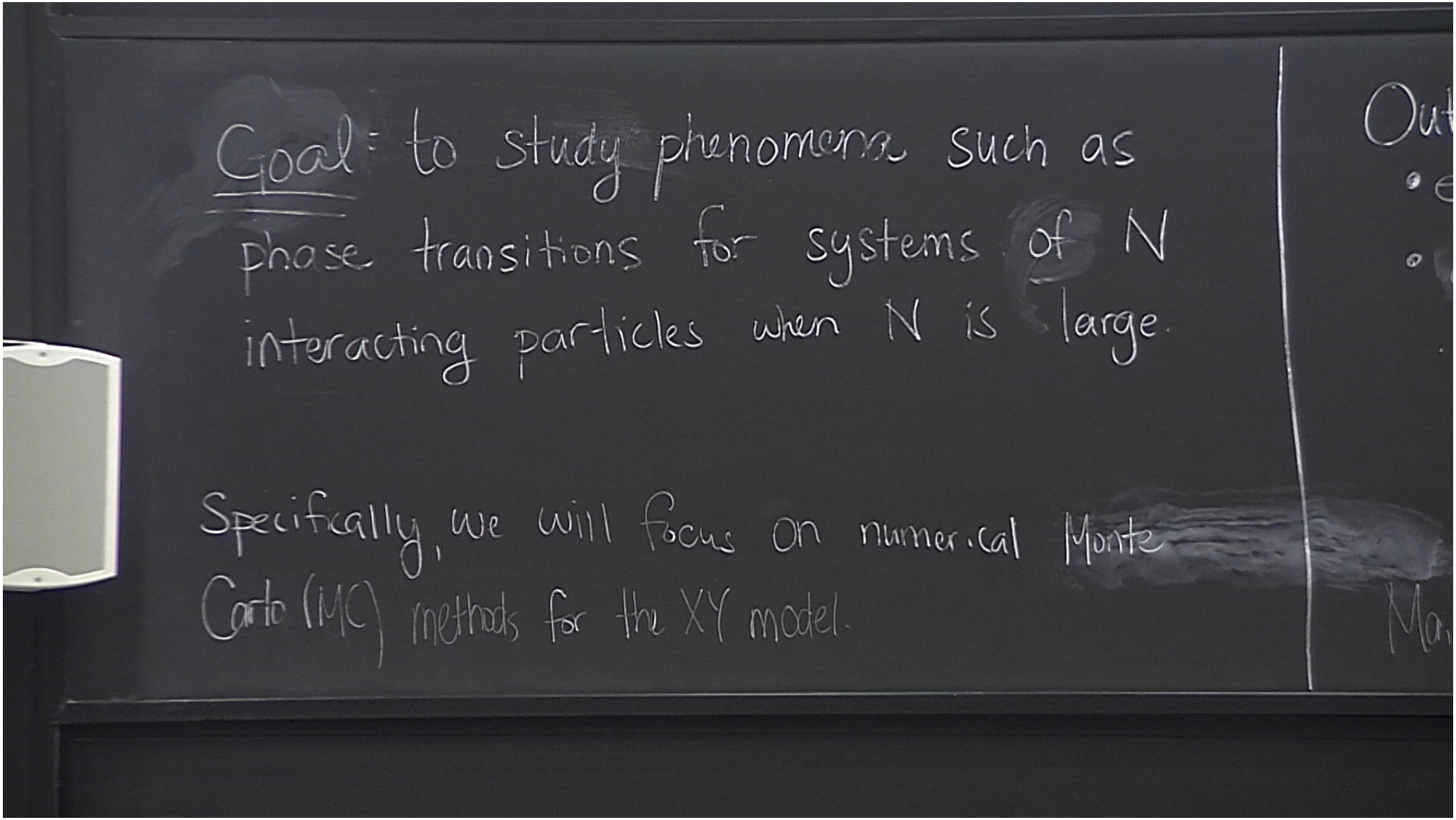
Title: PSI 2019/2020 - Condensed Matter (Wang) - Lecture 16

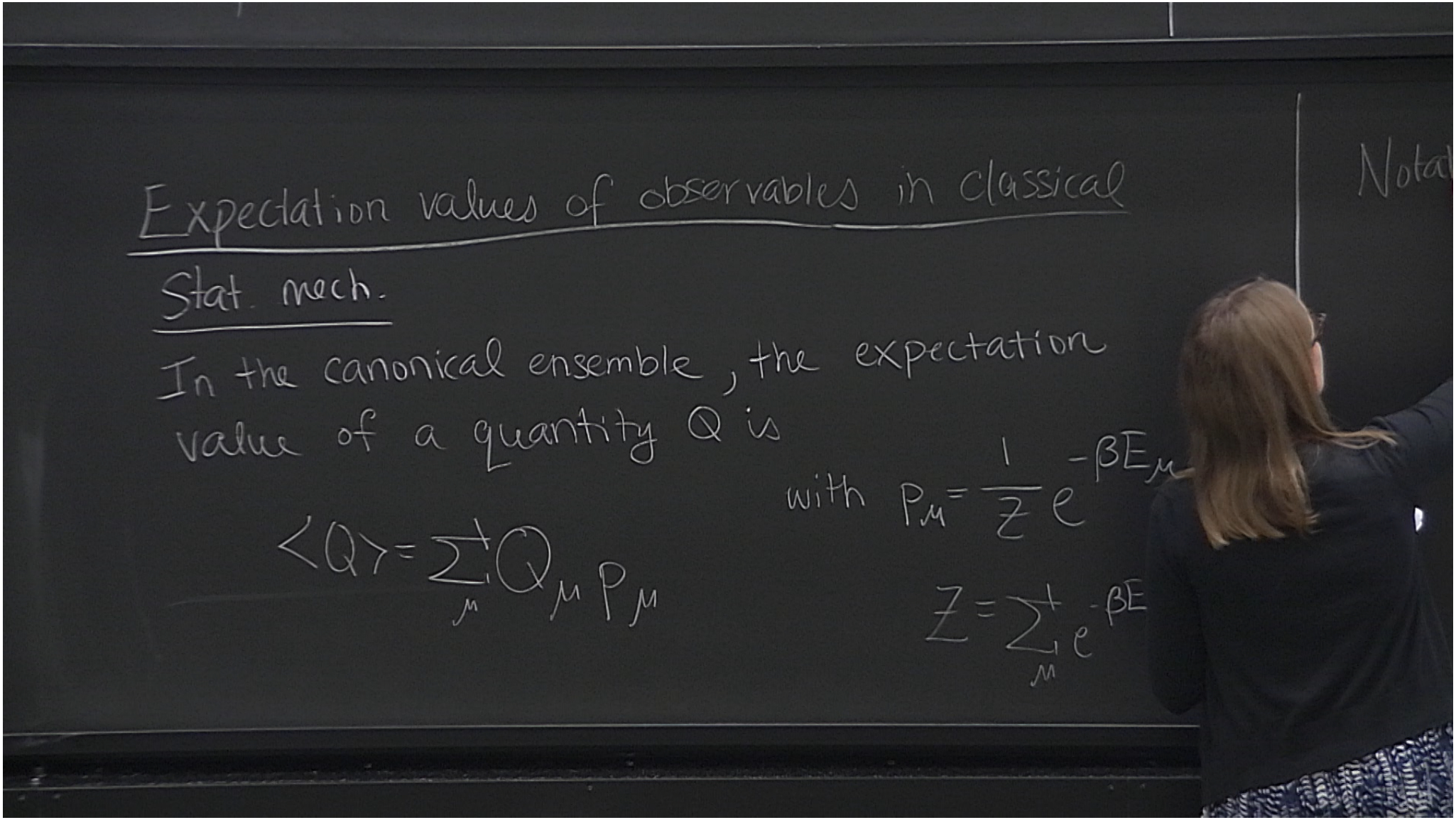
Speakers: Chong Wang

Collection: PSI 2019/2020 - Condensed Matter (Wang)

Date: December 06, 2019 - 10:45 AM

URL: http://pirsa.org/19120009


Goal: to study phenomena such as phase transitions for systems of N interacting particles when N is large.
Specifically, we will focus on numerical Monte Carlo (MC) methods for the XY model.


Expectation values of observables in classical
Stat. mech.
In the canonical ensemble, the expectation value of a quantity Q is
$\langle Q \rangle = \sum_{\mu}^{+} Q_\mu P_\mu$
with $P_\mu = \frac{1}{Z} e^{-\beta E_\mu}$
$Z = \sum_{\mu}^{+} e^{-\beta E}$
Nota

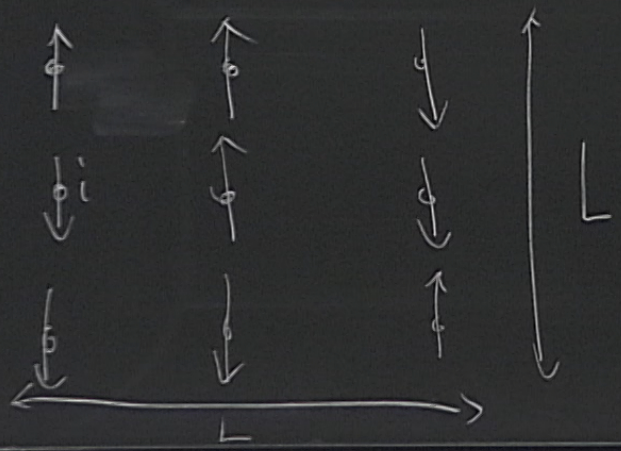
Notation:

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

We would like to study the behaviour of $\langle Q \rangle$ when $N \to \infty$

↳ # of particles

For example, consider how to evaluate the sums $\sum_{\mu}^{+}$ directly for an Ising model.



$$H = -J \sum_{\langle ij \rangle}^{+} s_i s_j$$

$$s_i = \pm 1$$

$$N = L^d$$

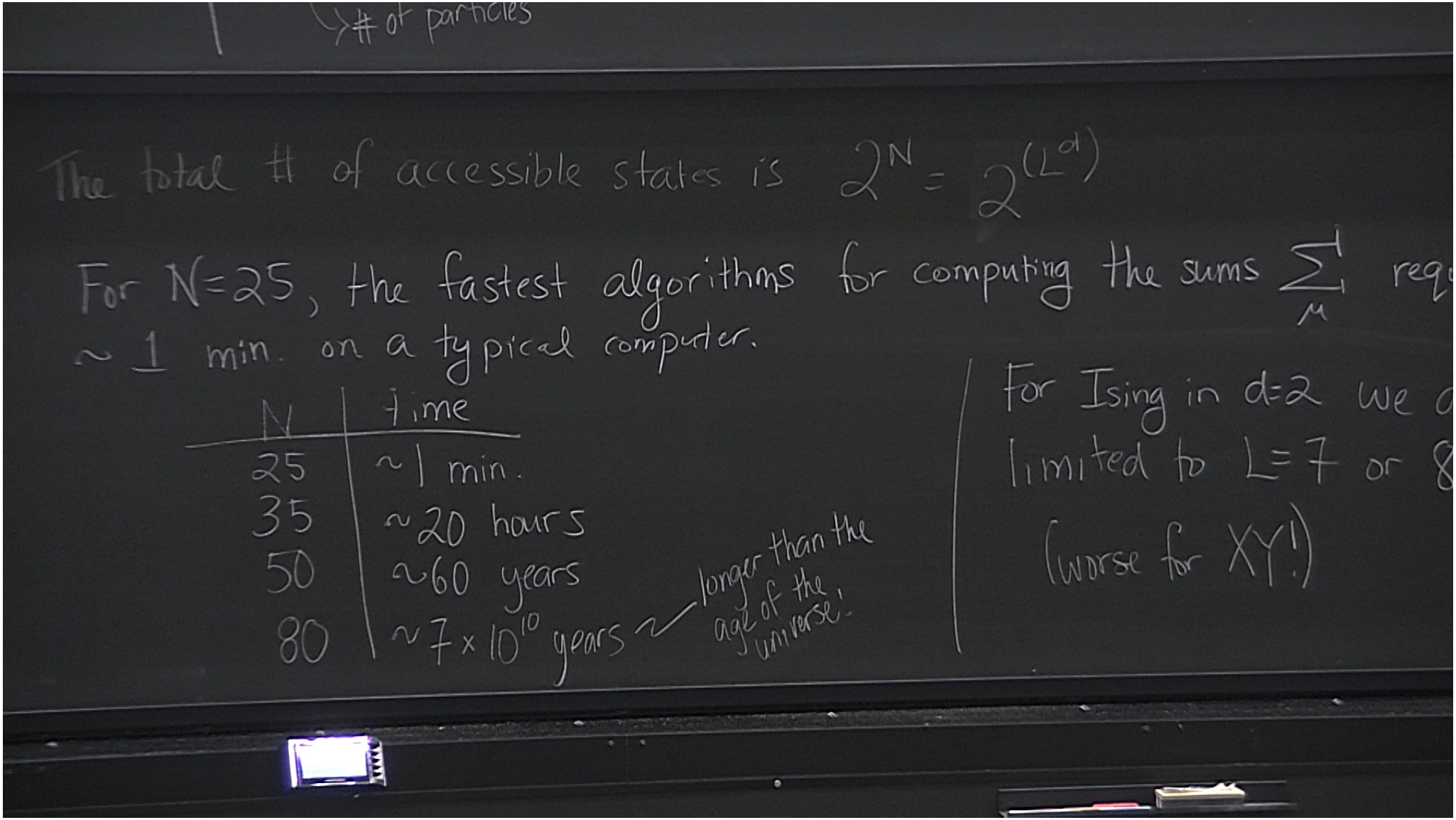
(Note: we have exact solutions for $d=1$ and $d=2$

# of particles

The total # of accessible states is $2^N = 2^{(L^d)}$

For N=25, the fastest algorithms for computing the sums $\sum_{\mu}^{1}$ req
~ 1 min. on a typical computer.

N	time
25	~1 min.
35	~20 hours
50	~60 years


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N | time
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80 | ~7×10^{10} years ~ longer than the age of the universe!
For Ising in d=2 we c
limited to L=7 or 8
(worse for XY!)

# of particles

Total # of accessible states is $2^N = 2^{(L^d)}$

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25	~1 min.
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For Ising in $d=2$ we are limited to $L=7$ or 8

(worse for XY!)

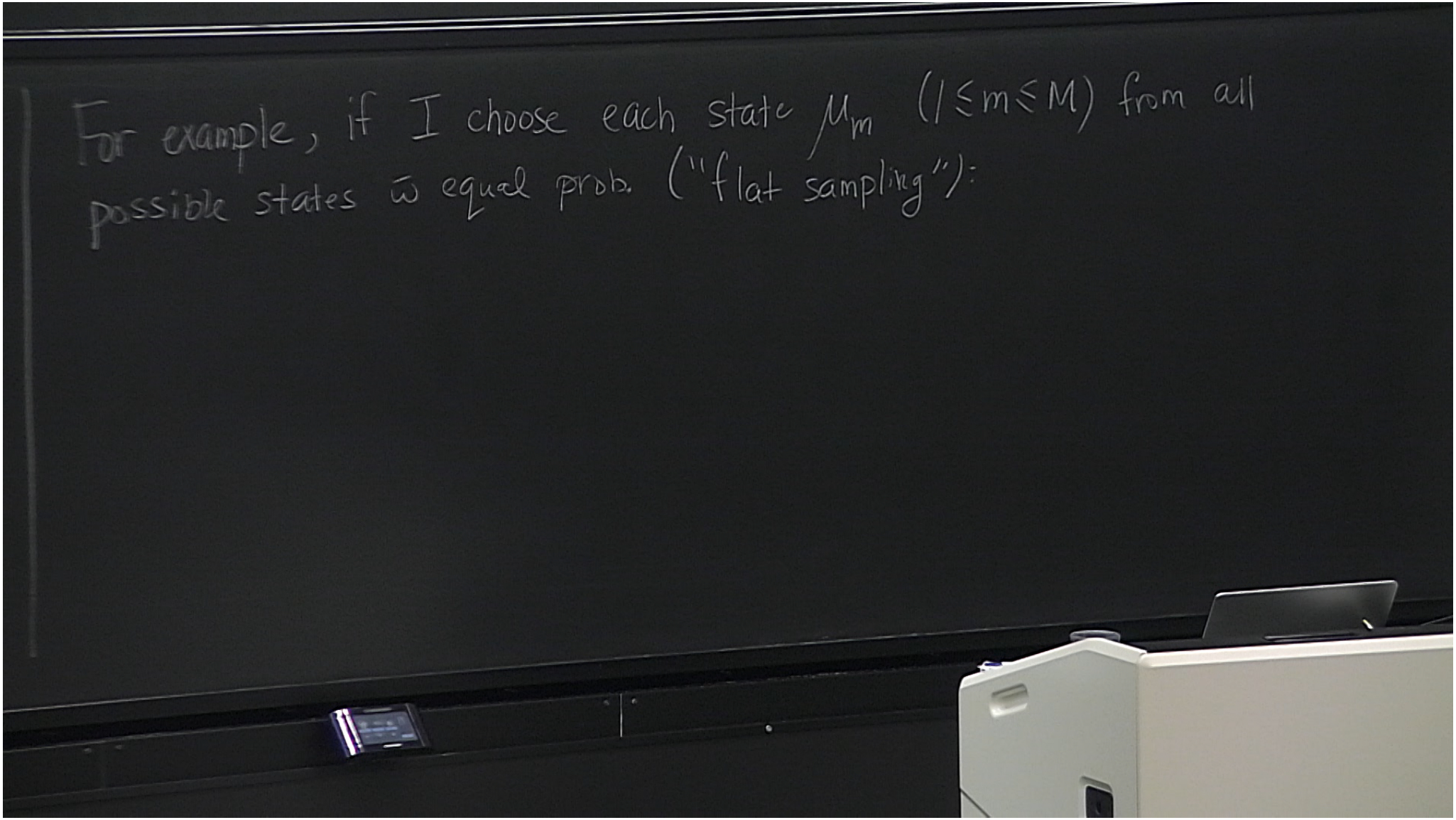
Classical MC methods

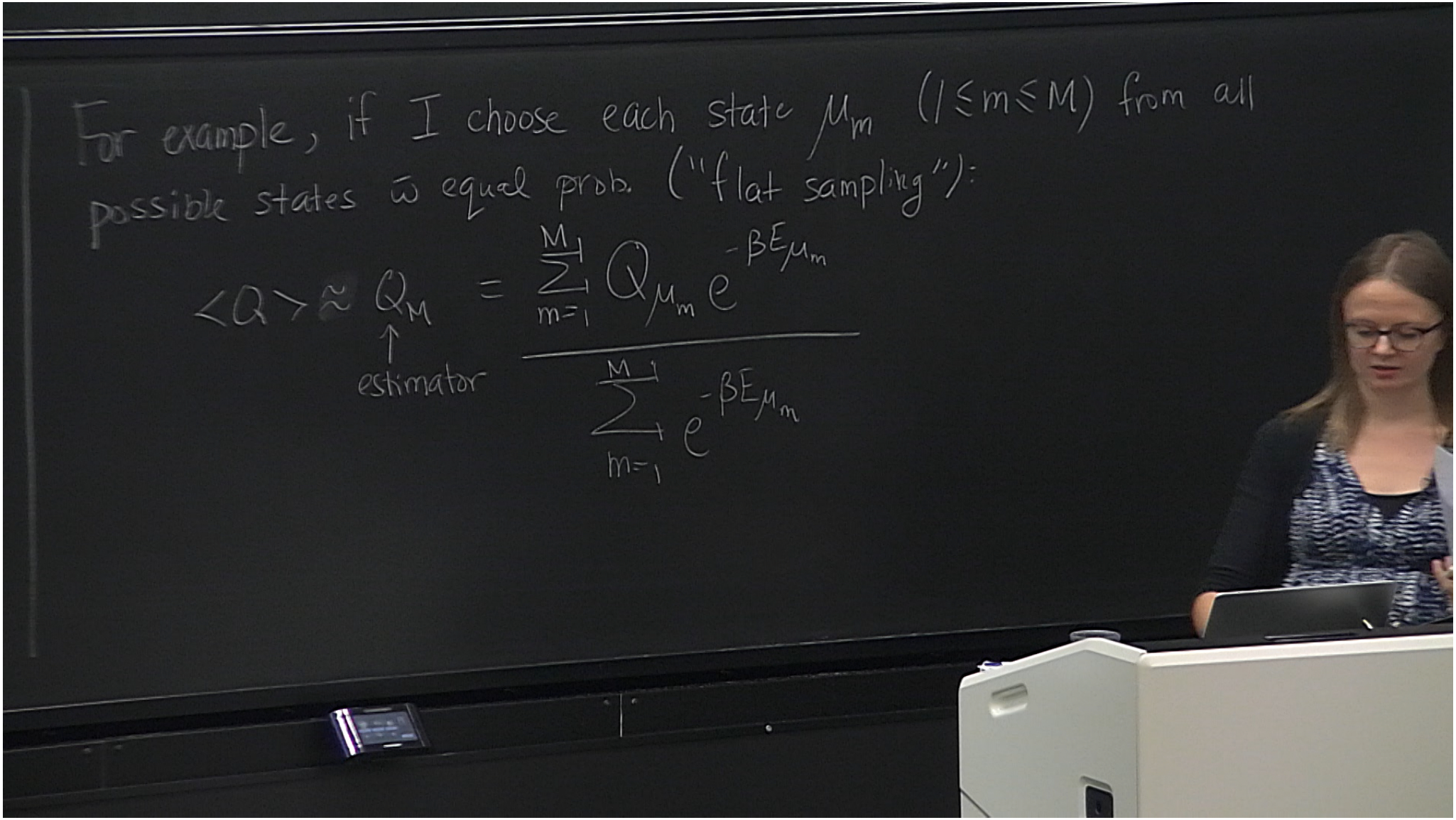
↳ addresses this exponential complexity by considering only M states
↳ ($M \ll N$ ideally)

$\mu_1, \mu_2, \cdots, \mu_M$

Selected at random.

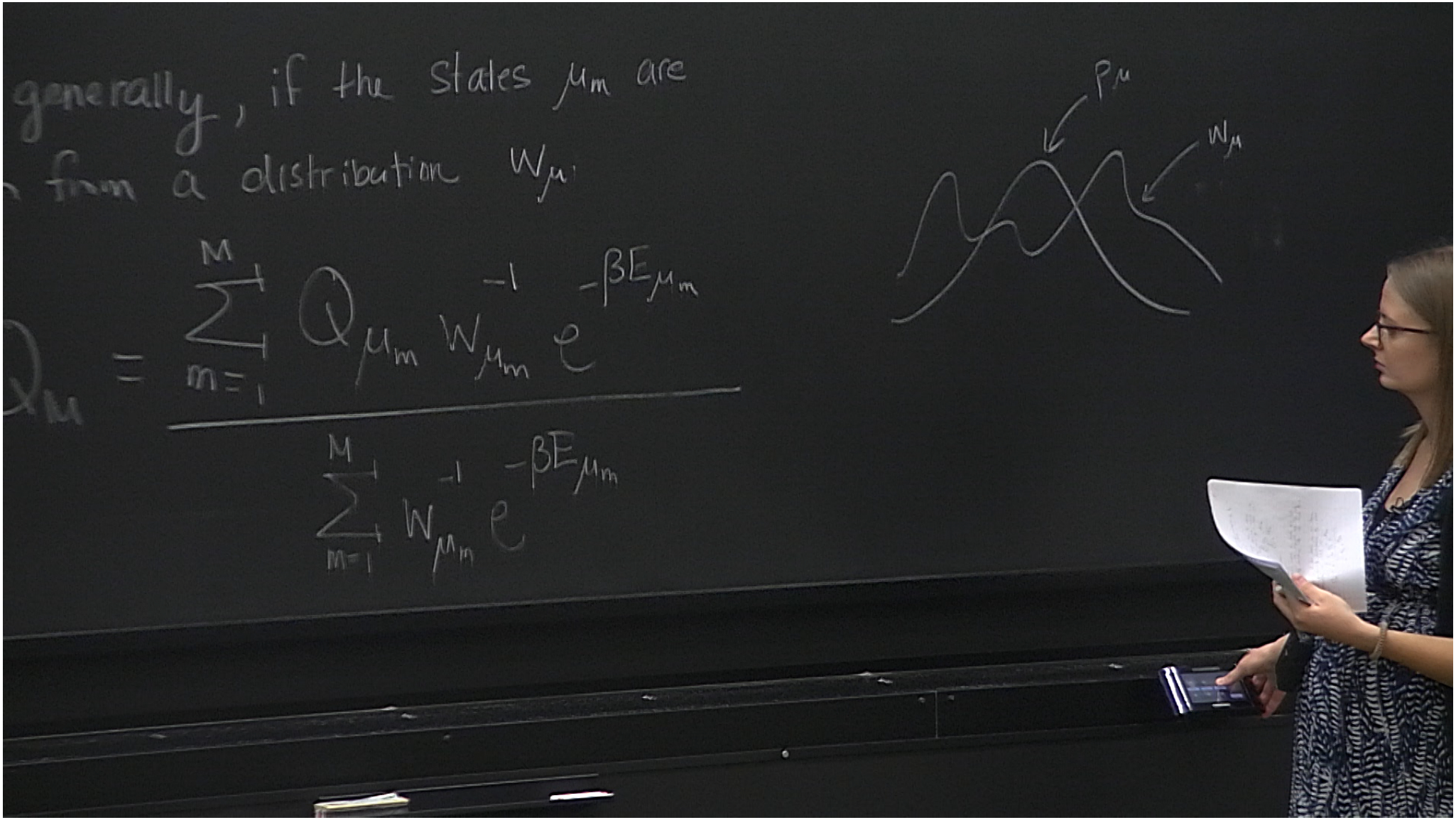
For example,

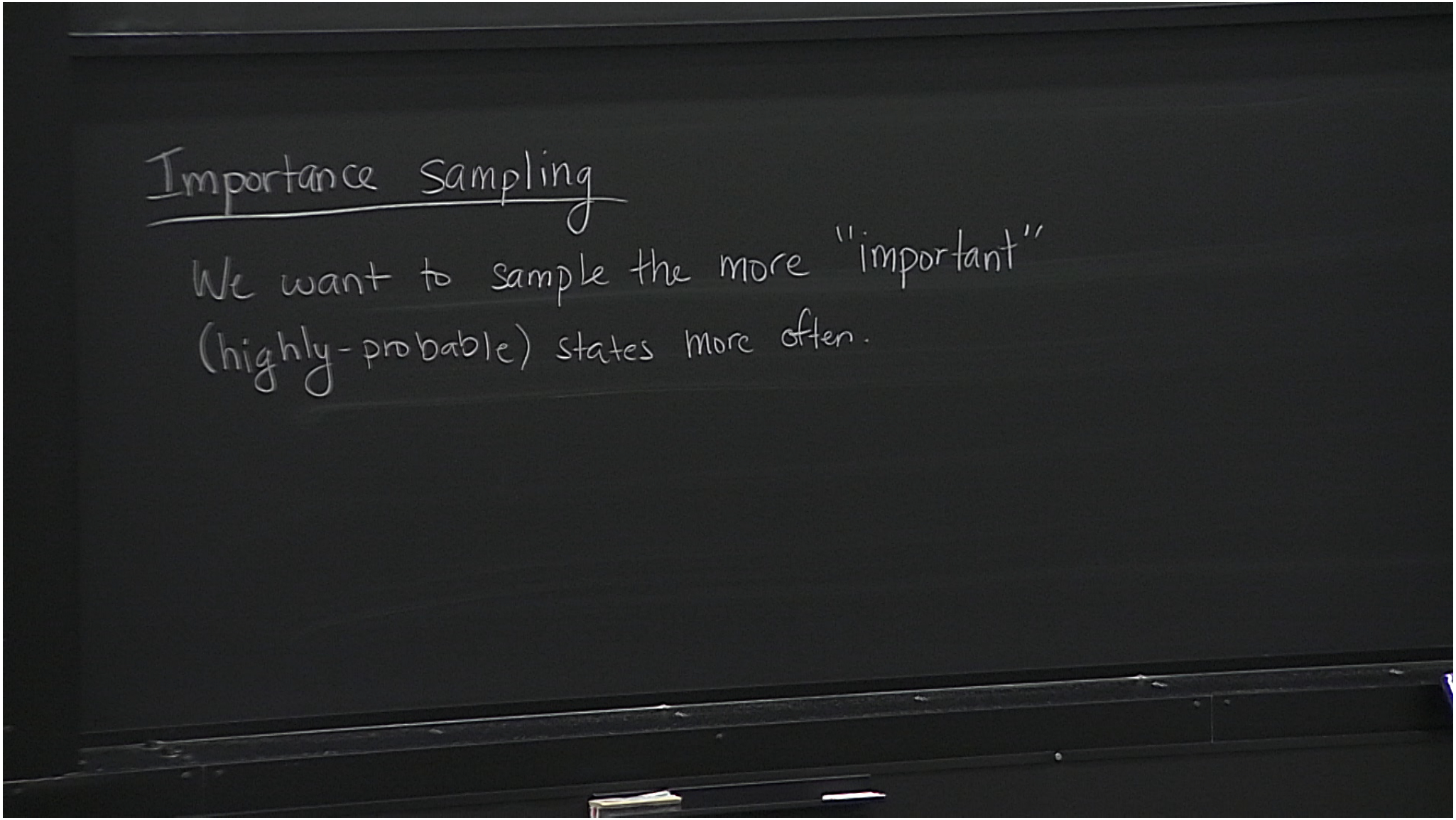

For example, if I choose each state μ_m $(1 \leq m \leq M)$ from all possible states $\bar{\omega}$ equal prob. ("flat sampling"):

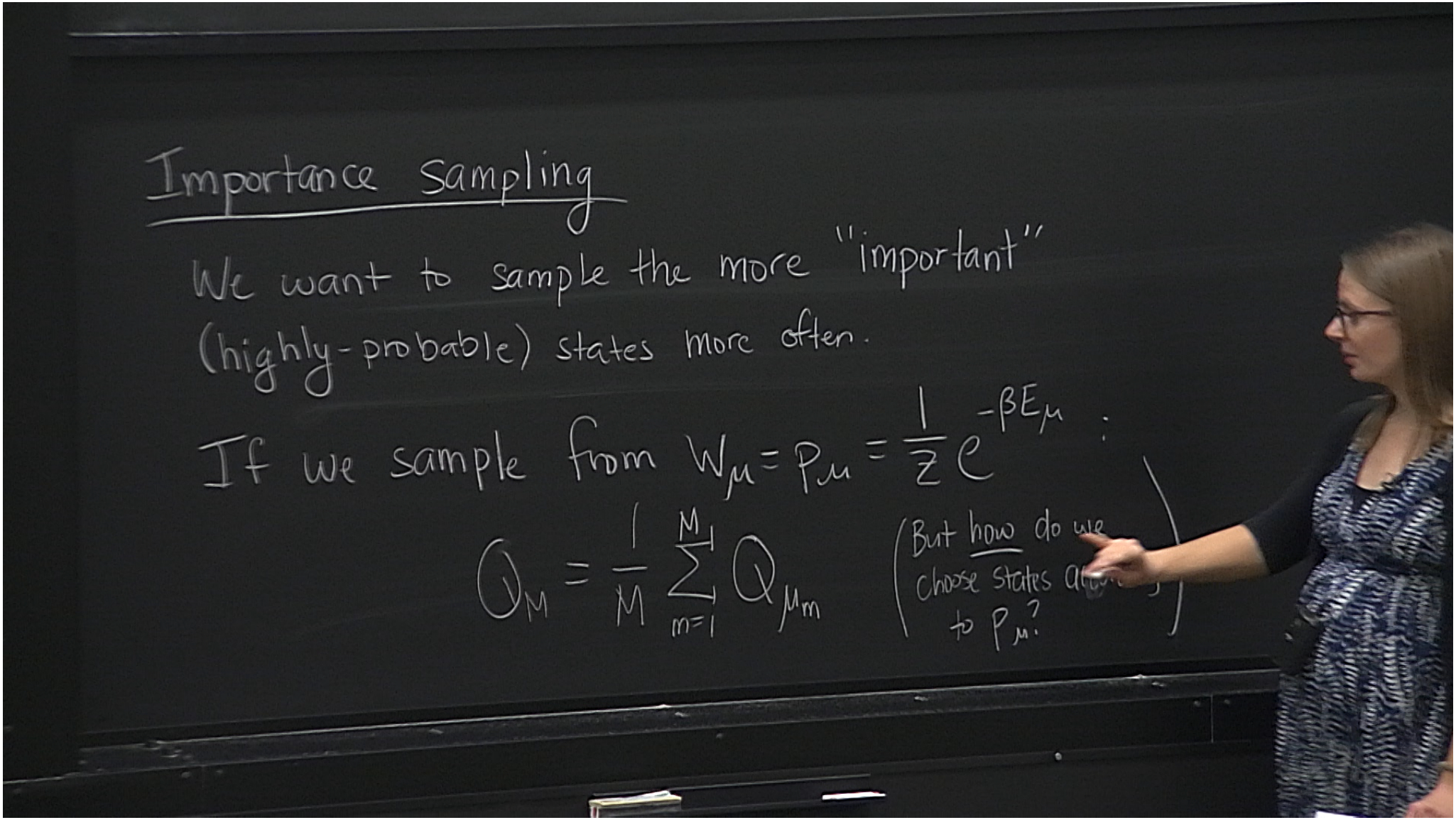

For example, if I choose each state μ_m $(1 \leq m \leq M)$ from all possible states $\bar{\omega}$ equal prob. ("flat sampling"):
$\langle Q \rangle \approx Q_M = \frac{\sum_{m=1}^{M} Q_{\mu_m} e^{-\beta E_{\mu_m}}}{\sum_{m=1}^{M} e^{-\beta E_{\mu_m}}}$
estimator

More generally, if the states μ_m are taken from a distribution W_μ:

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


generally, if the states μ_m are
from a distribution W_μ:
$$Q_\mu = \frac{\sum_{m=1}^{M} Q_{\mu_m}^{-1} W_{\mu_m} e^{-\beta E_{\mu_m}}}{\sum_{m=1}^{M} W_{\mu_m} e^{-\beta E_{\mu_m}}}$$
P_μ
W_μ


Importance sampling
We want to sample the more "important"
(highly-probable) states more often.


Importance sampling
We want to sample the more "important" (highly-probable) states more often.
If we sample from $W_\mu = P_\mu = \frac{1}{Z} e^{-\beta E_\mu}$:
$Q_M = \frac{1}{M} \sum_{m=1}^{M} Q_{\mu_m}$
(But how do we choose states according to P_μ?)

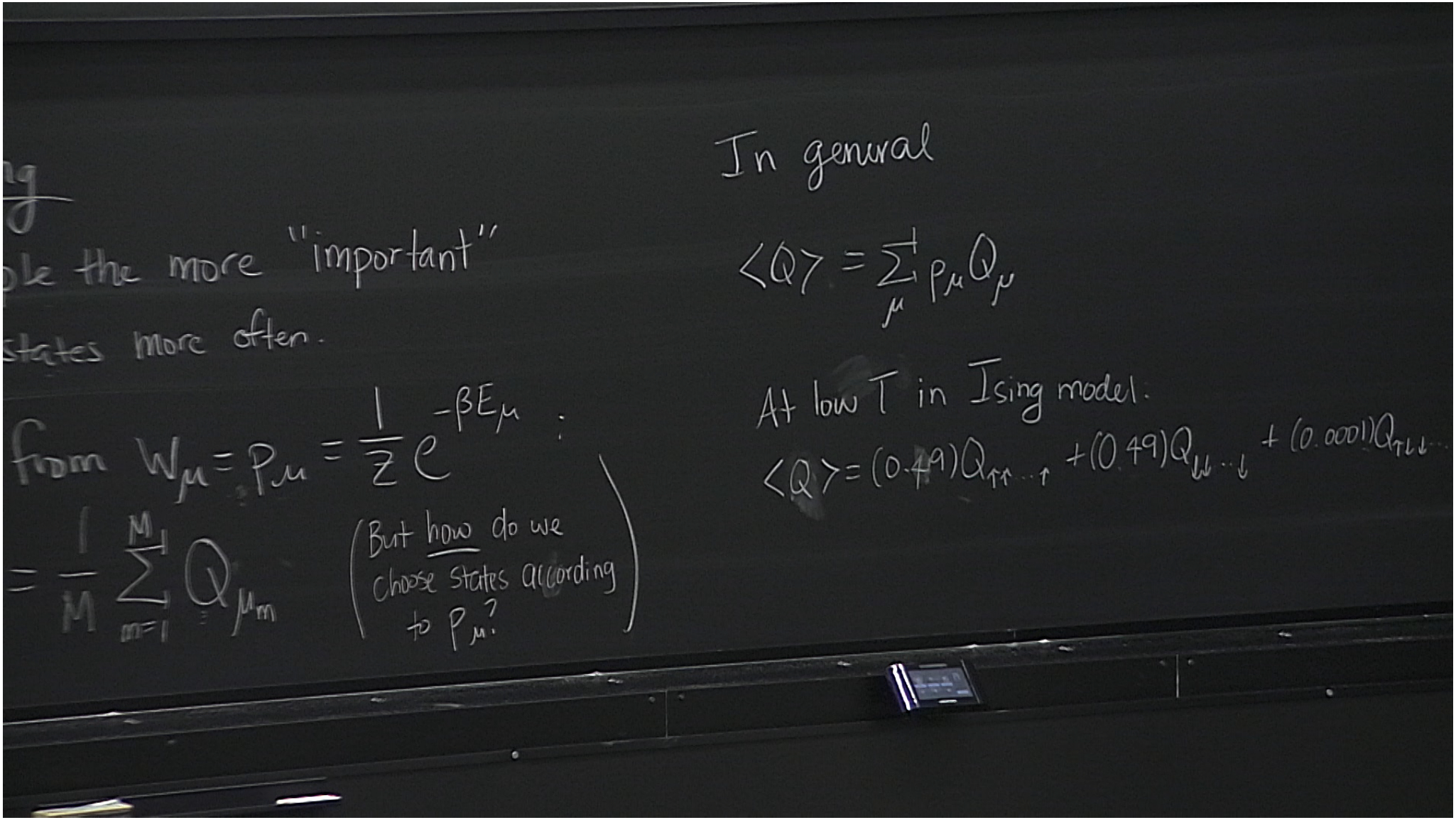
Importance Sampling

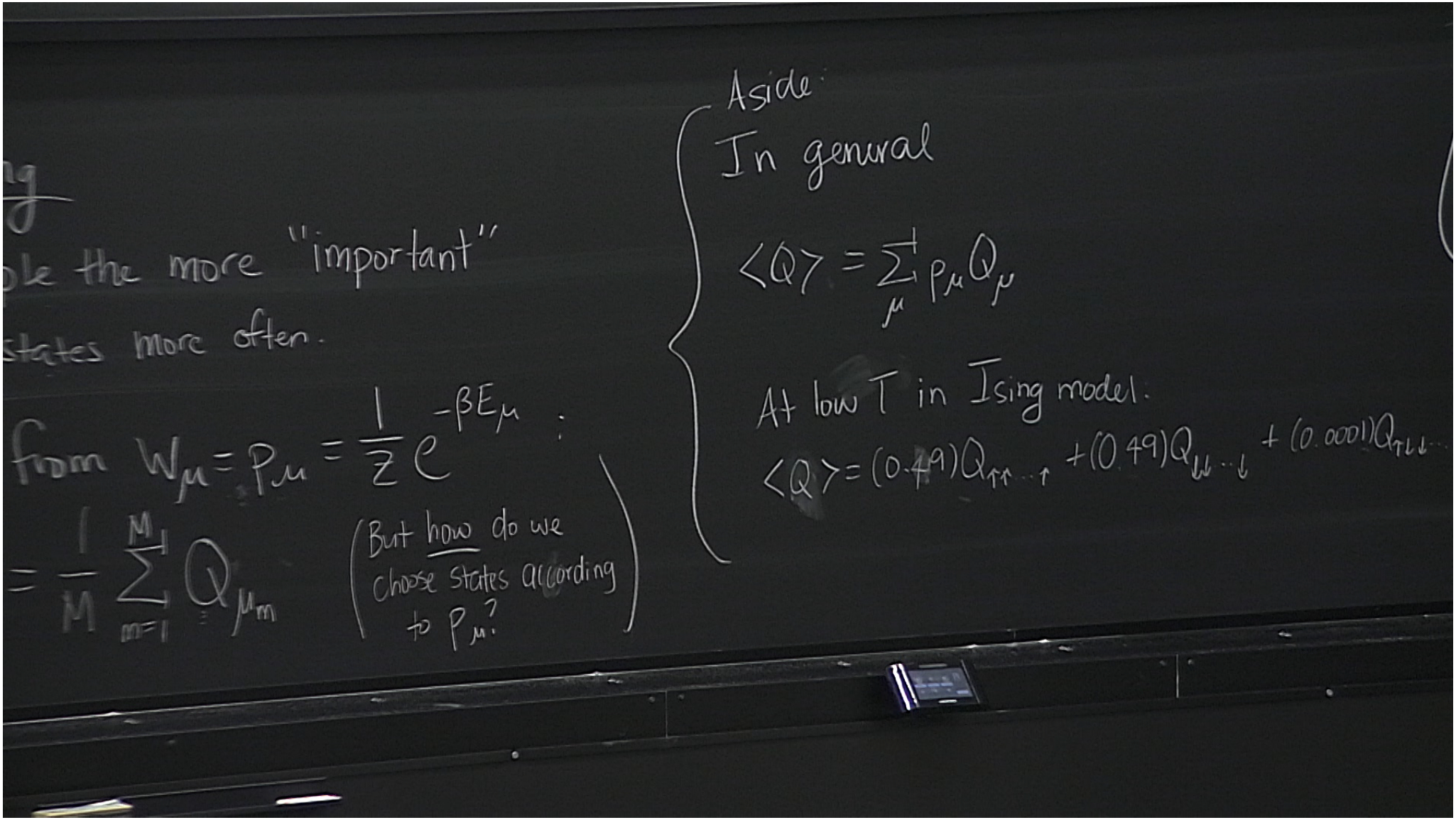
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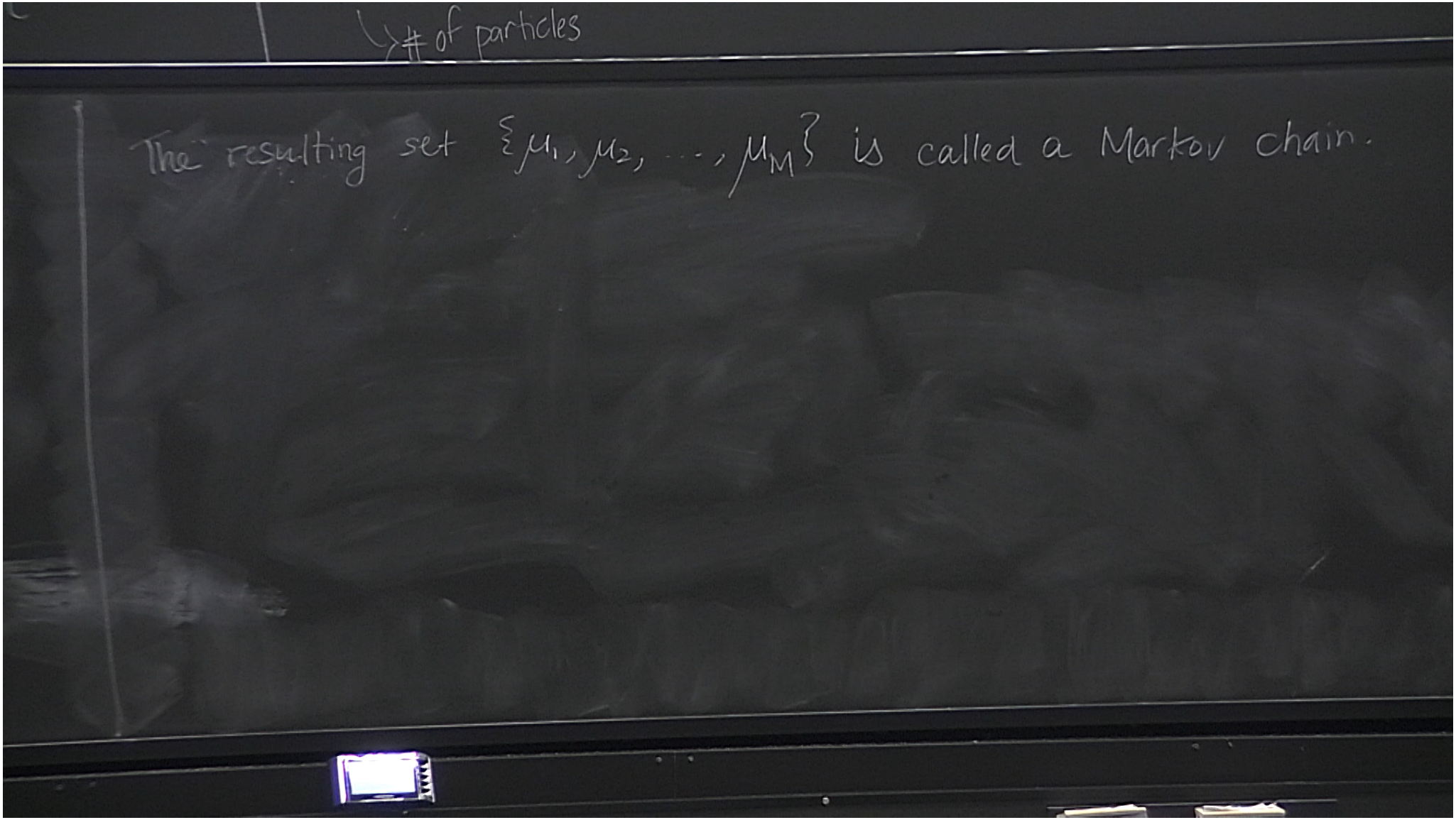

ng
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$= \frac{1}{M} \sum_{m=1}^{M} Q_{\mu_m}$
(But how do we choose states according to P_μ?)
In general
$\langle Q \rangle = \sum_\mu P_\mu Q_\mu$
At low T in Ising model.
$\langle Q \rangle = (0.49) Q_{\uparrow\uparrow\cdots\uparrow} + (0.49) Q_{\downarrow\downarrow\cdots\downarrow} + (0.0001) Q_{\uparrow\downarrow\cdots}$


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Aside:
In general
$\langle Q \rangle = \sum_\mu P_\mu Q_\mu$
At low T in Ising model.
$\langle Q \rangle = (0.49) Q_{\uparrow\uparrow\cdots\uparrow} + (0.49) Q_{\downarrow\downarrow\cdots\downarrow} + (0.0001) Q_{\uparrow\downarrow\cdots}$

Markov Chain Monte Carlo

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

- $T(\mu_m \to \mu_{m+1})$ depends only on μ_m and μ_{m+1} (not $\mu_1, \mu_2, \cdots, \mu_{m-1}$)
- $T(\mu_m \to \mu_{m+1})$ are time indep.
- $\sum_\nu T(\mu \to \nu) = 1$


↳ # of particles
The resulting set $\{\mu_1, \mu_2, \ldots, \mu_M\}$ is called a Markov chain.

$-\beta E_\mu$

$N \to \infty$

↳ # of particles

The resulting set $\{\mu_1, \mu_2, \ldots, \mu_M\}$ is called a Markov chain.

To reach states from the target dist. w_μ, we need to design an algorithm that satisfies two conditions.

(1) Ergodicity: Given <u>any</u> two states μ and ν, it must be possible (non-zero prob) to transition between them through some intermediate chain

- $T(\mu_m \to \mu_{m+1})$ are time indep.
- $\sum_\nu T(\mu \to \nu) = 1$

One way

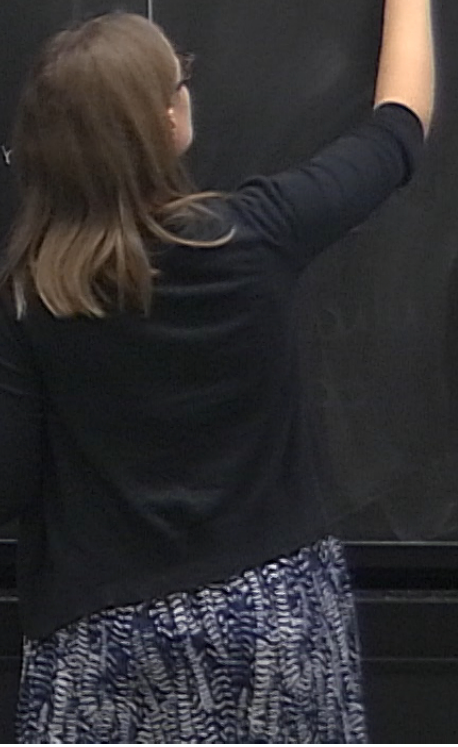
(2) Detailed Balance (DB)

The rate of transition into and out of any μ must be equal (otherwise W_μ would change $\bar{\omega}$ ti

For any μ $\sum_\nu W_\nu T(\nu \to \mu) - \sum_\nu W_\mu T(\mu \to \nu) = 0$

rate of transition into μ

rate of transition out of μ



One way to satisfy this condition is:

$$W_\mu T(\mu \to \nu) = W_\nu T(\nu \to \mu)$$ DB

When $W_\mu = \frac{1}{Z} e^{-\beta E_\mu}$

$$\frac{T(\mu \to \nu)}{T(\nu \to \mu)} = e^{-\beta(E_\nu - E_\mu)}$$

We have the freedom to chose the transition probs as long as their ratio is fixed.

...cst algorithm
...pical computer.
$(\sim 2^N)$

rate of transition into μ

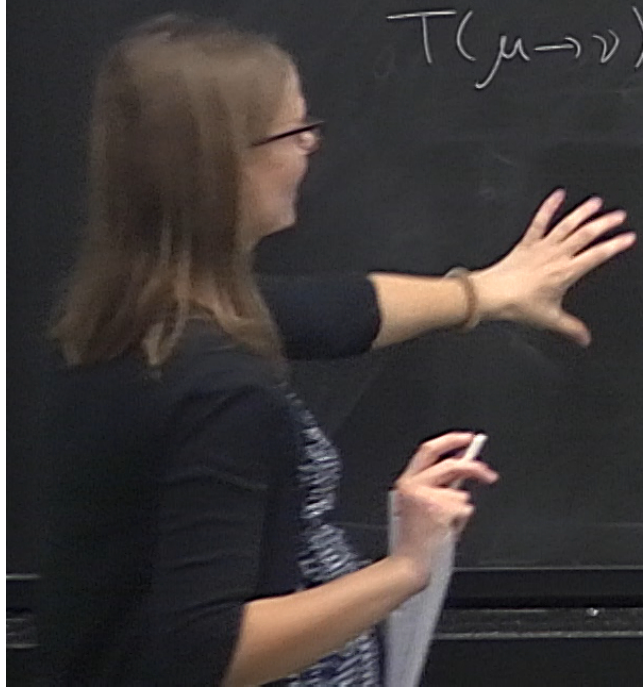
rate of transition out of μ

Let's introduce notation:

$$T(\mu \to \nu) = g(\mu \to \nu)\, A(\mu \to \nu)$$

Selection prob: prob of proposing a move to ν given initial state μ

acceptance prob: prob of accepting the move $\mu \to \nu$



We have the freedom to chose the transition probs as long as their ratio is fixed.

From DB:

$$\frac{A(\mu \to \nu)}{A(\nu \to \mu)} = \frac{g(\nu \to \mu) W_\nu}{g(\mu \to \nu) W_\mu}$$

We want the A's to be as close to 1 as possible so we sample more different states.

Metropolis Algorithm:

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

acceptance prob. is 1 for $\mu \to \nu$ or $\nu \to \mu$

XY model

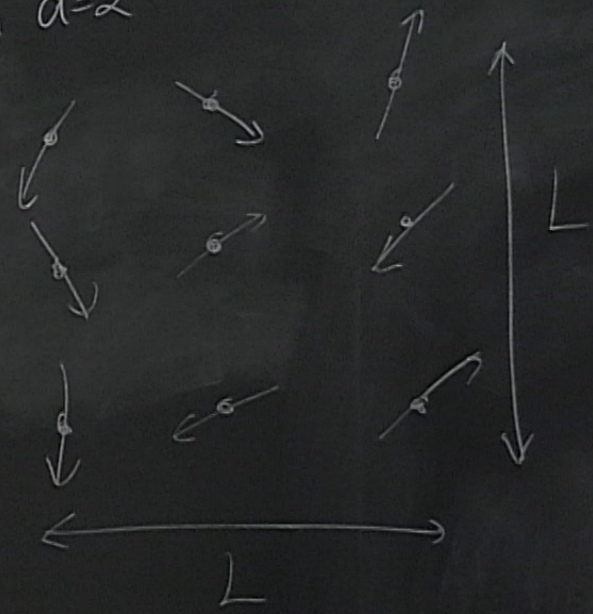
$$H = -J \sum_{\langle ij \rangle}^{'} \vec{S}_i \cdot \vec{S}_j$$

$$= -J \sum_{\langle ij \rangle}^{'} \cos(\theta_i - \theta_j)$$

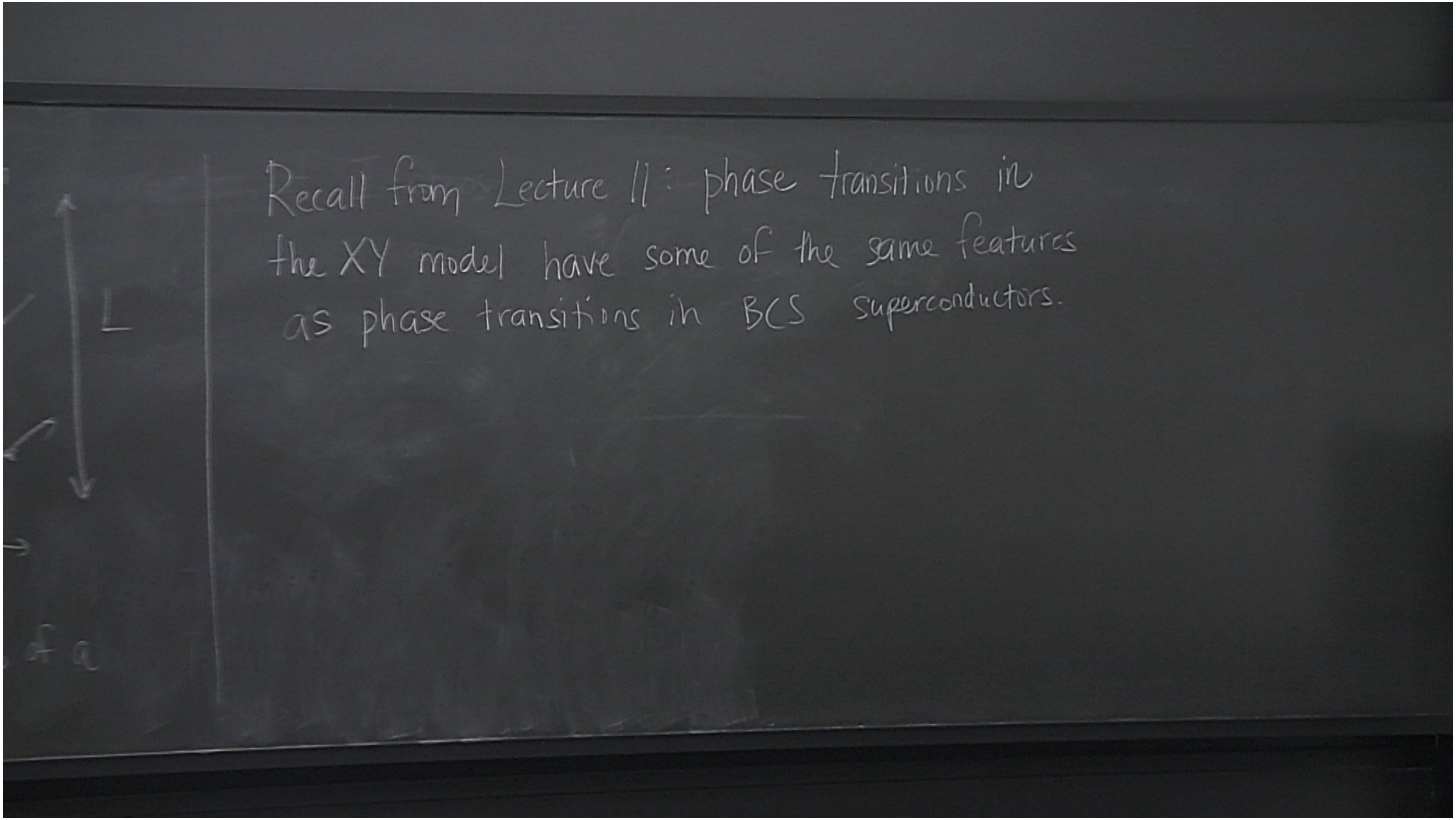
$$\vec{S}_i = (S_{ix}, S_{iy}) \; ; \; |\vec{S}_i| = 1$$

$$0 \leq \theta_i < 2\pi$$

In $d=2$:

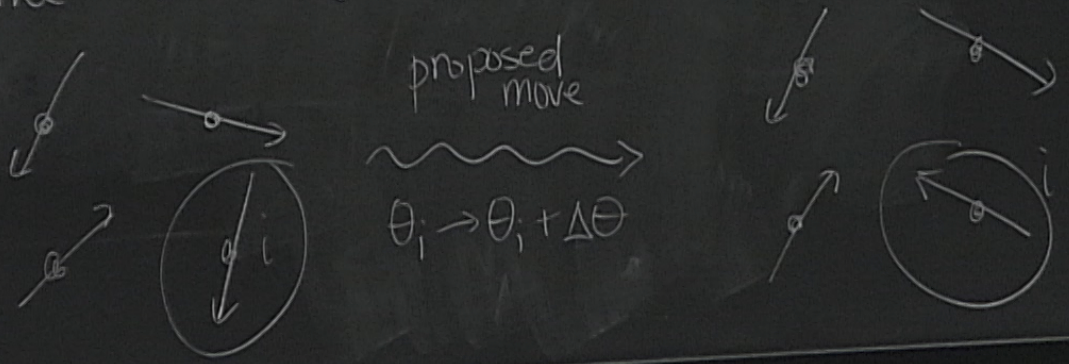


spins (rotors) on sites of a d-dim lattice


Recall from Lecture 11: phase transitions in the XY model have some of the same features as phase transitions in BCS superconductors.
L

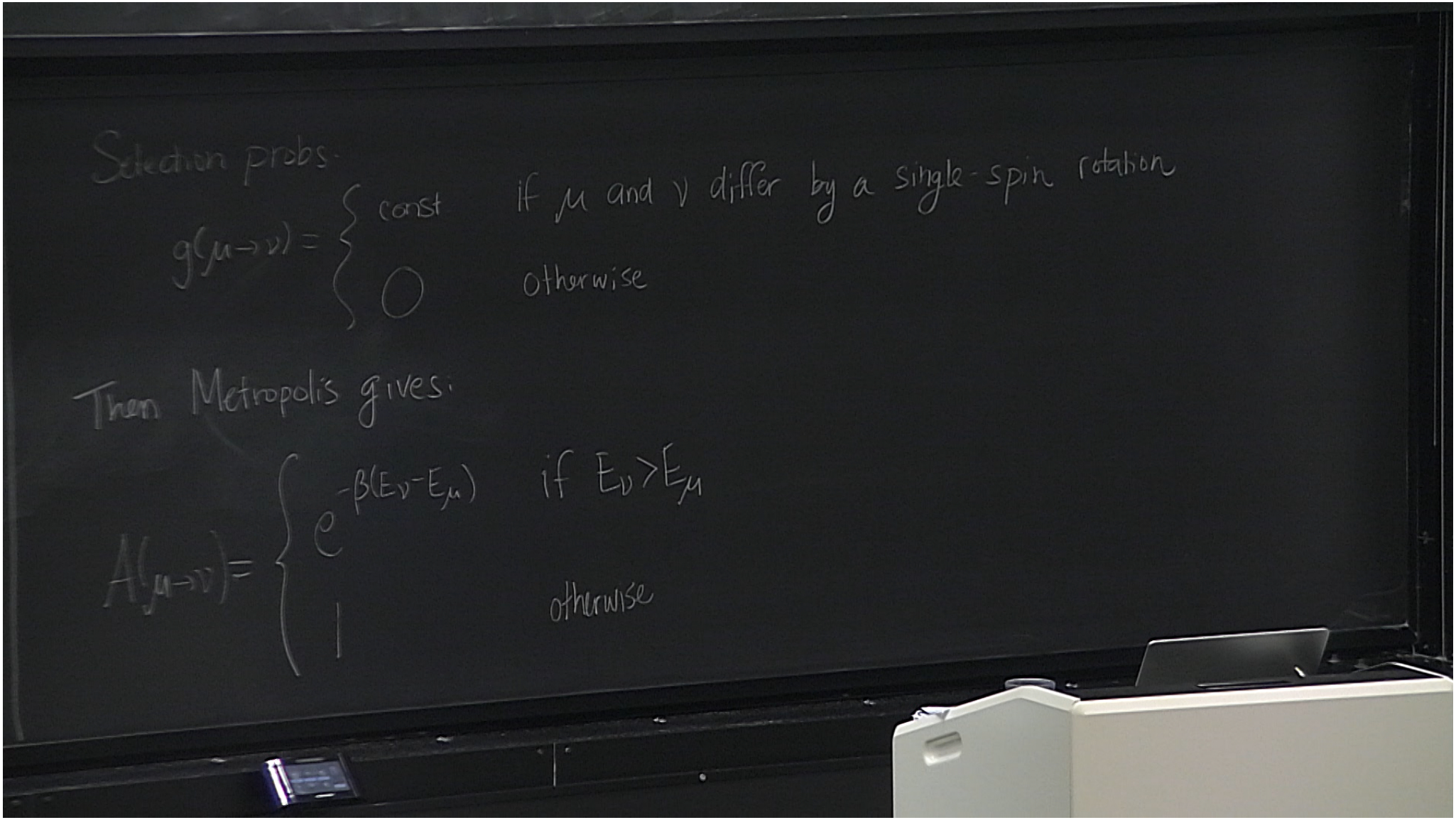
Single-spin-update algorithm for XY

Given state μ_m, generate μ_{m+1} by randomly rotating the rotor at site i ← random by some random $\Delta\theta$



Selection

$g(\mu$


Selection probs:
$g(\mu \to \nu) = \begin{cases} \text{const} & \text{if } \mu \text{ and } \nu \text{ differ by a single-spin rotation} \\ 0 & \text{otherwise} \end{cases}$
Then Metropolis gives:
$A(\mu \to \nu) = \begin{cases} e^{-\beta(E_\nu - E_\mu)} & \text{if } E_\nu > E_\mu \\ 1 & \text{otherwise} \end{cases}$

rate of transition into μ

rate of transition out of μ

Steps:

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

for any μ $\quad \sum_\nu W_\nu T(\nu \to \mu) - \sum_\nu W_\mu T(\mu \to \nu) = 0$

rate of transition into μ — rate of transition out of μ

We have the freedom to ch

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Note: better cluster algorithms exist
- ↳ Wolff
- ↳ Swendsen-Wang