Transition path sampling algorithm for discrete many-body systems

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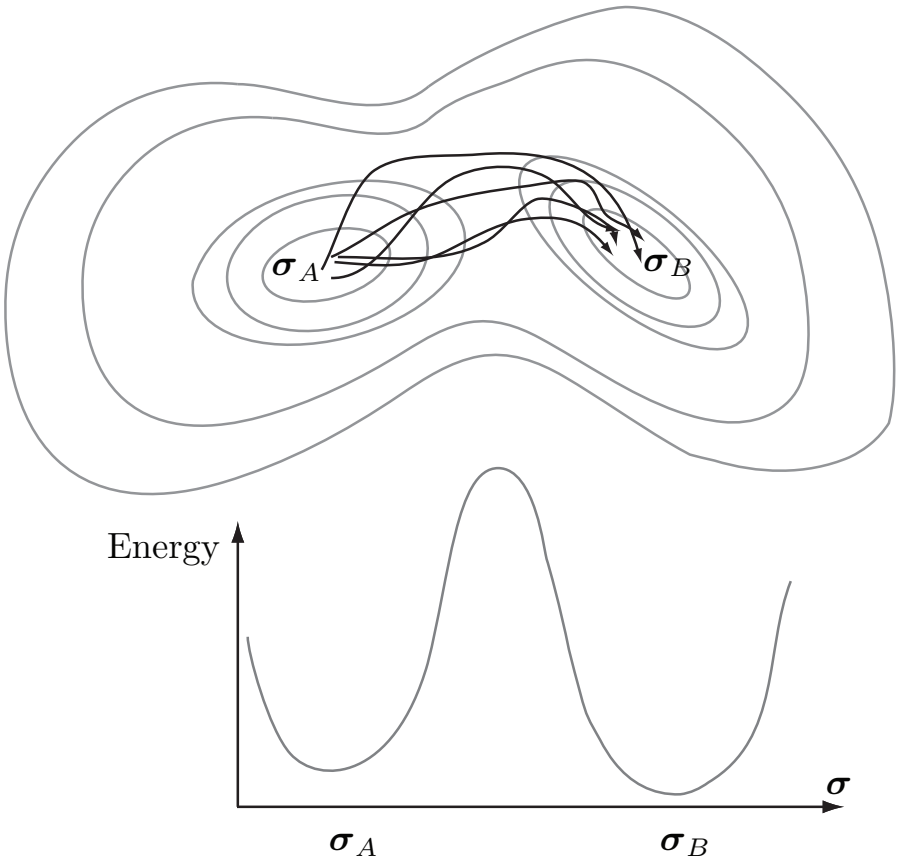
Outline

Metastable states and transition paths



Consider a stochastic system moving in a potential with at least two deep energy minima A and B:

- At low enough temperature, the system spends most of the time in state A or B
- Rare and quick transitions between the two states, with transition rate $k_{A\to B}$
- The transition can follow one of many possible transition paths, each path having a different weight
- The transition rate is determined by the **total** weight of the paths: both **energy** and **entropy** matter

For many-body systems, the problem of calculating $k_{A\to B}$ is extremely difficult.

The aim of this talk is to present an algorithm to compute $k_{A\to B}$ in generic stochastic systems with many discrete variables

A short review of the literature

The literature on this problem is, of course, immense. However, most algorithms are designed for continuous systems. Some of the approaches that have been used are:

- **Mapping on a one-dimensional problem**: identify one (or a set of) "reaction coordinate" that parametrizes well the dominant transition path. Use the standard Kramers theory for the reduced problem.

  - Difficult to take into account the effect of entropy (multiplicity of transition paths)
  - Sometimes the reaction coordinate cannot be identified
  - Necessarily approximate

  Example: the "string method" of E. Vanden-Eijnden et al. PRB 2002

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- **Shooting methods**: cut the barrier crossing problem in a series of smaller barrier crossings that can be sampled efficiently.
  - ◇ Construct a series of interfaces $\Sigma_0, \Sigma_1, \ldots, \Sigma_{\mathcal{N}}$ separating state A and B
  - ◇ "Shoot" a number of random walkers from state A
  - ◇ Count the fraction of walkers that reach the closest interface to A (Σ_0) in a given time
  - ◇ Select a set of such walkers, and "shoot" again starting from them.
  - ◇ Count how many of such walkers reach Σ_1 before going back to A, in a given time
  - ◇ Repeat starting from Σ_1, Σ_2, $\cdots$ until B is reached

  A very efficient method, but
  - requires some information on the transition path to construct the interfaces efficiently
  - a correct sampling might require a lot of interfaces

  Example: "Forward flux sampling", R.J.Allen, D.Frenkel et al. JCP 2006

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The literature on this problem is, of course, immense. However, most algorithms are designed for continuous systems. Some of the approaches that have been used are:

- **Current sampling**: consider a system of particles with continuous coordinates r_i, undergoing Langevin dynamics. The probability $P(\{r_i\}, t)$ satisfies the associated Fokker-Planck equation:

$$\frac{\partial P}{\partial t} = -H_{FP} P = -\sum_i \frac{\partial J_i}{\partial r_i} \qquad \text{with} \qquad J_i = \frac{1}{\gamma m_i}\left(k_B T \frac{\partial}{\partial r_i} + \frac{\partial V}{\partial r_i}\right)$$

  One can also write an equation for the current:

$$\frac{\partial J_i}{\partial t} = -H_{FP} J_i - \sum_j \frac{\partial^2 V}{\partial r_i \partial r_j} J_j$$

  If the system is initialized in state A, $P(\{r_i\}, t = 0) \sim P_A(\{r_i\})$, then on a short time scale the current will converge to a stationary current that describes the probability flow out of A. From this one can extract the transition rate and the transition paths.

  In practice, this is done by a Monte Carlo simulation of the equation for the current through a system of "walkers" that evolve with standard Langevin dynamics but are cloned or killed with a rate proportional to the last term in the current equation.

  - very efficient to identify transition paths
  - the calculation of the transition rate might suffer from the "sign problem"

  J.Kurchan et al. JSP 2006 & 2011, JCP 2011

A short review of the literature

The literature on this problem is, of course, immense. However, most algorithms are designed for continuous systems. Some of the approaches that have been used are:

- **Transition path sampling**:
  - ◇ Construct the probability $\mathcal{P}[x(t)]$ that describes the weight of a given path $x(t)$
  - ◇ Add the constraint that paths start in A and end in B to obtain $\mathcal{P}_{AB}[x(t)]$
  - ◇ Construct a Monte Carlo sampling of paths from $\mathcal{P}_{AB}[x(t)]$
  - ◇ Use this sampling to compute the transition probability as a function of time

  - A totally unbiased and exact method
  - Only requires the knowledge of the dynamics and the two states A and B
  - Gives very detailed information on the transition paths
  - A thermodynamic integration is needed to compute the transition rate
  - However, sampling might now be easy

  Example: C. Dellago, D. Chandler et al. JCP 1998

  So far, this method has been implemented only for continuous systems.
  The aim of this work is to present an implementation of this idea for discrete systems.

Outline

Definitions: two-state model

A two-state model is described by:

$$\partial_t \begin{pmatrix} p_A(t) \\ p_B(t) \end{pmatrix} = \begin{pmatrix} -k_{A\to B} & k_{B\to A} \\ k_{A\to B} & -k_{B\to A} \end{pmatrix} \cdot \begin{pmatrix} p_A(t) \\ p_B(t) \end{pmatrix}$$

The evolution operator has:
- one zero eigenvalue, corresponding to the steady-state solution
- one non-zero eigenvalue $\Delta = k_{A\to B} + k_{B\to A}$, the "energy gap"

The probability to be in B at time t given that the system was in A at time $t = 0$ is

$$Z_{AB}(t) = \frac{k_{A\to B}}{k_{A\to B}+k_{B\to A}} \left[1 - e^{-(k_{A\to B}+k_{B\to A})t}\right] .$$

The probability that the system has passed at least once by B after a time t, given that it started in A, is:

$$Z^*_{AB}(t) = 1 - e^{-k_{A\to B}t}.$$

The mean first passage time is:

$$\mathrm{MFPT}_{A\to B} = \int_0^\infty dt\, t\, \frac{dZ^*_{AB}}{dt} = \frac{1}{k_{A\to B}}.$$

At "short" times $k_{A\to B}t \ll 1$ we have $Z_{AB}(t) \approx Z^*_{AB}(t) \approx k_{A\to B}t$.

Our aim is to be able to compute $Z_{AB}(t)$ for a complex many-body system, and extract from it the rate $k_{A\to B}$.

Ising spin systems

The method works for general discrete stochastic systems, but let's consider an example for concreteness:

- A system of N spins $\boldsymbol{\sigma} = \{\sigma_i\}$, with Hamiltonian $H(\boldsymbol{\sigma}) = -\sum_{i=1}^{N} \tilde{h}_i \sigma_i - \sum_{i,j} J_{ij} \sigma_i \sigma_j$.
- Master equation for $p_t(\boldsymbol{\sigma})$: $\partial_t p_t(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} \left[w_{\boldsymbol{\sigma};\boldsymbol{\sigma}'} p_t(\boldsymbol{\sigma}') - w_{\boldsymbol{\sigma}';\boldsymbol{\sigma}} p_t(\boldsymbol{\sigma}) \right]$
- One spin flip at a time: $\boldsymbol{\sigma}_{\updownarrow i} = \{\boldsymbol{\sigma}_{\setminus i}, -\sigma_i\}$ is the configuration $\boldsymbol{\sigma}$ with spin i flipped.
- Energy variation: $\Delta E = H(\boldsymbol{\sigma}) - H(\boldsymbol{\sigma}_{\updownarrow i}) = -2 h_i \sigma_i$ with $h_i = \tilde{h}_i + \sum_{j(\neq i)} J_{ij} \sigma_j$.
- $w_{\boldsymbol{\sigma};\boldsymbol{\sigma}_{\updownarrow i}} = w(\Delta E) = w(-2 h_i \sigma_i)$
- Simple Glauber dynamics with detailed balance: $w(\Delta E) = e^{-\beta \Delta E} w(-\Delta E)$
  Here we choose: $w(\Delta E) = w_0 e^{-\beta \Delta E / 2}$ with $w_0 = 1$ (unit of time).
- Then $\partial_t p_t(\boldsymbol{\sigma}) = \sum_i \left[e^{\beta h_i \sigma_i} p_t(\boldsymbol{\sigma}_{\updownarrow i}) - e^{-\beta h_i \sigma_i} p_t(\boldsymbol{\sigma}) \right]$

The single spin flip assumption is important to simplify the method
The fact that the flip rate only depends on a few "neighbors" is also important

Instead, detailed balance is not needed for the method to work!
Any (local) choice of the single spin flip rate is allowed

An example: the Curie-Weiss model

As a last example, consider the mean field Curie-Weiss model: $J_{ij} = 1/(2N), \forall i,j$ and $\widetilde{h}_i = 0$. Then $H(\boldsymbol{\sigma}) = M(\boldsymbol{\sigma})^2/(2N)$ depends only on global magnetization.

The free energy at constant $M = mN$ is:

$$\beta f(m) \equiv \lim_{N\to\infty} \frac{\beta}{N} F(mN) = -\frac{\beta}{2} m^2 + \frac{1+m}{2} \log \frac{1+m}{2} + \frac{1-m}{2} \log \frac{1-m}{2}$$

and has two minima at $\pm m^*$ for $T < 1$ separated by a barrier in $m = 0$.

One can write a reduced Master equation:

$$\partial_t p_t(M) = w_+(M-2)p_t(M-2) + w_-(M+2)p_t(M+2) - [w_-(M) + w_+(M)]p_t(M)$$

which is a simple one dimensional random walk in M space and can be easily diagonalized numerically up to $N = 400$.

An explicit calculation of the mean first passage time gives for $N \to \infty$:

$$\mathrm{MFPT}_{A\to B} = \frac{\pi}{\beta} \sqrt{\frac{1}{[1-\beta(1-(m^*)^2)](\beta-1)}}\, e^{\beta N[f(0)-f(m^*)]}$$

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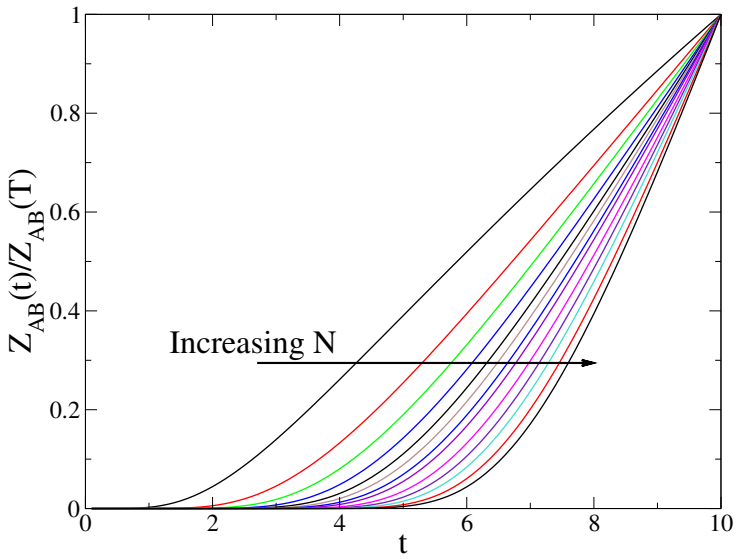
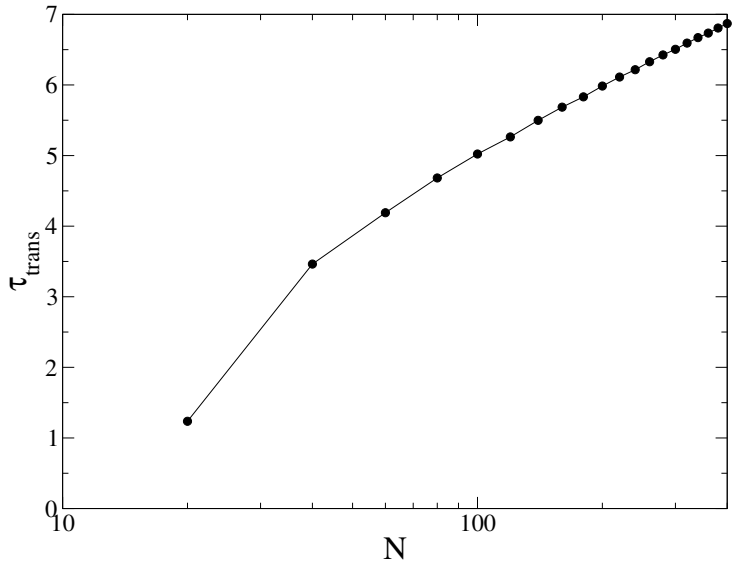
The function $Z_{AB}(t)$ can be computed numerically:

- At very short times, it is very small: a minimal time is required to perform the transition!
- At intermediate times $\tau_{\rm trans} \ll t \ll 1/k_{A\to B}$, it is linear: $Z_{AB}(t) \sim k_{A\to B} \times (t - \tau_{\rm trans})$
- The transient scales as $\tau_{\rm trans} \sim \log N$





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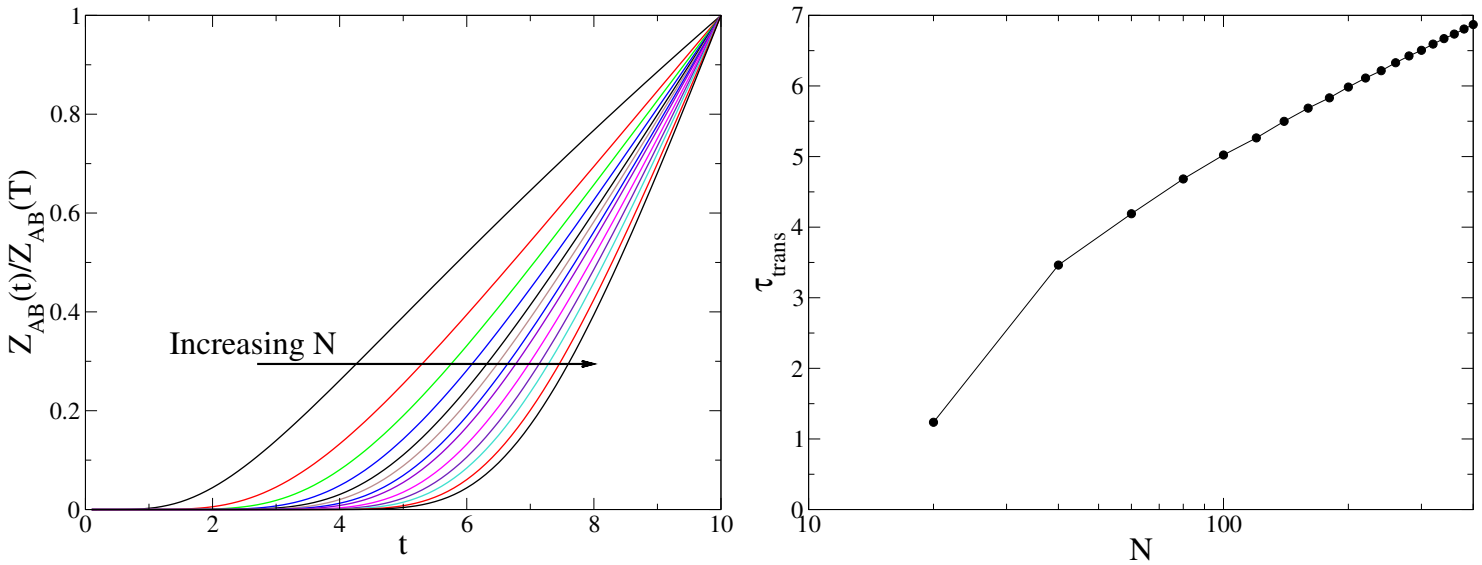


A simple argument: for large N, $\dot{m}(t) \sim -f'[m(t)] + \eta(t)/N$, where η is a white noise. Linearizing around $m = 0$, $\dot{m}(t) = |f''(0)|m(t) + \eta(t)/N$, then $\langle m(t)^2 \rangle \sim (\exp(2|f''(0)|t)/N^2$. Starting in $m = 0$ it takes a time $\sim \log N$ to leave the unstable point and go to either A or B. $\tau_{\rm trans}$ is dominated by the time it takes to make the transition from the top of the barrier
We have to measure $Z_{AB}(t)$ on a time scale $\tau_{\rm trans} \ll t \ll 1/k_{A\to B}$

Outline

The path action

Assign a probability $P_A(\boldsymbol{\sigma})$ to define the initial state and an indicator function $\chi_B(\boldsymbol{\sigma}) = 1$ if $\boldsymbol{\sigma} \in B$ and zero otherwise.
Probability for a given path $\boldsymbol{\sigma}(t)$ of the system of N spins that goes from $\boldsymbol{\sigma}_A \in A$ to $\boldsymbol{\sigma}_B \in B$, in discrete time over N_s steps, the total time being $\mathcal{T} = N_s dt$:

$$\mathbb{P}(\boldsymbol{\sigma}(t)) = P_A(\boldsymbol{\sigma}_A) \prod_{t=dt}^{N_s dt} \left[\left(1 - \sum_{\boldsymbol{\sigma}'} w_{\boldsymbol{\sigma}';\boldsymbol{\sigma}_t} dt \right) \delta_{\boldsymbol{\sigma}_t,\boldsymbol{\sigma}_{t+dt}} + w_{\boldsymbol{\sigma}_{t+dt};\boldsymbol{\sigma}_t} dt (1 - \delta_{\boldsymbol{\sigma}_t,\boldsymbol{\sigma}_{t+dt}}) \right] \chi_B(\boldsymbol{\sigma}_B)$$

Continuum limit for a path with M jumps labeled by $(t_m, \boldsymbol{\sigma}_m)$, $m = 0, \cdots, M$ and $\boldsymbol{\sigma}_m = \boldsymbol{\sigma}(t_m^+)$:

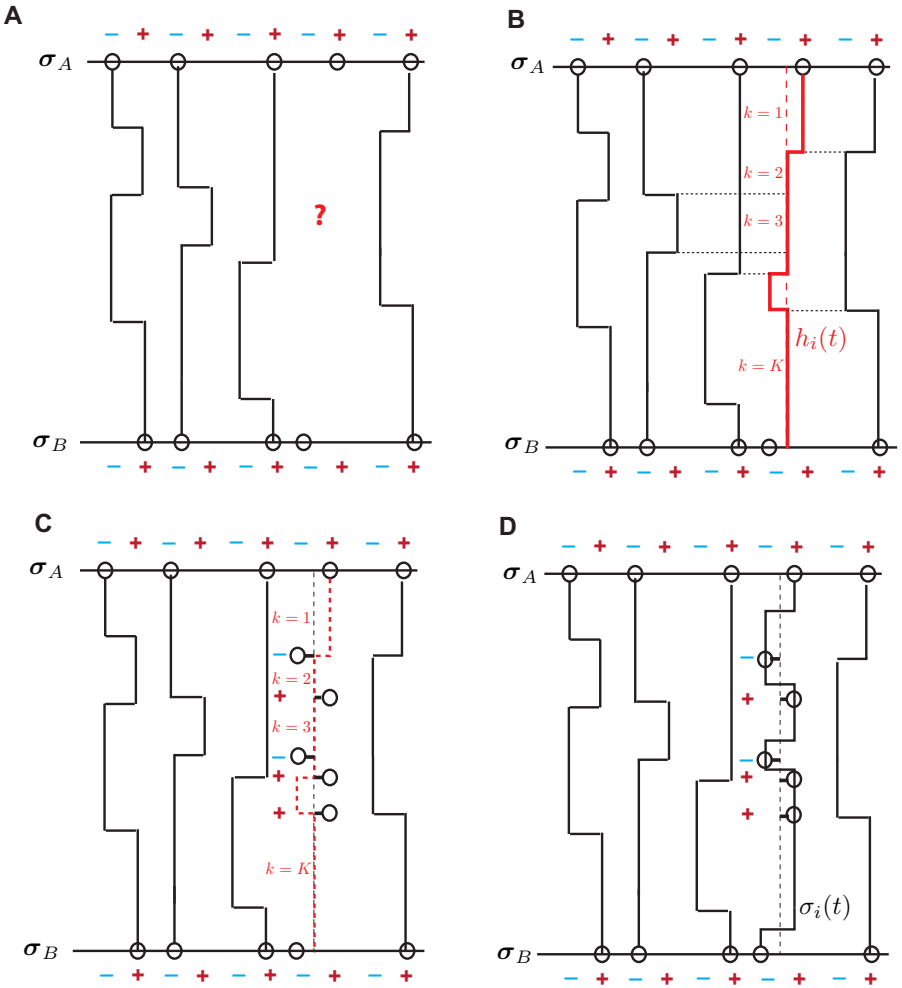
$$\mathrm{d}\mathbb{P}(\boldsymbol{\sigma}(t)) = P_A(\boldsymbol{\sigma}_A) \left\{ \prod_{m=1}^{M} \exp\left[-(t_m - t_{m-1}) \sum_{\boldsymbol{\sigma}} w_{\boldsymbol{\sigma};\boldsymbol{\sigma}^m} \right] \prod_{m=1}^{M-1} w_{\boldsymbol{\sigma}^{m+1},\boldsymbol{\sigma}^m} dt_m \right\} \chi_B(\boldsymbol{\sigma}_B)$$

Use the single-spin flip form of the rates and call i_m the spin that flips at time t_m and h_i^m the local field on spin i in configuration $\boldsymbol{\sigma}_m$:

$$\mathrm{d}\mathbb{P}(\boldsymbol{\sigma}(t)) = P_A(\boldsymbol{\sigma}_A) \left\{ \prod_{m=1}^{M} \exp\left[-(t_m - t_{m-1}) \sum_{i} w(2h_i^m \sigma_i^m) \right] \prod_{m=1}^{M-1} w(2h_{i_m}^m \sigma_{i_m}^m) dt_m \right\} \chi_B(\boldsymbol{\sigma}_B)$$

Heat bath sampling

Update one spin path at each step, according to the conditional probability $\mathrm{d}\mathbb{P}(\sigma_i(t)|\boldsymbol{\sigma}_{\setminus i}(t))$



A Delete one spin path i chosen at random

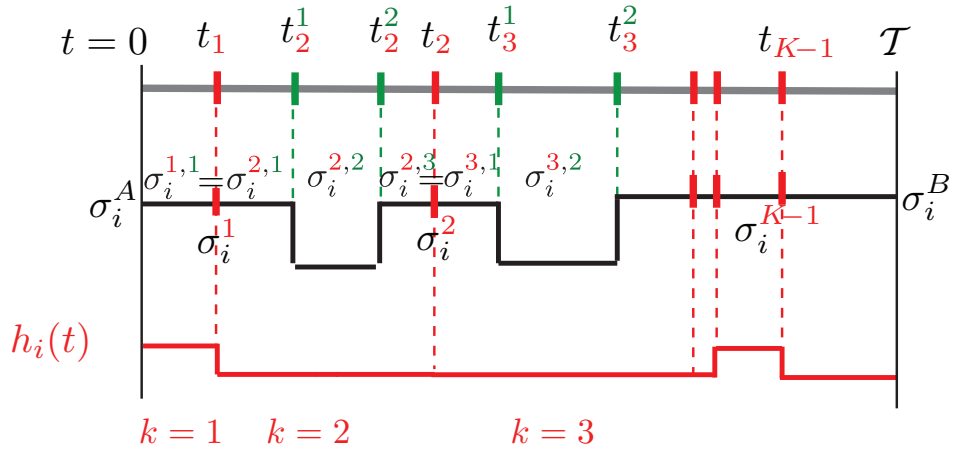
B The conditional probability for i depends on $h_i(t)$, the field of all other spins j. It also depends on the fields $\bar{h}_j$ that each of these spins feel in the absence of i. Divide the trajectory into K time intervals, denoted by k, on which these fields are constant.

C Draw a value of the spins at the boundaries of the K intervals.

D Draw the trajectory inside each of the intervals, with fixed boundaries.

F.Krzakala, A.Rosso, G.Semerjian, FZ, PRB 2008
F.Martinelli, M.Wouts, arXiv:1105.5970

The conditional probability

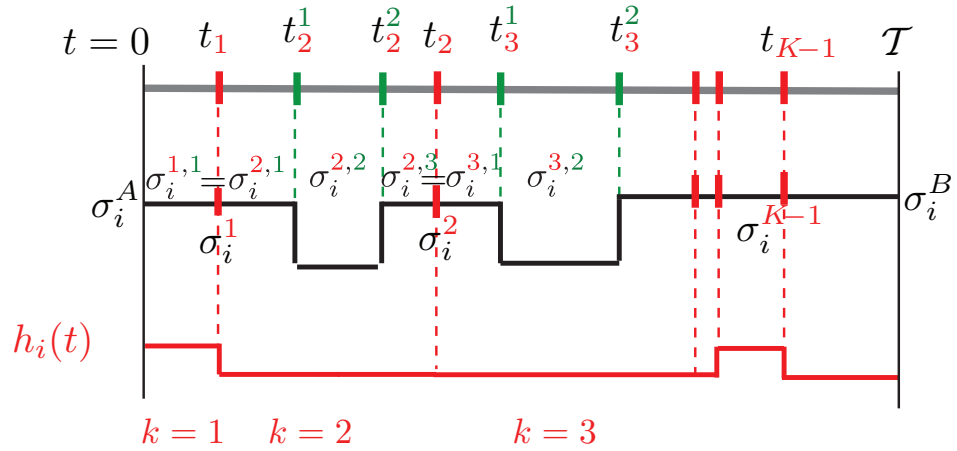


$$\mathrm{d}\mathbb{P}(\sigma_i(t)|\boldsymbol{\sigma}_{\setminus i}(t)) \propto P_A(\sigma_{A,i}|\boldsymbol{\sigma}_{A,\setminus i})$$

$$\times \prod_{k=1}^{K}\Big\{\prod_{\ell=1}^{l_k}\exp\big[-(t_k^\ell - t_k^{\ell-1})[w(2h_i^k\sigma_i^{k,\ell}) + \sum_{j\neq i} w(2\sigma_j^k(\bar{h}_j^k + J_{ji}\sigma_i^{k,\ell}))]\big]\prod_{\ell=1}^{l_k-1} w(2h_i^k\sigma_i^{k,\ell})dt_{k,\ell}\Big\}$$

$$\times \prod_{k=1}^{K-1} w[2\sigma_{j_k}^k(\bar{h}_{j_k}^k + J_{j_k i}\sigma_i^k)]\ \chi_B(\sigma_{B,i}|\boldsymbol{\sigma}_{B,\setminus i})$$

The conditional probability



Define the operator $\mathcal{L}_i^k$, a 2×2 matrix:

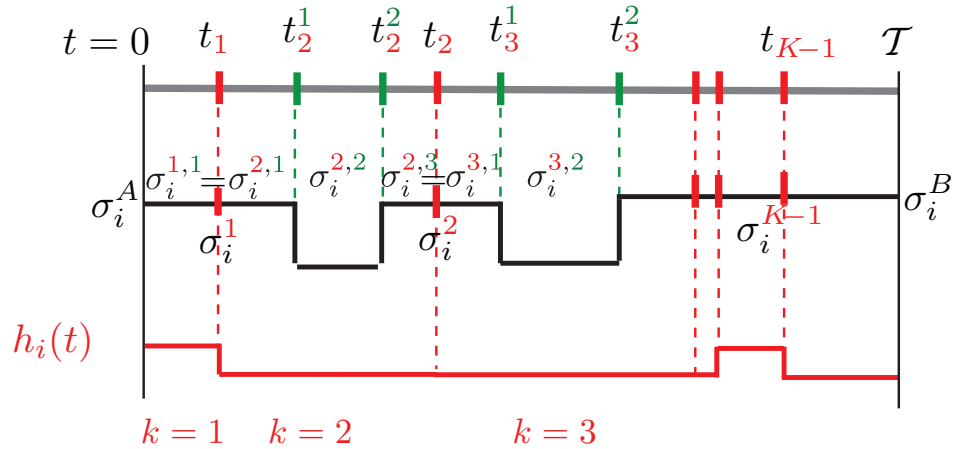
$$\langle\sigma'|\mathcal{L}_i^k|\sigma\rangle = \begin{cases} -w(2h_i^k\sigma) - \sum_{j\neq i} w(2\sigma_j^k(\bar{h}_j^k + J_{ji}\sigma)) & \text{for } \sigma' = \sigma \\ w(2h_i^k\sigma) & \text{for } \sigma' = -\sigma \end{cases}$$

then

$$\sum_{\text{paths}}^{\sigma_i^{k-1}\to\sigma_i^k} \left\{ \prod_{\ell=1}^{I_k} \exp\left[-(t_k^\ell - t_k^{\ell-1})[w(2h_i^k\sigma_i^{k,\ell}) + \sum_{j\neq i} w(2\sigma_j^k(\bar{h}_j^k + J_{ji}\sigma_i^{k,\ell}))]\right] \prod_{\ell=1}^{I_k} w(2h_i^k\sigma_i^{k,\ell})dt_{k,\ell} \right\}$$

$$= \langle\sigma_i^k|e^{(t_k-t_{k-1})\mathcal{L}_i^k)}|\sigma_i^{k-1}\rangle$$

The conditional probability



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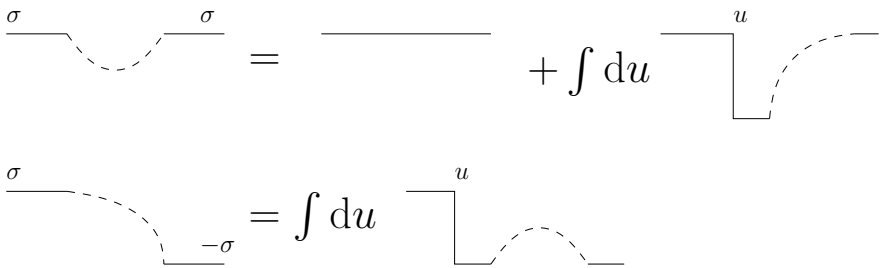
then

$$\mathbb{P}(\{\sigma_i^k\}|\boldsymbol{\sigma}_{\setminus i}(t)) \;\propto\; e^{h_i^A\sigma_i^A} \prod_{k=1}^{K} \langle\sigma_i^k|e^{(t_k-t_{k-1})\mathcal{L}_i^k)}|\sigma_i^{k-1}\rangle \left\{\prod_{k=1}^{K-1} w[2\sigma_{j_k}^k(\bar{h}_{j_k}^k + J_{j_k i}\sigma_i^k)]\right\} e^{h_i^B\sigma_i^B}$$

From this one dimensional chain representation we can draw easily the boundary values σ_i^k

Generate the trajectory inside each interval

Recursions between paths :



To generate a path of length λ, with $\sigma(0) = \sigma$, $\sigma(\lambda) = \sigma$

- with probability $\frac{e^{\lambda \langle \sigma | \mathcal{L} | \sigma \rangle}}{\langle \sigma | e^{\lambda \mathcal{L}} | \sigma \rangle}$, set $\sigma(t) = \sigma$ for $t \in [0, \lambda]$
- otherwise
  - draw $u \in [0, \lambda]$ with probability density proportional to $e^{u \langle \sigma | \mathcal{L} | \sigma \rangle} \langle -\sigma | e^{(\lambda - u)\mathcal{L}} | \sigma \rangle$
  - set $\sigma(t) = \sigma$ for $t \in [0, u]$
  - generate a path of length $\lambda - u$ with $\sigma(u) = -\sigma$, $\sigma(\lambda) = \sigma$

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- set $\sigma(t) = \sigma$ for $t \in [0, u]$
- generate a path of length $\lambda - u$ with $\sigma(u) = -\sigma$, $\sigma(\lambda) = -\sigma$

The calculation of the transition rate

Using this path Monte Carlo algorithm, we can compute averages over the measure $d\mathbb{P}(\boldsymbol{\sigma}(t)) = P_A[\boldsymbol{\sigma}(0)]\,\mathcal{P}[\boldsymbol{\sigma}(t)]\,\chi_B[\boldsymbol{\sigma}(\mathcal{T})]$ of all paths that go from A to B in time $\mathcal{T}$
How do we extract the rate from this?

The function $Z_{AB}(\mathcal{T})$ is the partition function associated with this measure:

$$Z_{AB}(\mathcal{T}) = \int d\mathbb{P}[\boldsymbol{\sigma}(t)] = \sum_{\boldsymbol{\sigma}(t)} P_A[\boldsymbol{\sigma}(0)]\,\mathcal{P}[\boldsymbol{\sigma}(t)]\,\chi_B[\boldsymbol{\sigma}(\mathcal{T})]$$

so we must use thermodynamic integration:

$$Z_{AB}(\mathcal{T},\mu(1)) = Z_{AB}(\mathcal{T},\mu(0))\; e^{\int_0^1 ds\, U_{AB}(\mathcal{T},\mu(s))\frac{d\mu}{ds}}$$

$$U_{AB}(\mathcal{T},\mu) = \frac{\partial \log Z_{AB}(\mathcal{T},\mu)}{\partial \mu}$$

where $\mu(s)$ is an interpolation path between $Z_{AB}(\mathcal{T},\mu(0))$, that is assumed to be easily calculable, and $Z_{AB}(\mathcal{T},\mu(1)) = Z_{AB}(\mathcal{T})$.

The choice of the optimal interpolation path depends on the system under investigation.

The calculation of the transition rate

In principle, we should perform a thermodynamic integration for each value of $\mathcal{T}$.

However, we can use this trick (*Dellago et al. JCP 1998*) for $\tau < \mathcal{T} \ll 1/k_{A\to B}$:

$$
\begin{aligned}
Z_{AB}(\tau) &= \sum_{\boldsymbol{\sigma}(t)} P_A[\boldsymbol{\sigma}(0)]\, \mathcal{P}[\boldsymbol{\sigma}(t)]\, \chi_B[\boldsymbol{\sigma}(\tau)] \\
&\approx \sum_{\boldsymbol{\sigma}(t)} P_A[\boldsymbol{\sigma}(0)]\, \mathcal{P}[\boldsymbol{\sigma}(t)]\, \chi_B[\boldsymbol{\sigma}(\tau)]\, \chi_B[\boldsymbol{\sigma}(\mathcal{T})] \\
&= Z_{AB}(\mathcal{T})\, \frac{\sum_{\boldsymbol{\sigma}(t)} P_A[\boldsymbol{\sigma}(0)]\, \mathcal{P}[\boldsymbol{\sigma}(t)]\, \chi_B[\boldsymbol{\sigma}(\tau)]\, \chi_B[\boldsymbol{\sigma}(\mathcal{T})]}{\sum_{\boldsymbol{\sigma}(t)} P_A[\boldsymbol{\sigma}(0)]\, \mathcal{P}[\boldsymbol{\sigma}(t)]\, \chi_B[\boldsymbol{\sigma}(\mathcal{T})]} \\
&= Z_{AB}(\mathcal{T})\, \langle \chi_B[\boldsymbol{\sigma}(\tau)] \rangle_{AB,\mathcal{T}}
\end{aligned}
$$

It allows to compute $Z_{AB}(\tau)$ using only one path MC simulation, once $Z_{AB}(\mathcal{T})$ is known. Sometimes it might be useful... but not always!

Outline

The 2d ferromagnetic Ising model

We consider the 2d Ising model on a square lattice with $J_{ij} = 1$ for nearest neighbors and zero otherwise, and $\widetilde{h}_i = 0$.

We work at $\beta = 1 > \beta_c = 0.4407$ where $m_{\rm eq} = 0.999275\ldots$.

We choose

$$P_A(\boldsymbol{\sigma}_A) = \frac{\exp\left(h_A M_A\right)}{\left(2\cosh h_A\right)^N} = \prod_{i=1}^{N} \frac{e^{h_A \sigma_i^A}}{2\cosh h_A}$$

$$\chi_B(\boldsymbol{\sigma}_B) = \exp\left[-h_B\left(M^* - M_B\right)\Theta\left(M^* - M_B\right)\right]$$

with $h_A = -3$ and $h_B = 1$, $M^* = [0.56N]$ so the system goes from the down (A) to the up (B) state.

Thermodynamic integration

The first idea was to start at $h_B = 0$: no constraint on the final state. Then $Z_{AB}(t) = 1$.
Then do the thermodynamic integration from $h_B = 0$ to the final h_B.

Does not work: the path system undergoes a first order transition along the integration path.
Around the transition it is very hard to equilibrate the system, due to histeresis.
Note that this was the proposal of *Dellago et al. JCP 1998*.

Thermodynamic integration

Then perform the integration starting from $\beta = 0$ and changing β up to $\beta = 1$.
At $\beta = 0$ spins are independent, then:

$$p_{up}(t) = \frac{1}{2}\left[1 + (2p_{up}(0) - 1)e^{-2t}\right] \text{ with } p_{up}(0) = e^{h_A}/(2\cosh(h_A)).$$

Probability that the system has magnetization M at time t:

$$P_t(M) = \binom{N}{\frac{N+M}{2}} p_{up}(t)^{(N+M)/2}(1 - p_{up}(t))^{(N-M)/2}$$

The partition function at $\beta = 0$ is:

$$Z_{AB}(\mathcal{T}, \beta = 0) = \sum_M P_{\mathcal{T}}(M)e^{-h_B(M^* - M)\theta(M^* - M)}$$

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Then perform the integration starting from $\beta = 0$ and changing β up to $\beta = 1$.
At $\beta = 0$ spins are independent, then:

$$p_{up}(t) = \frac{1}{2}\left[1 + (2p_{up}(0) - 1)e^{-2t}\right] \text{ with } p_{up}(0) = e^{h_A}/(2\cosh(h_A)).$$

Probability that the system has magnetization M at time t:

$$P_t(M) = \binom{N}{\frac{N+M}{2}} p_{up}(t)^{(N+M)/2}(1 - p_{up}(t))^{(N-M)/2}$$

The partition function at $\beta = 0$ is:

$$Z_{AB}(\mathcal{T}, \beta = 0) = \sum_M P_{\mathcal{T}}(M) e^{-h_B(M^* - M)\theta(M^* - M)}$$

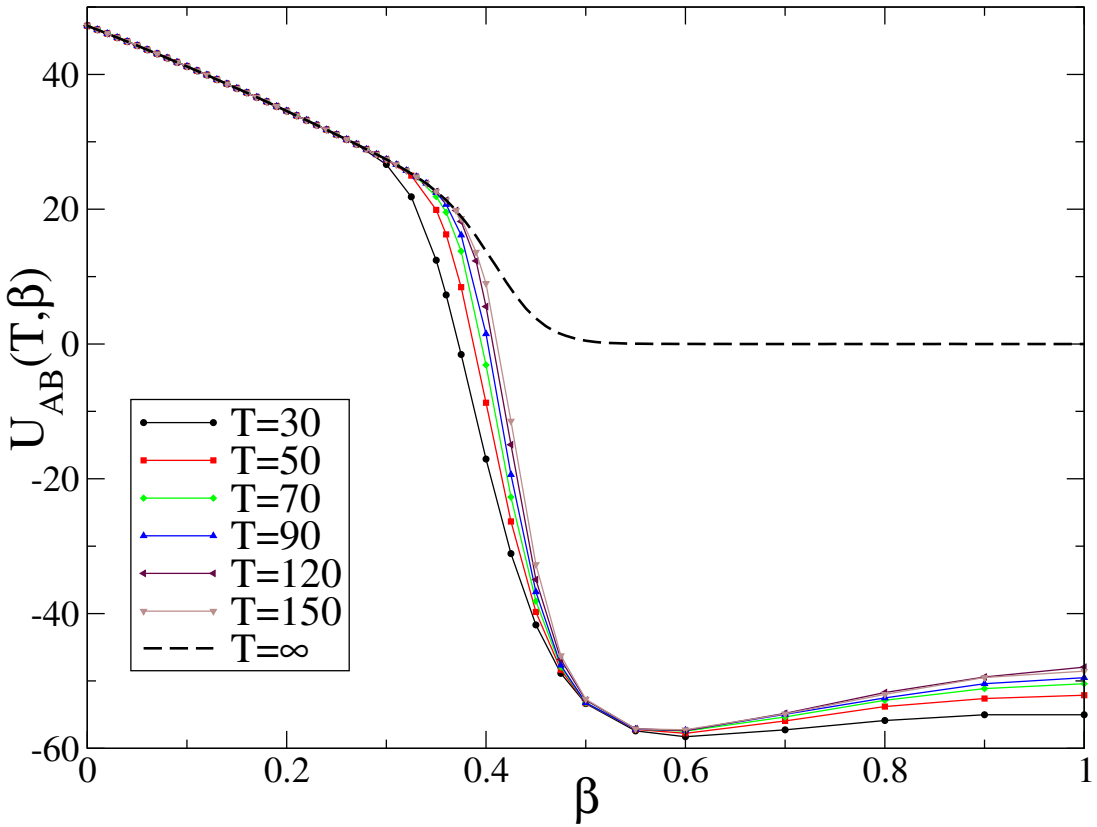
We have:

$$U_{AB}(\mathcal{T}, \beta) = \frac{\partial \log Z_{AB}(\mathcal{T}, \beta)}{\partial \beta} = \left\langle \sum_{k=1}^{L}(t_k - t_{k-1}) \sum_i w(2h_i^k \sigma_i^k) h_i^k \sigma_i^k - \sum_{k=1}^{L-1} h_{i_k}^k \sigma_{i_k}^k \right\rangle_{AB,\mathcal{T},\beta}$$

$$Z_{AB}(\mathcal{T}, \beta) = Z_{AB}(\mathcal{T}, \beta = 0)\ e^{\int_0^\beta d\beta'\ U_{AB}(\mathcal{T}, \beta')}$$

Thermodynamic integration

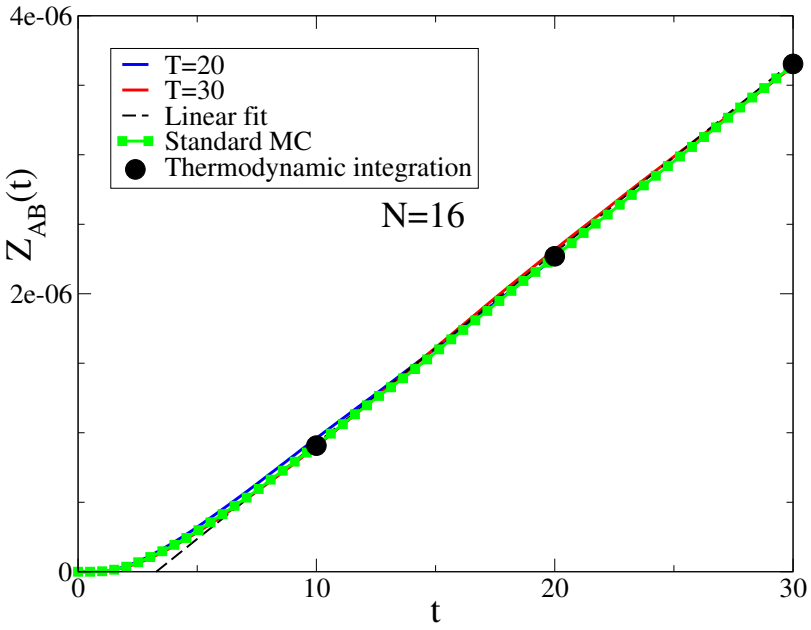
$$Z_{AB}(\mathcal{T},\beta) = Z_{AB}(\mathcal{T},\beta=0)\ e^{\int_0^\beta d\beta'\ U_{AB}(\mathcal{T},\beta')}$$

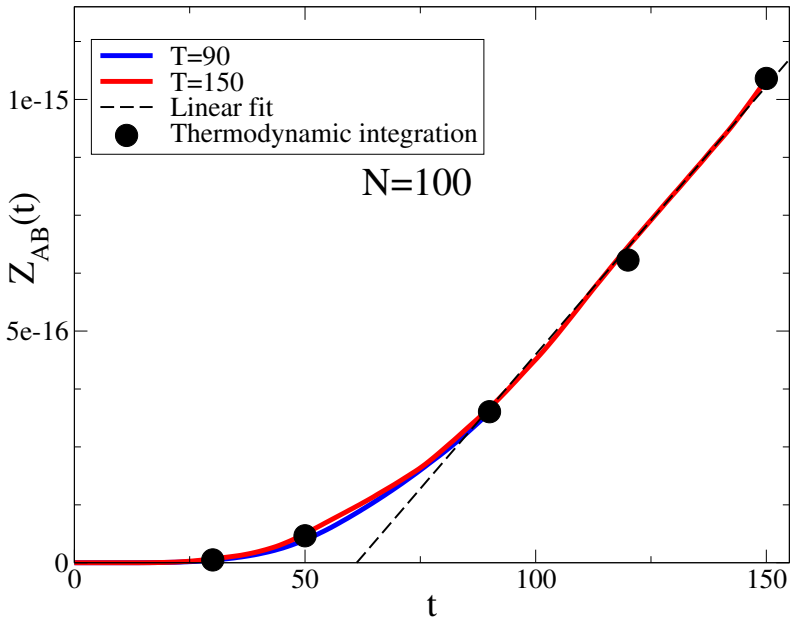


A single point for $N = 81$ and $\mathcal{T} = 150$ needed a CPU time $\sim$ 500 hours (one month).
We need 12 points for $Z_{AB}(\mathcal{T})$: 1 year of CPU time.

The limit $\mathcal{T} \to \infty$ can be calculated via a standard Monte Carlo: very useful for small β

The function $Z_{AB}(t)$



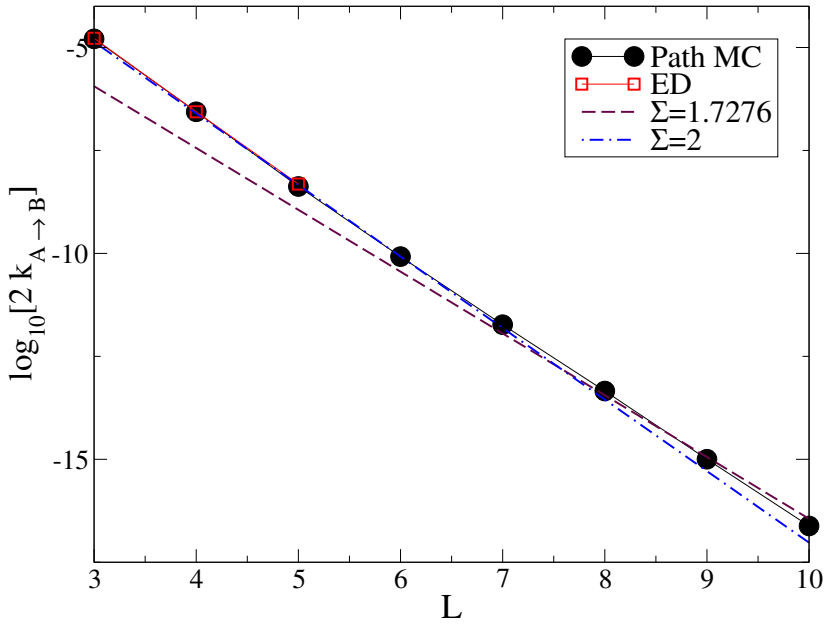


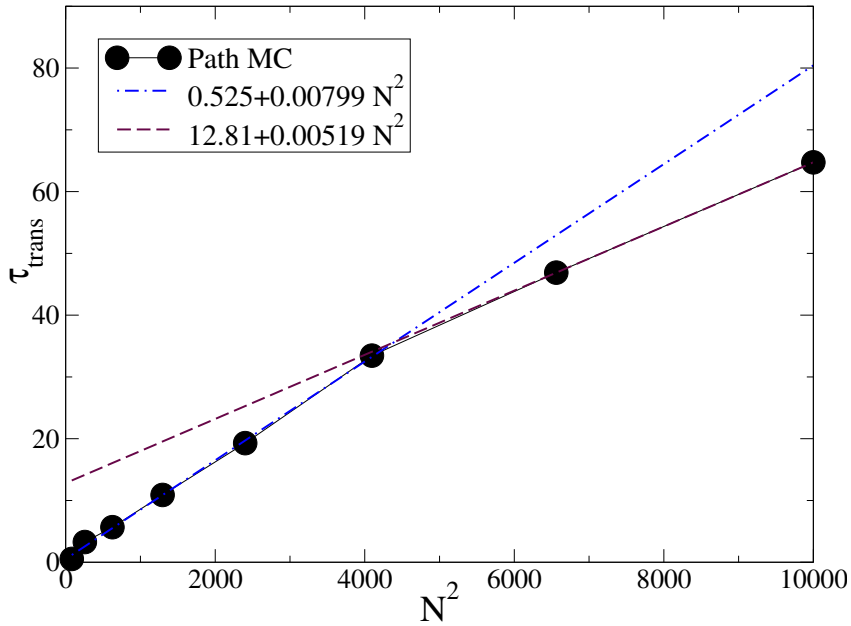
Black dots: thermodynamic integration
Red and blue lines: results from *Dellago et al.* trick

Green points are obtained via standard Monte Carlo to check the accuracy of the method

For large t: $Z_{AB}(t) = k_{A\to B} \times (t - \tau_{\rm trans})$

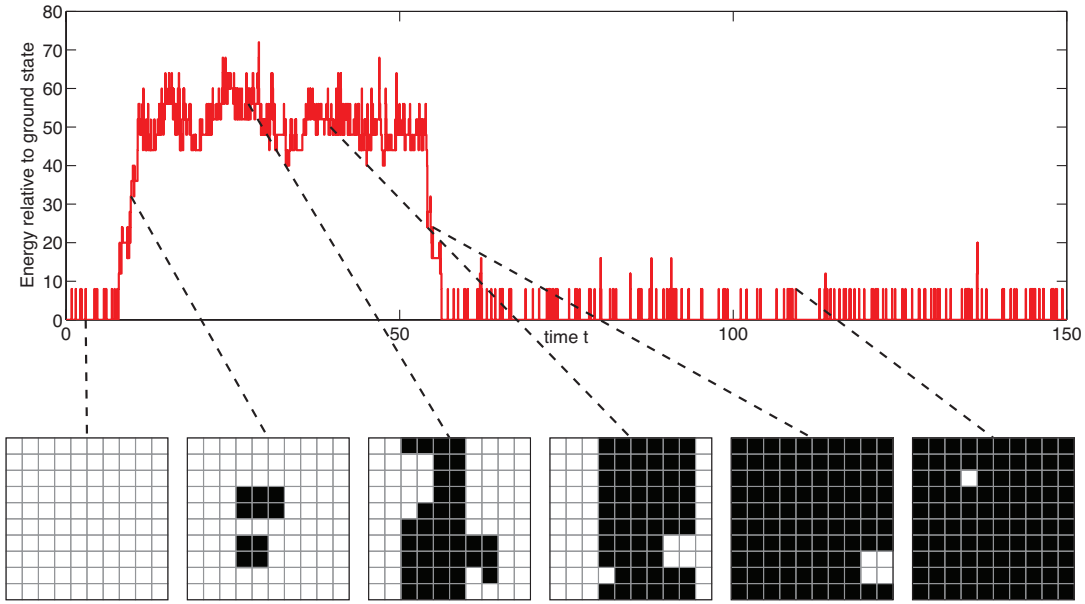
Transition rate and transient time





- Transition rate $k_{A\to B} \sim \exp(-2\Sigma L)$
- Transient time $\tau_{\mathrm{trans}} \propto N^2$
- A change in prefactors around $L = 8$

A typical transition path

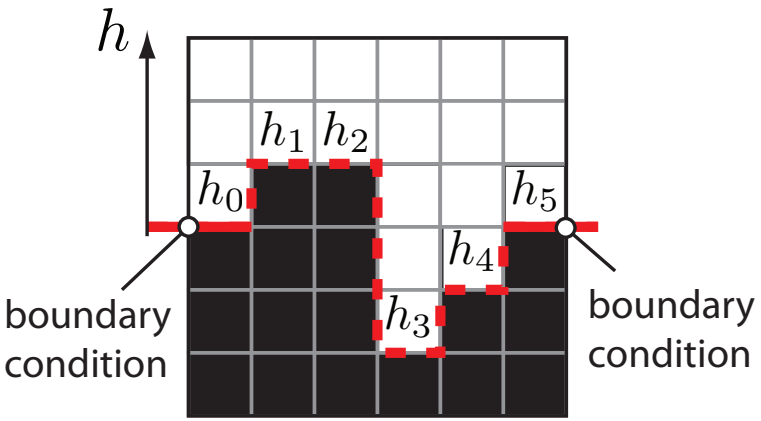


- The transition state is a stripe of $+$ spins in the $-$ background
- Explains the exponential factor $\exp(-2\Sigma L)$ (*F.Martinelli, JSP 1994*)
- Once the stripe is formed, its growth is an unbiased random walk:
  - ◇ One move of the interface requires diffusion of a kink on a length L: takes a time $\sim N$
  - ◇ Moving the interface by L requires N such steps: $N \times N = N^2$

A simple model for the interface

Assume that the height of the interface is a single valued function h_i

E. Muller-Hartmann and J. Zittarz, Z. Phys. B 1977



$H_I = 2L + 2\sum_{i=1}^{L+1} |h_i - h_{i-1}|$ with $h_0 = h_{L+1} = 0$.

$$Z_I = e^{-2\beta L} \sum_{h_1 \cdots h_L} e^{-2\beta \sum_{i=1}^{L+1} |h_i - h_{i-1}|} = e^{-2\beta L} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left(\frac{e^{4\beta} - 1}{e^{4\beta} + 1 - 2e^{2\beta} \cos(k)} \right)^{L+1} \equiv e^{-L\Sigma}$$

Asymptotic results:

- For small L and large β, $h_i = 0$ dominates: $\Sigma = 2\beta$
- For $L \to \infty$, via a saddle point at $k = 0$: $\Sigma = 2\beta + \log(\tanh(\beta))$
  (this is the correct result obtained by Onsager!)
- The crossover length increases with β and diverges for $\beta \to \infty$
- At $\beta = 1$, the crossover is roughly around $L \sim 10$, consistent with our data

Outline

Conclusions

- A new algorithm to perform constrained path sampling of discrete many-body systems
- Based on the Transition Path Sampling strategy of Dellago, Chandler et al. and on the Quantum Monte Carlo heat bath algorithm of Krzakala et al.
- Works for generic stochastic processes with local interactions; detailed balance is not necessary
- Combined with thermodynamic integration, can be used to compute transition rates
- Gives detailed information on:
  - ◇ the typical transition paths
  - ◇ the time-dependent transition probability $Z_{AB}(t)$
  - ◇ the transition rate $k_{A\to B}$
  - ◇ the transient time $\tau_{\rm trans}$, related to the barrier crossing time
- An application to the 2d Ising ferromagnetic model gives consistent results