Title: PSI 2018/2019 - Statistical Mechanics - Lecture 12

Date: Oct 29, 2018 10:45 AM

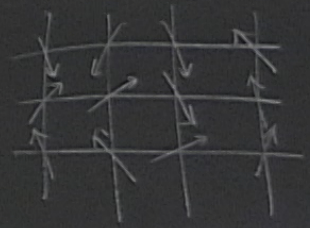
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Abstract:

Goal: to study phenomena such as phase transitions for systems of N interacting particles when N is large.

Specifically, today we will develop numerical Monte Carlo (MC) methods to study the XY model on a 2d lattice

$$H = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \quad ; \; 0 \leq \theta_i < 2\pi$$



Outline for today:

- Expectation values of observable quantities in classical stat. mech.
- Classical Monte Carlo (MC) methods
  - ↳ Importance sampling
  - ↳ Markov chain MC
  - ↳ Metropolis algorithm, single-spin-update algorithm
  - ↳ Data analysis practices: equilibration, measurement correlations

→ Metropolis algorithm, single-spin-update algorithm

↳ Data analysis practices: equilibration, measurement correlations

Expectation values of observables

In the canonical ensemble at fixed T, the expectation value of a quantity Q is:

$$\langle Q \rangle = \sum_{\mu}^{1} Q_\mu P_\mu$$

$$P_\mu = \frac{1}{Z} e^{-\beta E_\mu}, \quad Z = \sum_{\mu}^{1} e^{-\beta E_\mu}$$

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- $\beta = \frac{1}{k_B T}$ (set $k_B = 1$)
- μ represents a microstate of the system
- E_μ is the energy of state μ

rion

(set $k_B = 1$)

rts a microstate

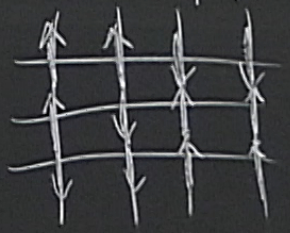
ystem

he energy of state μ

We would like to study
$\langle Q \rangle$ in the limit $N \to \infty$.

For example, consider the Ising model

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j \qquad \sigma_i = \pm 1$$



exact solutions known in $d=1$ and $d=2$

rion

(set $k_B=1$)

nts a microstate

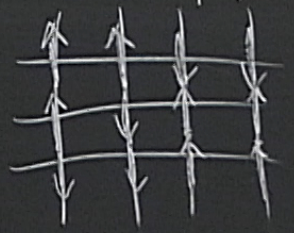
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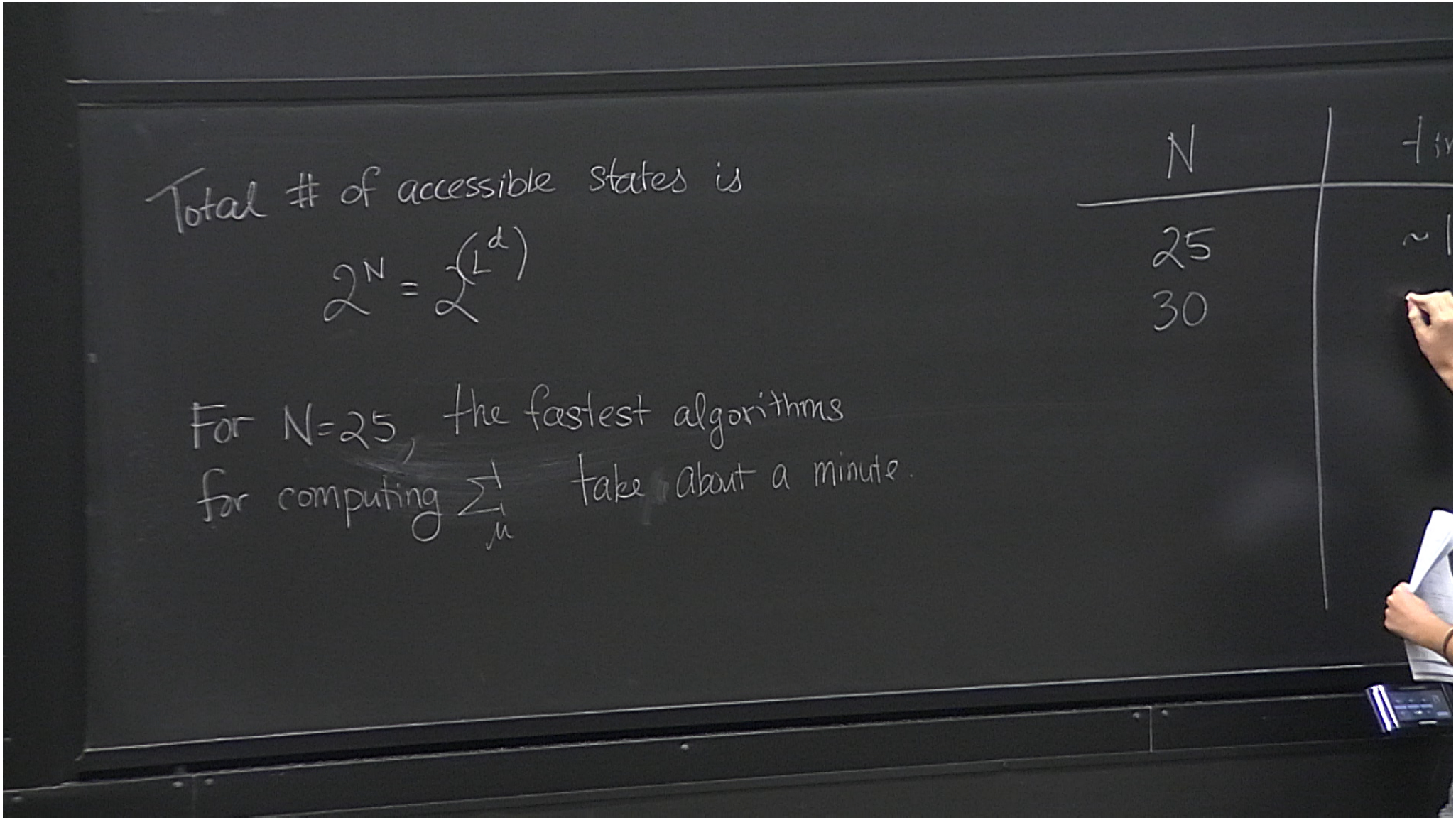
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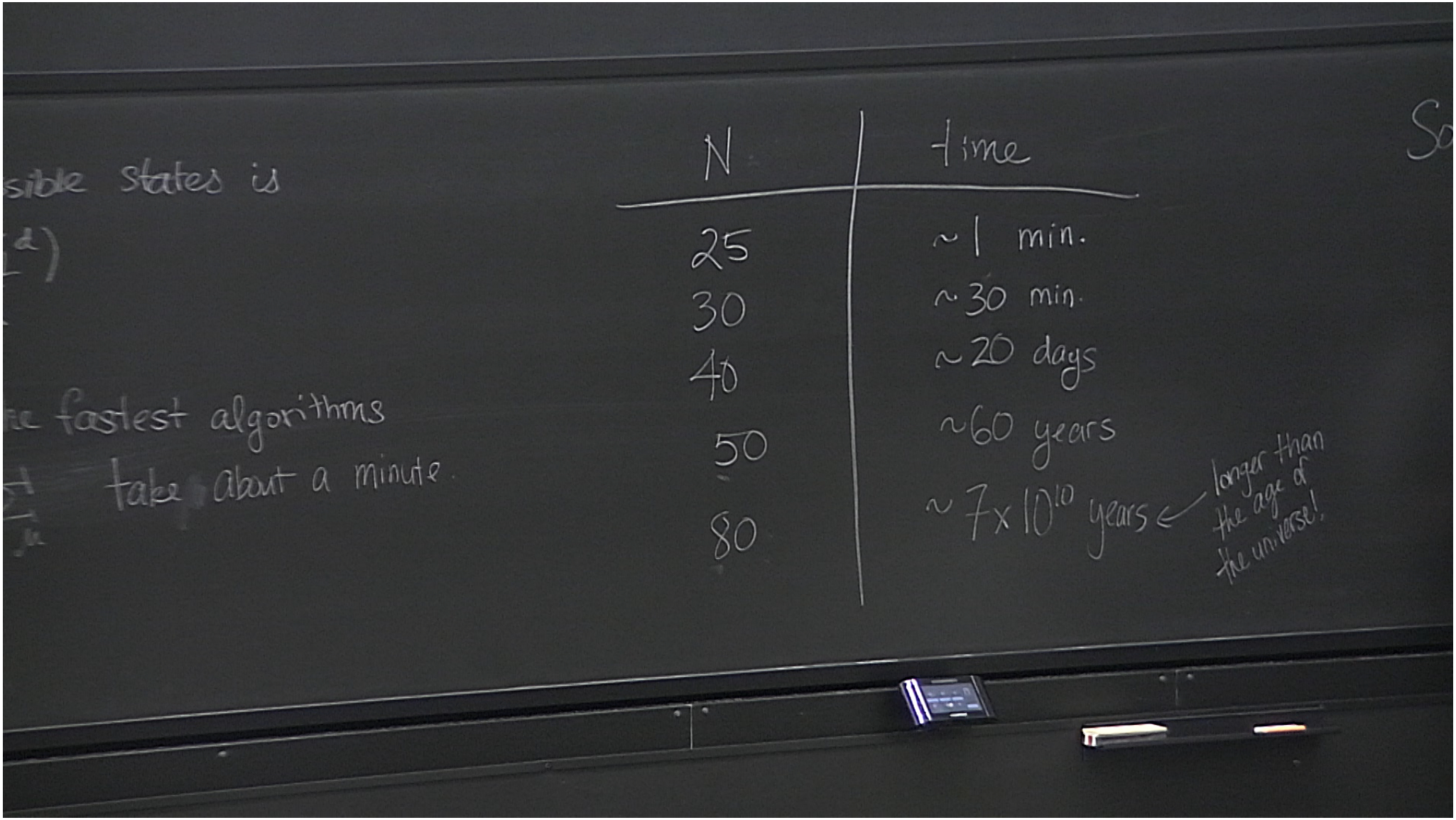
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exact solutions known in $d=1$ and $d=2$


Total # of accessible states is
$2^N = 2^{(L^d)}$
For N=25, the fastest algorithms
for computing $\sum_{\mu}^{\dagger}$ take about a minute.
N
25
30


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fastest algorithms
take about a minute.
N
time
25
~1 min.
30
~30 min.
40
~20 days
50
~60 years
80
~7x10^10 years
longer than the age of the universe!

Classical MC Methods

↳ addresses the exponential complexity by consider only M states

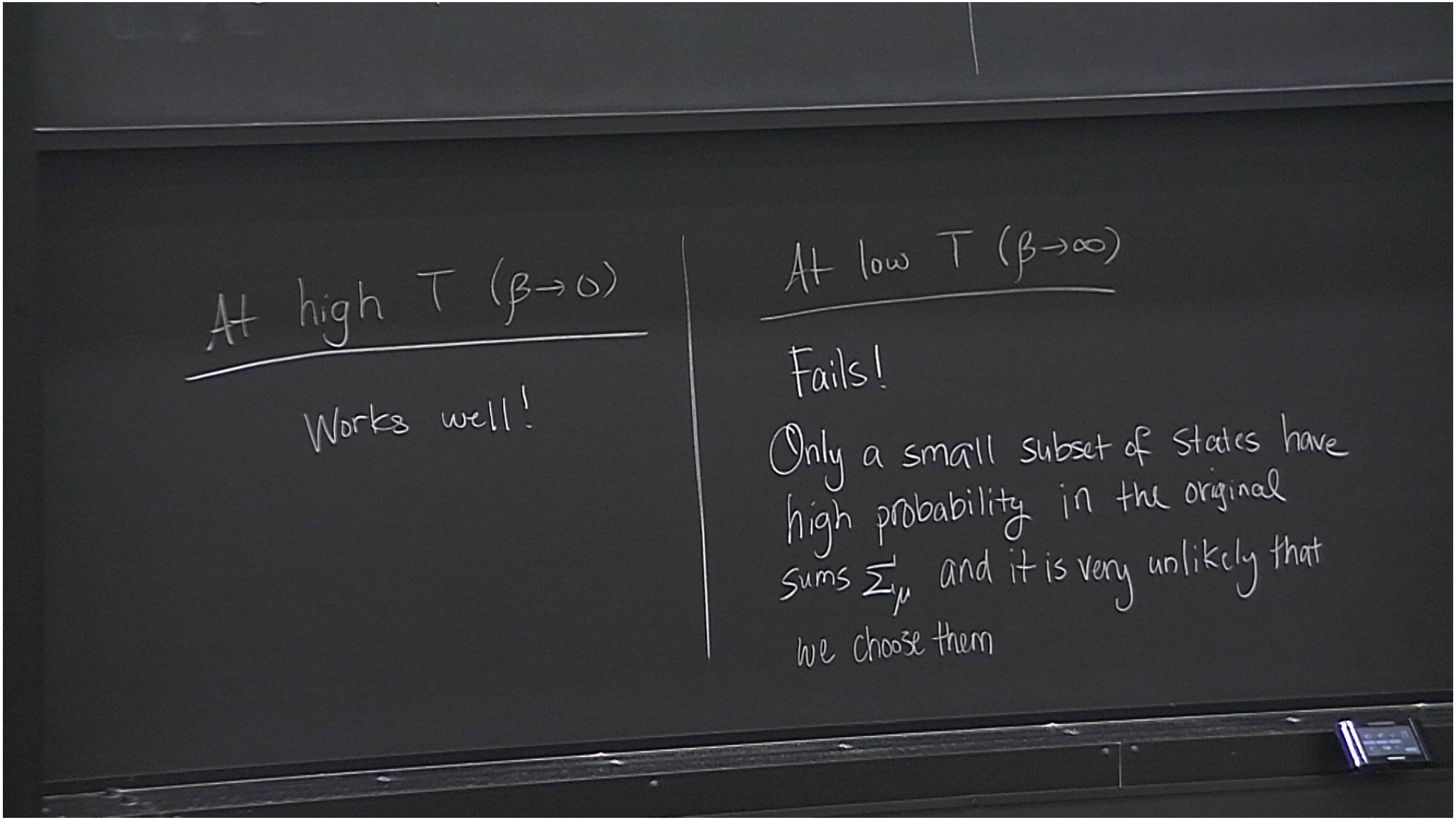
$\mu_1, \mu_2, \ldots, \mu_M$

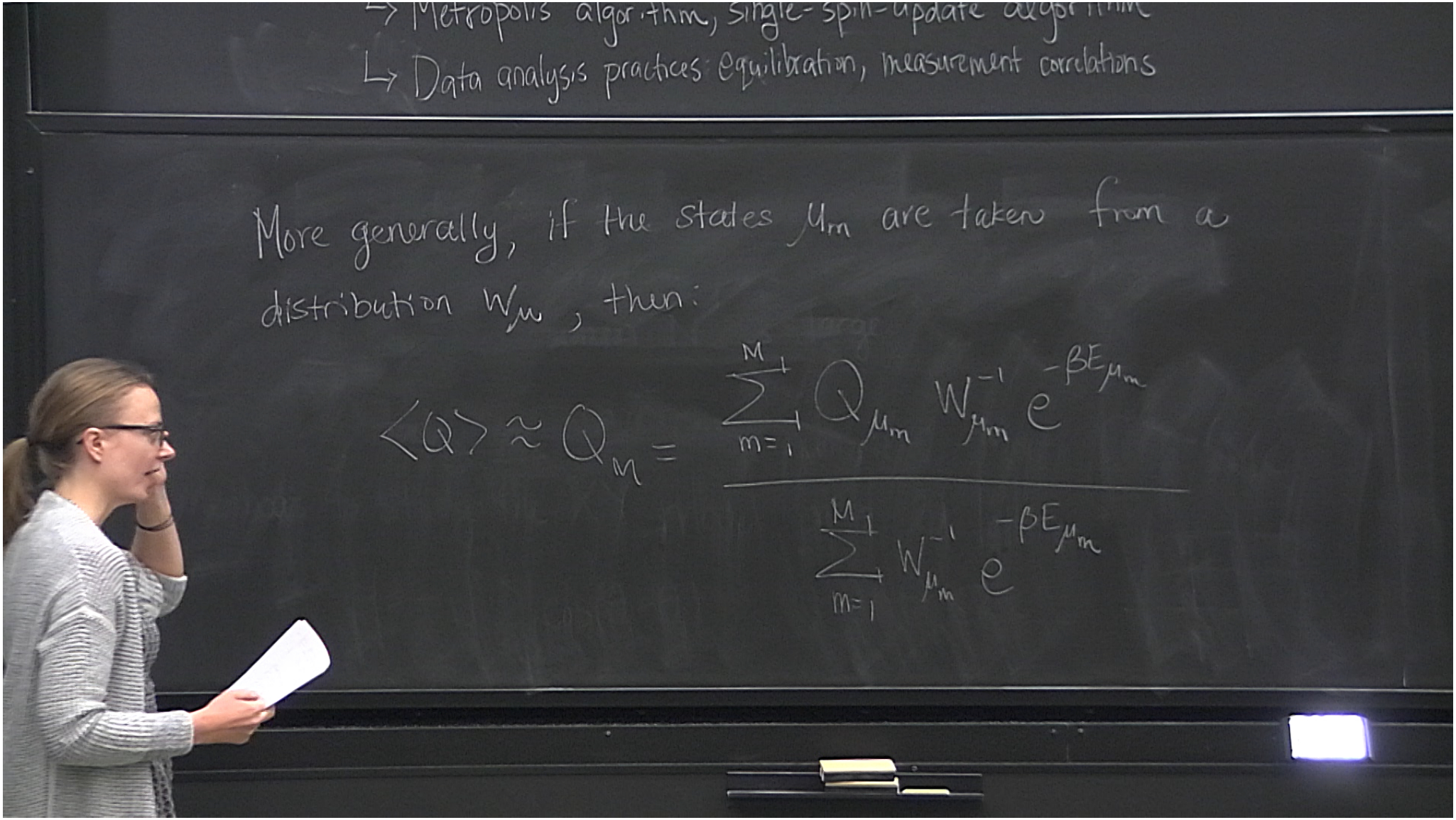
selected at random

For example, if we choose M states μ_m $(1 \leq m \leq M)$ from all possible states with equal probability ("flat sampling"):

$$\langle Q \rangle \simeq Q_M = \frac{\sum_{m=1}^{M} Q_{\mu_m} e^{-\beta E_{\mu_m}}}{\sum_{m=1}^{M} e^{-\beta E_{\mu_m}}}$$

"estimator"


At high T ($\beta \to 0$)
Works well!
At low T ($\beta \to \infty$)
Fails!
Only a small subset of states have high probability in the original sums Σ_μ and it is very unlikely that we choose them


↳ Metropolis algorithm, single-spin-update algorithm
↳ Data analysis practices: equilibration, measurement correlations
More generally, if the states μ_m are taken from a distribution W_μ, then:
$$\langle Q \rangle \approx Q_M = \frac{\sum_{m=1}^{M} Q_{\mu_m} W_{\mu_m}^{-1} e^{-\beta E_{\mu_m}}}{\sum_{m=1}^{M} W_{\mu_m}^{-1} e^{-\beta E_{\mu_m}}}$$

→ Metropolis algorithm, single-spin-update algorithm

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We

Importance sampling

We would like to sample the "important" (highly probable) states more frequently.

For example, if $W_\mu = P_\mu = e^{-\beta E_\mu}/Z$:

$$\langle Q \rangle \approx Q_M = \frac{1}{M} \sum_{m=1}^{M} Q_{\mu_m}$$

But how do we choose states according to P_μ?

We would like to study $\langle Q \rangle$ in the limit $N \to \infty$

Markov chain MC

Idea: given state μ_m, move to the next state μ_{m+1} according to the transition prob $T(\mu_m \to \mu_{m+1})$, where:

- $T(\mu_m \to \mu_{m+1})$ only depends on μ_m and μ_{m+1} (not earlier $\mu_1, \mu_2, \ldots$)
- $T(\mu_m \to \mu_{m+1})$ doesn't depend on time
- $\sum_\nu T(\mu \to \nu) = 1$

The resulting set $\{\mu_1, \mu_2, \cdots, \mu_M\}$ is called a Markov chain of states

We must satisfy two conditions:

(1) Ergodicity: Given two states μ and ν, it must be possible to transition between them (with non-zero prob.) through some chain of intermediate states

$\cdots, \mu_{m-1})$

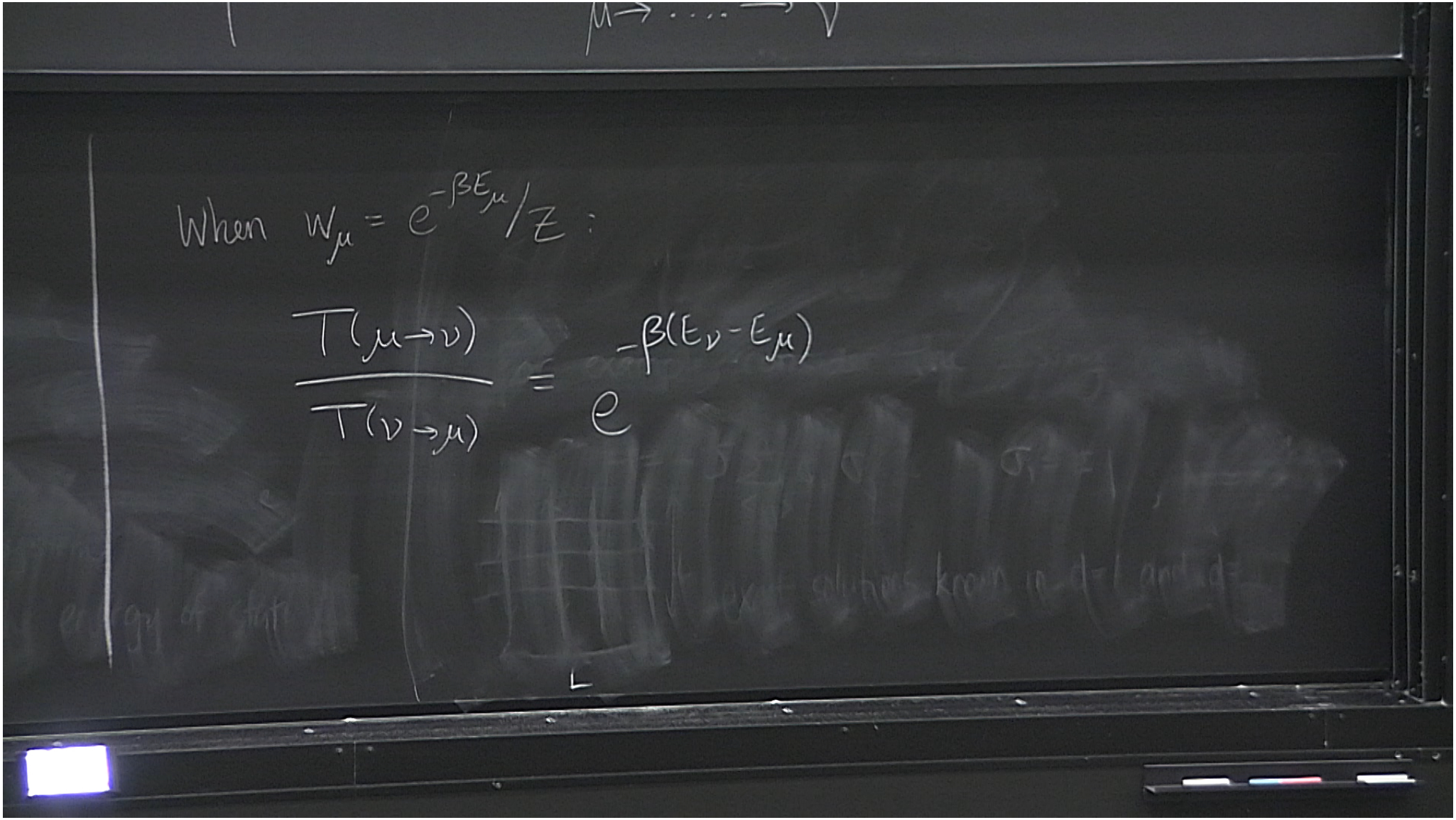
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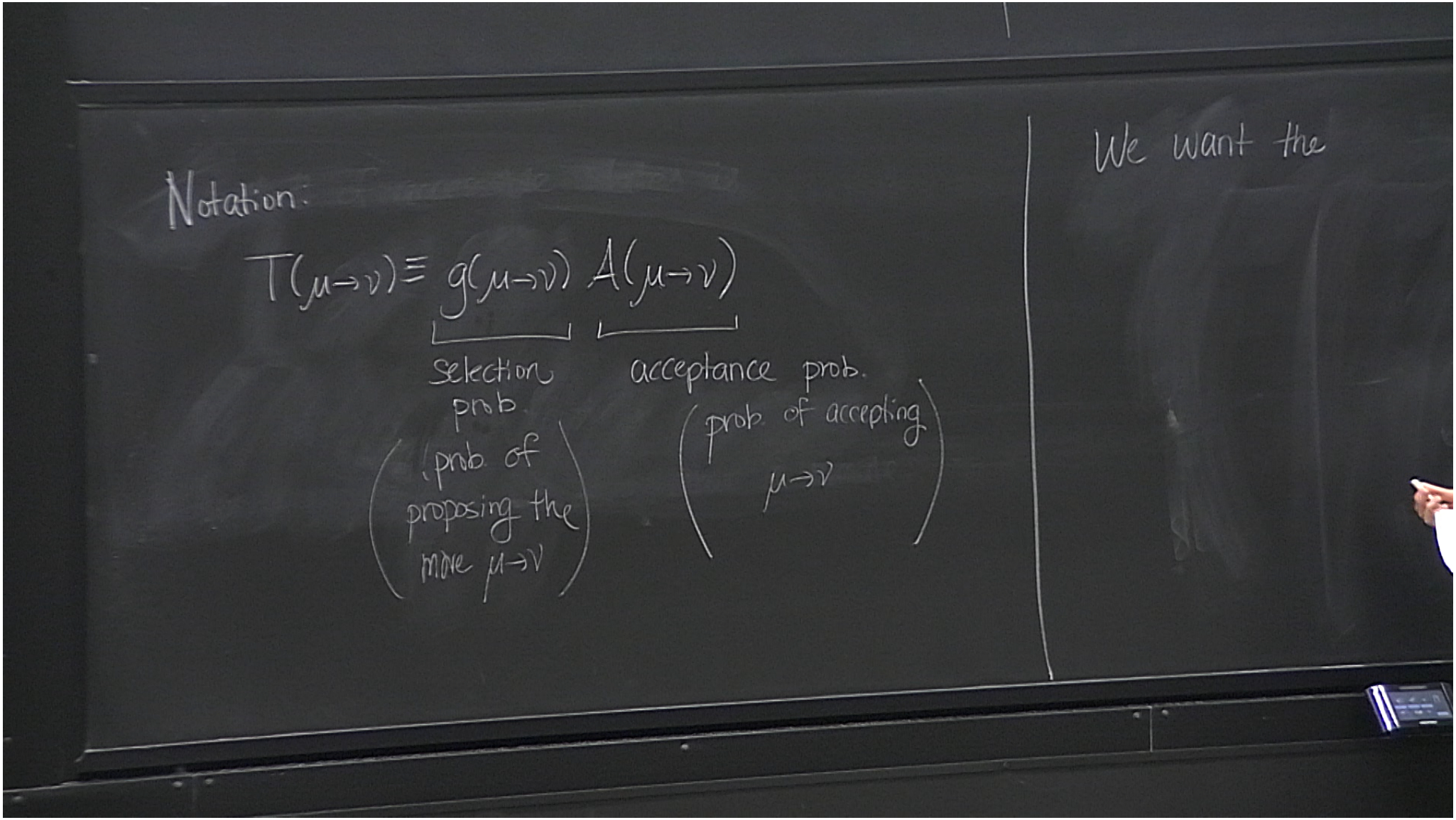
(2) Detailed balance (DB):

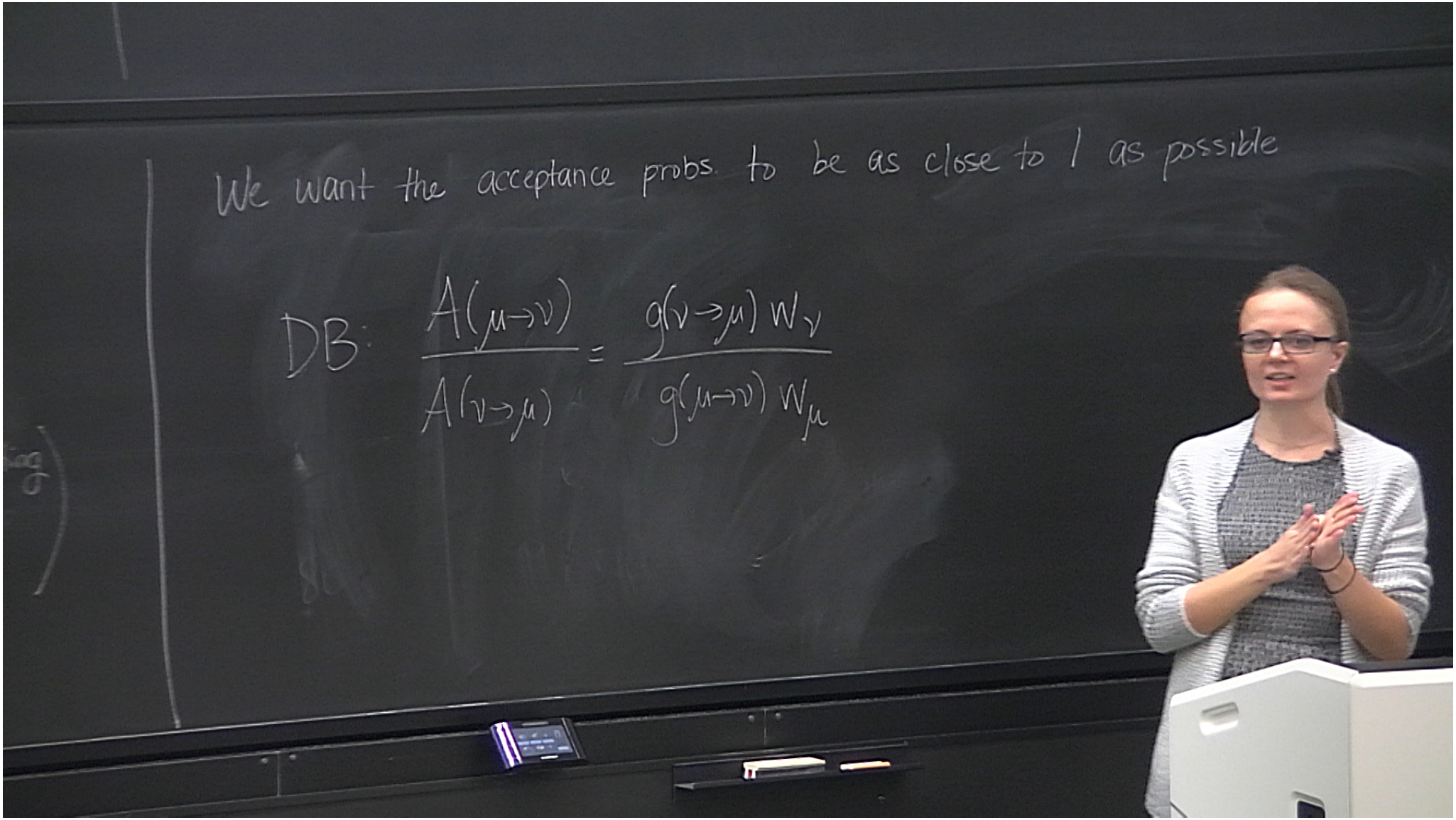
$$\underbrace{\sum_\nu W_\nu \, T(\nu \to \mu)}_{\text{rate of transition into } \mu} - \underbrace{\sum_\nu W_\mu \, T(\mu \to \nu)}_{\text{rate of transition out of } \mu} = 0 \qquad \forall \mu$$

One way to have this:

$$\boxed{W_\mu \, T(\mu \to \nu) = W_\nu \, T(\nu \to \mu)} \quad \text{DB}$$


When $W_\mu = e^{-\beta E_\mu}/Z$:
$\frac{T(\mu \to \nu)}{T(\nu \to \mu)} = e^{-\beta(E_\nu - E_\mu)}$


Notation:
$T(\mu \to \nu) \equiv g(\mu \to \nu)\, A(\mu \to \nu)$
selection prob
(prob. of proposing the move $\mu \to \nu$)
acceptance prob.
(prob. of accepting $\mu \to \nu$)
We want the


We want the acceptance probs. to be as close to 1 as possible
DB: $\frac{A(\mu \to \nu)}{A(\nu \to \mu)} = \frac{g(\nu \to \mu) W_\nu}{g(\mu \to \nu) W_\mu}$

Aside: weighted sums

$\sum_{u}^{t} p_u s_u$

$S = \{1, 2, 4, 8, 9\}$

$P = \{\frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}\}$

① Strategy: select from S uniformly at random N times

$y = \{8, 2, 1, 9, 1, 2, 4, 2, \ldots\}$



Aside: weighted sums

$\bar{s} = \sum_{\mu}^{t} p_\mu s_\mu$ $\quad s = \{1, 2, 4, 8, 9\}$

$= \frac{1+2+4+8+9}{5}$ $\quad p = \left\{\frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}\right\}$

(1) Strategy: select from s uniformly at random N times

$y = \{8, 2, 1, 9, 1, 2, 4, 2, \ldots\}$

$\sum_{\mu}^{t} y_\mu / N$ is a good approx for $\bar{s}$

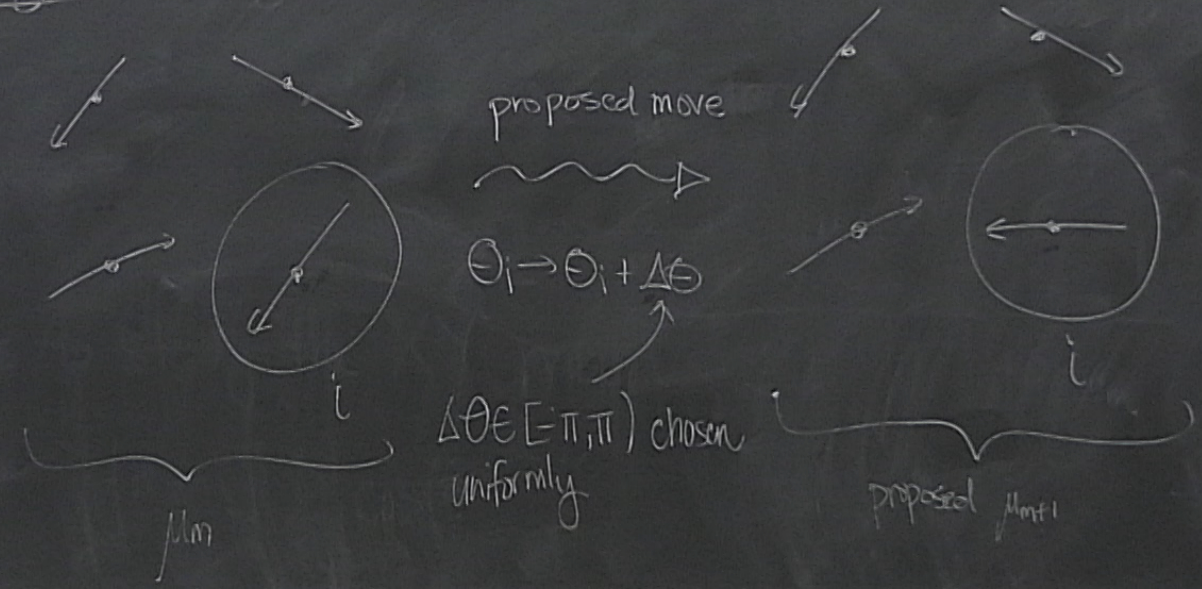
(2) Use weight



depend on time

$\sum_\nu T(\mu \to \nu) = 1$

Single-spin-update algorithm for the XY model



Selection

$g(\mu$

Selection probs.:

$$g(\mu \to \nu) = \begin{cases} \text{const.} & \text{if } \mu \text{ and } \nu \text{ differ by one spin rotation} \\ 0 & \text{otherwise} \end{cases}$$

Using Metropolis:

$$A(\mu \to \nu) = \begin{cases} e^{-\beta(E_\nu - E_\mu)} & \text{if } E_\nu > E_\mu \\ 1 & \text{otherwise} \end{cases}$$

$\mu \to \ldots \to \nu$

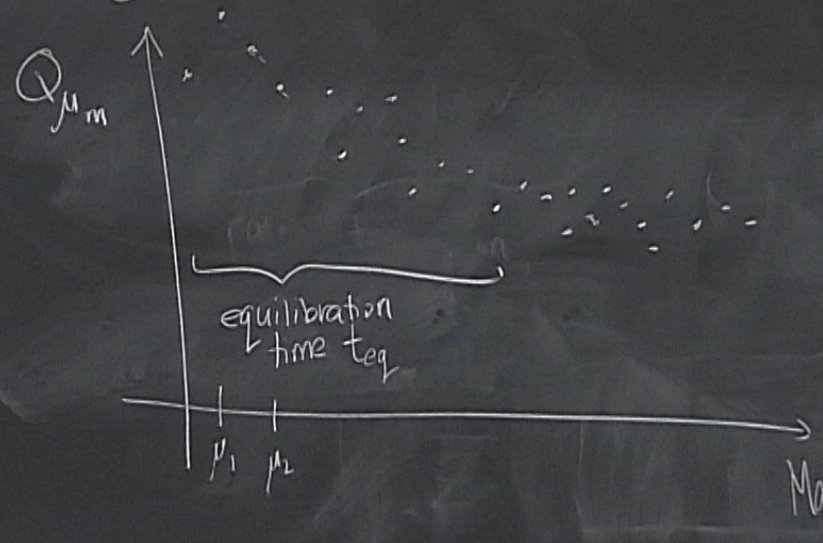
Single-spin-update Metropolis alg. for XY

1) Generate a random state μ_1 $(m=1)$
2) Choose site i of the lattice at random $(1 \leq i \leq N)$
3) Choose a random angle $\Delta\theta \in [-\pi, \pi)$
4) Calculate the energy diff ΔE associated with the move $\theta_i \rightarrow \theta_i + \Delta\theta$
5) Generate a random number $r \in [0,1)$ from a uniform distribution
6) If $\Delta E \leq 0$ OR $r < e^{-\beta \Delta E}$, accept the move to get μ_{m+1}
   Otherwise, reject the move $(\mu_{m+1} = \mu_m)$

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Otherwise, reject the move. ($\mu_{m+1} = \mu_m$)

Plotting some quantity vs. "Markov time"



So we use

Metropolis Algorithm

Ensure that $A = 1$ for $\mu \to \nu$ or $\nu \to \mu$

$$A(\mu \to \nu) = \min\left(1, \frac{g(\nu \to \mu)}{g(\mu \to \nu)} \frac{W_\nu}{W_\mu}\right)$$

For single-spin-updates, μ_m and μ_{m+1} are highly correlated.

As a result, we do (at least) a "sweep" of $O(N)$ proposed updates before adding μ_{m+1} to our samples.

μ_m and μ_{m+1} are separated by $O(N)$ proposed updates