Markov Chain Monte Carlo

PHYS 246 class 9

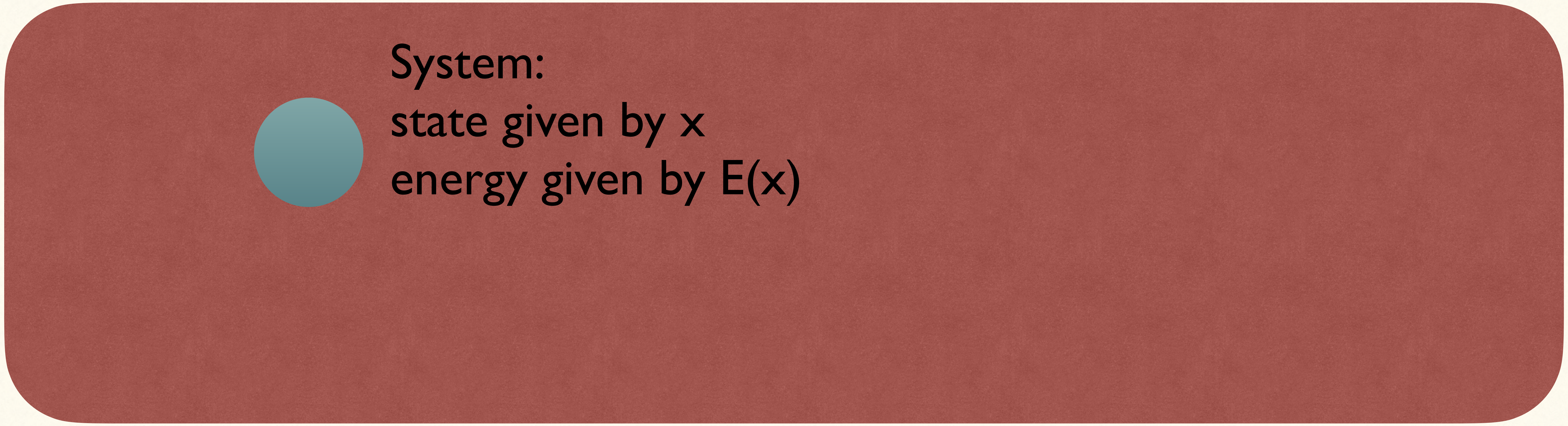
https://lkwagner.github.io/IntroductionToComputationalPhysics/intro.html

Announcements/notes

```
from google.colab import drive
drive.mount('/content/drive')
!cp /content/drive/MyDrive/Colab\ Notebooks/Dynamics.ipynb ./
!jupyter nbconvert --to HTML "Dynamics.ipynb"
```

- Hope your spring break was great!
- 'Random walks' is due tonight.
- Reminder that we will prioritize help on *this* week's work today.
- Thanks to Surkhab for filling in last class!

Statistical mechanics



Environment at temperature T

Boltzmann:

$$\rho(x) = \frac{e^{-\frac{E(x)}{kT}}}{\int e^{-\frac{E(x)}{kT}} dx} \equiv \frac{e^{-\frac{E(x)}{kT}}}{Z}$$

Averages:

$$\langle O(x) \rangle = \int O(x) \rho(x) dx$$

Monte Carlo integration

Boltzmann:

$$\rho(x) = \frac{e^{-\frac{E(x)}{kT}}}{\int e^{-\frac{E(x)}{kT}} dx} \equiv \frac{e^{-\frac{E(x)}{kT}}}{Z}$$

Averages:

$$\langle O(x) \rangle = \int O(x)\rho(x)dx$$

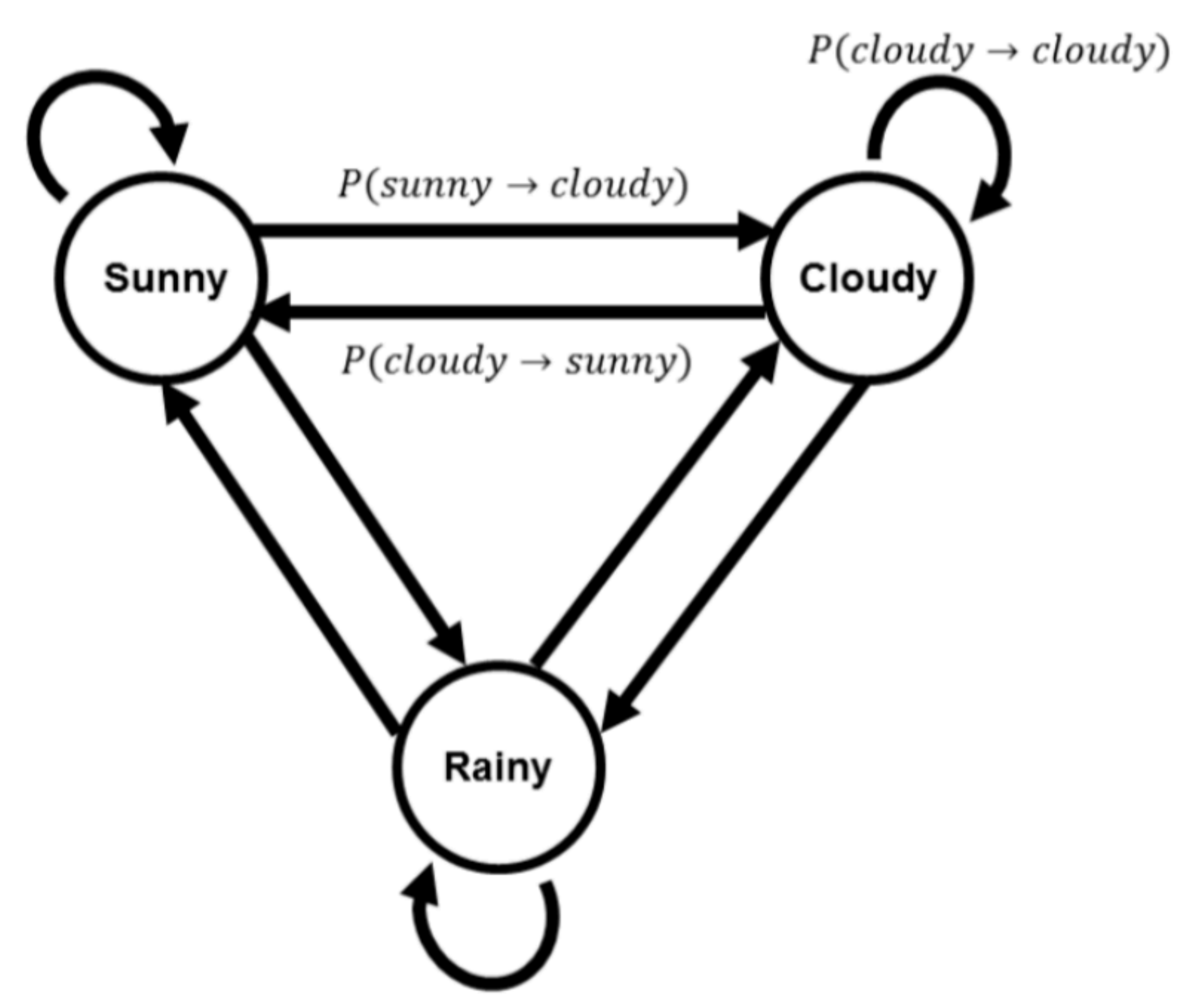
x might be very high dimensional!

$$\langle O(x) \rangle = \int O(x)\rho(x)dx = \langle O(x) \rangle_{x \sim \rho}$$

Expectation value

Sample average where x is drawn from ρ

Markov chains



We will use Markov chains to generate x from the Boltzmann distribution.

Markov chains are random processes that only depend on the current state.

Almost everything can be written as a Markov chain..

Metropolis algorithm: simple case

If you are in state A:
With probability 0.5, move to state B
With probability 0.5, stay in state A

If you are in state B:
With probability 1, move to state A

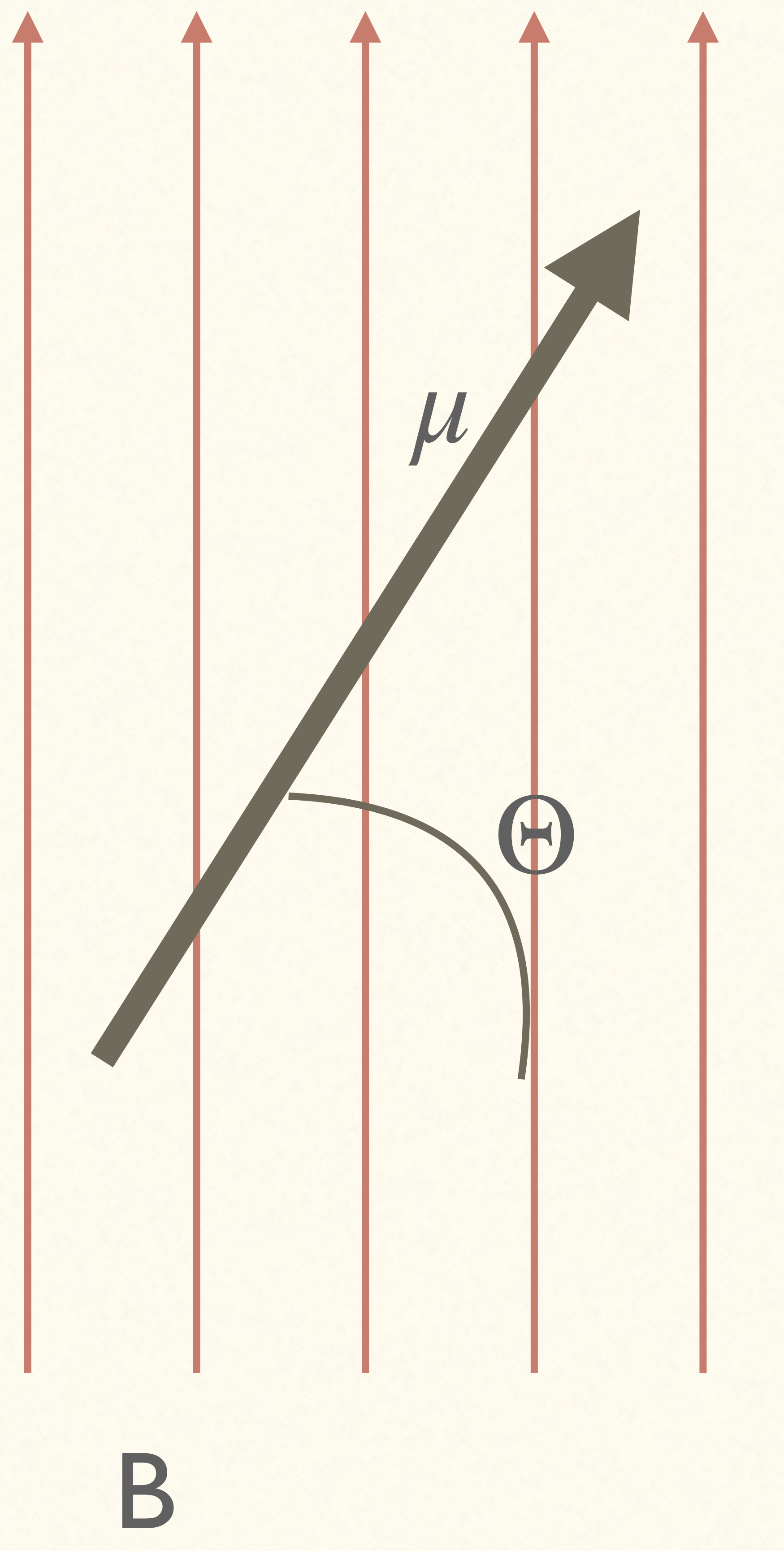
Question: what is the probability distribution we will sample?

Metropolis: general case

Looping over i

1. Start at point x_i
2. Choose point t at random (note some caveats)
3. x_{i+1} is set to t with probability $\min\left(1, \frac{\rho(t)}{\rho(x_i)}\right)$, otherwise $x_{i+1} = x_i$

Example 1: Classical dipole



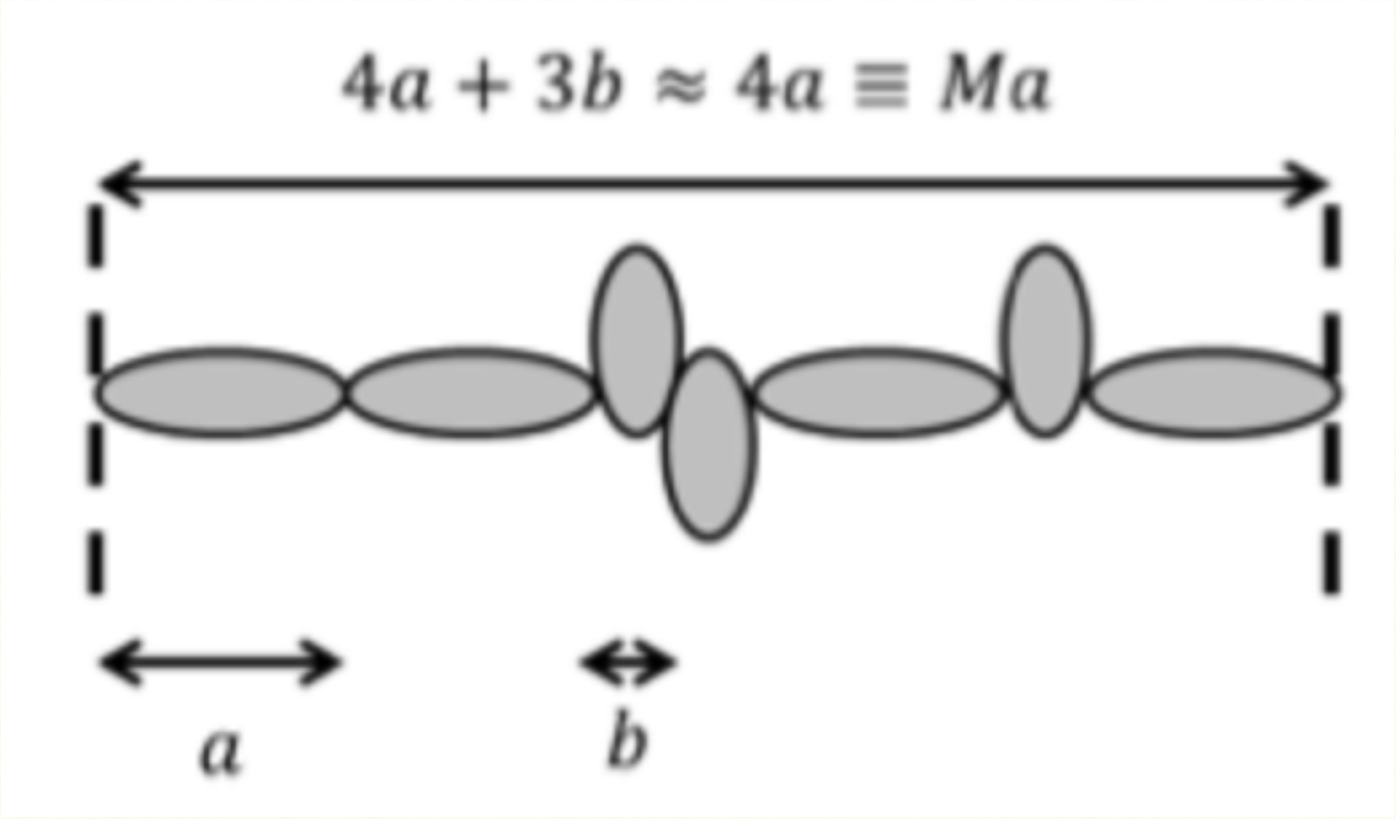
Variable: Θ
Energy: $E(\Theta) = -\mu B \cos\Theta$
Observable: $m(\Theta) = \cos(\Theta)$

$$\langle m \rangle = \frac{1}{Z}\int e^{-E(\Theta)/kT} m(\Theta) d\Theta$$

What do we expect to see at high temperature?
Low temperature?

Example 11: Rubber band

Rubber band model



Variable: $S = [0,1,1,0,\ldots]$
Observable: $M(S) = a \sum_i s_i$

Energy: $E(S) = \epsilon M(S)$

Suppose ϵ is negative.
What happens at high temperature? Low temperature?

Notes and tricks

We work with unitless numbers $h = \dfrac{\mu B}{kT}$ and $\dfrac{\epsilon}{kT}$, which are the only things that change the physics. High temperature is small h and low temperature is large h.

Make sure that if you reject a move, you average the old position again.