Title: Date:

7. Quantum spin system II or quantum Monte Carlo II

* You know why we go from $d \to d+1$
* You know why we would want to use continuous-time Monte Carlo schemes.
* You can derive cluster updates for various quantum spin models

7.1 World line representations for quantum lattice models

We are now acquainted with the problem, that given a set of degrees of freedom, the partition sum Z is not just a sum over their possible configurations but that

$$Z = \operatorname{tr} e^{-\beta H}$$

is a potentially complicated operator expression. Furthermore, the expression for an observable like the magnetization m

$$\langle m \rangle = \operatorname{tr}\left[\hat{m}\, e^{-\beta H}\right] / Z$$

is not just sampling over configurations as $\hat{m}$ might induce transitions between different quantum states:

Title: Date:

Imagine $H|\lambda\rangle = \lambda|\lambda\rangle \Rightarrow$

$$Z = \mathrm{tr}\, e^{-\beta H} = \sum_\lambda \langle\lambda| e^{-\beta H} |\lambda\rangle$$
$$= \sum_\lambda e^{-\lambda\beta}$$

But generically $\hat{m}|\lambda\rangle \neq m|\lambda\rangle$ but $m|\lambda\rangle = \sum_m a_m |\lambda_m\rangle$. Therefore, the first step of any quantum Monte-Carlo procedure is to map the system to an equivalent classical system

$$Z = \mathrm{tr}\, e^{-\beta H} = \sum_c w(c)$$
$$\langle m\rangle = \frac{1}{Z}\, \mathrm{tr}\, m\, e^{-\beta H} = \frac{1}{Z} \sum_c m(c)\, w(c)$$
$$= \sum_c m(c)\, P(c)$$

with $P(c) = \frac{w(c)}{Z}$ and the sum runs over configurations c of an artificial system. We have seen such a mapping for particles in free space in the framework of path-integral quantum Monte-Carlo. As an introduction to lattice problems we discuss a single quantum mechanical spin-$\frac{1}{2}$.

7.2 A spin-$\frac{1}{2}$ in a magnetic field

The Hamiltonian for a single quantum mechanical spin-$\frac{1}{2}$ in a longitudinal field h and a transverse field Γ is given by

$$\mathcal{H} = \mathcal{H}_z + \mathcal{H}_x = -hS^z - \Gamma S^x .$$

Using a basis set in which the z-component of the spin-operator S^z is diagonal

$$\{ |\tfrac{1}{2}\rangle, |-\tfrac{1}{2}\rangle \},$$

the spin operators S^x and S^z are given by the Pauli matrices

$$S^x = \frac{\hbar}{2}\sigma^x = \begin{pmatrix} 0 & \hbar/2 \\ \hbar/2 & 0 \end{pmatrix},$$

$$S^z = \frac{\hbar}{2}\sigma^z = \begin{pmatrix} \hbar/2 & \\ & -\hbar/2 \end{pmatrix}.$$

For simplicity, we set $\hbar = 1$, the Hamiltonian becomes

$$\mathcal{H} = \begin{pmatrix} -h/2 & \Gamma/2 \\ \Gamma/2 & h/2 \end{pmatrix}.$$

7.2.1 Discrete time path integral

As we did with path-integrals for free particles we discretize "imaginary time" β. As we will later take the limit $\Delta_\tau \to 0$, it is sufficient to take the lowest order Trotter approximation.

Title: Date:

As usual we divide β into M time steps $\Delta_\tau = \beta/M$, arriving at a discrete time approximation of the quantum transfer matrix $e^{-\Delta_\tau H}$

$$e^{-\Delta_\tau H} = \mathcal{U} + \mathcal{O}(\Delta_\tau^2)$$

where we introduced the transfer matrix

$$\mathcal{U} = \mathbb{1} - \Delta_\tau H = \begin{pmatrix} 1 + \frac{\Delta_\tau h}{2} & \frac{\Delta_\tau \Gamma}{2} \\ \frac{\Delta_\tau \Gamma}{2} & 1 - \frac{\Delta_\tau h}{2} \end{pmatrix}.$$

Note the we just used the lowest order Taylor expansion versus a more sophisticated Trotter-Suzuki scheme.

In the discrete time path integral formulation, we evaluate the operator exponential $e^{-\beta H}$ by writing the trace as a sum over all basis states $|i\rangle$. Inserting M sums over a complete sets of states

$$\mathbb{1} = \sum_i |i\rangle\langle i|$$

we obtain

$$Z = \operatorname{tr} e^{-\beta H} = \operatorname{tr}\left(e^{-\Delta_\tau H}\right)^M = \operatorname{tr}\left[\mathcal{U} + \mathcal{O}(\Delta_\tau^2)\right]^M$$

$$= \sum_{i_1,\dots,i_M} \langle i_1|\mathcal{U}|i_2\rangle\langle i_2|\mathcal{U}|i_3\rangle\langle i_3| \dots \langle i_M|\mathcal{U}|i_1\rangle + \mathcal{O}(\Delta_\tau)$$

Title: Date:

This expression is identical to the partition sum of a one-dimensional chain of classical Ising spins $\sigma_i = \pm 1$ of length M at inverse temperature β_{cl}

$$\mathcal{H}_{cl} = -J_{cl} \sum_{i=1}^{M} \sigma_i \sigma_{i+1} - h_{cl} \sum_i \sigma_i + E_0$$

with periodic boundary conditions $\sigma_{M+1} = \sigma_1$ and the following relations

$$\beta_{cl} J_{cl} = -\frac{1}{2} \log(\Delta_\tau \Gamma / 2),$$

$$\beta_{cl} h_{cl} = \log(1 + \Delta_\tau h / 2) \approx \Delta_\tau h / 2,$$

$$\beta_{cl} E_0 = M \beta_{cl} J_{cl}.$$

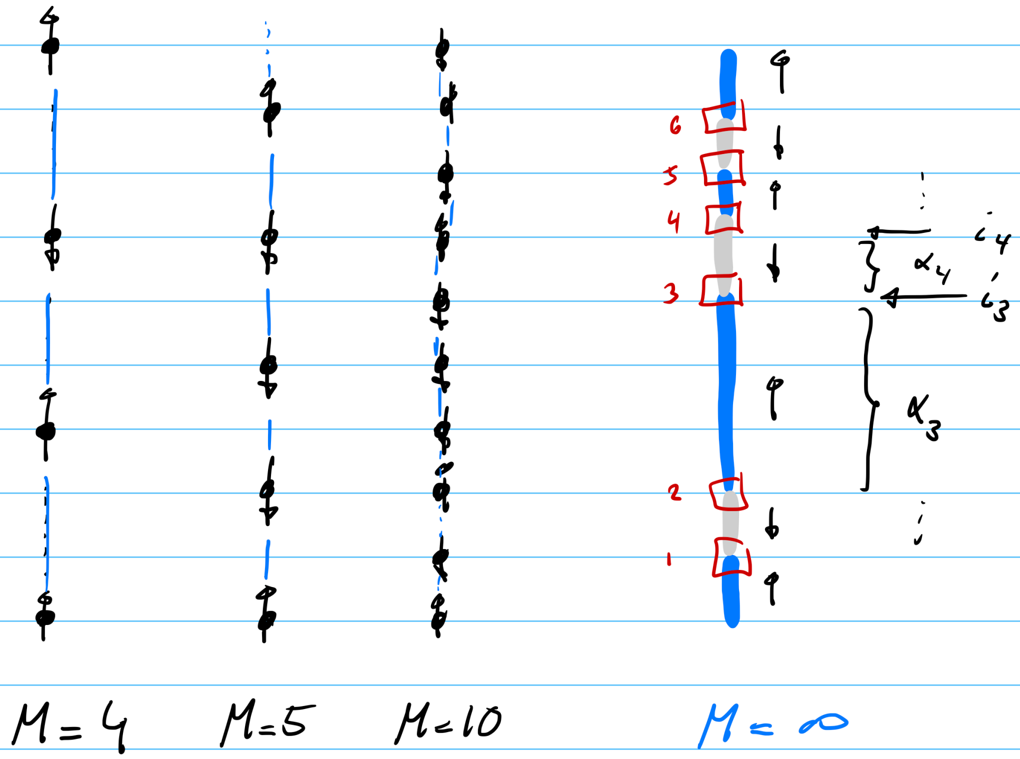
Therefore any Monte-Carlo algorithm for the classical Ising model, including cluster-updates, can be used for the simulation. Similarly, any d-dimensional quantum Ising model

$$H = -J \sum_{\langle ij \rangle} S_i^z S_j^z - h \sum_i S_i^z - \Gamma \sum_i S_i^x$$

can be mapped to an anisotropic d+1 dimensional classical Ising model.

7.2.2. Continuous time path integral

Instead of working with discrete time steps Δ_τ, modern world-line algorithms work directly in the continuum with $\Delta_\tau \to 0$ or $M \to \infty$. Let us try to understand what happens in this limit.



Each time we reduce Δ_τ or increase M, we have more spins in the β-direction of our spin lattice model. However, while the number of spins diverge, the number of domain walls remains finite!

Why? The coupling between neighboring spins

$$\beta_{cl} J_{cl} = -\log\left(\Delta_\tau \Gamma/2\right) \to \infty \quad \text{for } \Delta_\tau \to 0$$

becomes infinitely large. The ratio of spin pairs that are antiparallel vs. parallel is given by

Title: Date:

the Boltzmann factor

$$e^{-2\beta_{cl} J_{cl}} = \frac{\Delta_\tau \Gamma}{2}.$$

It is proportional to Δ_τ and hence goes down for $M \to \infty$. The average number of domain walls is given by

$$M \cdot e^{-2\beta_{cl} J_{cl}} = M \frac{\Delta_\tau \Gamma}{2} = \frac{\beta \Gamma}{2}$$

and hence finite in the $\Delta_\tau \to 0$ limit.

Since the number of domain walls n remains finite while the number of spins M diverges, we want to store the values α_j of the spins in the j'th domain $j = 1, \dots, n$, and the location of the last spin of the j'th domain i_j.

In this notation we have

$$\langle i_1 | \mathcal{U} | i_2 \rangle \langle i_2 | \mathcal{U} | i_3 \rangle \dots \langle i_M | \mathcal{U} | i_1 \rangle$$

$$= (1 + \Delta_\tau h \alpha_1)^{i_1 - 1} \langle \alpha_1 | \mathcal{U} | \alpha_2 \rangle (1 + \Delta_\tau h \alpha_2)^{i_2 - i_1 - 1} \dots$$

$$\dots (1 + \Delta_\tau h \alpha_n)^{(i_n - i_{n-1} - 1)} \langle \alpha_n | \mathcal{U} | \alpha_1 \rangle (1 + \Delta_\tau h \alpha_1)^{M - i_n}.$$

Identifying $\tau_j = i_j \Delta_\tau$ and $E_j = -h\alpha_j$ we realize that

$$\langle \alpha_j | \mathcal{U} | \alpha_{j+1} \rangle = -\Delta_\tau \langle \alpha_j | H_x | \alpha_{j+1} \rangle$$

Title: Date:

or $|\alpha_i\rangle \neq |\alpha_{i+1}\rangle$. We then take $\Delta_\tau \to 0$ to end up with

$$(-1)^n e^{-\tau_1 E_1} \langle \alpha_1 | H^x | \alpha_2 \rangle e^{-(\tau_2-\tau_1)E_2} \cdots$$

$$\cdots e^{-(\tau_n-\tau_{n-1})E_n} \langle \alpha_n | H^x | \alpha_1 \rangle e^{-(\beta-\tau_1)E_1} d\tau_1 \cdots d\tau_n .$$

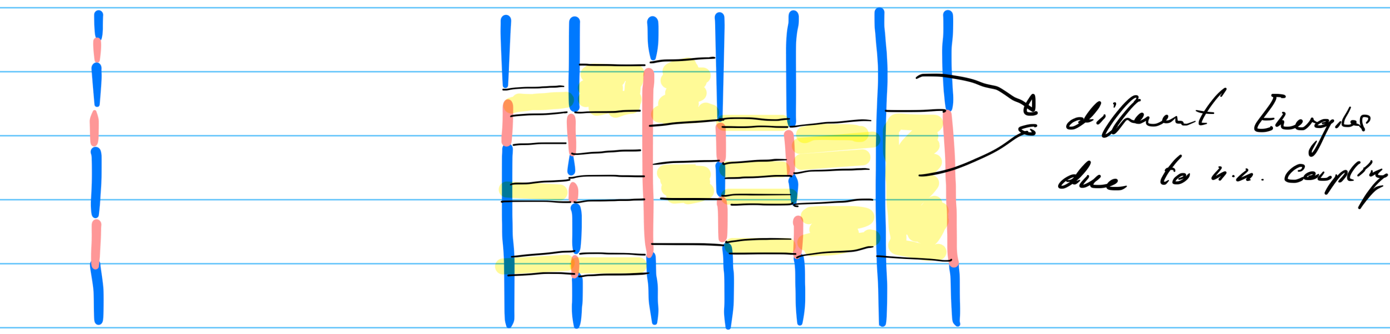
Integrating this weight over all possible locations for the domain walls and summing over all possible numbers n of such domain walls gives us the final continuous time representation

$$\boxed{\begin{aligned} Z = & \sum_{\alpha_0 = \pm 1} \langle \alpha_0 | e^{-\beta E_0} | \alpha_0 \rangle + \\ & \sum_{n=1}^{\infty} \sum_{(\alpha_1, \dots, \alpha_n)} (-1)^n \int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \, e^{-\tau_1 E_1} \langle \alpha_1 | H^x | \alpha_2 \rangle \\ & \times e^{-(\tau_2-\tau_1)E_2} \cdots e^{-(\tau_n-\tau_{n-1})E_n} \langle \alpha_n | H^x | \alpha_1 \rangle \\ & \times e^{-(\beta-\tau_1)E_1} . \end{aligned}}$$

7.3 More complicated models: the XXZ chain

For the transverse field Ising model, the world lines were just "colored" segments of straight lines: one color for $|\uparrow\rangle$ and another for $|\downarrow\rangle$, and we stored the location of the domain walls:

Title: Date:



zero-d TFIM one-d TFIM

In cases where the total magnetization is conserved, our world lines become simpler, as they cannot just change color as above.

We consider the Hamiltonian

$$H = - \sum_{\langle ij \rangle} \left[J_z S_i^z S_j^z + \frac{J_{xy}}{2} \left(S_i^+ S_j^- + S_j^+ S_i^- \right) \right].$$

We start again by discretizing $\beta = M \Delta_\tau$:

$$e^{-\beta H} = \left(e^{-\Delta_\tau H} \right)^M = \left(1 - \Delta_\tau H \right)^M + O(\Delta_\tau)$$

For $M \to \infty$ this becomes exact. As usual, we write

$$Z = \operatorname{tr} e^{-\beta H} = \sum_{i_1, \ldots, i_M} \langle i_1 | 1 - \Delta_\tau H | i_2 \rangle \langle i_2 | 1 - \Delta_\tau H | i_3 \rangle \ldots$$

$$\langle i_M | 1 - \Delta_\tau H | i_1 \rangle$$

$$= \sum_{i_1, \ldots, i_M} P_{i_1, \ldots, i_M}$$

Title: Date:

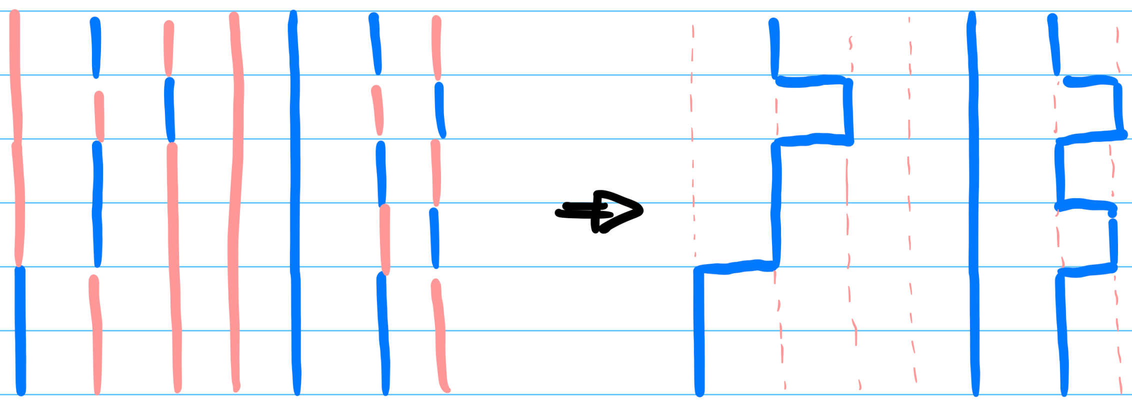
For measurements we find similarly

$$\langle A \rangle = \sum_{i_1, \dots, i_M} \frac{\langle i_1 | A(1-\Delta_\tau H) | i_2 \rangle}{\langle i_1 | 1 - \Delta_\tau H | i_2 \rangle} P_{i_2, \dots, i_M} .$$

As before, we could sample this d+1-dimensional spin-$\frac{1}{2}$ problem over all classical configurations $i_1, \dots, i_M$. The probabilities would be given by

$$\langle i_n | \mathbb{1} - \Delta_\tau H | i_{n+1} \rangle .$$

But now we realize something! $\mathbb{1}$ doesn't change any spin, so there $\langle i_n | \stackrel{!}{=} \langle i_{n+1} |$. Moreover $\Delta_\tau H$ also only mediates matrix elements between states where $|i_n\rangle$ and $|i_{n+1}\rangle$ differ by one spin-flip $S_i^+ S_j^-$! All classical configurations $i_1, \dots, i_M$ that do not fulfill this condition, have exactly zero weight. Therefore we only need to consider world lines like



Finally, the continuum limes $\Delta_\tau \to 0$. Again, instead

Title: Date:

of storing all spins at all M time slices, we only store the minimal information of where and in which direction the blue lines bend. Or in other words, where spin flip-flops occur.

From

$$(1-\Delta_\tau H)^M$$

we see, that the probability of H acting at a given time is proportional to $\frac{1}{M}$, and hence, the total number of spin flip-flops will stay finit under $M \to \infty$.