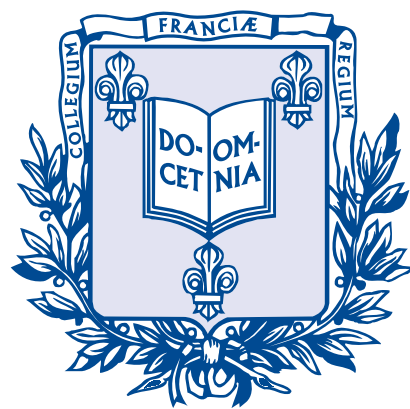


# Continuous-time quantum Monte Carlo algorithms for impurity models

Michel Ferrero

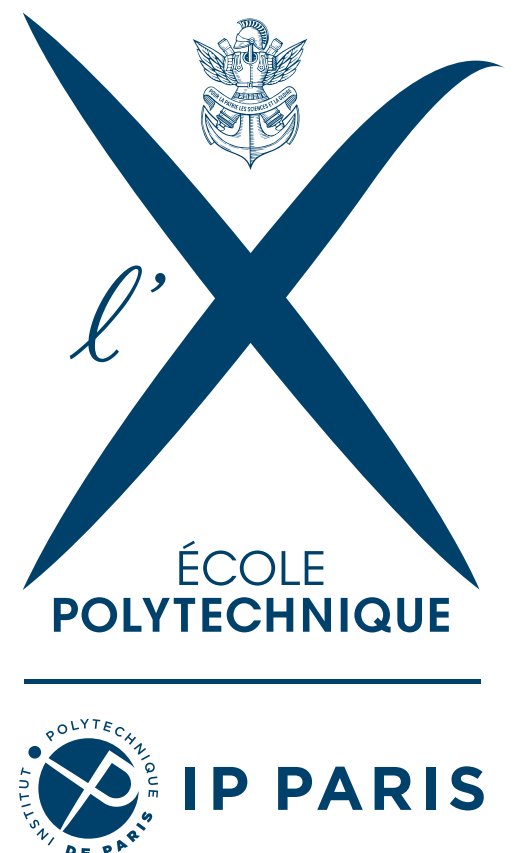
Ecole Polytechnique and Collège de France

Summer School on Computational Quantum Materials  
Jouvence, May 29, 2026



COLLÈGE  
DE FRANCE  
— 1530 —

<https://doc.quantum2026.ccs.usherbrooke.ca/ctqmc>



- **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

# 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)

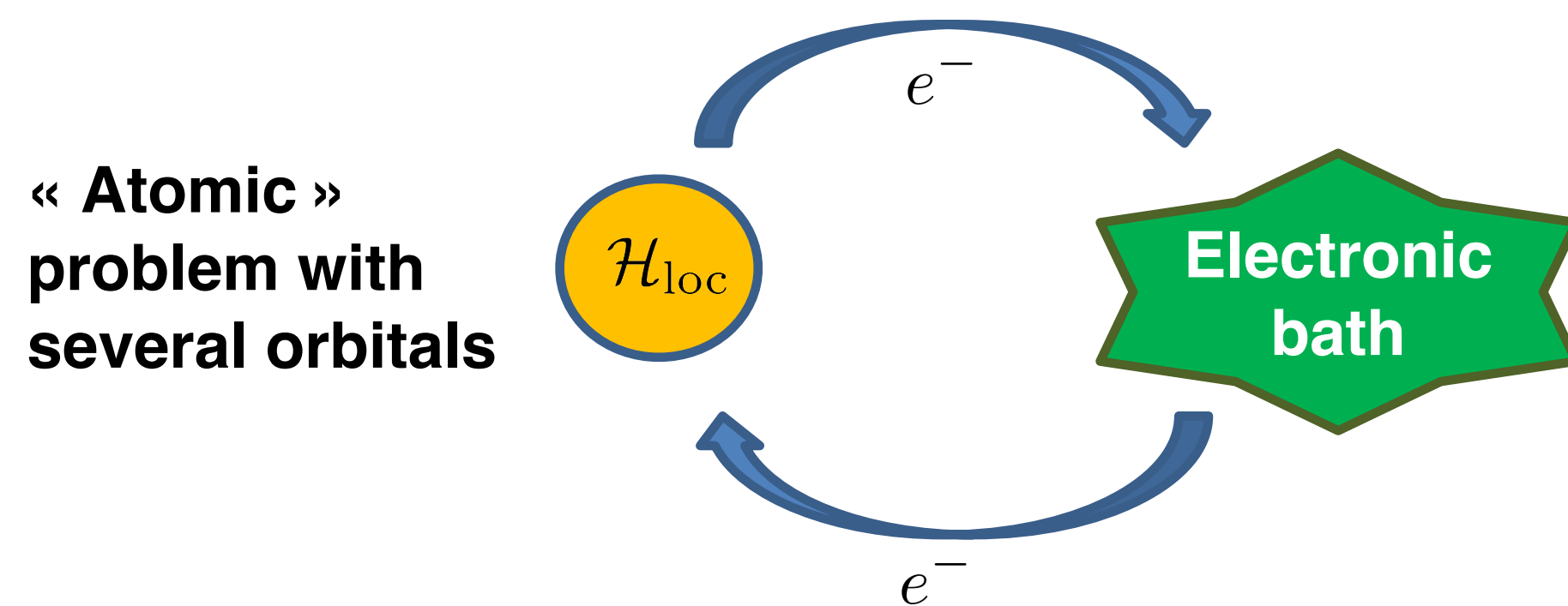
Write a perturbation series expansion in the hybridization function

# 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://triqs.github.io/ctint>

# 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

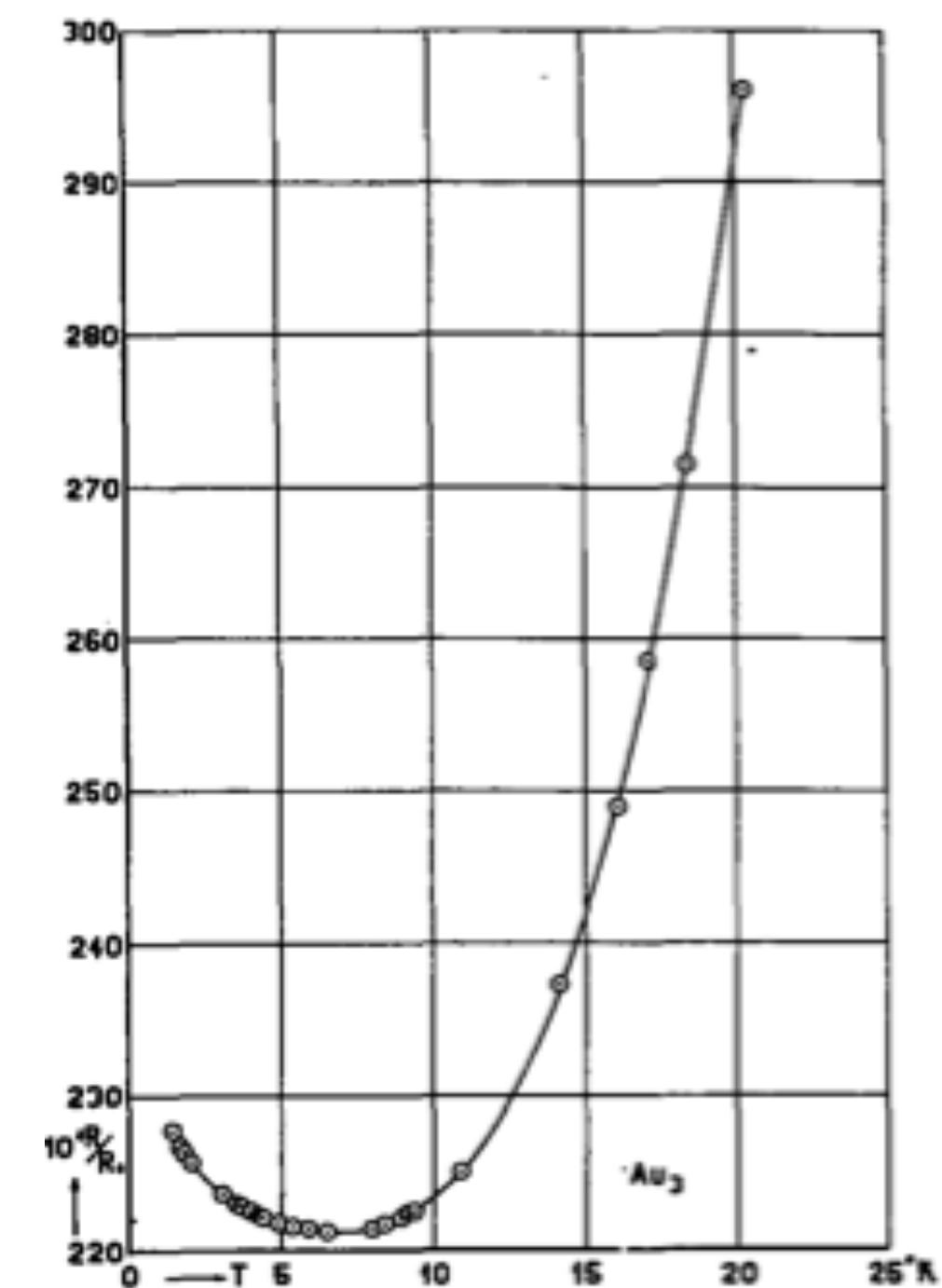
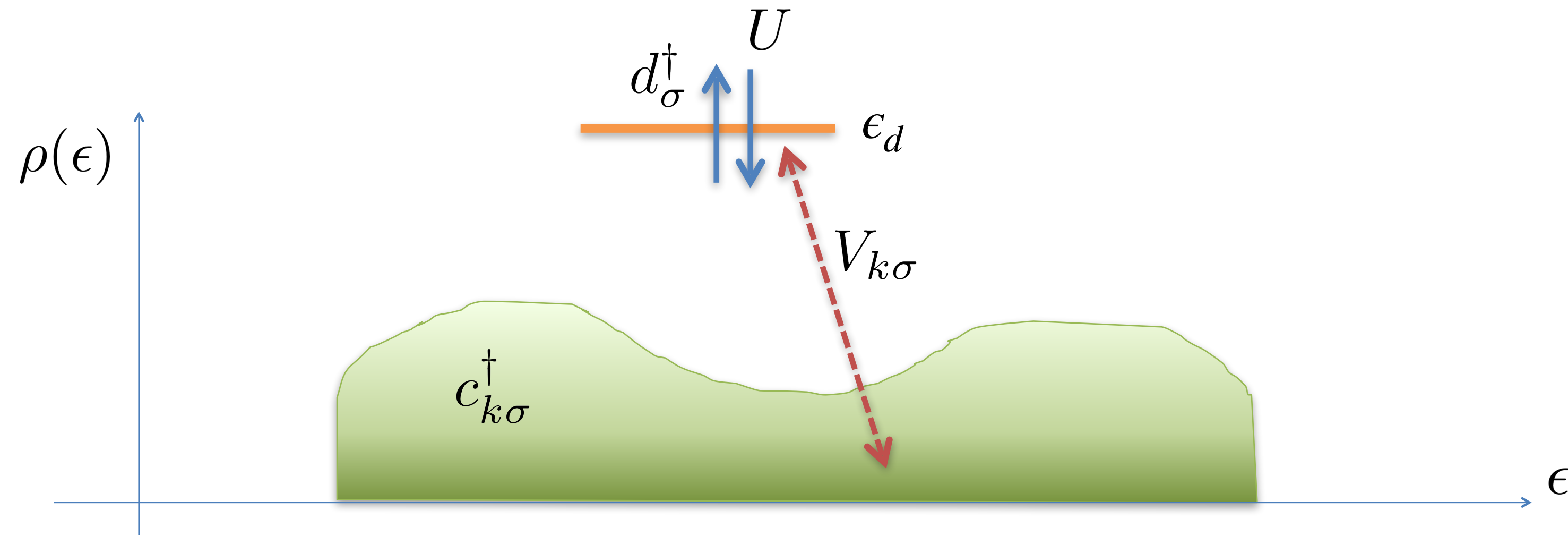


Fig. 1. Electrical resistance of Au<sub>3</sub>.

*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:



$$\mathcal{H} = \underbrace{\sum_{\sigma=\uparrow,\downarrow} \epsilon_0 d_\sigma^\dagger d_\sigma + U n_{d\uparrow} n_{d\downarrow}}_{\text{local many-body interaction}} + \underbrace{\sum_{k,\sigma} V_{k\sigma} c_{k\sigma}^\dagger d_\sigma + \text{h.c.}}_{\text{hybridization to the bath}} + \underbrace{\sum_{k,\sigma} \epsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma}}_{\text{free bath states}}$$

local many-body  
interaction

hybridization to  
the bath

free bath  
states

# The Anderson model

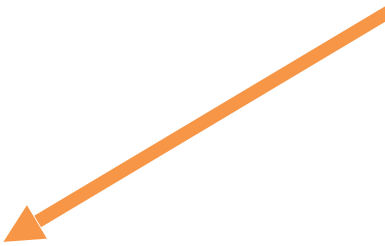
- When  $U = 0$ , the Anderson model can be solved
- Its non-interacting Green function is then

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

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  $\Delta$
- 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!

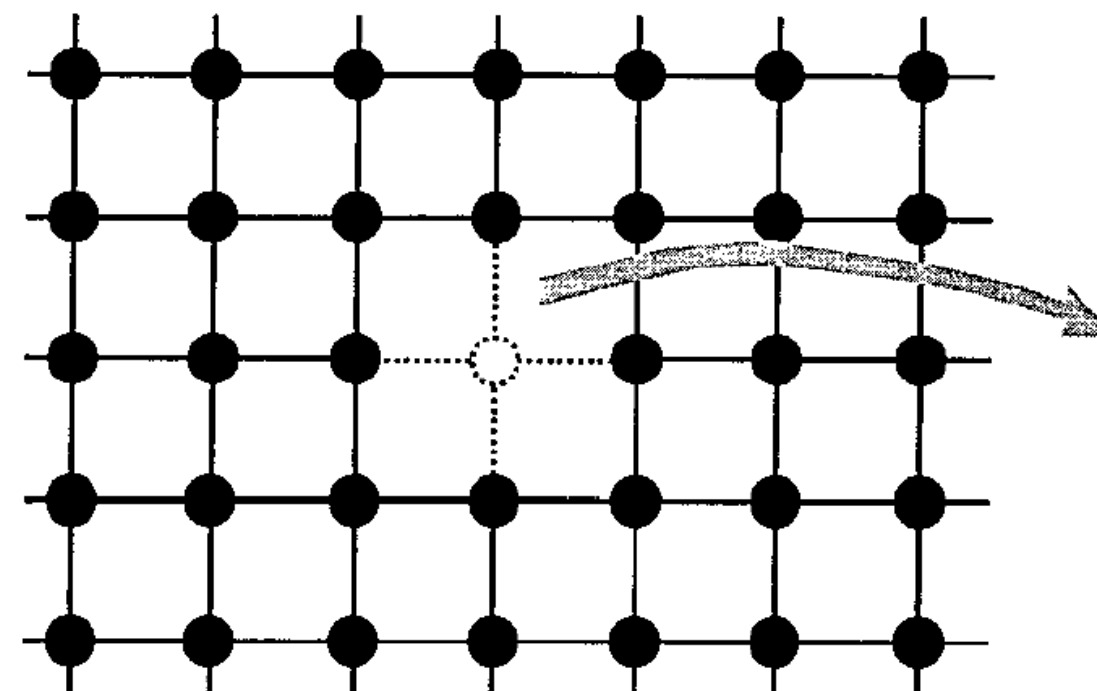
# Our goal: solve the DMFT equations

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

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



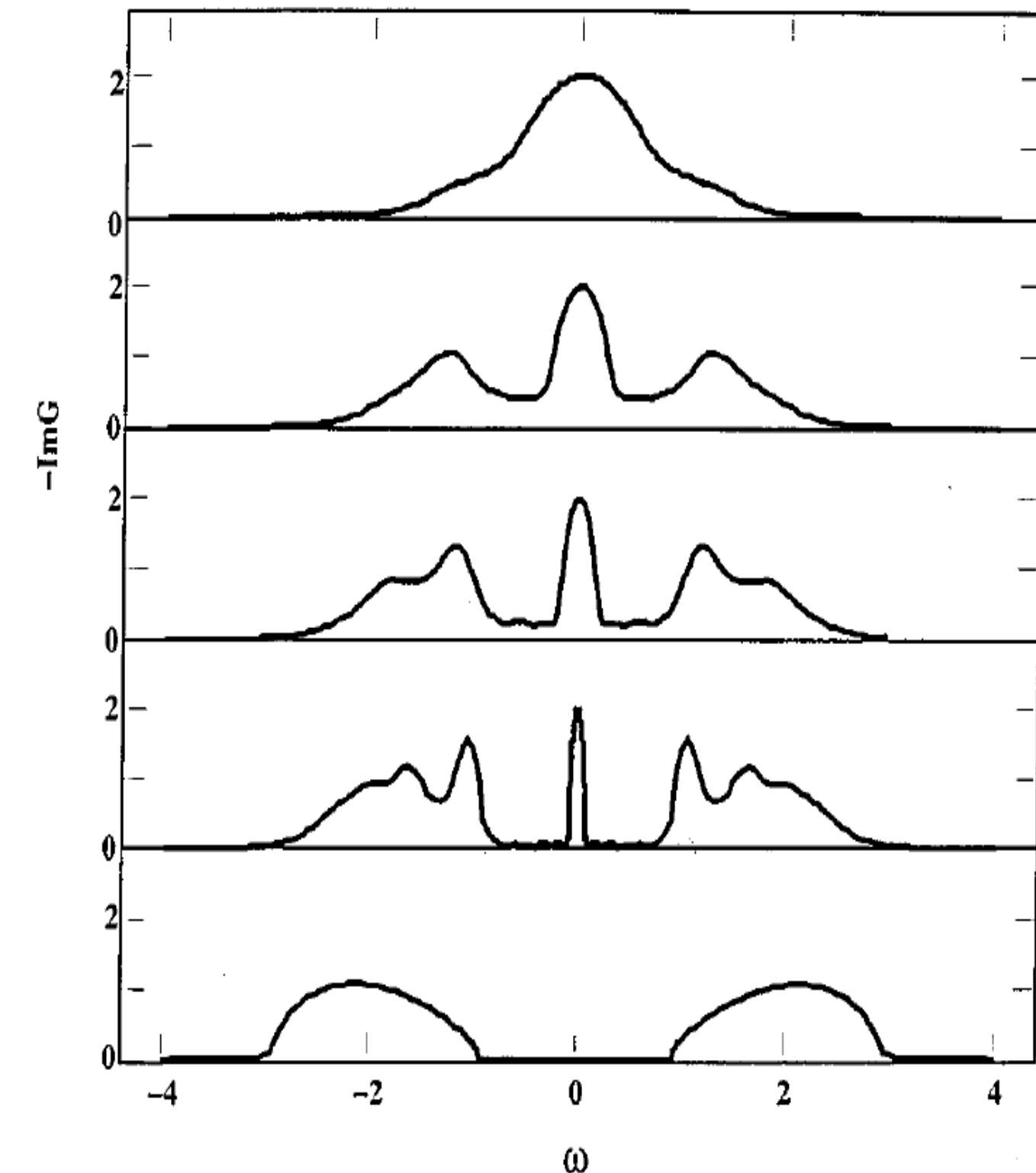
Anderson impurity model



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**

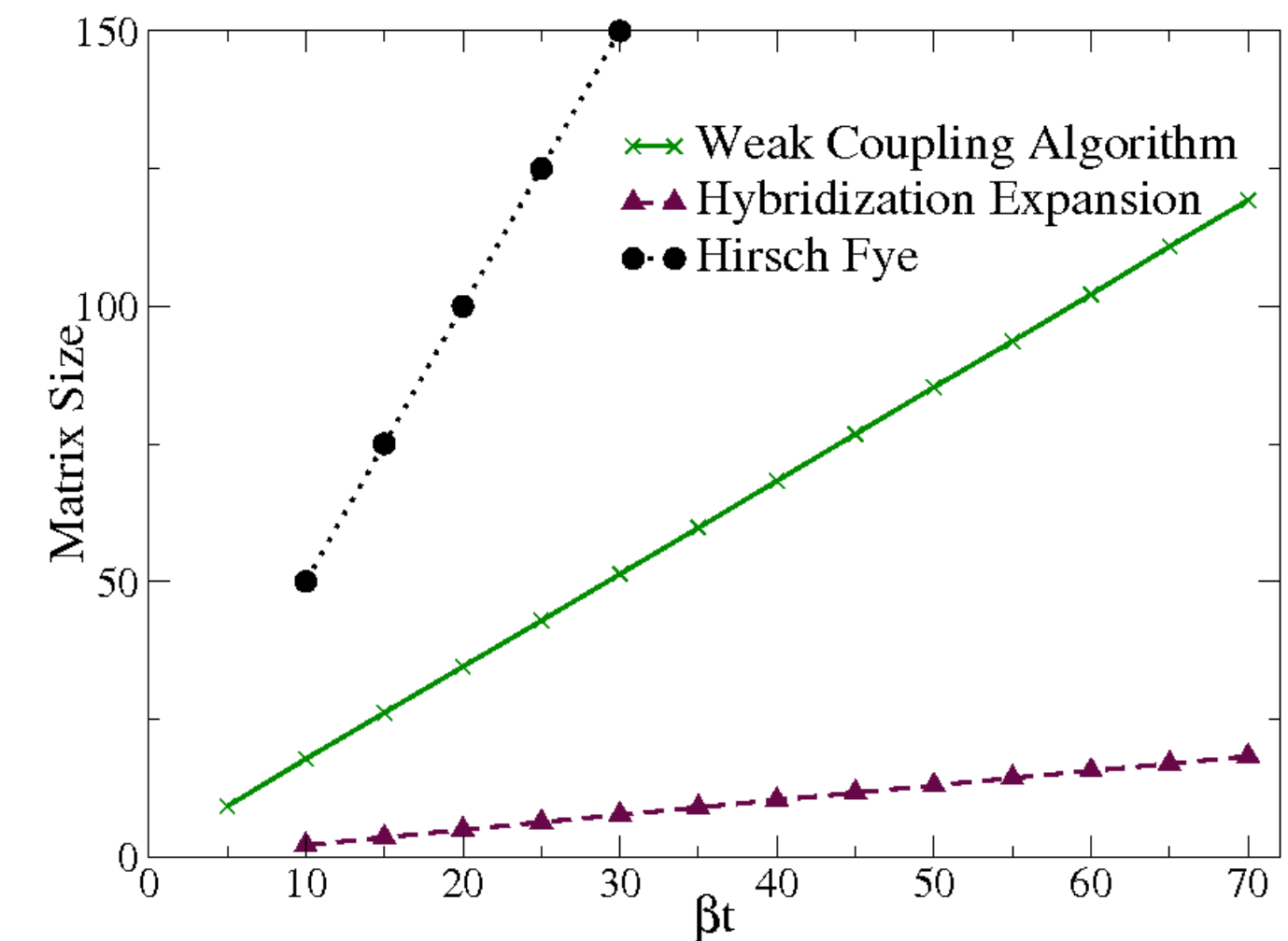


# Continuous-time quantum Monte Carlo algorithms

- 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

# 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

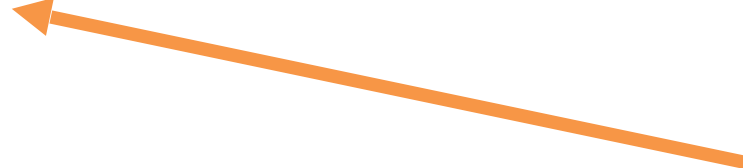
$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_I$$

- **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  $\Delta$

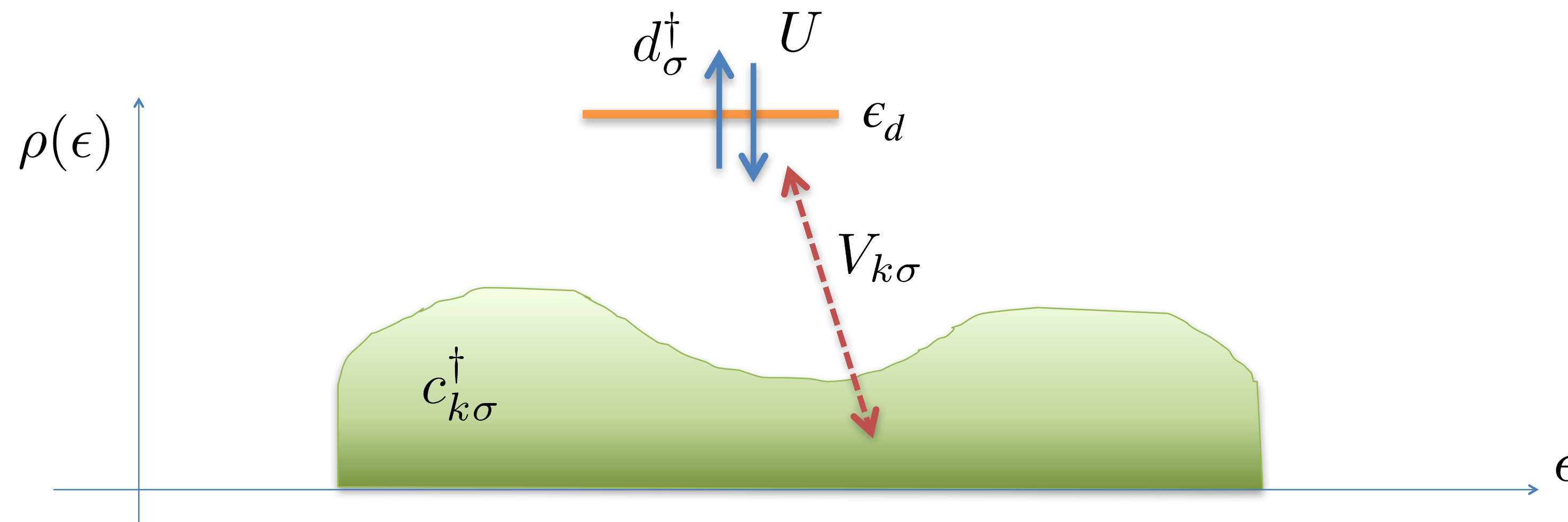
We want to compute "  $Z = \sum_n a_n \Delta^n$  "

# 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

# 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)



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

# Interaction expansion CT-QMC

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

$$\hat{A}(\tau) = e^{\tau\mathcal{H}_0} A e^{-\tau\mathcal{H}_0} \quad \text{Interaction picture}$$

- 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:

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

- Pushing the integration limits to  $\tau$  and introducing the time-ordering operator  $T_{\tau}$

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

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

# Interaction expansion CT-QMC

- We want to compute the partition function

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

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

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

we obtain

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

# Interaction expansion CT-QMC

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

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

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

$$M_{\sigma}^{(n)} = \begin{pmatrix} G_{0\sigma}(0^-) & G_{0\sigma}(\tau_1 - \tau_2) & \cdots & G_{0\sigma}(\tau_1 - \tau_n) \\ G_{0\sigma}(\tau_2 - \tau_1) & G_{0\sigma}(0^-) & \cdots & G_{0\sigma}(\tau_2 - \tau_n) \\ \vdots & \vdots & \ddots & \vdots \\ G_{0\sigma}(\tau_n - \tau_1) & G_{0\sigma}(\tau_n - \tau_2) & \cdots & G_{0\sigma}(0^-) \end{pmatrix} \quad G_0(i\omega_n) = \frac{1}{i\omega_n - \epsilon_d - \Delta(i\omega_n)}$$

# Interaction expansion CT-QMC

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

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

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

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

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

We want to compute the integrals stochastically

# Monte Carlo elements

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

- Monte Carlo sum  $\sum_{\mathcal{C}}^{\text{MC}} \equiv \sum_n \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n$
- Configuration  $\mathcal{C} = \{n, \tau_1, \dots, \tau_n\}$
- Probability distribution  $\rho(\mathcal{C}) = |w(\mathcal{C})|$  with  $w(\mathcal{C}) = \frac{(-U)^n}{n!} \det M_\uparrow^{(n)} \det M_\downarrow^{(n)}$  Very different from the Boltzmann weight!
- Compute 
$$K_\sigma(i\omega_n) = \frac{\sum_{\mathcal{C}}^{\text{MC}} \sum_{ij} e^{i\omega_n(\tau_i - \tau_j)} \left[ M_\sigma^{(n)} \right]_{ij}^{-1} \text{sign}(w(\mathcal{C}))}{\sum_{\mathcal{C}}^{\text{MC}} \text{sign}(w(\mathcal{C}))}$$

# 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

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

- 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

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

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

$$U n_{\uparrow} n_{\downarrow} = \frac{U}{2} \sum_{s=\uparrow, \downarrow} (n_{\uparrow} - \alpha_{s\uparrow}) (n_{\downarrow} - \alpha_{s\downarrow}) + \underbrace{\frac{U}{2} (n_{\uparrow} + n_{\downarrow})}_{\text{we absorb this term in the chemical potential}} + \text{const} \quad \alpha_{s\sigma} = \frac{1}{2} + (2\delta_{s\sigma} - 1)\delta$$

we absorb this term in the chemical potential

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

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

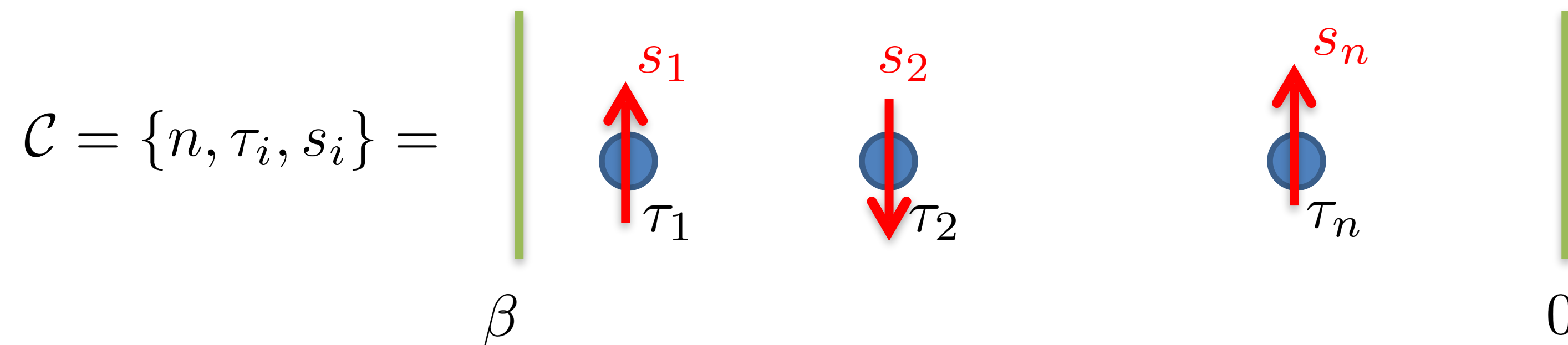
we now have an extra sum over auxiliary spins

tuning  $\delta$  can help the sign problem a lot

# Monte Carlo elements after trick

- MC sum:
 
$$\sum_{\mathcal{C}}^{\text{MC}} = \sum_n \int_{\tau_1 > \dots > \tau_n} d\tau_1 \cdots d\tau_n \sum_{s_1} \cdots \sum_{s_n}$$

- 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.

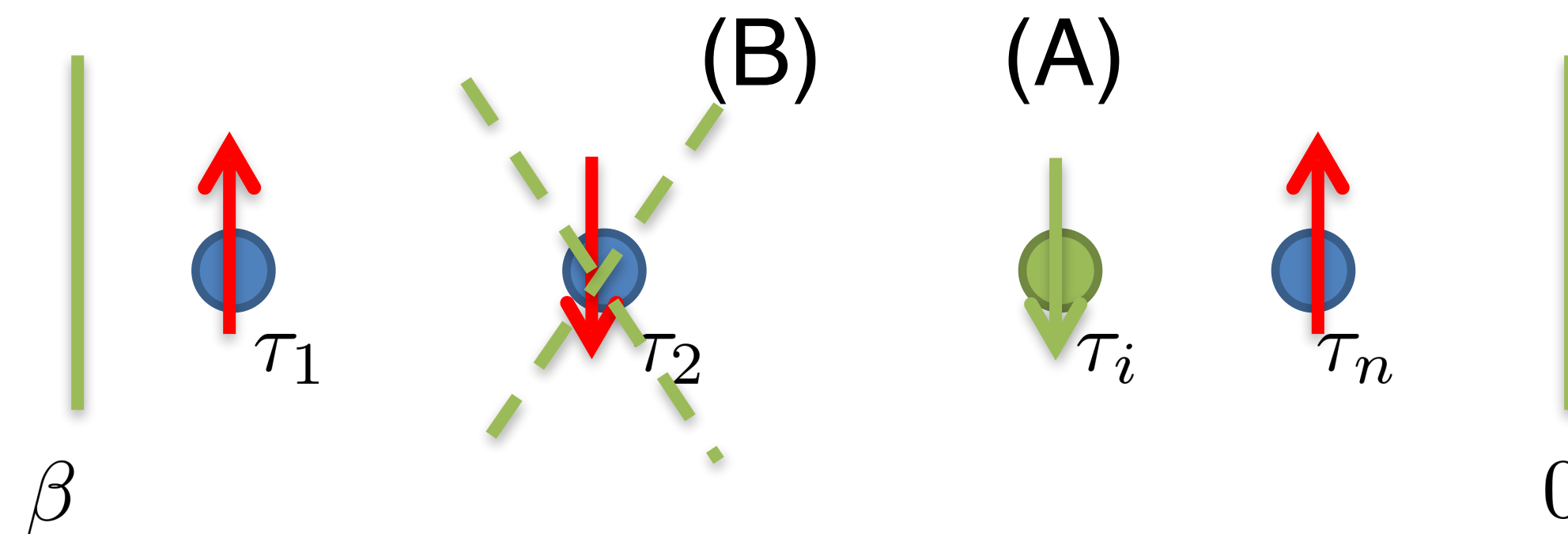


- The weight of every diagram is given by the absolute value of

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

# Generating diagrams

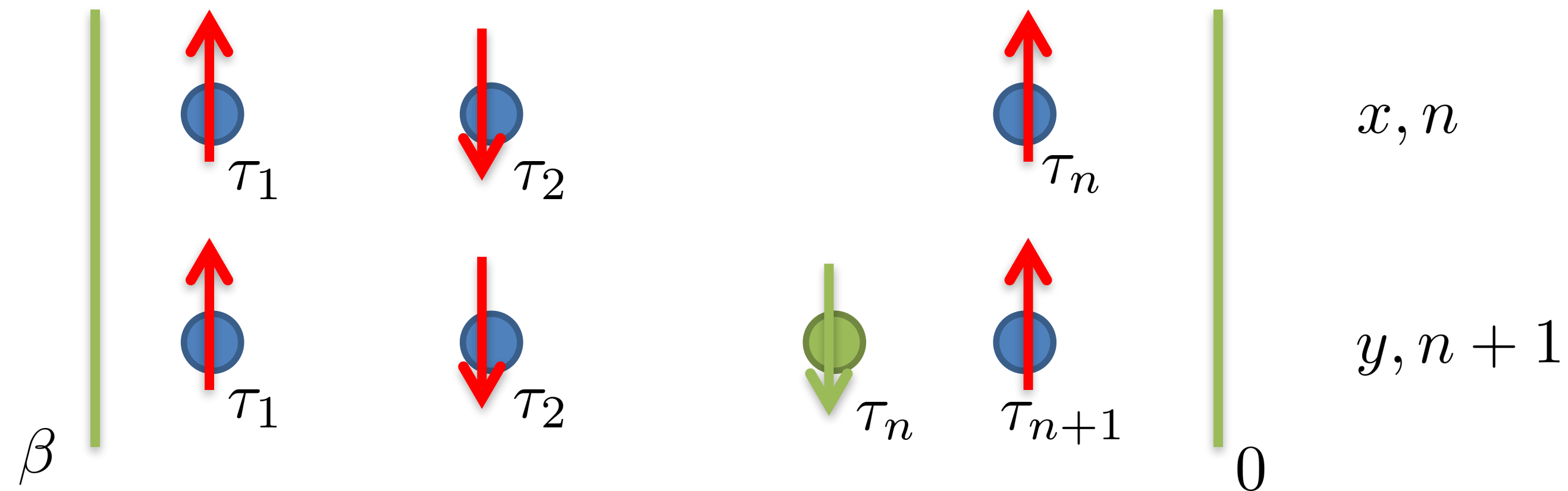
- We need to create a Markov chain of diagrams
- We can propose any changes to go from one diagram to another. A simple solution is to use two “moves”:
- **An insertion of a vertex**: we pick a random imaginary time and insert a vertex with a spin randomly up or down (A)
- **A removal of a vertex**: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



# Insertion of a vertex

- What is the acceptance rate?

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



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

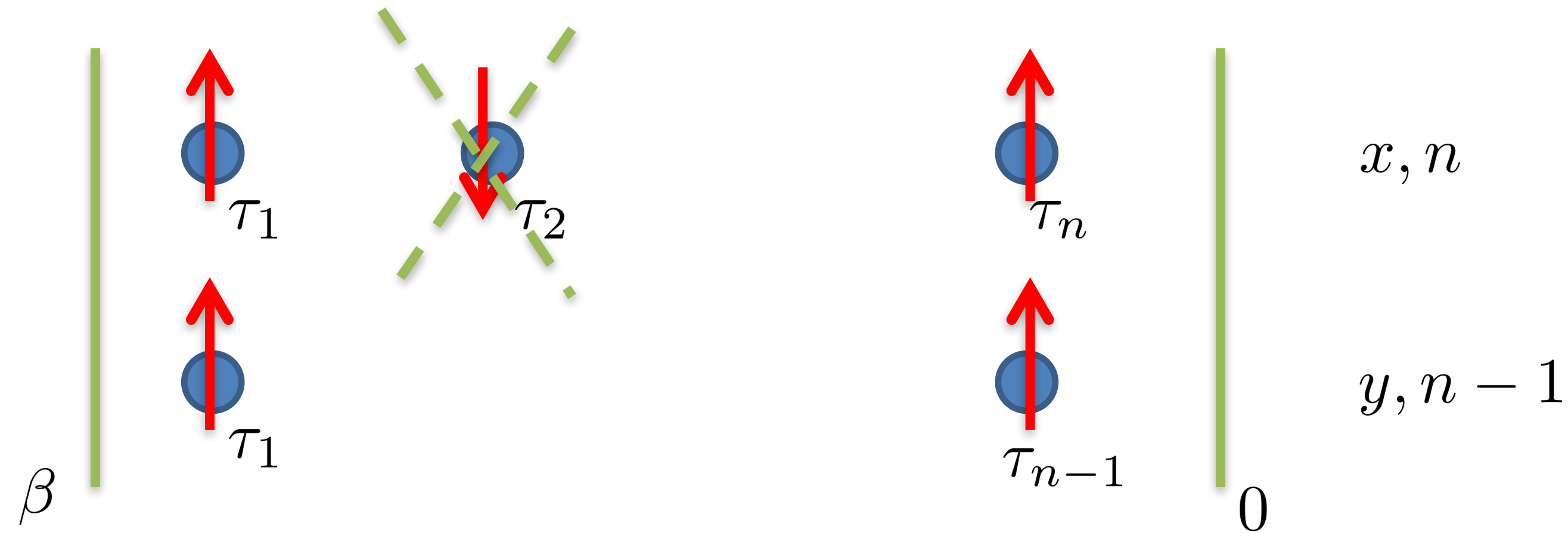
$$P_{y,x}\rho(y) = \frac{1}{2} \times \frac{1}{n+1} \times \left| \left( \frac{-U}{2} \right)^{n+1} \det D_{n+1}^\uparrow \det D_{n+1}^\downarrow \prod_{i=1}^{n+1} d\tau_i \right|$$

- 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:

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

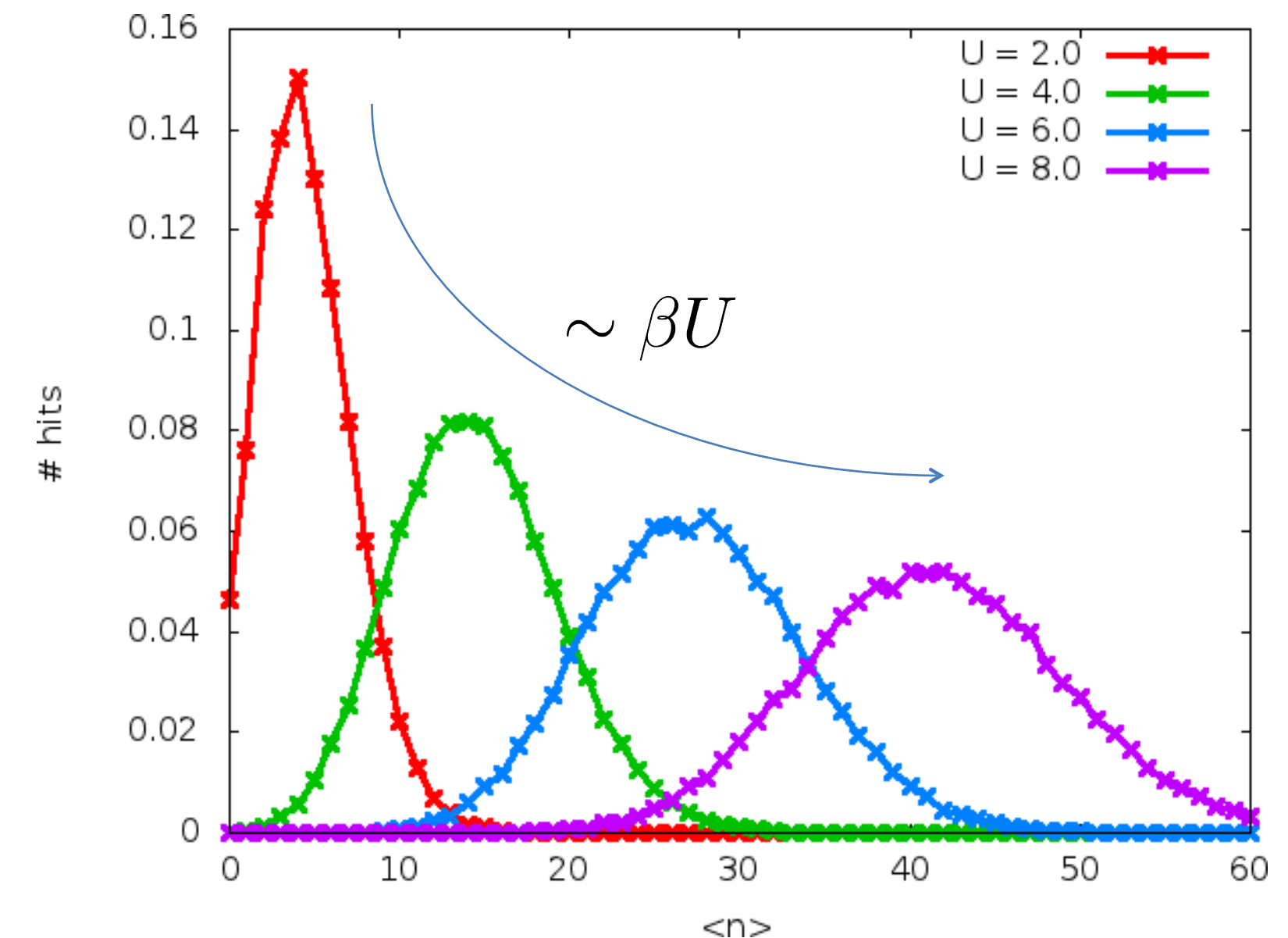
# Computational effort

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

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

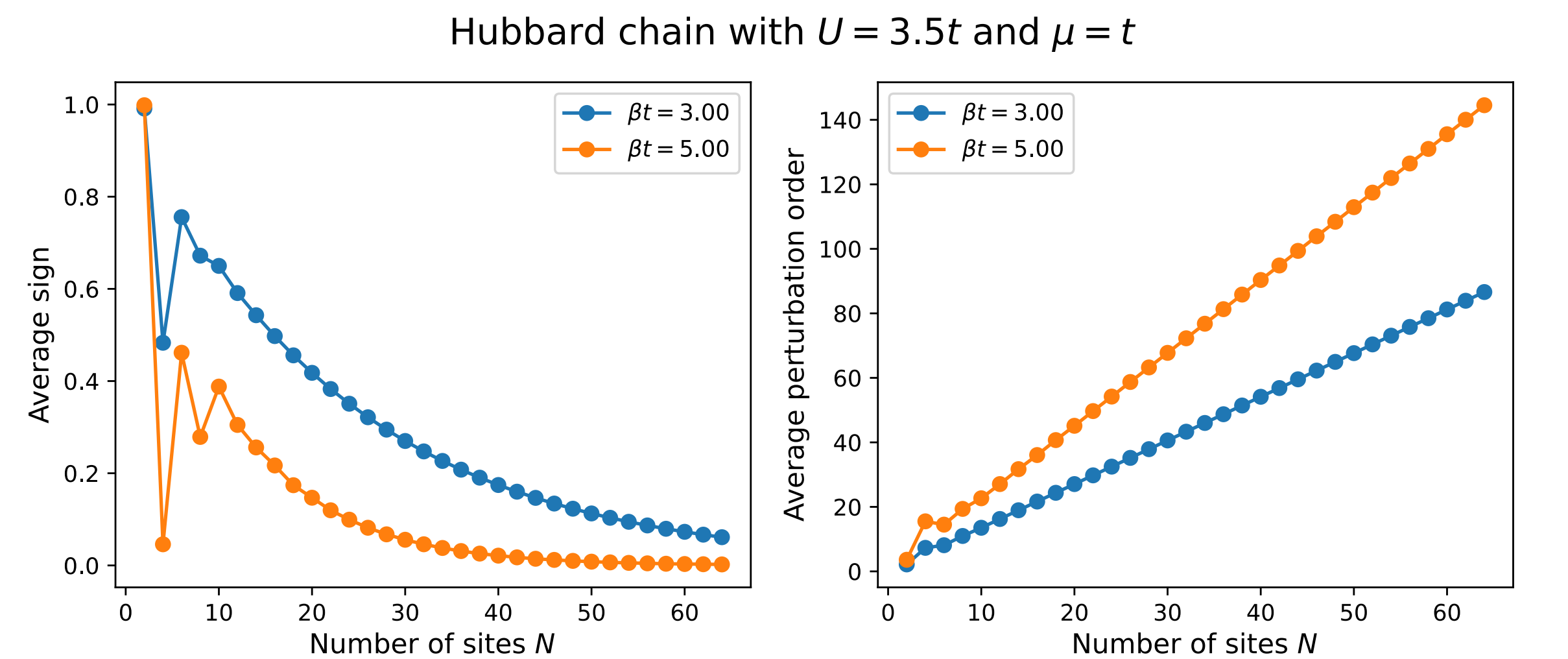
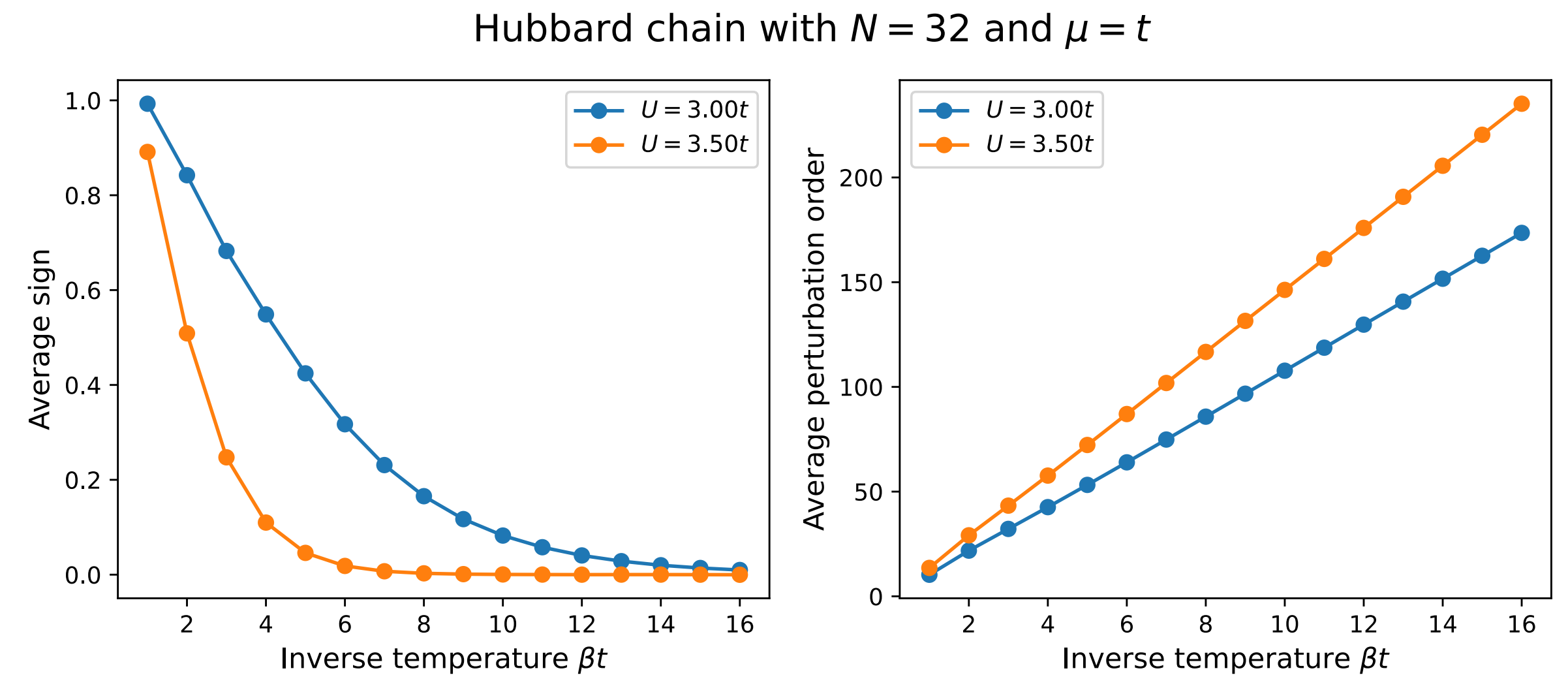
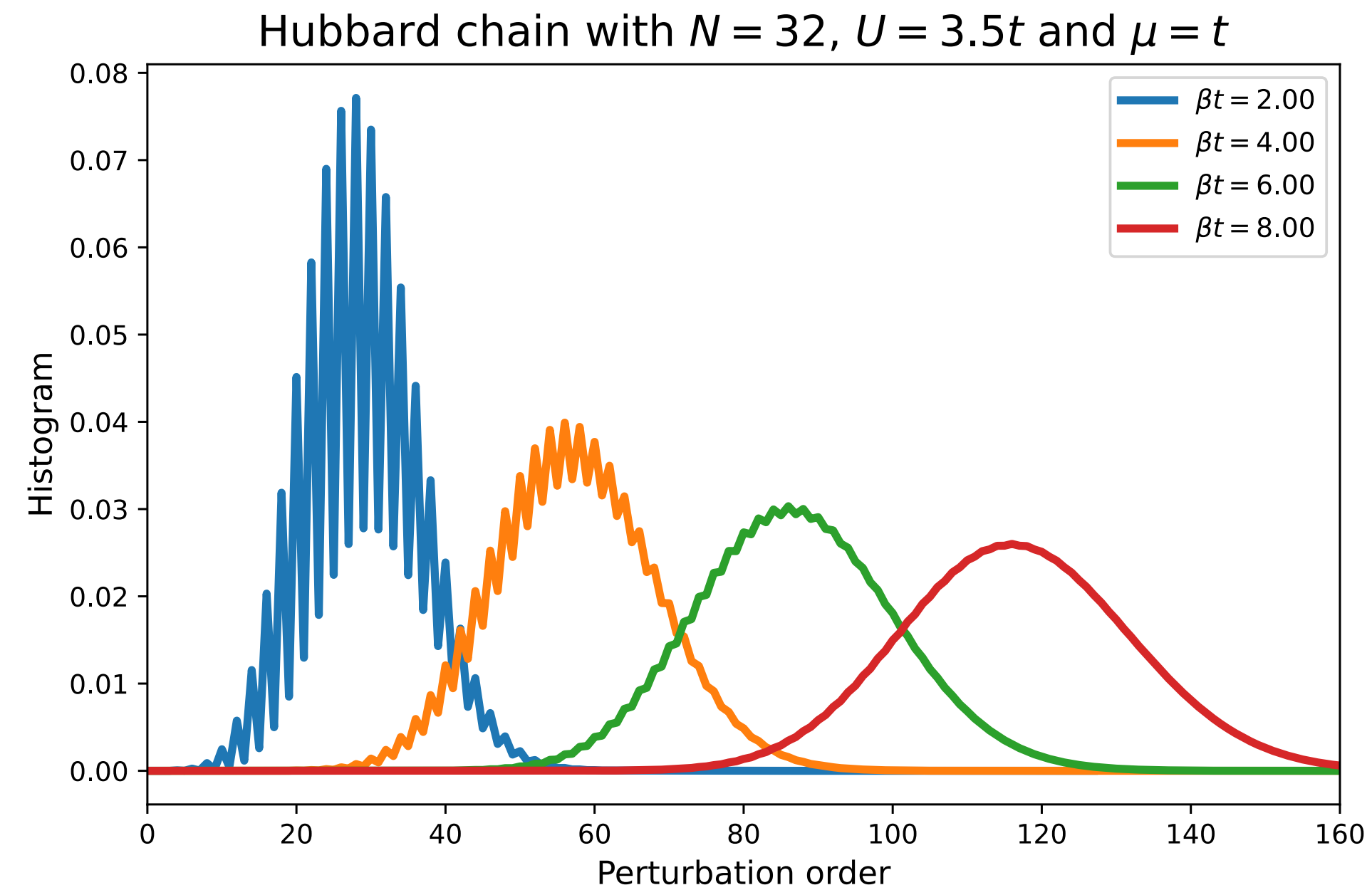
$$G_\sigma(i\omega_n) \sim G_{0\sigma}(i\omega_n) - \frac{1}{\beta Z} G_{0\sigma}^2(i\omega_n) \sum_{\mathcal{C}}^{\text{MC}} \sum_{ij} [D_n^\sigma]_{ij}^{-1} e^{i\omega_n(\tau_i - \tau_j)} \times \text{sign}(w(\mathcal{C}))$$

- 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

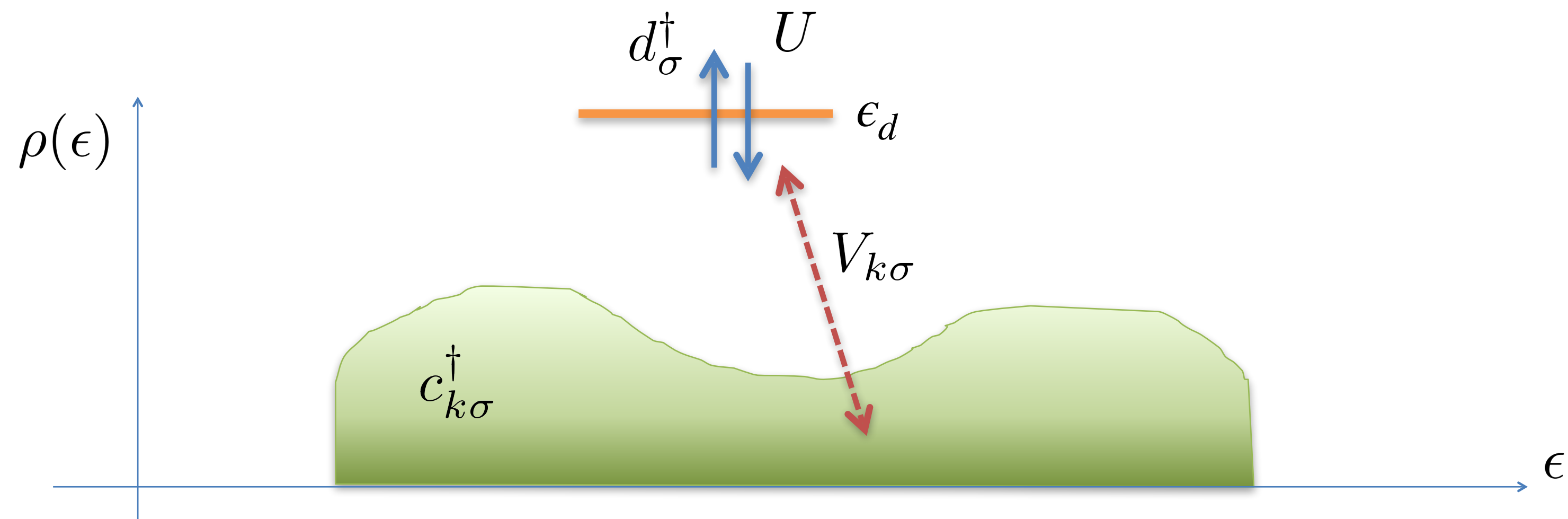


# Continuous-time quantum Monte Carlo algorithms

- 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)



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

# Hybridization expansion CT-QMC

- We work in the imaginary-time formalism

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

- The action for the Anderson model:

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

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

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

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

← action of the atomic problem

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

← “perturbation”

# Hybridization expansion CT-QMC

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

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

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

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

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

$$\langle A \rangle_{\text{loc}} = \frac{1}{Z_{\text{loc}}} \text{Tr} e^{-\beta \mathcal{H}_{\text{loc}}} \leftarrow \text{Hamiltonian of the local problem}$$

# Hybridization expansion CT-QMC

- Inserting the expression of the hybridization action we get

$$Z = \sum_{n_{\uparrow}, n_{\downarrow}=0}^{\infty} \left\langle T_{\tau} \prod_{\sigma} \frac{(-1)^{n_{\sigma}}}{n_{\sigma}!} (\hat{S}_{\text{hyb}}^{\sigma})^{n_{\sigma}} \right\rangle_{\text{loc}} \int_0^{\beta} d\tau d\tau' d_{\sigma}^{\dagger}(\tau) \Delta_{\sigma}(\tau - \tau') d_{\sigma}(\tau')$$

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

Sum over many  
(continuous)  
variables

Product of  
hybridization  
functions

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

Trace involving  
both spin up  
and down  
operators

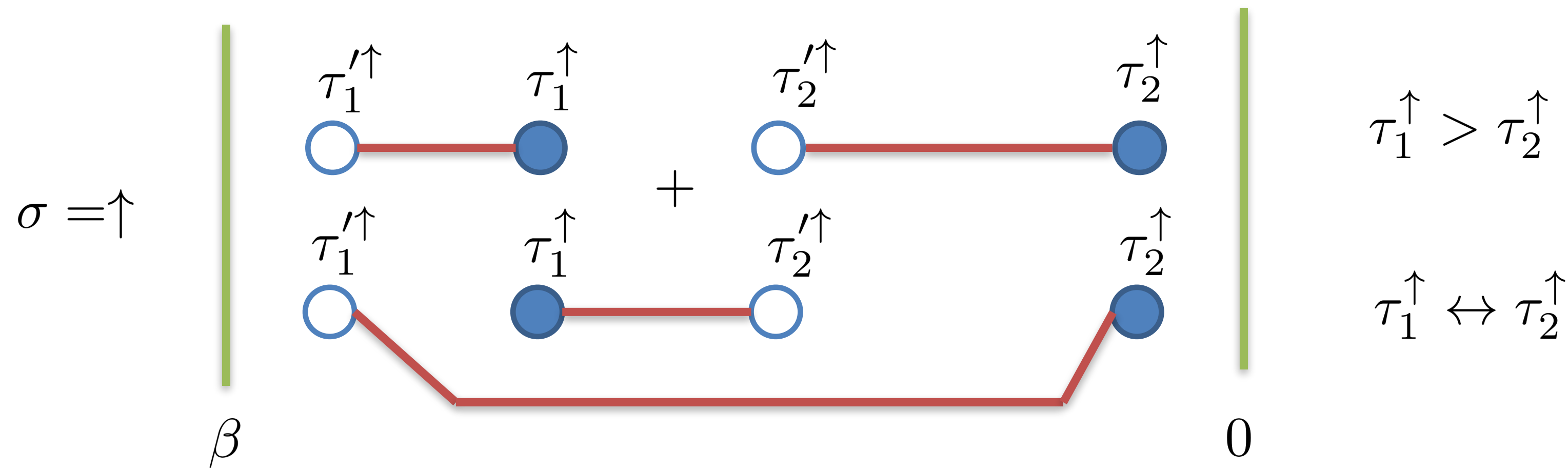
$$\text{Tr} \left[ e^{-\beta \mathcal{H}_{\text{loc}}} T_{\tau} \prod_{i=1}^{n_{\uparrow}} d_{\uparrow}^{\dagger}(\tau_i^{\uparrow}) d_{\uparrow}(\tau_i^{\prime\uparrow}) \prod_{i=1}^{n_{\downarrow}} d_{\downarrow}^{\dagger}(\tau_i^{\downarrow}) d_{\downarrow}(\tau_i^{\prime\downarrow}) \right]$$

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



# Trick: resumming diagrams

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



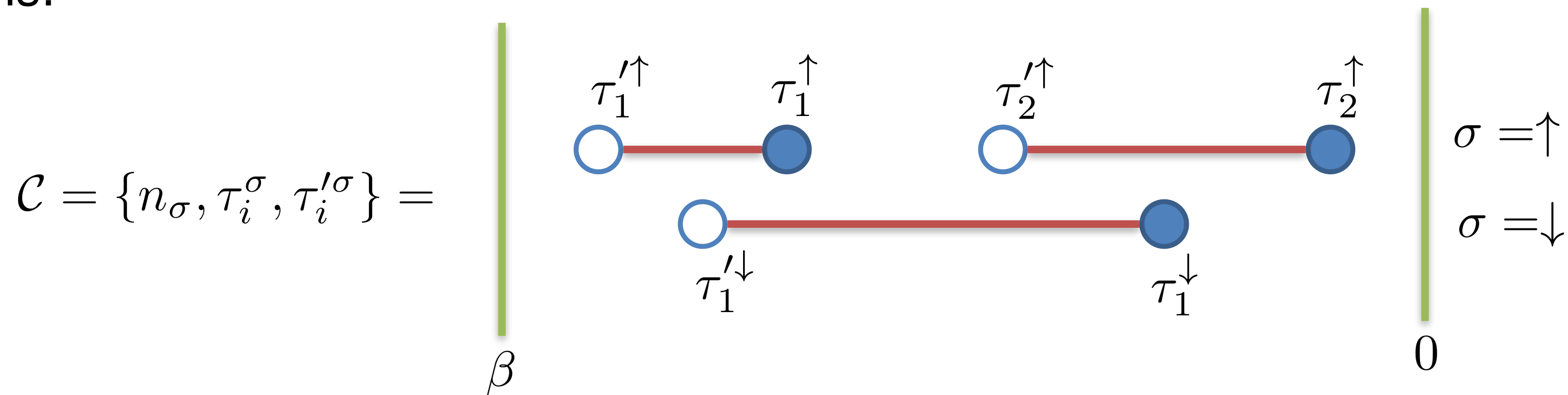
$$\begin{aligned}
 & \text{Tr} \left[ e^{-\beta \mathcal{H}_{\text{loc}}} d_\uparrow^\dagger(\tau_1^\uparrow) d_\uparrow(\tau_1'^\uparrow) d_\uparrow^\dagger(\tau_2^\uparrow) d_\uparrow(\tau_2'^\uparrow) \right] \times \frac{1}{2} \Delta_\uparrow(\tau_1^\uparrow - \tau_1'^\uparrow) \Delta_\uparrow(\tau_2^\uparrow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

# Hybridization expansion Monte Carlo

- MC sum:

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

- Diagrams:



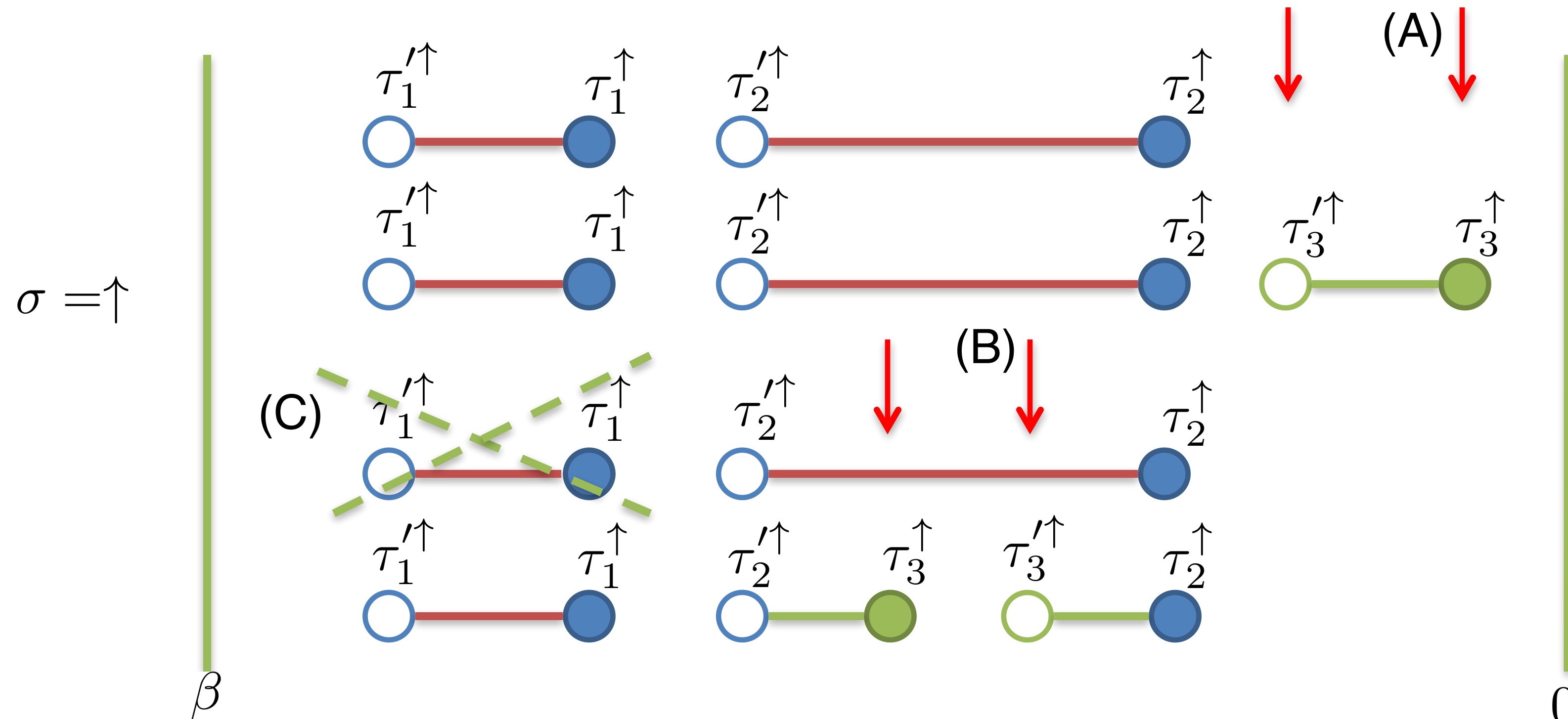
- Weight:

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

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

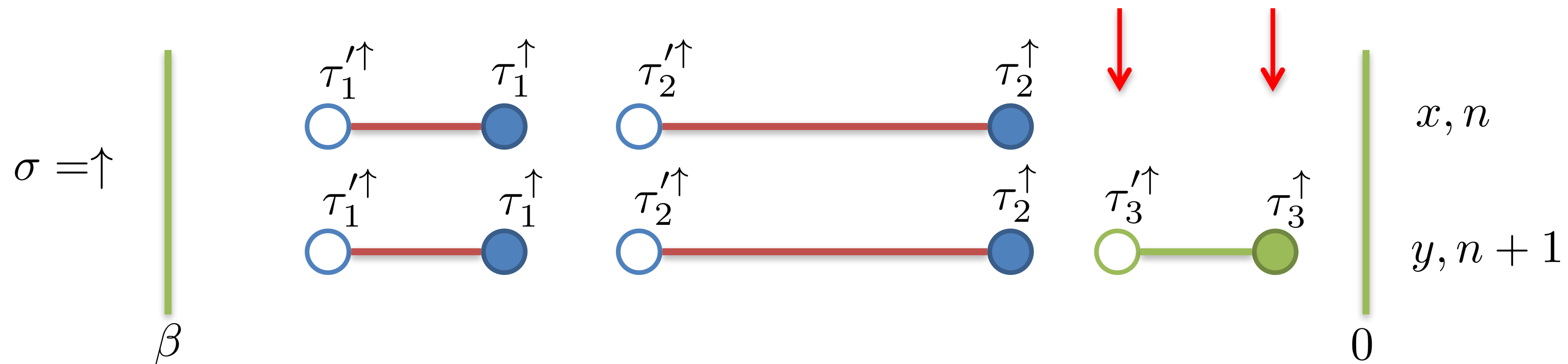
# Generating diagrams

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



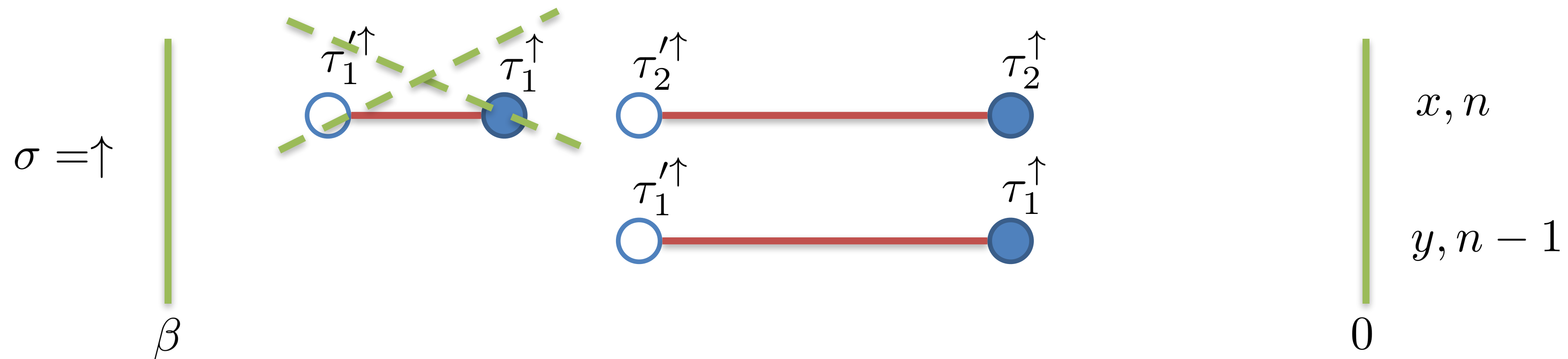
$$P_{x,y} \rho(x) = \frac{1}{2} \times \frac{d\tau_{n+1}}{\beta} \frac{d\tau'_{n+1}}{l_{\max}} \times \left| \text{Tr} \mathcal{C}_x \det \Delta_{\mathcal{C}_x} \prod_{i=1}^n d\tau_i d\tau'_i \right|$$

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

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

# Removal of a link

- What is the acceptance rate for this move?  $A_{x,y} = \min \left[ 1, \frac{P_{y,x} \rho(y)}{P_{x,y} \rho(x)} \right]$



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

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

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

# Measuring the Green function

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

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

- How do we get the Green's function?

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

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

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

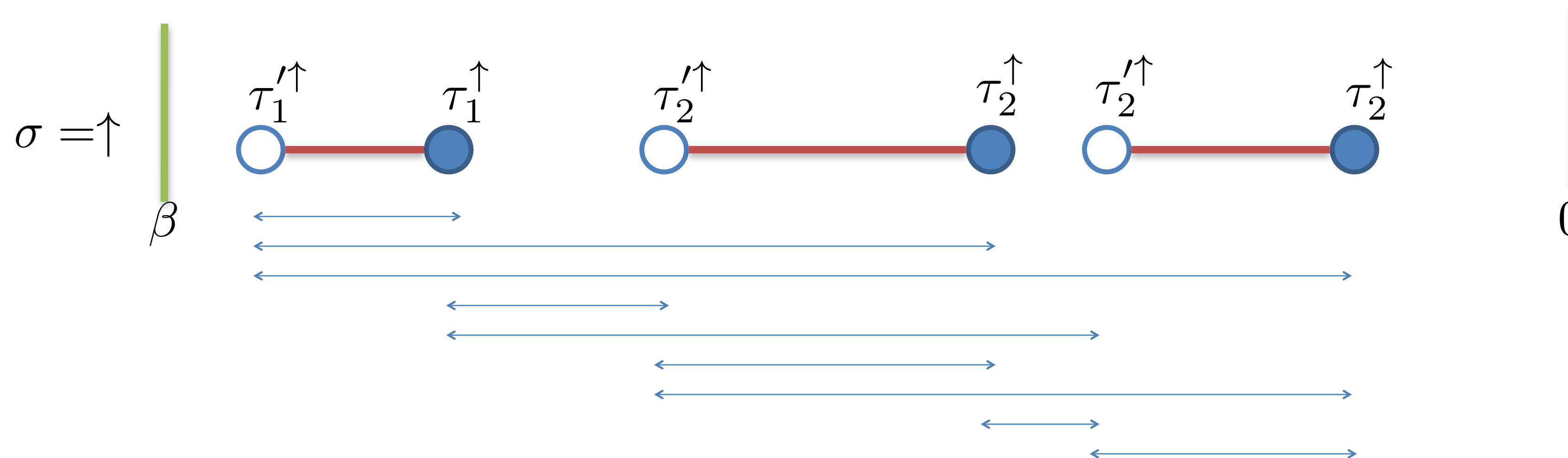
- Measure:

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

# Measuring the Green function

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

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



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

# Measuring using Legendre polynomials

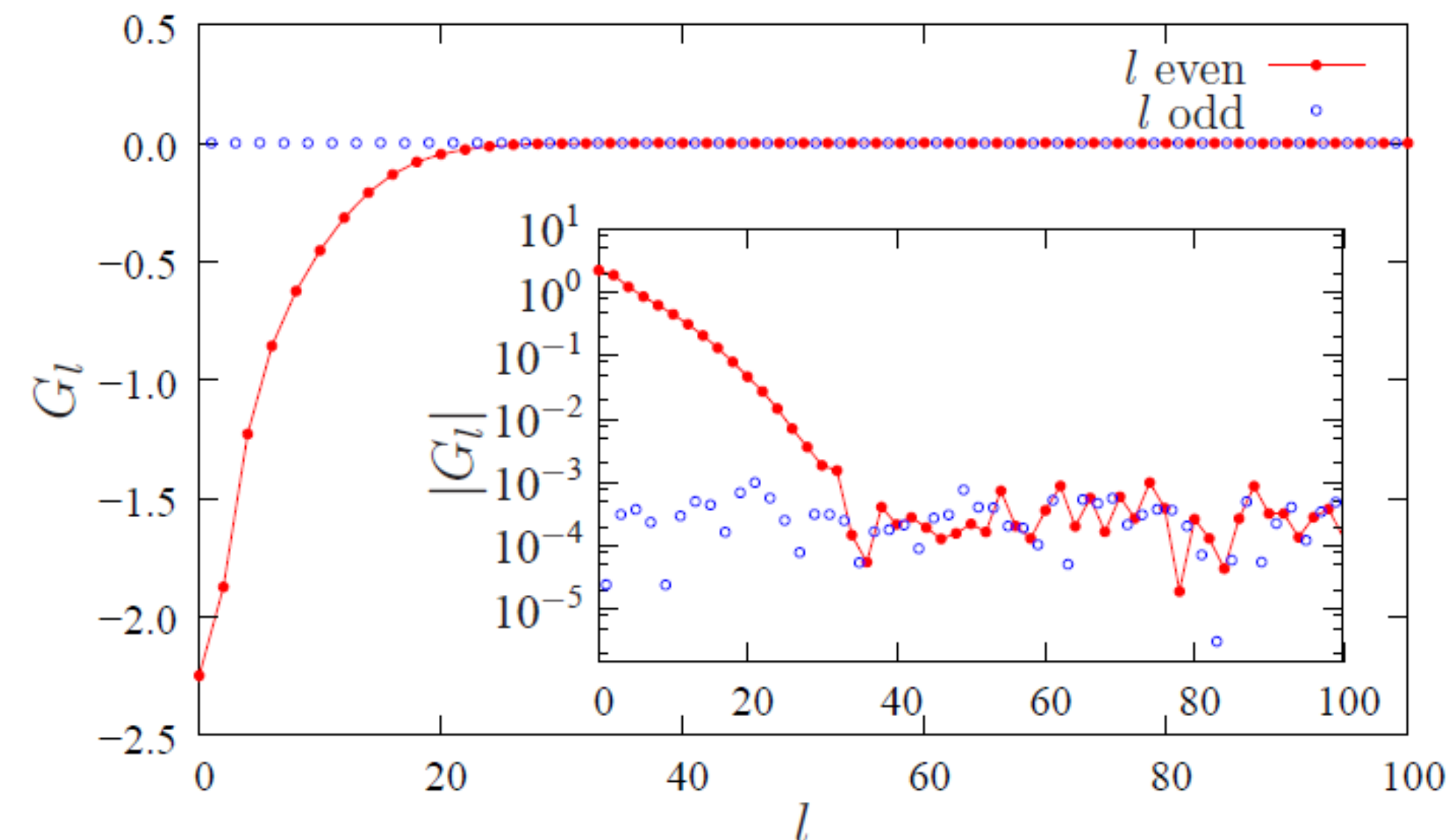
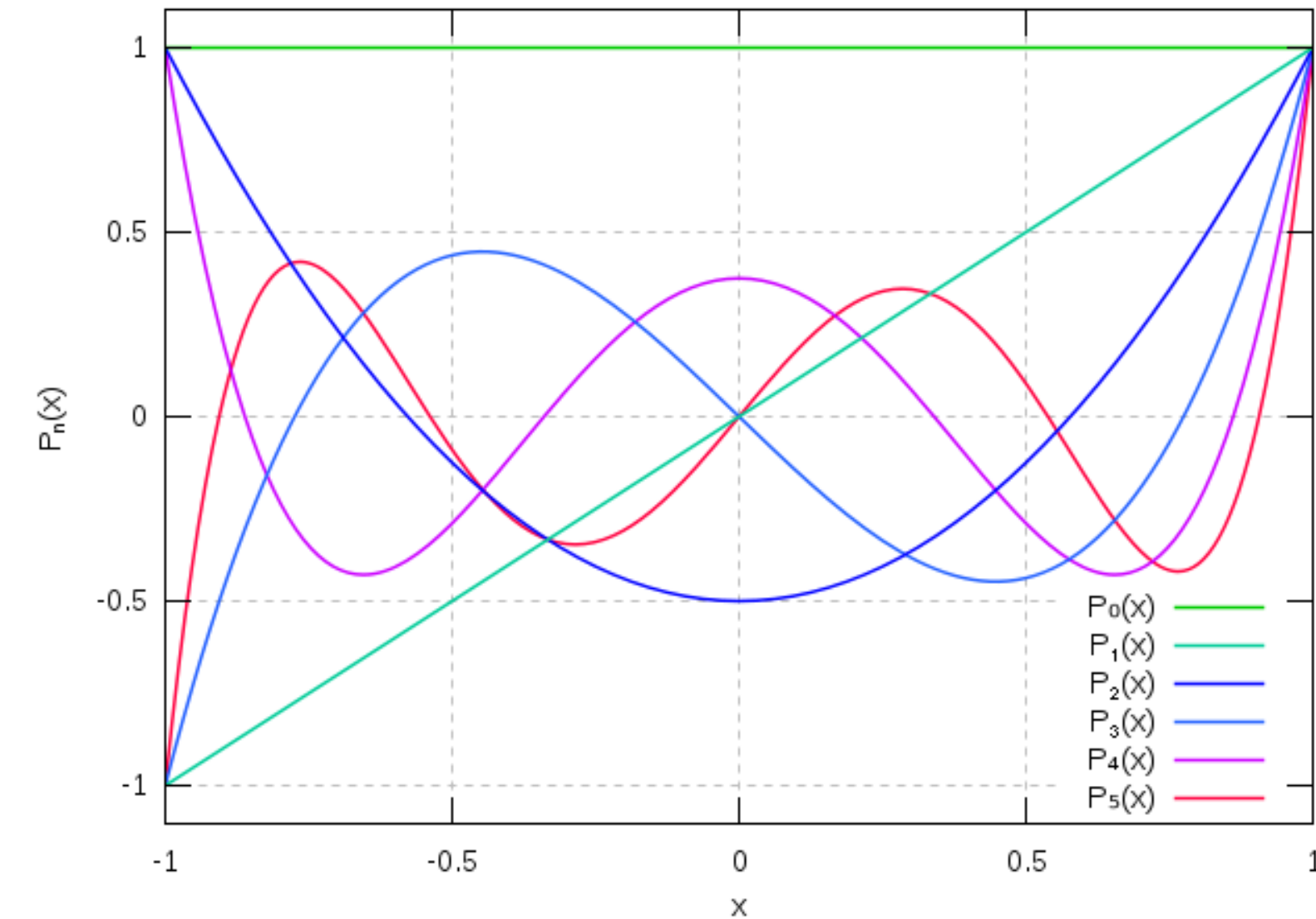
L. Boehnke et al., PRB (2011)

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

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

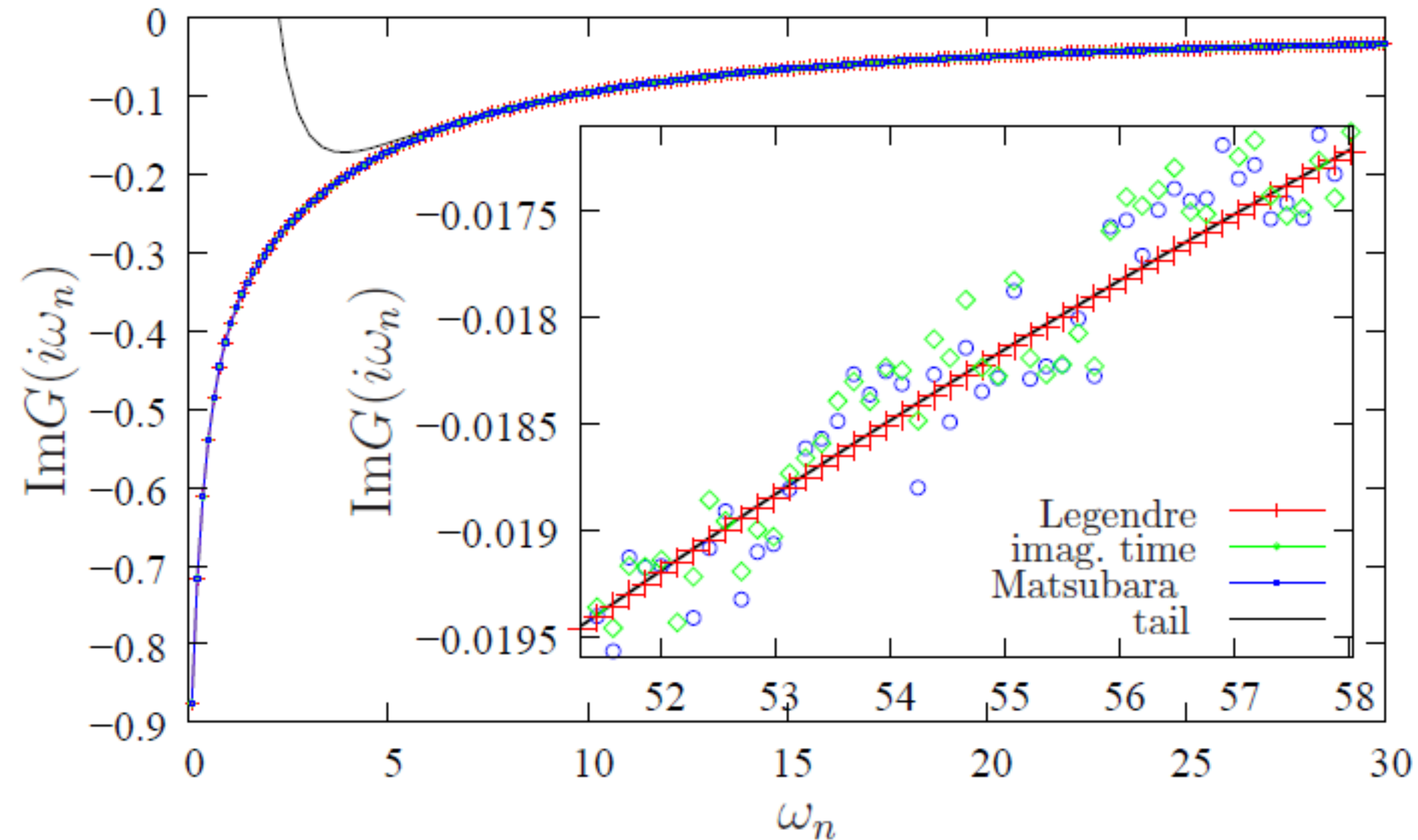
$$G(\tau) = \sum_{l \geq 0} \frac{\sqrt{2l+1}}{\beta} P_l[x(\tau)] G_l$$

- The coefficients  $G_l$  in this basis decay very quickly



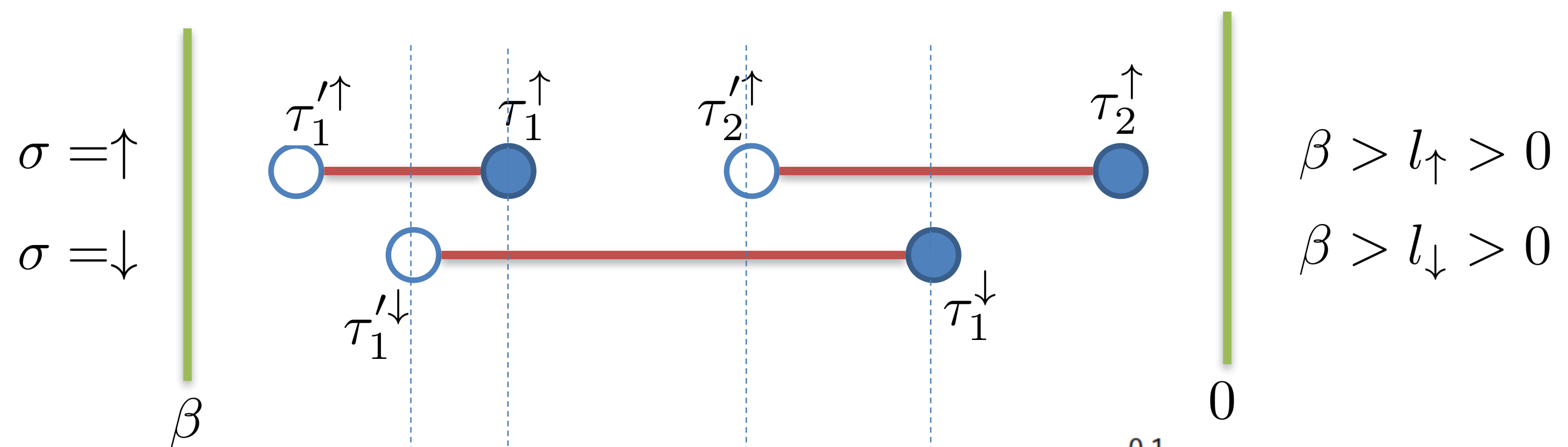
# Legendre basis acting as a filter

- 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

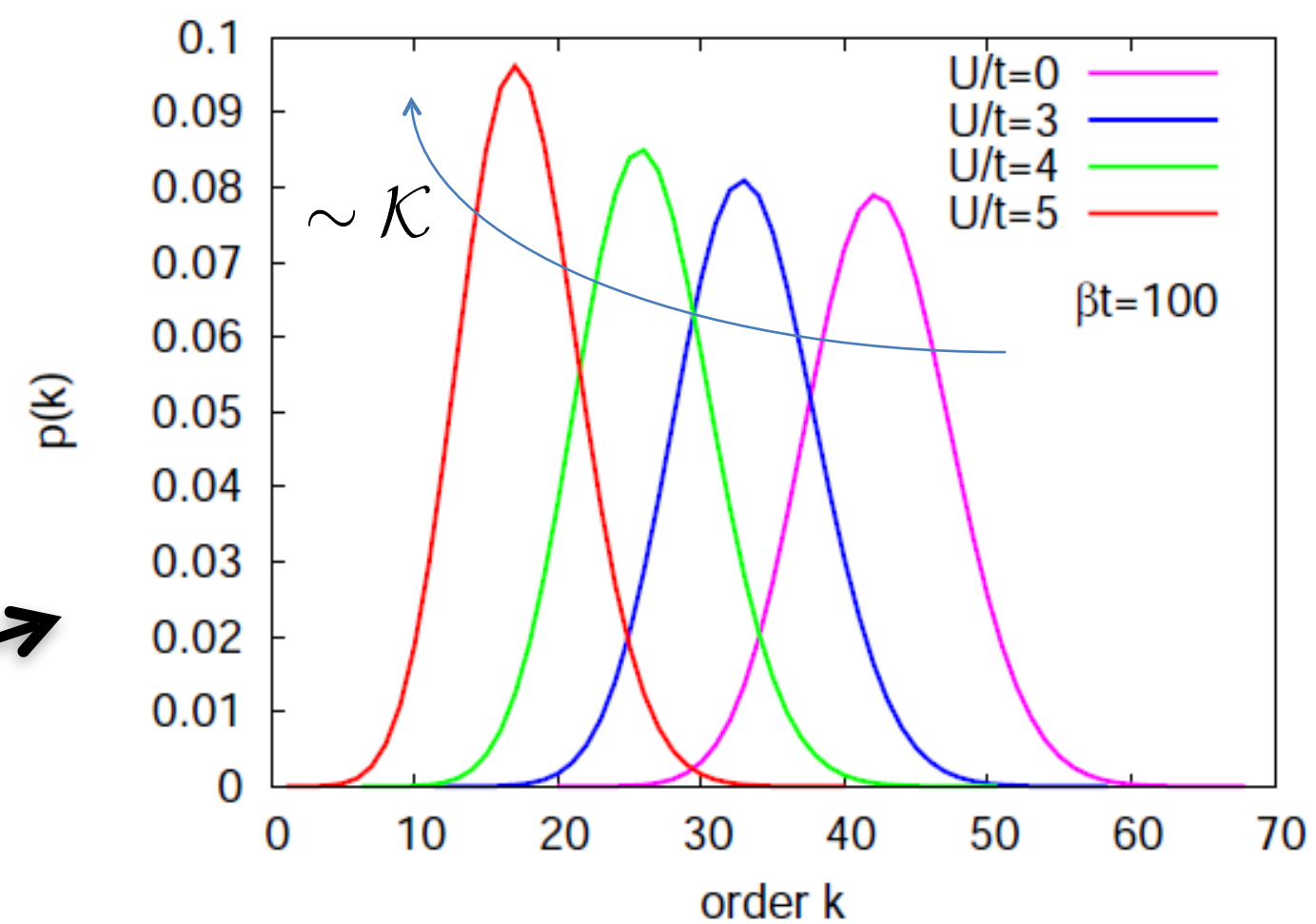
- Can the contribution of a diagram be computed quickly?
- Determinants can be updated quickly (Sherman-Morrison)
- For simple Hamiltonians, the trace is very easy



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

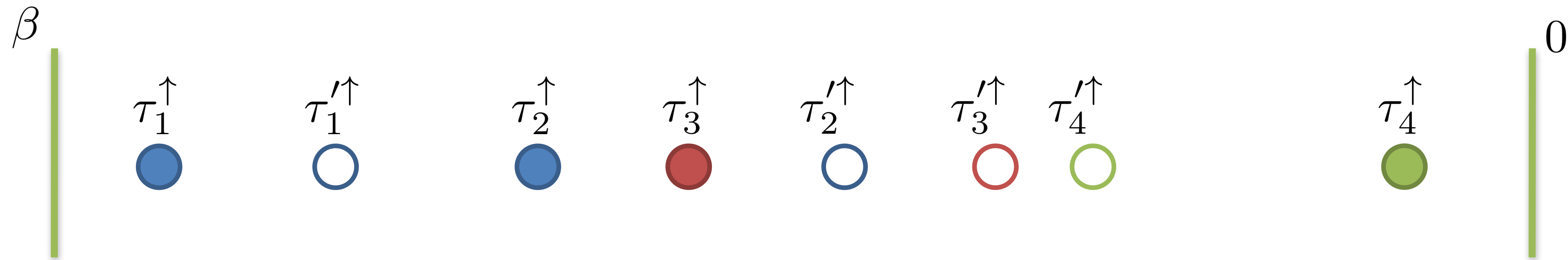
- Computational effort grows in

$\mathcal{O}(n^3)$   $\rightarrow$



# 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  $\Rightarrow$  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 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!