Title: Lecture - Statistical Physics, PHYS 602

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Subject: Condensed Matter, Other

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∂t continuity equation, generic fluid

but $\nabla \cdot (\rho v) = \frac{\partial \rho}{\partial x^a} v^a = \frac{\partial \rho}{\partial x^a} \dot{X}^a$

so $\boxed{\frac{\partial \rho}{\partial t} + \{\rho, H\} = 0}$ (Hamilton's equations specifically) (Liouville)

$\boxed{\{\rho, H\} = 0}$ equilibrium $\frac{\partial \rho}{\partial t} = 0$

At

At equilibrium, we can write:

$$\rho(q,p) = \rho[H(q,p)]$$

Gibbs/Shannon Entropy ← connected to Boltzmann entropy (Tutorial 1)

Allows to define entropy (S) from weights (ρ) of the microstates

For $P_\lambda = \frac{\rho_\lambda}{\sum_\lambda \rho_\lambda}$ (λ state), the Gibbs Entropy is

$$\boxed{S = -k \sum_\lambda P_\lambda \ln(P_\lambda)}$$

Continuous versio

state $\sum_\lambda P_\lambda$, The Gibbs Entropy

$$\boxed{S = -k \sum_\lambda P_\lambda \ln(P_\lambda)}$$

$$P(q,p) = \frac{\rho(p,q)}{\int_M \rho(q,p)\, d^N q\, d^N p}$$

← not dimensionless

$$S = -k \int_M P(q,p) \ln\left(P(q,p) W_0\right) d^N q\, d^N p$$

↑ fundamental volume of phase space)

(Tutorial 2)

fundamental volume of phase space (Tutorial 2)

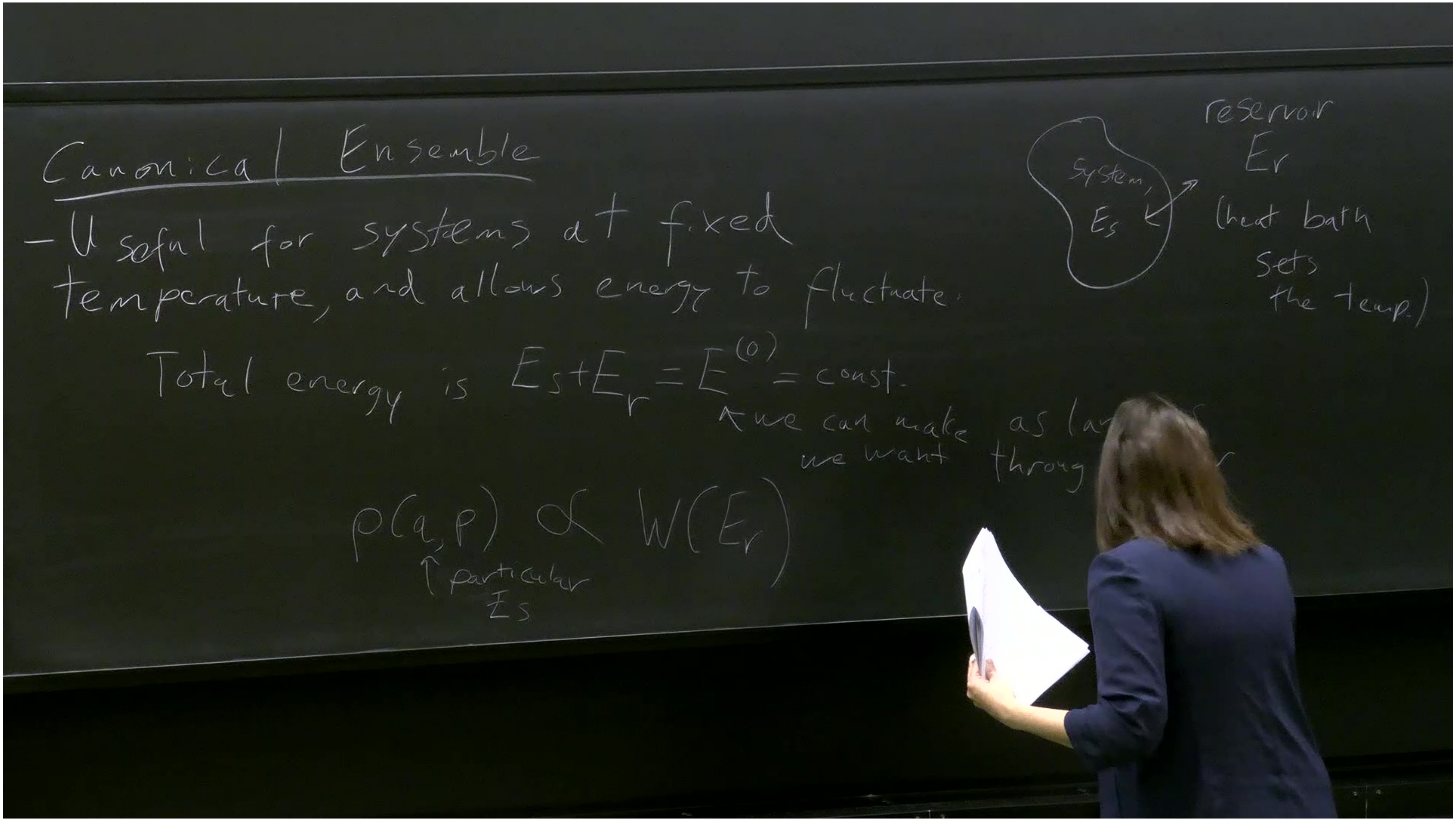
W is total number of microstates

$$S = -k\int_M P(q,p)\ln\left(P(q,p)\,W_0\right) d^Nq\, d^Np$$

$$P(q,p) = \frac{1}{W}$$

$$= -k\ln\left(\frac{1}{W}W_0\right)\underbrace{\int_M P(q,p)\,d^Nq\, d^Np}_{1}$$

$$\boxed{S = k\ln\left(\frac{W}{W_0}\right)}$$


Canonical Ensemble
- Useful for systems at fixed temperature, and allows energy to fluctuate.
Total energy is $E_s + E_r = E^{(0)} = \text{const.}$
we can make as
we want
$\rho(q,p) \propto W(E_r)$
particular E_s
System, E_s
reservoir E_r
(heat bath sets the temp.)

because for each q,p state, we need $W(E_r)$ to get the full weight of syst res

To get a convergent series, we expand in terms of $\ln(\rho(p,q))$ about $E_r = E^{(0)}$ (since $E^{(0)} - E_r$ is small)

$$\ln(\rho(p,q)) \simeq \ln(W(E^{(0)})) + \underbrace{\left.\frac{\partial \ln W(E)}{\partial E}\right|_{E=E^{(0)}}}_{\frac{1}{k}\frac{\partial S}{\partial E}} (E_r - E^{(0)}) + \dots$$

$\ln(\rho(p,q))$ about $E_r = E^{(0)}$

(since $E^{(0)} - E_r$ is small)

$$\ln(\rho(p,q)) \simeq \ln(W(E^{(0)})) + \frac{\partial \ln W(E)}{\partial E}\bigg|_{E=E^{(0)}} (E_r - E^{(0)}) + \dots$$

$$\frac{1}{k}\frac{\partial S}{\partial E} \qquad \frac{1}{T}$$

$$\ln(\rho(p,q)) = \text{const.} - \beta E_s$$

And
$$P(q,p) = \frac{e^{-\beta H(q,p)}}{Z}$$

$$\ln(e^{-\beta H(q,p)}) + \ln(W_0/Z) \quad \checkmark$$

$$\rho(q,p) \propto e^{-\beta H(q,p)}$$

Gibbs Entropy

$$S = -\frac{k}{Z}\int_M e^{-\beta H(q,p)} \ln\left(e^{-\beta H(q,p)} W_0/Z\right) d^N q\, d^N p$$

For continuous q, p:

$$Z = \int_M e^{-\beta H(q,p)} d^N q\, d^N p$$

$$\boxed{S = k\beta \langle E \rangle + k \ln\left(\frac{Z}{W_0}\right)}$$

$$S = k\beta \langle E \rangle + k \ln\left(\frac{Z}{W_0}\right)$$

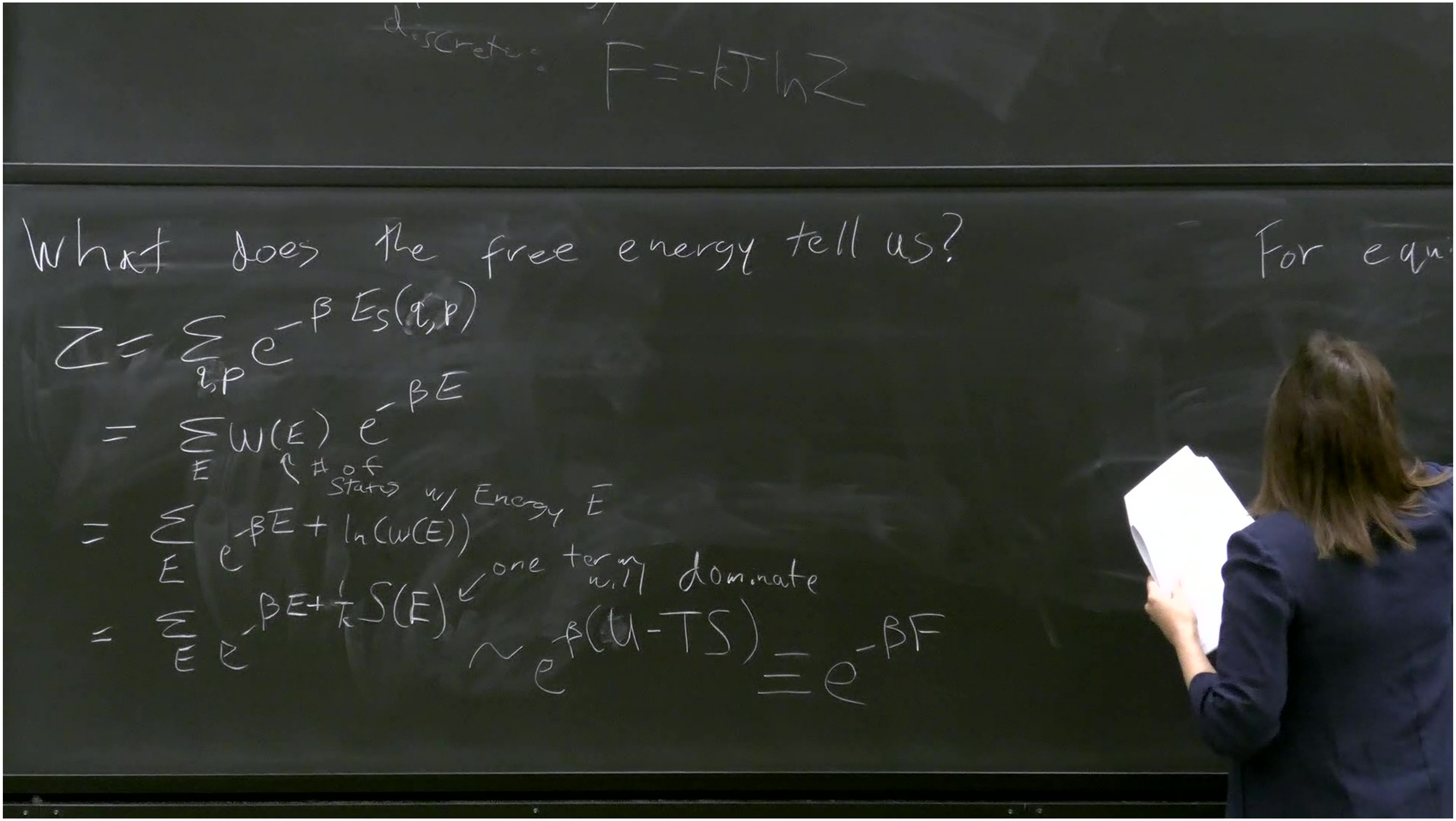
$$\boxed{S = -\left(\frac{\partial F}{\partial T}\right)_E}$$

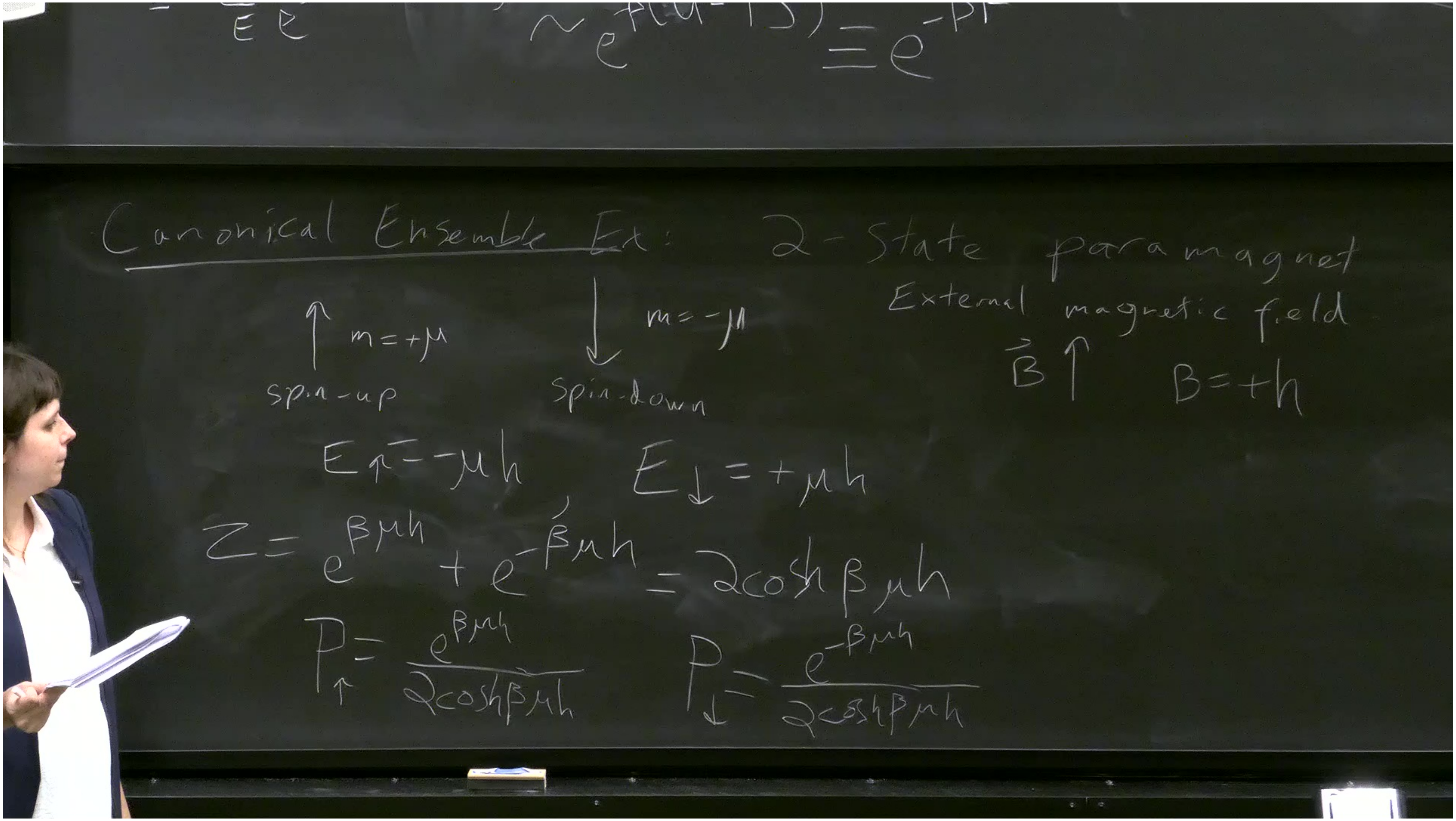
To get to a thermodynamic potential:

$$\boxed{F = U - TS = -kT \ln\left(\frac{Z}{W_0}\right)}$$

helmholtz free energy

discrete: $F = -kT \ln Z$


discrete: $F=-kT\ln Z$
What does the free energy tell us?
For equ
$Z = \sum_{q,p} e^{-\beta E_s(q,p)}$
$= \sum_E W(E)\, e^{-\beta E}$
# of States w/ Energy E
$= \sum_E e^{-\beta E + \ln(W(E))}$
one term will dominate
$= \sum_E e^{-\beta E + \frac{1}{k} S(E)} \sim e^{-\beta(U-TS)} = e^{-\beta F}$


Canonical Ensemble Ex: 2-State paramagnet
External magnetic field
$\vec{B}\uparrow$ $B=+h$
$\uparrow$ $m=+\mu$
spin-up
$\downarrow$ $m=-\mu$
spin-down
$E_\uparrow=-\mu h$, $E_\downarrow=+\mu h$
$Z=e^{\beta\mu h}+e^{-\beta\mu h}=2\cosh\beta\mu h$
$P_\uparrow=\frac{e^{\beta\mu h}}{2\cosh\beta\mu h}$
$P_\downarrow=\frac{e^{-\beta\mu h}}{2\cosh\beta\mu h}$

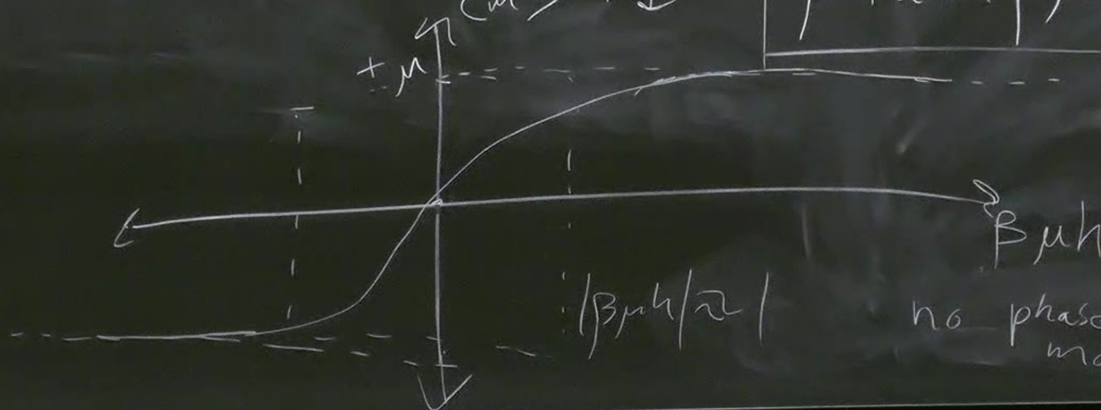
agnet
field
th

Expectations:

high temp – lots of fluctuations in spin $\qquad \beta = \frac{1}{kT}$

low temp – spin should be aligned with mag field

$$\langle m \rangle = \mu P_{\uparrow} - \mu P_{\downarrow} = \boxed{\mu \tanh \beta\mu h} = \langle m \rangle$$



no phase transition system is always magnetized for finite h.

agnet
field
th

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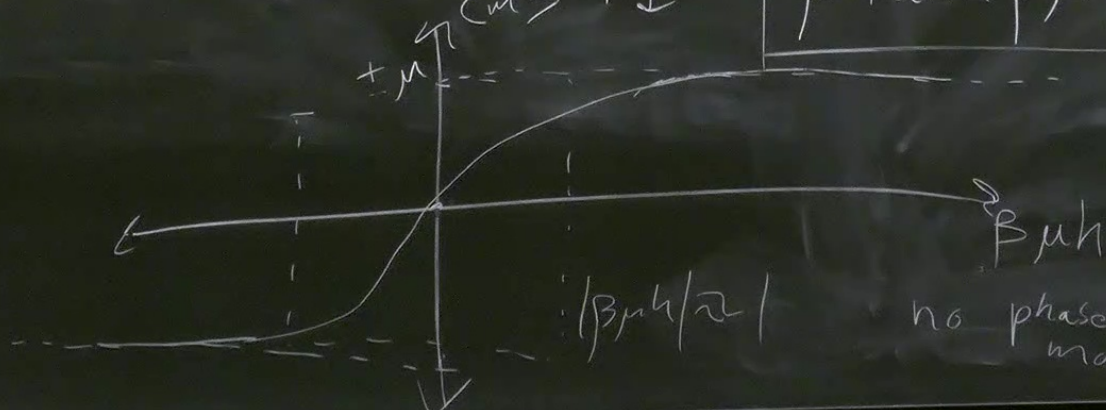
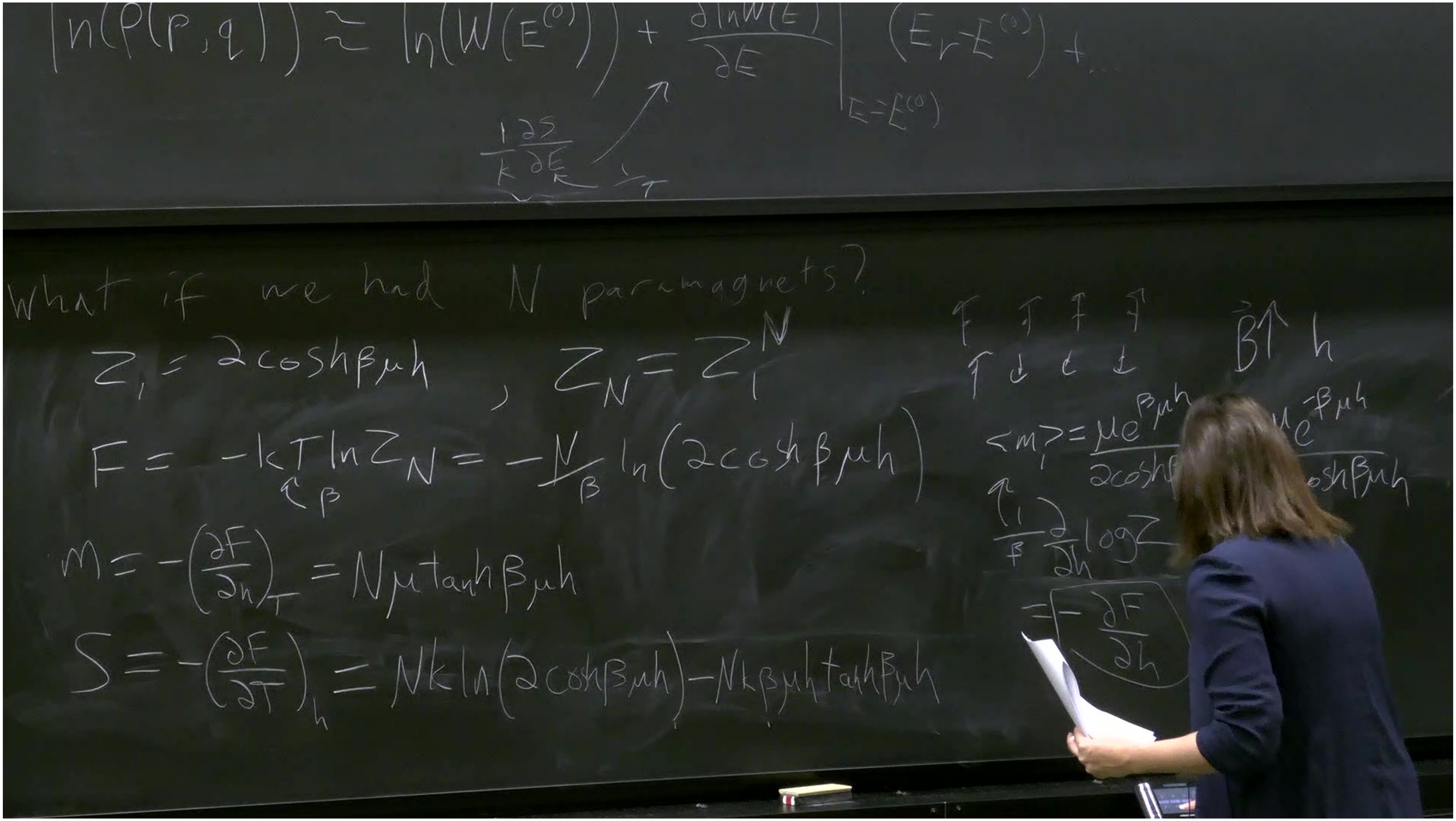
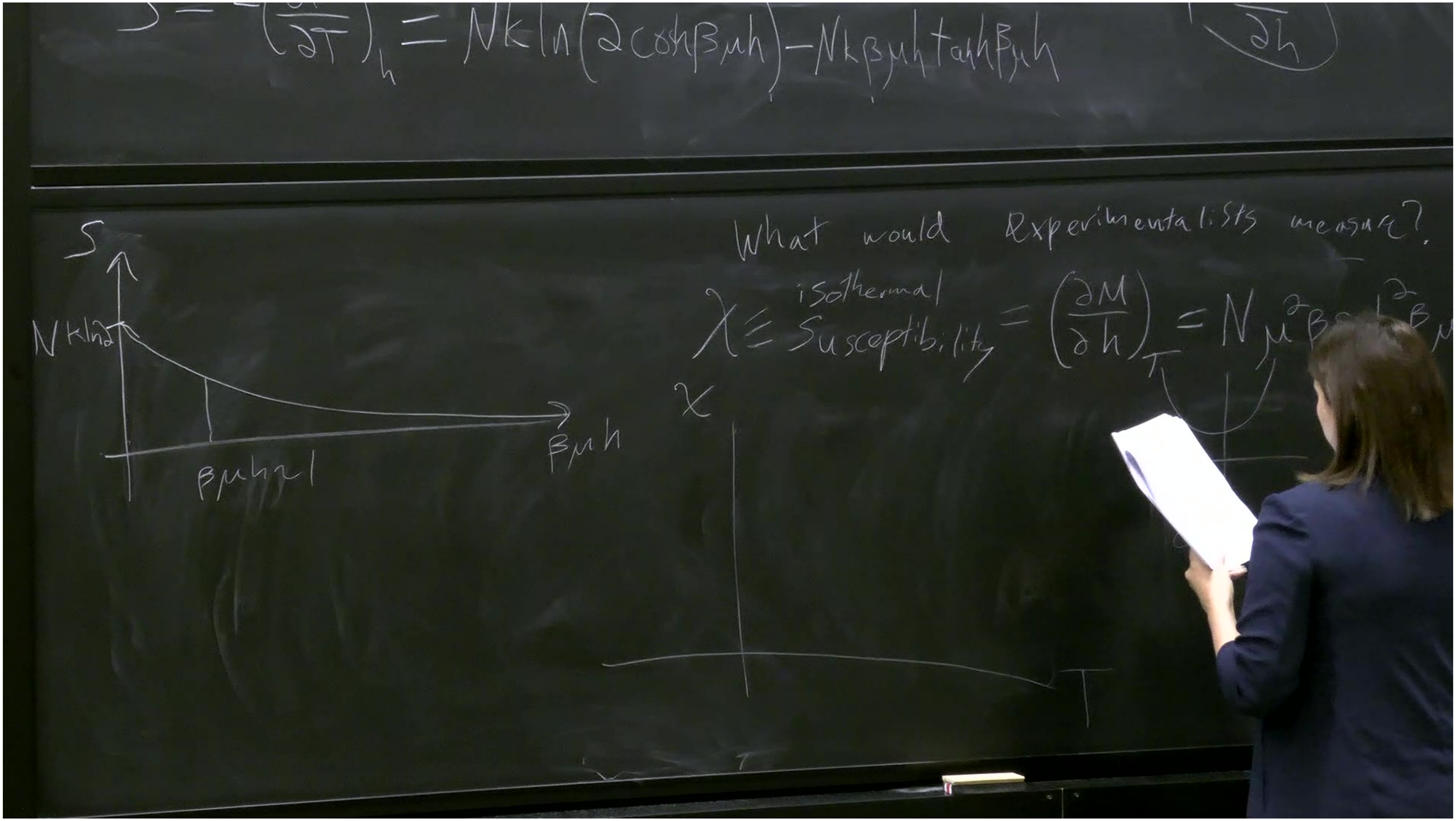


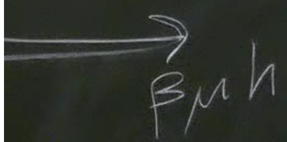
no phase transition system is always magnetized for finite h.

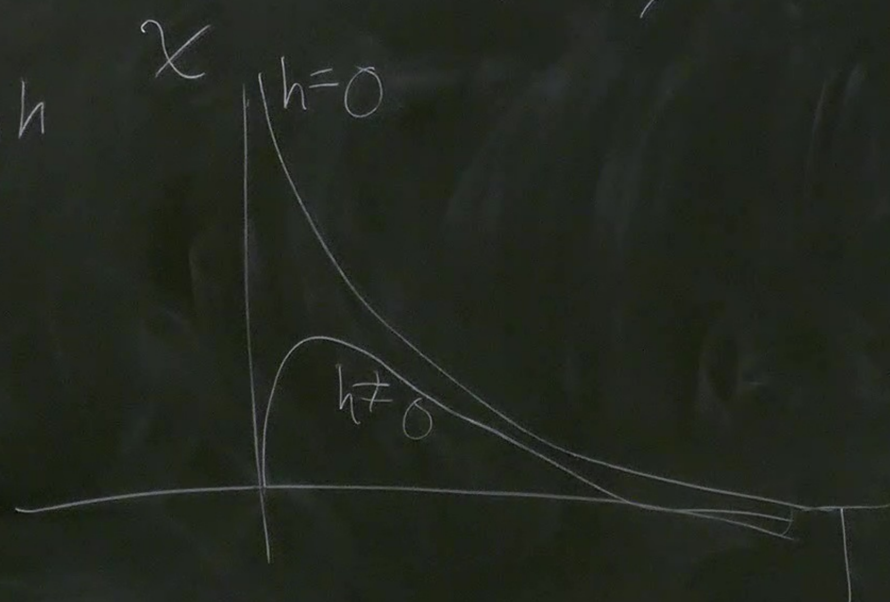

$\ln(\rho(p,q)) \simeq \ln(W(E^{(0)})) + \left.\frac{\partial \ln W(E)}{\partial E}\right|_{E=E^{(0)}} (E_r - E^{(0)}) + \ldots$
$\frac{1}{k}\frac{\partial S}{\partial E}$
$\frac{1}{T}$
What if we had N paramagnets?
$Z_1 = 2\cosh\beta\mu h \quad , \quad Z_N = Z_1^N$
$F = -kT \ln Z_N = -\frac{N}{\beta} \ln(2\cosh\beta\mu h)$
β
$M = -\left(\frac{\partial F}{\partial h}\right)_T = N\mu \tanh\beta\mu h$
$S = -\left(\frac{\partial F}{\partial T}\right)_h = Nk\ln(2\cosh\beta\mu h) - Nk\beta\mu h \tanh\beta\mu h$
$\vec{B}\uparrow h$
$\langle m_1 \rangle = \frac{\mu e^{\beta\mu h} - \mu e^{-\beta\mu h}}{2\cosh\beta\mu h}$
$\frac{1}{\beta}\frac{\partial}{\partial h}\log Z_1$
$= -\frac{\partial F}{\partial h}$

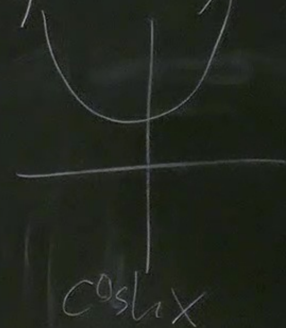

= Nk ln(2 cosh βμh) − Nkβμh tanh βμh
S
Nk ln2
βμh≈1
βμh
What would experimentalists measure?
χ ≡ isothermal Susceptibility = (∂M/∂h)_T = Nμ²β
χ
T

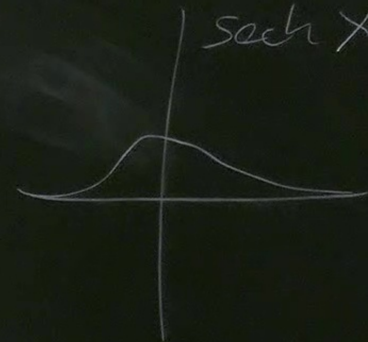
What would experimentalists measure?

$$\chi \equiv \text{isothermal Susceptibility} = \left(\frac{\partial M}{\partial h}\right)_T = N\mu^2\beta\,\mathrm{sech}^2\beta\mu h$$

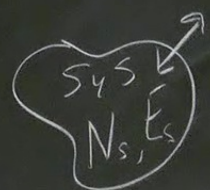








Grand Canonical Ensemble



res
N_r, E_r

$$N_s + N_r = N^{(0)} \qquad N_s \ll N^{(0)}$$

$$E_s + E_r = E^{(0)} \qquad E_s \ll E^{(0)}$$

$$P_s \propto W(E_r, N_r)$$

$$\ln P_S \propto \ln W(N^{(0)}, E^{(0)}) + \left(\frac{\partial \ln W}{\partial N}\right)_{N=N^{(0)}} (N_S - N^{(0)})$$

$$+ \left(\frac{\partial \ln W}{\partial E}\right)\Bigg|_{E=E^{(0)}} (E_S - E^{(0)}) + \ldots$$

chemical potential

$$\simeq \text{const.} + \frac{\mu}{kT} N_S - \frac{1}{kT} E_S$$

$$\rho \propto e^{\mu/kT\, N - \beta E}$$

canonical ensemble

$$\mathcal{Z} = \sum_{N=0}^{\infty} e^{\beta\mu N} Z_N$$

grand canonical ensemble

$$PV = \Phi = U - TS - \mu N = kT \ln \mathcal{Z}$$