Lecture 20

Exam average $45/60 \sim$ A-

$30/60 \sim$ low B-

We've been discussing quantum systems

Compared to classical: $\rho(p,q) \to \hat{\rho}$

$\int d\omega \to \mathrm{Tr}$

In practice, $\hat{\rho} \to e^{-\beta E_n}$

subtleties of $\hat{\rho}$ don't come up

Today, turn to fundamental difference between classical & quantum: how indistinguishability handled

Consider quantum system of N non-interacting particles

$$\hat{H} = \sum_{i=1}^{N} \hat{H}_i$$

$\hat{H}_i$ acts on particle i

typically $\hat{H}_i(\hat{q}_i, \hat{p}_i)$

Schrodinger eqn

$$\hat{H} \psi\{q\} = E \psi\{q\}$$

has separable solution

$$\psi_0\{q\} = \prod_{i=1}^{N} u_{\varepsilon_i}(q_i)$$

where $\hat{H}_i u_{\varepsilon_i} = \varepsilon_i u_i$ single-particle state

Say n_ε particles in state ε

Then $\psi_0\{q\} = \prod_{m=1}^{n_1} u_1(m) \prod_{m=n_1+1}^{n_1+n_2} u_2(m) \ldots$

Know that for distinguishable particles,
each set $\{n_\varepsilon\}$ corresponds to

$$W\{n_\varepsilon\} = \frac{N!}{n_1! n_2! \ldots} \quad \text{different states}$$

For classical identical particles, take $W \to \frac{1}{n_1! n_2! \ldots}$

$\Leftrightarrow$ assume no two particles ever in same state

For quantum identical particles, can't make this assumption.

Instead, demand each set $\{n_\varepsilon\}$ corresponds to one state

$$W\{n_\varepsilon\} = 1$$

ie, once you specify # of particles in each state, you're done, can't say anything else

Actually, more to it

Introduce permutation operator P

$P\{q\} \Rightarrow$ rearrangement of q's

have $N!$ different P's

Note any P can be composed of 2-particle exchanges

$$P_{ij}\{\ldots, q_i, \ldots q_j, \ldots\} = \{\ldots q_j \ldots q_i \ldots\}$$

If $P =$ product of even # of P_{ij}'s

say P even

Else $P =$ odd

For identical particles, demand physical ψ

= eigenstate of P's

$$P\psi = \lambda\psi$$

where $P\psi(\{q\}) \equiv \psi(P\{q\})$

Since $P_{ij}P_{ij} = 1$ & all P composed from P_{ij}'s

must have $\lambda^2 = 1$

$\Rightarrow \lambda = \pm 1$

<u>Bosons</u> = particles with integer spin

$\lambda = +1$ always

Then $$\psi_B\{q\} = A\sum_P P\psi_0\{q\}$$

= symmetric superposition of all possible permutations.

$A =$ normalization

clearly $P\psi_B\{q\} = \psi_B\{q\}$ for any P

Fermions: particles with half-integer spin

$\lambda = -1$ for two-particle exchanges

Then $\psi_F\{q\} = A \sum_P \delta_P P \psi_0\{q\}$

$$\delta_P = +1 \text{ for } P \text{ even}$$
$$= -1 \text{ for } P \text{ odd}$$

Immediately get Pauli exclusion principle:

Can't have two fermions in same quantum state

Say $\psi_F \propto u_\xi(q_i) u_\xi(q_j)$

Then $P_{ij} \psi_F = u_\xi(q_j) u_\xi(q_i) = \psi_F$

but also need $P_{ij} \psi_F = -\psi_F$

So $\psi_F = -\psi_F \Rightarrow \psi_F = 0$ no state

So really, for bosons have $W\{n_\xi\} = 1$

for fermions have $W\{n_\xi\} = 1$ if all $n_\xi = 0$ or 1

$= 0$ else

Want to determine what impact this has on ensemble

Show two derivations

First: microcanonical

Math a little flaky, but connects to previous work

In microcanonical, have

$$N = \sum_\varepsilon n_\varepsilon$$

$$E = \sum_\varepsilon n_\varepsilon \varepsilon \qquad \text{fixed}$$

Want to calculate number of corresponding microstates

$$\Omega = \sum_{\{n_\varepsilon\}} W\{n_\varepsilon\}$$

Sum constrained by N + E

As before, argue that

$$\ln \Omega \approx \ln W\{n_e^*\}$$

where $\{n_e^*\}$ = distribution with largest W

but that doesn't make sense, all W's the same!

Address by lumping nearby states together into "cells" j

g_j = # of states in cell j

ε_j = avg energy of states in cell j

n_j = # of particles in cell j

Assume that spread of energies w/in cell is small enough to neglect

Also assume all $g_j, n_j \gg 1$

Still have $\sum_j n_j = N$

$$\sum n_j \varepsilon_j = E$$

$$\Omega = \sum_{\{n_j\}} W\{n_j\}$$

but now $W\{n_j\} = \prod_j w(j)$

where $w(j)$ = # of ways to rearrange particles in cell j

Figure out $w(j)$:

Bosons: # of ways to put n_j identical particles into g_j distinct states

Use box & line argument:

particles

possible arrangement: $| \circ \circ | \circ | \ldots | \circ \circ \circ |$

state 1 2 ... g_j

$$\text{\# of arrangements} = \frac{(n_j+g_j-1)!}{n_j!\,(g_j-1)!}$$

$$\approx \frac{(n_j+g_j)!}{n_j!\,g_j!} = w_B(j)$$

$$= \binom{n_j+g_j}{n_j}$$

Fermions: $w(j) =$ # of ways to choose n_j states to be occupied out of g_j states total

$$= \binom{g_j}{n_j} = \frac{g_j!}{n_j!(g_j-n_j)!} = w_F(j)$$

Then we get

$$S = k \ln \Omega$$
$$\approx k \ln W\{n_j^*\}$$
$$= k \sum_j \ln w(j)$$

Note: $\ln \binom{a}{b} = a \ln a - a - b \ln b + b$
$$- (a-b)\ln(a-b) + a - b$$
$$= a \ln a - b \ln b - (a-b)\ln(a-b)$$

So $\ln w_B \approx (n+g)\ln(n+g) - n \ln n - g \ln g$

$\ln w_F = g \ln g - n \ln n - (g-n)\ln(g-n)$

Be clever, write

$$\ln w_j = n_j \ln\left(\frac{g_j}{n_j} - a\right) - \frac{g_j}{a}\ln\left(1 - a\frac{n_j}{g_j}\right)$$

$a = -1$ boson

$a = +1$ fermion

boson $\ln w = n \ln\left(\frac{g}{n}+1\right) + g \ln\left(1+\frac{n}{g}\right)$

$= n \ln(g+n) - n \ln n + g \ln(g+n) - g \ln g$

$= (n+g)\ln(n+g) - n\ln n - g \ln g$

You can check fermion

So, we want to maximize $S = k \sum_j \ln w_j$

subject to constraints $\sum n_j = N$

$\sum n_j \varepsilon_j = E$

Use Lagrange multipliers α, β

$$\frac{\partial}{\partial n_j}\left[\sum_j n_j \ln\left(\frac{g_j}{n_j} - a\right) - \frac{g_j}{a}\ln\left(1 - a\frac{n_j}{g_j}\right) - \alpha n_j - \beta \varepsilon_j n_j \right] = 0$$

$$\ln\left(\frac{g_j}{n_j} - a\right) + \underbrace{n_j\left(\frac{-\frac{g_j}{n_j^2}}{\frac{g_j}{n_j} - a}\right)}_{-\frac{g_j}{g_j - n_j a}} - \underbrace{\frac{g_j}{a}\left(\frac{-\frac{a}{g_j}}{1 - a\frac{n_j}{g_j}}\right)}_{-\frac{g_j}{g_j - a n_j}} - \alpha - \beta\varepsilon_j = 0$$

cancel

$$\ln\left(\frac{g_j}{n_j} - a\right) = \alpha + \beta \varepsilon_j$$

$$\boxed{n_j = n_j^* = \frac{g_j}{e^{\alpha + \beta\varepsilon_j} + a}}$$

Since $n_j \propto g_j$, seems reasonable to take

$$g_j \to 1$$

get $n_\varepsilon^* = \dfrac{1}{e^{\alpha + \beta\varepsilon} + a}$ = occupation # of single state w/ energy ε

Correct, but not well justified.

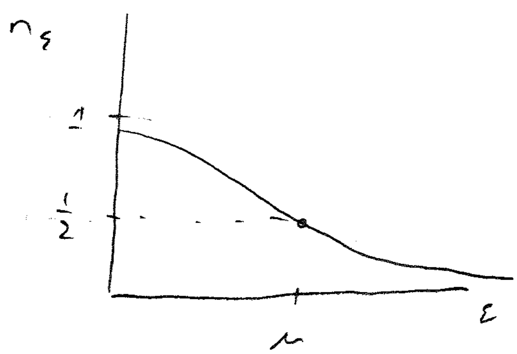
Give more secure derivation next time

Notes:

- As before, identify $\beta = \frac{1}{kT}$ $\quad \alpha = -\frac{\mu}{kT}$

Fermi-Dirac distribution $(a = +1)$

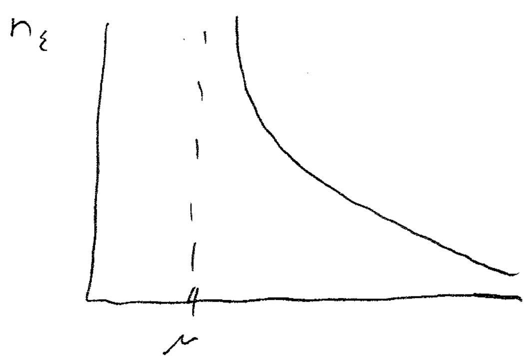
$$n_\varepsilon = \frac{1}{e^{\beta(\varepsilon - \mu)} + 1}$$



n_ε never exceeds 1, as required

Bose-Einstein distribution $(a = -1)$

$$n_\varepsilon = \frac{1}{e^{\beta(\varepsilon - \mu)} - 1}$$



$\to \infty$ as $\varepsilon \to \mu$

Require $\mu < \varepsilon_{min}$ always

Compare classical: Maxwell-Boltzmann

$$n_\varepsilon = e^{\beta(\mu-\varepsilon)} \qquad \text{obtain with } a = 0$$

In between BE & FD

Also see that if $e^{\beta(\varepsilon-\mu)} \gg 1$,

a is negligible

all distributions $\rightarrow$ Maxwell-Boltzmann limit

$=$ limit where $n_\varepsilon \ll 1$

makes sense

quantum statistical effects only significant when particles likely to be in same quantum state