Continuous-time quantum Monte Carlo algorithms for impurity models

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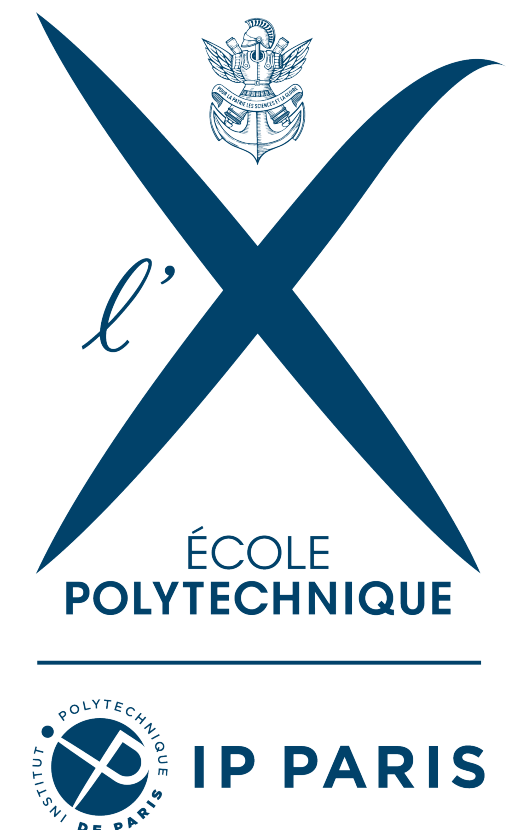
TRIQS Summer School
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https://mferrero.github.io/triqs_2023

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 algorithms

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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.

« **Atomic** » **problem with several orbitals**

$\mathcal{H}_{\rm loc}$

e^-

e^-

Electronic bath
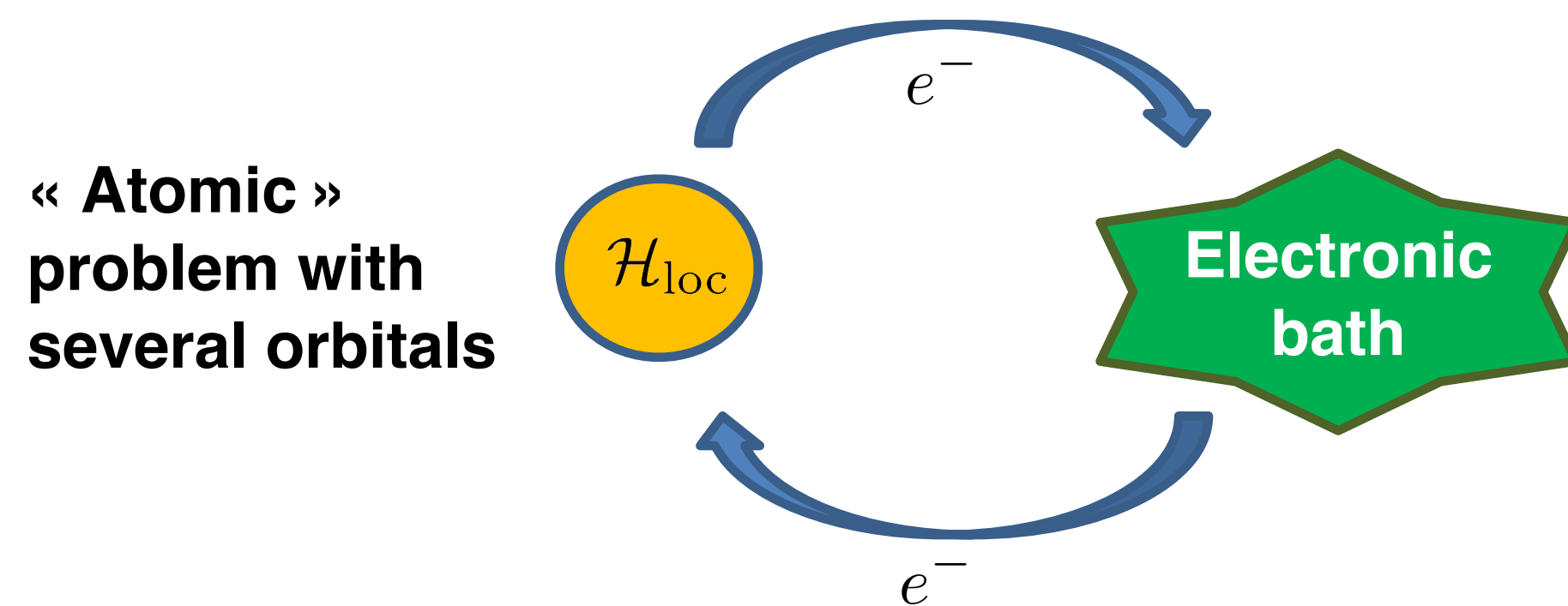
- Impurity models have a long history, e.g. the Kondo problem

- Lead to the development of models and methods

300

290

280

270

260

250

240

230

10%
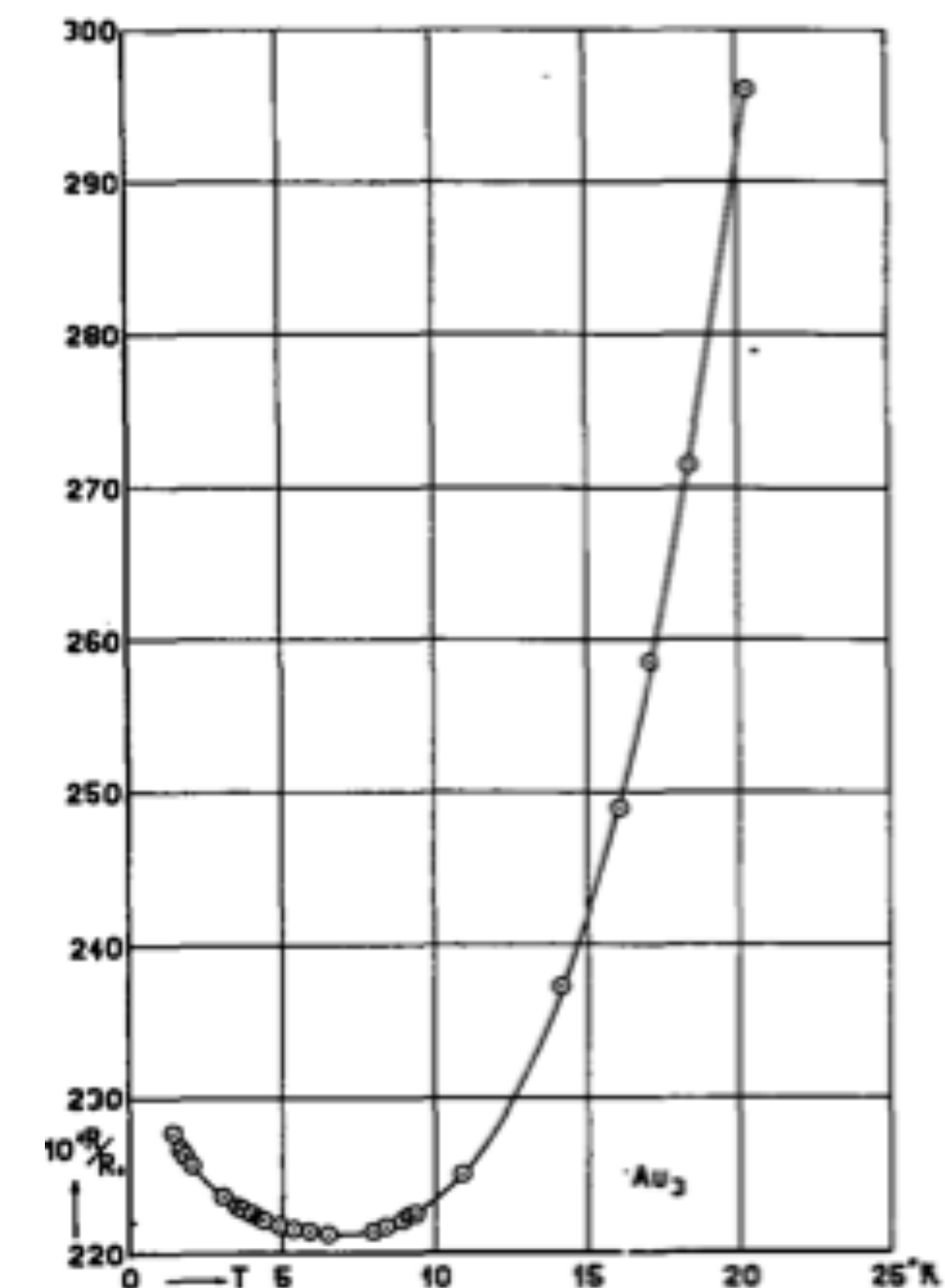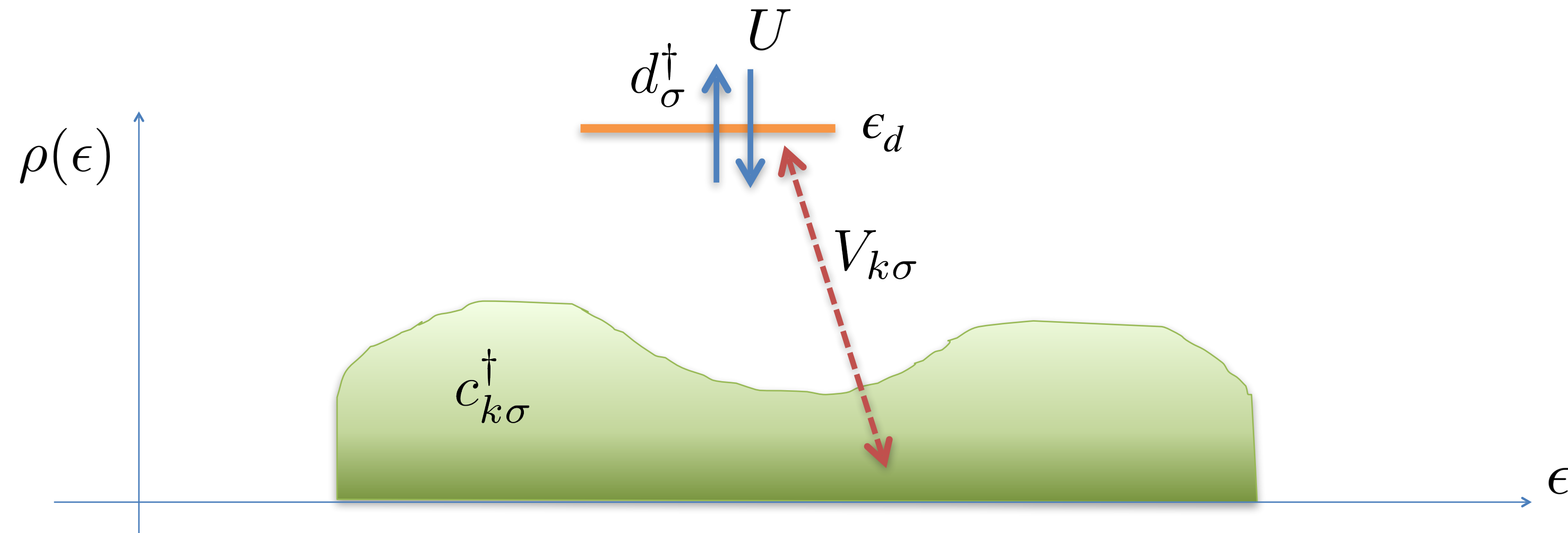
220

0 ——T 5   10   15   20   25°K

'Au₃

Fig. 1. Electrical resistance of Au₃.

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:

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

local many-body interaction   hybridization to the bath   free bath states
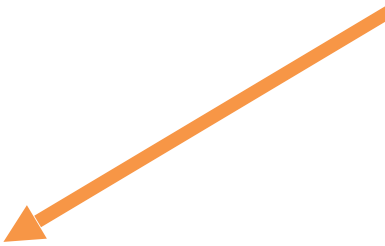
The Anderson model

- 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
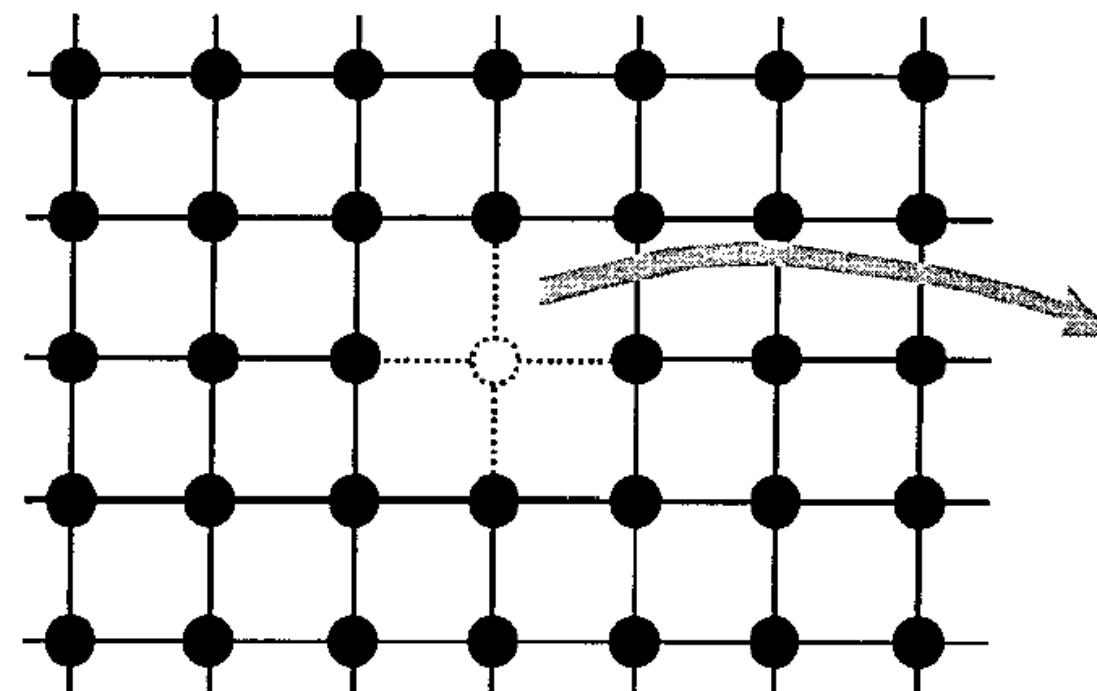
  – And many more…

- 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
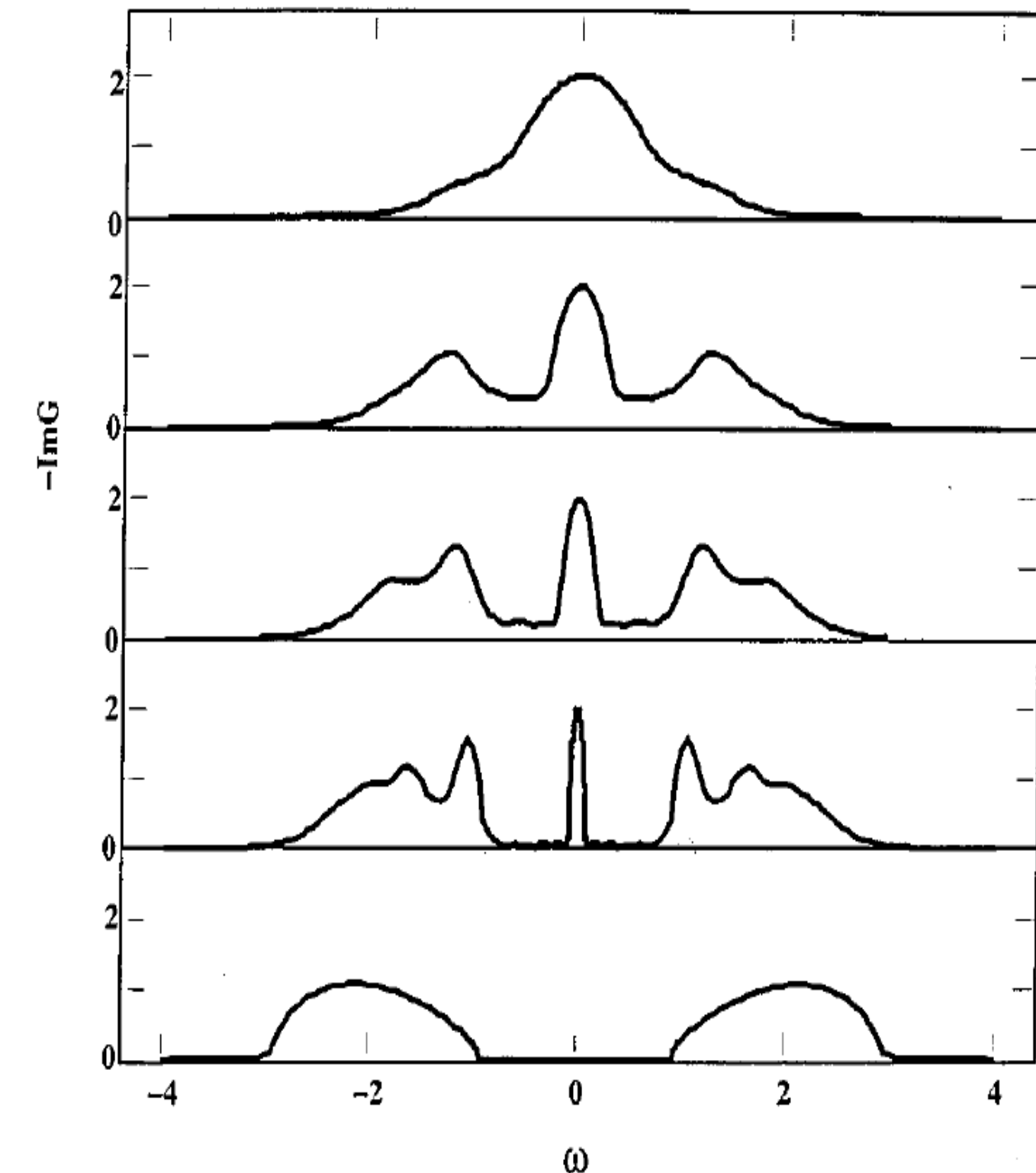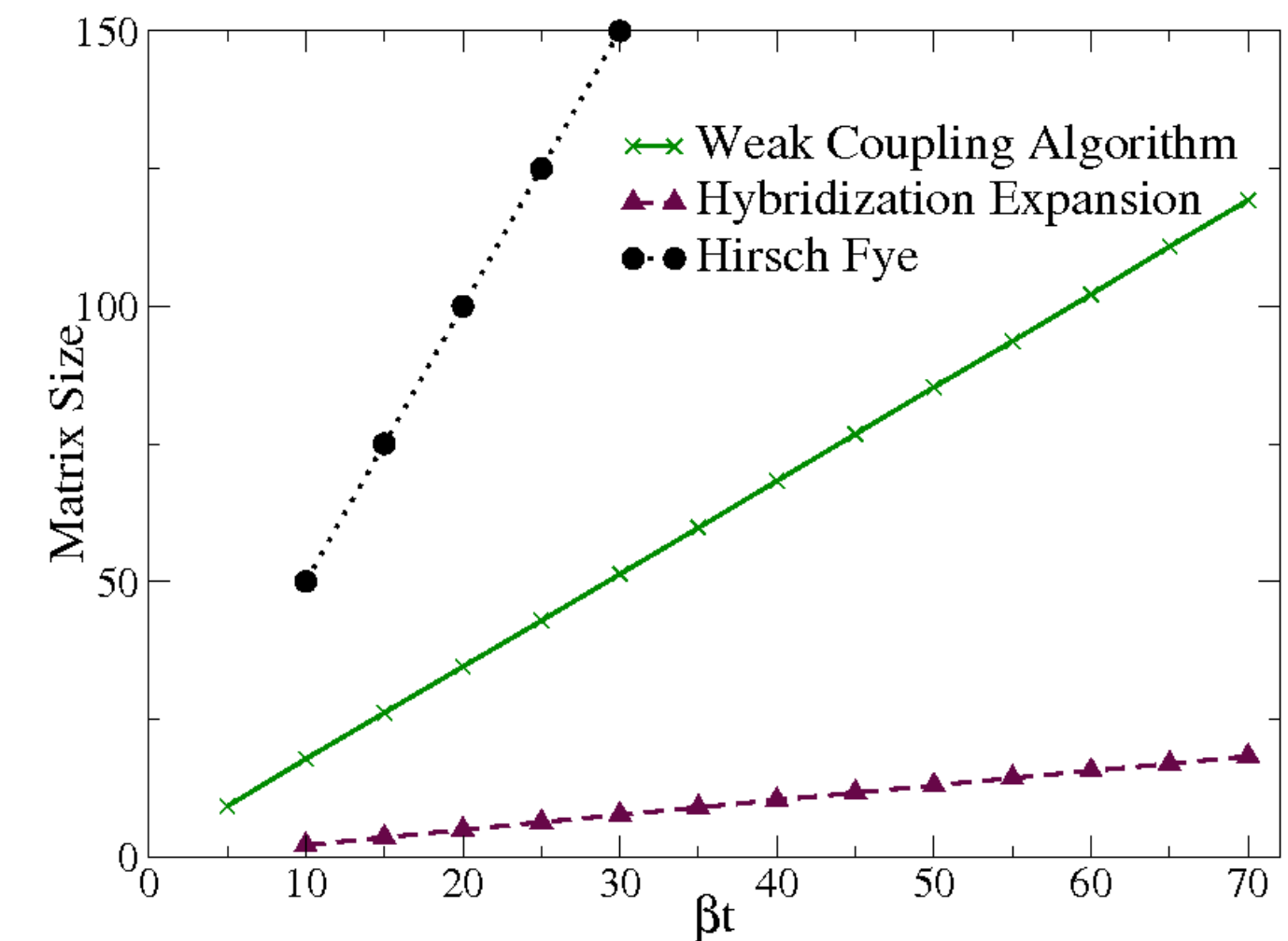
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Continuous-time quantum Monte Carlo methods

- **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 <u>series expansion</u> 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**

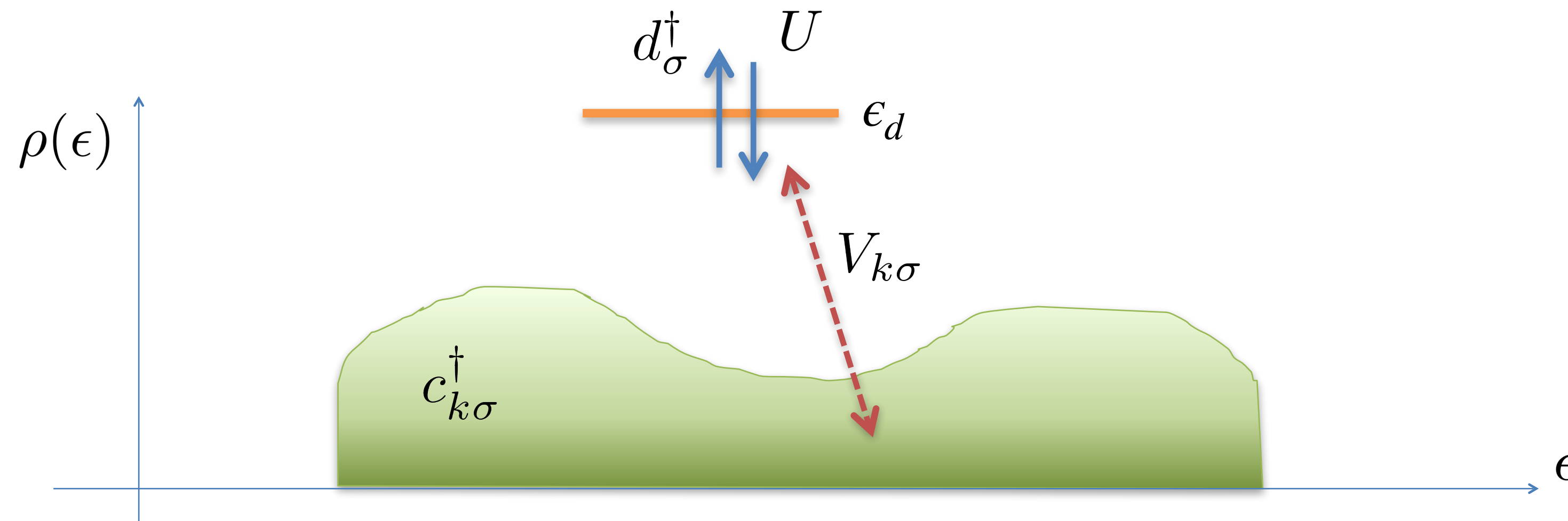   - H_0 is the "atomic limit" and H_I is the hybridization to the bath Δ

    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)

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

Interaction expansion CT-QMC

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

- 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

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

- 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:

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

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

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

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

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

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

Interaction expansion CT-QMC

- We want to compute the partition function

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

- 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

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

Interaction expansion CT-QMC

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

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

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

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

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

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

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

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

$$\mathcal{C} = \{n, \tau_1, \ldots, \tau_n\}$$

Very different from the Boltzmann weight!

- Probability distribution $\quad \rho(\mathcal{C}) = |w(\mathcal{C})| \quad$ with $\quad w(\mathcal{C}) = \frac{(-U)^n}{n!} \det M_\uparrow^{(n)} \det M_\downarrow^{(n)}$

- 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

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

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

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

we absorb this term in
the chemical potential

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

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

$$\left\langle T_{\tau}(n_{d\downarrow}(\tau_1) - \alpha_{s_1\downarrow}) \cdots (n_{d\downarrow}(\tau_n) - \alpha_{s_n\downarrow}) \right\rangle_0$$
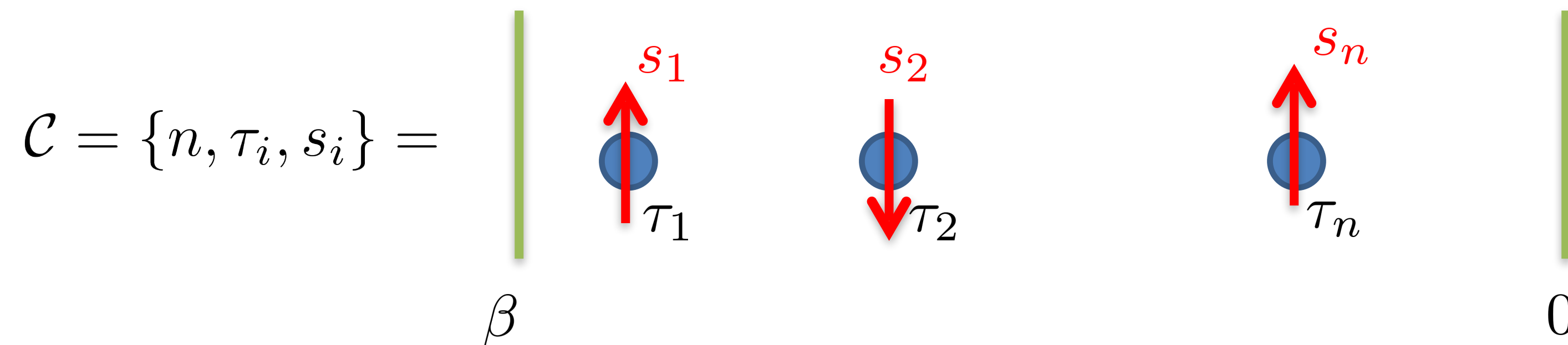
we now have an extra
sum over auxiliary spins

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

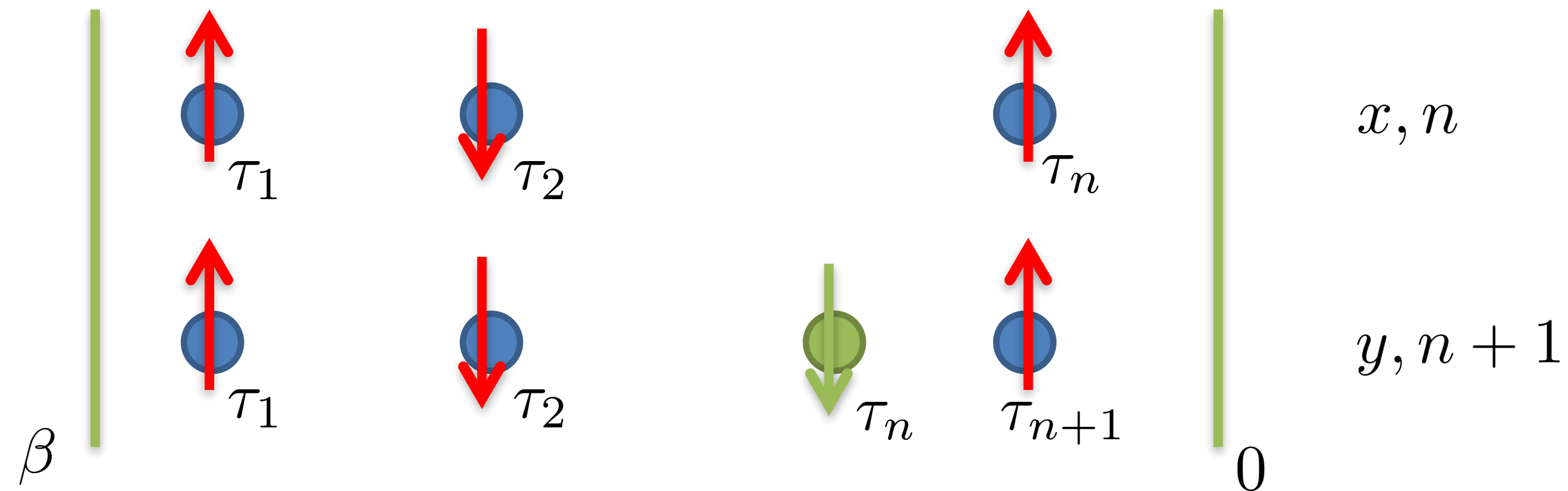- We need to create a Markov chain of diagrams

- 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)
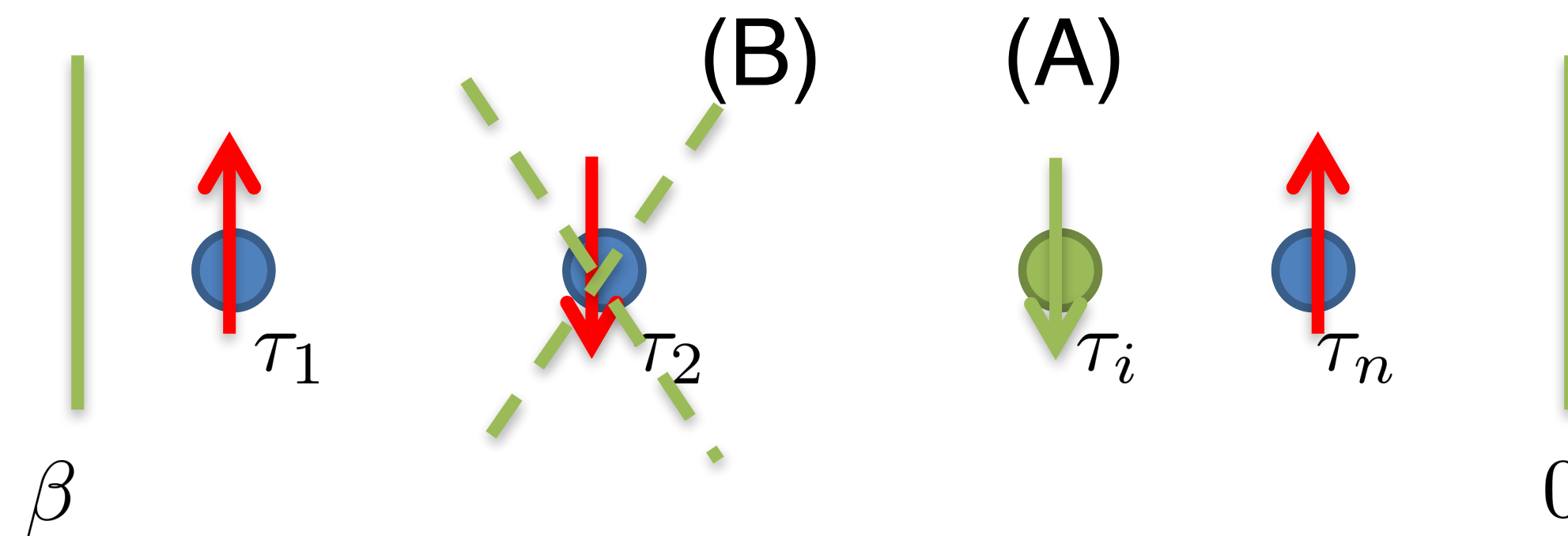
Insertion of a vertex

- What is the acceptance rate?

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

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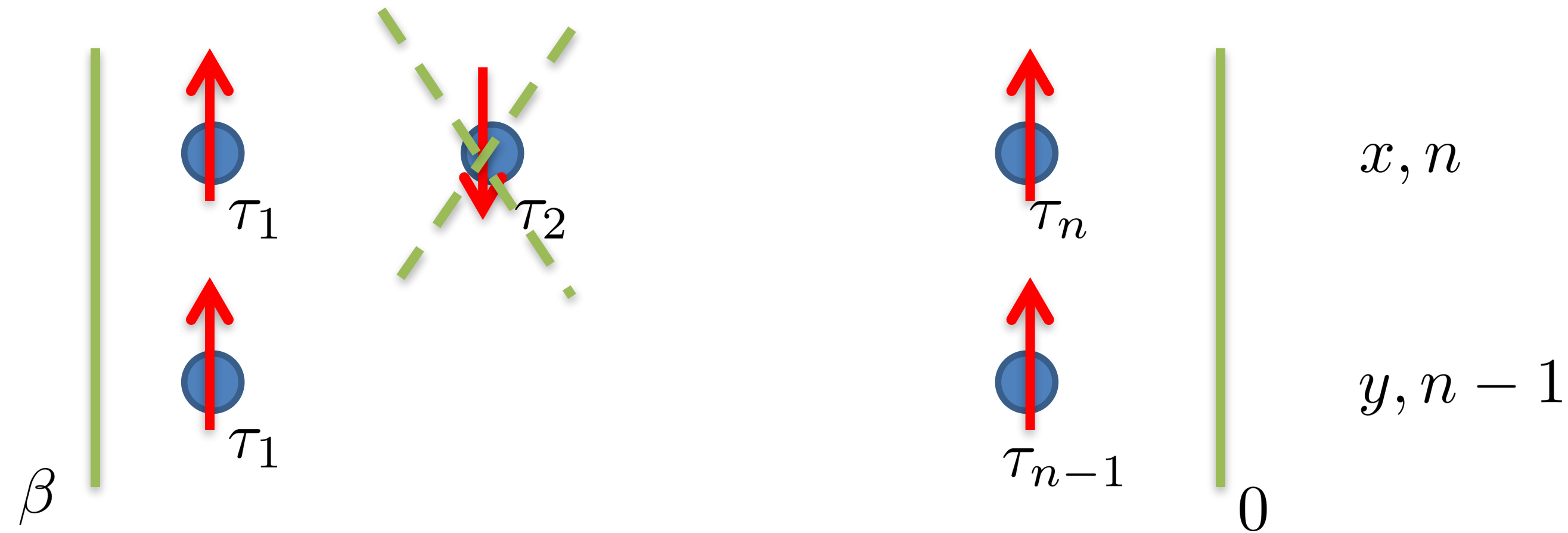
$$P_{y,x}\rho(y) = \frac{1}{2} \times \frac{1}{n+1} \times \left|\left(\frac{-U}{2}\right)^{n+1} \det D_{n+1}^\uparrow \det D_{n+1}^\downarrow \prod_{i=1}^{n+1} d\tau_i\right|$$

- 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)

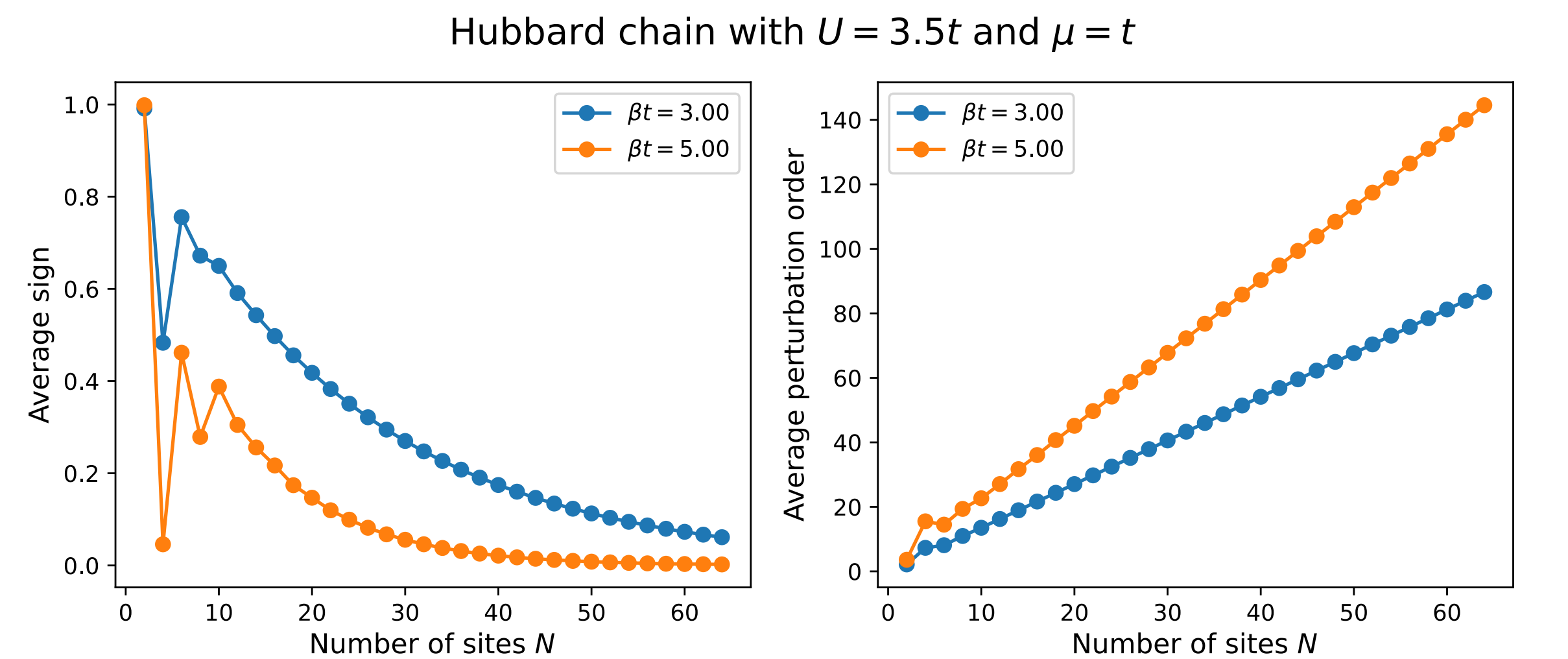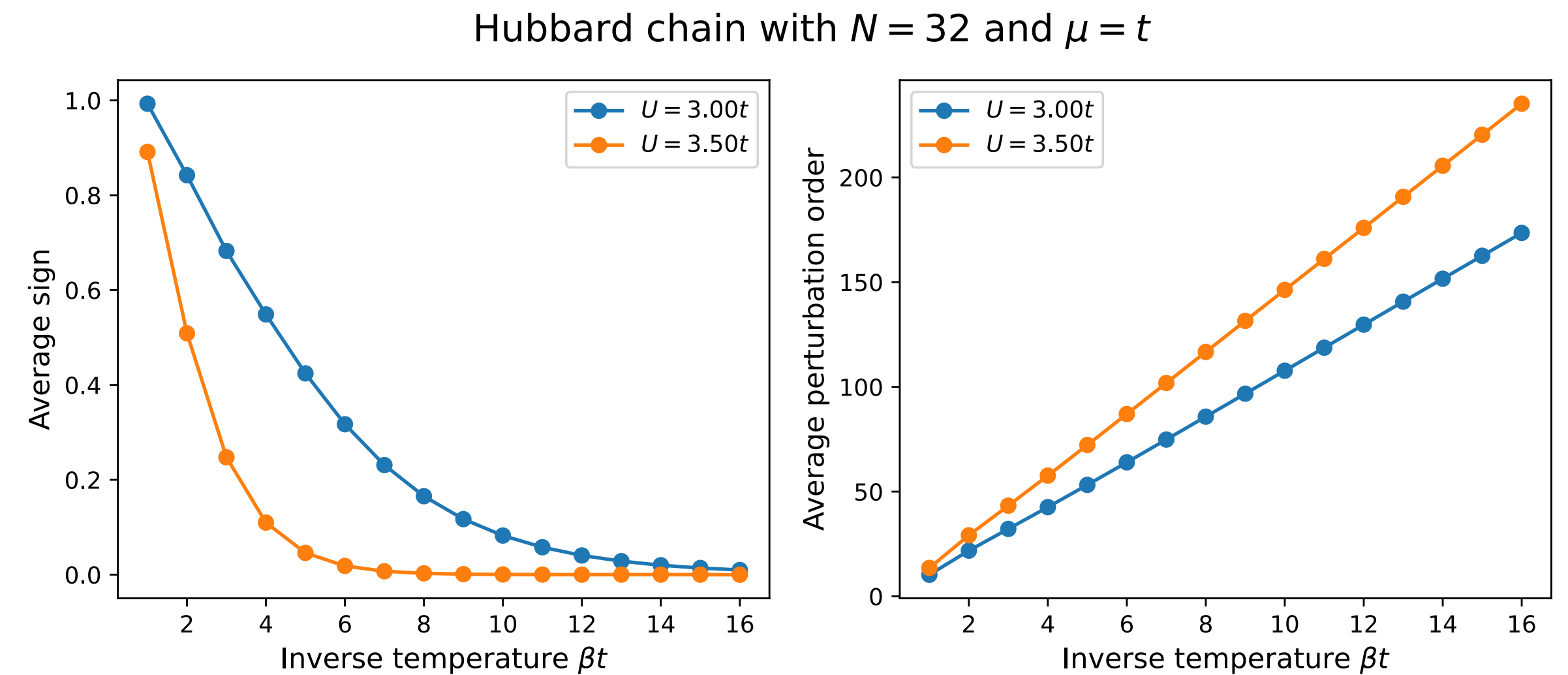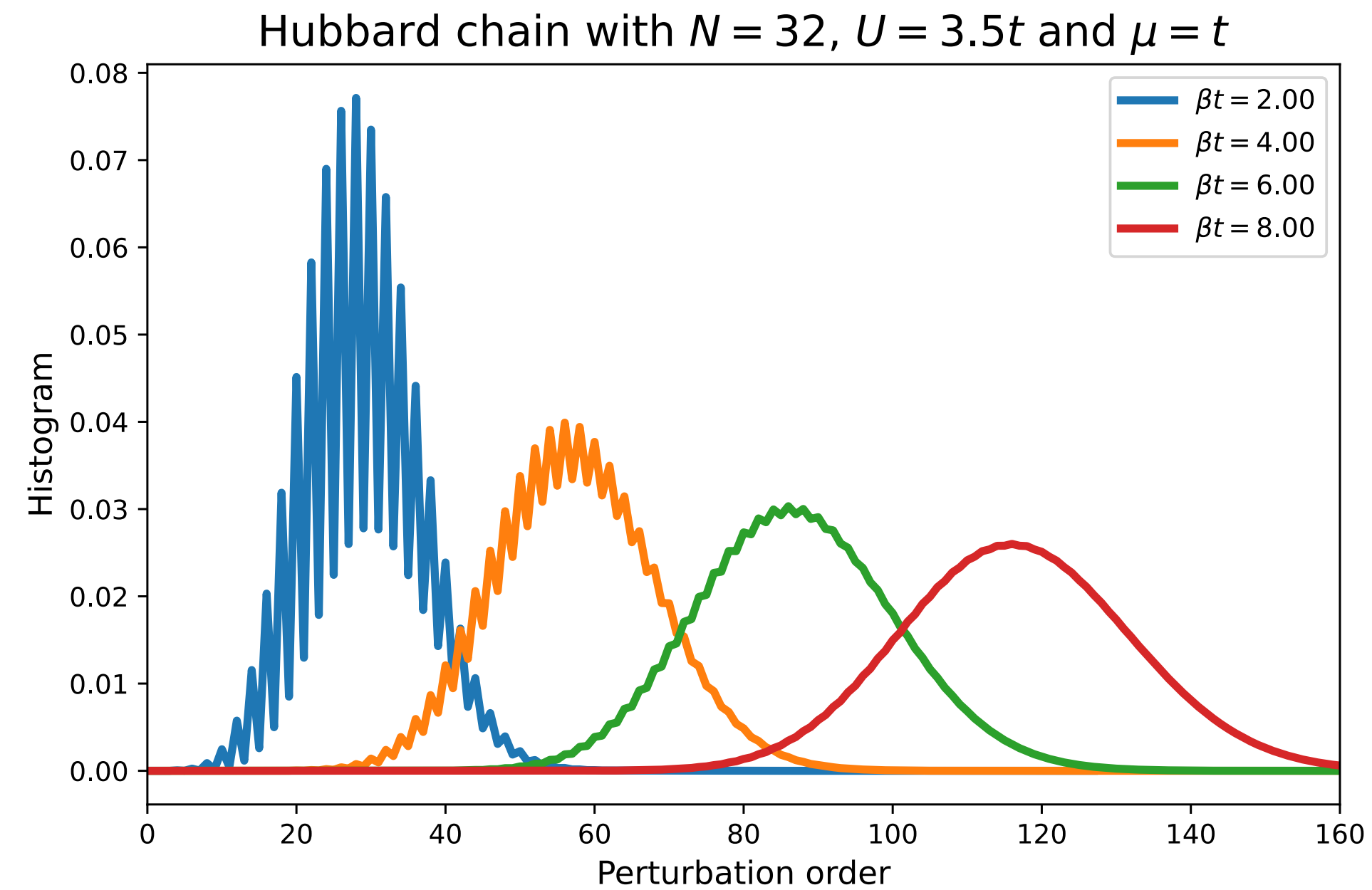$$Z = Z_0 \int_{\mathcal{C}} \left(\frac{-U}{2} \right)^n \det D_n^\uparrow \det D_n^\downarrow$$

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

- 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 $\mathcal{O}(n^3)$
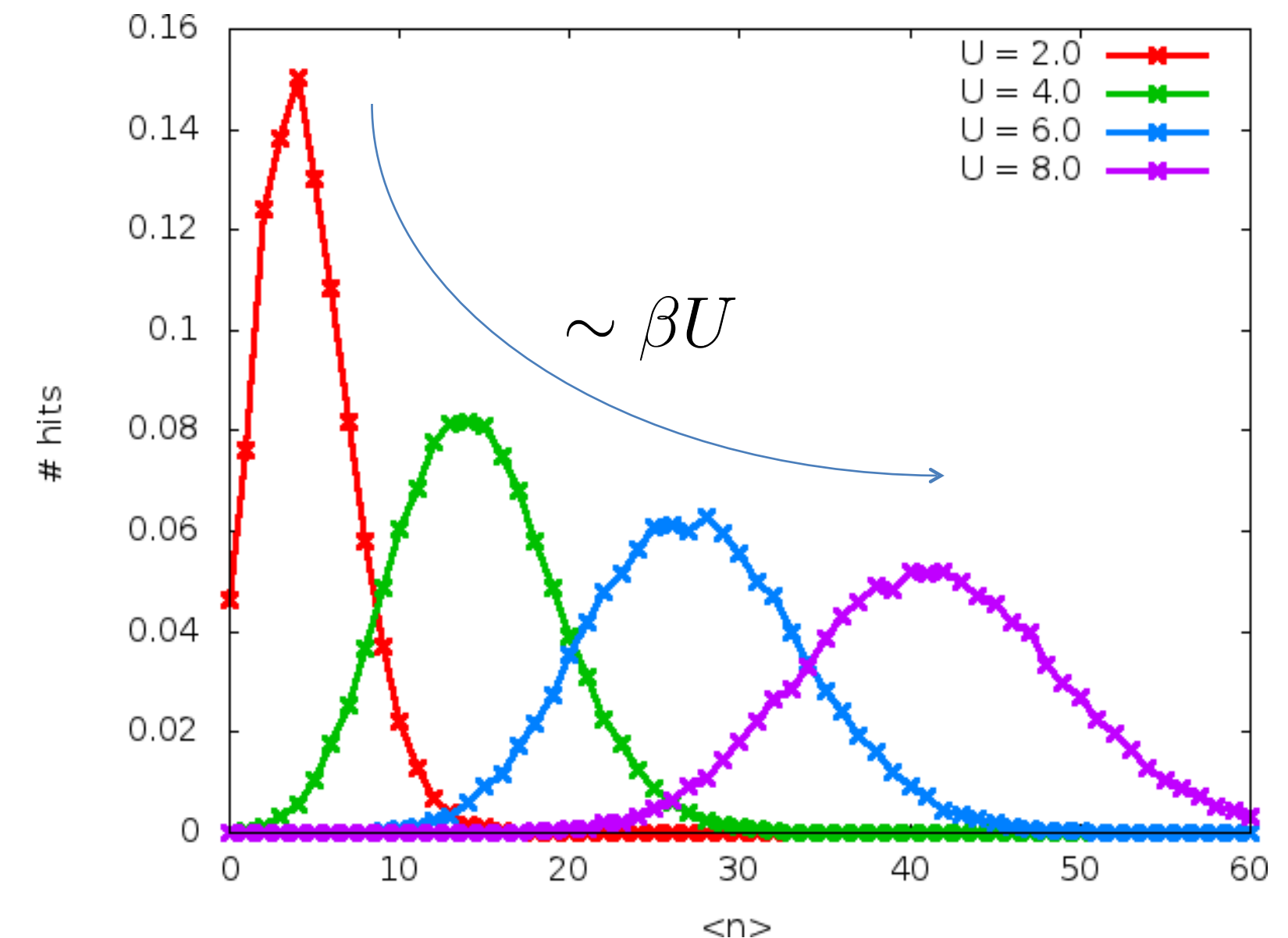
Sign problem in the generic case

- Simple investigation on Hubbard chain

Hubbard chain with $N = 32$, $U = 3.5t$ and $\mu = t$

Hubbard chain with $N = 32$ and $\mu = t$

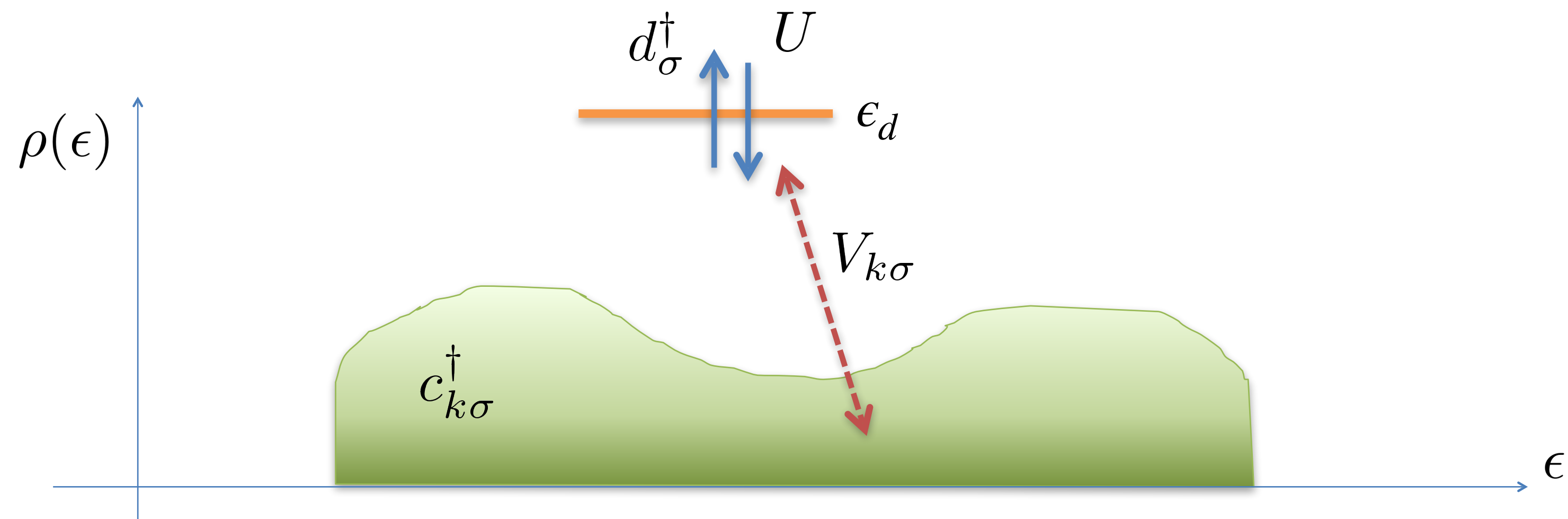Hubbard chain with $U = 3.5t$ and $\mu = t$

Continuous-time quantum Monte Carlo algorithms

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  Historical importance of quantum impurity problems and algorithmic developments

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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

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

- 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 $\quad S = S_{\text{loc}} + \sum_\sigma S_{\text{hyb}}^\sigma$

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

action of the atomic problem

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

"perturbation"

Hybridization expansion CT-QMC

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

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

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

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

average over the atomic state

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

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

Hamiltonian of the local problem

Hybridization expansion CT-QMC

- Inserting the expression of the hybridization action we get

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

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

Sum over many (continuous) variables

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

Product of hybridization functions

$$\prod_\sigma \frac{(-1)^{n_\sigma}}{n_\sigma!} \prod_{i=1}^{n_\sigma} \Delta_\sigma(\tau_i^\sigma - \tau_i'^\sigma) \quad \times$$
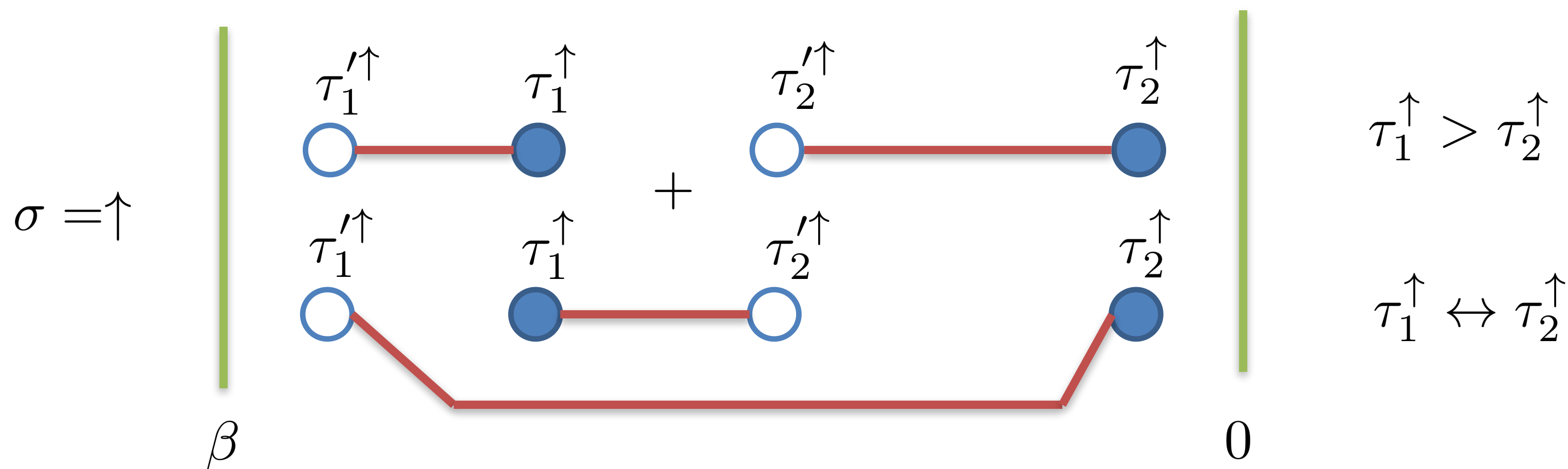
Trace involving both spin up and down operators

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

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

Hybridization expansion CT-QMC

- MC sum:

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

- Diagrams:

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

- Weight:

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

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

- 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 $\{\tau_i^\uparrow\}$
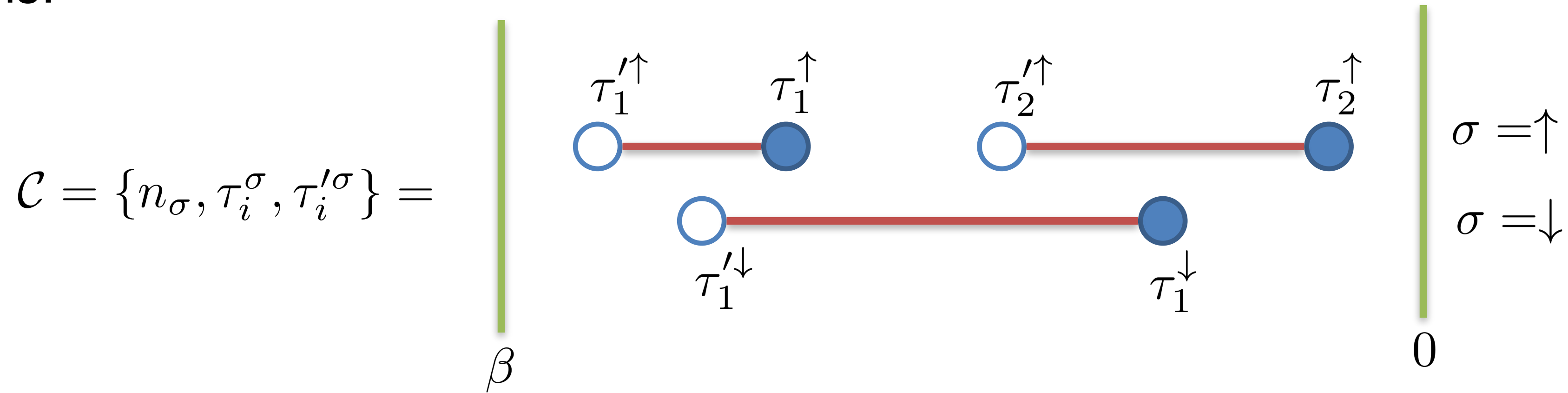

$$\mathrm{Tr}\left[e^{-\beta\mathcal{H}_{\mathrm{loc}}}d_\uparrow^\dagger(\tau_1^\uparrow)d_\uparrow(\tau_1'^\uparrow)d_\uparrow^\dagger(\tau_2^\uparrow)d_\uparrow(\tau_2'^\uparrow)\right] \times \frac{1}{2}\Delta_\uparrow(\tau_1^\uparrow - \tau_1'^\uparrow)\Delta_\uparrow(\tau_2^\uparrow - \tau_2'^\uparrow)$$

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

$$=$$

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

Hybridization expansion Monte Carlo

- MC sum:

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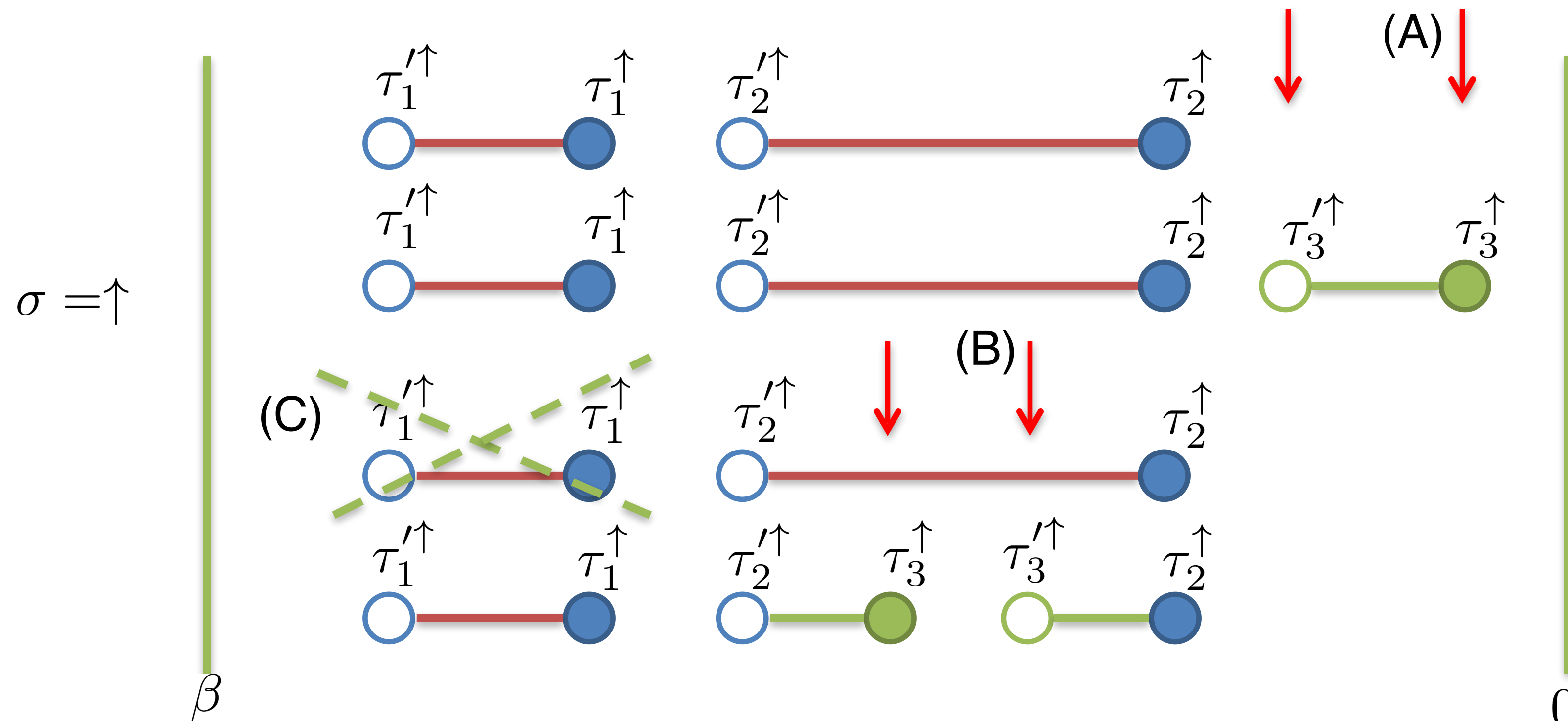
- Diagrams:

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

- Weight:

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

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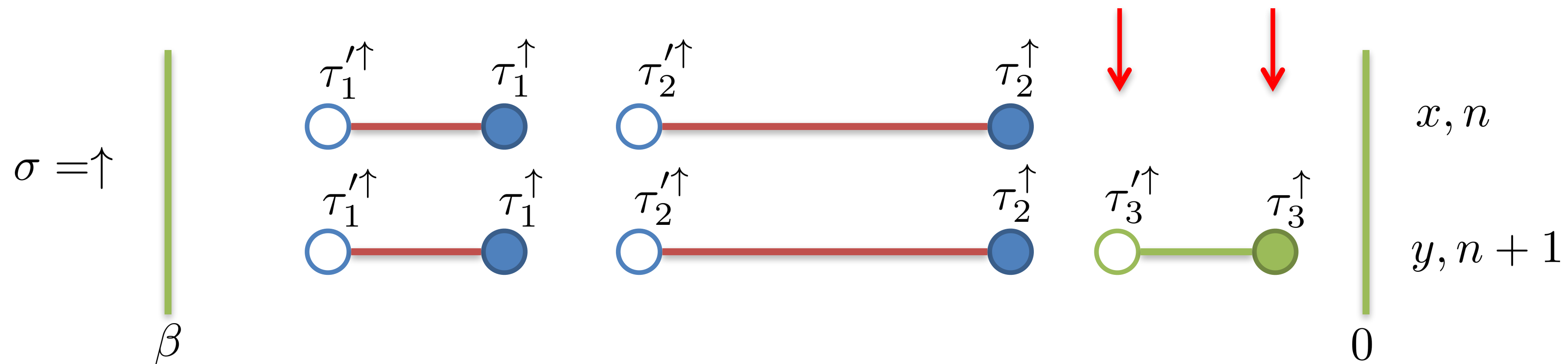
Generating diagrams

- 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?

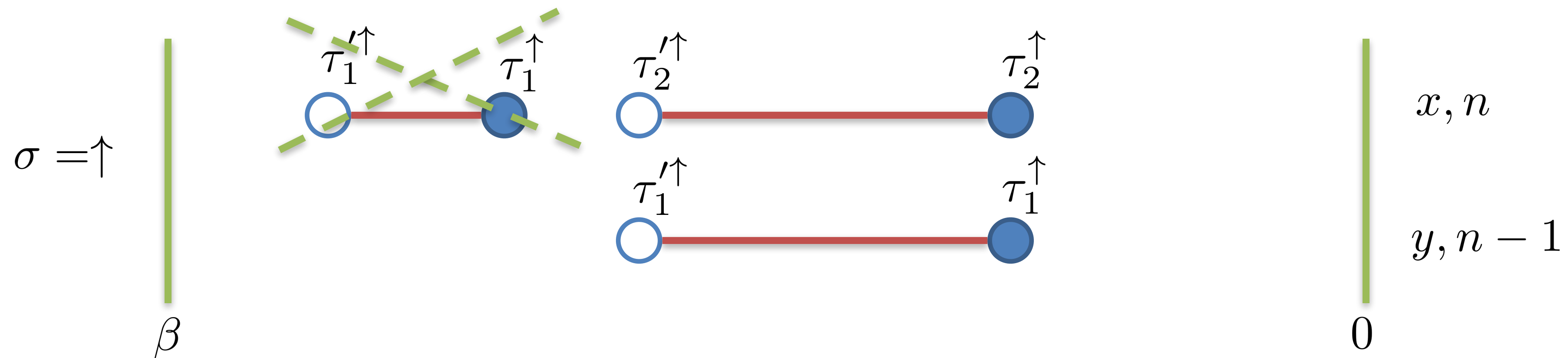$$A_{x,y} = \min\left[1, \frac{P_{y,x}\rho(y)}{P_{x,y}\rho(x)}\right]$$

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

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

- 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?

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

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

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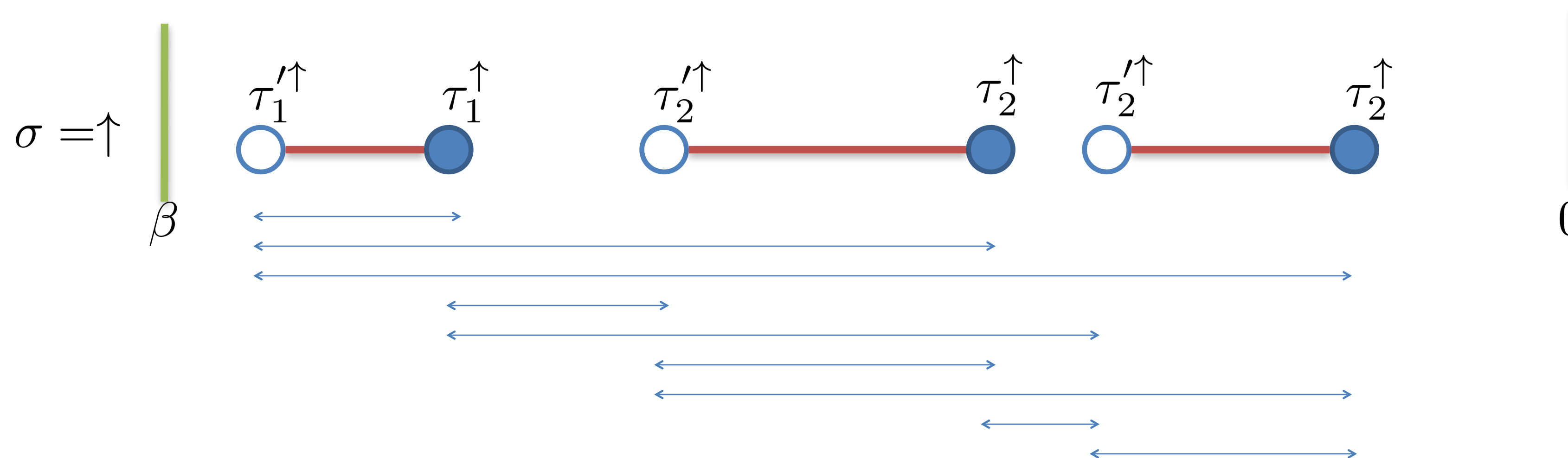
- Measure: $\quad G_\sigma(\tau) \sim \frac{-1}{Z\beta} \sum_{\mathcal{C}}^{\mathrm{MC}} \sum_{k,l} \delta(\tau_k^\sigma - \tau_l'^\sigma + \tau) \times [\Delta_{\sigma \mathcal{C}}^{-1}]_{k,l} \times \mathrm{sign}(w(\mathcal{C}))$

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
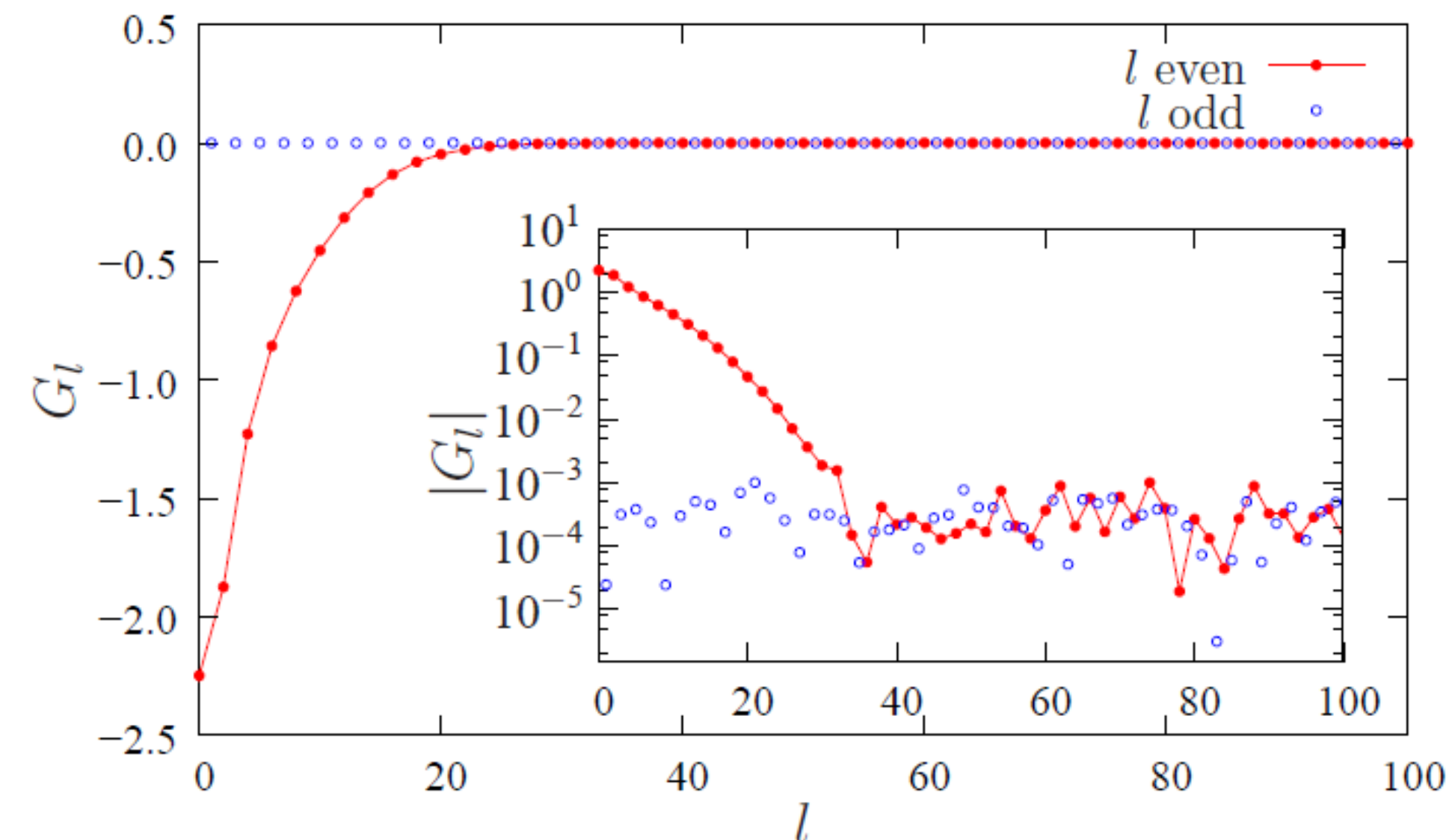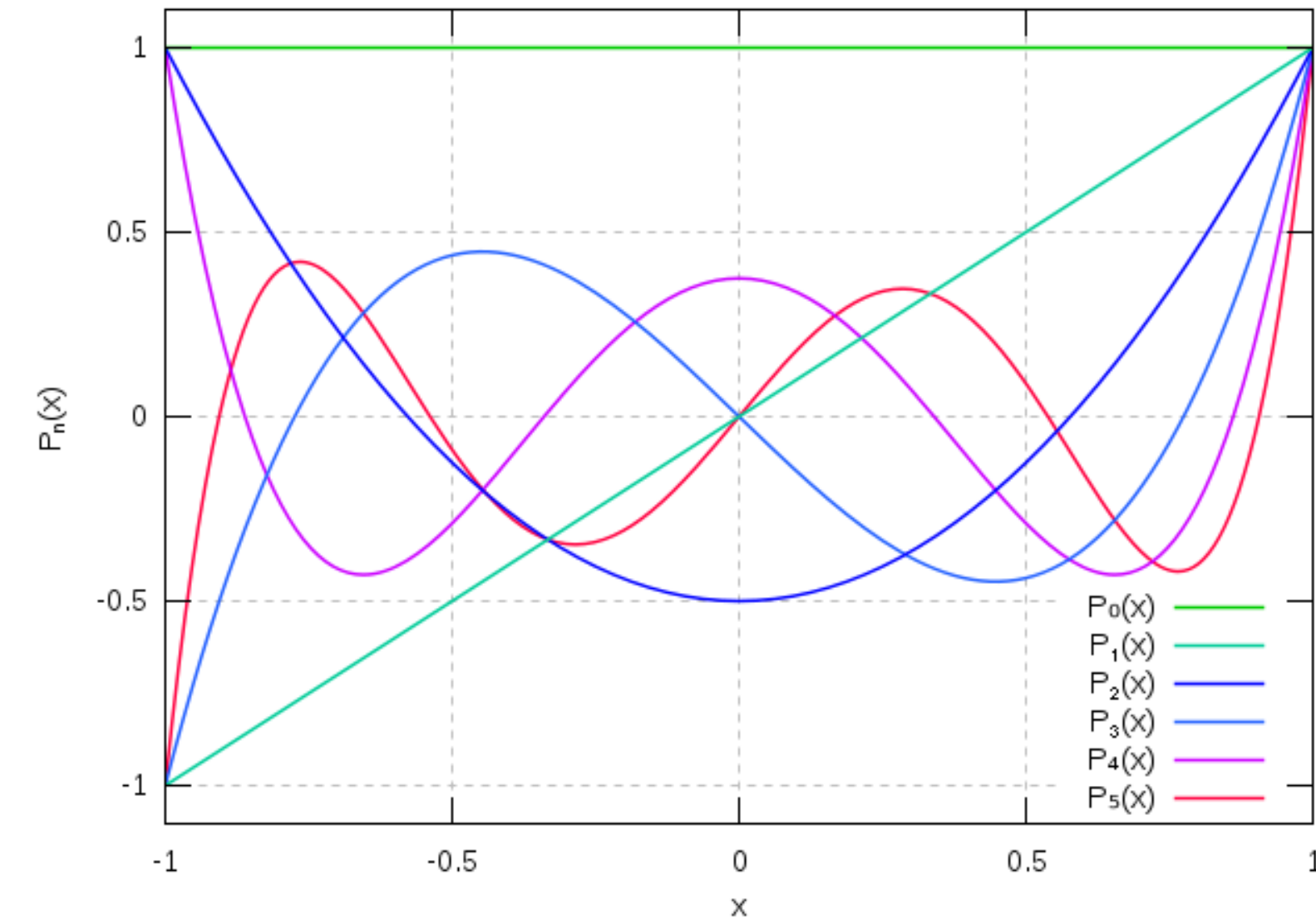
Measuring using Legendre polynomials

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

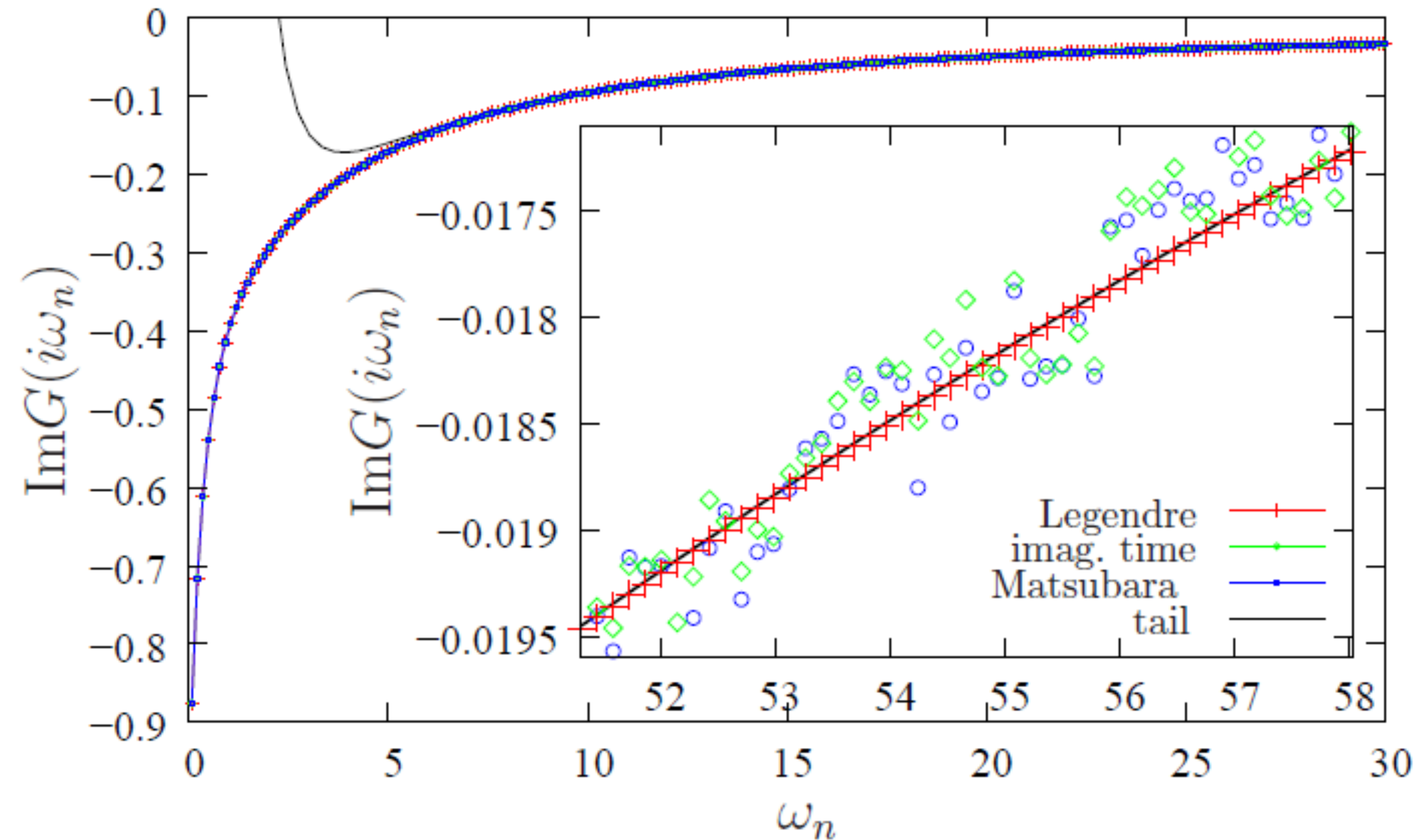- We can express the imaginary-time Green's function in this basis

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

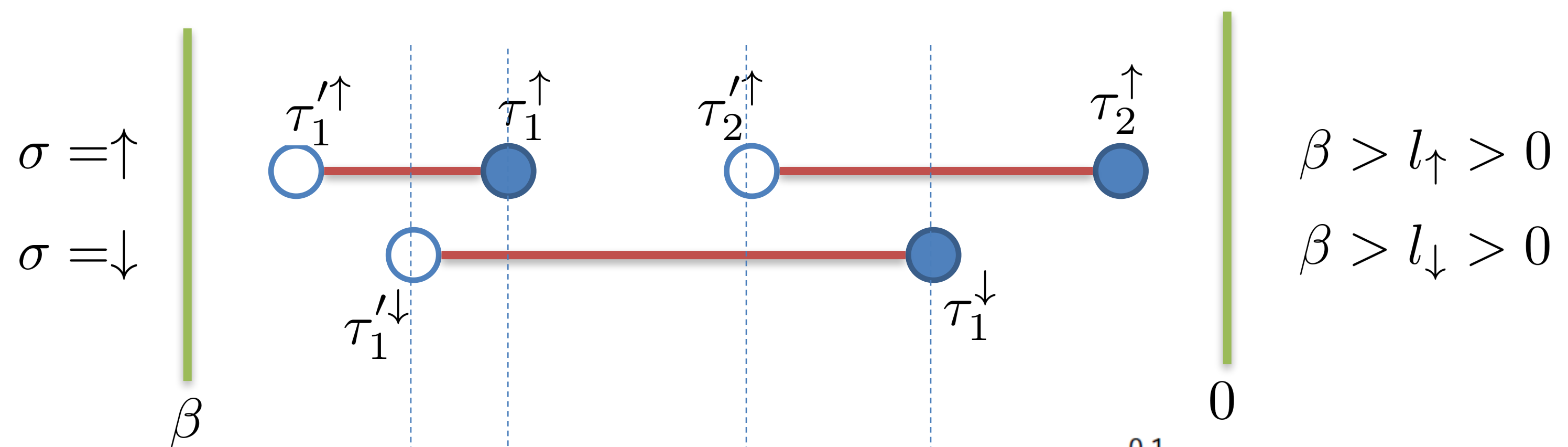- The coefficients G_l in this basis decay very quickly

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:
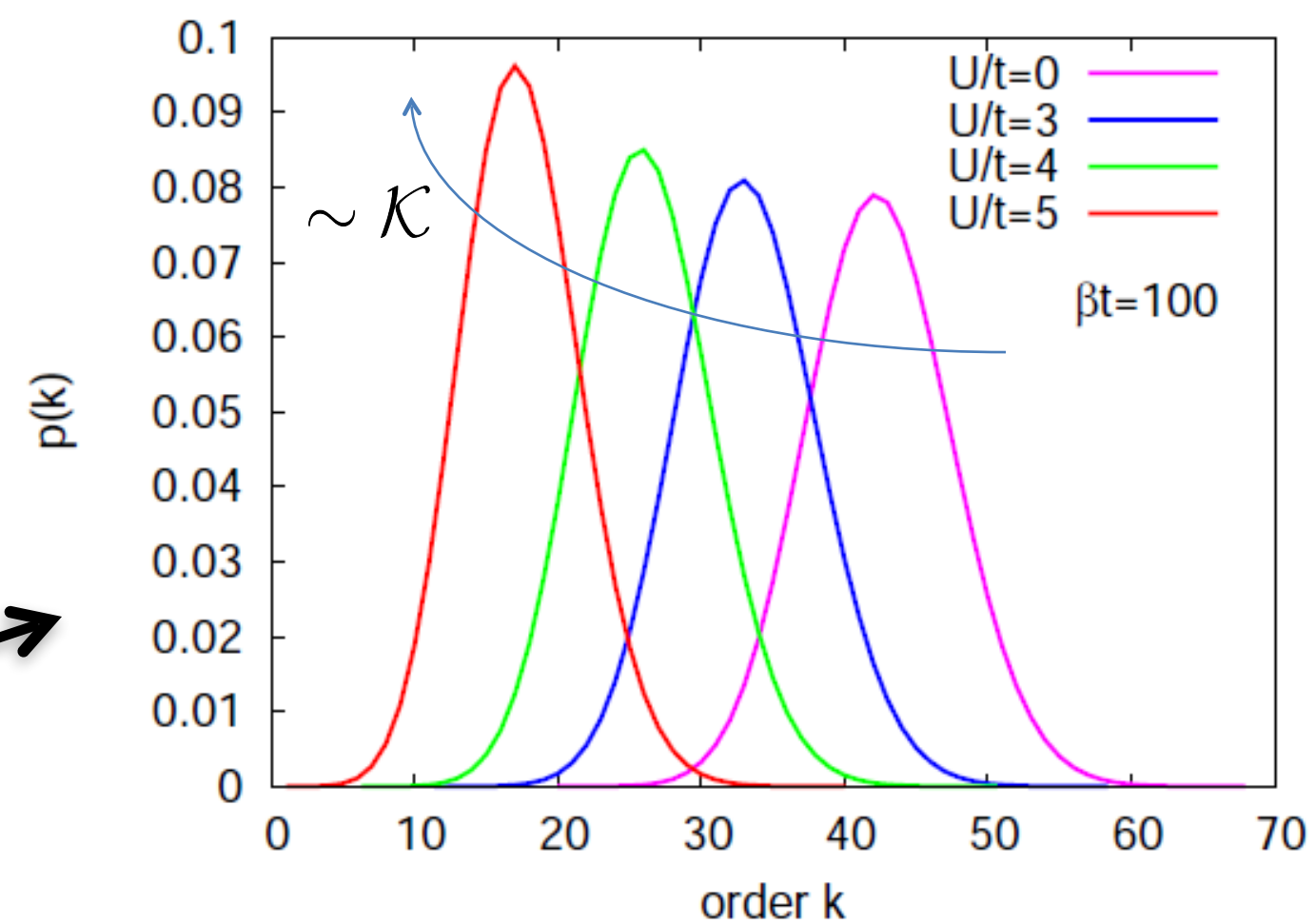
Computational effort

- Can the contribution of a diagram be computed quickly?

- Determinants can be updated quickly (Sherman-Morrison)

- For simple Hamiltonians, the trace is very easy

$$\sigma = \uparrow$$

$$\tau_1'^{\uparrow} \qquad \tau_1^{\uparrow} \qquad \tau_2'^{\uparrow} \qquad \tau_2^{\uparrow}$$

$$\sigma = \downarrow$$

$$\tau_1'^{\downarrow} \qquad \tau_1^{\downarrow}$$

$$\beta > l_\uparrow > 0$$

$$\beta > l_\downarrow > 0$$

$$\beta$$

$$0$$

overlap: l_1 l_2

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

- Computational effort grows in

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

$\sim \mathcal{K}$

p(k)

U/t=0
U/t=3
U/t=4
U/t=5

βt=100

order k

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
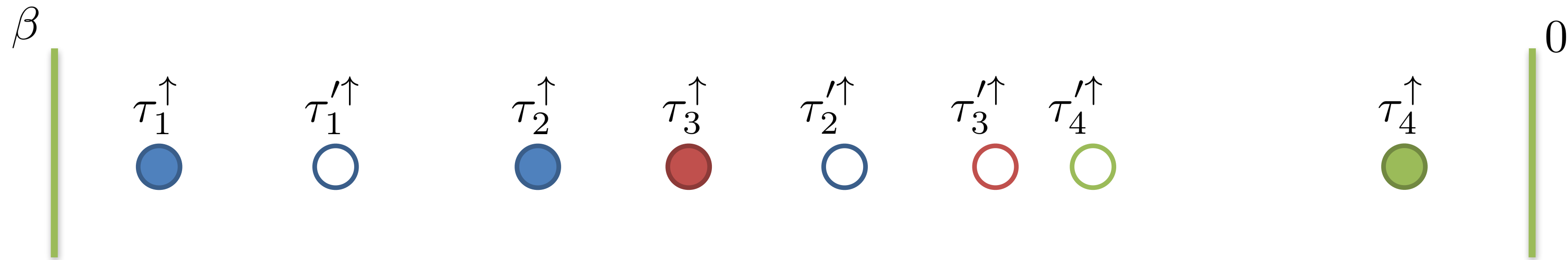
- The main drawback is that there is no longer a quick way to compute the trace

- 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!

Thank you for your attention!