Monte Carlo simulations.

observable: $O(\vec{x})$

$$\langle O \rangle = \frac{\int O(\vec{x})\, e^{-\beta H(\vec{x})}\, d\vec{x}}{\int e^{-\beta H(\vec{x})}\, d\vec{x}} \qquad \int e^{-\beta H(\vec{x})}\, d\vec{x} = Z$$

– efficient sampling $\quad P(\vec{x})$

$$\langle O \rangle = \frac{\int P^{-1}(\vec{x})\, \frac{O(\vec{x})}{P^{-1}(\vec{x})}\, e^{-\beta H(\vec{x})}\, d\vec{x}}{\int e^{-\beta H(\vec{x})}\, d\vec{x}}$$

the most likely states are those that maximize the Boltzmann distribution

$$p(\vec{x}) = \frac{e^{-\beta H(\vec{r})}}{Z}$$

$$\langle O \rangle = \int O(\vec{x}) \cdot p^{-1}(\vec{x}) \, d\vec{x} =$$

$$= \int O^{*}(\vec{x}) \, d\vec{x}$$

$$\langle O \rangle = \frac{1}{N} \sum_{i=1}^{N} O^{*}(\vec{x}_i)$$

We must generate state given by the distribution $p(\vec{x})$

- Select a dynamics that brings the system to the equilibrium.

- Markov process
- transition probabilities ω

$$\omega(\vec{x}_i \to \vec{x}_j) \geq 0$$

$$\sum_i \omega(\vec{x}_i \to \vec{x}_j) = 1$$

- Detailed Balance Condition

$$P_{eq}(\vec{x}_i)\, w(\vec{x}_i \to \vec{x}_j) = P_{eq}(\vec{x}_j) \cdot w(\vec{x}_j \to \vec{x}_i)$$

$$\frac{w(\vec{x}_i \to \vec{x}_j)}{w(\vec{x}_j \to \vec{x}_i)} = \frac{P_{eq}(\vec{x}_j)}{P_{eq}(\vec{x}_i)} = e^{-\beta[H(\vec{x}_j) - H(\vec{x}_i)]} = e^{-\beta \Delta H_{ij}}$$

canonical

$$P_{eq}(\vec{x}) \sim e^{-\beta H(\vec{x})}$$

METROPOLIS CHOICE!

$$
w(\vec{x}_i \to \vec{x}_j) = \begin{cases} A\, e^{-\beta \Delta H_{ij}} & \Delta H_{ij} > 0 \\ A & \Delta H_{ij} \le 0 \end{cases}
$$

for simplicity $A = 1$

2d Ising Model

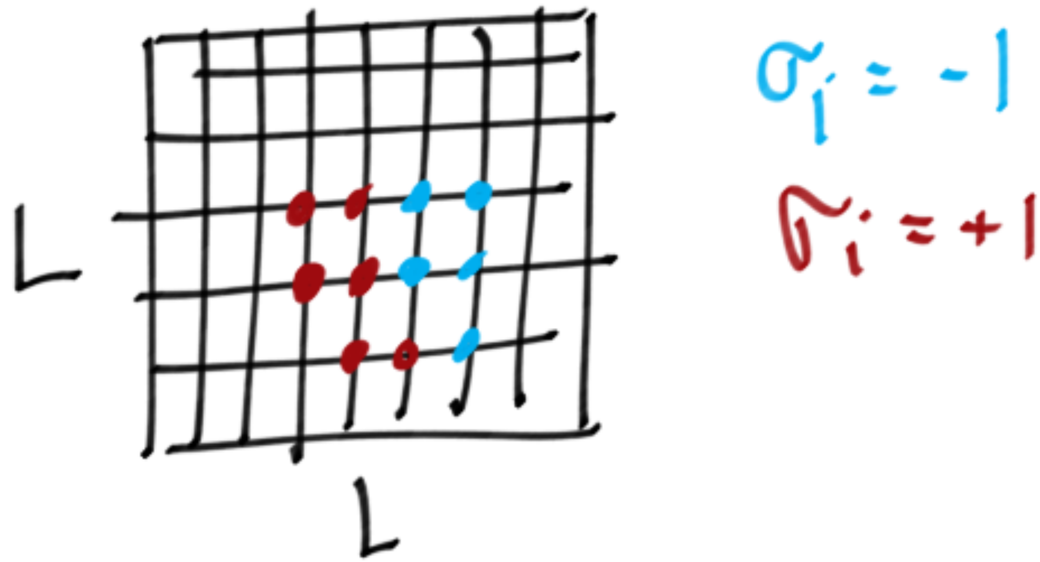
$$H(\sigma) = -\sum_{\langle ij \rangle} J_{ij}\,\sigma_i \sigma_j - \mu \sum_i h_i \sigma_i$$

$$J_{ij} = J$$

$$H(\sigma) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

$$\boxed{\sigma_i = \begin{cases} +1 \\ -1 \end{cases}}$$

- 2d square lattice of size L



- Number of spins $N = L^2$
- set the system temperature T (J/k_B)
- Metropolis MC
  1. thermalization (10^3)
  2. take measures

$$e^{-\beta \Delta H} = e^{-\frac{\Delta H}{k_B T}} = e^{-\frac{J}{k_B T}\Delta H^*}$$

$$e^{-\frac{\Delta H^*}{T}}$$

T in units of J/k_B

Evaluate:

- System energy $\langle H \rangle$ vs $T\ (J/k_B)$
- Specific heat

$$C_V = \frac{\partial}{\partial T}\langle H\rangle = \frac{\beta}{T}\left(\langle H^2\rangle - \langle H\rangle^2\right)$$

C_V vs $T\ (J/k_B)$

- Magnetization:

$$\langle M\rangle = \frac{1}{N}\sum_i \sigma_i$$

$\langle M\rangle$ vs $T\ (J/k_B)$

- Magnetic susceptibility

$$\chi = \frac{\partial \langle M \rangle}{\partial H} = \beta \left(\langle M^2 \rangle - \langle M \rangle^2 \right)$$

χ vs T (J/k_B)

Variables.

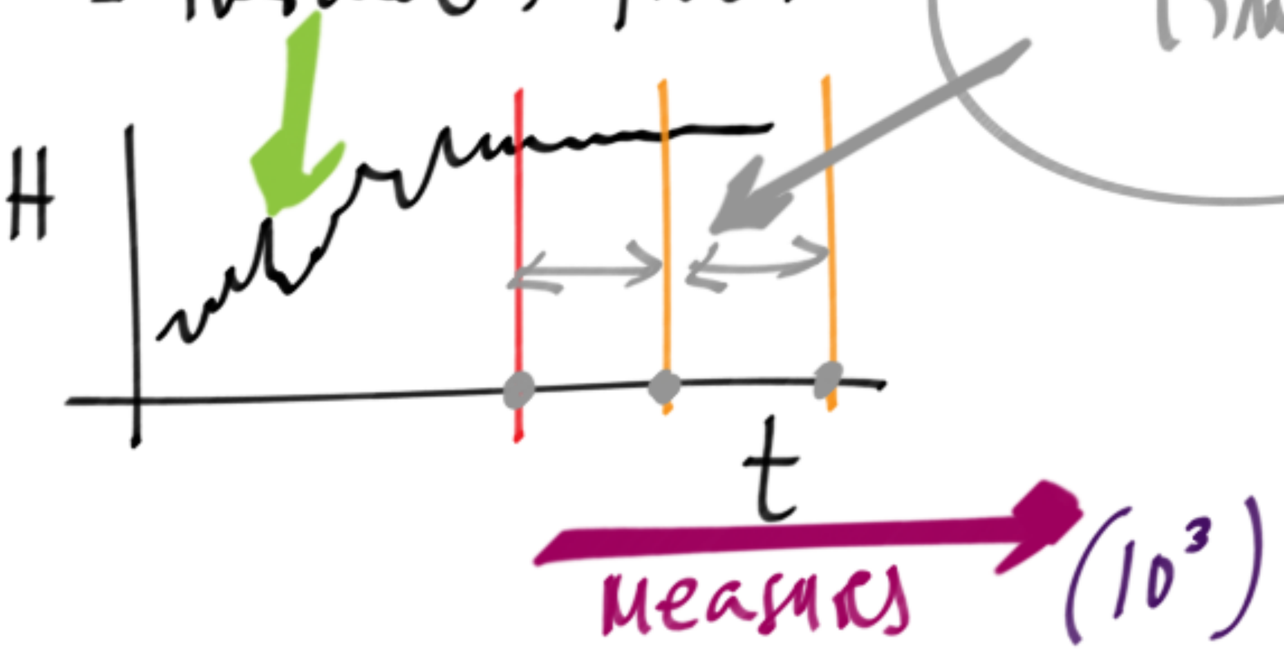
$$T\,(J/k_B) \in [0,5] \quad , \quad \Delta T = 0{,}1$$

$$L = (4, 8, 16, 32, 64)$$

Check!

- thermalization.

Correlation time



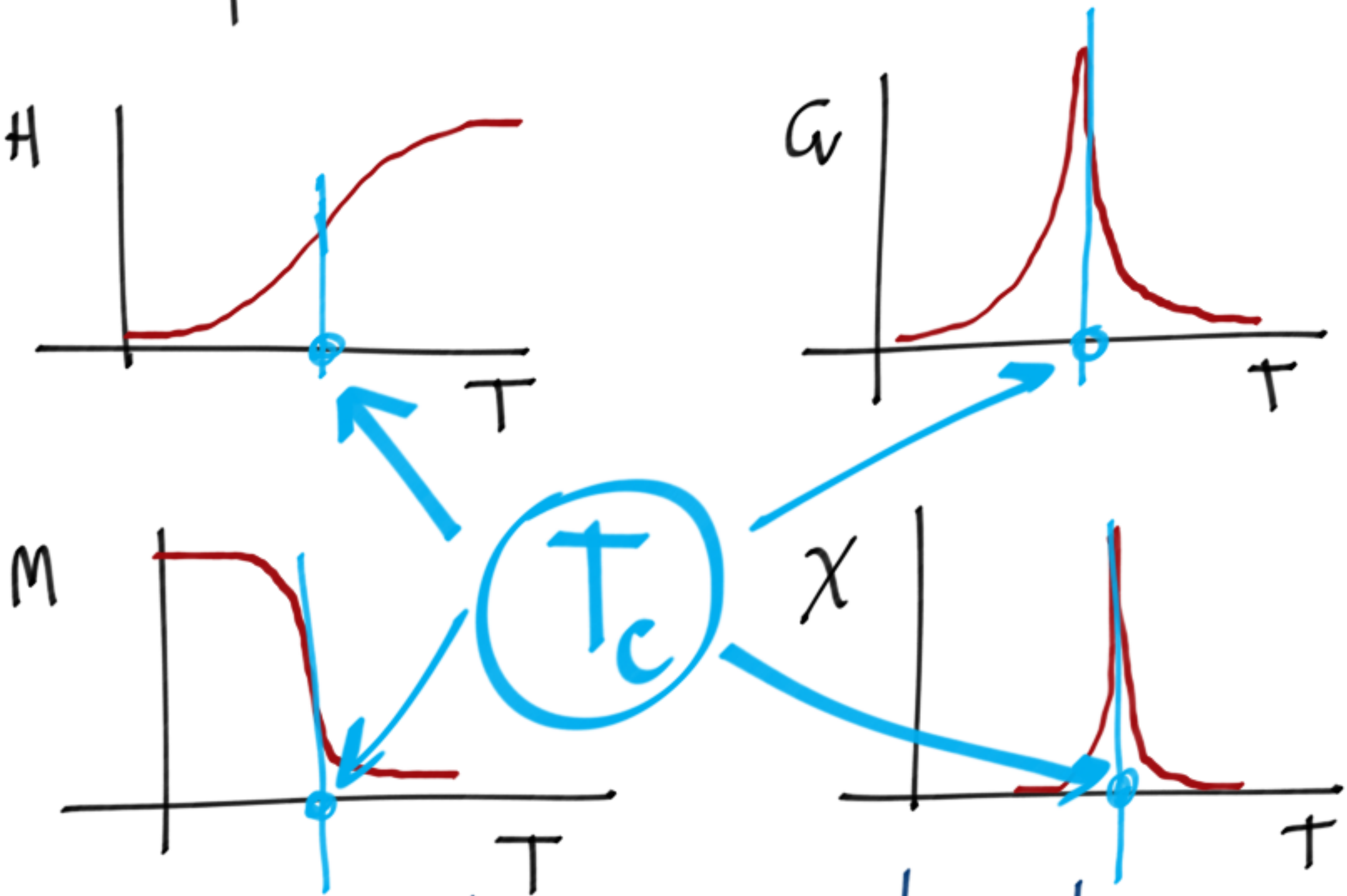
Estimate the correlation time

$$\chi(t) = \int dt' \left[M(t') M(t+t') - \langle M \rangle^2 \right] \sim$$

$$\sim e^{-t/t_c}$$

$$t_c = \int_0^\infty dt \, \frac{\chi(t)}{\chi(0)}$$

Expected Results.



continuum phase transition

theoretical Results (Onsager's)

- $T_c = \dfrac{2J}{k_B \ln(1+\sqrt{2})} = 2{,}269 \; J/k_B$

- $\langle M \rangle = \left\{ 1 - \left[\sinh(2\beta J) \right]^{-4} \right\}^{1/8}$

- $\langle H \rangle = -J \coth(2\beta J) \left[1 + \cdots \right]$

- $\dfrac{C_V}{k_B} = \dfrac{2}{\pi} \left(\dfrac{2J}{kT} \right)^2 \left[-\ln\left(1 - \dfrac{T}{T_c}\right) + \ln\left(\dfrac{kT_c}{2J}\right) - \left(1 + \dfrac{\pi}{4}\right) \right]$

near T_c

CRITICAL EXPONENTS

$$\tau = \frac{T - T_c}{T_c}$$

$\langle M \rangle \sim |\tau|^{\beta}$ $\quad$ $\beta = 1/8$

$C_V \sim |\tau|^{-\alpha}$ $\quad$ $\alpha = 0$ (log. divergence)

$\chi \sim |\tau|^{-\gamma}$ $\quad$ $\gamma = 7/4$

CORRELATION LENGTH

$$\langle (\sigma_i - \langle\sigma\rangle)(\sigma_j - \langle\sigma\rangle) \rangle \sim e^{-\frac{|i-j|}{\xi}}$$

$$\xi \sim |\tau|^{-\nu} \qquad \nu = 1$$

FINITE SIZE EFFECTS

Because of finite system size:

$$\boxed{\xi \sim L} \leftarrow \text{close to } T_c$$

$$\xi \sim |\tau|^{-\nu} \rightarrow L^{-1/\nu} \sim |\tau|$$

$$\chi \sim |\tau|^{-\gamma} \rightarrow \chi \sim \left[L^{-1/\nu}\right]^{-\gamma} = L^{\gamma/\nu}$$

Similarly

$$M \sim |\tau|^{\beta} \rightarrow L^{-\beta/\nu}$$

SCALING

$$\chi = L^{\gamma/\nu} f(L^{\frac{1}{\nu}} \tau)$$

$$\chi L^{-\gamma/\nu} = f(L^{1/\nu} \tau)$$

DATA COLLAPSE!

Universal scaling function

BEYOND METROPOLIS .... (close to T_c)

(local dynamics)

WOLFF ALGORITHM (global dynamics)

* CRITICAL SLOWING DOWN $\quad t_c \to \infty$ as $T \to T_c$

1. choose a spin at random. (SEED)
2. nn spins parallel to the SEED define the perimeter
3. Choose a perimeter spin
   - generate a flat Random Number η
   - Evaluate bond strength $\quad P = 1 - \exp\left(-\frac{2J}{kT}\right)$
   - If $\eta \leq P$ the bond is formed and spin clusters

     add nn spins to the perimeter list
   - REPEAT UNTIL NO PERIMETER SPINS REMAIN
   - Flip ALL the spins of the CLUSTER