LECTURE 4:

BASICS OF MONTE CARLO SIMULATIONS

GOAL:

calculate expectation values

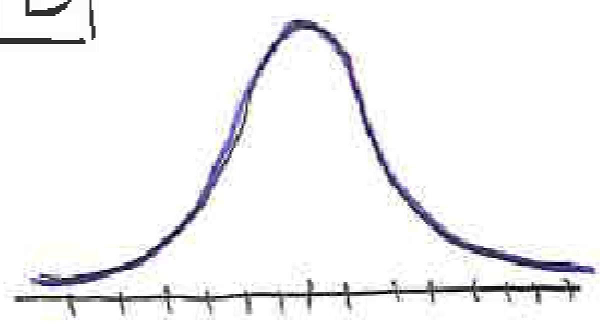
$$\langle O \rangle = \int \prod_x d\phi(x)\; O[\phi]\; e^{-S} / Z$$

$$Z = \int \prod_x d\phi(x)\; e^{-S}$$

$N_s^3 N_t$ points
N_F field components

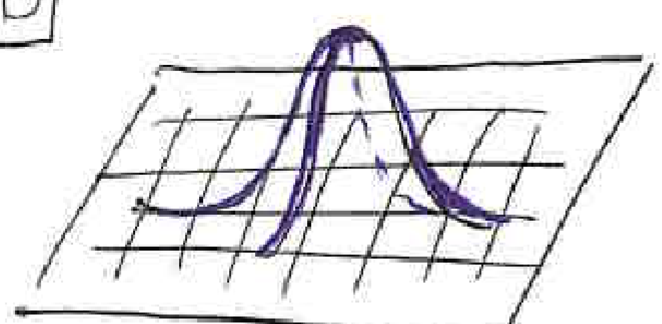
$\Big\}$ $N_s^3 N_t N_F$ dimensional integral

$\boxed{1D}$



N fn. evaluations

$\boxed{2D}$



N^2 fn. evaluations

N^{64^4} fn. evaluations ↯

MONTE CARLO METHODS

random field configurations

if uniform distributed $\rightarrow$ just as bad as quadrature

IMPORTANCE SAMPLING

take random configs $\Phi_1, \dots, \Phi_N$

with probability

$$W[\Phi] \propto e^{-S[\Phi]}$$

obtain expectation values as

$$\langle O \rangle = \lim_{N\to\infty} \underbrace{\frac{1}{N} \sum_i O[\Phi_i]}_{\overline{O}_N}$$

def. of an expectation value

$$\mathrm{Var}(\overline{O}_N) = \frac{1}{N^2}\, N\, \mathrm{Var}(O) = \frac{\mathrm{Var}(O)}{N} \quad \text{(indep. samples)}$$

stat. error of average $\sim \frac{1}{\sqrt{N}}$

TYPES OF SAMPLING

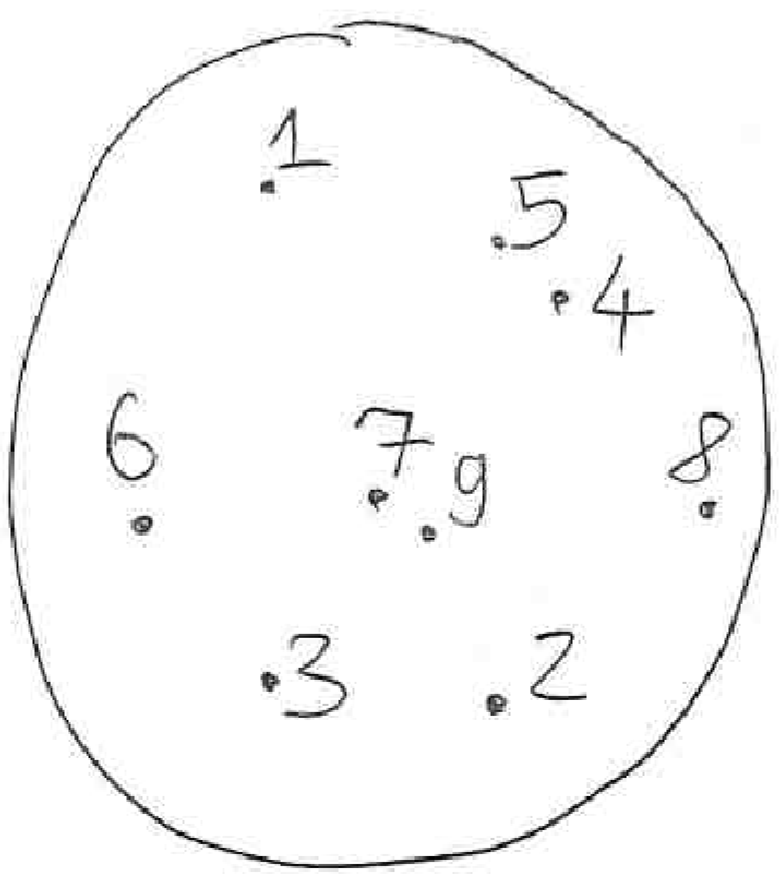
DIRECT

* independent samples
* can be done in 1D for an arbitrary distribution
* in many dim.s only for simple distributions

  e.g. ∘ Gaussians $e^{-\frac{1}{2}\phi_i M_{ij} \phi_j}$

  ∘ uniform point on sphere S^n

  ...



* more complicated MC algorithms also feature direct sampling as an intermediate step

MARKOV CHAIN

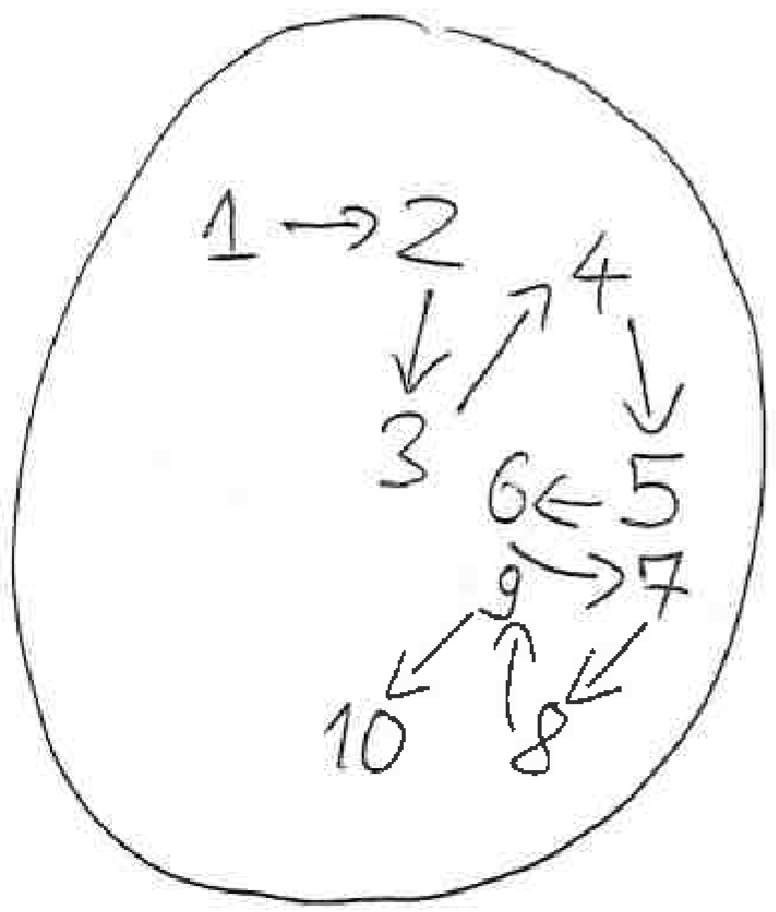
MCMC = Markov Chain Monte Carlo

$$\Phi_1 \to \Phi_2 \to \Phi_3 \to \dots$$

defined by transition probabilities $P(\Phi_{i+1} \leftarrow \Phi_i)$

* with a proper choice of the transition probabilities, can sample from arbitrarily complicated multidim. prob. distributions

BUT: if we don't take enough steps, the chain will remember where it started



the samples are not independent

autocorrelation fn.

$$C_A(\tau) = \langle A_n A_{n+\tau} \rangle - \langle A_n \rangle \langle A_{n+\tau} \rangle$$

$$\neq 0$$

BASICS OF MCMC ALGORITHMS

TRANSITION PROBABILITIES $P[\Phi_{i+1} \leftarrow \Phi_i]$

IF THE CURRENT PROB. DISTR. IS $W[\Phi]$

AFTER ONE STEP $W'[\Phi'] = \int D\Phi \; P[\Phi' \leftarrow \Phi] \, W[\Phi]$

OR IN MATRIX NOTATION $W' = PW$

CONDITIONS FOR CORRECTNESS

(0) $0 \le P(\Phi' \leftarrow \Phi) \le 1 \quad \forall \Phi, \Phi'$ it is a probability

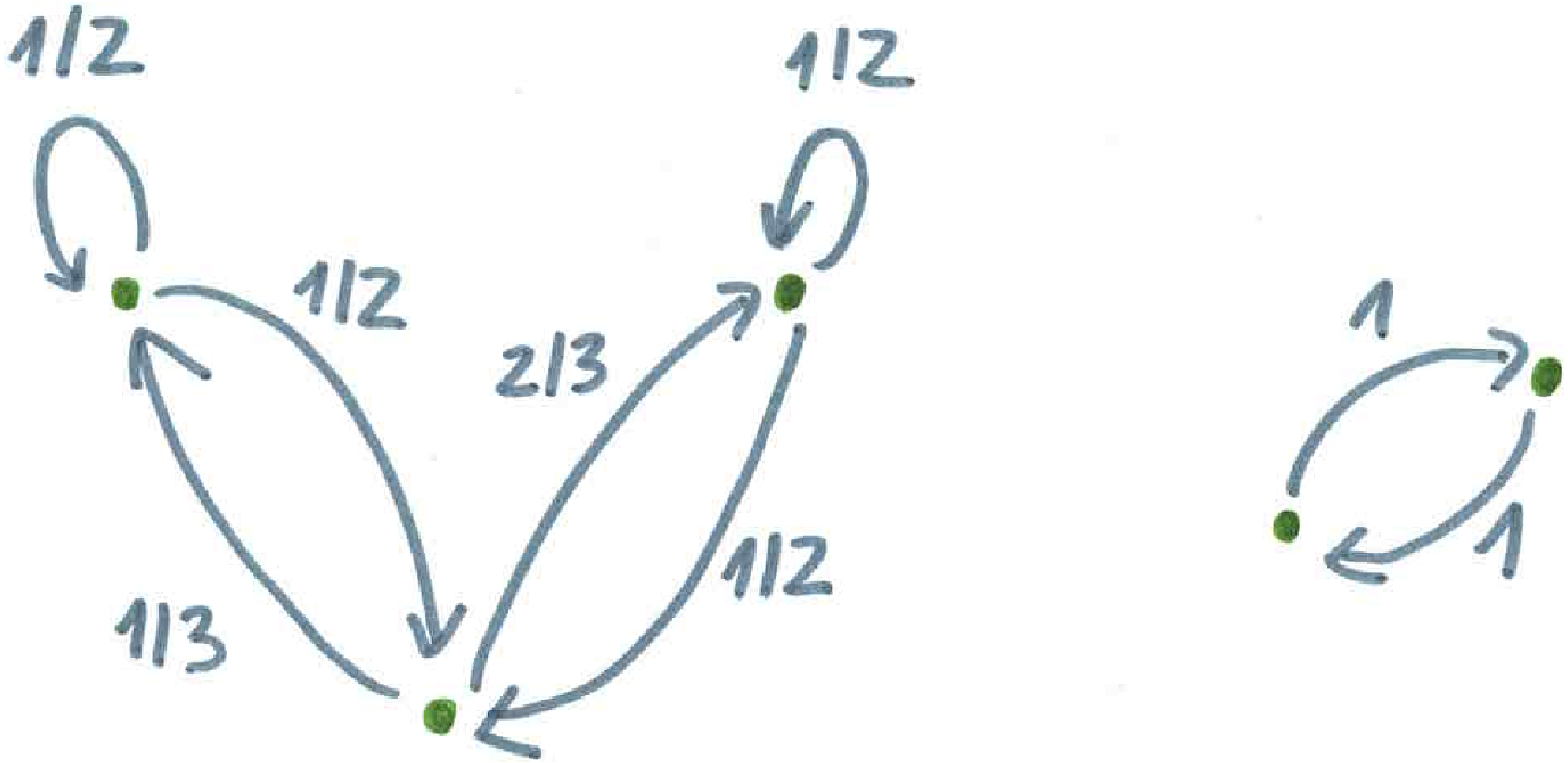
(1) normalization $\int D\Phi' \, P(\Phi' \leftarrow \Phi) = 1$

$$\Rightarrow \int D\Phi' \, W'[\Phi'] = \int D\Phi \, W[\Phi]$$

(2) ergodicity two types

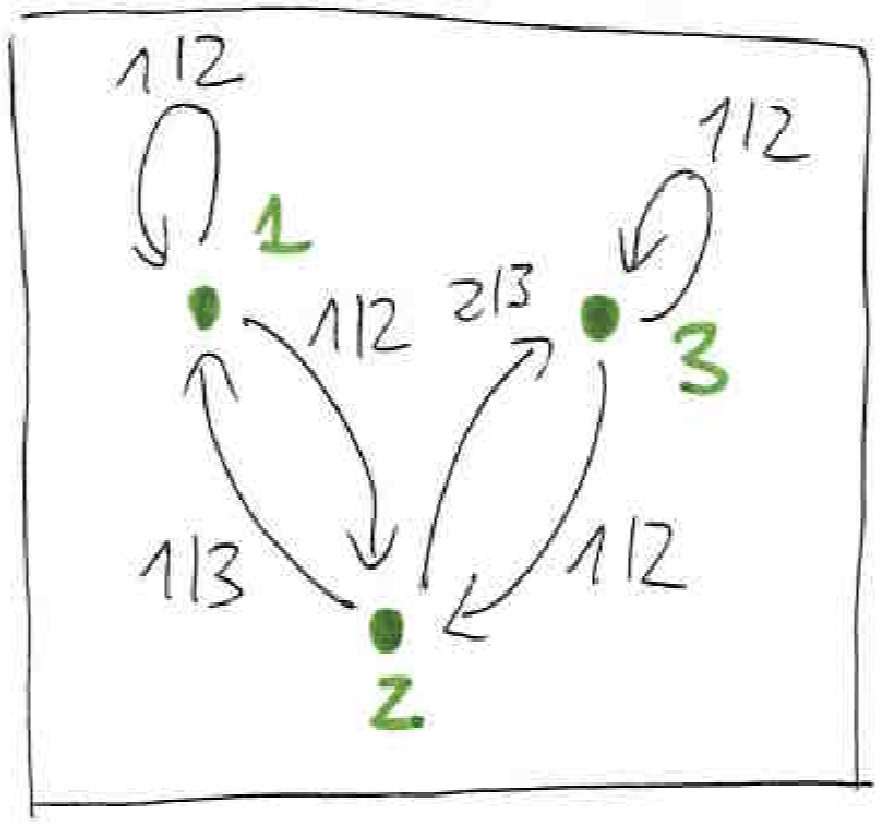
STRONG $P(\Phi' \leftarrow \Phi) > 0 \quad \forall \Phi', \Phi$ WEAK $P^k(\Phi' \leftarrow \Phi) > 0$ for some k

EXAMPLE OF A NON-ERGODIC MC



THE CONFIGURATIONS DECOMPOSE INTO GROUPS

STARTING FROM ONE YOU WILL NEVER GET TO THE OTHER



$P(1 \leftarrow 1) = 1/2$

$P(2 \leftarrow 1) = 1/2$

$P(3 \leftarrow 1) = 0$

$P(1 \leftarrow 2) = 1/3$

$P(2 \leftarrow 2) = 0$

$P(3 \leftarrow 2) = 2/3$

$P(1 \leftarrow 3) = 0$

$P(2 \leftarrow 3) = 1/2$

$P(3 \leftarrow 3) = 1/2$

$$P = \begin{pmatrix} 1/2 & 1/3 & 0 \\ 1/2 & 0 & 1/2 \\ 0 & 2/3 & 1/2 \end{pmatrix}$$

suppose I start from state $1 \Rightarrow W_0 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$

<u>1 step</u> $P W_0 = \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}$

<u>2 steps</u> $P^2 W_0 = \begin{pmatrix} 5/12 \\ 1/4 \\ 1/3 \end{pmatrix}$

<u>5 steps</u> $\begin{pmatrix} 0.2396 \\ 0.3438 \\ 0.4167 \end{pmatrix}$

$\vdots$

$\boxed{\exists \text{ equilibrium distribution}}$

$\boxed{\text{Claim: unique for all ergodic tr. mat.}}$

different starting point

$W_0 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$

<u>1 step</u> $\begin{pmatrix} 1/3 \\ 0 \\ 2/3 \end{pmatrix}$

$\vdots$

many steps $\rightarrow$ same

i.e. as $k \to \infty$ the columns of P^k will become the same

<u>Q:</u> How to choose P so that I have the eq. distr. that I want?

③ GLOBAL BALANCE / CORRECT EQUILIBRIUM DISTR.

$$W_{eq}[\Phi] = \int D\Phi' \, P[\Phi \leftarrow \Phi'] \, W_{eq}[\Phi']$$

$$\boxed{\underbrace{\int D\Phi' \, P[\Phi' \leftarrow \Phi]}_{1} \, W_{eq}[\Phi] = \int D\Phi' \, P[\Phi \leftarrow \Phi'] \, W_{eq}[\Phi']}$$

a <u>sufficient, but not necessary</u> condition is

DETAILED BALANCE

$$\boxed{P[\Phi' \leftarrow \Phi] \, W_{eq}[\Phi] = P[\Phi \leftarrow \Phi'] \, W_{eq}[\Phi']}$$

THE METROPOLIS ALGORITHM

1. choose a config. Φ' with some proposal probability $T_0[\Phi' \leftarrow \Phi]$
2. accept proposal w. prob. $T_A(\Phi' \leftarrow \Phi) = \min\left\{1, \frac{T_0[\Phi \leftarrow \Phi']}{T_0[\Phi' \leftarrow \Phi]} \frac{W[\Phi']}{W[\Phi]}\right\}$
3. goto 1

the full transition prob. is $P[\Phi' \leftarrow \Phi] = T_0(\phi' \leftarrow \phi)\, T_A(\phi' \leftarrow \phi)$

detailed balance $\quad P(\Phi' \leftarrow \Phi)\, e^{-S[\Phi]} \stackrel{?}{=} P(\phi \leftarrow \phi')\, e^{-S[\phi']}$

$$
\begin{aligned}
P(\phi' \leftarrow \phi)\, e^{-S[\phi]} &= T_0(\phi' \leftarrow \phi) \min\left\{1, \frac{T_0(\phi \leftarrow \phi')}{T_0(\phi' \leftarrow \phi)} \frac{e^{-S[\phi']}}{e^{-S[\phi]}}\right\} e^{-S[\phi]} \\
&= \min\left(T_0(\phi' \leftarrow \phi)\, e^{-S[\phi]},\ T_0(\phi \leftarrow \phi')\, e^{-S[\phi']}\right\} \\
&= \min\left\{1, \frac{T_0(\phi' \leftarrow \phi)}{T_0(\phi \leftarrow \phi')} \frac{e^{-S[\phi]}}{e^{-S[\phi']}}\right\} e^{-S[\phi']}\, T_0[\phi \leftarrow \phi'] = P(\phi \leftarrow \phi')\, e^{-S[\phi']}
\end{aligned}
$$

$\square$

COMMENTS:

1. DON'T NEED TO NORMALIZE W_{eq}

   DON'T NEED TO CALCULATE Z : IMPORTANT

2. THE ACCEPT/REJECT STEP GUARANTEES DETAILED BALANCE

   THE PROPOSAL STEP MUST GUARANTEE ERGODICITY

SPEC. CASE

$$T_0(\phi' \leftarrow \phi) = T_0(\phi \leftarrow \phi')$$

$$\Rightarrow T_A(\phi' \leftarrow \phi) = \min\{1, e^{-\Delta S}\} \qquad \Delta S = S[\phi'] - S[\phi]$$

LOCAL UPDATES

IF proposal of T_0 local change & action is local

$\Rightarrow$ calculation of ΔS is only $O(1)$

(say the contrib. of the 2d neighbors of the updated field)

EXPONENTIAL AUTOCORRELATION TIME

HOW FAST DOES THE MARKOV CHAIN APPROACH EQUIL.?

For an ergodic Markov matrix
There is 1 eigenvalue $\lambda_1 = 1$
all others are $\lambda < 1$

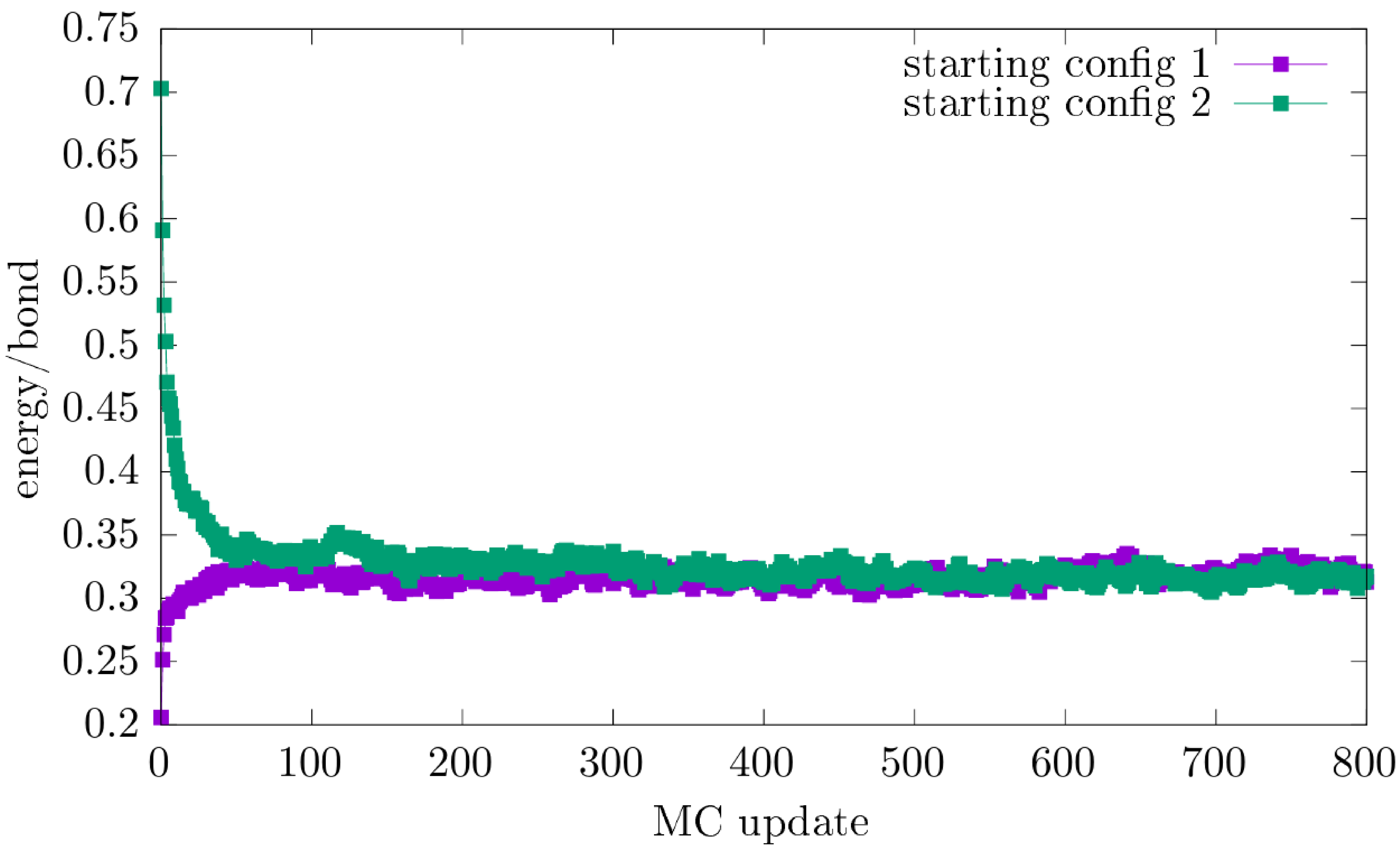
$$P^k = 1\, \underbrace{P_1}_{\substack{\text{projection to the} \\ \lambda=1 \text{ subspace}}} + \lambda_2^k P_2 + \lambda_3^k P_3 + \dots$$

$$P^k W_0 = W_{eq} + \underbrace{\lambda_2^k}_{e^{-k/\tau_{exp}}} P_2 W_0 + \dots$$

<u>exponential autocorrelation time</u> $\frac{1}{\tau_{exp}} = -\ln \lambda_2$

slowest timescale in the MC "dynamics"

THERMALIZATION



CRITICAL SLOWING DOWN

near a 2nd order PhTr $\qquad \tau_{exp} \sim \xi^{z}$

z = dynamical critical exponent, depends on the dynamics (i.e. the update algorithm)

STATISTICAL ERRORS & INTEGRATED AUTOCORR. TIME

$$\mathrm{Var}(\overline{O}_N) = \left\langle \frac{1}{N^2}\sum_{i,j=1}^{N}(O_i - \langle O\rangle)(O_j - \langle O\rangle)\right\rangle = \frac{1}{N^2}\sum_{i,j=1}^{N}\underbrace{\langle (O_i - \langle O\rangle)(O_j - \langle O\rangle)\rangle}_{C_O(|i-j|)}$$

$$= \frac{1}{N^2}\sum_{t=-N+1}^{N-1}\sum_{i=1}^{N-|t|} C_O(|t|) = \frac{1}{N^2}\sum_{t=-N+1}^{N-1}(N-|t|)C_O(|t|) = \sum_{t=-N}^{N}\frac{N-|t|}{N^2}C_O(|t|)$$

$$= \frac{C_O(0)}{N}\sum_{t=-N}^{N}\Gamma_O(|t|)\left(1-\frac{|t|}{N}\right) \underset{\text{large } N}{\approx} \frac{\mathrm{Var}(O)}{N}\,2\underbrace{\left(\frac{1}{2}+\sum_{t=1}^{N}\Gamma_O(|t|)\right)}_{\equiv \tau_{int,O}} = \frac{\mathrm{Var}(O)}{N}\,2\tau_{int,O}$$

$$\boxed{\Gamma_O(t) = \frac{C_O(t)}{C_O(0)}}$$

$\Rightarrow$ # of effectively independent data $\quad N_{indep} = \dfrac{N}{2\tau_{int,O}}$

suppose the autocorr. fn. is a single exponential

$$\Gamma(t) \sim e^{-t/\tau_{exp}}$$

$$\tau_{int} = \frac{1}{2}\left(1+2\sum_{t=1}^{\infty} e^{-t/\tau_{exp}}\right) = \frac{1}{2}\left[1+\frac{2e^{-1/\tau_{exp}}}{1-e^{-1/\tau_{exp}}}\right] \underset{\tau_{exp}\gg 1}{\approx} \frac{1}{2}\left[1+\frac{2-\frac{2}{\tau_{exp}}}{\frac{1}{\tau_{exp}}}\right] = \frac{1}{2}(2\tau_{exp}-1) \approx \tau_{exp}$$

if (more realistically) we have more exponentials

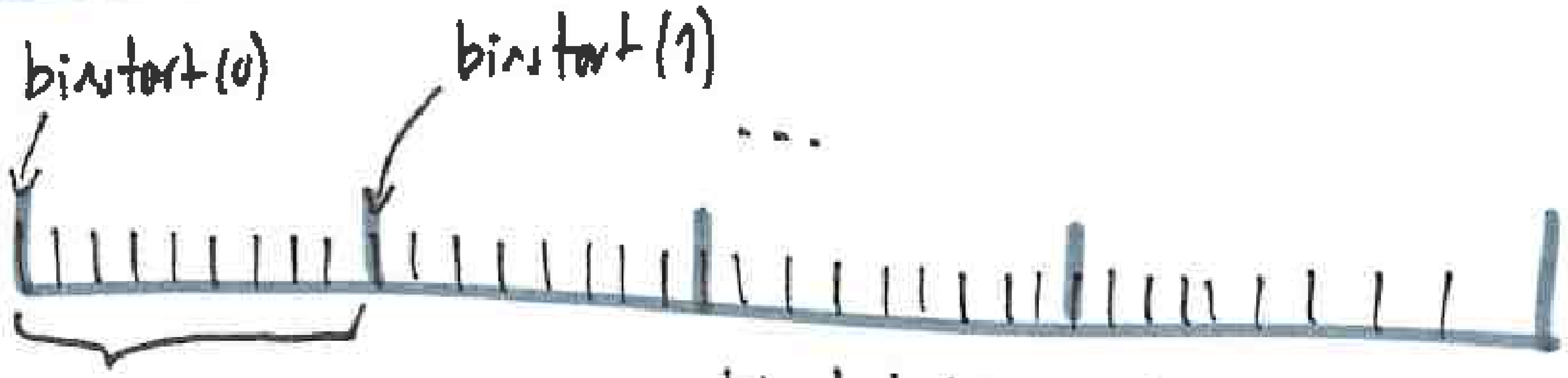
$$\Gamma(t) = \sum_{n=1}^{K} c_n e^{-t/\tau_n}$$

assume $\tau_1 = \tau_{exp} > \tau_2 > \ldots > \tau_K \gg 1$

$\sum_c c_n = 1$ since $\Gamma(0) = 1$

$$\tau_{int} \approx \sum_n c_n \tau_n < \tau_1 = \tau_{exp}$$

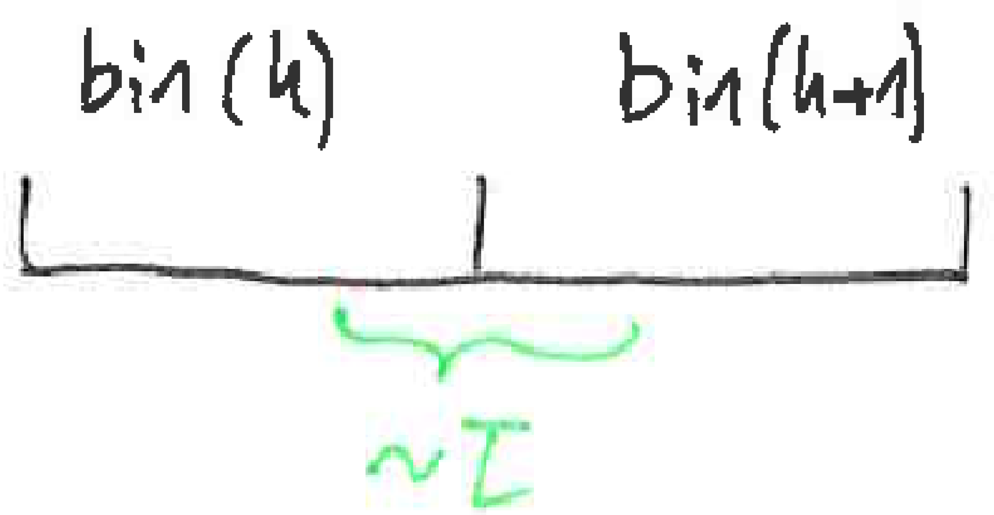
BINNING / DATA BUNCHING



$$O_{\substack{bin\\average}}^{(k)} = \frac{1}{N_{binsize}} \sum_{i=binstart(k)}^{binstart+binsize-1} O_i$$

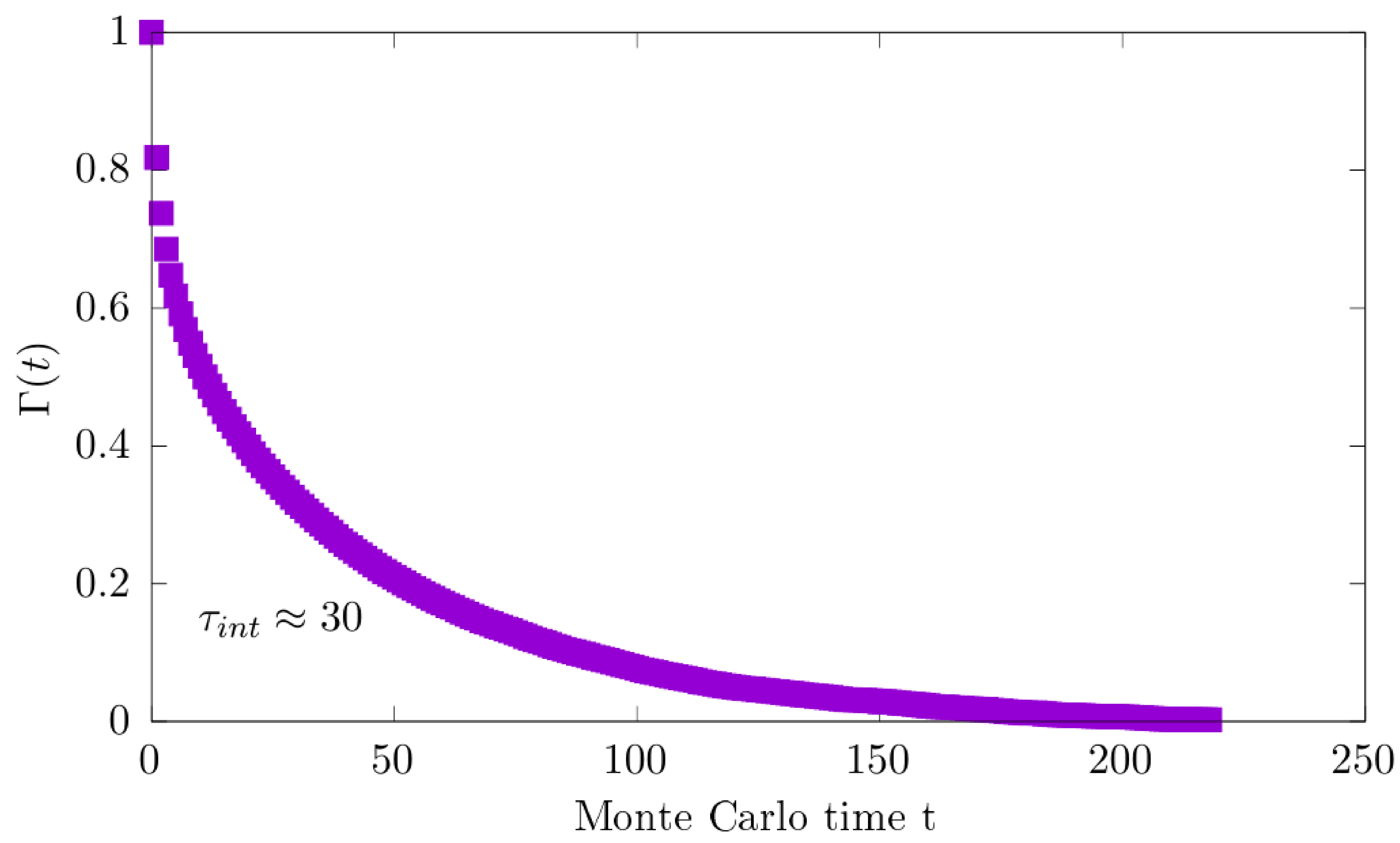
if $N_{binsize} \gg \tau_{int}$

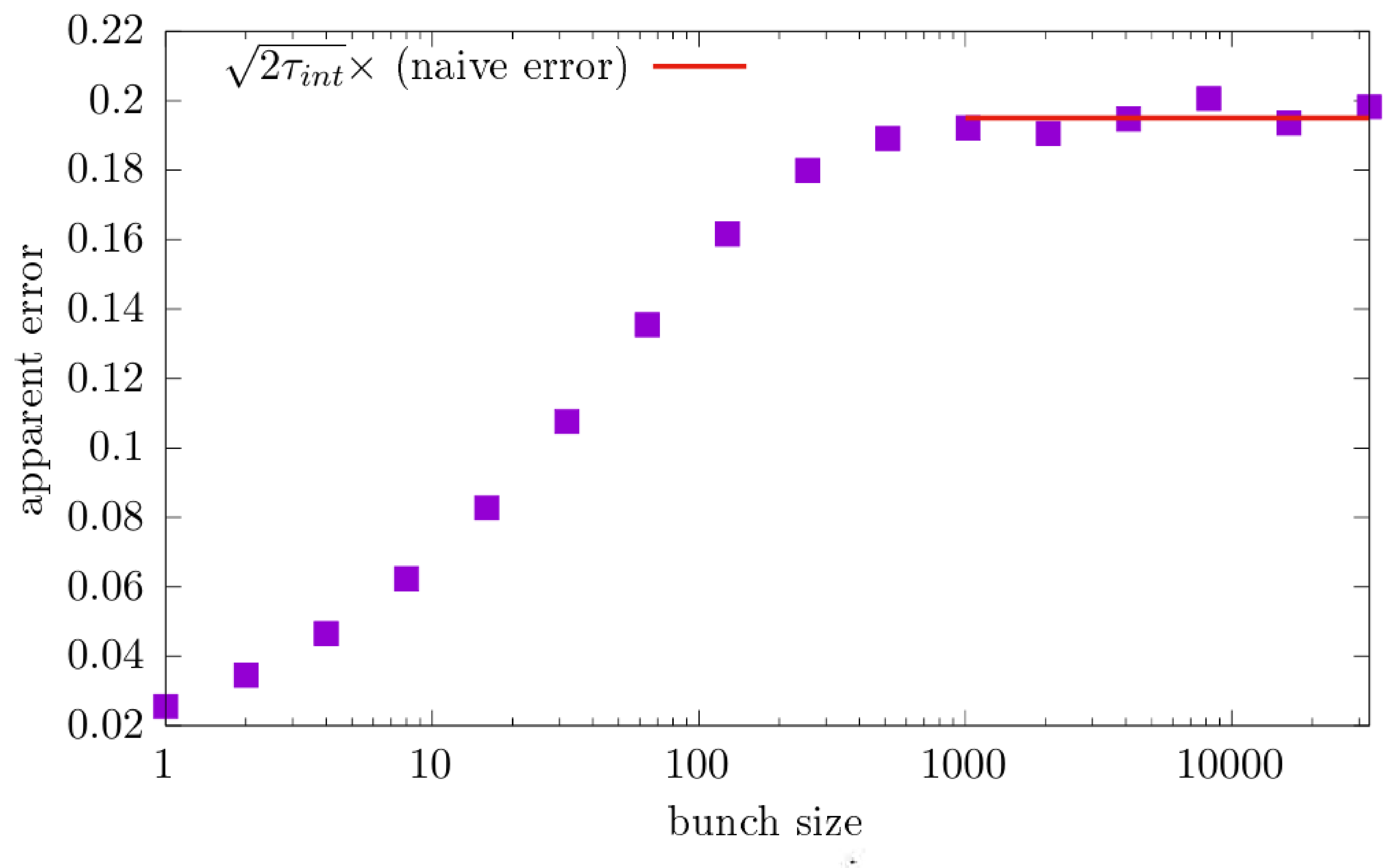
$\Rightarrow O_{\substack{bin\\average}}^{(k)}$ are to a good approx. uncorrelated



simplest analysis method:

* make bins, pretend they are uncorrelated
* check what happens when you change the binsize.





STRUCTURE OF A BASIC MC PROGRAM

INITIALIZATION

init. random num generator
init. tables (e.g. neighbor indices)
init. field configurations

LOOP OVER THERMALIZATION UPDATES

for ($n=1 \ldots n_{therm}$)
  update config
end for

LOOP OVER MC UPDATES W. MEASUREMENTS

for ($n=1 \ldots n_{measure}$)
  for ($k=1 \ldots n_{discarded}$)
    update config
  end for

  measure observables (magnetization, correlation fns, ...), write to output file
end for

write final config & status of random generator for future restart

A SHORTCUT

$$M_{spontaneous} = \underbrace{\lim_{H\to 0^+} \lim_{N_{spins}\to\infty}}_{\text{quite invonvenient, mostly not done}} \frac{1}{N_{spins}}\langle M\rangle \qquad N_{spins} = N$$

quite invonvenient, mostly not done (except for cases like spin glasses, where the ordering is hard to understand)

<u>what can be done at $H=0$?</u> There are a few options

$$M_{rms} = \sqrt{\langle M^2\rangle}\,\frac{1}{N} \qquad M_{||} = \langle |M|\rangle \frac{1}{N} \qquad M_{corr} = \sqrt{\langle \sigma(0)\,\sigma(L/2)\rangle}\,\frac{1}{N}$$

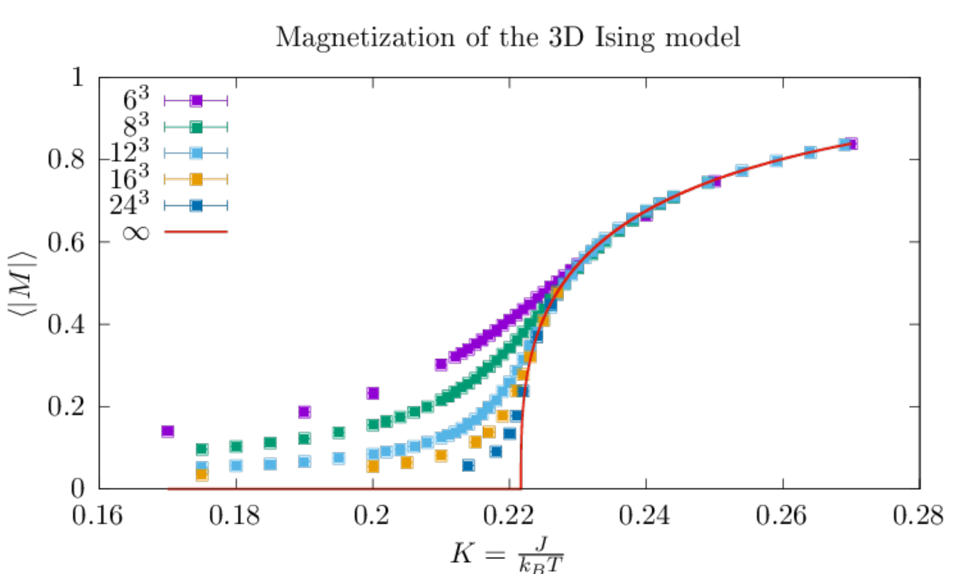
in the thermodynamic limit all of these will agree

<u>susceptibility:</u> can use:

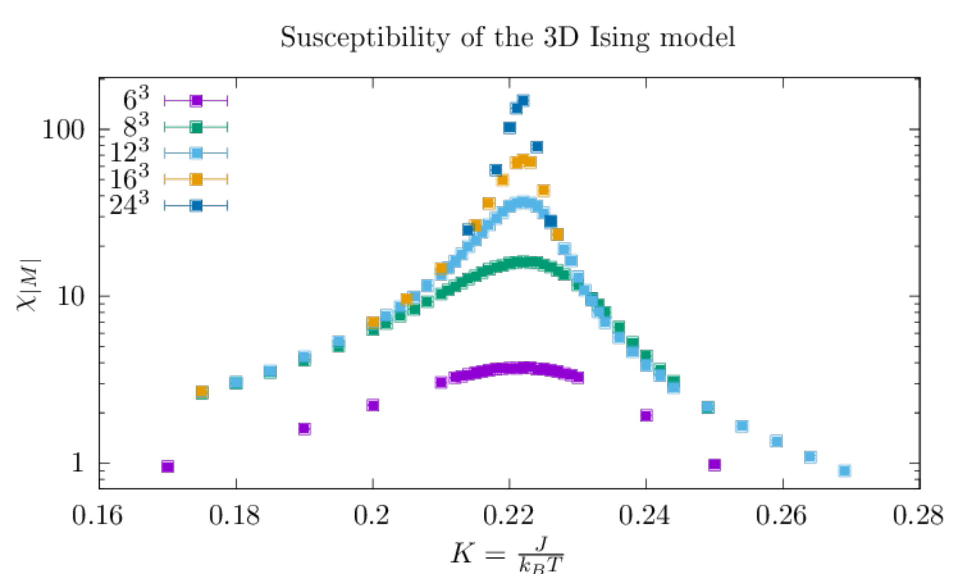
$$\chi_{|M|} = \frac{1}{N}\left(\langle M^2\rangle - \langle |M|\rangle^2\right)$$

of course for the energy, can simply use

$$\chi_E = \frac{1}{N}\left(\langle E^2\rangle - \langle E\rangle^2\right)$$



Magnetization of the 3D Ising model
6^3
8^3
12^3
16^3
24^3
∞
1
0.8
0.6
0.4
0.2
0
0.16
0.18
0.2
0.22
0.24
0.26
0.28
$\langle|M|\rangle$
$K = \frac{J}{k_B T}$



Susceptibility of the 3D Ising model
6^3
8^3
12^3
16^3
24^3
100
10
1
$\chi_{|M|}$
0.16
0.18
0.2
0.22
0.24
0.26
0.28
$K = \frac{J}{k_B T}$

FINITE-SIZE SCALING NEAR A 2ND ORDER PhTr

suppose $\langle O \rangle_\infty \sim |t|^{-\beta}$ where $t = \frac{T-T_c}{T_c}$ reduced temperature

<u>scaling ansatz:</u> $\langle O \rangle_L \sim L^{w} \hat{f}_0(L/\xi)$ i.e. finite volume effects are dictated by how many corr. lengths fit in a volume

some function

$\xi \sim |t|^{-\nu}$ $\Leftarrow$ def. of critical exponent ν $\Rightarrow \frac{L}{\xi} \sim L\, t^{\nu} \sim (L^{1/\nu} t)^{\nu}$

let $\hat{f}_0(L/\xi) = f_0(L^{1/\nu} t)$

in order for $\langle O_L \rangle \sim L^{w} f_0(L^{1/\nu} t) \sim t^{-\beta}$

we need $f_0(x) \sim x^{-c}$ (as $x \to \infty$) with $c = \beta$ so that we have $t^{-\beta}$

and $w = \frac{\beta}{\nu}$ so that we have L^0

$\Rightarrow \langle O_L \rangle \sim L^{\frac{\beta}{\nu}} f_0(L^{1/\nu} t)$

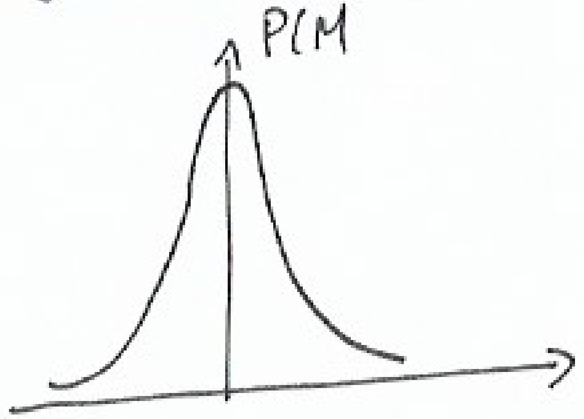
at the critical temperature $(t=0)$ $\langle O_L \rangle \sim L^{\beta/\nu} \underbrace{f_0(0)}_{\text{number}}$

RULE OF THUMB if at $L=\infty$ $\langle O \rangle \sim |t|^{-\beta} \sim \xi^{\beta/\nu}$

than at $L=$ finite and $t=0$ $\langle O \rangle_L \sim L^{\beta/\nu}$

PROBABILITY DISTR. OF THE ORDER PARAM. (M)

symmetric phase



close to a Gaussian

variance ~ susceptibility

near T_c

scaling ansatz

$$P(M,L) \cong L^a \hat{P}\left(L^b M, \frac{L}{\xi}\right)$$

normalization

$$\int dM\, P(M,L) = 1$$

$$\parallel$$

$$L^{a-b} \int dz\, \hat{P}\left(z, \frac{L}{\xi}\right) = 1$$

$$\boxed{a=b}$$

match def. of crit. exponents

$\boxed{T \to T_c^+}$

$$L^d \chi = \int dM\, M^2 P(M,L)$$

$$= L^{-2a} \int dz\, z^2\, \hat{P}(z, L/\xi)$$

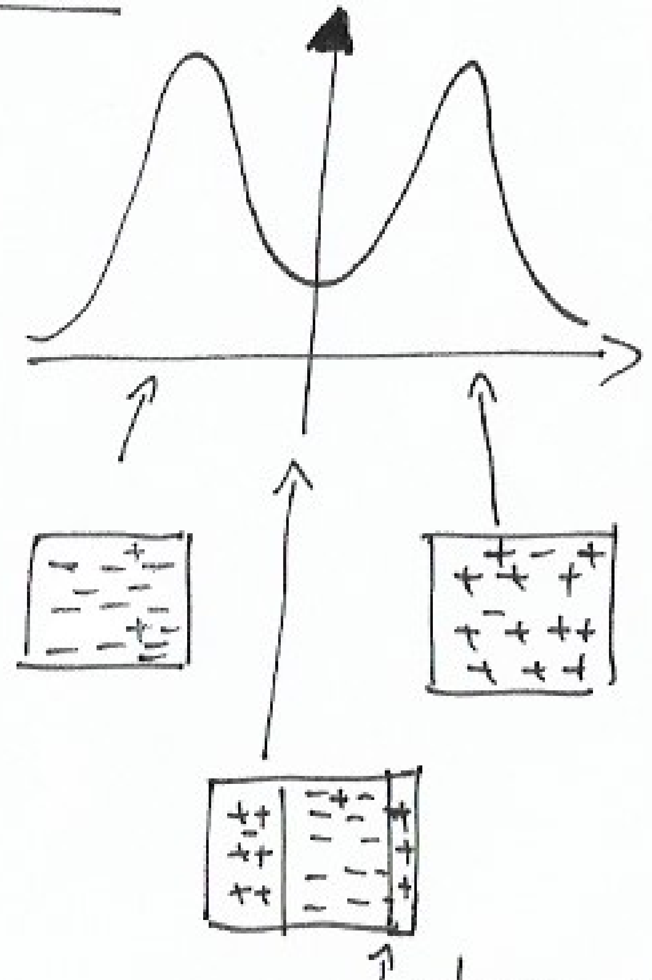
$$\sim L^{-2a} \sim L^{\frac{\gamma}{\nu}+d}$$

$$a = -\frac{1}{2}\left(\frac{\gamma}{\nu} + d\right)$$

$$\langle M^{2n} \rangle \sim L^{-2na}$$

broken phase

bimodal



at large volumes turns to a double delta fn.

$$P(M) \simeq \frac{1}{2}\left[\delta(M - M_0) + \delta(M + M_0)\right]$$

BINDER CUMULANT

$$\frac{\langle M^4\rangle}{\langle M^2\rangle^2} = B$$

symmetric phase

$P(M)$ almost Gaussian

$$\xrightarrow[L\to\infty]{} 3$$

at T_c

we expect

$\approx$ const.

as a fn. of volume

near T_c we expect

$$B \approx \frac{\int dz\, \hat{P}(z, L/\xi)\, z^4}{\left[\int dz\, \hat{P}(z, L/\xi)\, z^2\right]^2}$$

$$= F(L/\xi) = \hat{f}\left[L^{\frac{1}{\nu}}(K-K_c)\right]$$

broken phase

$$P(M) \approx \frac{1}{2}\left[\delta(M-M_0) + \delta(M+M_0)\right]$$

$$\xrightarrow[L\to\infty]{} 1$$