$$\Rightarrow \sum_{\substack{j=1 \\ j \neq i}}^{N} \left[w_{j \to i} n_j - w_{i \to j} n_i \right] = 0$$

Can make sure that this holds by choosing $w_{j \to i}$ such that

$$w_{j \to i} n_j = w_{i \to j} n_i \quad \text{for all } i \text{ and } j$$

"detailed balance"

$$w_{j \to i} = w_{i \to j} \frac{n_i}{n_j} = w_{i \to j} \frac{n_i}{n_j} = w_{i \to j} e^{-\beta(E_i - E_j)}$$

do not need to know partition function $Z(T)$!

3/4
3/11

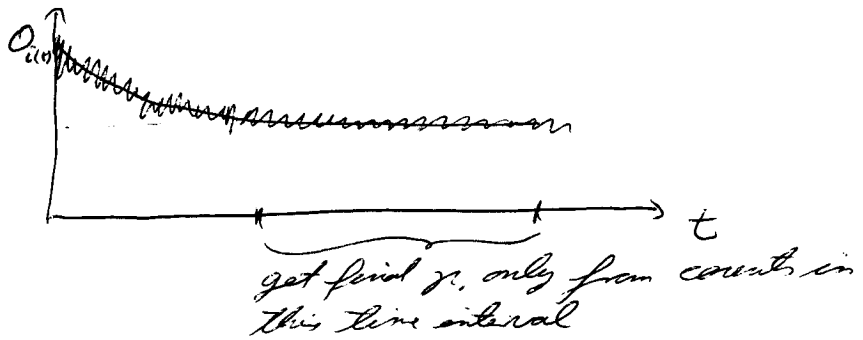
In practice:

- Choose most $w_{i \to j}$ to be zero as long as
  - if $w_{i \to j} = 0$ then also $w_{j \to i} = 0$
  - it is possible for the system to go from any i to any j through intermediate states
- Choose $w_{i \to j} = \begin{cases} 1 & E_j \leq E_i \\ e^{-\beta(E_j - E_i)} & E_i < E_j \end{cases}$ *
- Look at time evolution of a single system instead of an ensemble

Metropolis algorithm:

- Choose random state i
- Repeat for $T \gg 1$ time steps
  - Choose a random state j among all states with $w_{i\to j} > 0$
  - if $E_j \le E_i$ make j the new state i
  - if $E_j > E_i$ choose random number $r \in [0,1]$ If $r < e^{-\beta(E_j - E_i)}$ make j the new state i, otherwise stay at i
- n_i = # of time steps during which i is the current state
- $p_i \approx \frac{n_i}{T}$

Choose T by looking at observable O



VII.1.2 Ising model

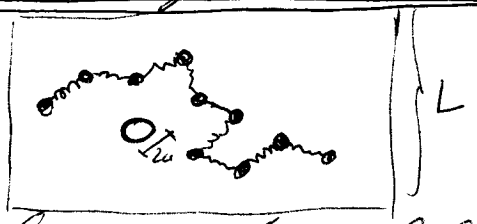
N spins on a lattice $i \to (s_1, \dots, s_N)$ $\quad s_n \in \{\pm 1\}$

$$E_{(s_1,\dots,s_N)} = -J \sum_{n=1}^{N'} \sum_{\substack{m \text{ neighbor} \\ \text{of } n}} s_n s_m$$

Choose $w_{(s_1,\dots,s_N)\to(s_1',\dots,s_N')} = 0$ unless $(s_1,\dots,s_N)$ and $(s_1',\dots,s_N')$ differ only in one spin.

- Choose N random numbers $r_1, \dots, r_N$ between 0 and 1 (uniform) and initialize $s_n = +1$ if $r_n < \frac{1}{2}$, $s_n = -1$ if $r_n > \frac{1}{2}$
- Calculate magnetization $M(t=0) = \sum_{n=1}^{N} s_n$
- Repeat $T \gg 1$ times
  - pick random spin $n \in \{1, \dots, N\}$
  - calculate $S = \sum_{m \text{ neighbors}} s_m$ and $\Delta E = -\frac{J}{2} S((-s_n) - s_n) = J S s_n$
  - if $\Delta E \leq 0$ update $M \to M - 2s_n$, $s_n \to -s_n$
  - if $\Delta E > 0$ choose random numb $r \in [0,1]$, if $r < e^{-\beta \Delta E}$ update $M \to M - 2s_n$, $s_n \to -s_n$

VII.1.3 Polymer and attractive defect



polymer = chain of N beads connected by springs of length ℓ.
configuration: $(\vec{r}_1, \dots, \vec{r}_N)$ = positions of all the N beads
attractive defect: Energy gain ϵ for each bead with $|\vec{r}_n| \leq a$

$$\Rightarrow H(\vec{r}_1, \dots, \vec{r}_N) = \sum_{n=1}^{N-1} \frac{k}{2} (|\vec{r}_{n+1} - \vec{r}_n| - \ell)^2 - \epsilon \sum_{n=1}^{N} \delta_{|\vec{r}_n| \leq a}$$

choose $W_{(\vec{r}_1, \dots, \vec{r}_N) \to (\vec{r}_1', \dots, \vec{r}_N')} = 0$ unless $\vec{r}_1, \dots, \vec{r}_N$ differ in only one position and difference in that position is inside a cube of length $2\Delta r$

- Choose random initial position $\vec{r}_n$ within simulation box
- Calculate $R^2 = \sum_{i=1}^{N} \vec{r}_i^{\,2}$
- Repeat for $T \gg 1$ steps
  - choose random label $n \in \{1, \ldots, N\}$
  - choose random vector $\vec{\delta}$ within cube of size $2\Delta r$
  - if $\vec{r}_n + \vec{\delta}$ is inside simulation box
    + Calculat $\Delta E \equiv \frac{k}{2}\big[(|\vec{r}_{n+1} - \vec{r}_n - \vec{\delta}| - \ell)^2 + (|\vec{r}_n + \vec{\delta} - \vec{r}_{n-1}| - \ell)^2 - (|\vec{r}_{n+1} - \vec{r}_n| - \ell)^2 - (|\vec{r}_n - \vec{r}_{n-1}| - \ell)^2 \big] - \epsilon\left(\delta_{|\vec{r}_n + \vec{\delta}| \le a} - \delta_{|\vec{r}_n| \le a}\right)$
      (with appropriate modification if $n = 1$ or $n = N$)
    + if $\Delta E \le 0$ update $R^2 \to R^2 - \vec{r}_n^{\,2} + (\vec{r}_n + \vec{\delta})^2$, $\vec{r}_n \to \vec{r}_n + \vec{\delta}$
    + if $\Delta E > 0$ choose random number $r \in [0, 1[$. If $r < e^{-\beta \Delta E}$ update $R^2 \to R^2 - \vec{r}_n^{\,2} + (\vec{r}_n - \vec{\delta})^2$, $\vec{r}_n \to \vec{r}_n + \vec{\delta}$

VII.2 Summary

concepts:

detailed balance

Metropolis algorithm

facts:

$$w_{i \to j} = \begin{cases} 1 & \Delta E \le 0 \\ e^{-\beta \Delta E} & \Delta E > 0 \end{cases}$$

unbinding transition of polymer from defect

tools:

Master equation

3/11