

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

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∂_t

continuity equation, generic fluid

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

$A+$

↪ 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 equilibrium, we can write

$$p(q, p) = p[-H(q, p)]$$

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

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

For $P_{\text{state}} = \frac{p_a}{\sum_a p_a}$, the Gibbs Entropy is

$$S = -k \sum_a P_a \ln(P_a)$$

Continuous version

state $\sum_i P_i$ the Gibbs entropy

$$S = -k \sum_i P_i \ln(P_i)$$

$$P(q, p) = \frac{\rho(q, p)}{\int_M \rho(q, p) d^N q d^N p} \leftarrow \text{not dimensionless}$$

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

↑
fundamental volume
of phase space
(Tutorial 2)

\uparrow
 fundamental volume
 of phase space
 (Tutorial 2)

$$S = -k \int_{\mu} P(q, p) \ln(P(q, p) W_0) d^N q d^N p$$

$$= -k \ln\left(\frac{1}{W} W_0\right) \int_{\mu} P(q, p) d^N q d^N p$$

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

W is total
 number of
 microstates

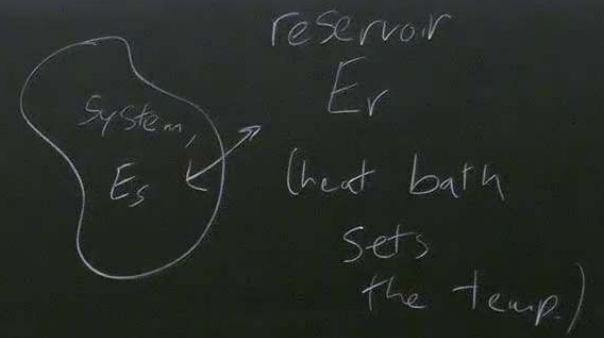
Canonical Ensemble

- 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 large as we want through

$\rho(q, p) \propto W(E_r)$
↑ particular E_s



because for each q, p state, we need $W(E_r)$ to get the full weight of $\text{Sys} + \text{res}$.

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

$$\ln(P(p, q)) \approx \ln(W(E^{(0)})) + \left. \frac{\partial \ln W(E)}{\partial E} \right|_{E=E^{(0)}} (E_r - E^{(0)}) + \dots$$

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

$\ln(p(p, q))$ about $E_r = E^{(0)}$ (since $E^{(0)} - E_r$ is small)

$$\ln(p(p, q)) \approx \ln(W(E^{(0)})) + \left. \frac{\partial \ln W(E)}{\partial E} \right|_{E=E^{(0)}} (E_r - E^{(0)}) + \dots$$

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

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

And $P(a, p) = \frac{e^{-\beta H(a, p)}}{Z}$ $\ln(e^{-\beta H(a, p)}) + \ln\left(\frac{W_0}{Z}\right)$

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

For continuous q, p :

Gibbs Entropy

$$S = -k \int \frac{1}{Z} e^{-\beta H(a, p)} \ln\left(\frac{e^{-\beta H(a, p)}}{W_0/Z}\right) d^N q d^N p$$

$$Z = \int_M e^{-\beta H(a, p)} d^N q d^N p \quad \left| \quad S = k\beta \langle E \rangle + k \ln\left(\frac{Z}{W_0}\right)\right.$$

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

To get to a thermodynamic potential:

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

↑ helmholtz
free energy

discrete: $F = -kT \ln Z$

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

discrete

$$F = -kT \ln Z$$

What does the free energy tell us?

For eqn

$$Z = \sum_{q,p} e^{-\beta E_s(q,p)}$$

$$= \sum_E W(E) e^{-\beta E}$$

$$= \sum_E e^{-\beta E + \ln(W(E))}$$

↑ # of States w/ Energy E

$$= \sum_E e^{-\beta E + \frac{1}{k} S(E)}$$

one term will dominate

$$\sim e^{-\beta(U-TS)} \equiv e^{-\beta F}$$

$$- \frac{1}{k_B T} \ln Z \sim e^{\beta \langle U \rangle} = e^{-\beta \langle H \rangle}$$

Canonical Ensemble Ex: 2-State paramagnet



$$E_{\uparrow} = -\mu h \quad E_{\downarrow} = +\mu h$$

$$Z = e^{\beta \mu h} + e^{-\beta \mu h} = 2 \cosh \beta \mu h$$

$$P_{\uparrow} = \frac{e^{\beta \mu h}}{2 \cosh \beta \mu h} \quad P_{\downarrow} = \frac{e^{-\beta \mu h}}{2 \cosh \beta \mu h}$$

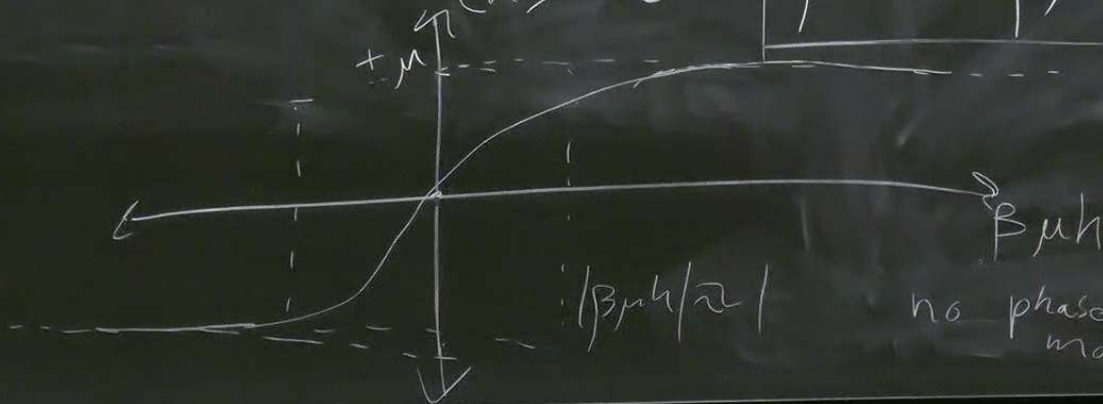
magnet
field
+h

Expectations:
high temp - lots of fluctuations
in spin

$$\beta = \frac{1}{kT}$$

low temp - spin should be aligned with
mag field

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



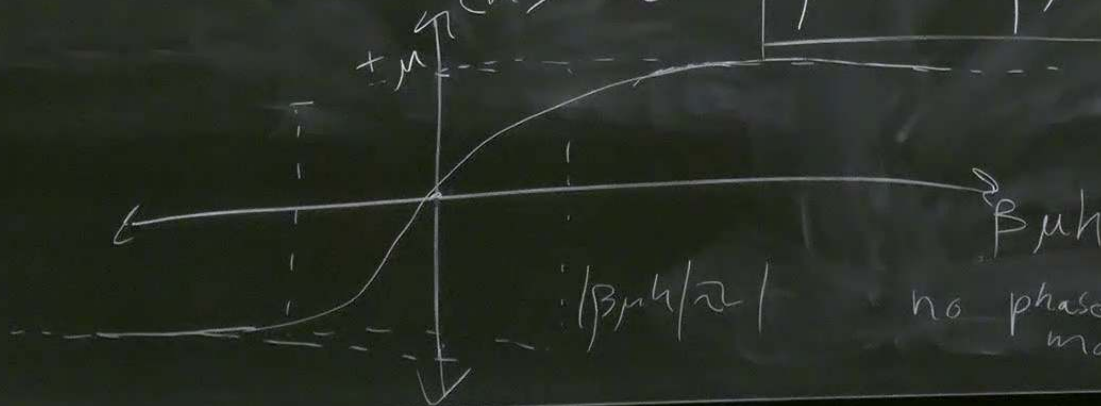
no phase transition system is always
magnetized for finite h .

magnet
field
+h

Expectations:
high temp - lots of fluctuations
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$$\beta = \frac{1}{kT}$$

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



no phase transition system is always
magnetized for finite h .

$$\ln(P(p, q)) \approx \ln(W(E^{(0)})) + \left. \frac{\partial \ln W(E)}{\partial E} \right|_{E=E^{(0)}} (E_r - E^{(0)}) + \dots$$

$\frac{1}{k} \frac{\partial S}{\partial E} \uparrow$

What if we had N paramagnets?

$$Z_1 = 2 \cosh \beta \mu h, \quad Z_N = Z_1^N$$

$$F = -kT \ln Z_N = -\frac{N}{\beta} \ln(2 \cosh \beta \mu h)$$

$$M = -\left(\frac{\partial F}{\partial h}\right)_T = N \mu \tanh \beta \mu h$$

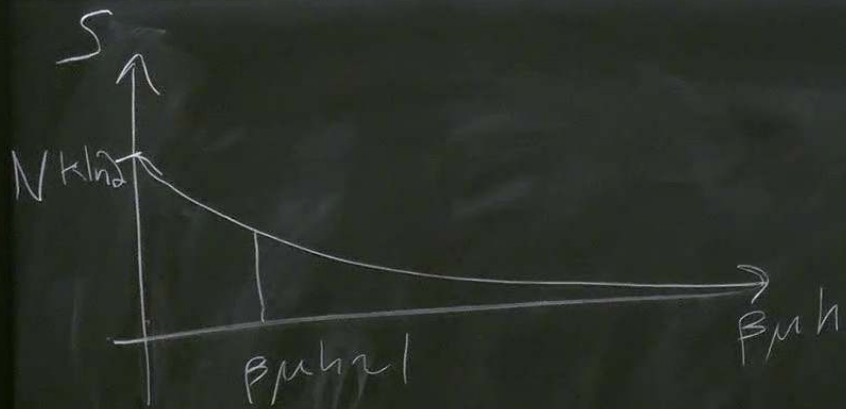
$$S = -\left(\frac{\partial F}{\partial T}\right)_h = Nk \ln(2 \cosh \beta \mu h) - Nk \beta \mu h \tanh \beta \mu h$$

$\uparrow \uparrow \uparrow \uparrow$
 $\uparrow \downarrow \downarrow \downarrow$
 $\vec{B} \uparrow h$

$$\langle m \rangle = \frac{\mu e^{\beta \mu h} - \mu e^{-\beta \mu h}}{2 \cosh \beta \mu h}$$

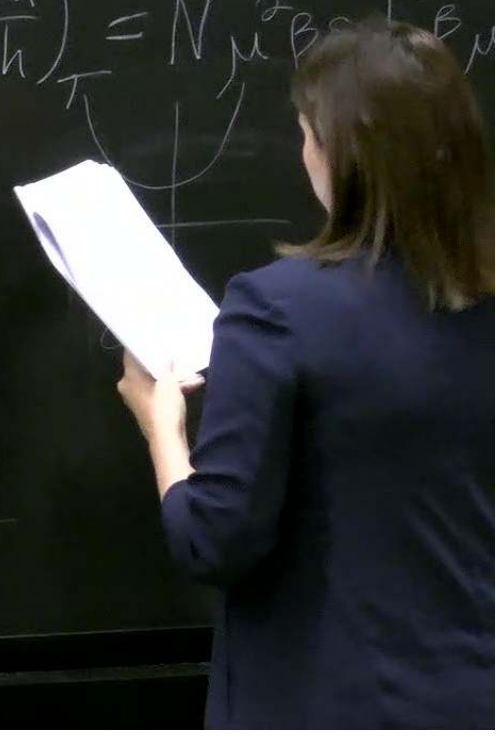
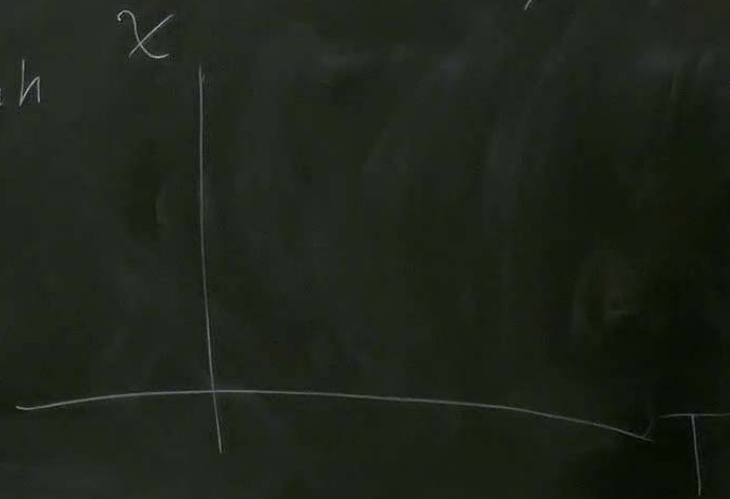
$$\frac{1}{F} \frac{\partial \log Z}{\partial h} = -\frac{\partial F}{\partial h}$$

$$S = - \left(\frac{\partial M}{\partial T} \right)_h = Nk \ln(2 \cosh \beta \mu h) - Nk \beta \mu h \tanh \beta \mu h$$



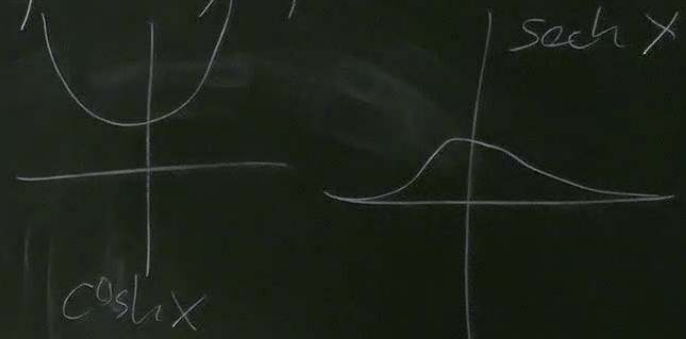
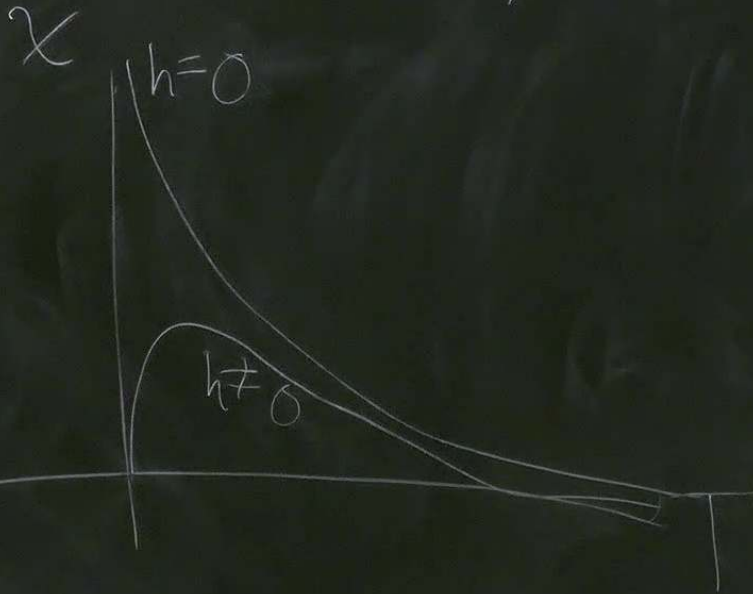
What would experimentalists measure?

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



What would experimentalists measure?

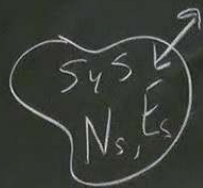
$$\chi \equiv \text{isothermal Susceptibility} = \left(\frac{\partial M}{\partial h} \right)_T = N \mu^2 \beta \operatorname{sech}^2 \beta \mu h$$



EE

$$\sim e^{-\beta(E - \mu N)} = e^{-\beta E + \beta \mu N}$$

Grand Canonical Ensemble



res
 N_r, E_r

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

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

$$N_s \ll N^{(0)}$$

$$E_s \ll E^{(0)}$$

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

$\ln P_S \propto \ln W(N, E) + \left(\frac{\partial \ln W}{\partial N} \right)_{N=N^{(0)}} (N_S - N^{(0)})$
 $+ \left(\frac{\partial \ln W}{\partial E} \right)_{E=E^{(0)}} (E_S - E^{(0)}) + \dots$
 $\approx \text{const.} + \frac{\mu \downarrow \text{chemical potential}}{kT} N_S - \frac{1}{kT} E_S$
 $P \propto e^{\frac{\mu}{kT} N - \beta E}$

$Z = \sum_{N=0}^{\infty} e^{\beta \mu N} Z_N \leftarrow \text{canonical ensemble}$
 \uparrow
 grand canonical ensemble
 $PV = \Phi = U - TS - \mu N = kT \ln Z$