

# Continuous-time quantum Monte Carlo algorithms for impurity models



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# Outline

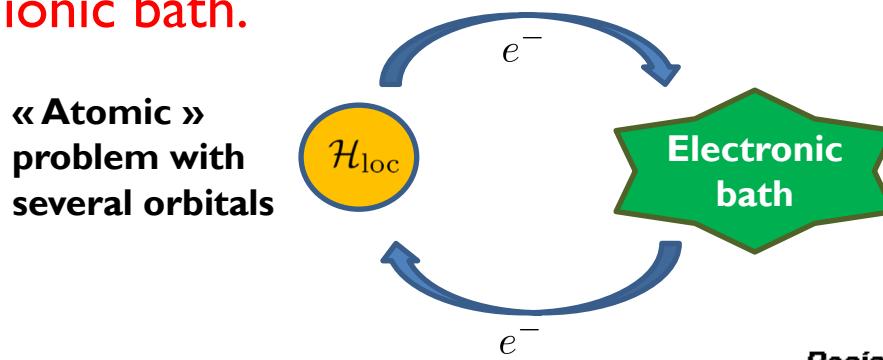
- Motivation: Quantum impurity problems
- Continuous-time quantum Monte Carlo (CT-QMC) methods
- The interaction-expansion algorithm (CT-INT)
- The hybridization-expansion algorithm (CT-HYB)

# References

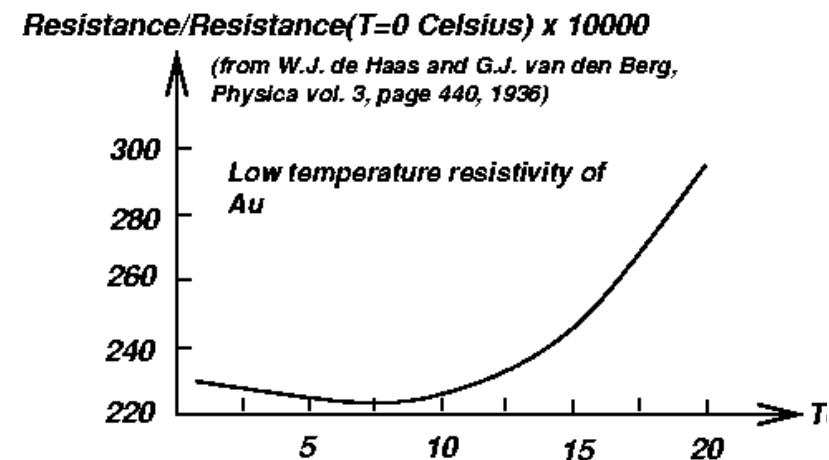
- Quantum impurity problems: *A. C. Hewson, “The Kondo Problem to Heavy Fermions”, Cambridge University Press*
- CT-QMC solvers: *E. Gull et al., RMP (2011)*
  - The interaction-expansion algorithm  
*Rubtsov et al., PRB (2005) and Rubtsov and Lichtenstein, JETP Lett. (2004)*
  - The hybridization-expansion 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.ipht.cnrs.fr/applications/cthyb>

# 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**.

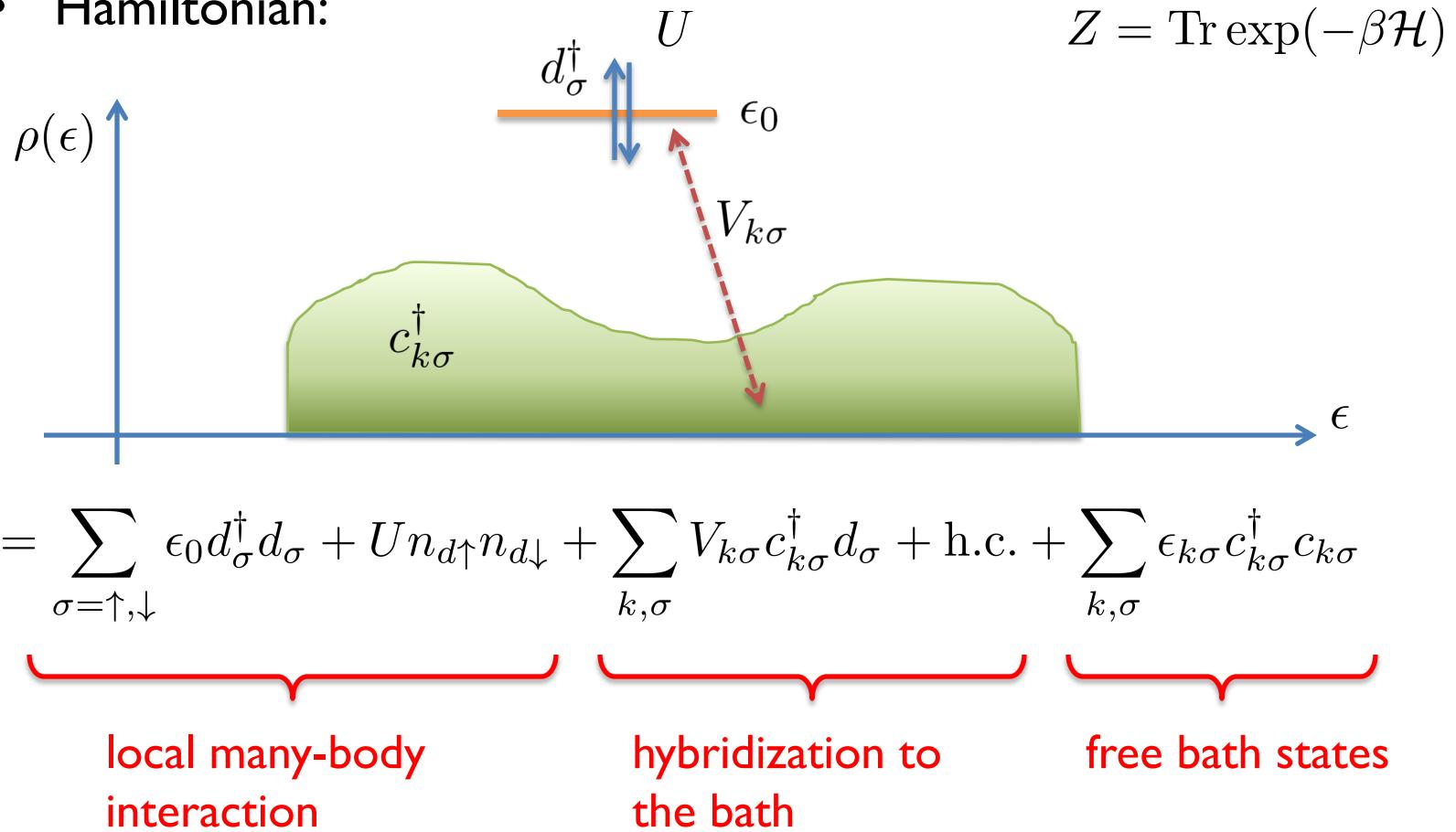


- Impurity models have a long history  
e.g. the Kondo problem
- Lead to the development of models  
and methods



# The Anderson model

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



# Action for the Anderson model

- After integrating out the fermionic bath:  
$$S = - \sum_{\sigma} \int_0^{\beta} d\tau d\tau' d_{\sigma}^{\dagger}(\tau) G_{0\sigma}^{-1}(\tau - \tau') d_{\sigma}(\tau') + \int_0^{\beta} d\tau U n_{d\uparrow}(\tau) n_{d\downarrow}(\tau)$$
  
$$G_{0\sigma}^{-1}(i\omega_n) = i\omega_n - \epsilon_0 - \Delta_{\sigma}(i\omega_n)$$
 ← non-interacting Green's function  
$$\Delta_{\sigma}(i\omega_n) = \sum_k \frac{|V_{k\sigma}|^2}{i\omega_n - \epsilon_{k\sigma}}$$
 ← hybridization function: describes the transition between the bath and the orbital

Remember:  $G_{0\sigma}$  contains the information about the structure of the bath!

- Generic case (several orbitals or sites):

$$S = - \sum_{a,b} \int_0^{\beta} d\tau d\tau' d_a^{\dagger}(\tau) G_{0,ab}^{-1}(\tau - \tau') d_b(\tau') + \int_0^{\beta} d\tau \mathcal{H}_{\text{loc}}(\{d_a^{\dagger}, d_a\})(\tau)$$

$$G_{0,ab}^{-1}(i\omega_n) = i\omega_n \delta_{ab} + t_{ab} - \Delta_{ab}(i\omega_n)$$

# 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**
- All have pros and cons!

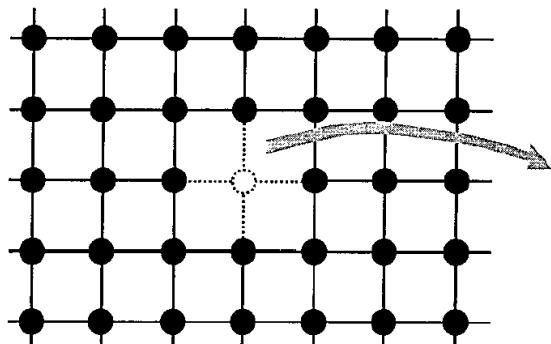
# Our goal: Solve the DMFT equations

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



## Action of auxiliary impurity model

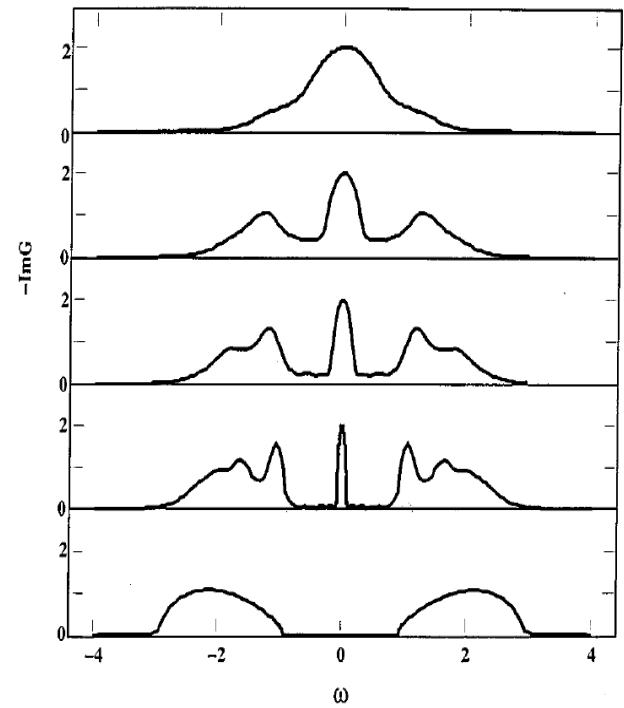
$$S = - \sum_{\sigma} \int_0^{\beta} d\tau d\tau' d_{\sigma}^\dagger(\tau) \textcolor{red}{G_{0\sigma}^{-1}(\tau - \tau')} d_{\sigma}(\tau') + \int_0^{\beta} d\tau U n_{d\uparrow}(\tau) n_{d\downarrow}(\tau)$$



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**



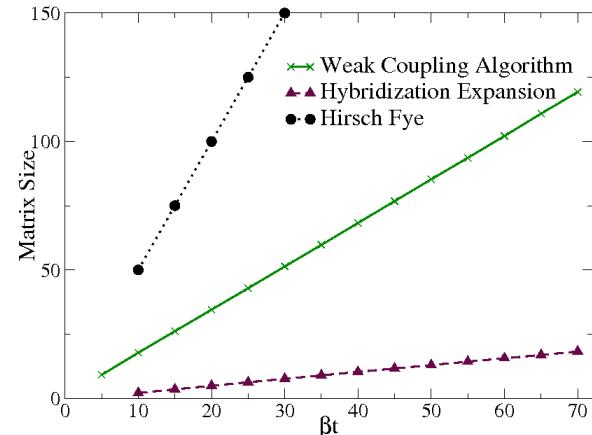
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- Motivation: Quantum impurity problems
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- The interaction-expansion algorithm (CT-INT)
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# Continuous-time quantum Monte Carlo methods

- 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

$$Z = \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \dots$$



- Sample the contributions stochastically (Monte Carlo)
- Compute quantities of interest (Green's function, ...)

# Monte Carlo: a quick summary

- The Monte Carlo is a method to compute sums:

$$\sum_x p(x)f(x), \quad \text{where } p(x) > 0, \quad \sum_x p(x) = 1$$

- The idea is to generate stochastically a large set of  $x_i$  such that the probability to find a given  $x_n$  is  $p(x_n)$
- The original sum is replaced by an average over the set  $\{x_i\}$

$$\sum_x p(x)f(x) \sim \frac{1}{N} \sum_{i=1}^N f(x_i)$$

- Note that  $x$  should be understood as a set of variables  $x = (\tau, \sigma, \dots)$
- One can think of  $x$  as a “configuration” in a phase space
- Example: classical Ising model

# Markov chain

- How do we generate configurations with the correct distribution?
- We don't sample independent configurations, but generate a **Markov chain**:  $x_1 \rightarrow x_2 \rightarrow x_3 \rightarrow x_4 \rightarrow \dots$
- The transition probability  $W_{x,y}$  to go from configuration  $x$  to a configuration  $y$  must satisfy:

- Normalization:

$$\sum_y W_{x,y} = 1$$

- Ergodicity: one must be able to reach any configuration
  - Stationary distribution, balance condition:

$$\frac{d}{dt} p(x) = 0 \quad \rightarrow \quad \sum_{y \neq x} p(y) W_{y,x} - \sum_{y \neq x} p(x) W_{x,y} = 0$$

- Detailed balance (sufficient but not necessary):  $\frac{W_{x,y}}{W_{y,x}} = \frac{p(y)}{p(x)}$

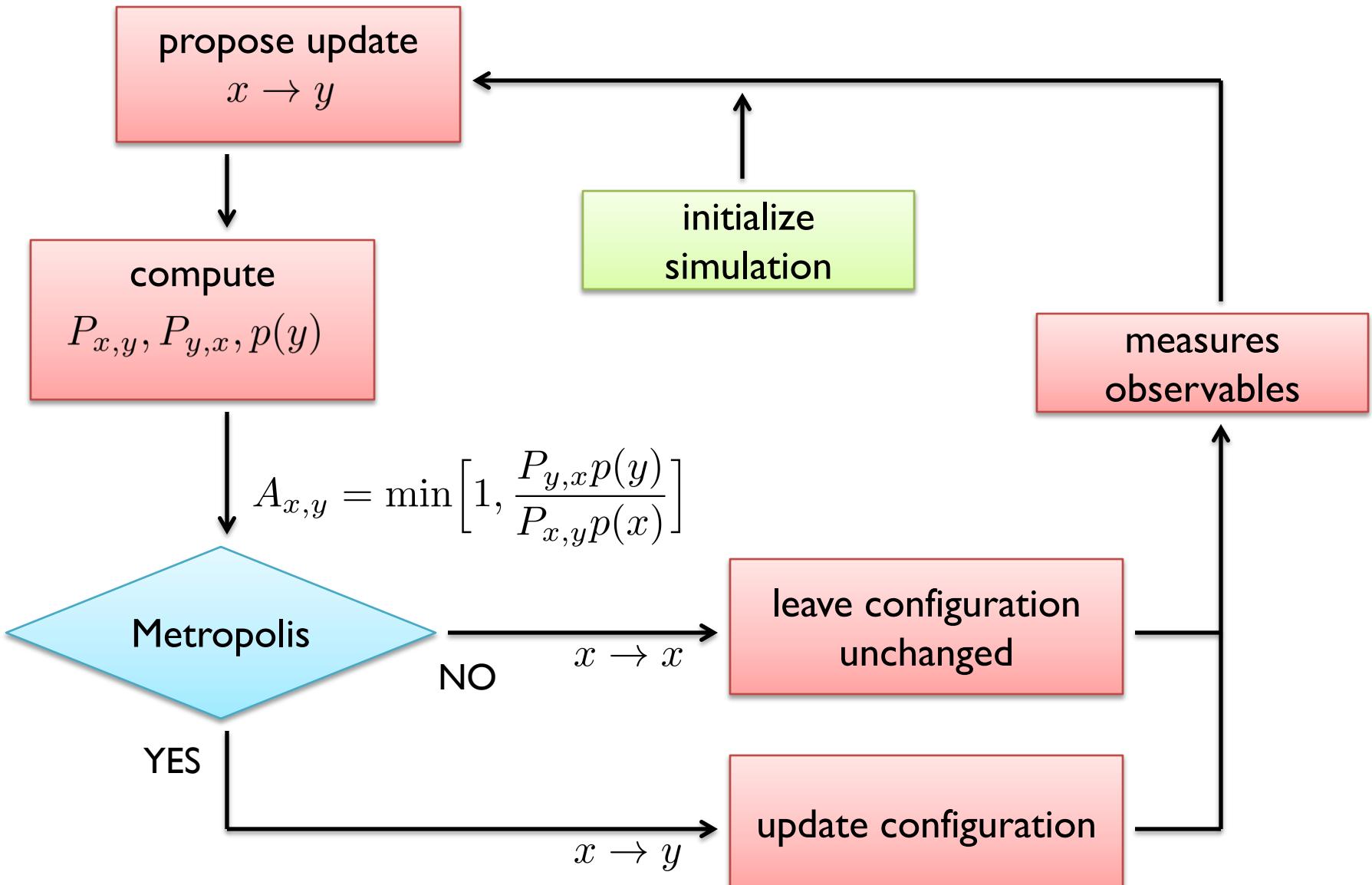
# Metropolis algorithm

- How do we get a transition probability satisfying these criteria?
- Proposal – rejection scheme:
  - Propose a change with a chosen proposal rate  $P_{x,y}$
  - Accept this proposal with a probability  $A_{x,y}$
  - Otherwise don't change the configuration
  - The total transition rate is  $W_{x,y} = A_{x,y}P_{x,y}$
- Metropolis algorithm:

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

- It satisfies the detailed balance and therefore the Markov chain will be distributed according to  $p(x)$

# A Metropolis Monte Carlo algorithm



# 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 would like to use  $w(x)$  as a probability. But what if it can be negative?
- We can use the absolute value instead:

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

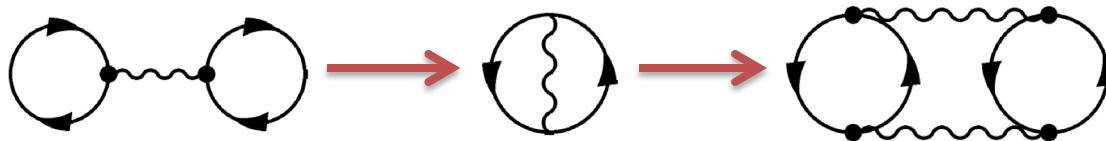
- If signs alternate the denominator is very small and there is a big variance! Gets worse at low temperatures, big systems...
- Fermionic problems very often suffer this sign problem!

# Continuous-time quantum Monte Carlo

- Partition function:

$$Z = \int_{\mathcal{C}} w(\mathcal{C}) \sim \sum_{\mathcal{C}}^{\text{MC}} \text{sign}(w(\mathcal{C}))$$

- Propose **configurations/diagrams** in a Markov chain:



- Accept these proposals with a rate (Metropolis) such that the diagrams appear with probability density  $|w(\mathcal{C})|$
- From the generated configurations, compute the observables you are interested in

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

- The different versions of continuous-time Monte Carlo solvers correspond to different choices of writing the partition function

# Getting a series expansion for the partition function

- Write the action in two parts

$$S = S_A + S_B$$

$S_A$  ← We can solve this action

$S_B$  ← This is the “perturbation”

- Express the partition function as

$$Z = \int \mathcal{D}[d^\dagger, d] e^{-S_A} e^{-S_B} = \int \mathcal{D}[d^\dagger, d] e^{-S_A} \sum_n \frac{(-1)^n}{n!} S_B^n$$

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

we get  $Z = Z_A \sum_n \frac{(-1)^n}{n!} \underbrace{\left\langle T_\tau S_B^n \right\rangle}_A$

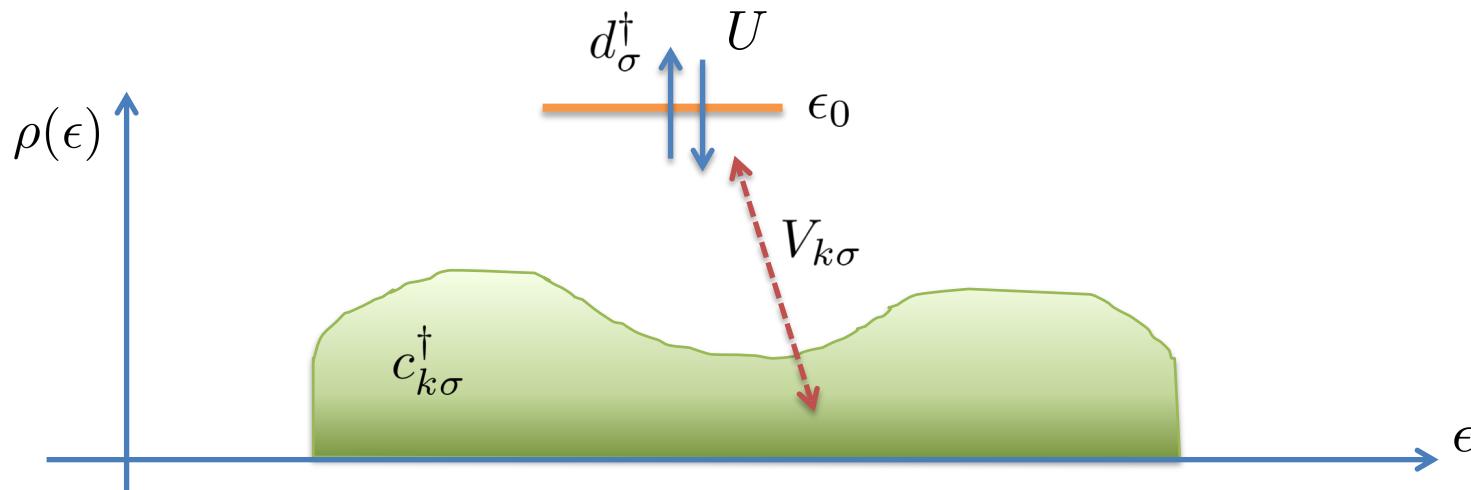
This is an average over the states described by the action A. It generally involves sums and integrals over imaginary time and can have a diagrammatical representation.

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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 cont'd

- 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:

$$S = - \underbrace{\sum_{\sigma} \int_0^{\beta} d\tau d\tau' d_{\sigma}^\dagger(\tau) G_{0\sigma}^{-1}(\tau - \tau') d_{\sigma}(\tau')}_{S_0} + \int_0^{\beta} d\tau U n_{d\uparrow}(\tau) n_{d\downarrow}(\tau)$$

“perturbation”

$S_0 \leftarrow$  action of the non-interacting problem

- The partition function can be written as

$$Z = \int \mathcal{D}[d^\dagger, d] e^{-S_0} \exp \left( \int_0^{\beta} d\tau (-U) n_{d\uparrow}(\tau) n_{d\downarrow}(\tau) \right)$$

this will produce a time-ordered average over the non-interacting state

## Interaction expansion cont'd

- We write a series expansion for the exponential

$$\begin{aligned} Z &= Z_0 \left\langle T_\tau \exp \left( \int_0^\beta d\tau (-U) n_{d\uparrow}(\tau) n_{d\downarrow}(\tau) \right) \right\rangle_0 \quad \text{average over the non-interacting state} \\ &= Z_0 \left\langle T_\tau \sum_n \frac{(-U)^n}{n!} \left( \int_0^\beta d\tau n_{d\uparrow}(\tau) n_{d\downarrow}(\tau) \right)^n \right\rangle_0 \\ &= Z_0 \sum_n \int_0^\beta d\tau_1 \cdots d\tau_n \frac{(-U)^n}{n!} \left\langle T_\tau n_{d\uparrow}(\tau_1) n_{d\downarrow}(\tau_1) \cdots n_{d\uparrow}(\tau_n) n_{d\downarrow}(\tau_n) \right\rangle_0 \end{aligned}$$

- At this stage we have a perturbation expansion for the partition function of the type:
- However there is an obvious sign problem!

$$Z = \int_{\mathcal{C}} w(\mathcal{C}) \sim \sum_{\mathcal{C}}^{\text{MC}} \text{sign}(w(\mathcal{C}))$$

## Interaction expansion cont'd

- The trick is to rewrite the interaction differently

$$Un_{\uparrow}n_{\downarrow} = \frac{U}{2} \sum_{s=\uparrow,\downarrow} (n_{\uparrow} - \alpha_{s\uparrow})(n_{\downarrow} - \alpha_{s\downarrow}) + \frac{U}{2} (n_{\uparrow} + n_{\downarrow}) + \text{const}$$

$$\alpha_{s\sigma} = \frac{1}{2} + (2\delta_{s\sigma} - 1)\delta$$

we absorb this term in  
the chemical potential

- We eventually get (up and down spins decouple)

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

- By tuning  $\delta$  we can improve the sign problem a lot!

## Interaction expansion cont'd

- In the end we have

$$Z = Z_0 \sum_n \int d\tau_1 \cdots d\tau_n \sum_{s_1} \cdots \sum_{s_n}$$

Sum over many (some continuous) variables

$$\frac{(-U)^n}{n!2^n} \left\langle T_\tau (n_{d\uparrow}(\tau_1) - \alpha_{s_1\uparrow}) \cdots (n_{d\uparrow}(\tau_n) - \alpha_{s_n\uparrow}) \right\rangle_0$$

Product of two non-interacting averages

$$\left\langle T_\tau (n_{d\downarrow}(\tau_1) - \alpha_{s_1\downarrow}) \cdots (n_{d\downarrow}(\tau_n) - \alpha_{s_n\downarrow}) \right\rangle_0$$

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

- A Monte Carlo “configuration” is described by  $\mathcal{C} = \{n, \tau_i, s_i\}$
- Now we need to find a way to compute the averages

# Computing the averages

- The averages are on a non-interacting state. Therefore we can use Wick's theorem
- With this definition of the Green's function

$$G_{0\sigma}(\tau) = -T_\tau \langle c_\sigma(\tau) c_\sigma^\dagger(0) \rangle_0$$

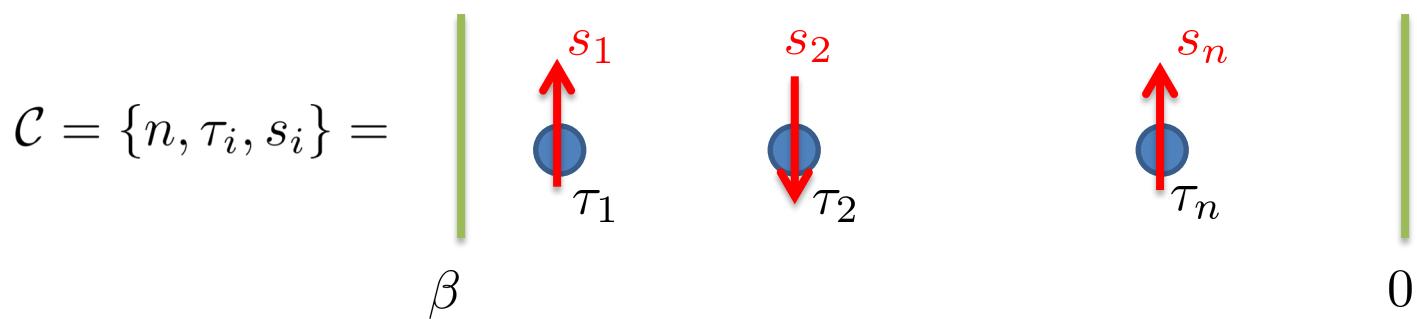
we get

$$\begin{aligned} \left\langle (n_{d\sigma}(\tau_1) - \alpha_{s_1\sigma}) \cdots (n_{d\sigma}(\tau_n) - \alpha_{s_n\sigma}) \right\rangle_0 &= \det D_n^\sigma = \\ \begin{vmatrix} G_{0\sigma}(0^-) - \alpha_{s_1\sigma} & G_{0\sigma}(\tau_1 - \tau_2) & \cdots & \cdots \\ G_{0\sigma}(\tau_2 - \tau_1) & G_{0\sigma}(0^-) - \alpha_{s_2\sigma} & G_{0\sigma}(\tau_2 - \tau_3) & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & G_{0\sigma}(\tau_n - \tau_{n-1}) & G_{0\sigma}(0^-) - \alpha_{s_n\sigma} \end{vmatrix} \end{aligned}$$

and  $Z = Z_0 \sum_n \int d\tau_1 \cdots d\tau_n \sum_{s_1} \cdots \sum_{s_n} \frac{(-U)^n}{n!2^n} \det D_n^\uparrow \det D_n^\downarrow$

# Monte Carlo elements

- 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.

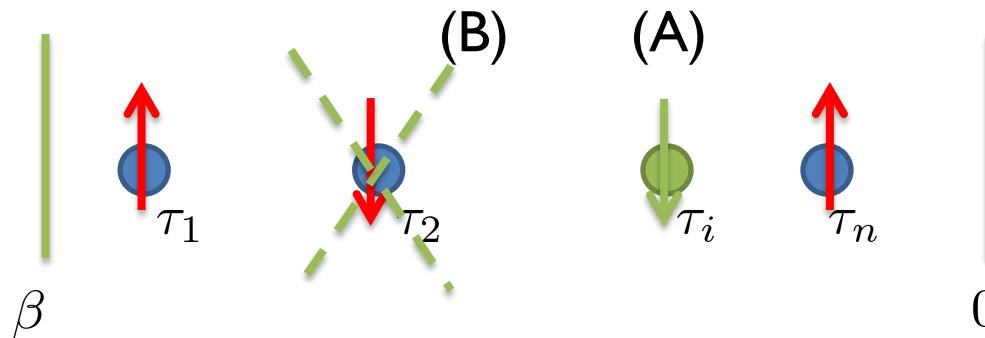


- The weight of every diagram is given by

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

# Generating diagrams

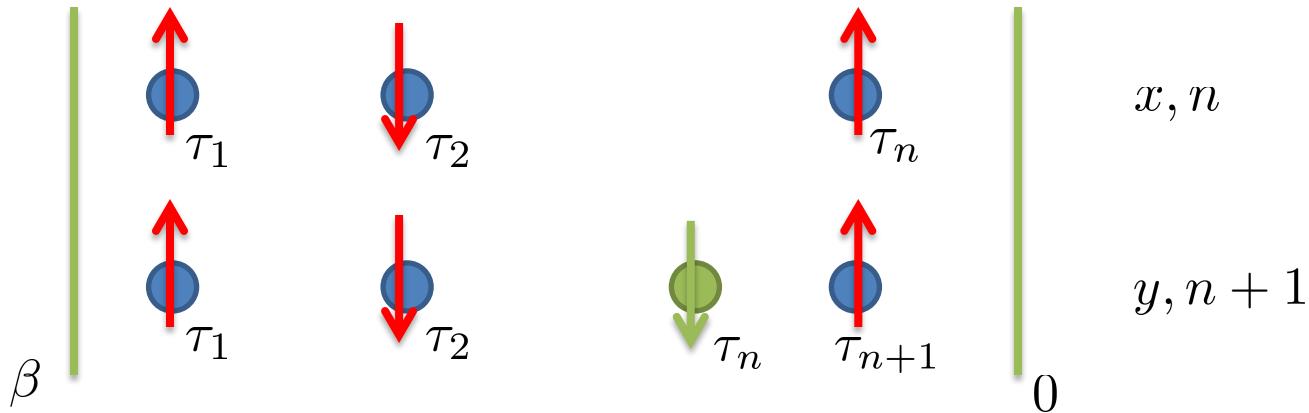
- We need to create a Markov chain of diagrams
- We can propose any changes to go from one diagram to another. A simple solution is to use two “moves”:
- **An insertion of a vertex:** we pick a random imaginary time and insert a vertex with a spin randomly up or down (A)
- **A removal of a vertex:**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



# Insertion of a vertex

- What is the acceptance rate?

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



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

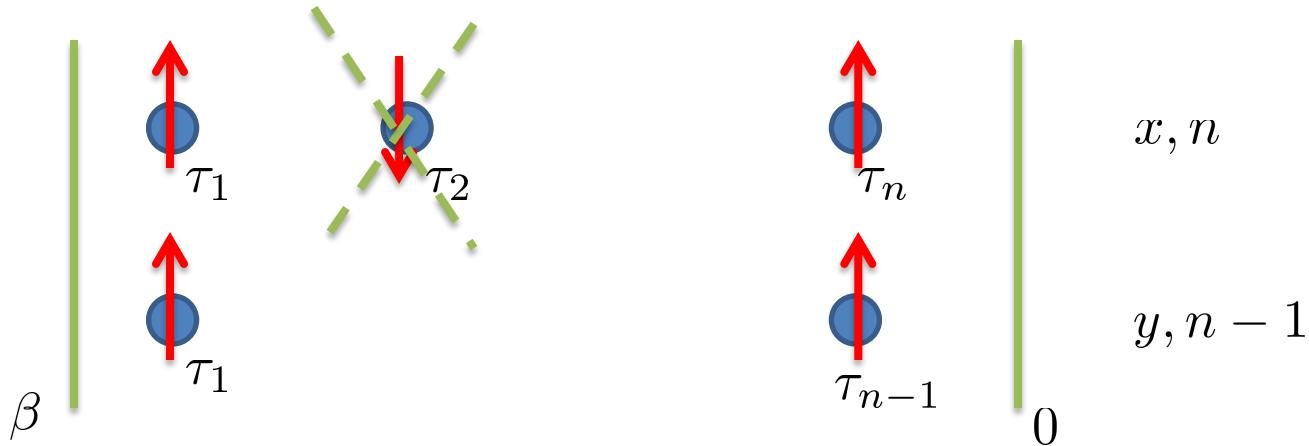
$$P_{y,x}\rho(y) = \frac{1}{2} \times \frac{1}{n+1} \times \left| \left( \frac{-U}{2} \right)^{n+1} \det D_{n+1}^\uparrow \det D_{n+1}^\downarrow \prod_{i=1}^{n+1} d\tau_i \right|$$

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

# Measuring the Green's function

- We know how to generate a distribution corresponding to the terms in the partition function
- Now we just need to find how to measure the Green's function from this distribution

$$G(\tau) = -T_\tau \langle d(\tau) d^\dagger(0) \rangle = \frac{1}{Z} \int \mathcal{D}[d^\dagger, d] e^{-S} d^\dagger(0) d(\tau)$$

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

$$G_{0\sigma}^{-1}(\tau - \tau') = (\partial_{\tau-\tau'} - \epsilon_0) \delta(\tau - \tau') - \Delta_\sigma(\tau - \tau')$$

- We finally see that  $G_\sigma(\tau) = -\frac{1}{\beta} \frac{\delta \ln Z}{\delta \Delta_\sigma(-\tau)}$

# Measuring the Green's function cont'd

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

- The functional derivative eventually gives:

$$G_{\sigma}(i\omega_n) = G_{0\sigma}(i\omega_n) - \frac{1}{\beta} G_{0\sigma}^2(i\omega_n) \times \int_{\mathcal{C}} \sum_{ij} [D_n^{\sigma}]_{ij}^{-1} e^{i\omega_n(\tau_i - \tau_j)} \left(\frac{-U}{2}\right)^n \det D_n^{\uparrow} \det D_n^{\downarrow}$$

- So we see that we need to compute the following Monte Carlo average to get the Green's function

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

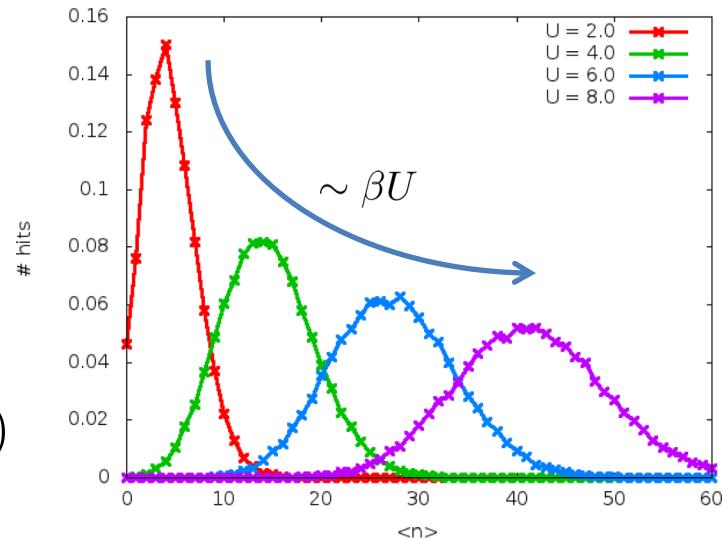
# Computational effort

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

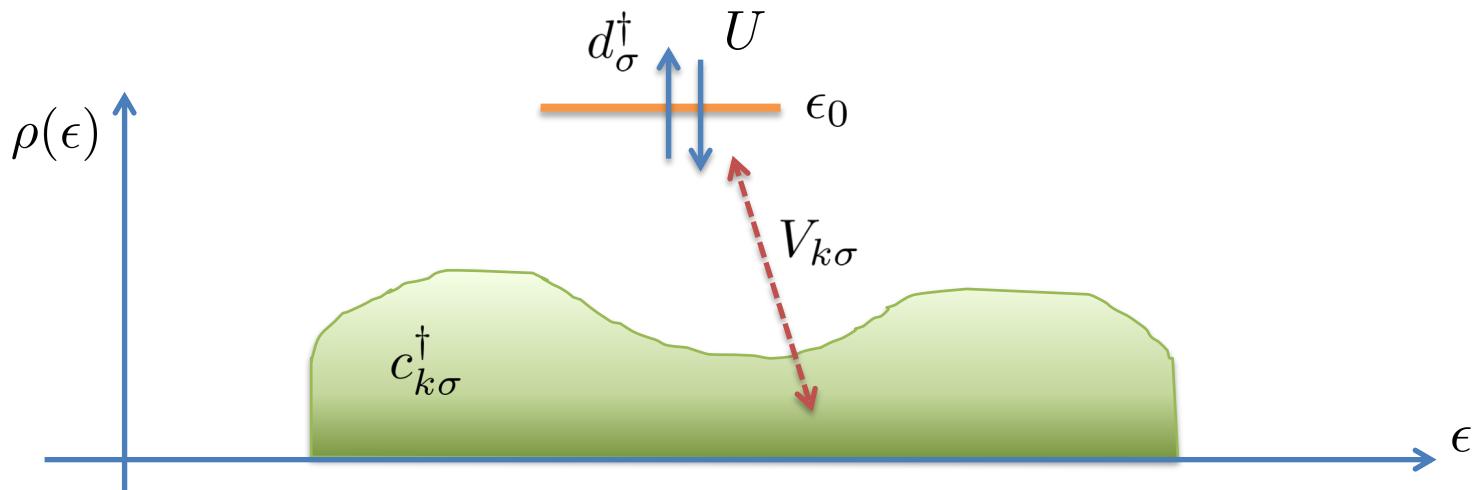


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# Hybridization-expansion CT-QMC

- 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 cont'd

- 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:

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

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

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

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

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

← action of the atomic problem

← “perturbation”

## Hybridization expansion cont'd

- 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!

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

average over the atomic state

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

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

Hamiltonian of the local problem

# Hybridization expansion cont'd

- Inserting the expression of the hybridization action we get

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

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

Sum over many  
(continuous) variables

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

Product of  
hybridization  
functions

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

X

Trace involving both spin up and down operators

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

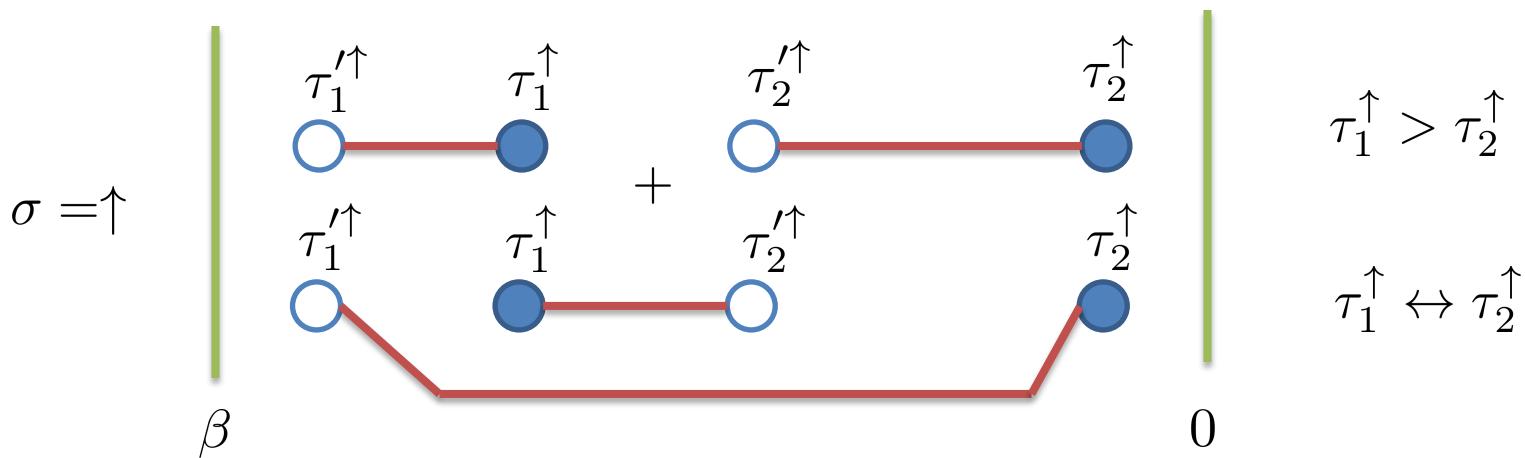
$$Z = \int_{\mathcal{C}} w(\mathcal{C}) \sim \sum_{\mathcal{C}}^{\text{MC}} \text{sign}(w(\mathcal{C})) \quad \langle f \rangle = \frac{1}{Z} \int_{\mathcal{C}} w(\mathcal{C}) f(\mathcal{C}) \sim \frac{1}{Z} \sum_{\mathcal{C}}^{\text{MC}} f(\mathcal{C}) \text{sign}(w(\mathcal{C}))$$

# Hybridization expansion cont'd

- MC sum:  $\sum_{\mathcal{C}}^{\text{MC}} = \sum_{n_\uparrow, n_\downarrow=0}^{\infty} \int_0^\beta d\tau_1^\uparrow \dots d\tau_{n_\uparrow}^{\prime\uparrow} \int_0^\beta d\tau_1^\downarrow \dots d\tau_{n_\downarrow}^{\prime\downarrow}$
- Diagrams:  
 $\mathcal{C} = \{n_\sigma, \tau_i^\sigma, \tau_i'^\sigma\} =$
- Weight:  $w(\mathcal{C}) = \prod_{\sigma} \frac{(-1)^{n_\sigma}}{n_\sigma!} \prod_{i=1}^{n_\sigma} \Delta_\sigma(\tau_i^\sigma - \tau_i'^\sigma) \times \text{Tr} \left[ e^{-\beta \mathcal{H}_{\text{loc}}} T_\tau \prod_{i=1}^{n_\uparrow} d_\uparrow^\dagger(\tau_i^\uparrow) d_\uparrow(\tau_i'^\uparrow) \prod_{i=1}^{n_\downarrow} d_\downarrow^\dagger(\tau_i^\downarrow) d_\downarrow(\tau_i'^\downarrow) \right]$
- Unfortunately these diagrams have alternating signs  $\Rightarrow$  problems!

# 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  $\{\tau_i^\uparrow\}$



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

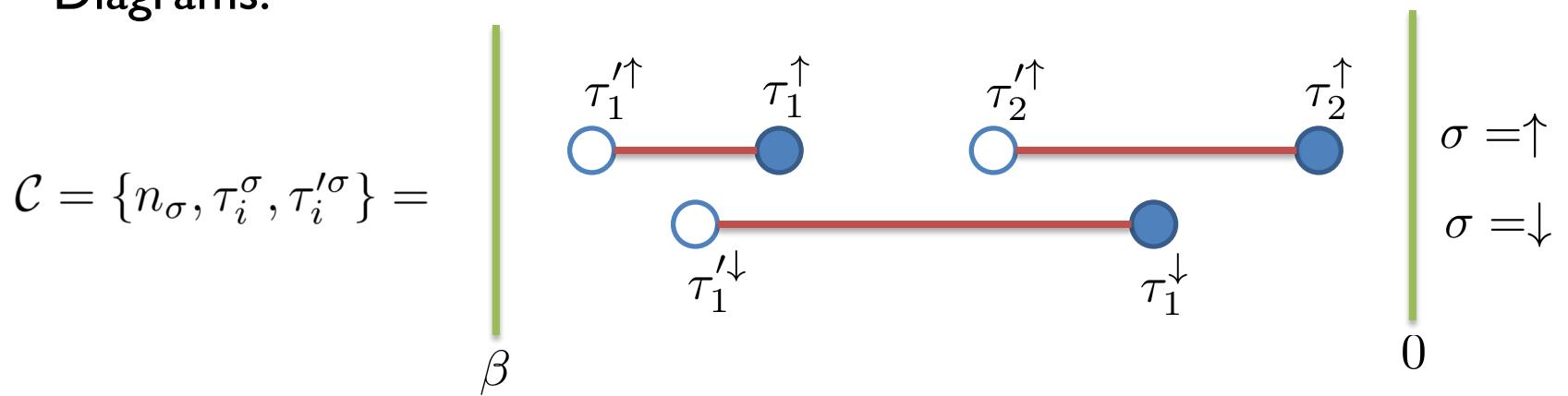
$$(-1) \text{Tr} \left[ e^{-\beta \mathcal{H}_{\text{loc}}} d_\uparrow^\dagger(\tau_1^\uparrow) d_\uparrow(\tau_1'^\uparrow) d_\uparrow^\dagger(\tau_2^\uparrow) d_\uparrow(\tau_2'^\uparrow) \right] \times \frac{1}{2} \Delta_\uparrow(\tau_2^\uparrow - \tau_1'^\uparrow) \Delta_\uparrow(\tau_1^\uparrow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

=

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

# Hybridization expansion Monte Carlo

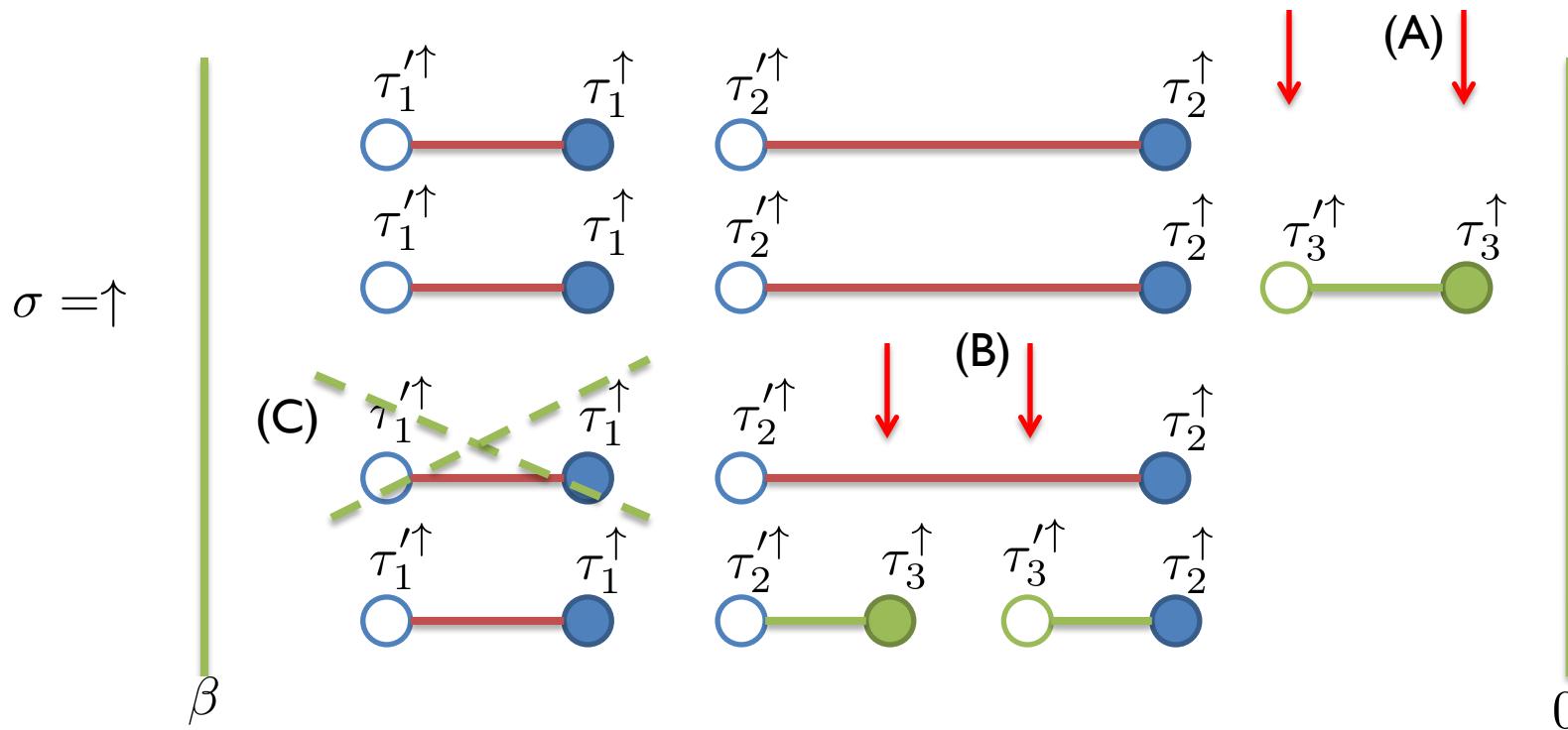
- MC sum:  $\sum_{\mathcal{C}}^{\text{MC}} = \sum_{n_{\uparrow}, n_{\downarrow}=0}^{\infty} \int_{\substack{\tau_1^{\uparrow} > \dots > \tau_n^{\uparrow} \\ \tau'_1{}^{\uparrow} > \dots > \tau'_n{}^{\uparrow}}} d\tau_1^{\uparrow} \dots d\tau_n^{\uparrow} \int_{\substack{\tau_1^{\downarrow} > \dots > \tau_n^{\downarrow} \\ \tau'_1{}^{\downarrow} > \dots > \tau'_n{}^{\downarrow}}} d\tau_1^{\downarrow} \dots d\tau_n^{\downarrow}$
- Diagrams:



- Weight:  $w(\mathcal{C}) = \prod_{\sigma} (-1)^{n_{\sigma}} \det_{1 \leq k, l \leq n_{\sigma}} \Delta_{\sigma}(\tau_k^{\sigma} - \tau_l'^{\sigma}) \times \text{Tr} [e^{-\beta \mathcal{H}_{\text{loc}}} T_{\tau} \prod_{i=1}^{n_{\uparrow}} d_{\uparrow}^{\dagger}(\tau_i^{\uparrow}) d_{\uparrow}(\tau_i'^{\uparrow}) \prod_{i=1}^{n_{\downarrow}} d_{\downarrow}^{\dagger}(\tau_i^{\downarrow}) d_{\downarrow}(\tau_i'^{\downarrow})]$

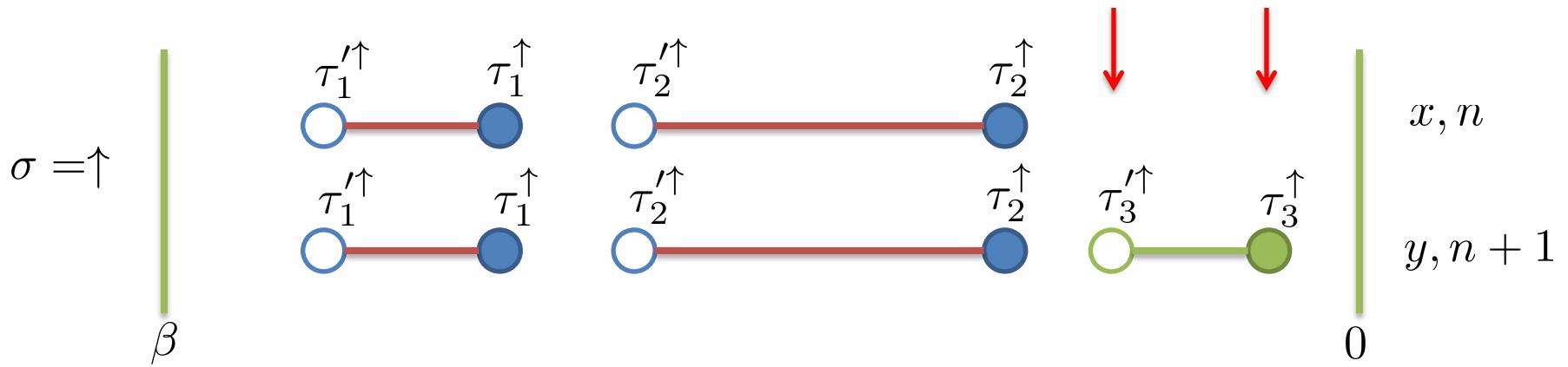
# Generating diagrams

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



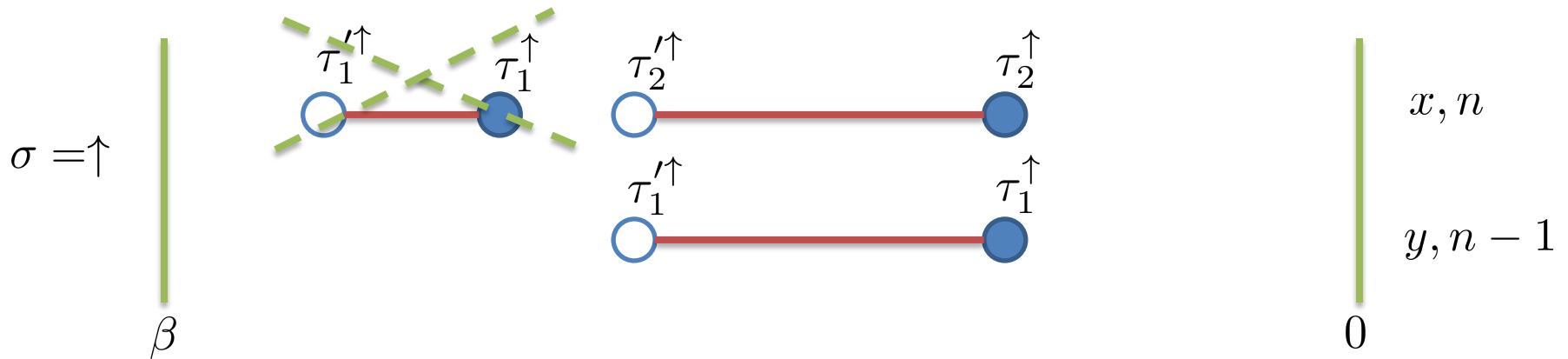
$$P_{x,y}\rho(x) = \frac{1}{2} \times \frac{d\tau_{n+1}}{\beta} \frac{d\tau'_{n+1}}{l_{\max}} \times \left| \text{Tr} \mathcal{C}_x \det \Delta_{\mathcal{C}_x} \prod_{i=1}^n d\tau_i d\tau'_i \right|$$

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

- 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's function

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

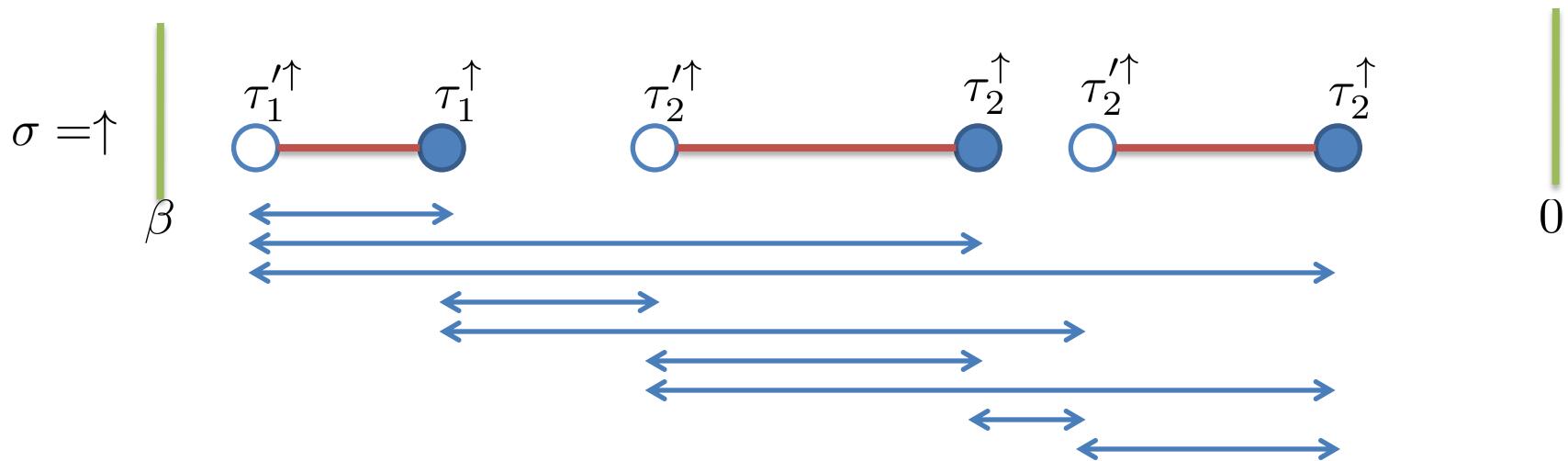
$$Z = \int_{\mathcal{C}} (-1)^{n_{\uparrow} + n_{\downarrow}} \det \Delta_{\uparrow \mathcal{C}} \det \Delta_{\downarrow \mathcal{C}} \text{Tr} \mathcal{C} = \int_{\mathcal{C}} w(\mathcal{C}) \sim \sum_{\mathcal{C}}^{\text{MC}} \text{sign}(w(\mathcal{C}))$$

- 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's function cont'd

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

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



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

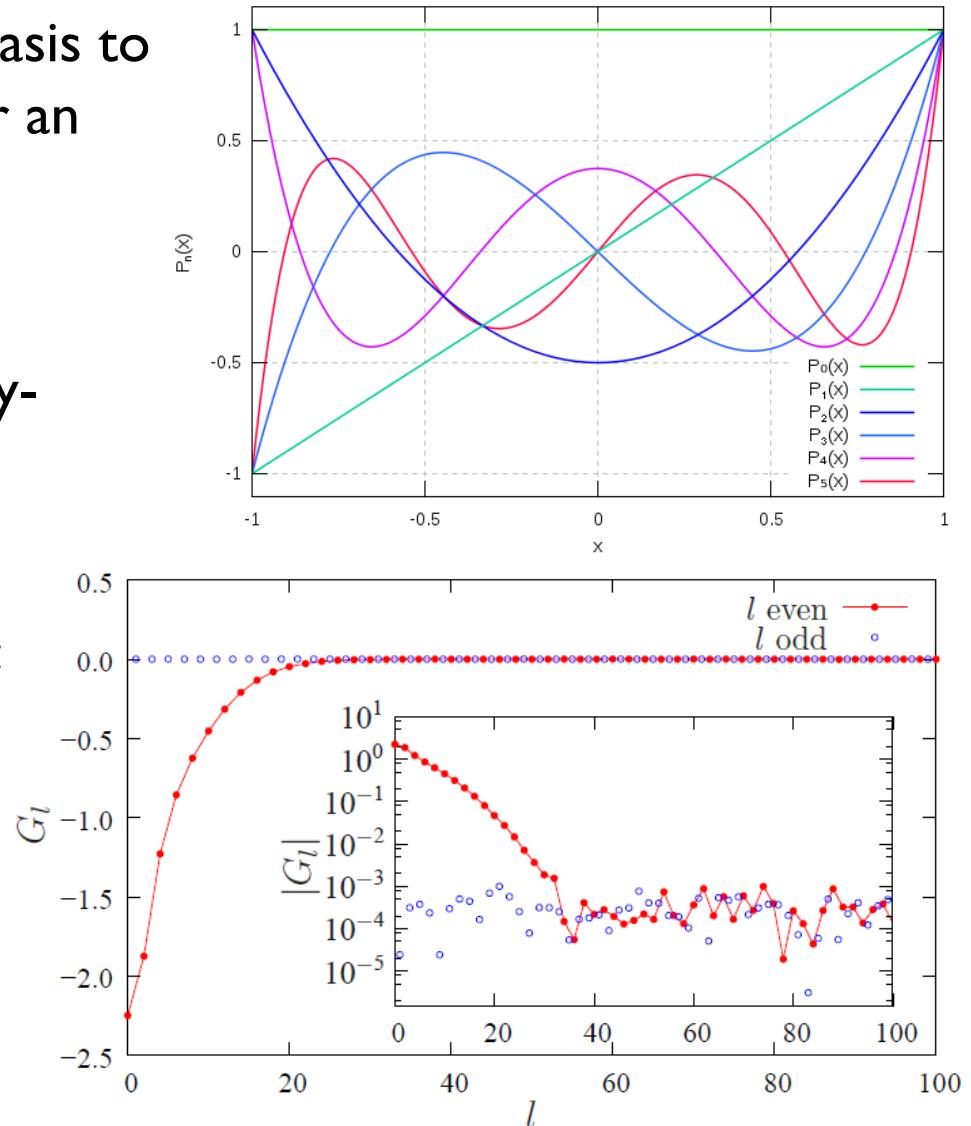
# Measuring using Legendre polynomials

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

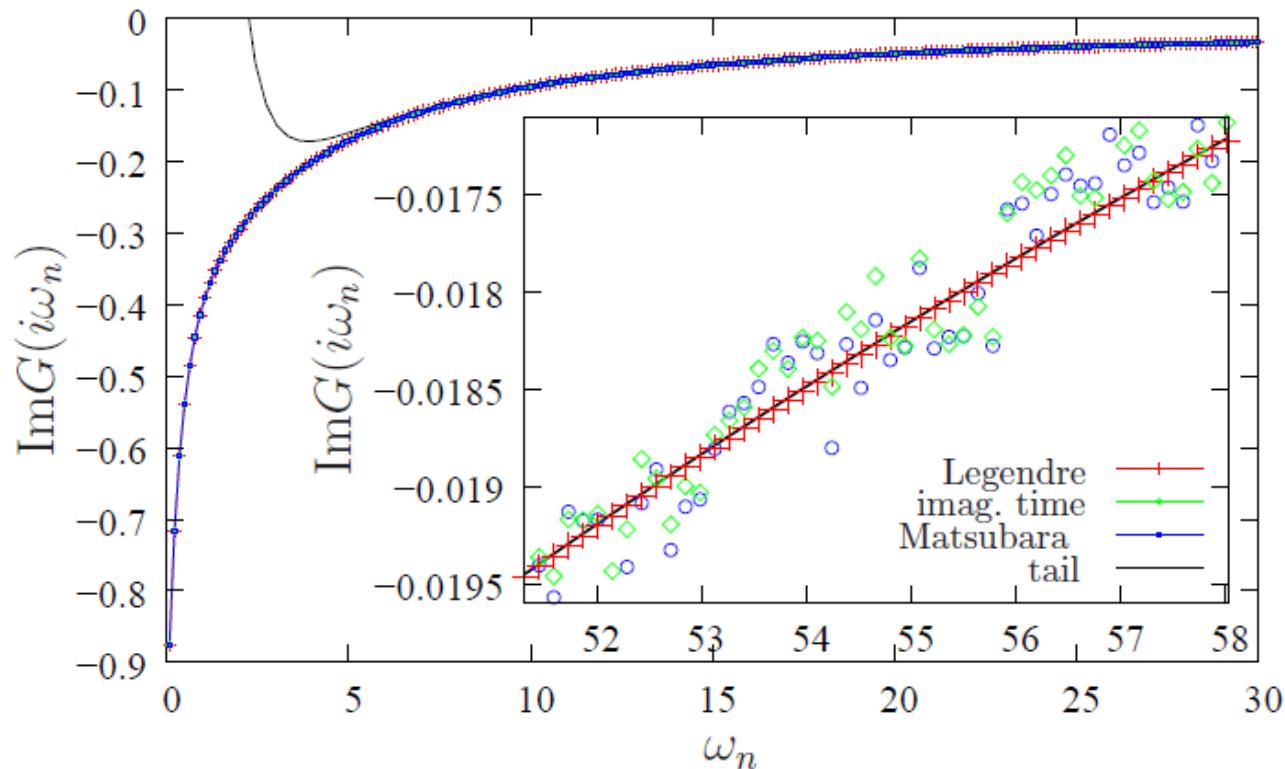
$$G(\tau) = \sum_{l \geq 0} \frac{\sqrt{2l+1}}{\beta} P_l[x(\tau)] G_l$$

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



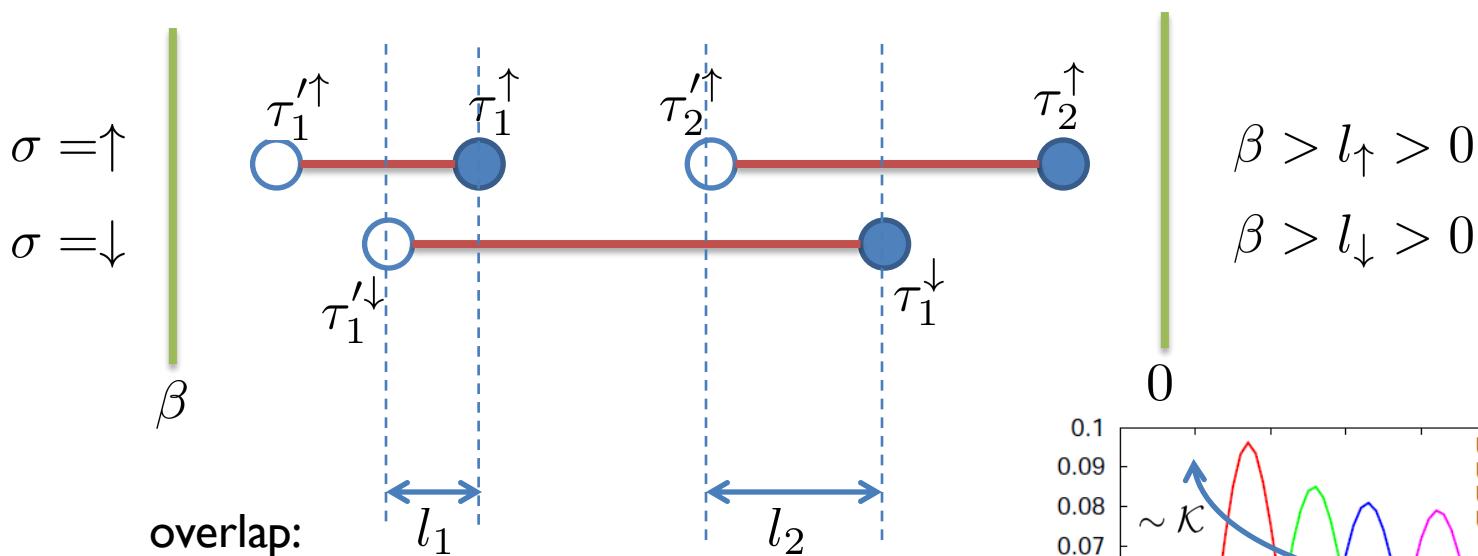
# Legendre basis acting as a noise filter

- 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:



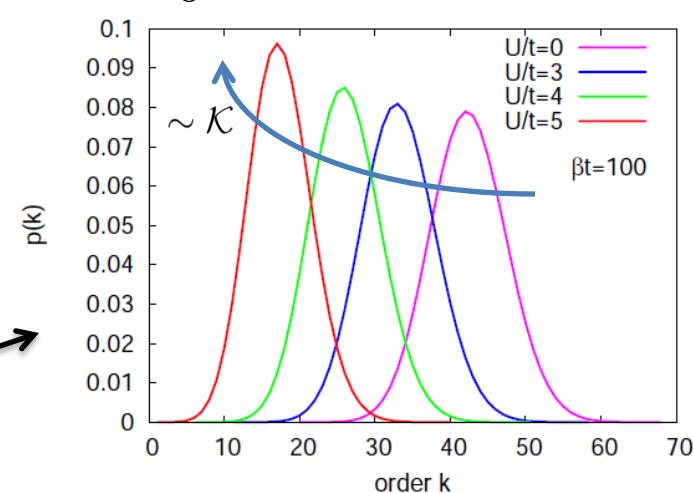
# Computational effort

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



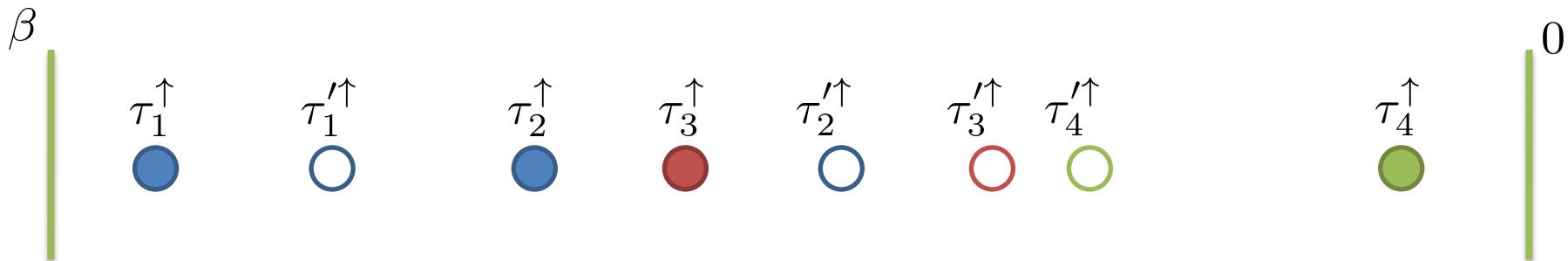
$$\text{Tr } \mathcal{C} = e^{(l_\uparrow + l_\downarrow)\mu - U(l_1 + l_2)}$$

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



# 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: real-time algorithms are being 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
- We will learn to use a CT-HYB solver this afternoon
- There are still limitations (sign problem, speed, ...) and more work has to be done!

Thank you for your attention!