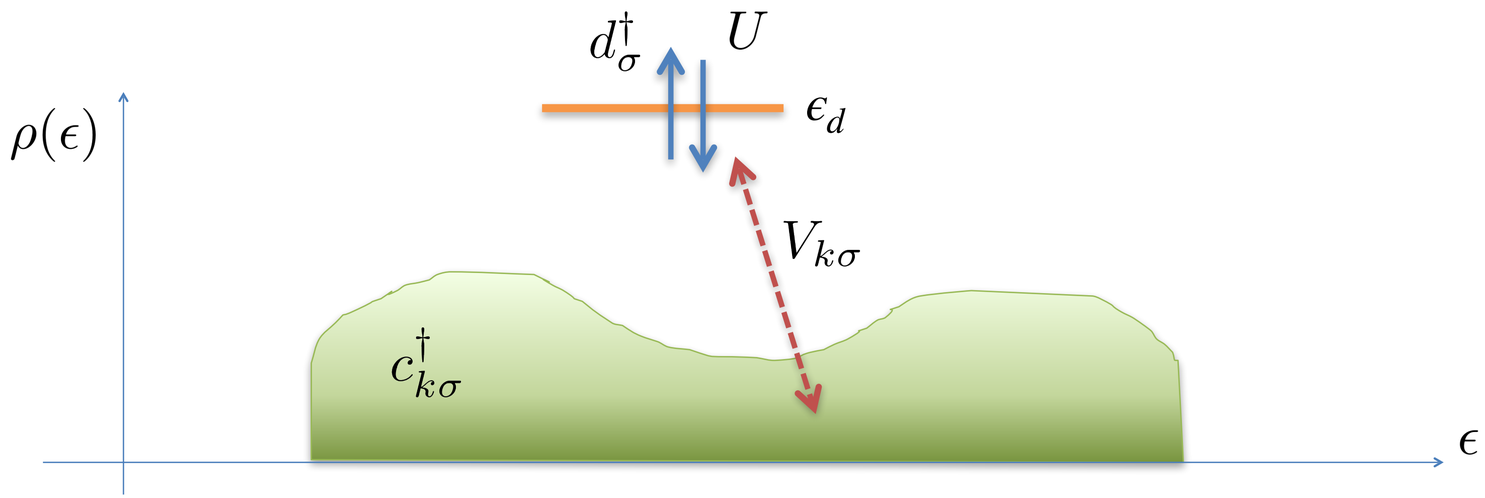
- The hybridization-expansion algorithm (CT-HYB)

  Write a perturbation series expansion in the hybridization function

Hybridization expansion CT-QMC

- We focus on the simplest Anderson model (can be generalized to multi-orbital problems)

- We want to derive an expansion around the atomic limit (expansion in the hybridization)



$$\mathcal{H} = \sum_{\sigma=\uparrow,\downarrow} \epsilon_0 d^\dagger_\sigma d_\sigma + U n_{d\uparrow} n_{d\downarrow} + \sum_{k,\sigma} V_{k\sigma} c^\dagger_{k\sigma} d_\sigma + \text{h.c.} + \sum_{k,\sigma} \epsilon_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma}$$

Hybridization expansion CT-QMC

- We work in the imaginary-time formalism

$$Z = \int \mathcal{D}[d^\dagger, d] e^{-S} \qquad \langle A \rangle = \frac{1}{Z} \int \mathcal{D}[d^\dagger, d] e^{-S} A$$

- The action for the Anderson model:

$$S = -\sum_\sigma \int_0^\beta d\tau d\tau' d_\sigma^\dagger(\tau) G_{0\sigma}^{-1}(\tau - \tau') d_\sigma(\tau') + \int_0^\beta d\tau U n_{d\uparrow}(\tau) n_{d\downarrow}(\tau)$$

$$G_{0\sigma}^{-1}(i\omega_n) = i\omega_n - \epsilon_0 - \Delta_\sigma(i\omega_n) \qquad \Delta_\sigma(i\omega_n) = \sum_k \frac{|V_{k\sigma}|^2}{i\omega_n - \epsilon_{k\sigma}}$$

- Rewrite the action as $S = S_{\mathrm{loc}} + \sum_\sigma S_{\mathrm{hyb}}^\sigma$

$$S_{\mathrm{loc}} = \int_0^\beta d\tau \Big[\sum_\sigma d_\sigma^\dagger(\tau)(-\partial_\tau + \epsilon_0) d_\sigma(\tau) + U n_{d\uparrow}(\tau) n_{d\downarrow}(\tau) \Big]$$

action of the atomic problem

$$S_{\mathrm{hyb}}^\sigma = \int_0^\beta d\tau d\tau' d_\sigma^\dagger(\tau) \Delta_\sigma(\tau - \tau') d_\sigma(\tau')$$

“perturbation”

Hybridization expansion CT-QMC

- We write a series expansion for the exponential of the perturbation

$$Z = \int \mathcal{D}[d^\dagger, d] e^{-S_{\rm loc} - \sum_\sigma S^\sigma_{\rm hyb}} = \int \mathcal{D}[d^\dagger, d] e^{-S_{\rm loc}} \prod_\sigma \left[\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(S^\sigma_{\rm hyb} \right)^n \right]$$

- Again an average appears but this time over the atomic state!

$$Z = \sum_{n_\uparrow, n_\downarrow = 0}^{\infty} \left\langle T_\tau \prod_\sigma \frac{(-1)^{n_\sigma}}{n_\sigma!} \left(\hat{S}^\sigma_{\rm hyb} \right)^{n_\sigma} \right\rangle_{\rm loc}$$

average over the atomic state

- This time, we cannot use Wick's theorem and those averages will have to be computed with

$$\left\langle A \right\rangle_{\rm loc} = \frac{1}{Z_{\rm loc}} {\rm Tr} e^{-\beta \mathcal{H}_{\rm loc}}$$

Hamiltonian of the local problem

Hybridization expansion CT-QMC

- Inserting the expression of the hybridization action we get

$$\int_0^\beta d\tau d\tau' d_\sigma^\dagger(\tau)\Delta_\sigma(\tau-\tau')d_\sigma(\tau')$$

$$Z = \sum_{n_\uparrow,n_\downarrow=0}^{\infty} \left\langle T_\tau \prod_\sigma \frac{(-1)^{n_\sigma}}{n_\sigma!} \left(\hat{S}_{\mathrm{hyb}}^\sigma\right)^{n_\sigma} \right\rangle_{\mathrm{loc}}$$

Sum over many (continuous) variables

$$Z = \sum_{n_\uparrow,n_\downarrow=0}^{\infty} \int_0^\beta d\tau_1^\uparrow \dots d\tau_{n_\uparrow}'^\uparrow \int_0^\beta d\tau_1^\downarrow \dots d\tau_{n_\downarrow}'^\downarrow$$

Product of hybridization functions

$$\prod_\sigma \frac{(-1)^{n_\sigma}}{n_\sigma!} \prod_{i=1}^{n_\sigma} \Delta_\sigma(\tau_i^\sigma - \tau_i'^\sigma) \times$$

Trace involving both spin up and down operators

$$\mathrm{Tr}\left[e^{-\beta\mathcal{H}_{\mathrm{loc}}} T_\tau \prod_{i=1}^{n_\uparrow} d_\uparrow^\dagger(\tau_i^\uparrow) d_\uparrow(\tau_i'^\uparrow) \prod_{i=1}^{n_\downarrow} d_\downarrow^\dagger(\tau_i^\downarrow) d_\downarrow(\tau_i'^\downarrow)\right]$$

$$Z = \int_{\mathcal{C}} w(\mathcal{C}) \sim \sum_{\mathcal{C}}^{\mathrm{MC}} \mathrm{sign}(w(\mathcal{C})) \qquad \langle f \rangle = \frac{1}{Z}\int_{\mathcal{C}} w(\mathcal{C}) f(\mathcal{C}) \sim \frac{1}{Z}\sum_{\mathcal{C}}^{\mathrm{MC}} f(\mathcal{C})\,\mathrm{sign}(w(\mathcal{C}))$$

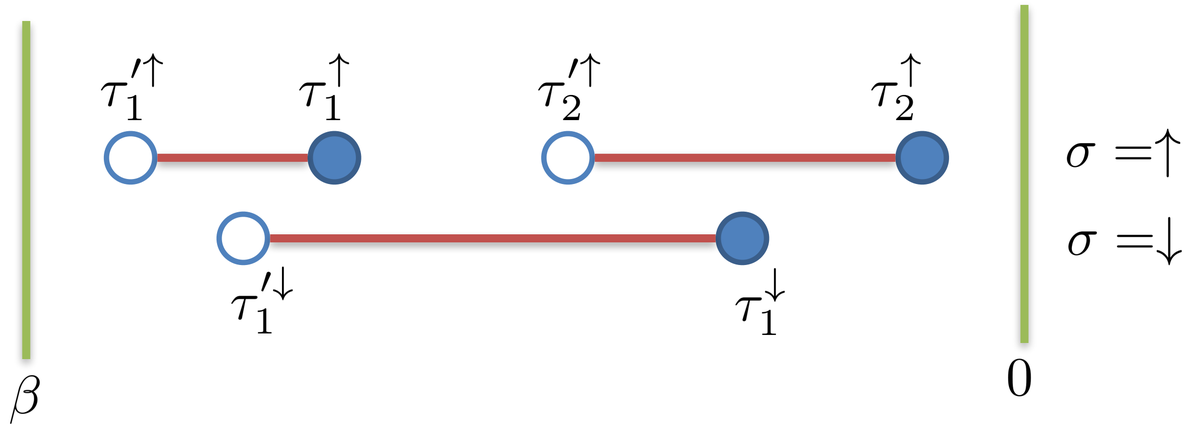
Hybridization expansion CT-QMC

- MC sum:

$$\sum_{\mathcal{C}}^{\mathrm{MC}} = \sum_{n_\uparrow, n_\downarrow = 0}^{\infty} \int_0^\beta d\tau_1^\uparrow \dots d\tau_{n_\uparrow}'^\uparrow \int_0^\beta d\tau_1^\downarrow \dots d\tau_{n_\downarrow}'^\downarrow$$

- Diagrams:

$$\mathcal{C} = \{n_\sigma, \tau_i^\sigma, \tau_i'^\sigma\} =$$



- Weight:

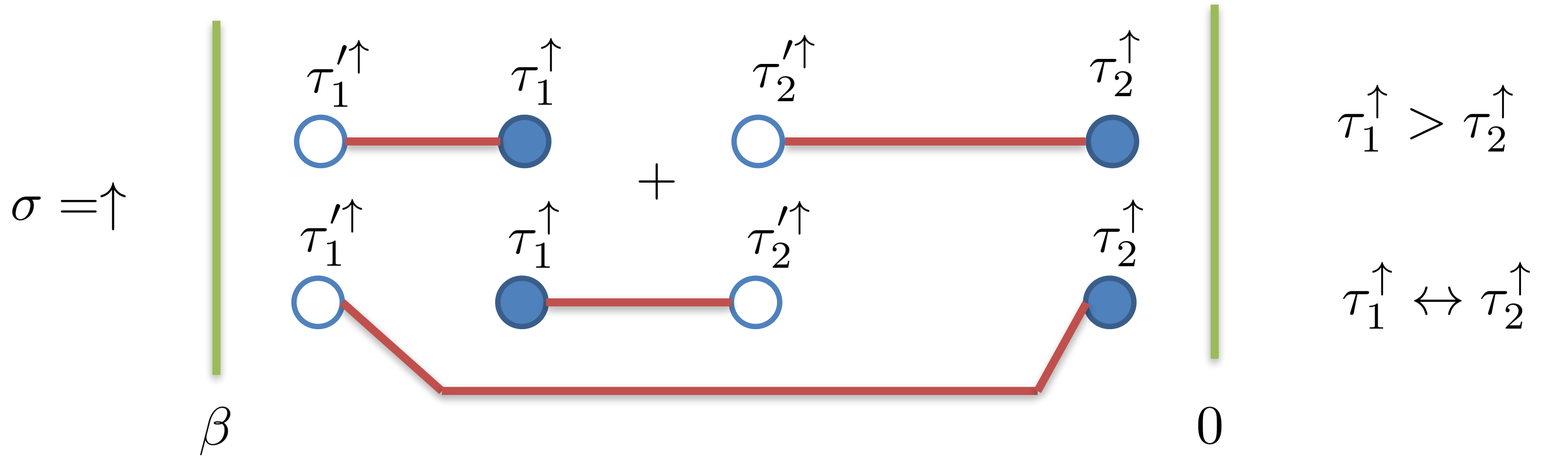
$$w(\mathcal{C}) = \prod_\sigma \frac{(-1)^{n_\sigma}}{n_\sigma!} \prod_{i=1}^{n_\sigma} \Delta_\sigma(\tau_i^\sigma - \tau_i'^\sigma) \quad \times$$

$$\mathrm{Tr}\left[e^{-\beta \mathcal{H}_{\mathrm{loc}}} T_\tau \prod_{i=1}^{n_\uparrow} d_\uparrow^\dagger(\tau_i^\uparrow) d_\uparrow(\tau_i'^\uparrow) \prod_{i=1}^{n_\downarrow} d_\downarrow^\dagger(\tau_i^\downarrow) d_\downarrow(\tau_i'^\downarrow)\right]$$

- Unfortunately these diagrams have alternating signs ⇒ problems!

Trick: resumming diagrams

- The idea is to resum diagrams into a determinant. We start from a diagram where $\tau_1^\uparrow > \ldots > \tau_{n_\uparrow}^\uparrow$ and sum all the permutations of $\{\tau_i^\uparrow\}$



$$\mathrm{Tr}\left[e^{-\beta\mathcal{H}_{\mathrm{loc}}} d_\uparrow^\dagger(\tau_1^\uparrow) d_\uparrow(\tau_1'^\uparrow) d_\uparrow^\dagger(\tau_2^\uparrow) d_\uparrow(\tau_2'^\uparrow)\right] \times \frac{1}{2}\Delta_\uparrow(\tau_1^\uparrow - \tau_1'^\uparrow)\Delta_\uparrow(\tau_2^\uparrow - \tau_2'^\uparrow)$$

$$(-1)\mathrm{Tr}\left[e^{-\beta\mathcal{H}_{\mathrm{loc}}} d_\uparrow^\dagger(\tau_1^\uparrow) d_\uparrow(\tau_1'^\uparrow) d_\uparrow^\dagger(\tau_2^\uparrow) d_\uparrow(\tau_2'^\uparrow)\right] \times \frac{1}{2}\Delta_\uparrow(\tau_2^\uparrow - \tau_1'^\uparrow)\Delta_\uparrow(\tau_1^\uparrow - \tau_2'^\uparrow)$$

$$=$$

$$\mathrm{Tr}\left[e^{-\beta\mathcal{H}_{\mathrm{loc}}} d_\uparrow^\dagger(\tau_1^\uparrow) d_\uparrow(\tau_1'^\uparrow) d_\uparrow^\dagger(\tau_2^\uparrow) d_\uparrow(\tau_2'^\uparrow)\right] \times \frac{1}{2} \det_{1\leq k,l\leq 2} \Delta_\uparrow(\tau_k^\uparrow - \tau_l'^\uparrow)$$

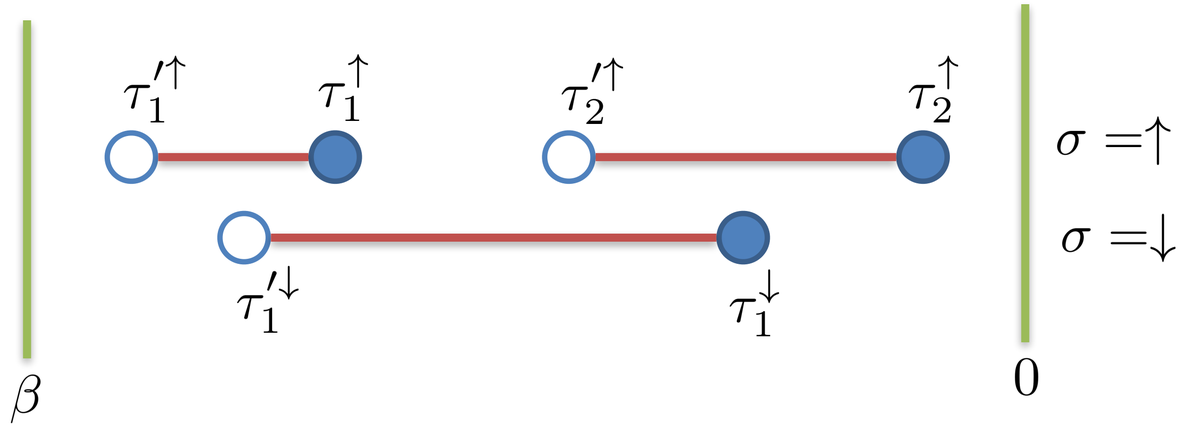
Hybridization expansion Monte Carlo

- MC sum:

$$\sum_{\mathcal{C}}^{\mathrm{MC}} = \sum_{n_\uparrow, n_\downarrow = 0}^{\infty} \int_{\substack{\tau_1^\uparrow > \ldots > \tau_n^\uparrow \\ \tau_1'^\uparrow > \ldots > \tau_n'^\uparrow}} d\tau_1^\uparrow \ldots d\tau_n'^\uparrow \int_{\substack{\tau_1^\downarrow > \ldots > \tau_n^\downarrow \\ \tau_1'^\downarrow > \ldots > \tau_n'^\downarrow}} d\tau_1^\downarrow \ldots d\tau_{n_\downarrow}'^\downarrow$$

- Diagrams:

$$\mathcal{C} = \{n_\sigma, \tau_i^\sigma, \tau_i'^\sigma\} =$$



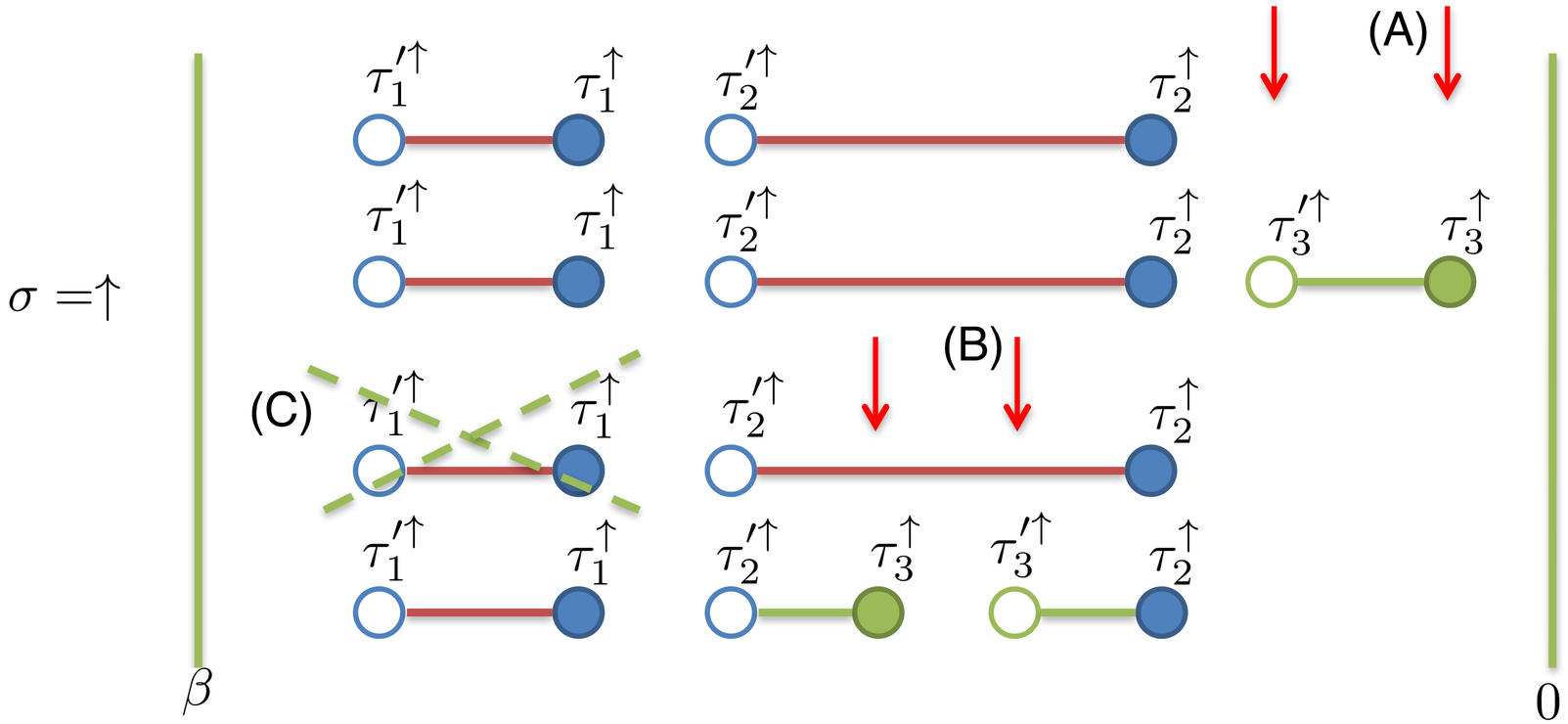
- Weight:

$$w(\mathcal{C}) = \prod_\sigma (-1)^{n_\sigma} \det_{1 \le k,l \le n_\sigma} \Delta_\sigma(\tau_k^\sigma - \tau_l'^\sigma) \quad \times$$

$$\mathrm{Tr}\left[e^{-\beta \mathcal{H}_{\mathrm{loc}}} T_\tau \prod_{i=1}^{n_\uparrow} d_\uparrow^\dagger(\tau_i^\uparrow) d_\uparrow(\tau_i'^\uparrow) \prod_{i=1}^{n_\downarrow} d_\downarrow^\dagger(\tau_i^\downarrow) d_\downarrow(\tau_i'^\downarrow)\right]$$

Generating diagrams

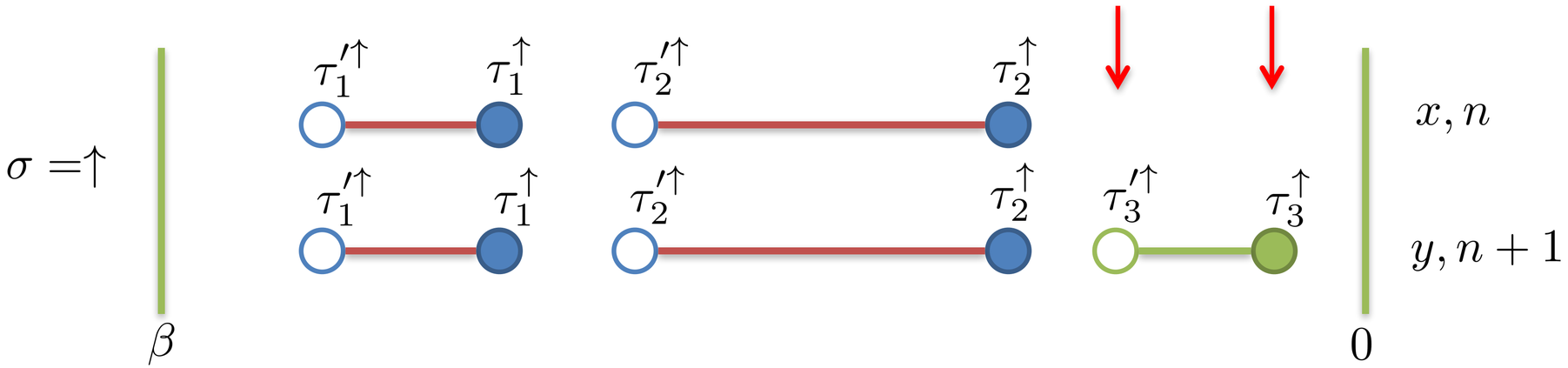
- New diagrams are generated with two “moves”:
- Insertion of an (anti)-link: chose a spin flavor and pick two random imaginary times such that there is no operator between them. Either construct a link (A) or an anti-link (B)
- Removal of a link: chose a spin flavor and remove a random link (C)



Insertion of an (anti-)link

- What is the acceptance rate for this move?

$$A_{x,y} = \min\left[1, \frac{P_{y,x}\rho(y)}{P_{x,y}\rho(x)}\right]$$



$$P_{x,y}\rho(x) = \frac{1}{2} \times \frac{d\tau_{n+1}}{\beta} \frac{d\tau'_{n+1}}{l_{\max}} \times \left|\mathrm{Tr}\mathcal{C}_x \det \Delta_{\mathcal{C}_x} \prod_{i=1}^{n} d\tau_i d\tau'_i\right|$$

$$P_{y,x}\rho(y) = \frac{1}{2} \times \frac{1}{n+1} \times \left|\mathrm{Tr}\mathcal{C}_y \det \Delta_{\mathcal{C}_y} \prod_{i=1}^{n+1} d\tau_i d\tau'_i\right|$$

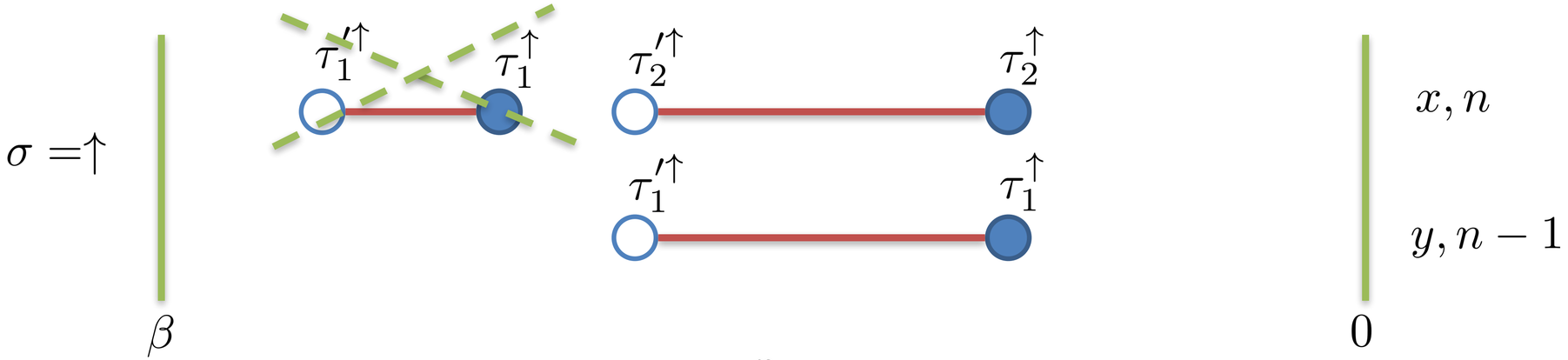
- Accept with probability:

$$A_{x,y} = \min\left[1, \frac{\beta l_{\max}}{n+1} \times \left|\frac{\mathrm{Tr}\mathcal{C}_y \det \Delta_{\mathcal{C}_y}}{\mathrm{Tr}\mathcal{C}_x \det \Delta_{\mathcal{C}_x}}\right|\right]$$

Removal of a link

- What is the acceptance rate for this move?

$$A_{x,y} = \min\left[1, \frac{P_{y,x}\rho(y)}{P_{x,y}\rho(x)}\right]$$



$$P_{x,y}\rho(x) = \frac{1}{2} \times \frac{1}{n} \times \left|\mathrm{Tr}\mathcal{C}_x \det \Delta_{\mathcal{C}_x} \prod_{i=1}^{n} d\tau_i d\tau_i'\right|$$

$$P_{y,x}\rho(y) = \frac{1}{2} \times \frac{d\tau_n}{\beta}\frac{d\tau_n'}{l_{\max}} \times \left|\mathrm{Tr}\mathcal{C}_y \det \Delta_{\mathcal{C}_y} \prod_{i=1}^{n-1} d\tau_i d\tau_i'\right|$$

- Accept with probability:

$$A_{x,y} = \min\left[1, \frac{n}{\beta l_{\max}} \times \left|\frac{\mathrm{Tr}\mathcal{C}_y \det \Delta_{\mathcal{C}_y}}{\mathrm{Tr}\mathcal{C}_x \det \Delta_{\mathcal{C}_x}}\right|\right]$$

Measuring the Green function

- We know how to sample diagrams with weights corresponding to their contribution in the partition function.

$$Z = \int_{\mathcal{C}} (-1)^{n_\uparrow + n_\downarrow} \det \Delta_{\uparrow\mathcal{C}} \det \Delta_{\downarrow\mathcal{C}} \mathrm{Tr}\mathcal{C} = \int_{\mathcal{C}} w(\mathcal{C}) \sim \sum_{\mathcal{C}}^{\mathrm{MC}} \mathrm{sign}(w(\mathcal{C}))$$

- How do we get the Green's function?

$$G_\sigma(\tau) = -\frac{1}{\beta} \frac{\delta \log Z}{\delta \Delta_\sigma(-\tau)}$$

$$G_\uparrow(\tau) = \frac{-1}{Z\beta} \int_{\mathcal{C}} \frac{\delta \det \Delta_{\uparrow\mathcal{C}}}{\delta \Delta_\uparrow(-\tau)} \times (-1)^{n_\uparrow + n_\downarrow} \det \Delta_{\downarrow\mathcal{C}} \mathrm{Tr}\mathcal{C}$$

$$G_\uparrow(\tau) = \frac{-1}{Z\beta} \int_{\mathcal{C}} \sum_{k,l} \delta(\tau_k^\uparrow - \tau_l'^\uparrow + \tau) [\Delta_{\uparrow\mathcal{C}}^{-1}]_{k,l} \times \underbrace{(-1)^{n_\uparrow + n_\downarrow} \det \Delta_{\uparrow\mathcal{C}} \det \Delta_{\downarrow\mathcal{C}} \mathrm{Tr}\mathcal{C}}_{w(\mathcal{C})}$$

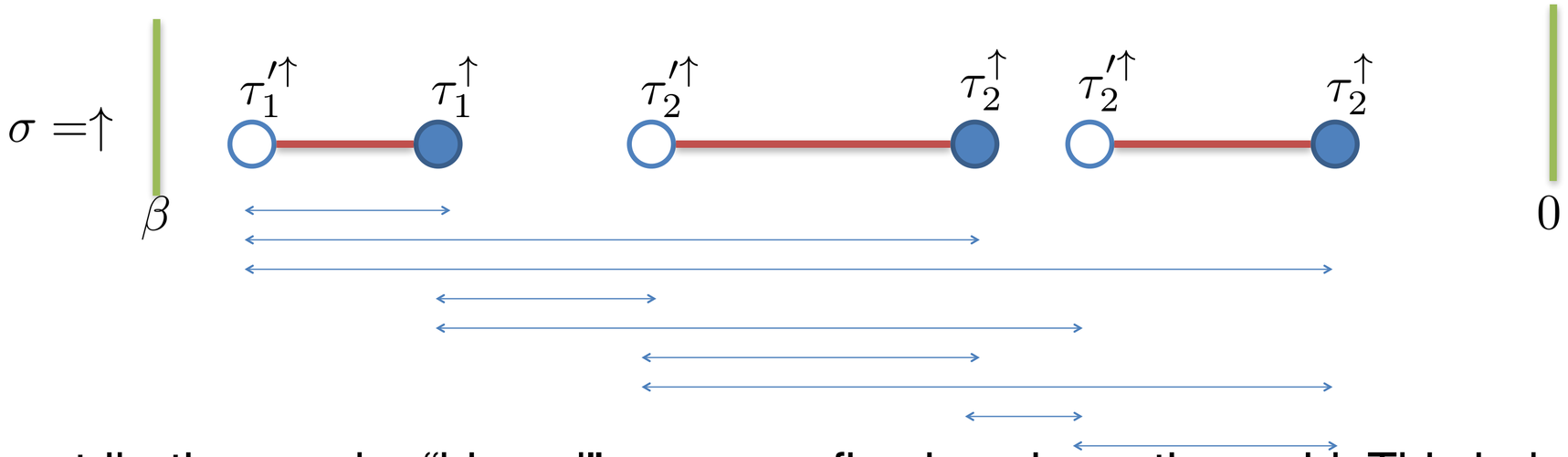
- Measure:

$$G_\sigma(\tau) \sim \frac{-1}{Z\beta} \sum_{\mathcal{C}}^{\mathrm{MC}} \sum_{k,l} \delta(\tau_k^\sigma - \tau_l'^\sigma + \tau) \times [\Delta_{\sigma\mathcal{C}}^{-1}]_{k,l} \times \mathrm{sign}(w(\mathcal{C}))$$

Measuring the Green function

- Each configuration give contributions for a discrete set of imaginary times:

$$G_\sigma(\tau) \sim \frac{-1}{Z\beta} \sum_{\mathcal{C}}^{\mathrm{MC}} \sum_{k,l} \delta(\tau_k^\sigma - \tau_l'^\sigma + \tau) \times [\Delta_{\sigma\mathcal{C}}^{-1}]_{k,l} \times \mathrm{sign}(w(\mathcal{C}))$$



- These contribution can be “binned” on a very fine imaginary-time grid. This induces high frequency noise in Matsubara frequencies

Measuring using Legendre polynomials

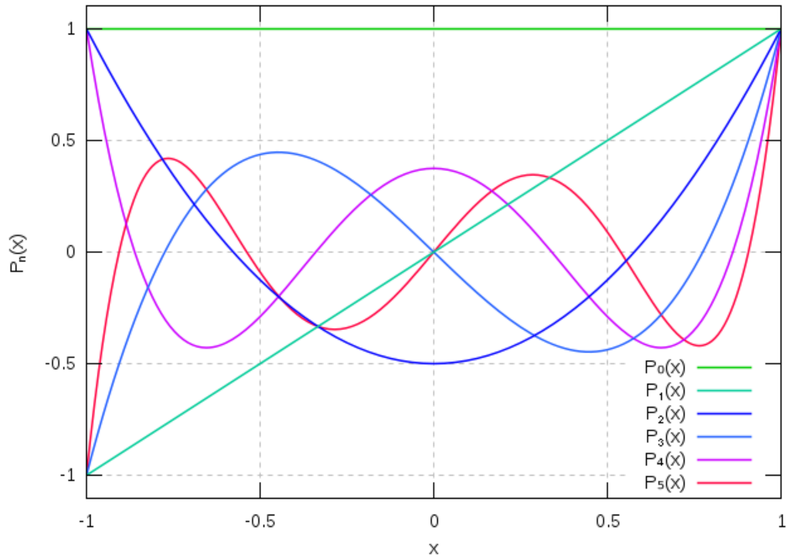
L. Boehnke et al., PRB (2011)

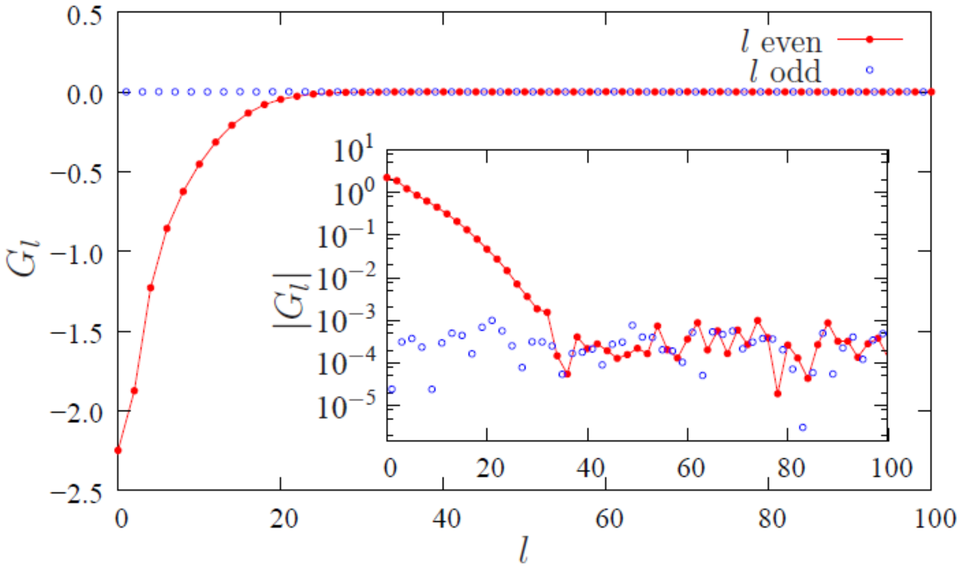
- Legendre polynomials are a basis to express function defined over an interval

- We can express the imaginary-time Green's function in this basis

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

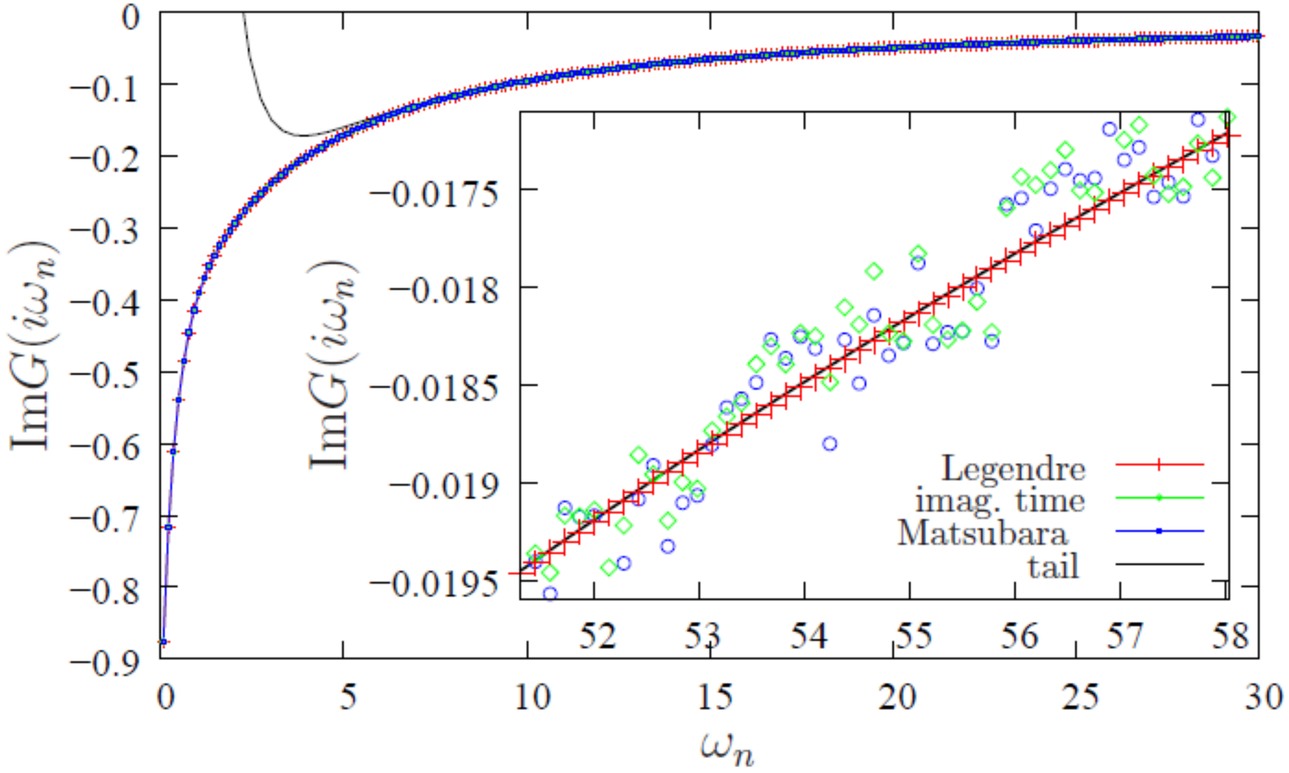
- The coefficients G_l in this basis decay very quickly





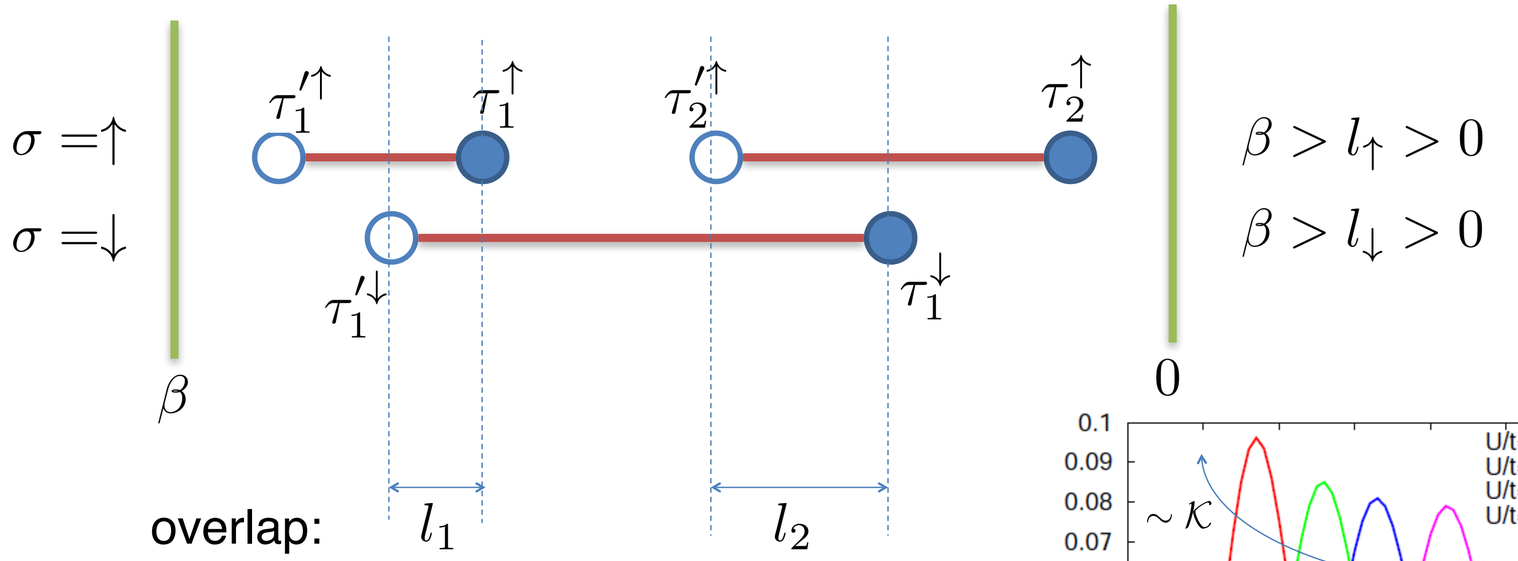
Legendre basis acting as a filter

- The noise in the Matsubara frequencies can be reduced by truncating the Legendre coefficients that are zero within their error bars
- A typical outcome of this procedure:



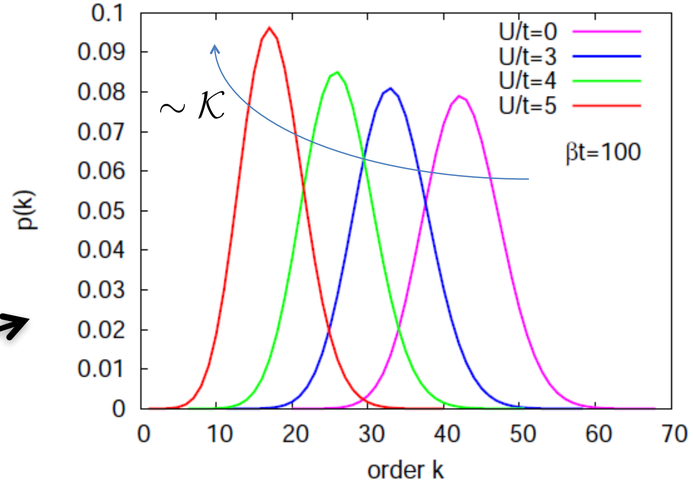
Computational effort

- Can the contribution of a diagram be computed quickly?
- Determinants can be updated quickly (Sherman-Morrison)
- For simple Hamiltonians, the trace is very easy



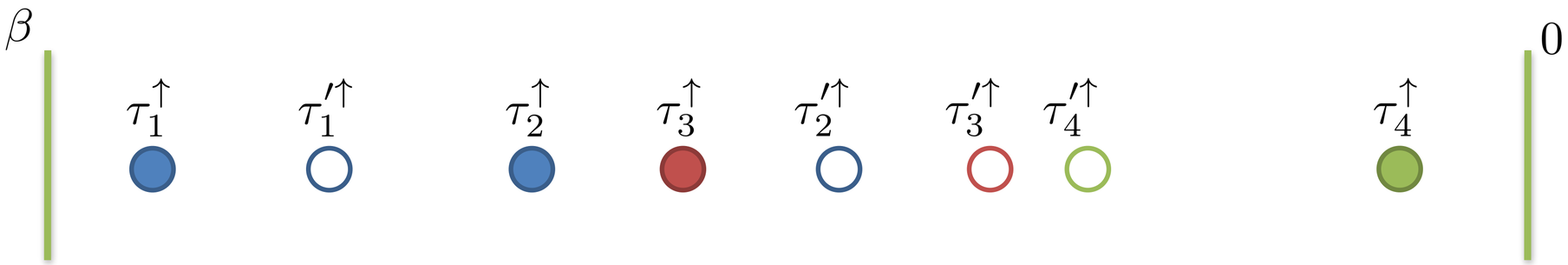
$$\mathrm{Tr}\, \mathcal{C} = e^{(l_\uparrow + l_\downarrow)\mu - U(l_1 + l_2)}$$

- Computational effort grows in $\mathcal{O}(n^3)$



What about non density-density Hamiltonians?

- The hybridization expansion algorithm can be modified for generic Hamiltonians
- Configurations are a set of creation / destruction operators of different flavor on a single imaginary-time line



- The main drawback is that there is no longer a quick way to compute the trace
- Operators are matrices that must be multiplied and traced over all atomic states
- The number of these atomic states quickly becomes large with several orbitals

CT-INT versus CT-HYB

- CT-INT & CT-AUX: series in the interaction
  - Many orbitals, weak coupling, high temperatures
  - Mainly density-density Hamiltonians
  - Average perturbation order $\sim \beta U$

- CT-HYB: series in the hybridization function
  - Good at low temperatures, strong coupling
  - Can treat generic Hamiltonians
  - Hard to treat many orbitals
  - Average perturbation order is the kinetic energy

Pros and cons of the CT-QMC algorithms

- Pros:
  - Faster than earlier algorithms like Hirsch-Fye
  - Monte Carlo ⇒ can easily be parallelized
  - Flexible Hamiltonians
  - Good scaling with number of orbitals if density-density
- Limitations:
  - Many orbitals difficult with generic Hamiltonian
  - They are in imaginary time, so one needs to do analytical continuation, and this is a very delicate procedure!
  - Note: some real-time and DMRG algorithms have been developed
  - Sign problem

Summary

- Continuous-time quantum Monte Carlo algorithms have allowed for progress in computing the properties of strongly-correlated systems
  - Lower temperatures
  - Generic Hamiltonians, new approaches (e.g cluster DMFT, …)
  - Larger number of orbitals / sites

- The idea of the algorithms is to sample stochastically the diagrams of a series expansion of the partition function

- According to one's need, different expansions can be used

- There are still limitations (sign problem, speed, …) and more work has to be done!

Thank you for your attention!