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 (CT-INT)
    Rubtsov et al., PRB (2005) and Rubtsov and Lichtenstein, JETP Lett. (2004)
  - The hybridization-expansion algorithm (CT-HYB)
    Werner and Millis, PRB (2006) and Werner et al., PRL (2006)

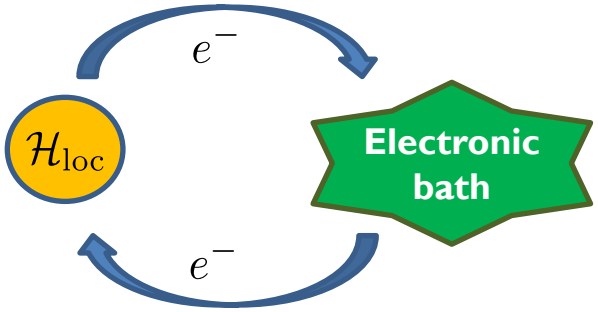
- Dynamical mean-field theory: *A. Georges et al., RMP (1996)*

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

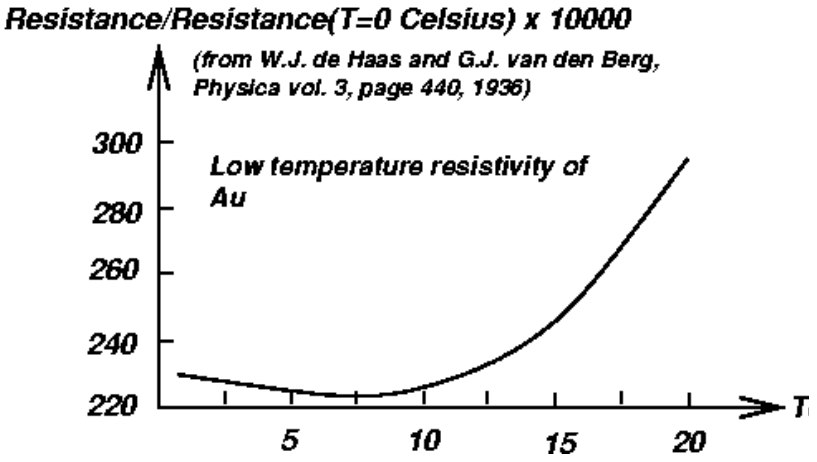
Quantum impurity problems

- 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



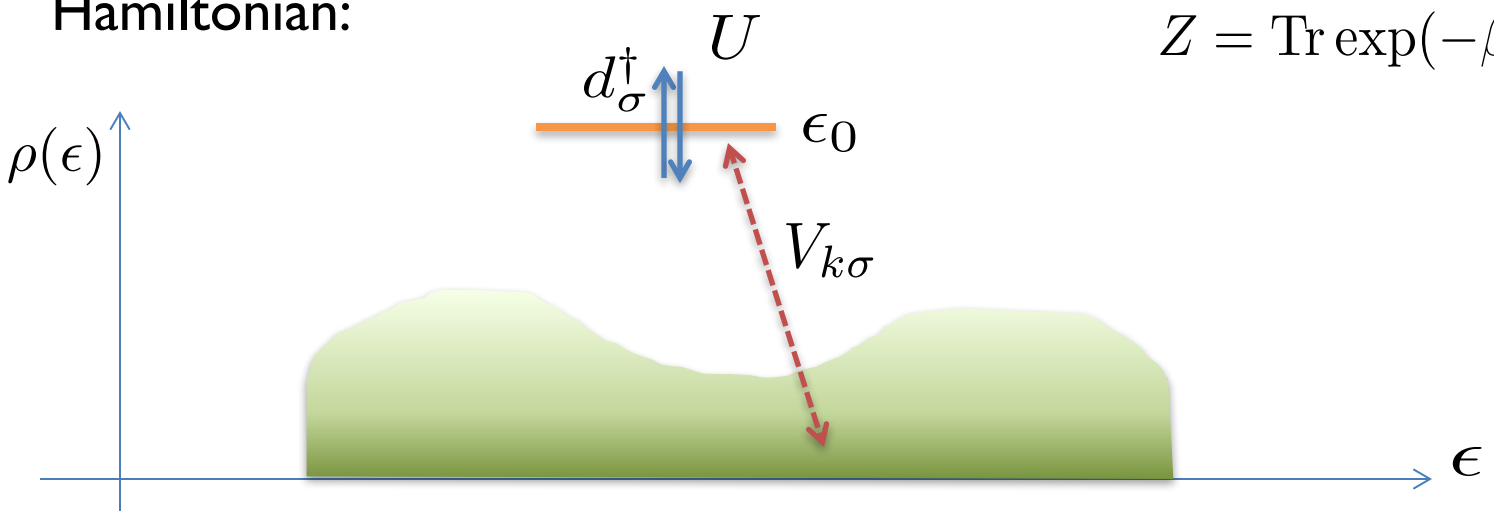
- Impurity models have a long history e.g. the Kondo problem
- Lead to the development of models and methods



The Anderson model

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

$$Z = \mathrm{Tr}\exp(-\beta\mathcal{H})$$



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

local many-body interaction

hybridization to the bath

free bath states

Action for the Anderson model

- After integrating out the fermionic bath: $Z = \int \mathcal{D}[d^\dagger, d] e^{-S}$

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

$$G_{0\sigma}^{-1}(i\omega_n) = i\omega_n - \epsilon_0 - \Delta_\sigma(i\omega_n)$$ ← 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):

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

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

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!

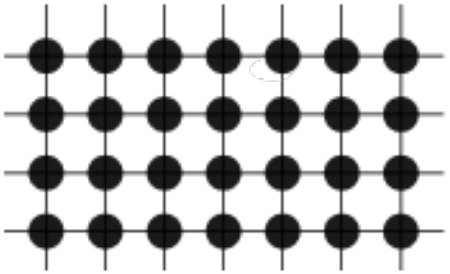
Our goal: Solve the DMFT equations

A. Georges and G. Kotliar, PRB (1992)

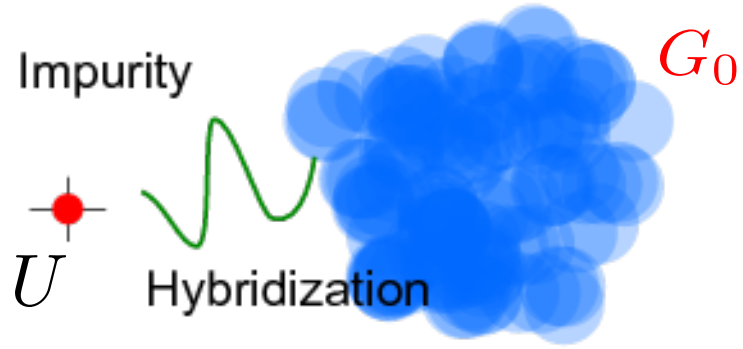
- The dynamical mean-field theory makes an approximation of a lattice model using an auxiliary quantum impurity problem

Lattice Hubbard model

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



Auxiliary Anderson impurity model



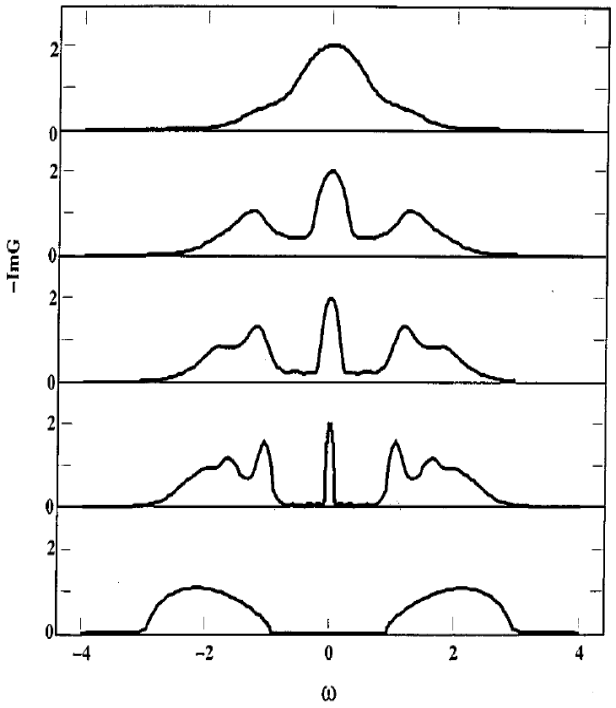
The impurity model is described by the following action:

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

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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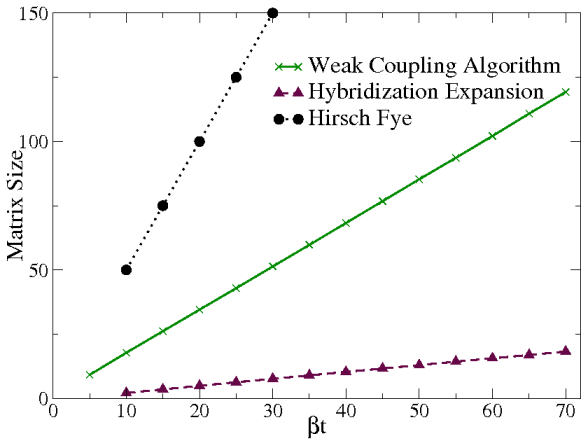
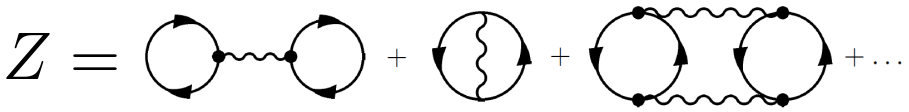
Continuous-time quantum Monte Carlo methods

- 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 series expansion of the partition function



  - 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:

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

- 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 $x = (\tau, \sigma, \ldots)$
- 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: $x_1 \to x_2 \to x_3 \to x_4 \to \ldots$
- 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): $$\frac{W_{x,y}}{W_{y,x}} = \frac{p(y)}{p(x)}$$

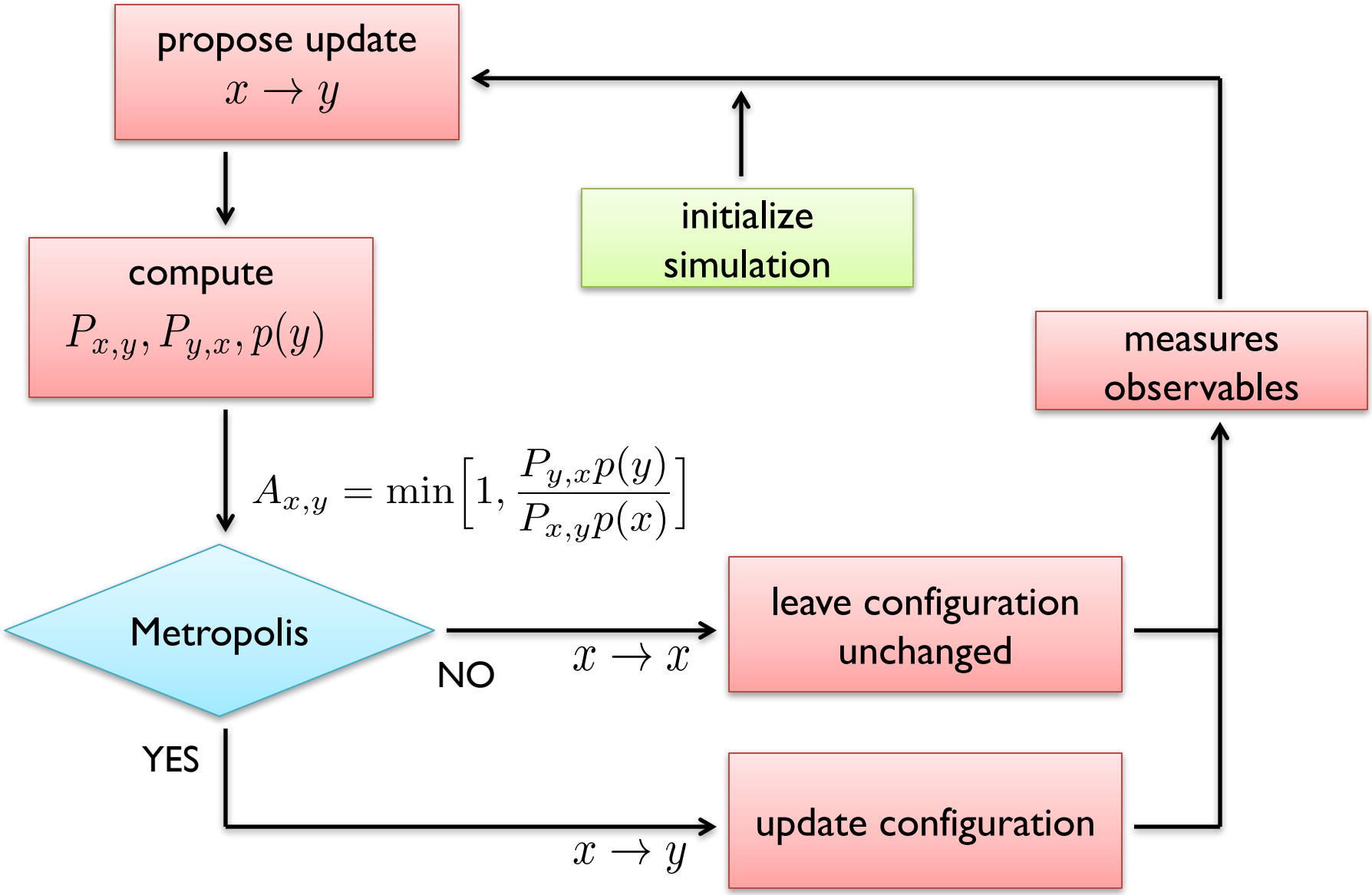
Metropolis algorithm

- 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:

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

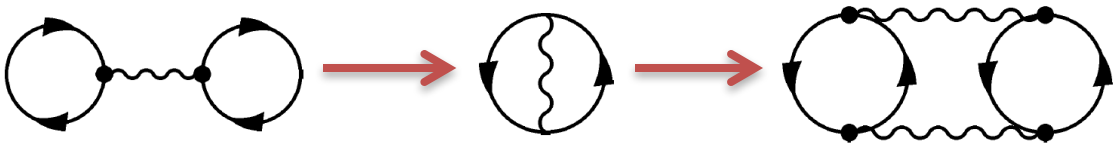
- We would like to use $w(x)$ as a probability. But what if it can be negative?
- We can use the absolute value instead:

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

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

Continuous-time quantum Monte Carlo

- Partition function: $$Z = \int_{\mathcal{C}} w(\mathcal{C}) \sim \sum_{\mathcal{C}}^{\mathrm{MC}} \mathrm{sign}(w(\mathcal{C}))$$
- Propose configurations/diagrams in a Markov chain:



- Accept these proposals with a rate (Metropolis) such that the diagrams appear with probability density $\left|w(\mathcal{C})\right|$
- From the generated configurations, compute the observables you are interested in $$\langle f \rangle = \frac{1}{Z} \int_{\mathcal{C}} w(\mathcal{C}) f(\mathcal{C}) \sim \frac{1}{Z} \sum_{\mathcal{C}}^{\mathrm{MC}} f(\mathcal{C}) \,\mathrm{sign}(w(\mathcal{C}))$$
- 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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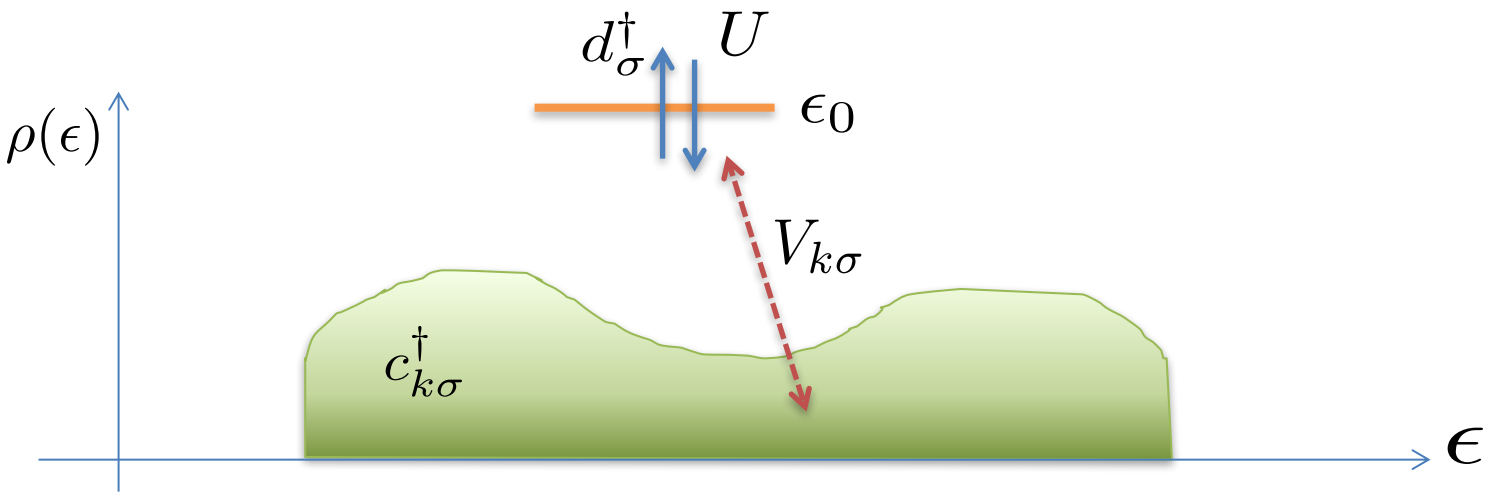
Interaction-expansion CT-QMC

- 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)



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

Interaction expansion 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:

"perturbation"

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

S_0 ← action of the non-interacting problem

- The partition function can be written as

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

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

Interaction expansion cont'd

- We write a series expansion for the exponential

$$
\begin{aligned}
Z &= Z_0 \Big\langle T_\tau \exp\Big(\int_0^\beta d\tau (-U) n_{d\uparrow}(\tau) n_{d\downarrow}(\tau) \Big) \Big\rangle_0 \\
&= Z_0 \Big\langle T_\tau \sum_n \frac{(-U)^n}{n!} \Big(\int_0^\beta d\tau n_{d\uparrow}(\tau) n_{d\downarrow}(\tau) \Big)^n \Big\rangle_0 \\
&= Z_0 \sum_n \int_0^\beta d\tau_1 \cdots d\tau_n \frac{(-U)^n}{n!} \Big\langle T_\tau n_{d\uparrow}(\tau_1) n_{d\downarrow}(\tau_1) \cdots n_{d\uparrow}(\tau_n) n_{d\downarrow}(\tau_n) \Big\rangle_0
\end{aligned}
$$

average over the non-interacting state

- At this stage we have a perturbation expansion for the partition function of the type:

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

- However there is an obvious sign problem!

Interaction expansion cont'd

- The trick is to rewrite the interaction differently

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

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

we absorb this term in the chemical potential

- We eventually get (up and down spins decouple)

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

- By tuning δ we can improve the sign problem a lot!

Interaction expansion cont'd

- In the end we have

Sum over many (some continuous) variables

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

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

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

Product of two non-interacting averages

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

- 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

$$\left\langle (n_{d\sigma}(\tau_1) - \alpha_{s_1\sigma}) \cdots (n_{d\sigma}(\tau_n) - \alpha_{s_n\sigma}) \right\rangle_0 = \det D_n^\sigma =$$

$$\begin{vmatrix} G_{0\sigma}(0^-) - \alpha_{s_1\sigma} & G_{0\sigma}(\tau_1 - \tau_2) & \cdots & \cdots \\ G_{0\sigma}(\tau_2 - \tau_1) & G_{0\sigma}(0^-) - \alpha_{s_2\sigma} & G_{0\sigma}(\tau_2 - \tau_3) & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & G_{0\sigma}(\tau_n - \tau_{n-1}) & G_{0\sigma}(0^-) - \alpha_{s_n\sigma} \end{vmatrix}$$

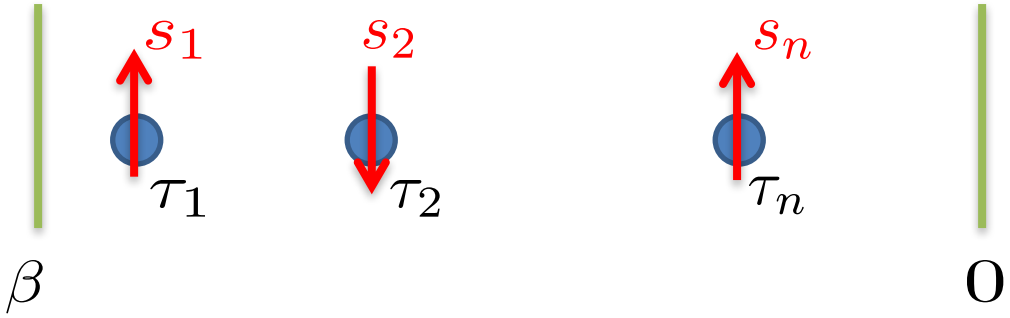
and $$Z = Z_0 \sum_n \int d\tau_1 \cdots d\tau_n \sum_{s_1} \cdots \sum_{s_n} \frac{(-U)^n}{n! 2^n} \det D_n^\uparrow \det D_n^\downarrow$$

Monte Carlo elements

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

- 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.

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

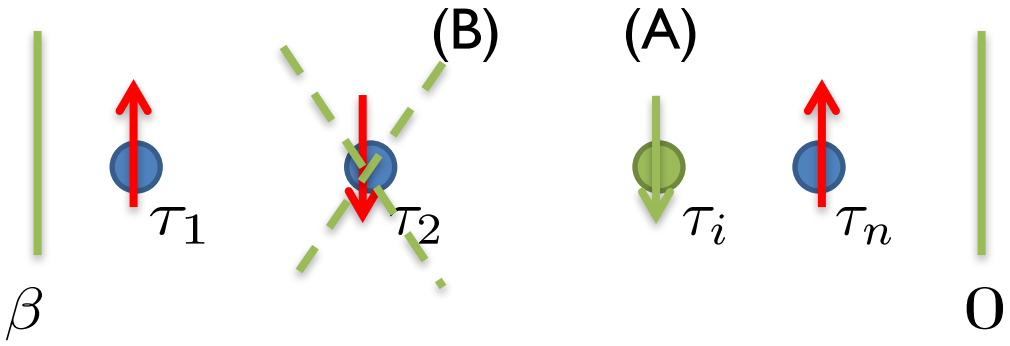


- The weight of every diagram is given by

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

Generating diagrams

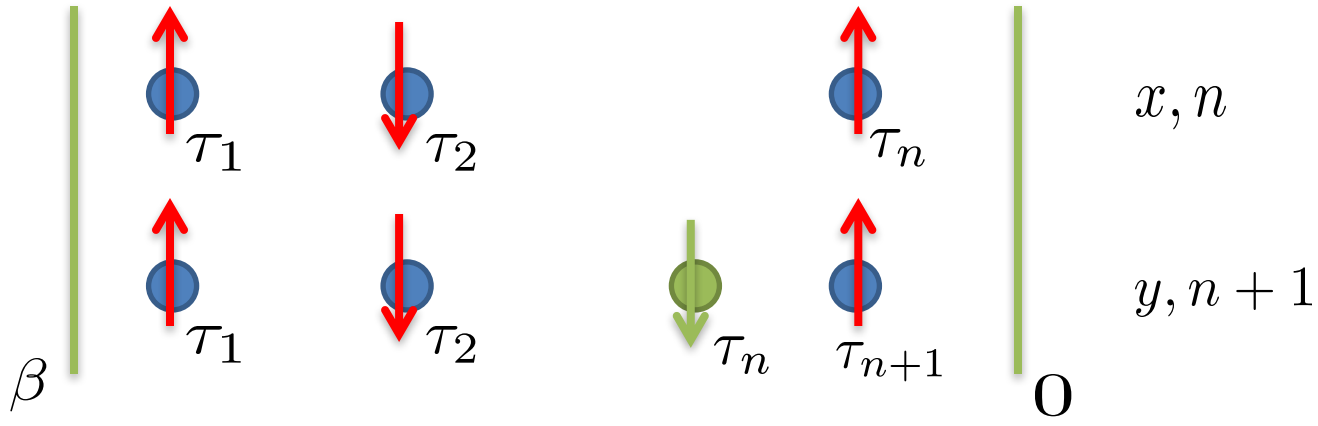
- We need to create a Markov chain of diagrams
- We can propose any changes to go from one diagram to another. A simple solution is to use two "moves":
- An insertion of a vertex: we pick a random imaginary time and insert a vertex with a spin randomly up or down (A)
- A removal of a vertex: pick a random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



Insertion of a vertex

- What is the acceptance rate?

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



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

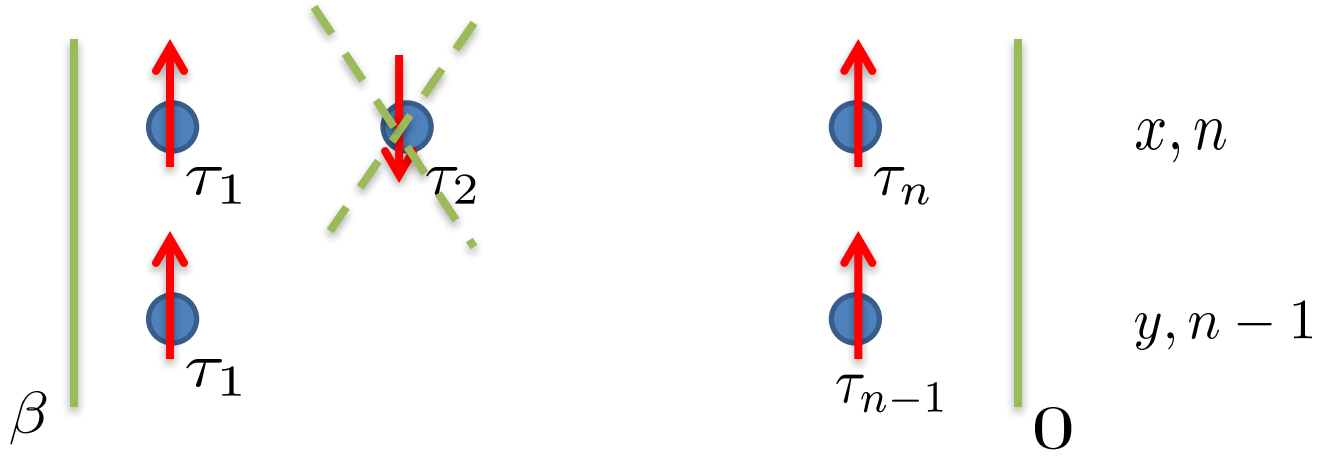
$$P_{y,x}\rho(y) = \frac{1}{2} \times \frac{1}{n+1} \times \left| \left(\frac{-U}{2}\right)^{n+1} \det D_{n+1}^{\uparrow} \det D_{n+1}^{\downarrow} \prod_{i=1}^{n+1} d\tau_i \right|$$

- 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

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

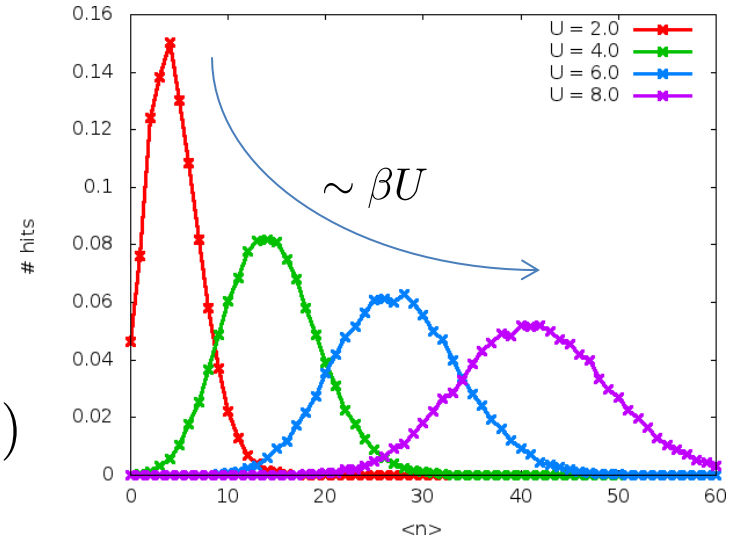
Computational effort

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

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

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

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

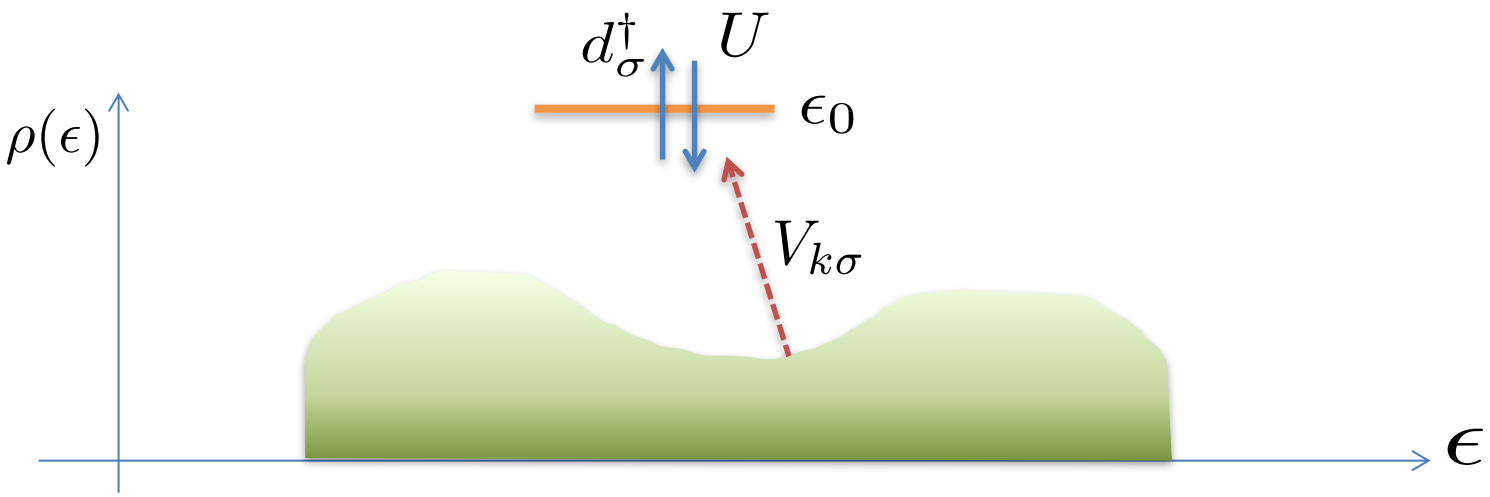


Outline

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

Hybridization-expansion CT-QMC

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



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

Hybridization expansion 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:

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

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

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

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

action of the atomic problem

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

"perturbation"

Hybridization expansion cont'd

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

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

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

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

average over the atomic state

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

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

Hamiltonian of the local problem

Hybridization expansion cont'd

- Inserting the expression of the hybridization action we get

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

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

Sum over many (continuous) variables

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

Product of hybridization functions

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

Trace involving both spin up and down operators

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

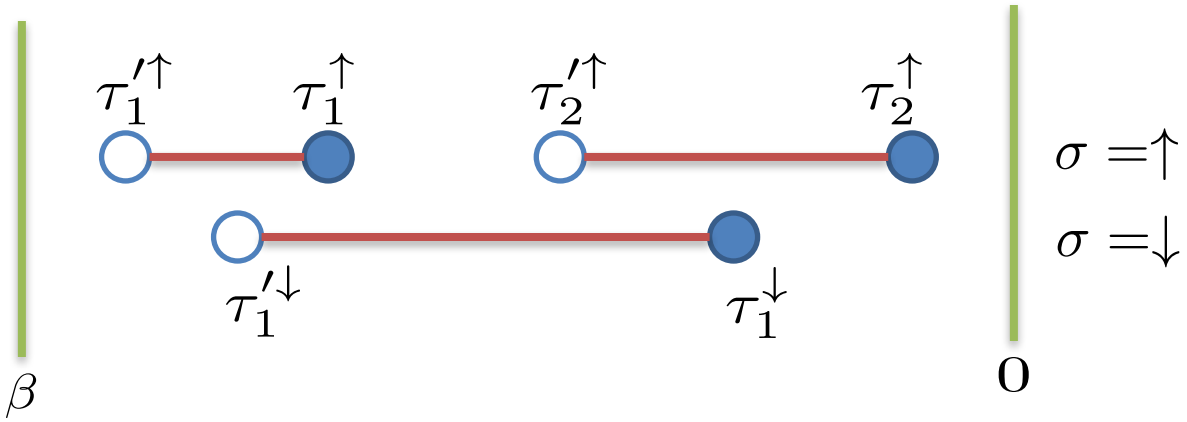
$$Z = \int_{\mathcal{C}} w(\mathcal{C}) \sim \sum_{\mathcal{C}}^{\rm MC} \mathrm{sign}(w(\mathcal{C})) \qquad \langle f \rangle = \frac{1}{Z}\int_{\mathcal{C}} w(\mathcal{C}) f(\mathcal{C}) \sim \frac{1}{Z}\sum_{\mathcal{C}}^{\rm MC} f(\mathcal{C})\,\mathrm{sign}(w(\mathcal{C}))$$

Hybridization expansion cont'd

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

- Diagrams:

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

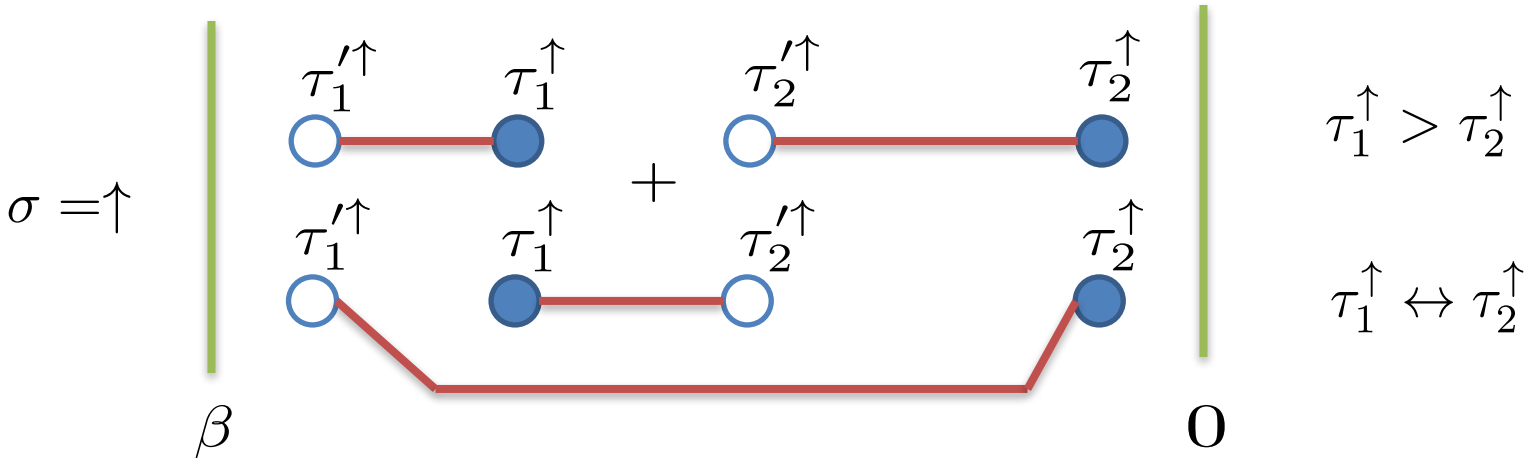


- Weight: $$w(\mathcal{C}) = \prod_\sigma \frac{(-1)^{n_\sigma}}{n_\sigma!} \prod_{i=1}^{n_\sigma} \Delta_\sigma(\tau_i^\sigma - \tau_i'^\sigma) \quad \times$$
$$\mathrm{Tr}\left[e^{-\beta \mathcal{H}_{\mathrm{loc}}} T_\tau \prod_{i=1}^{n_\uparrow} d_\uparrow^\dagger(\tau_i^\uparrow) d_\uparrow(\tau_i'^\uparrow) \prod_{i=1}^{n_\downarrow} d_\downarrow^\dagger(\tau_i^\downarrow) d_\downarrow(\tau_i'^\downarrow)\right]$$

- Unfortunately these diagrams have alternating signs $\Rightarrow$ 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 $\{\tau_i^\uparrow\}$



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

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

$$=$$

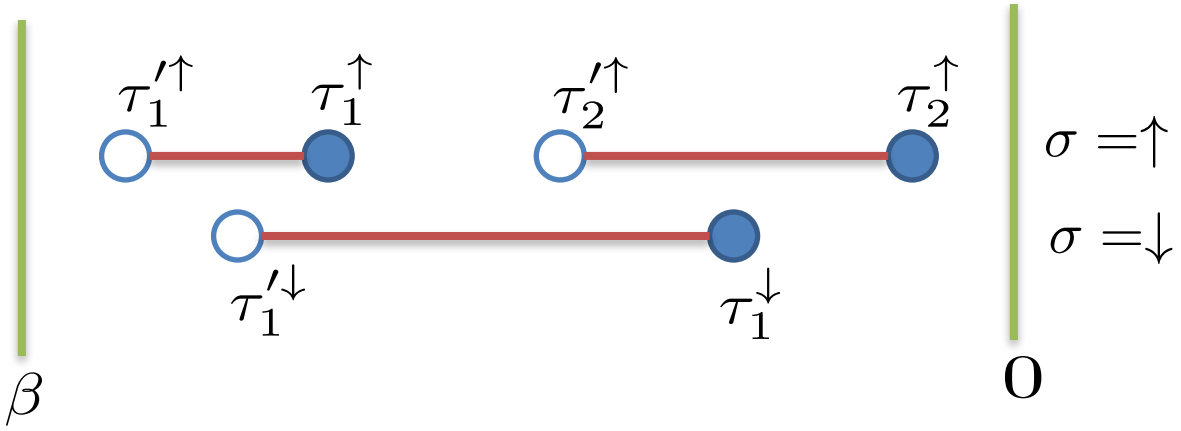
$$\mathrm{Tr}\left[e^{-\beta\mathcal{H}_{\mathrm{loc}}} d_\uparrow^\dagger(\tau_1^\uparrow) d_\uparrow(\tau_1'^\uparrow) d_\uparrow^\dagger(\tau_2^\uparrow) d_\uparrow(\tau_2'^\uparrow)\right] \times \frac{1}{2} \det_{1\leq k,l\leq 2} \Delta_\uparrow(\tau_k^\uparrow - \tau_l'^\uparrow)$$

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:

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

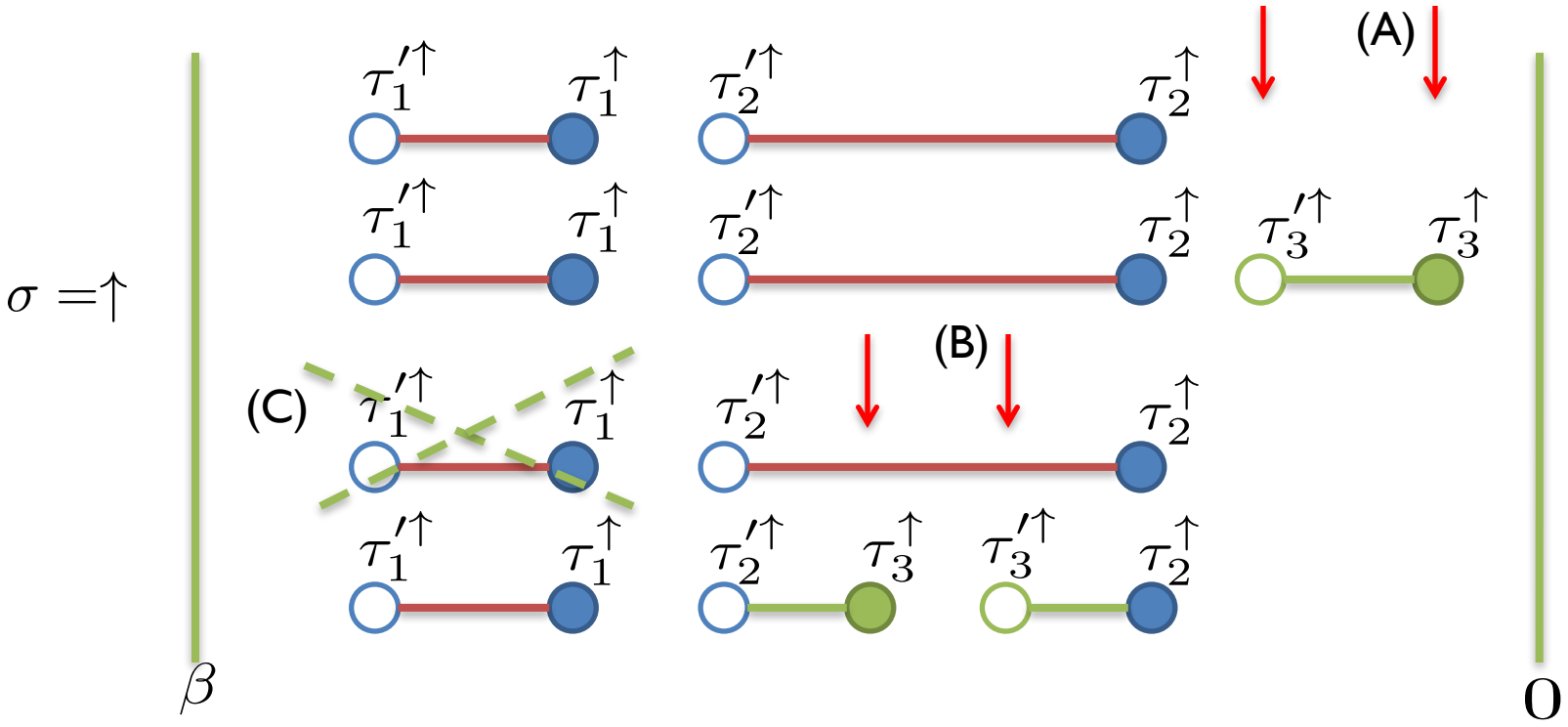


- Weight: $$w(\mathcal{C}) = \prod_\sigma (-1)^{n_\sigma} \det_{1 \le k,l \le n_\sigma} \Delta_\sigma(\tau_k^\sigma - \tau_l'^\sigma) \times$$

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

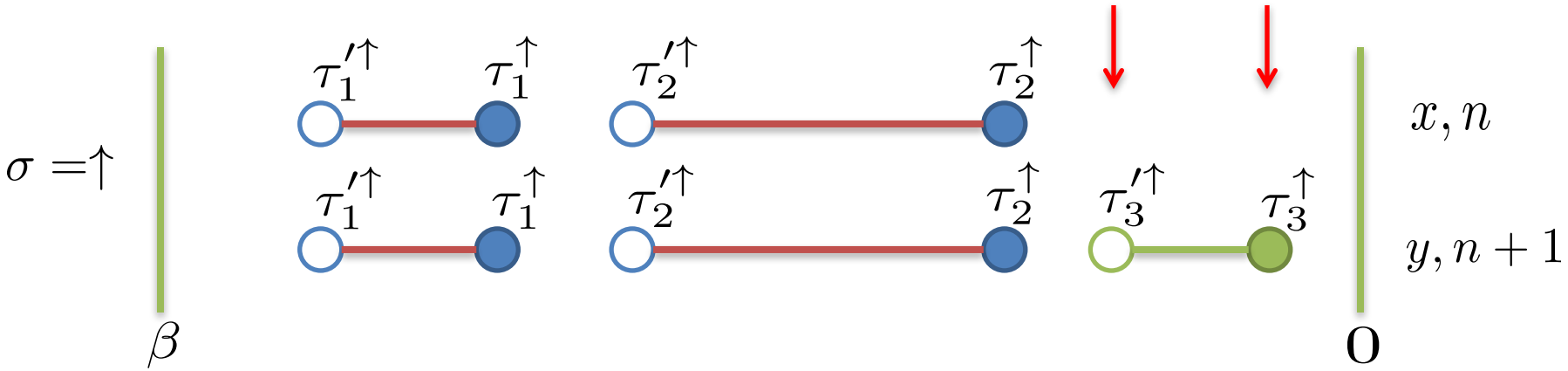
Generating diagrams

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



Insertion of an (anti)-link

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



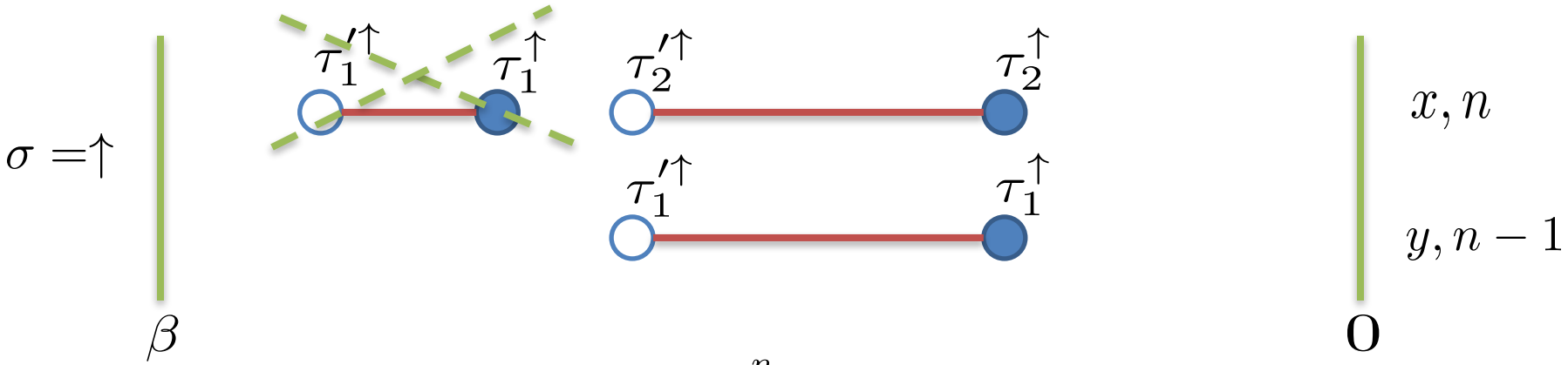
$$P_{x,y}\rho(x) = \frac{1}{2} \times \frac{d\tau_{n+1}}{\beta}\frac{d\tau'_{n+1}}{l_{\max}} \times \left|\mathrm{Tr}\mathcal{C}_x \det \Delta_{\mathcal{C}_x} \prod_{i=1}^{n} d\tau_i d\tau'_i\right|$$

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

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

Removal of a link

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



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

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

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

Measuring the Green's function

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

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

- How do we get the Green's function?

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

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

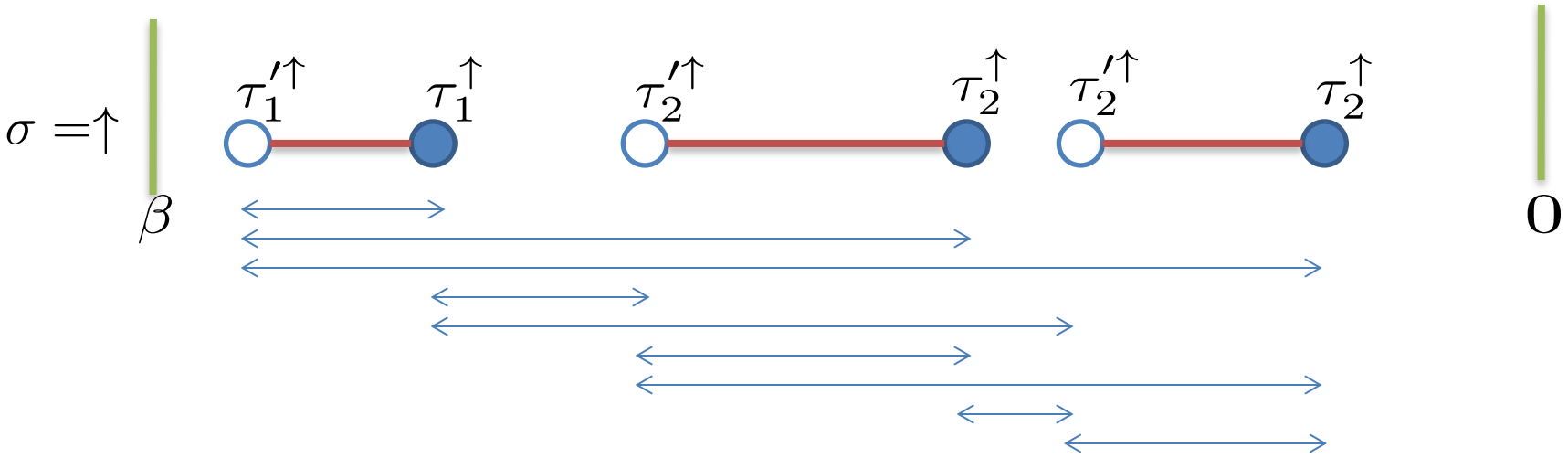
$$G_\uparrow(\tau) = \frac{-1}{Z\beta} \int_{\mathcal{C}} \sum_{k,l} \delta(\tau_k^\uparrow - \tau_l'^\uparrow + \tau) [\Delta_{\uparrow\mathcal{C}}^{-1}]_{k,l} \times \underbrace{(-1)^{n_\uparrow + n_\downarrow} \det \Delta_{\uparrow\mathcal{C}} \det \Delta_{\downarrow\mathcal{C}} \mathrm{Tr}\mathcal{C}}_{w(\mathcal{C})}$$

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

Measuring the Green's function cont'd

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

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

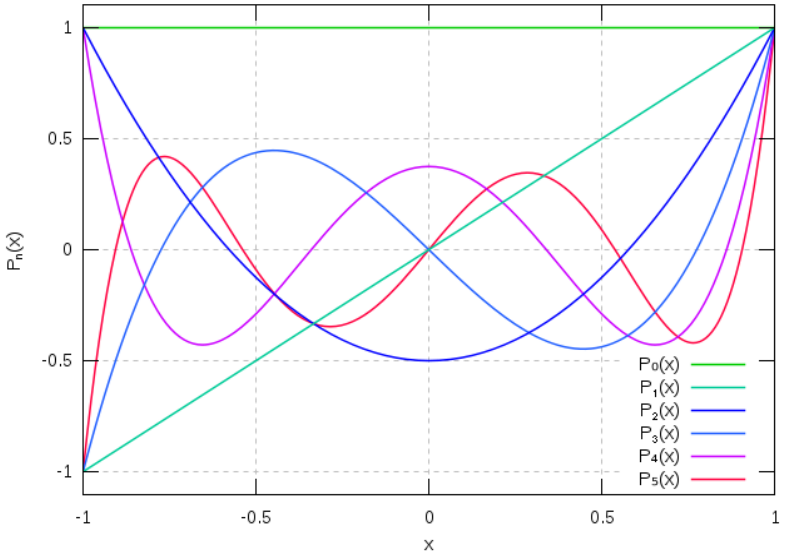


- These contribution can be "binned" on a very fine imaginary-time grid. This induces high frequency noise in Matsubara frequencies

Measuring using Legendre polynomials

L. Boehnke et al., PRB (2011)

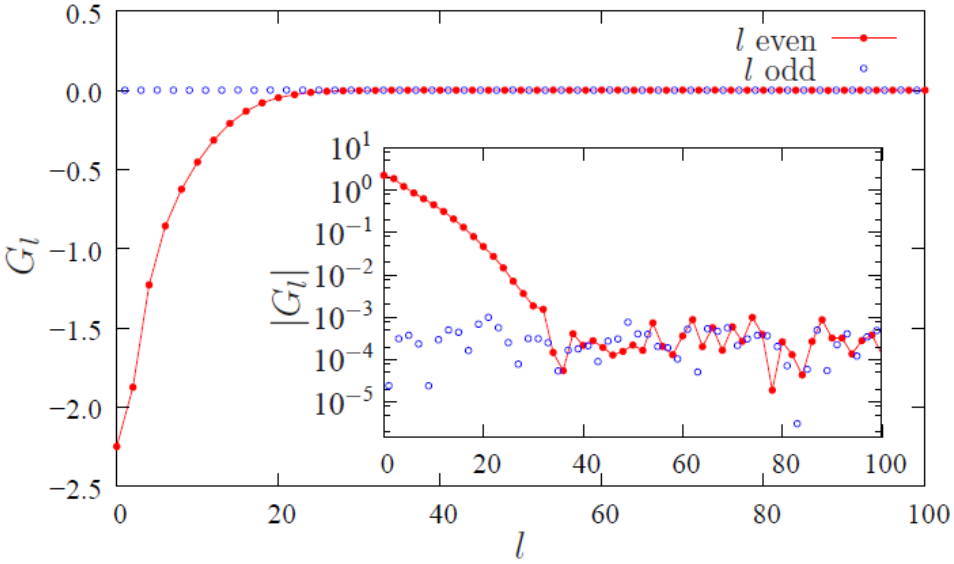
- Legendre polynomials are a basis to express function defined over an interval



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

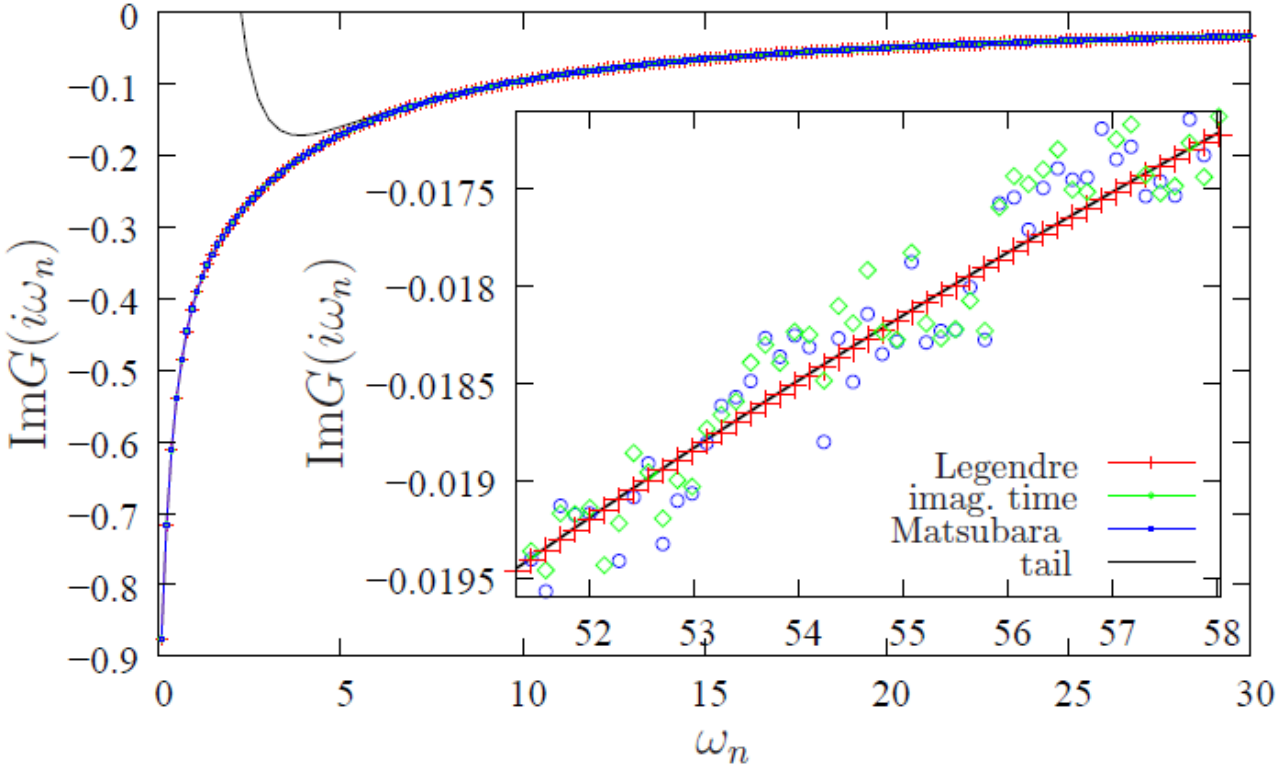
$$G(\tau) = \sum_{l \geq 0} \frac{\sqrt{2l+1}}{\beta} P_l[x(\tau)] G_l$$

- The coefficients G_l in this basis decay very quickly



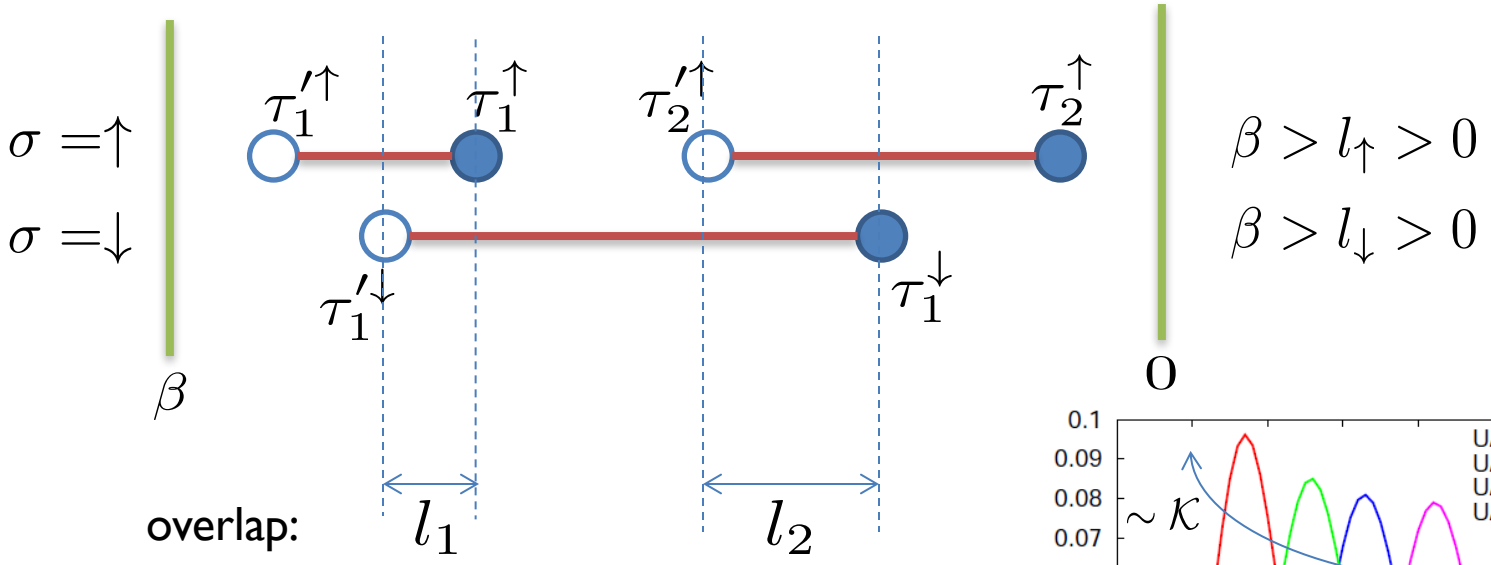
Legendre basis acting as a noise filter

- 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:



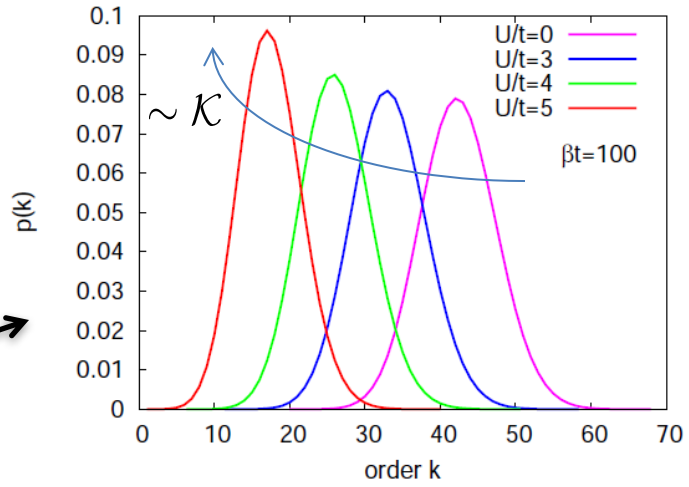
Computational effort

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



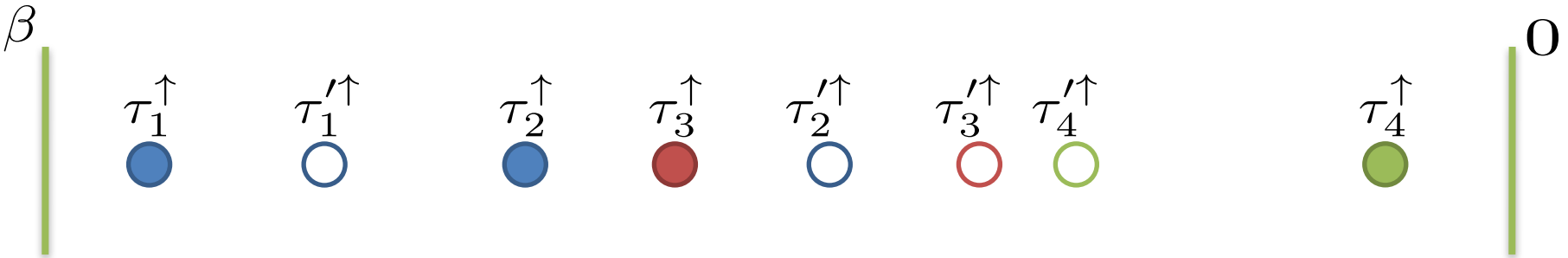
$$\mathrm{Tr}\,\mathcal{C} = e^{(l_\uparrow + l_\downarrow)\mu - U(l_1 + l_2)}$$

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



What about non density-density Hamiltonians?

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



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

CT-INT versus CT-HYB

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

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

Pros and cons of the CT-QMC algorithms

- Pros:
  - Faster than earlier algorithms like Hirsch-Fye
  - Monte Carlo $\Rightarrow$ 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 beeing 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 how to use a CT-HYB solver this afternoon
- There are still limitations (sign problem, speed, …) and more work has to be done!