Title: Statistical Physics Lecture - 111723

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Note:

I gave two formulations for the microcanonical ensemble:

$$\rho = \begin{cases} 1 & \text{if } E < H(q,p) < E + \delta E \\ 0 & \text{otherwise} \end{cases}$$

or

$$\rho(q,p) = \delta\left(H(q,p)/E - 1\right)$$

These give the same macroscopic results, but they are not equivalent at the microscopic level.

Ergodic Hypothesis

We've been discussing ensemble averages

$$\langle A \rangle_{ens} = \frac{\int_M A(q,p)\,\rho(q,p)\,d^N q\, d^N p}{\int_M \rho(q,p)\, d^N q\, d^N p}$$

- What do these correspond to experimentally?

averages

$(q,p)\, d^N q\, d^N p$

$d^N q\, d^N p$

-imentally?

- A time average of measurements of the system at times $t_1, t_2, \ldots, t_n$,

$$\langle A \rangle_{time} = \frac{1}{n} \sum_{l=1}^{n} A\big(q(t_l), p(t_l)\big)$$

trajectories governed by Hamilton's equations

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- At equilibrium, $\frac{\partial \rho}{\partial t} = 0$ and the ensemble average is indep. of time, so

$$\langle A \rangle_{ens} = \text{time average of } \left(\langle A \rangle_{ens} \right)$$

- Time averaging and ensemble averaging are completely independent, so we can also say:

$$\langle A \rangle_{ens} = \langle (\text{time average of } A) \rangle_{ens}$$

— Th

- The ergodic hypothesis is that

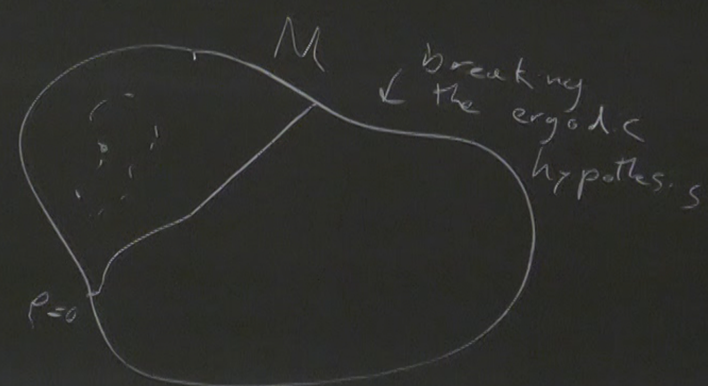
$\langle A \rangle_{time}$ over a sufficiently long time (with sufficently many measurements) must be the same for every member of the ensemble:

$$\langle A \rangle_{ens} = \langle A \rangle_{time} \quad \text{(when the time is long)}$$

So that we can have

$$\langle A \rangle_{ens} = A_{exp} \leftarrow \text{something we can obtain with exp}$$

The ergodic hypothesis (Boltzmann 1871) requires that the trajectory of any point, passes, in its time evolution, through every other point in the nonzero ρ phase space.



– Refinement: quasiergodic hypothesis – trajectory of any point traverses through the neighborhood of the relevant region. (ter Haar 1954, 1955, Farquhar 1964)

Working hypothesis – verify validity by comparing with experiment.

Quantum Gases

Here we'll model fermions and bosons in a pseudoclassical way using the canonical and grand canonical ensembles.

System of N noninteracting particles

ε_4 ——— n_4

ε_3 ——— n_3

ε_2 ——— n_2

ε_1 ——— n_1

ε_0 ——— n_0

$$E = \sum_\lambda n_\lambda \varepsilon_\lambda$$

number of particles with energy n_λ

So $N = \sum_\lambda n_\lambda$

$$Z_N = \sum_E e^{-\beta E} = \sum_{\{n_\lambda\}} g\{n_\lambda\}\, e^{-\beta \sum_\lambda n_\lambda \varepsilon_\lambda}$$

$$\{n_\lambda\} \leftarrow \{n_0, n_1, \ldots\} \leftarrow \sum_\lambda n_\lambda = N$$

Where: $g\{n_\lambda\} = 1$ for bosons

$$g\{n_\lambda\} = \begin{cases} 1 & \text{if all } n_\lambda = 0, 1 \\ 0 & \text{otherwise} \end{cases} \quad \text{for fermions}$$

$\{\, 0$ otherwise

Grand canonical Ensemble:

$$Z = \sum_{N=0}^{\infty} e^{\mu N/kT} Z_N = \sum_{N=0}^{\infty} \left[\sum_{\{n_\lambda\}} e^{\mu \sum_\lambda n_\lambda / kT} g\{n_\lambda\} e^{-\beta \sum_\lambda n_\lambda \varepsilon_\lambda} \right]$$

$$= \sum_{N=0}^{\infty} \left[\sum_{\{n_\lambda\}} g\{n_\lambda\} \prod_\lambda \left(e^{\mu/kT} e^{-\beta \varepsilon_\lambda} \right)^{n_\lambda} \right]$$

$$= \sum_{n_0, n_1, n_2 \ldots} g\{n\} \left(\left(e^{\mu/kT} e^{-\beta \varepsilon_0} \right)^{n_0} \left(e^{\mu/kT} e^{-\beta \varepsilon_1} \right)^{n_1} \ldots \right)$$

$$= \left[\sum_{n_0} g(n_0) \left(e^{\mu/kT} e^{-\beta \varepsilon_0} \right)^{n_0} \right] \left[\sum_{n_1} g(n_1) \left(e^{\mu/kT} e^{-\beta \varepsilon_1} \right)^{n_1} \right] \ldots\ldots$$

Bosons:

$$1 + x + x^2 + \dots = S$$

geometric series

$$- \quad x + x^2 + x^3 + \dots = xS$$

$$1 = S - xS$$

$$S = \frac{1}{1-x}$$

$$Z = \prod_{\lambda} \frac{1}{1 - e^{\mu/kT} e^{-\beta \varepsilon_\lambda}}$$

obtain with exp

$$+ e^{\mu/kT} e^{-\beta \varepsilon_\lambda})$$

$$Z = \begin{cases} \prod_\lambda \frac{1}{1 - e^{\beta\mu - \beta\varepsilon_\lambda}} & (B.E.) \\ \prod_\lambda \left(1 + e^{\beta\mu - \beta\varepsilon_\lambda}\right) & (F.D.) \end{cases}$$

Mean occupation number. $\langle n_\lambda \rangle$

$$\boxed{\langle n_\lambda \rangle = -\frac{1}{\beta}\frac{\partial}{\partial \varepsilon_\lambda} \ln(Z)} = -\frac{1}{\beta}\frac{\sum_{N,\{n_\lambda\}} (-\beta) n_\lambda e^{\beta \sum_\lambda n_\lambda(\mu-\varepsilon_\lambda)}}{Z}$$

Fermions:

$$\langle n_\lambda \rangle = -\frac{1}{\beta}\left[\frac{\prod_{\lambda'\neq\lambda}\left(1+e^{\beta\mu-\beta\varepsilon_{\lambda'}}\right)\left(-\beta e^{\beta\mu-\beta\varepsilon_\lambda}\right)}{\prod_{\lambda'}\left(1+e^{\beta\mu-\beta\varepsilon_{\lambda'}}\right)}\right] = \frac{1}{e^{\beta(\varepsilon_\lambda-\mu)}+1}$$

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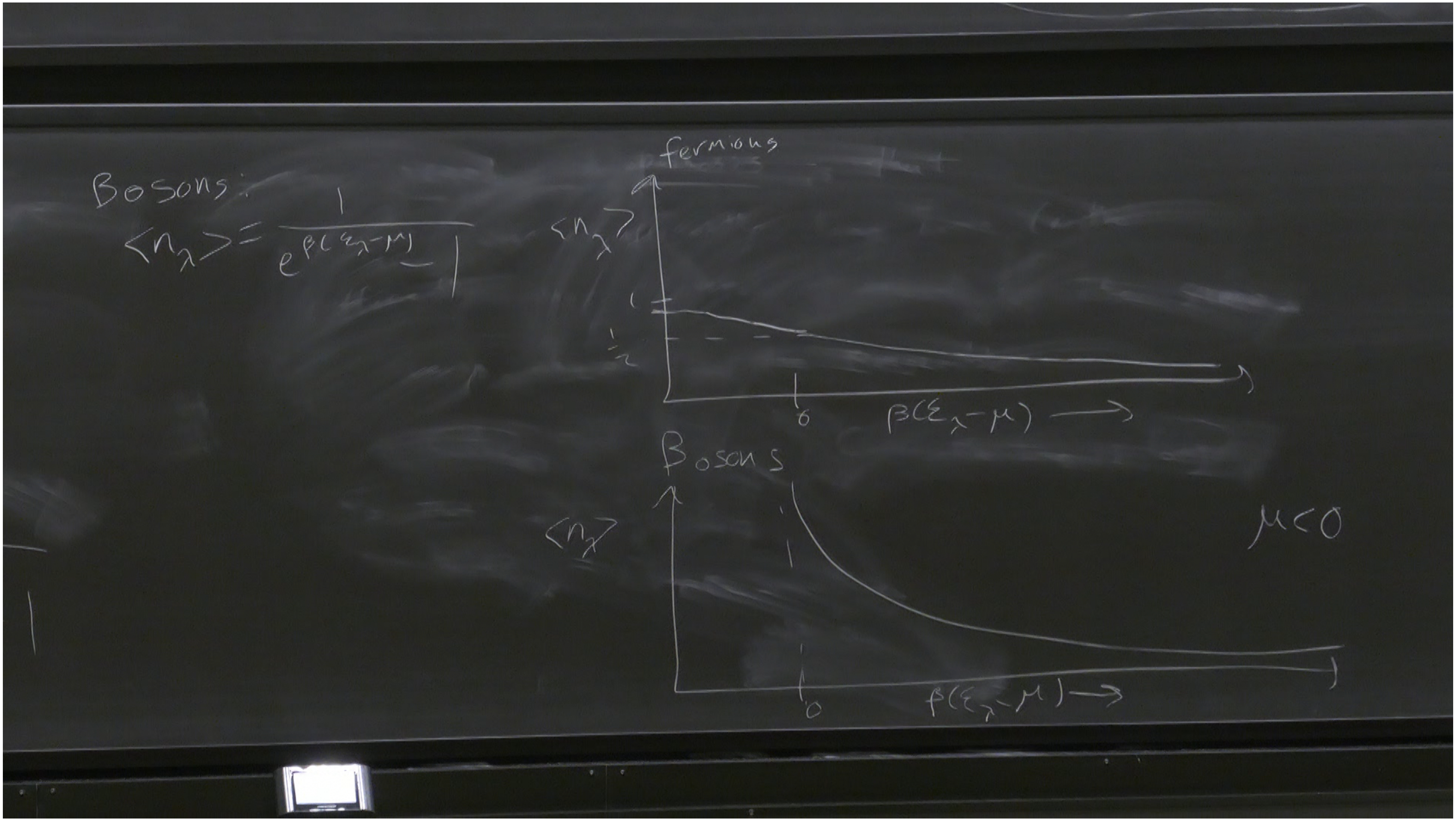
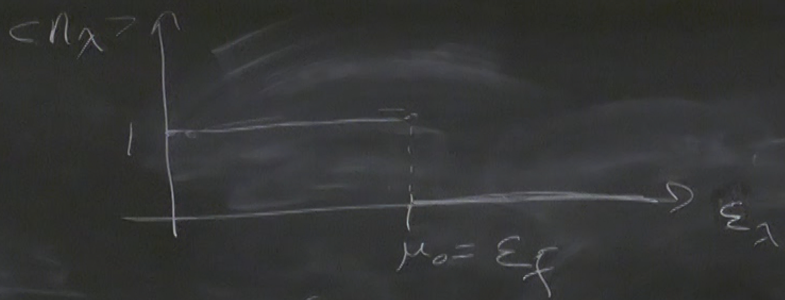

Bosons:
$\langle n_\lambda \rangle = \frac{1}{e^{\beta(\varepsilon_\lambda - \mu)} - 1}$
fermions
$\langle n_\lambda \rangle$
1
$\frac{1}{2}$
0
$\beta(\varepsilon_\lambda - \mu) \longrightarrow$
Bosons
$\langle n_\lambda \rangle$
$\mu < 0$
0
$\beta(\varepsilon_\lambda - \mu) \longrightarrow$

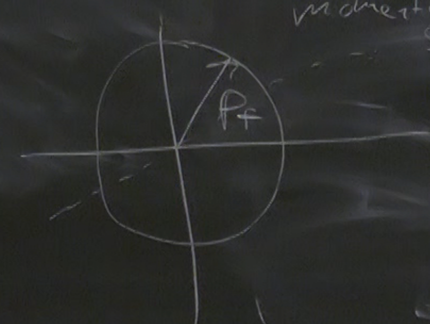


$$N = \int_0^{\varepsilon_f} d^3p\, d^3q = \int_0^{\varepsilon_f} a(\varepsilon)\, d\varepsilon = \frac{4}{3}\pi \frac{V}{h^3}(2m)^{3/2}\varepsilon_f^{3/2}$$

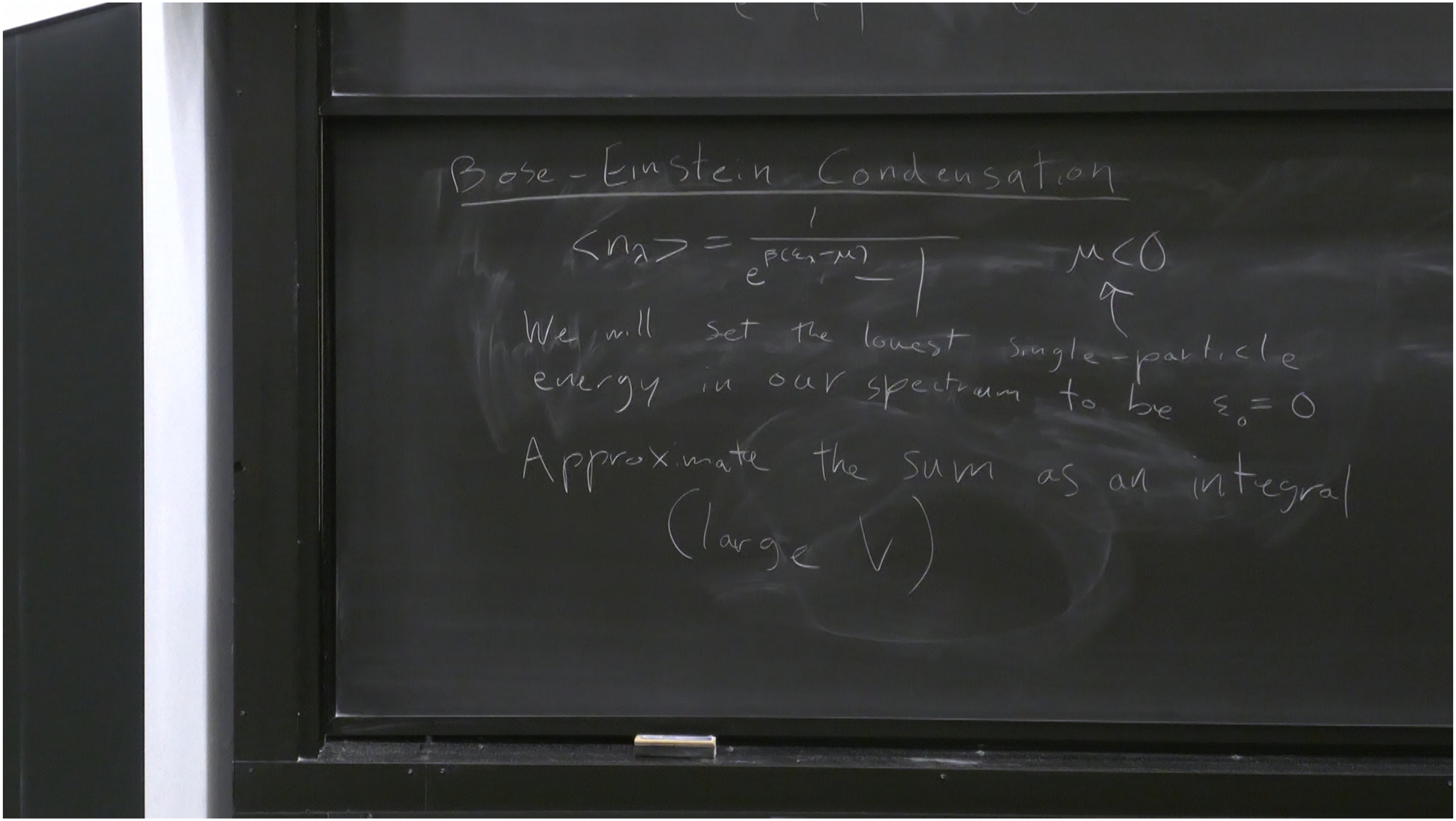
density of states

$$\varepsilon_f = \left(\frac{3N}{4\pi V}\right)^{2/3}\frac{h^2}{2m} = \frac{p_f^2}{2m}$$

momentum space



$Z =$


Bose-Einstein Condensation
$\langle n_\lambda \rangle = \frac{1}{e^{\beta(\epsilon_\lambda - \mu)} - 1}$
$\mu < 0$
We will set the lowest single-particle energy in our spectrum to be $\epsilon_0 = 0$
Approximate the sum as an integral
(large V)

$$= \frac{p_x^2}{2m}$$

$$N = \sum_\lambda \langle n_\lambda \rangle \approx \int \frac{1}{e^{\beta(\varepsilon-\mu)} - 1}\, d^3p\, d^3q$$

nonrelativistic particles

$$d^3p \to p^2\, dp\, d\Omega$$

$$\varepsilon = \frac{p^2}{2m}$$

$$\downarrow$$

$$p = \sqrt{2m\varepsilon}$$

$$\frac{d\varepsilon}{dp} = \frac{p}{m} \qquad d\varepsilon = \frac{p}{m}\, dp$$

$$p^2\, dp = m\sqrt{2m\varepsilon}\; d\varepsilon$$

ral

$$N = \underbrace{\frac{\pi V}{h^3}\int \frac{1}{e^{\beta(\varepsilon-\mu)}-1}(2m)^{3/2}\sqrt{\varepsilon}\,d\varepsilon}_{N_e \text{ (excited)}} + \underbrace{\frac{1}{e^{-\beta\mu}-1}}_{N_0}$$

Mathematical Identity:

$$\int_0^\infty \frac{x^{\nu-1}}{e^{-\beta\mu}e^{x}-1} = \Gamma(\nu)\left(e^{\beta\mu} + \frac{e^{2\beta\mu}}{2^\nu} + \frac{e^{3\beta\mu}}{3^\nu} + \dots\right)$$

So we can write

$$N_e = \frac{\mu V}{h^3 \beta^{3/2}} (2m)^{3/2} \int \frac{x^{1/2}}{e^{-\beta\mu} e^{x} - 1} \, dx$$

$$\boxed{x = \beta\varepsilon}$$

$$\nu = 3/2 \,, \quad \Gamma\left(\tfrac{3}{2}\right) = \frac{\sqrt{\pi}}{2}$$

$\mu \le 0$

$$N_e = \frac{\mu V}{h^3} (2mkT)^{3/2} \, \Gamma\left(\tfrac{3}{2}\right) \left(e^{\beta\mu} + \frac{e^{2\beta\mu}}{2^{3/2}} + \frac{e^{3\beta\mu}}{3^{3/2}} + \dots \right)$$

$$\le \frac{\mu V}{h^3} (2mkT)^{3/2} \, \Gamma\left(\tfrac{3}{2}\right) \zeta\left(\tfrac{3}{2}\right)$$

$\zeta\left(\tfrac{3}{2}\right) =$

$$\zeta\left(\tfrac{3}{2}\right) = 1 + \frac{1}{2^{3/2}} + \frac{1}{3^{3/2}} + \dots$$

can write

$$\frac{\mu V}{h^3 \beta^{3/2}} (2m)^{3/2} \int \frac{x^{1/2}\, dx}{e^{-\beta\mu} e^{x} - 1}$$

$$\nu = 3/2, \quad \Gamma\left(\tfrac{3}{2}\right) = \frac{\sqrt{\pi}}{2}$$

$\mu \le 0$

$$mkT)^{3/2}\, \Gamma\left(\tfrac{3}{2}\right)\left(e^{\beta\mu} + \frac{e^{2\beta\mu}}{2^{3/2}} + \frac{e^{3\beta\mu}}{3^{3/2}} + \dots\right)$$

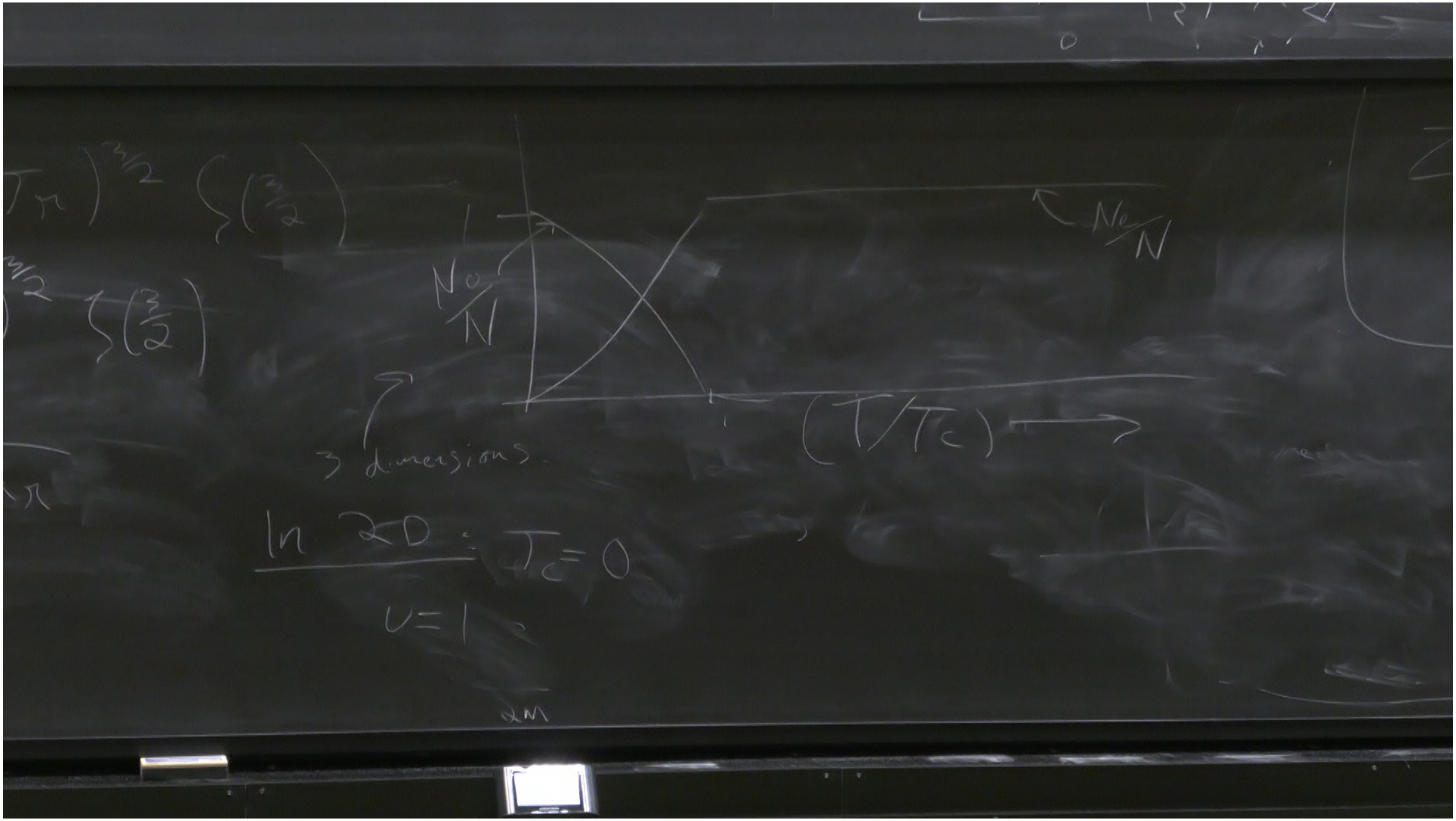
$$\le \frac{\mu V}{h^3} (2m\, kT)^{3/2}\, \Gamma\left(\tfrac{3}{2}\right) \zeta\left(\tfrac{3}{2}\right)$$

bounded!

$$N_0 = N - N_{e,max} = N - \frac{V}{2h^3}\left(2mkT\pi\right)^{3/2} \zeta\left(\frac{3}{2}\right)$$

$$N_{e\,max} = \frac{V}{2h^3}\left(2mkT_c\pi\right)^{3/2} \zeta\left(\frac{3}{2}\right)$$

$$T_c = \left(\frac{N\,2h^3}{\zeta(3/2)\,V}\right)^{2/3} \frac{1}{2mk\pi}$$


N_c/N
N_c/N
3 dimensions.
(T/T_c)
In 2D: $T_c = 0$
$\zeta(3/2)$
QM