Title: Lecture - Statistical Physics, PHYS 602

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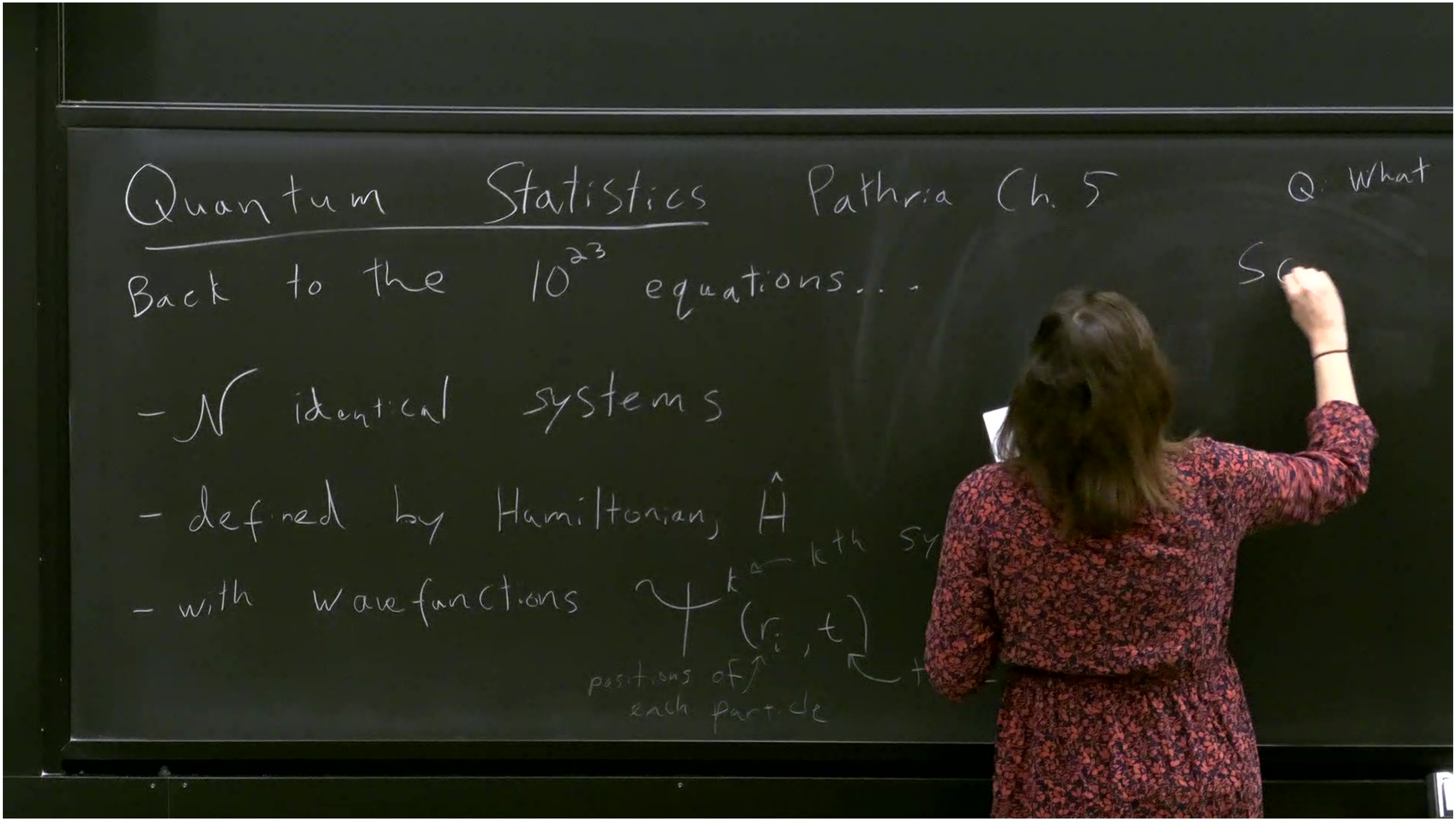
Collection/Series: Statistical Physics (Core), PHYS 602, October 7 - November 6, 2024

Subject: Condensed Matter, Other

Date: October 30, 2024 - 10:45 AM

URL: https://pirsa.org/24100018



Quantum Statistics   Pathria Ch. 5   Q: What

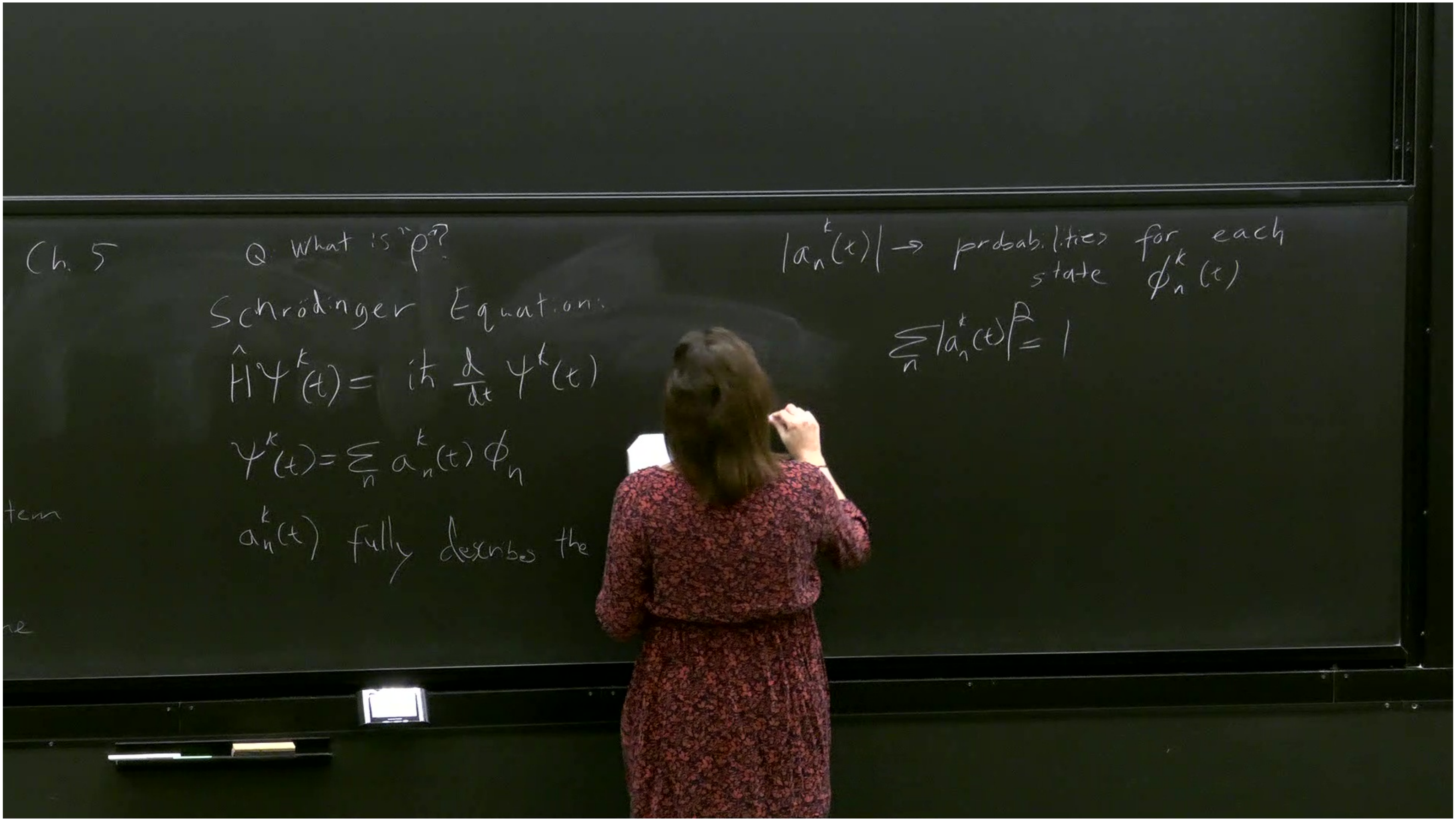
Back to the 10^{23} equations...   Sc

- N identical systems
- defined by Hamiltonian, $\hat{H}$
- with wavefunctions $\Psi^k(r_i, t)$

$k \leftarrow$ kth sy

$r_i \leftarrow$ positions of each particle

$t \leftarrow$ t



Ch. 5

Q. What is "ρ"?

Schrödinger Equation:

$$\hat{H}\Psi^k(t) = i\hbar \frac{d}{dt}\Psi^k(t)$$

$$\Psi^k(t) = \sum_n a_n^k(t)\,\phi_n$$

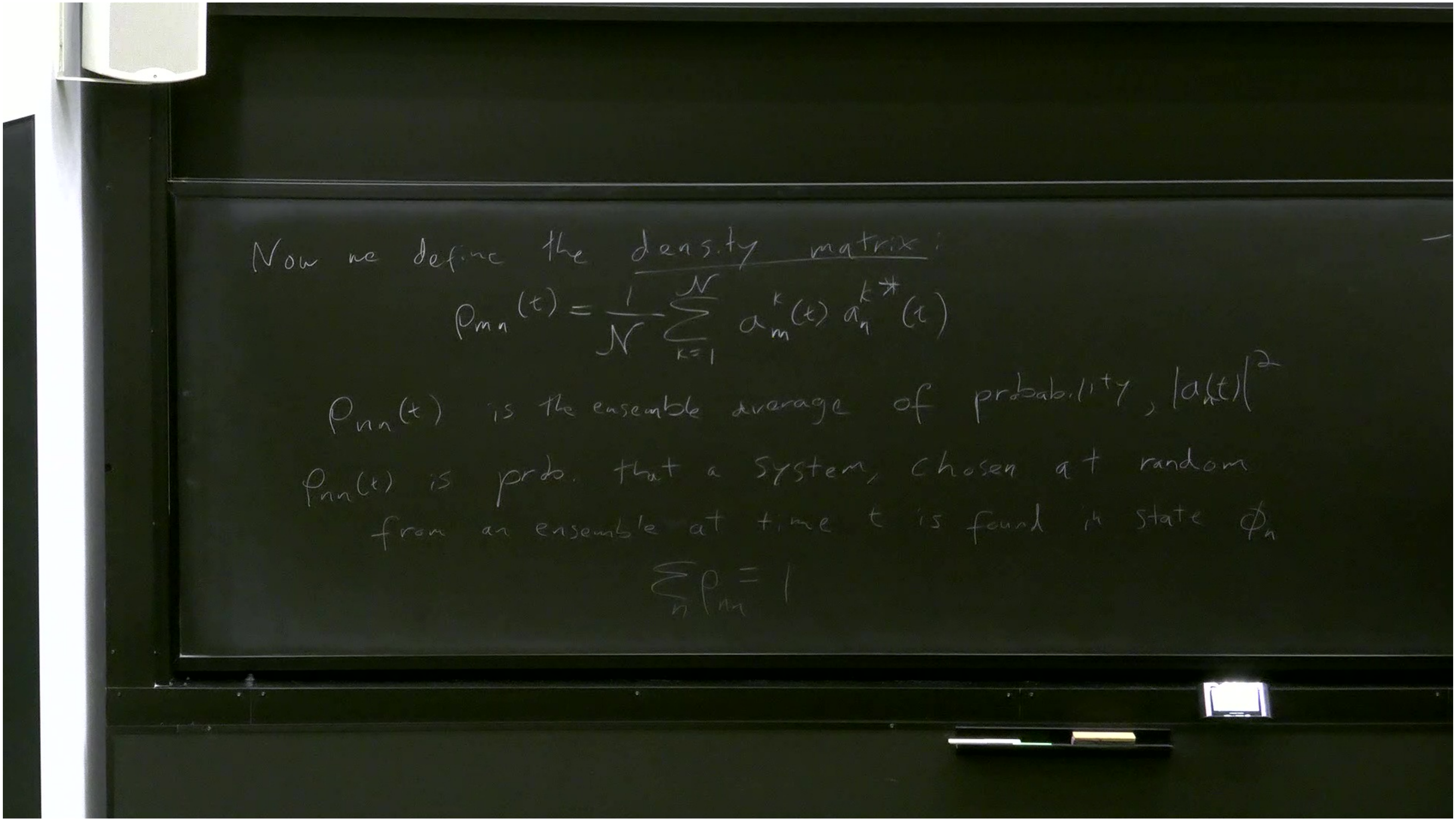
$a_n^k(t)$ fully describes the

$|a_n^k(t)| \rightarrow$ probabilities for each state $\phi_n^k(t)$

$$\sum_n |a_n^k(t)|^2 = 1$$

tem

ne



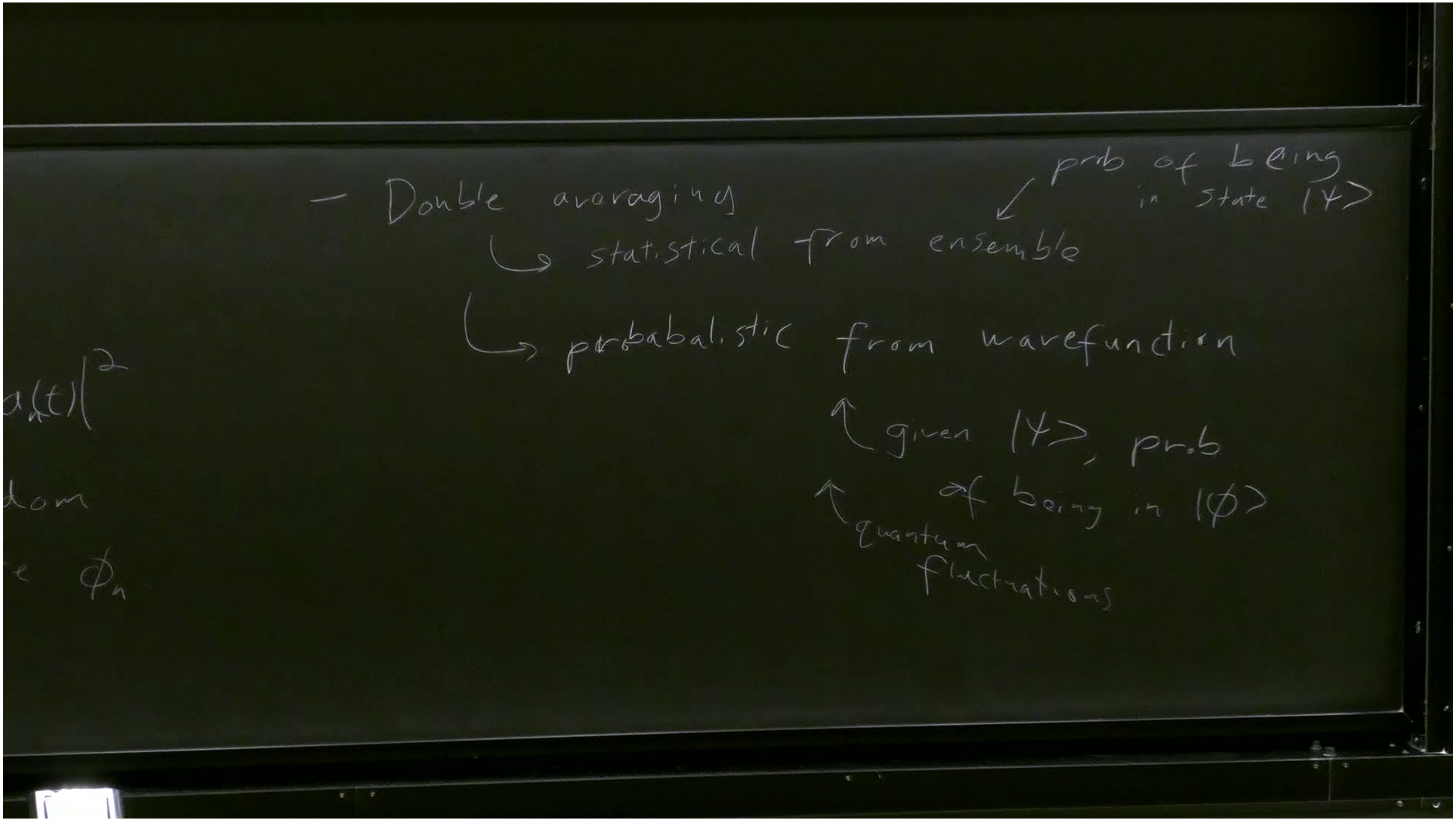
Now we define the density matrix:

$$\rho_{mn}(t) = \frac{1}{N} \sum_{k=1}^{N} a_m^k(t)\, a_n^{k*}(t)$$

$\rho_{nn}(t)$ is the ensemble average of probability, $|a_n(t)|^2$

$\rho_{nn}(t)$ is prob. that a system, chosen at random from an ensemble at time t is found in state ϕ_n

$$\sum_n \rho_{nn} = 1$$



$a_n(t)|^2$

dom

e ϕ_n

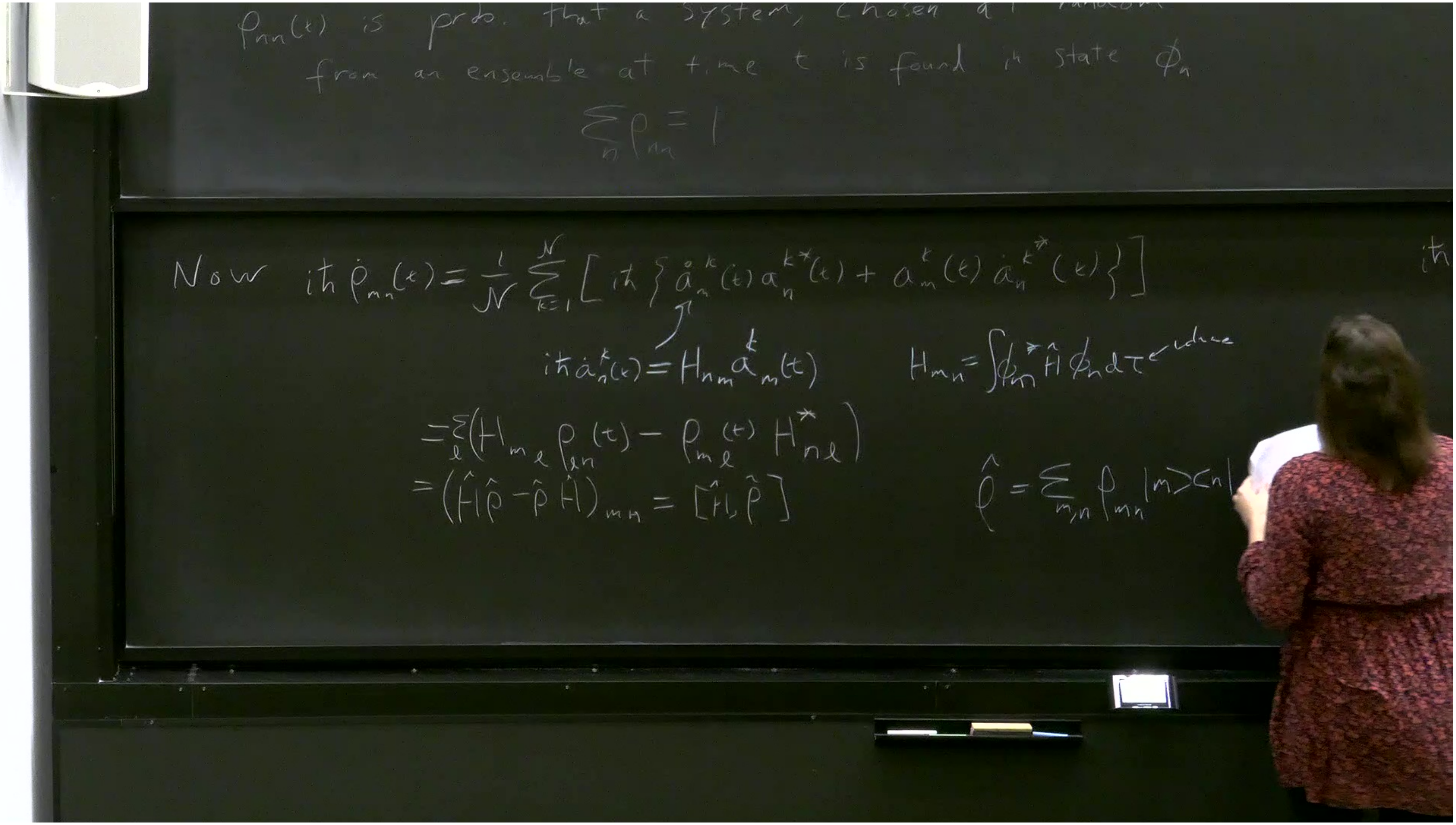
– Double averaging

↳ statistical from ensemble ↙ prob of being in state $|\psi\rangle$

↳ probabalistic from wavefunction

↑ given $|\psi\rangle$, prob of being in $|\phi\rangle$

↑ quantum fluctuations



$\rho_{nn}(t)$ is prob. that a system, chosen at random from an ensemble at time t is found in state ϕ_n

$$\sum_n \rho_{nn} = 1$$

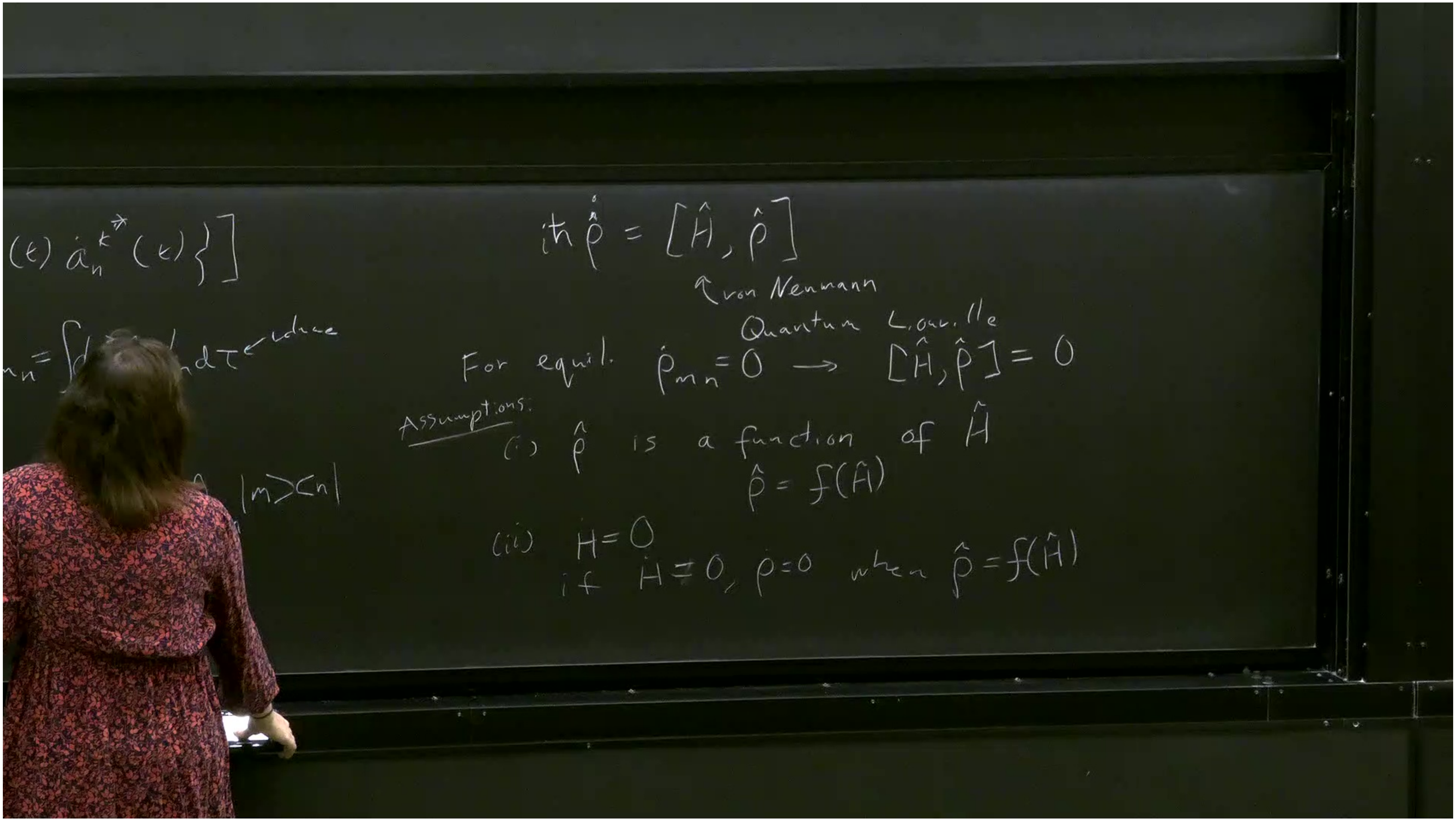
Now $$i\hbar\,\dot{\rho}_{mn}(t) = \frac{1}{\mathcal{N}}\sum_{k=1}^{\mathcal{N}}\left[i\hbar\left\{ \dot{a}_m^k(t)\, a_n^{k*}(t) + a_m^k(t)\, \dot{a}_n^{k*}(t)\right\}\right]$$ $i\hbar$

$$i\hbar\,\dot{a}_n^k(t) = H_{nm}\, a_m^k(t) \qquad H_{mn} = \int \phi_m^* \hat{H} \phi_n \, d\tau \leftarrow \text{value}$$

$$= \sum_l \left(H_{ml}\, \rho_{ln}(t) - \rho_{ml}(t)\, H_{nl}^* \right)$$

$$= (\hat{H}\hat{\rho} - \hat{\rho}\hat{H})_{mn} = [\hat{H}, \hat{\rho}]$$

$$\hat{\rho} = \sum_{m,n} \rho_{mn} |m\rangle\langle n|$$



$(t)\,\dot{a}_n^{k*}(t)\}]$

$_{mn} = \int d \quad d\tau$ ← volume

$|m\rangle\langle n|$

$$i\hbar\,\dot{\hat{\rho}} = [\hat{H}, \hat{\rho}]$$

↑ von Neumann

Quantum Liouville

For equil. $\dot{\rho}_{mn} = 0 \longrightarrow [\hat{H}, \hat{\rho}] = 0$

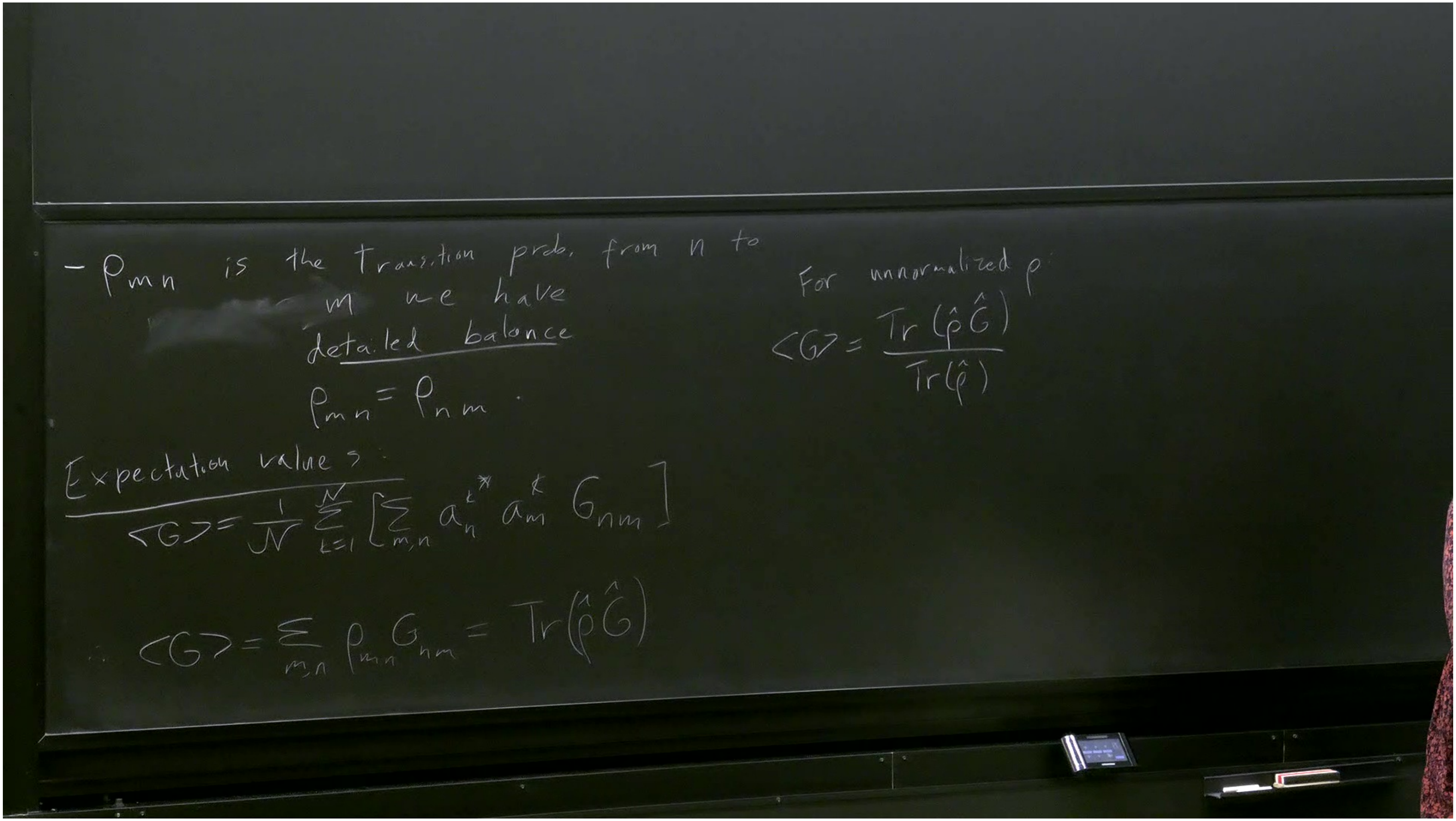
Assumptions:

(i) $\hat{\rho}$ is a function of $\hat{H}$

$\hat{\rho} = f(\hat{H})$

(ii) $\dot{H} = 0$

if $\dot{H} \neq 0$, $\dot{\rho} = 0$ when $\hat{\rho} = f(\hat{H})$



- ρ_{mn} is the transition prob. from n to m we have detailed balance

$$\rho_{mn} = \rho_{nm} .$$

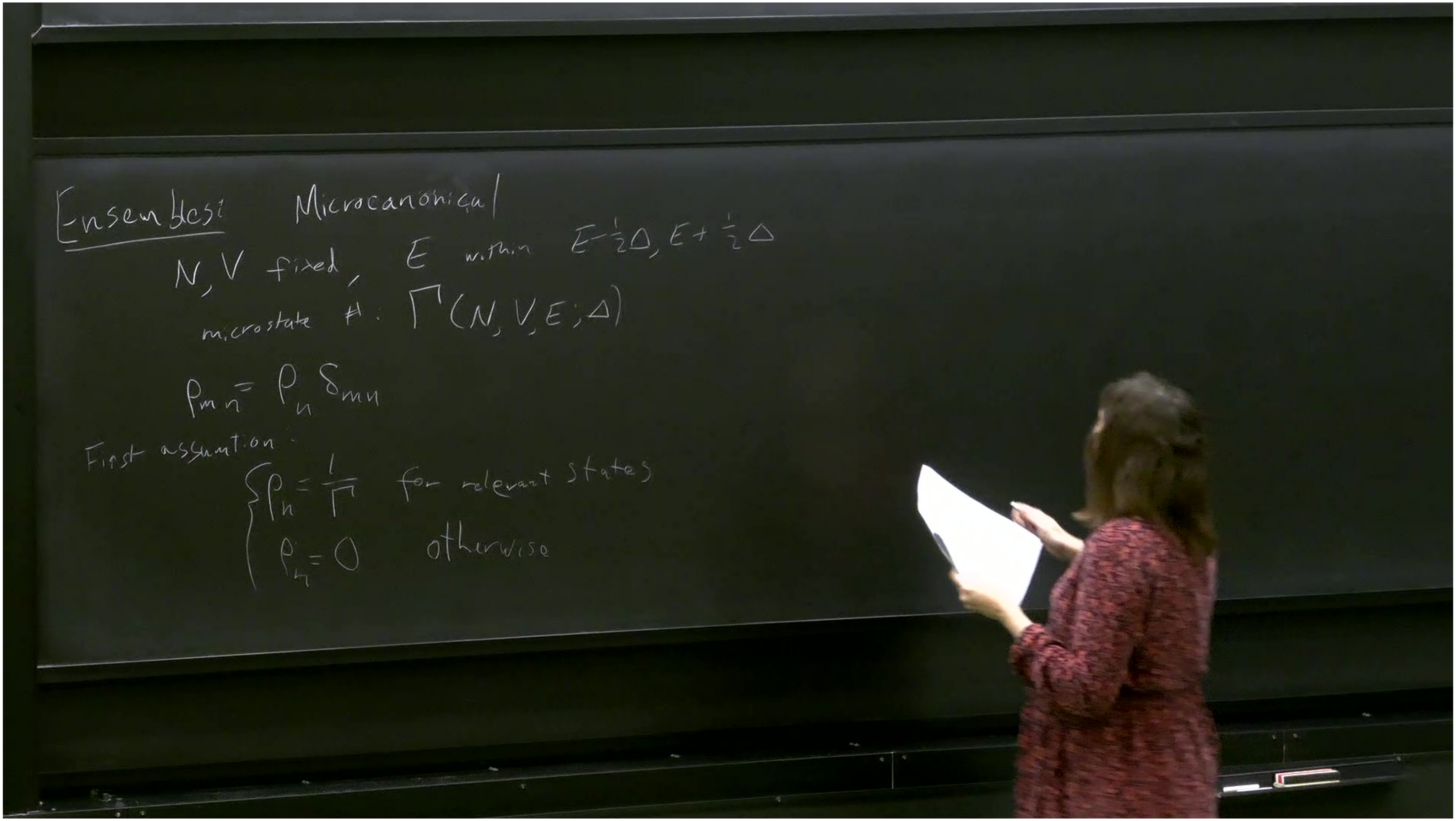
Expectation values:

$$\langle G \rangle = \frac{1}{N} \sum_{k=1}^{N} \left[\sum_{m,n} a_n^{k*} a_m^{k} G_{nm} \right]$$

$$\langle G \rangle = \sum_{m,n} \rho_{mn} G_{nm} = \mathrm{Tr}(\hat{\rho} \hat{G})$$

For unnormalized ρ:

$$\langle G \rangle = \frac{\mathrm{Tr}(\hat{\rho} \hat{G})}{\mathrm{Tr}(\hat{\rho})}$$



Ensembles: Microcanonical

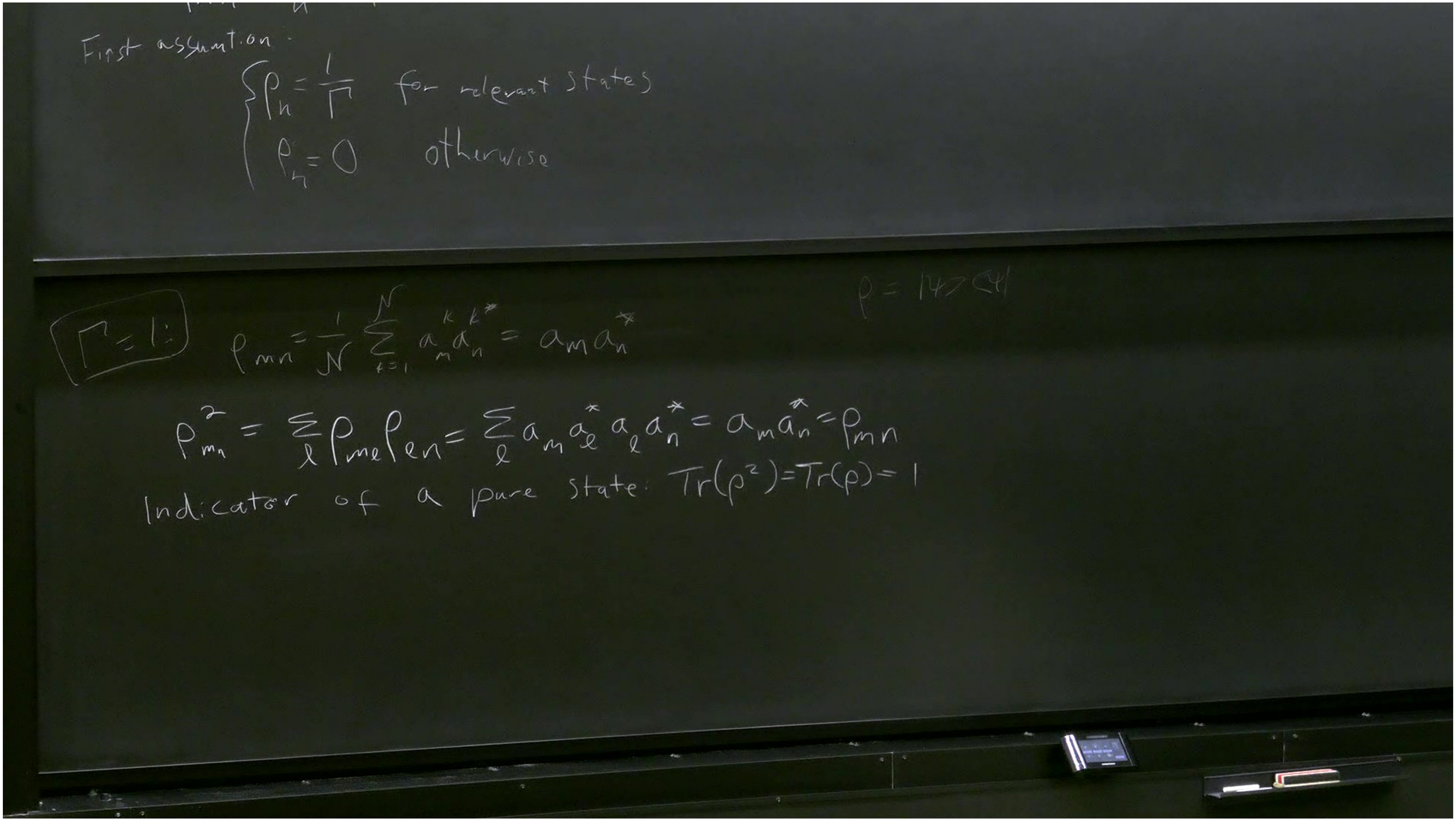
N, V fixed, E within $E-\frac{1}{2}\Delta, E+\frac{1}{2}\Delta$

microstate #: $\Gamma(N, V, E; \Delta)$

$$\rho_{mn} = \rho_n \delta_{mn}$$

First assumtion:

$$\begin{cases} \rho_n = \frac{1}{\Gamma} & \text{for relevant states} \\ \rho_n = 0 & \text{otherwise} \end{cases}$$



First assumtion:

$$\begin{cases} \rho_n = \frac{1}{\Gamma} & \text{for relevant states} \\ \rho_n = 0 & \text{otherwise} \end{cases}$$

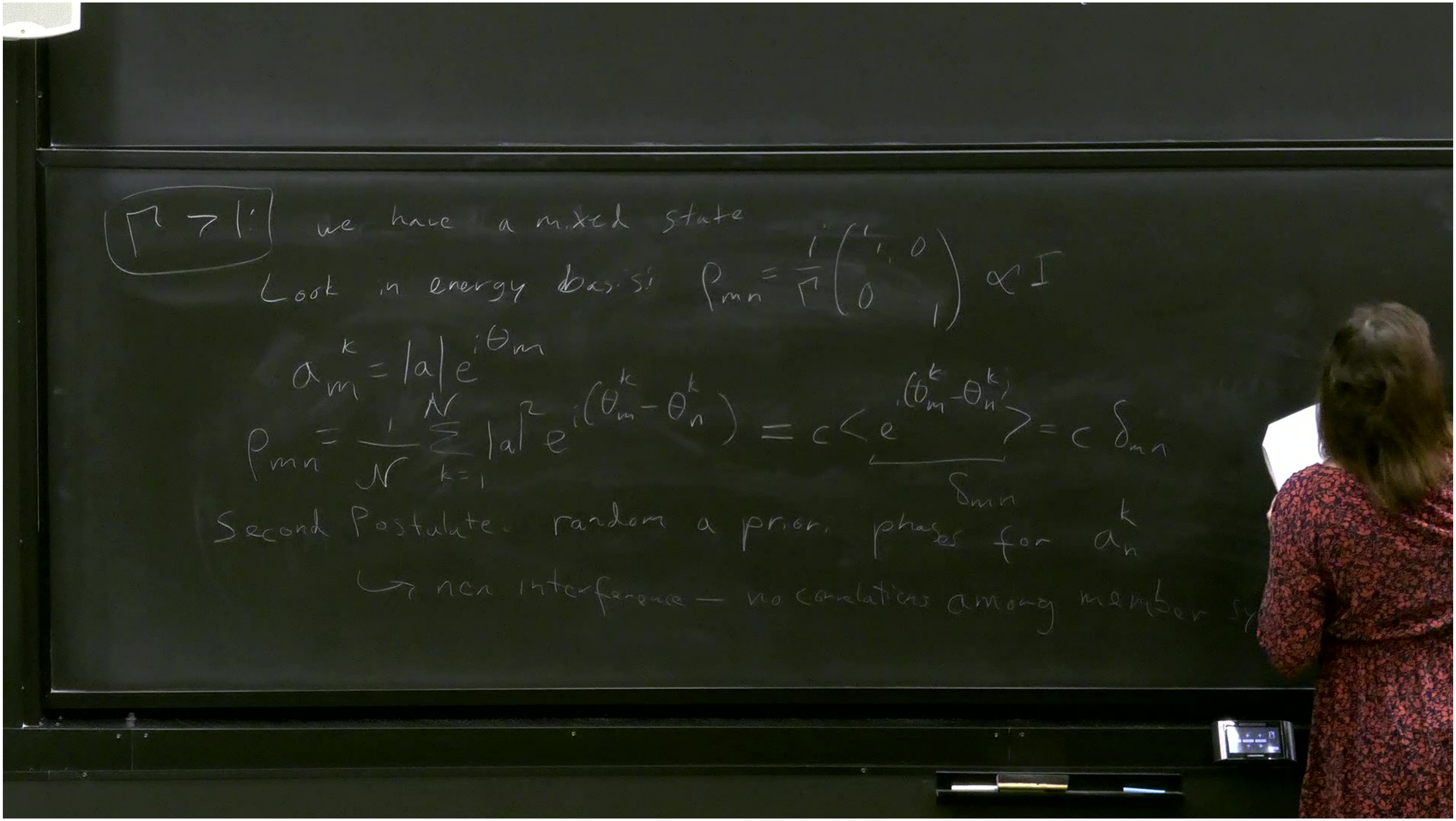
$\rho = |\psi\rangle\langle\psi|$

$\boxed{\Gamma = 1:}$

$$\rho_{mn} = \frac{1}{N} \sum_{k=1}^{N} a_m^k a_n^{k*} = a_m a_n^*$$

$$\rho_{mn}^2 = \sum_l \rho_{ml} \rho_{ln} = \sum_l a_m a_l^* a_l a_n^* = a_m a_n^* = \rho_{mn}$$

Indicator of a pure state: $Tr(\rho^2) = Tr(\rho) = 1$



$\boxed{\Gamma > 1:}$ we have a mixed state

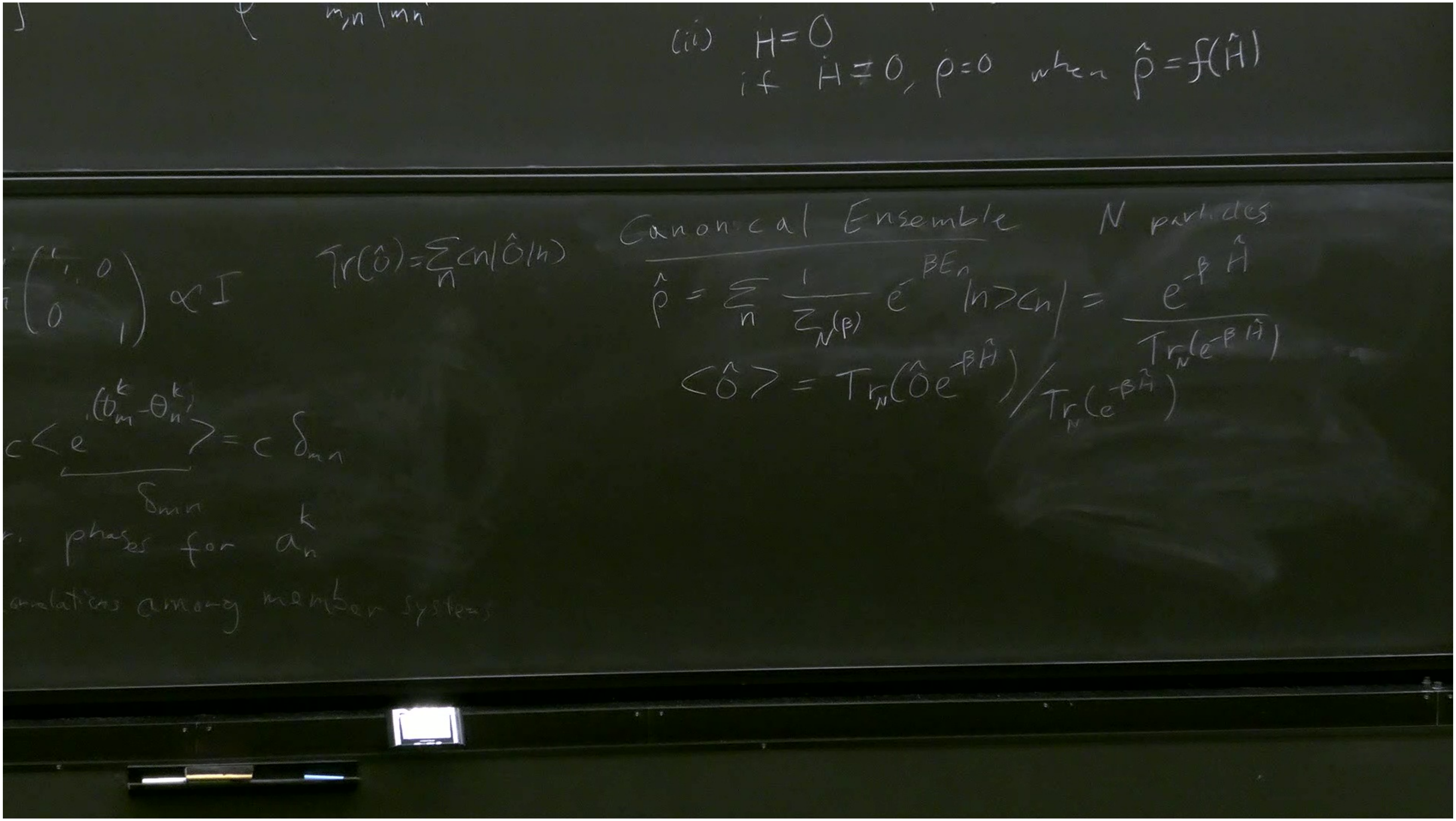
Look in energy basis: $\rho_{mn} = \frac{1}{\Gamma}\begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix} \propto I$

$$a_m^k = |a| e^{i\theta_m}$$

$$\rho_{mn} = \frac{1}{N}\sum_{k=1}^{N} |a|^2 e^{i(\theta_m^k - \theta_n^k)} = c\langle \underbrace{e^{i(\theta_m^k - \theta_n^k)}}_{\delta_{mn}} \rangle = c\,\delta_{mn}$$

Second Postulate: random a priori phases for a_n^k

↪ non interference — no correlations among member sy



(ii) $\dot{H}=0$

if $\dot{H} \neq 0$, $\dot{\rho}=0$ when $\hat{\rho}=f(\hat{H})$

$\begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix} \propto I$

$Tr(\hat{O}) = \sum_n \langle n|\hat{O}|n\rangle$

Canonical Ensemble

N particles

$$\hat{\rho} = \sum_n \frac{1}{Z_N(\beta)} e^{-\beta E_n} |n\rangle\langle n| = \frac{e^{-\beta \hat{H}}}{Tr_N(e^{-\beta \hat{H}})}$$

$$\langle \hat{O} \rangle = Tr_N(\hat{O} e^{-\beta \hat{H}}) / Tr_N(e^{-\beta \hat{H}})$$

$$c \underbrace{\langle e^{i(\theta_m^k - \theta_n^k)} \rangle}_{\delta_{mn}} = c\, \delta_{mn}$$

phases for a_n^k

correlations among member systems

(ii) $\dot{H}=0$

if $\dot{H} \neq 0$, $\dot{\rho}=0$ when $\hat{\rho} = f(\hat{H})$

$\begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix} \propto I$

$\mathrm{Tr}(\hat{O}) = \sum_n \langle n|\hat{O}|n\rangle$

$c\langle \underbrace{e^{i(\theta_m^k - \theta_n^k)}}_{\delta_{mn}} \rangle = c\,\delta_{mn}$

r. phases for a_n^k

correlations among member systems

Canonical Ensemble

N particles

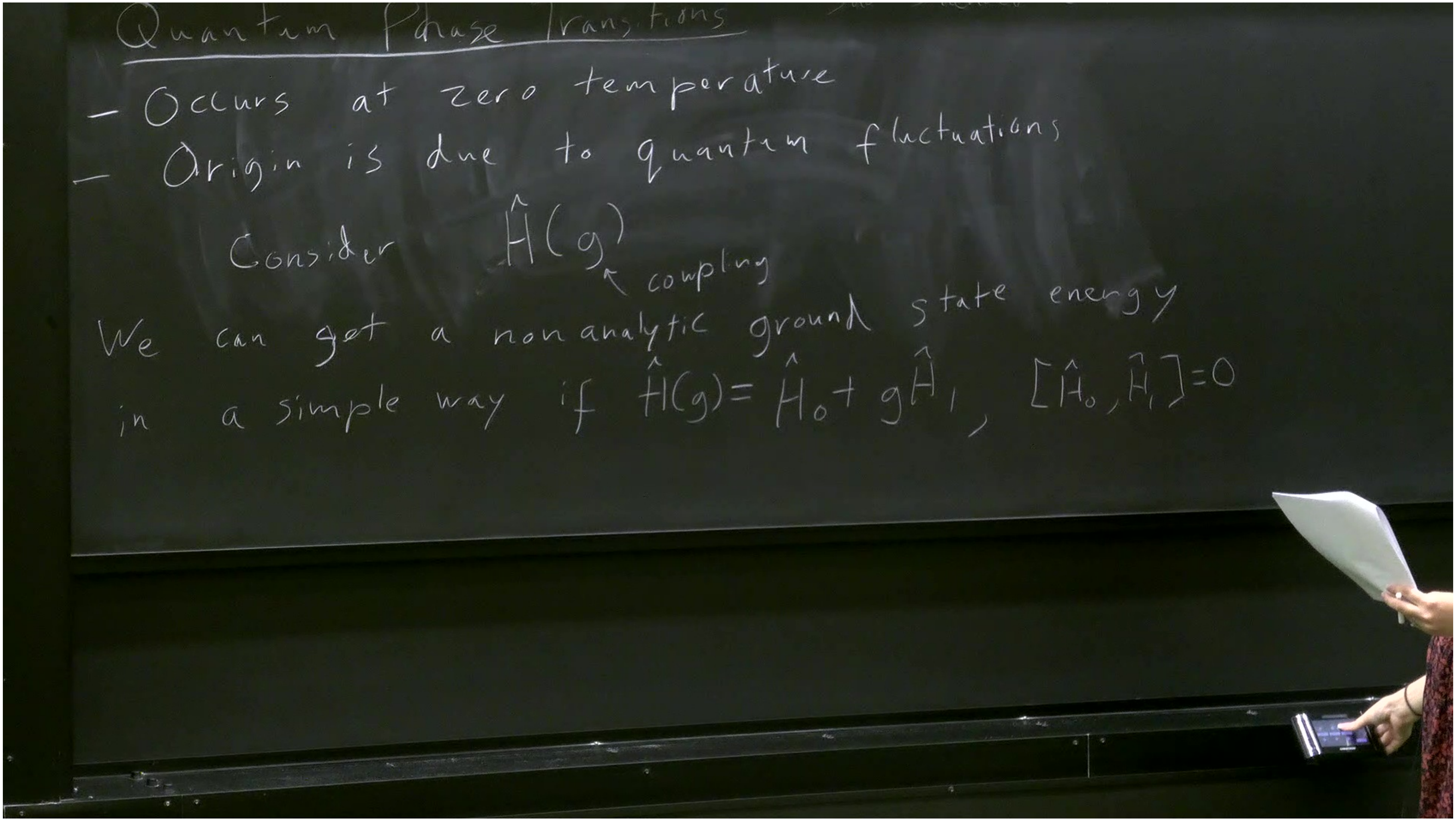
$$\hat{\rho} = \sum_n \frac{1}{Z_N(\beta)} e^{-\beta E_n} |n\rangle\langle n| = \frac{e^{-\beta \hat{H}}}{\mathrm{Tr}_N(e^{-\beta\hat{H}})}$$

$$\langle \hat{O} \rangle = \mathrm{Tr}_N(\hat{O} e^{-\beta\hat{H}}) / \mathrm{Tr}_N(e^{-\beta\hat{H}})$$

Grand Canonical Ensemble

$$\hat{\rho} = \frac{1}{Z(\beta,\mu)} e^{-\beta(\hat{H} - \mu\hat{N})}$$

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}(\hat{O} e^{-\beta\hat{H} + \beta\mu\hat{N}})}{\mathrm{Tr}(e^{-\beta\hat{H} + \beta\mu\hat{N}})}$$

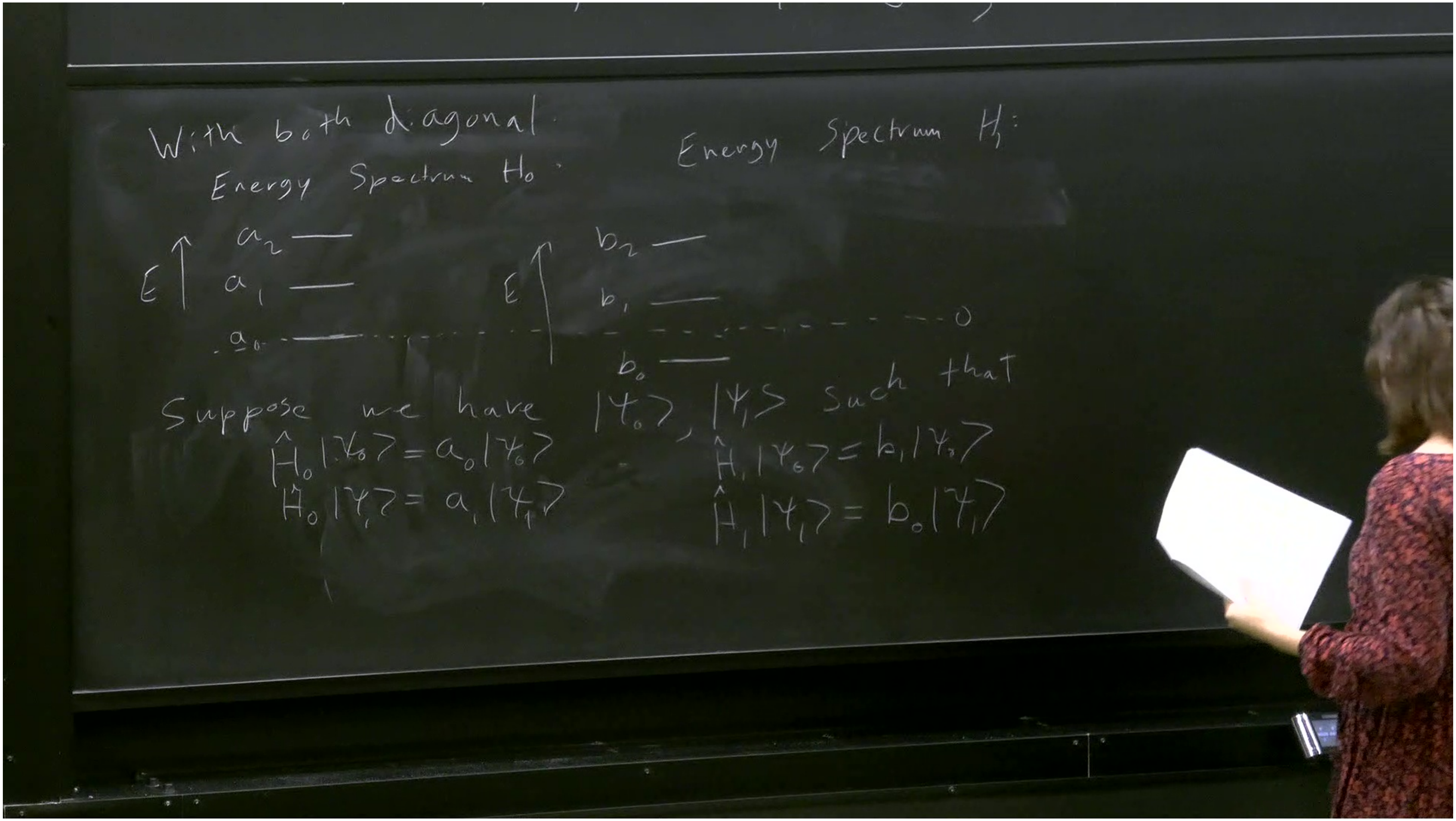


Quantum Phase Transitions

- Occurs at zero temperature
- Origin is due to quantum fluctuations

Consider $\hat{H}(g)$ $\nwarrow$ coupling

We can get a nonanalytic ground state energy in a simple way if $\hat{H}(g) = \hat{H}_0 + g\hat{H}_1$, $[\hat{H}_0, \hat{H}_1] = 0$



With both diagonal:

Energy Spectrum H_0:

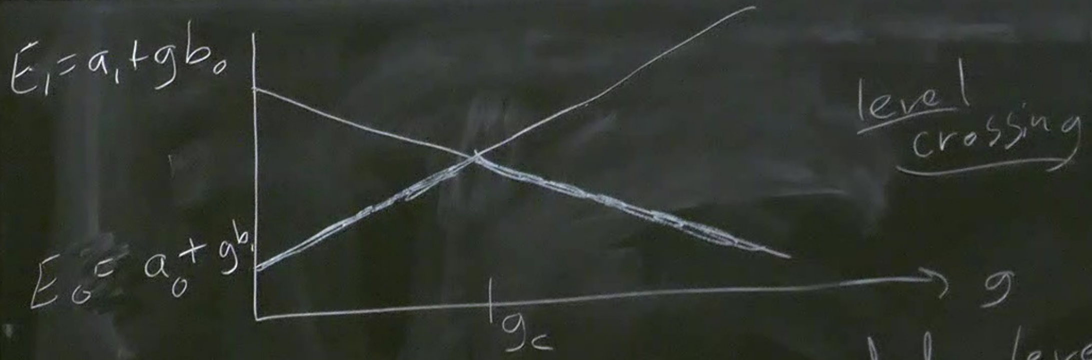
Energy Spectrum H_1:

Suppose we have $|\psi_0\rangle, |\psi_1\rangle$ such that

$$\hat{H}_0|\psi_0\rangle = a_0|\psi_0\rangle \qquad \hat{H}_1|\psi_0\rangle = b_1|\psi_0\rangle$$

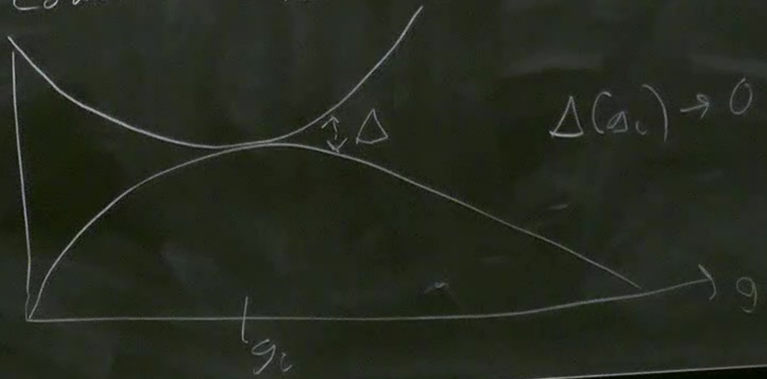
$$\hat{H}_0|\psi_1\rangle = a_1|\psi_1\rangle \qquad \hat{H}_1|\psi_1\rangle = b_0|\psi_1\rangle$$

$H_1|\psi_1\rangle = b_0|\psi_1\rangle$

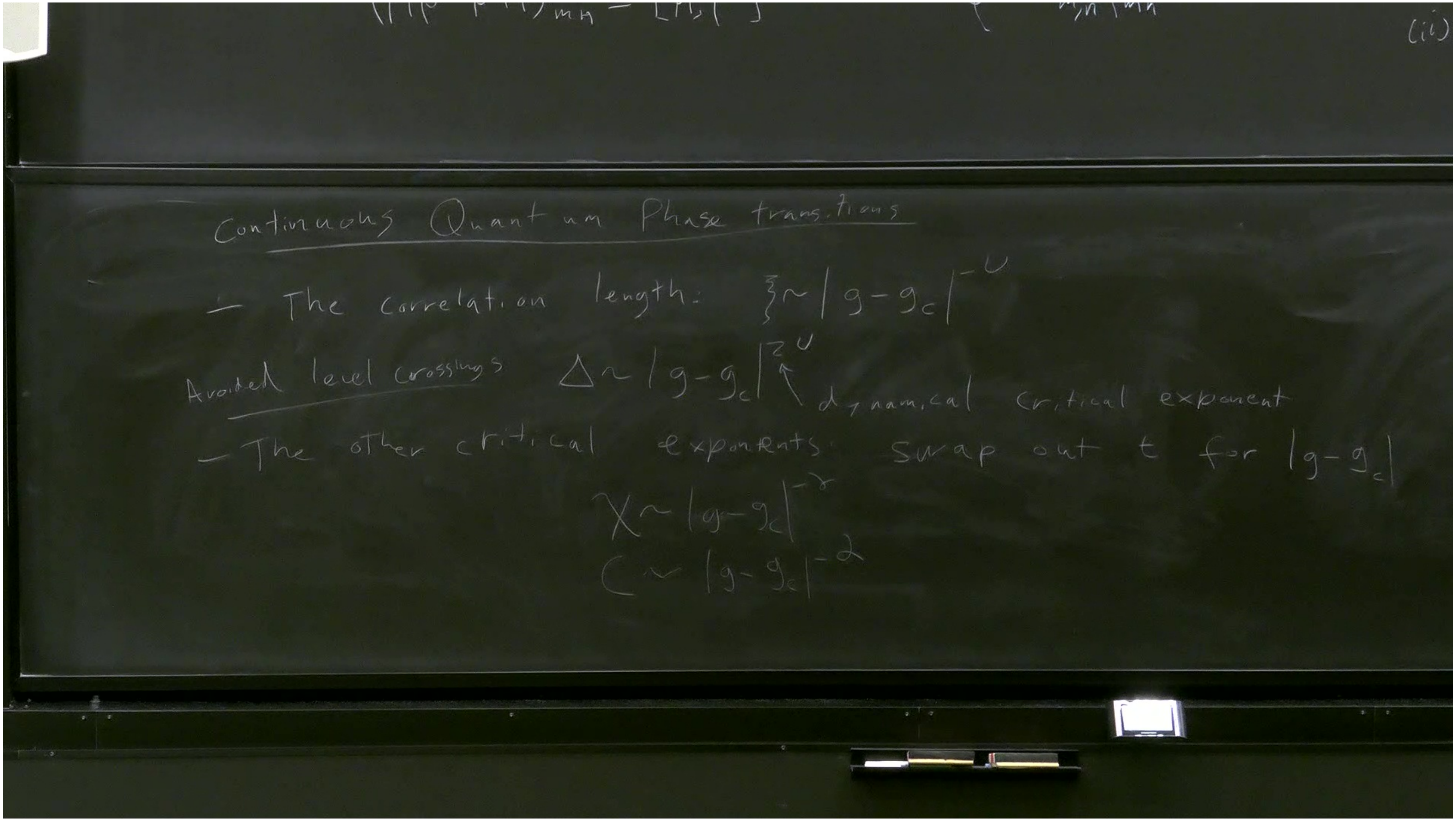


level crossing

— More common is an avoided level crossing



$\Delta(g_c) \to 0$ as $N \to \infty$



(ii)

Continuous Quantum Phase transitions

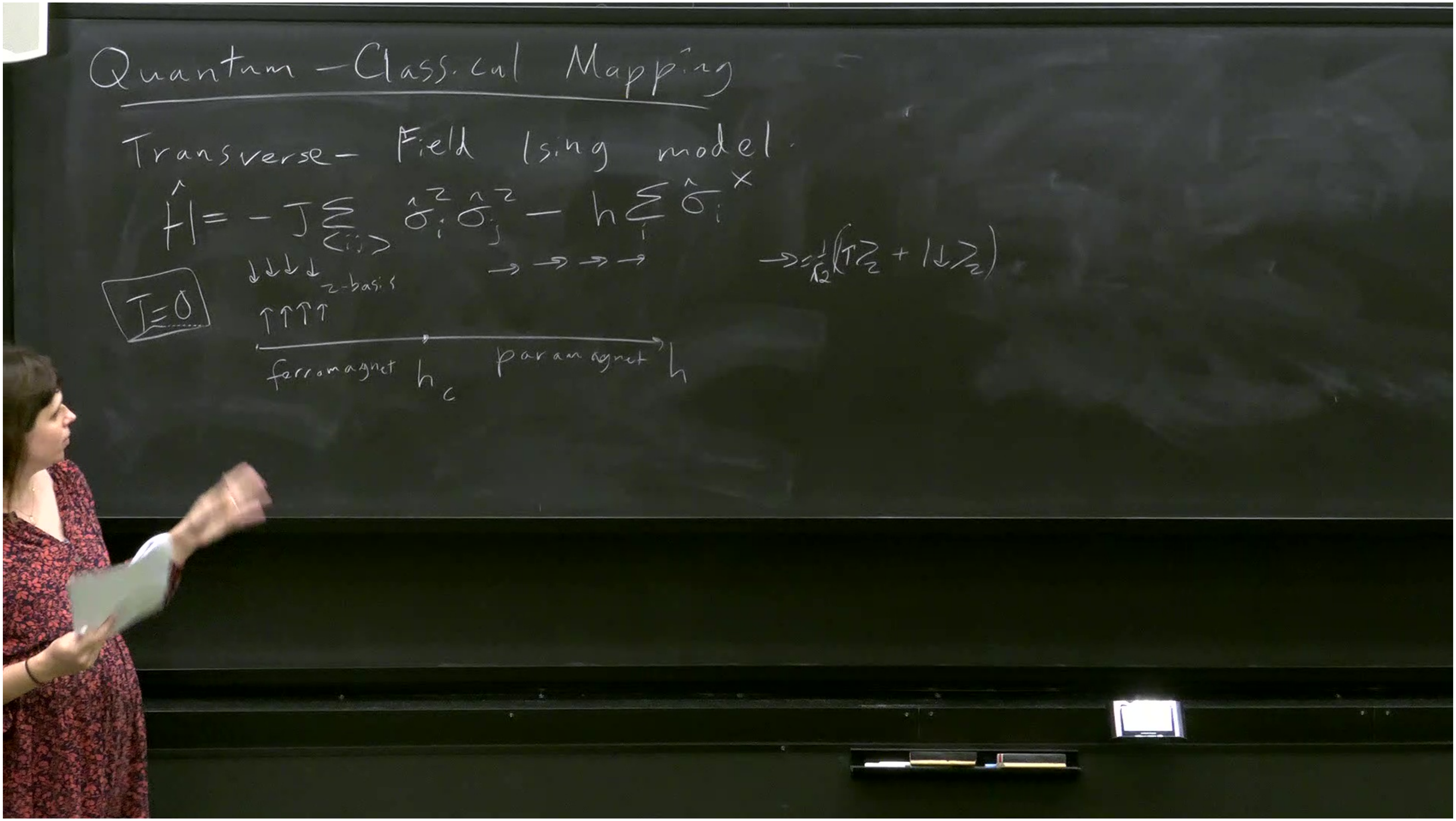
- The correlation length: $\xi \sim |g-g_c|^{-\nu}$

Avoided level crossings $\Delta \sim |g-g_c|^{z\nu}$ ↖ dynamical critical exponent

- The other critical exponents: swap out t for $|g-g_c|$

$$\chi \sim |g-g_c|^{-\gamma}$$

$$C \sim |g-g_c|^{-\alpha}$$



Quantum-Classical Mapping

Transverse-Field Ising model.

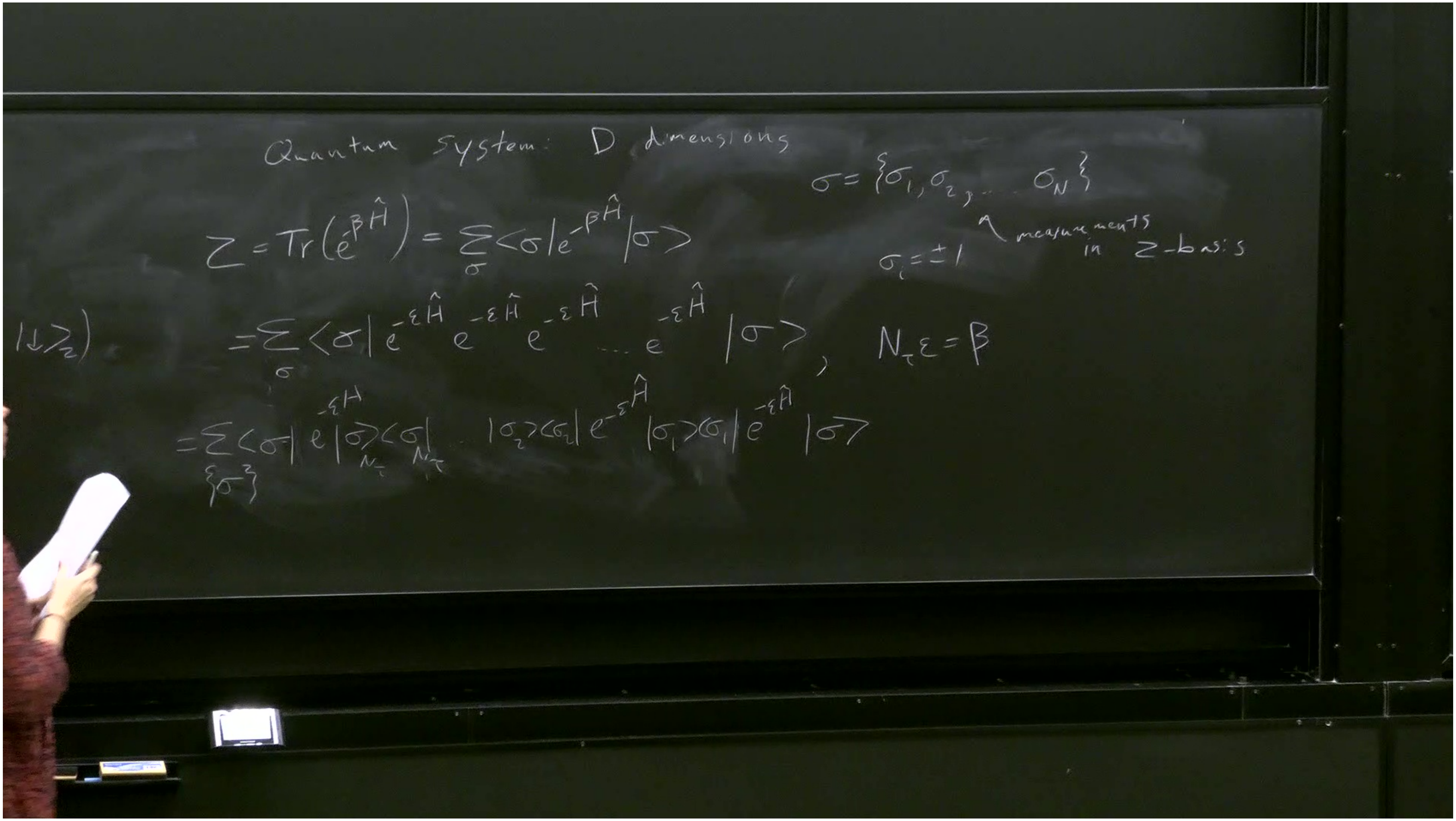
$$\hat{H} = -J\sum_{\langle ij\rangle}\hat{\sigma}_i^z\hat{\sigma}_j^z - h\sum_i \hat{\sigma}_i^x$$

$\boxed{J=0}$

$\downarrow\downarrow\downarrow\downarrow_{z\text{-basis}}$ $\qquad \rightarrow\rightarrow\rightarrow\rightarrow \qquad \rightarrow = \frac{1}{\sqrt{2}}(|\uparrow\rangle_z + |\downarrow\rangle_z)$

$\uparrow\uparrow\uparrow\uparrow$

ferromagnet h_c paramagnet h



Quantum system: D dimensions

$\sigma = \{\sigma_1, \sigma_2, \dots \sigma_N\}$

measurements in Z-basis

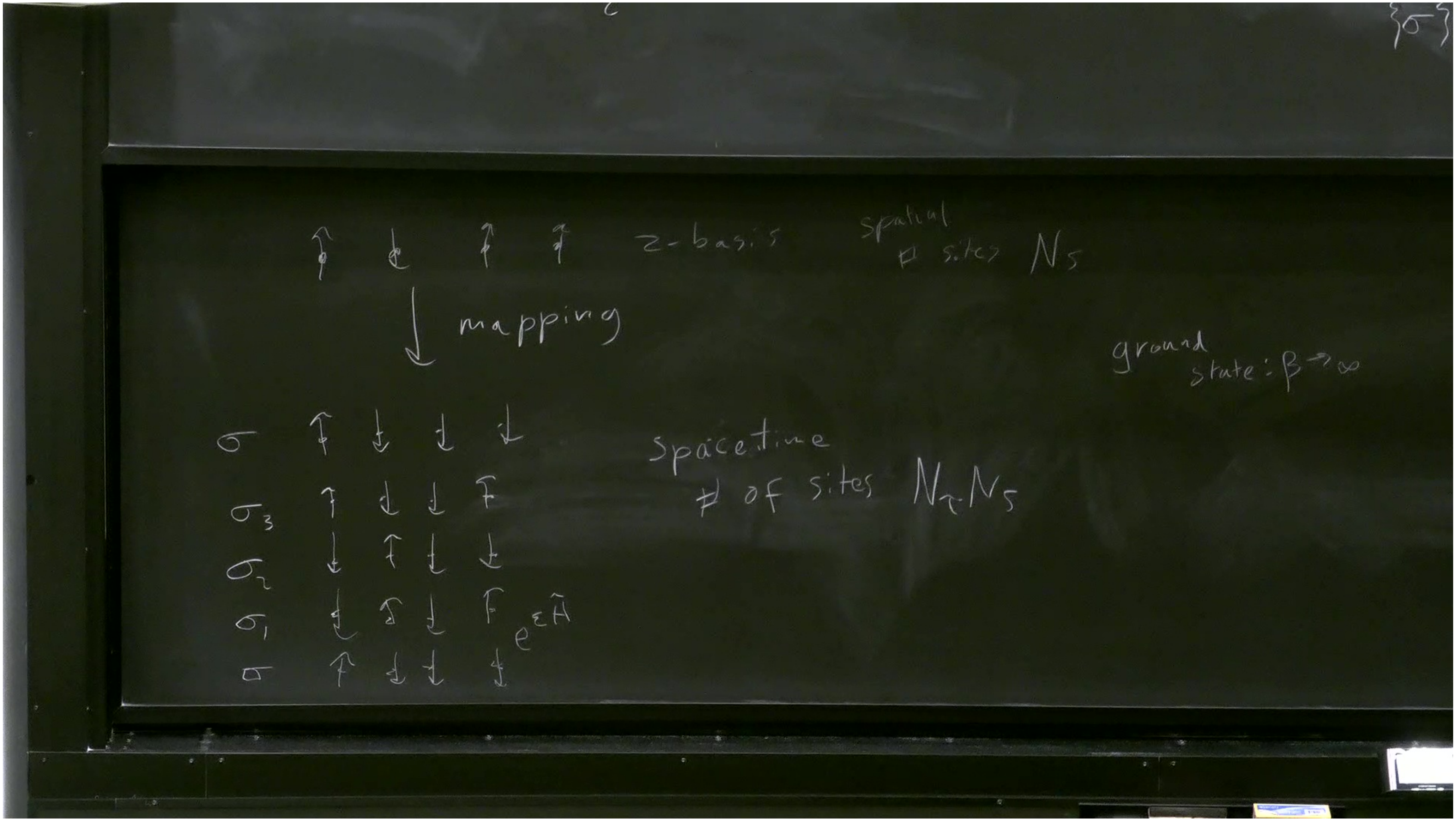
$\sigma_i = \pm 1$

$$Z = \mathrm{Tr}(e^{-\beta \hat{H}}) = \sum_{\sigma} \langle \sigma | e^{-\beta \hat{H}} | \sigma \rangle$$

$|\downarrow\rangle_2)$

$$= \sum_{\sigma} \langle \sigma | e^{-\varepsilon \hat{H}} e^{-\varepsilon \hat{H}} e^{-\varepsilon \hat{H}} \cdots e^{-\varepsilon \hat{H}} | \sigma \rangle, \quad N_\tau \varepsilon = \beta$$

$$= \sum_{\{\sigma\}} \langle \sigma | e^{-\varepsilon H} | \sigma_{N_\tau} \rangle \langle \sigma_{N_\tau} | \cdots | \sigma_2 \rangle \langle \sigma_2 | e^{-\varepsilon \hat{H}} | \sigma_1 \rangle \langle \sigma_1 | e^{-\varepsilon \hat{H}} | \sigma \rangle$$



$\{\sigma\}$

$\uparrow \; \downarrow \; \uparrow \; \uparrow$ z-basis

spatial
sites N_s

$\downarrow$ mapping

ground state: $\beta \to \infty$

$\sigma \quad \uparrow \; \downarrow \; \downarrow \; \downarrow$

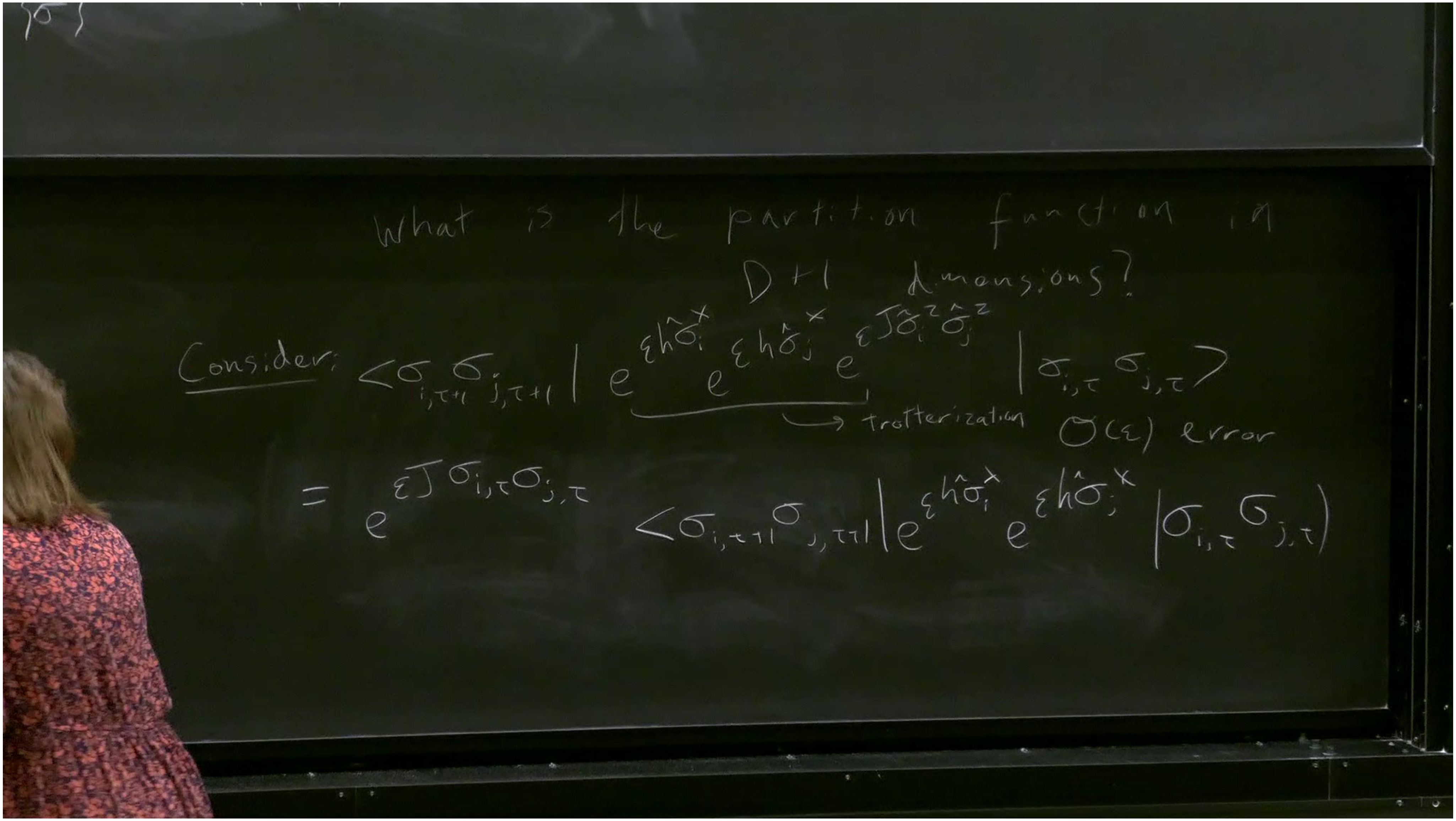
$\sigma_3 \quad \uparrow \; \downarrow \; \downarrow \; \uparrow$

$\sigma_2 \quad \downarrow \; \uparrow \; \downarrow \; \downarrow$

$\sigma_1 \quad \downarrow \; \uparrow \; \downarrow \; \uparrow \quad e^{\varepsilon \hat{H}}$

$\sigma \quad \uparrow \; \downarrow \; \downarrow \; \downarrow$

Spacetime
# of sites $N_\tau \cdot N_s$



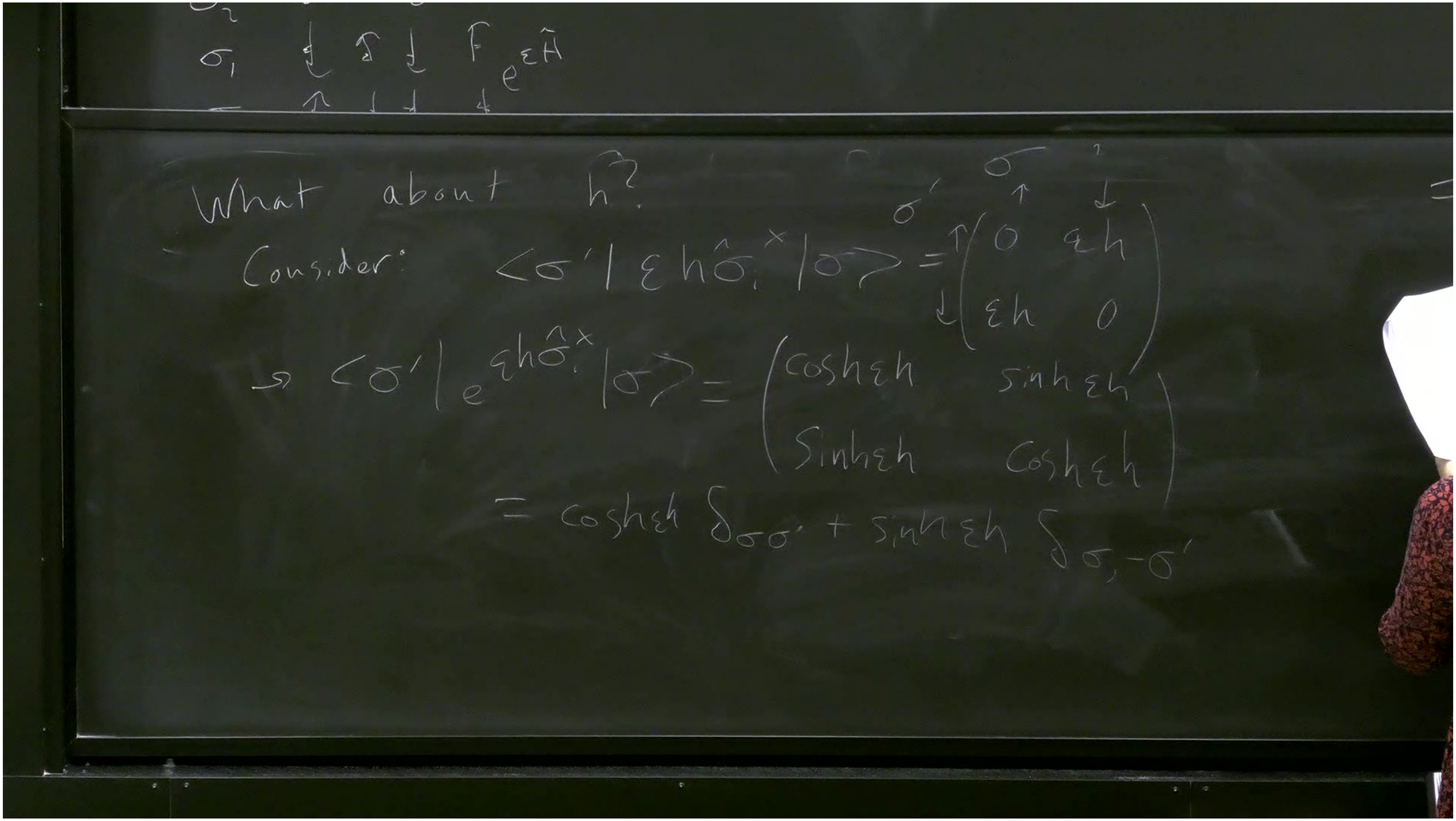
$\{\sigma\}$

What is the partition function in D+1 dimensions?

Consider: $$\langle \sigma_{i,\tau+1}\,\sigma_{j,\tau+1} \,|\, \underbrace{e^{\varepsilon h \hat{\sigma}_i^x}\, e^{\varepsilon h \hat{\sigma}_j^x}\, e^{\varepsilon J \hat{\sigma}_i^z \hat{\sigma}_j^z}} \,|\, \sigma_{i,\tau}\,\sigma_{j,\tau} \rangle$$

$\hookrightarrow$ trotterization $\mathcal{O}(\varepsilon)$ error

$$= e^{\varepsilon J \sigma_{i,\tau}\sigma_{j,\tau}} \quad \langle \sigma_{i,\tau+1}\,\sigma_{j,\tau+1} | e^{\varepsilon h \hat{\sigma}_i^x}\, e^{\varepsilon h \hat{\sigma}_j^x} | \sigma_{i,\tau}\,\sigma_{j,\tau})$$



σ_2

$\sigma_1 \quad \downarrow \quad \uparrow \quad \downarrow \quad \uparrow \quad e^{\varepsilon \hat{H}}$

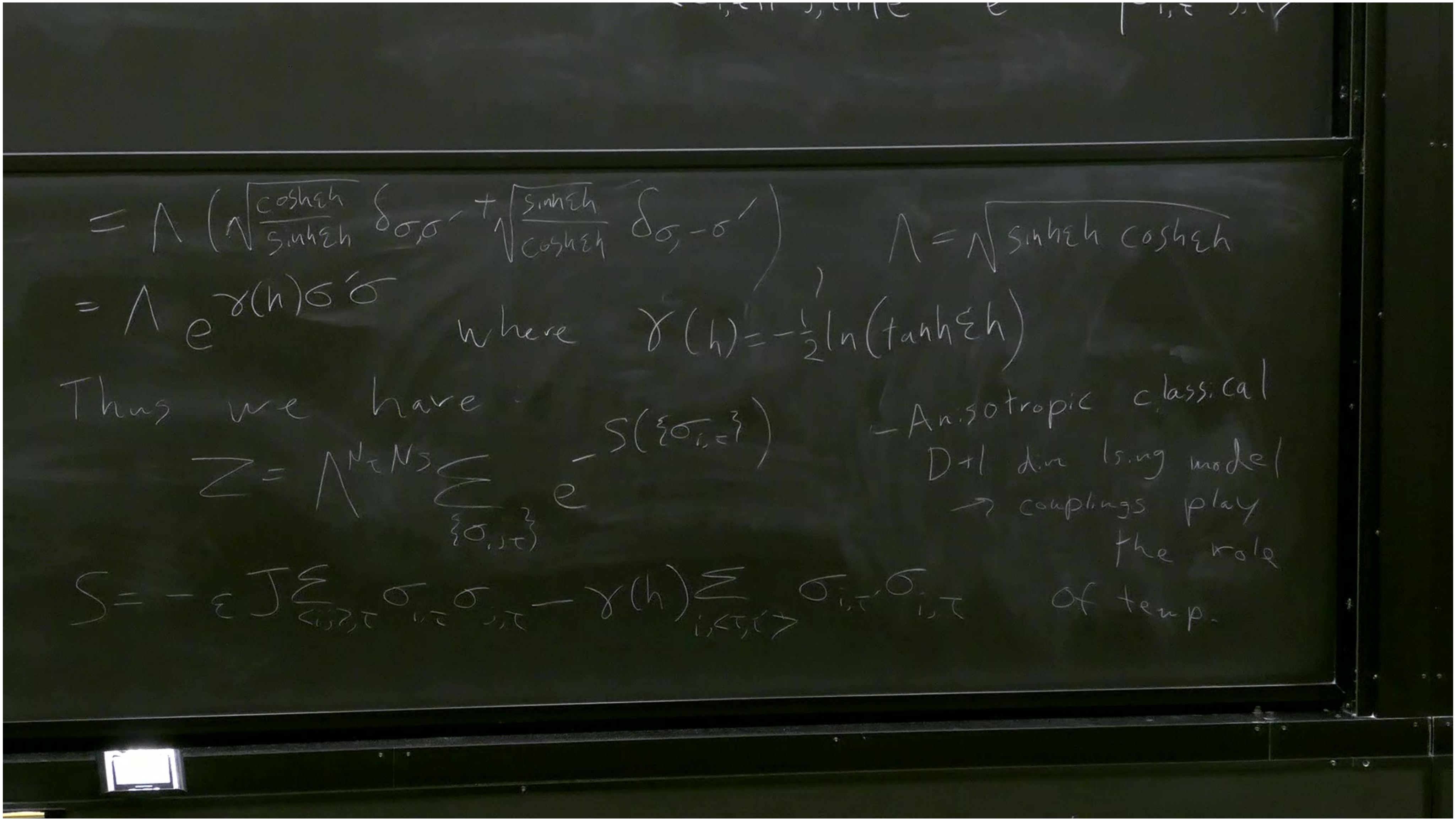
$\uparrow \quad \downarrow \quad \downarrow \quad \downarrow$

What about $\hat{h}$?

Consider: $\langle \sigma' | \varepsilon h \hat{\sigma}_i^x | \sigma \rangle = \begin{array}{c|cc} \sigma' \backslash \sigma & \uparrow & \downarrow \\ \hline \uparrow & 0 & \varepsilon h \\ \downarrow & \varepsilon h & 0 \end{array}$

$\rightarrow \langle \sigma' | e^{\varepsilon h \hat{\sigma}_i^x} | \sigma \rangle = \begin{pmatrix} \cosh \varepsilon h & \sinh \varepsilon h \\ \sinh \varepsilon h & \cosh \varepsilon h \end{pmatrix}$

$= \cosh \varepsilon h \, \delta_{\sigma \sigma'} + \sinh \varepsilon h \, \delta_{\sigma, -\sigma'}$



$$= \Lambda \left(\sqrt{\frac{\cosh \epsilon h}{\sinh \epsilon h}}\, \delta_{\sigma,\sigma'} + \sqrt{\frac{\sinh \epsilon h}{\cosh \epsilon h}}\, \delta_{\sigma,-\sigma'} \right) \qquad \Lambda = \sqrt{\sinh \epsilon h \cosh \epsilon h}$$

$$= \Lambda\, e^{\gamma(h)\sigma'\sigma} \quad \text{where} \quad \gamma(h) = -\frac{1}{2}\ln(\tanh \epsilon h)$$

Thus we have:

$$Z = \Lambda^{N_\tau N_s} \sum_{\{\sigma_{i,\tau}\}} e^{-S(\{\sigma_{i,\tau}\})}$$

$$S = -\epsilon J \sum_{\langle ij \rangle,\tau} \sigma_{i,\tau}\sigma_{j,\tau} - \gamma(h) \sum_{i,\langle \tau,\tau' \rangle} \sigma_{i,\tau'}\sigma_{i,\tau}$$

– Anisotropic classical D+1 dim Ising model

→ couplings play the role of temp.