VI Quantum Monte-Carlo

Until now we always aimed for representations of the many-body wave functions.

However, if we are only interested in observables, we don't necessarily need representations of $|\Psi\rangle$.

Instead, we can rewrite expectation values as:

$$\langle \hat{O} \rangle = \mathrm{Tr}\{\hat{\rho}\,\hat{O}\}$$

$$= \sum_{\sigma_1 \dots \sigma_L} \sum_{\sigma_1' \dots \sigma_L'} \langle \sigma_1 \dots \sigma_L | \hat{\rho} | \sigma_1' \dots \sigma_L' \rangle \langle \sigma_1' \dots \sigma_L' | \hat{O} | \sigma_1 \dots \sigma_L \rangle$$

Let us assume $\hat{O}$ is diagonal in the chosen basis:

$$\langle \sigma_1' \dots \sigma_L' | \hat{O} | \sigma_1 \dots \sigma_L \rangle = \delta_{\sigma_1' \sigma_1} \cdots \delta_{\sigma_L' \sigma_L} \; O(\sigma_1 \dots \sigma_L)$$

$$\Rightarrow \langle \hat{O} \rangle = \sum_{\sigma_1 \dots \sigma_L} p(\sigma_1 \dots \sigma_L) \; O(\sigma_1 \dots \sigma_L)$$

where $p(\sigma_1 \dots \sigma_L)$ is the prob. to find the configuration $(\sigma_1 \dots \sigma_L)$.

Assume now, that we where able to create samples $\underline{\sigma} \in \mathcal{D}^L$ where $\mathcal{D}$ is the set of configurations per degree of freedom σ_j, distributed according to $p(\underline{\sigma})$. Let us draw N samples $\{\underline{\sigma}^n\}_{n=1\dots N}$ then:

$$\langle \hat{O} \rangle \approx \frac{1}{N} \sum_{n=1}^{N} O(\underline{\sigma}^n) \equiv \bar{O}_N$$

is an approx. to $\langle \hat{O}_N \rangle$ in the state $\hat{\rho}$.

Now perform $M \in \mathbb{N}$ repititions of the estimation:

$$\langle \bar{O}_N \rangle = \frac{1}{M} \sum_{m=1}^{M} \bar{O}_{N,m}$$

which has the estimated error:

$$\langle \delta \bar{O}_N \rangle = \sqrt{\mathrm{Var}[N, \hat{O}]}$$

$$= \sqrt{\frac{1}{M} \sum_{m=1}^{M} \left(\bar{O}_{N,m} - \langle \bar{O}_N \rangle \right)^2}$$

Note that the repeated sampling is required to estimate $\langle \delta \bar{O}_N \rangle$, since a direct estimation of $(\langle \bar{O} - \langle \hat{O} \rangle \rangle)^2$ would require knowledge of $\langle \hat{O} \rangle$.

Now we have:

$$\frac{1}{M}\sum_{m=1}^{M}\left(\bar{O}_{N,m}-\langle\bar{O}_N\rangle\right)^2=\frac{1}{N^2}\sum_{n,n'=1}^{N}\frac{1}{M}\sum_{m=1}^{M}\left(O_m(\underline{\sigma}_n)-\langle\bar{O}_N\rangle\right)\left(O_m(\underline{\sigma}_{n'})-\langle\bar{O}_N\rangle\right)$$

We now demand that the samples $\underline{\sigma}_n$ are drawn independently. Then we have in the limit $M\to\infty$:

$$\mathrm{Var}[N,\hat{O}]\overset{M\to\infty}{=}\frac{1}{N^2}\sum_{n=1}^{N}\int d\underline{\sigma}_n\left(O(\underline{\sigma}_n)p(\underline{\sigma}_n)-\langle\bar{O}_N\rangle\right)^2$$

$$+\frac{1}{N^2}\sum_{n\neq n'}^{N}\int d\underline{\sigma}_n\, d\underline{\sigma}_{n'}\left(O(\underline{\sigma}_n)p(\underline{\sigma}_n)-\langle\bar{O}_N\rangle\right)\left(O(\underline{\sigma}_{n'})p(\underline{\sigma}_{n'})-\langle\bar{O}_N\rangle\right)$$

$$=\langle(\hat{O}-\langle\hat{O}\rangle)^2\rangle/N$$

$$+\frac{1}{N^2}\sum_{n=1}^{N}\Big[\underbrace{\int d\underline{\sigma}_n\left(O(\underline{\sigma}_n)p(\underline{\sigma}_n)-\langle\bar{O}_N\rangle\right)}_{0}\Big]^2$$

$$=\mathrm{Var}(\hat{O})/N$$

$$\Rightarrow\langle\delta\bar{O}_N\rangle=\bar{O}\pm\sqrt{\frac{\mathrm{Var}(\hat{O})}{N}}$$

The error scales as $\frac{1}{\sqrt{N}}$!

Remarks:

(i) For this estimation we need independent samples: $p(\underline{\sigma}_i,\underline{\sigma}_j)=p(\underline{\sigma}_i)\,p(\underline{\sigma}_j)$

(ii) For independent samples, we can use central limit theorem, i.e. the errors $\bar{O} - \langle \bar{O}_N \rangle$ is normal distributed for M large. Then 1σ ($\approx 68\%$) of all samples $\langle \bar{O}_N \rangle$ are in the interval $\pm \langle \delta \bar{O}_N \rangle$

(iii) Evaluating $O(\underline{\sigma})$ typically only scales $\sim \mathcal{O}(L^\alpha)$ with α small integer!

Now the question remains:

How to generate independent samples distributed according to $p(\underline{\sigma})$?

Idea: Choose $\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z_\beta}$ with $\beta \geq 0$ the inverse temperature $\beta = \frac{1}{T}$ ($k_B \equiv 1$).

(a) Given a sample $\underline{\sigma}$, we can in most practical situations evaluate $H(\underline{\sigma})$ very cheaply.

(b) From a sample $\underline{\sigma}$, we can create another sample $\underline{\sigma}'$ by noting that the ratio $\frac{p(\underline{\sigma}')}{p(\underline{\sigma})}$

is given by $e^{-\beta H(\underline{\sigma}')}/e^{-\beta H(\underline{\sigma})}$.

(c) Imagine a system is in configuration $\underline{\sigma}$. The prob. is $p(\underline{\sigma})$ & the prob. it transitions into $\underline{\sigma}'$ is given by:

$$p(\underline{\sigma}') \propto \frac{p(\underline{\sigma}')}{p(\underline{\sigma})} p(\underline{\sigma}) \equiv p(\underline{\sigma} \to \underline{\sigma}') \, p(\underline{\sigma})$$

Since $p(\underline{\sigma} \to \underline{\sigma}')$ only requires evaluation of $H(\underline{\sigma}')$ & $H(\underline{\sigma})$, it should be simple to sample trajectories:

$$\underline{\sigma}_1 \to \underline{\sigma}_2 \to \underline{\sigma}_3 \to \cdots$$

Now all we need to ensure is:

- $\underline{\sigma}_{n > n_0}$ created this way are independent for some n_0
- $\underline{\sigma}_{n > n_0}$ are drawn according to the desired $p(\underline{\sigma}) = e^{-\beta H(\underline{\sigma})}/Z_\beta$

VI.1 Markov chain & Metropolis algorithm

Let $\sigma_n, \sigma_m \in \mathcal{D}^L$ be configurations & W_{nm} the prob. that the transition $\sigma_n \to \sigma_m$ occurs.

P_{mn} describes a Markov process, if:

(i) $W_{nm} \geq 0$ for all n, m

(ii) $\sum_m W_{nm} = 1$

Important: Prob. to transition from $\sigma_n \to \sigma_m$ must <u>only</u> depend on σ_n!

We need a certain type of Markov process:

(i) <u>all</u> configurations must be reachable from any other configuration: $W^n_{nm} > 0$, $n \in \mathbb{N}$

(ii) We want to map probability distributions to probability distributions under W_{nm}:

$$p(\sigma_m) = \sum_n W_{nm}\, p(\sigma_n)$$

Because $1 = \sum_n p(\underline{\sigma}_m) = \sum_n \underbrace{\left(\sum_m W_{nm}\right)}_{1} p(\underline{\sigma}_n)$

$$= \sum_n p(\underline{\sigma}_n) = \underline{1}$$

There is an important consequence of these restrictions:

Denote by $\underline{P} = (p(\underline{\sigma}_1)\ p(\underline{\sigma}_2)\ \cdots\ p(\underline{\sigma}_D))$ where $D = |\Omega|^L$ the number of all possible configurations. Then W_{nm} can be treated as a matrix & :

$$\underline{\underline{W}}^T \cdot \underline{P} = \underline{P}$$

from condition (ii). Thus, the stationary distribution of $\underline{\underline{W}}^T$ is just the desired probability distribution $p(\underline{\sigma})$!

It can be reached starting from any configuration & successive evolution under

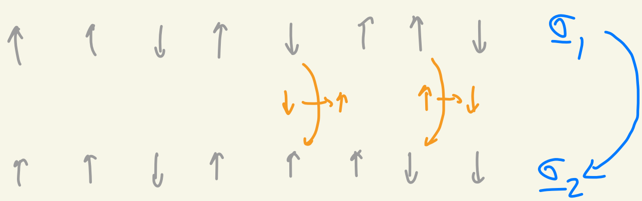
$\underline{\underline{W}}^T$ generates $p(\underline{\sigma})$ (Power-method !!!).

Now we can easily formalize our initial idea:

If W_{nm} satisfies $p(\underline{\sigma}_n)\, W_{nm} = p(\underline{\sigma}_m)\, W_{mn}$, then $\underline{P}(\underline{\sigma})$ is the stationary distribution of W_{nm}.

This implies: $$\frac{p(\underline{\sigma}_n)}{p(\underline{\sigma}_m)} = \frac{W_{mn}}{W_{nm}}$$ (compare this to $p(\underline{\sigma}_n \to \underline{\sigma}_m)$)

Sketch for $\mathcal{D} = \{\uparrow, \downarrow\}$:



with prob. $\min\left(1, \frac{P(\underline{\sigma}_2)}{P(\underline{\sigma}_1)}\right)$

Simplest realization: Flip only one spin "i"

$$W^{[i]}_{nm} = \left(\prod_{j \neq i} \delta_{\sigma_{j,n}, \sigma_{j,m}}\right) w_i(\sigma_i \to \bar{\sigma}_i)$$

We can show easily that varying i from $1, \dots, L$, this is a Markow process with stationary distribution $P(\sigma_{1,n}, \dots, \sigma_{L,n})$. Then we obtain

$$\frac{w_i(\uparrow \to \downarrow)}{w_i(\downarrow \to \uparrow)} = \frac{P(\sigma_{1,n}, \dots, \sigma_{i,n} = \downarrow, \dots, \sigma_{L,n})}{P(\sigma_{1,n}, \dots, \sigma_{i,n} = \uparrow, \dots, \sigma_{L,n})}$$

VI.1 Local Monte-Carlo algorithms

Markov processes with a desired stationary distribution $p(\underline{\sigma})$ can be constructed by updating only one degree of freedom at a time. Consider spin-$\frac{1}{2}$ degrees of freedom on a d-dimensional cubic lattice with L spins along each direction: $V = L^d$ spins.

The transition probabilities should satisfy detailed balance:

$$p(\underline{\sigma}_n) W_{nm} = p(\underline{\sigma}_m) W_{mn}$$

$$\Rightarrow \sum_m p(\underline{\sigma}_n) W_{nm} = \sum_m p(\underline{\sigma}_m) W_{mn}$$

$$= p(\underline{\sigma}_n) \sum_m W_{nm} = p(\underline{\sigma}_n)$$

i.e. detailed balance for W_{nm} w.r.t. $p(\underline{\sigma}_n)$ implies that $p(\underline{\sigma})$ is the stationary distr.!

We decompose W_{nm} into local updates:

$$W(\underline{\sigma}_n \to \underline{\sigma}_m) = \prod_{j \in V} w_{nm}^{[j]}$$

where j labels the V sites on the hypercube.

Here, $w_{nm}^{[j]}$ means keep all spins fixed except for site j:

$$w_{nm}^{[j]} = \left(\prod_{i \neq j} \delta_{\sigma_{i,n}\, \sigma_{i,m}} \right) w(\sigma_{j,n} \to \sigma_{j,m}) .$$

If $w_{nm}^{[j]}$ satisfy detailed balance:

$$p(\sigma_{1,n}, \dots, \sigma_{j,n}, \dots \sigma_{V,n})\, w_{nm}^{[j]} = p(\sigma_{1,n}, \dots, \sigma_{j,m}, \dots, \sigma_{V,n})\, w_{mn}^{[j]}$$

& $\omega^{[j]}_{nm}$ is Markov-process: $\sum_{\sigma_{jm}} \omega^{[j]}_{nm} = 1$, then

for V subsequent updates $\sigma_{1n} \to \sigma_{1m}$, $\sigma_{2n} \to \sigma_{2m}$, ...

we get:

site 1:

$$p(\sigma_{1m}, \ldots, \sigma_{Vm})\, \omega^{[1]}_{mn} = p(\sigma_{1n}, \sigma_{2m}, \ldots, \sigma_{Vm})\, \omega^{[1]}_{nm}$$

$$\Rightarrow p(\sigma_{1m}, \ldots, \sigma_{Vm}) \frac{\omega^{[1]}_{mn}}{\omega^{[1]}_{nm}} = p(\sigma_{1n}, \sigma_{2m}, \ldots, \sigma_{Vm})$$

site 2:

$$p(\sigma_{1m}, \ldots, \sigma_{Vm})\, \omega^{[2]}_{mn} \frac{\omega^{[1]}_{mn}}{\omega^{[1]}_{nm}} = p(\sigma_{1n}, \sigma_{2n}, \sigma_{3m}, \ldots, \sigma_{Vm})\, \omega^{[2]}_{nm}$$

$\vdots$

site V:

$$p(\sigma_{1m}, \ldots, \sigma_{Vm}) \frac{\prod_{j=1}^{V} \omega^{[j]}_{mn}}{\prod_{j=1}^{V} \omega^{[j]}_{nm}} = p(\sigma_{1n}, \ldots, \sigma_{Vn})$$

$$\Rightarrow \sum_{\sigma_{1m} \ldots \sigma_{Vm}} p(\sigma_{1m}, \ldots, \sigma_{Vm}) \prod_{j=1}^{V} \omega^{[j]}_{mn} = p(\sigma_{1n}, \ldots, \sigma_{Vn}) \sum_{\sigma_{1m} \ldots \sigma_{Vm}} \prod_{j=1}^{V} \omega^{[j]}_{nm}$$

using $\sum_{\sigma_{jm}} \omega^{[j]}_{nm}$, i.e. $\omega^{[j]}_{nm}$ is Markov: $= p(\sigma_{1n}, \ldots, \sigma_{Vn})$

$\Rightarrow$ stationary distribution is again $p(\underline{\sigma})$.

Question:

How to choose now $\omega^{[j]}_{nm}$?

Easy, only have to fulfill Markov-conditions & detailed balance!

Note: The state space per site is small!

For spin-$\frac{1}{2}$: $n \in \{\uparrow, \downarrow\}$

Heat-bath update

$\omega^{[j]}_{nm}$ is chosen such that final state m is independent on initial state n:

$$\left.\begin{aligned} \omega^{[j]}_{\uparrow\uparrow} &= \omega^{[j]}_{\downarrow\uparrow} \\ \omega^{[j]}_{\uparrow\downarrow} &= \omega^{[j]}_{\downarrow\downarrow} \end{aligned}\right\} \quad \omega^{[j]}_{nm} = \frac{e^{-\beta H(\sigma_{1m}, \ldots, \sigma_{jm}, \ldots, \sigma_{Vn})}}{\sum_{\sigma_{jm}=\uparrow,\downarrow} e^{-\beta H(\sigma_{1n}, \ldots, \sigma_{jm}, \ldots, \sigma_{Vn})}}$$

Clearly we have detailed balance:

$$\frac{p(\sigma_{1n},\dots,\sigma_{jn},\dots,\sigma_{Vn})}{p(\sigma_{1m},\dots,\sigma_{jm},\dots,\sigma_{Vn})} = \frac{e^{-\beta H(\sigma_{1n},\dots,\sigma_{jn},\dots,\sigma_{Vn})}}{e^{-\beta H(\sigma_{1n},\dots,\sigma_{jm},\dots,\sigma_{Vn})}} = \frac{w^{[j]}_{mn}}{w^{[j]}_{nm}}$$

& Markov-process: $\sum_{\sigma_{jn}} w^{[j]}_{nm} = 1$.

Metropolis update

Heat bath has a problem: It chooses new config. independent on previous config. What if σ_n is a very unlikely config? Heat bath does not care when determining $w^{[j]}_{nm}$. This can be cured taking prob. of σ_n into account:

$$w^{[j]}_{\sigma_{jn}\sigma_{jm}} = \min\left(1, \frac{p(\sigma_{1n},\dots,\sigma_{jm},\dots,\sigma_{Vn})}{p(\sigma_{1n},\dots,\sigma_{jn},\dots,\sigma_{Vn})}\right)$$

If $p(\sigma_{1n},\dots,\sigma_{jn},\dots,\sigma_{Vn}) < p(\sigma_{1n},\dots,\sigma_{jm},\dots,\sigma_{Vn})$

then the new config is choosen for sure!

For spin-$\frac{1}{2}$:

$$\omega^{[j]}_{\sigma_n,\bar{\sigma}_n} = \min\left(1, \frac{e^{-\beta H(\sigma_{1n},\dots,\bar{\sigma}_{jn},\dots,\sigma_{Vn})}}{e^{-\beta H(\sigma_{1n},\dots,\sigma_{jn},\dots,\sigma_{Vn})}}\right)$$

with $\bar{\sigma} = \begin{cases} \downarrow & \text{if } \sigma = \uparrow \\ \uparrow & \text{if } \sigma = \downarrow \end{cases}$

Prove detailed balance & Markov-properties as exercise :-).

VI.2 Autocorrelation time

We saw that we need statistically independent samples $\underline{\sigma}_n$ to properly estimate the std.-dev.

For local updates $(\sigma_{1n},\dots,\sigma_{jn},\dots,\sigma_{Vn}) \to (\sigma_{1n},\dots,\bar{\sigma}_{jn},\dots\sigma_{Vn})$ this is surely not the case.

So how many Markov-steps do we have to take until $\underline{\sigma}_n$ & $\underline{\sigma}_m$ are independent?

Consider again the variance of an observable $\hat{O}$ for N samples $\{\underline{\sigma}_n\}$ in M independent realizations:

$$\mathrm{Var}[N, \hat{O}] = \left\langle \left(\frac{1}{N} \sum_{n=1}^{N} \left(O[\underline{\sigma}_n] - \langle \bar{O}_N \rangle \right) \right)^2 \right\rangle$$

where $\langle \cdot \rangle$ refers to the average over the M realizations. We now define the autocorrelation

$$\Gamma_{\hat{O}}(n-m) = \left\langle \left(O[\underline{\sigma}_n] - \langle \bar{O}_N \rangle \right) \left(O[\underline{\sigma}_m] - \langle \bar{O}_N \rangle \right) \right\rangle$$

$$\Rightarrow \mathrm{Var}[N, \hat{O}] = \frac{1}{N^2} \sum_{n,m=1}^{N} \Gamma_{\hat{O}}(n-m)$$

$$\overset{M\to\infty}{=} \frac{1}{N} \mathrm{Var}(\hat{O}) + \frac{1}{N^2} \sum_{n \neq m = 1}^{N} \Gamma_{\hat{O}}(n-m)$$

The second vanishes for independent samples $\underline{\sigma}_n, \underline{\sigma}_m$ (see $\underline{\mathrm{VI}}.\underline{1}$) but in practice it's finite.

For large $|n-m|$ we get for Markov-chains:

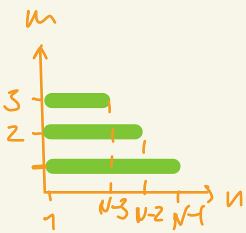
$$\Gamma_{\hat{O}}(n-m) \sim e^{-|n-m|/\tau} \quad , \quad \tau \in \mathbb{R}^+$$

(it can be shown that $\tau = -\frac{1}{\ln \lambda_1}$ where $\lambda_1 < 1$ is the second largest eigenvalue of W_{nm})!

Using $\Gamma_{\hat{O}}(n-m) = \Gamma_{\hat{O}}(|n-m|)$ we get:

$$\sum_{n \neq m = 1}^{N} \Gamma_{\hat{O}}(|n-m|) = 2 \sum_{n<m}^{N} \Gamma_{\hat{O}}(n-m)$$

$$= 2 \sum_{n=1}^{N-1} \sum_{m=n+1}^{N} \Gamma_{\hat{O}}(n-m)$$



$$= 2 \sum_{n=1}^{N} \sum_{m=1}^{N-n} \Gamma_{\hat{O}}(m)$$

$$= 2 \sum_{n=1}^{N-1} (N-n) \Gamma_{\hat{O}}(n)$$

$$\Rightarrow Var[\hat{O}, N] = \frac{Var(\hat{O})}{N} \left(1 + 2 \sum_{n=1}^{N} \left(1 - \frac{n}{N}\right) \frac{\Gamma_{\hat{O}}(n)}{Var(\hat{O})} \right)$$

$$= \frac{Var(\hat{O})}{N} \left(1 + \tau_m \right)$$

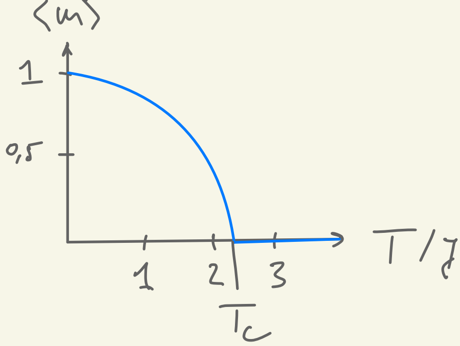
Thus, the estimator for uncorrelated samples $\frac{Var(\hat{O})}{N}$ is corrected by τ_m!

VI.3 Cluster Monte-Carlo algorithms

Systems at temperatures $T \approx T_c$ where T_c is the critical temp. of a continuous phase transition, exhibit universal behavior. In particular the correlation length's diverge: $\xi \sim |T-T_c|^{-\nu}$.

Example:

2D-Ising model: $\hat{H} = -J \sum_{\langle i,j \rangle} \hat{S}_i^z \hat{S}_j^z$



$$\langle m \rangle = \frac{1}{L^2} \sum_{j=1}^{L^2} \langle \hat{S}_j^z \rangle$$

$$T_c/J = \frac{2}{\ln(1+\sqrt{2})} \approx 2{,}269$$

Correlation function:

$$\langle (\delta \hat{S}^z)^2 \rangle = \langle \hat{S}_i^z \hat{S}_j^z \rangle - \langle \hat{S}_i^z \rangle \langle \hat{S}_j^z \rangle \sim \begin{cases} c\, e^{-|i-j|/\xi} & , |T-T_c| \gg 0 \\ |T-T_c|^{-\nu} & , |T-T_c| \approx 0 \end{cases}$$

What does this mean for local updates?

Critical slow-down

For Metropolis update the acceptance prob is

$$p_{\sigma\bar\sigma}^{[j]} = \min\left(1, \frac{e^{\beta J \sum_i' \sigma_{n_i} \bar\sigma_{n_j}}}{e^{\beta J \sum_i' \sigma_{n_i} \sigma_{n_j}}}\right)$$

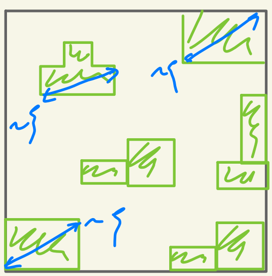
Only if "j" is at boundary of clusters we get large accept.-prob. Since $\hat H$ is invariant under $\sigma_j \to \bar\sigma_j$ for all j, $p(\underline{\sigma}) = p(\underline{\bar\sigma})$ & we can estimate number of surface sites by covering $L^2/2$ area with patches of size ξ^2:

$$n_{\text{patches}} = \frac{L^2}{2\xi^2} \Longrightarrow \sim \frac{L}{\xi} \text{ boundary sites}$$

$\Rightarrow$ acceptance rate becomes

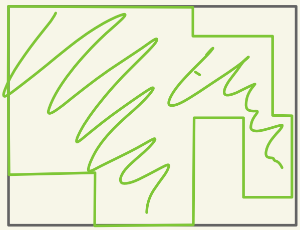
$$\sim p_{\sigma\bar\sigma}^{[j]} \frac{n_{\text{patches}}}{L^2} = p_{\sigma\bar\sigma}^{[j]} \frac{1}{L\xi}$$

(i) $|T - T_c| \gg 0$:



Green clusters have spins aligned $\uparrow$. Avg. size is $\sim \xi \ll L \Rightarrow \frac{1}{L\xi} \sim \mathcal{O}(1)$

(ii) $|T - T_c| \approx 0$:



Green clusters have spins aligned ↑. Avg. size is $\sim \xi \sim L \Rightarrow \frac{1}{L\xi} \sim \frac{1}{L^2}$

Close to critical temperature, the acceptance rate goes down $\sim \frac{1}{L^2} \Rightarrow \tau_m$ diverges :

$$\tau_m \sim |T - T_c|^{-z\nu} \sim \xi^z$$

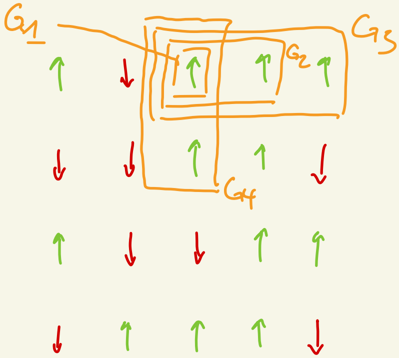
and here $z \approx 2$ (from above estimation: $\sim L^2$ samples to succesfully flip one spin).

Known as critical slow-down! But this not a problem of the method; Dependency on τ_m in observable estimation comes from W_{nm} being local! Idea: use global updates!

Cluster decomposition

We want to derive a Markov-process satisfying detailed balance such that more than 1 site can be updated without evaluating probabilities for too many different configurations!

Consider a configuration of spin-$\frac{1}{2}$ degrees of freedom:



Note:

We can label clusters of aligned spins to this configuration:

$$\mathcal{G}_{\underline{\sigma}} = \{ G_1, G_2, G_3, G_4, \dots \}$$

A configuration $\underline{\sigma}$ can be decomposed into various clusters! Let's identify clusters with graphs (here bond percolation graphs) & decompose $p(\underline{\sigma})$:

$$p(\underline{\sigma}) = \sum_{G \in \mathcal{G}} W(\underline{\sigma}, G) \quad \text{for all possible graphs } G \in \mathcal{G}.$$

The prob. to find a certain graph G in a given config $\underline{\sigma}$ is

$$P_{\underline{\sigma}}(G) = \frac{w(\underline{\sigma}, G)}{p(\underline{\sigma})} .$$

For the bond-percolation graphs we can factor w:

$$w(\underline{\sigma}, G) = V(G)\, \Delta(\underline{\sigma}, G)$$

where $V(G)$ is the prob. to find graph G out of <u>all</u> possible lattice-compatible graphs $\mathcal{G}$ & $\Delta(\underline{\sigma}, G)$ sorts out graphs incompatible with $\underline{\sigma}$:

$$\Delta(\underline{\sigma}, G) = \begin{cases} 1 & \text{if } G \in \mathcal{G}_{\underline{\sigma}} \\ 0 & \text{otherwise} \end{cases}$$

Now introduce a Markov process:

$$W_{nm}^{GG'} = w_{GG'}^{[\sigma_n]}\, w_{\sigma_n \sigma_m}^{[G']}$$

where : (i) $w_{GG'}^{[\sigma_n]}$ is transition amplitude from graph $G \to G'$ given σ_n

(ii) $w^{[G']}_{\underline{\sigma}_n \underline{\sigma}_m}$ is transition amplitude from config $\underline{\sigma}_n \to \underline{\sigma}_m$ given G'

Detailed balance:

(i) $P_{\underline{\sigma}_n}(G)\, w^{[\underline{\sigma}_n]}_{G G'} \overset{!}{=} P_{\underline{\sigma}_n}(G')\, w^{[\underline{\sigma}_n]}_{G' G}$

if we always choose a new graph G' then

$$w^{[\underline{\sigma}_n]}_{G G'} = 1 \Rightarrow \frac{P_{\underline{\sigma}_n}(G)}{P_{\underline{\sigma}_n}(G')} = \frac{V(G)}{V(G')} = \underline{1} \quad \checkmark$$

(ii) $P_G(\underline{\sigma}_n)\, w^{[G]}_{nm} \overset{!}{=} P_G(\underline{\sigma}_m)\, w^{[G]}_{mn}$

Here $P_G(\underline{\sigma}_n)$ is the prob. to have config $\underline{\sigma}_n$ & we can assign graph G from $\underline{\sigma}_n$:

$$P_G(\underline{\sigma}_n) = W(\underline{\sigma}_n, G)$$

$$\Rightarrow W(\underline{\sigma}_n, G)\, w^{[G]}_{nm} = W(\underline{\sigma}_m, G)\, w^{[G]}_{mn}$$

$$\Leftrightarrow \underbrace{\frac{V(G)\,\Delta(\underline{\sigma}_n, G)}{V(G)\,\Delta(\underline{\sigma}_m, G)}}_{1 \text{ because } \underline{\sigma}_n \,\&\, \underline{\sigma}_m \text{ compatible with}} = \frac{w^{[G]}_{mn}}{w^{[G]}_{nm}}$$

G, otherwise $\omega^{[G]}_{nm} = 0$ for all n, m!

We now only need to choose $\omega^{[G]}_{nm}$ to obey $p(\underline{\sigma}) = \sum_{G \in \mathcal{G}_{\underline{\sigma}}} V(G)$.

Consider graphs constructed from aligned, neighboring spins:

Spins \ Graph	○—○	○ ○	$p(\underline{\sigma})$
$\uparrow\uparrow$	$\Delta = 1$	$\Delta = 1$	$\sim e^{+\beta J}$
$\uparrow\downarrow$	$\Delta = 0$	$\Delta = 1$	$\sim e^{-\beta J}$
$\uparrow\downarrow$	$\Delta = 0$	$\Delta = 1$	$\sim e^{-\beta J}$
$\downarrow\downarrow$	$\Delta = 1$	$\Delta = 1$	$\sim e^{+\beta J}$

For $P_{\underline{\sigma}}(G) = \begin{cases} \left(e^{+\beta J} + e^{-\beta J}\right)/e^{\beta J} & \text{if } \uparrow\uparrow \text{ or } \downarrow\downarrow \\ 0 & \text{otherwise} \end{cases}$

For $\omega^{[G]}_{mn}$ flip cluster of connected spins (which keeps graph G intact) with $\omega^{[G]}_{nm} = \omega^{[G]}_{mn}$.

Examples discussed on sheet 4.

Remarks

(i) In the step $(\Sigma_n, G) \to (\Sigma_n, G')$ clusters are allowed to grow. Near $T=T_c$ this will happen almost surely since $P_\Sigma(G) \neq 0$ only for aligned spins

(ii) Away from $T=T_c$ large clusters are unlikely (only with prob. $\sim \frac{\xi^2}{L^2}$). Then updates can become very expensive

(iii) Observing τ_m & switching from local to cluster updates is good strategy!