remember last lecture:

$$\boxed{\frac{p_i(t+\Delta t)-p_i(t)}{\Delta t} = -\sum_{j\neq i} J_{ij}}$$ continuity equation

current $J_{ij} = \frac{1}{\Delta t}\left(-M_{ji}p_j + M_{ij}p_i\right) = -J_{ji}$

Example: random walk $\Big\}$ $M_{ij} = \frac{1}{2}\left(\delta_{j,i+1} + \delta_{j,i-1}\right)$

$\cdot 1/\Delta t$ $\qquad$ $\cdot 1/\Delta t$

$$p_i(t+\Delta t) - p_i(t) = \frac{1}{2}p_{i-1}(t) - p_i(t) + \frac{1}{2}p_{i+1}(t)$$

$\Delta t \to 0$ $\qquad \partial_t p_i(t) = \frac{1}{2\Delta t}\left(p_{i-1}(t) - 2p_i(t) + p_{i+1}(t)\right)$

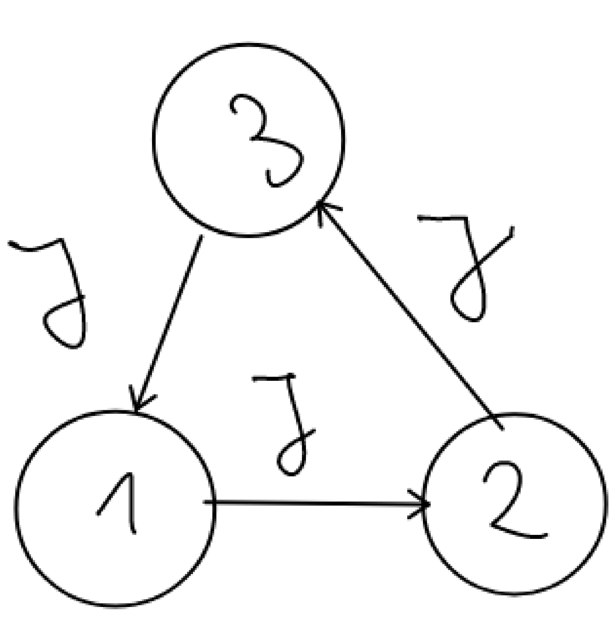
$N \to \infty$ $\qquad \partial_t p(x,t) = D\,\partial_x^2 p(x,t)$ diffusion law

equilibrium:

$$\vec{p}_{st}^{\,T}(t+\Delta t) = \boxed{\vec{p}_{st}^{\,T}(t)\cdot M = \vec{p}_{st}^{\,T}(t)}$$ (remember fixed point)

does not change anymore

$\Rightarrow \sum_{j\neq i} J_{ij} = 0$ $\quad$ ↯ we can still have circular currents like



stationary, but not yet equilibrium

we also need $\boxed{J_{ij} = 0}$

But how? Metropolis-Algorithm!

$$\boxed{M_{ij} = V_{ij}A_{ij} \text{ with } A_{ij} = \min\left(1, \frac{p_j}{p_i}\right) \text{ for } i\neq j}$$

interpretation: suggest new state j & accept probability $V_{ij} > 0$ & A_{ij}

additionally $V_{ij} = V_{ji}$ and $\sum_{j \neq i} V_{ij} = 1$

finally diagonal $\boxed{M_{ii} = 1 - \sum_{j \neq i} V_{ij} \min\left(1, \frac{P_j}{P_i}\right)}$

example: for $i = 1, \ldots, W$ $V_{ij} = V_{ji} = \frac{1}{W-1}$

12.3. Monte Carlo Simulation

remember Canonical ensemble with partion function

$$Z(T) = \sum_i e^{-\beta \mathcal{H}(i)}$$

$\mathcal{H}(i)$: Hamiltonian $\hat{=}$ energy of state

$\beta = 1/(k_B \cdot T)$

k_B = Boltzmann constant

⇝ probability for particle in state i

$$\boxed{P_B(i) = \frac{1}{Z} e^{-\beta \mathcal{H}(i)}}$$

We can now compute expectation values of arbitrary observables $\mathcal{O}$ as

$$\langle O \rangle = \sum_i P_B(i) \cdot \mathcal{O}(i) = \sum_i \frac{1}{Z} e^{-\beta \mathcal{H}(i)} \mathcal{O}(i)$$

use MC methods to compute, example

12.4. Ising model

lattice of spins (small magnets)

$\uparrow \quad \uparrow \quad \downarrow \quad \downarrow \quad \dots$ two states $\uparrow$ $S_n = 1$

$\downarrow$ $S_n = -1$

$\frac{\hbar}{2} S_n$ are eigenvalues of spin operator $\hat{S}_n^{(z)}$

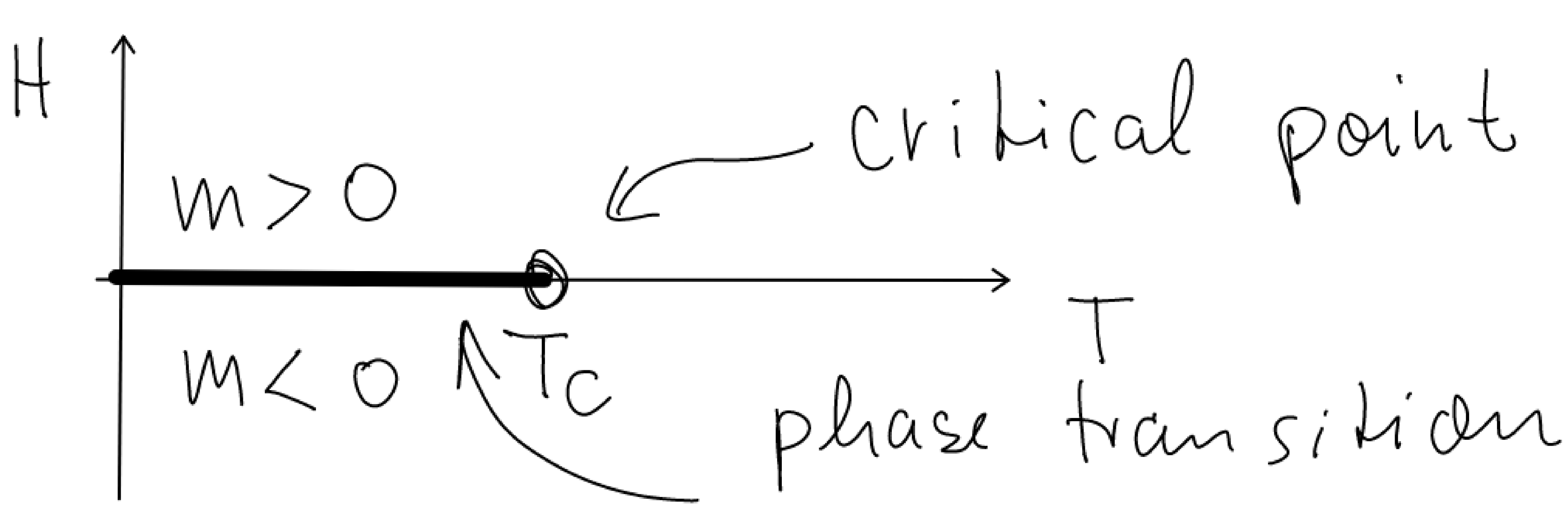
$$\boxed{\mathcal{H} = -\frac{1}{2} \underbrace{\sum_{n \neq m} J_{nm} S_n S_m}_{\text{coupling between spins}} - \underbrace{H}_{\text{external magnetic field}} \sum_{n=1}^{N} S_n}$$

$$J_{ij} = \begin{cases} J > 0 & i,j \text{ nearest neighbors} \\ 0 & \text{otherwise} \end{cases}$$

Consider the state $\{S_n\} = (s_1, \dots, s_N)$ with

$$\mathcal{H}(s_1, \dots, s_N) = -J \sum_{(n,m)\ \text{n.n.}} S_n S_m - H \sum_{n=1}^{N} S_n$$

- It has the partition function
$$Z(N, H, T) = \sum_{S_1 = \pm 1} \dots \sum_{S_N = \pm 1} e^{-\beta \mathcal{H}(s_1, \dots, s_n)}$$
- important observables are
  1) average energy $E = \langle \mathcal{H} \rangle$
  2) magnetization $M = \langle \sum_n S_n \rangle$
  3) specific heat capacity $C = \frac{\partial E}{\partial T} = \frac{1}{k_B T^2} \left(\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 \right)$
- in 2-dim. phase transition



T_C = Curie temperature

below ferro, above para magn.

$N = 100 \times 100 = 10^4$ states $\rightsquigarrow$ MC with importance sampling from Metropolis alg.

$$\boxed{A_{ij} = \min\left(1, \frac{P_B(j)}{P_B(i)}\right) = \min\left(1, e^{-\beta \underbrace{(\mathcal{H}(j) - \mathcal{H}(i))}_{\Delta E}}\right)} \quad (1)$$

Simulation step:

1) suggest $i \to j$ with $V_{ij} = V_{ji} \left(= \frac{1}{N-1}\right)$
2) accept with probability A_{ij} from (1)
   - compute $\Delta E = \mathcal{H}(j) - \mathcal{H}(i)$

   $\Delta E < 0$, accept always

   $\Delta E > 0$: 2a) get random $p \in [0,1]$

   2b) $p < e^{-\beta \Delta E}$ ✓ accept, × reject

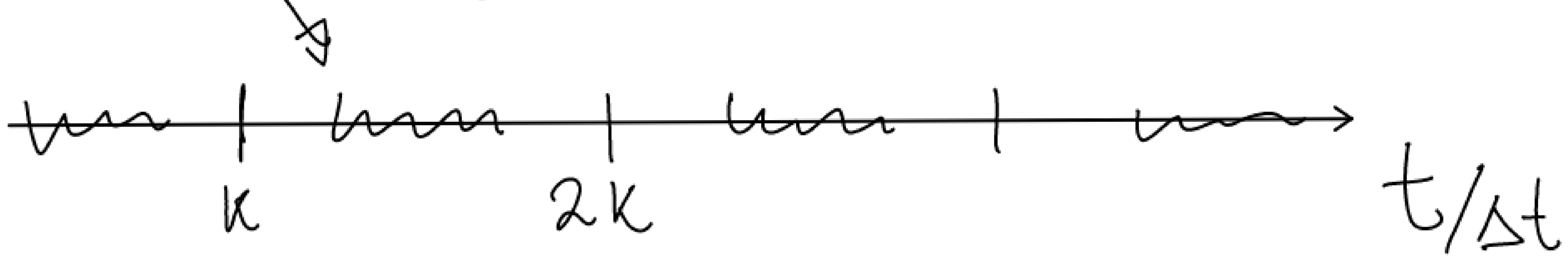
3) go back to 1)

4) average of L steps (measurement)

$$\langle O \rangle_{MC} = \frac{1}{L} \sum_{n=1}^{L} O(i(n\Delta t)) = \langle O \rangle$$

better $n \cdot K \cdot \Delta t$

forget last state



Complete simulation

a) set inital state for $t = 0$

b) simulate many steps to go to equilibrium
(forget initial state)

c) measurement