Quantum Statistics

$N \gg 1$ particles

(e.g. condensed matter)

Cannot specify the wavefcns and states of every particle

$\Rightarrow$ statistical mechanics (incomplete but useful information about the system)

microstate - detailed microscopic config. of the system

macrostate - characterized by a probability distribution of ensemble of microstates

thermal equilibrium : e.g. total energy E stays fixed, particles exchange energy $\Rightarrow$ system goes to "thermal" equilibrium
Total energy E is described by absolute temperature T

Basic postulate of statistical mechanics :
any microstate with same total energy is equally probable

Quantum stat. mech : bosons, fermions are expected to behave differently

Consider N quantum particles, weakly interacting.
Individually, single particle energy spectrum $\{E_m\}$
due to some ext. potential (e.g. SHO)
Particles exchange energy, but total E is fixed.

quantum state

Basic question: avg. number of particles in state m in thermal equilibrium?

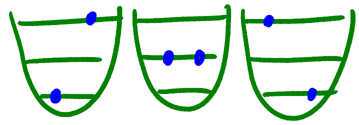
① $N=2$ in simple harmonic oscillator (SHO)

$E_m = \hbar\omega(m+\frac{1}{2})$, $m = 0, 1, \ldots$ quant. number m (n_m - # part.)

Let the total $E = 3\hbar\omega$

$E = \hbar\omega(m_1 + m_2 + 1)$, $\Rightarrow$ $m_1 + m_2 = 2$ ($m_{1,2}$ – quant number for particles 1, 2)

microstates :
(with same energy)



3 cases : a) non-identical

identical $\begin{cases} \text{b) bosons} \\ \text{c) fermions (ignore spin degen.)} \end{cases}$

microstate label	occupancy part. in each state: m=0	m=1	m=2	multipart. wavefcn $\psi_{m_1}(1)\psi_{m_2}(2)$	configuration $\{n_m\}$
α					
β					
γ					
...					

Find probabilities $p_\alpha, p_\beta, \dots$?

Find $\overline{n_m}$?

a) non-identical

	m=0	m=1	m=2		
α		1,2		$\psi_1(1)\psi_1(2)$	$\{0,2,0\}$
β	1		2	$\psi_0(1)\psi_2(2)$	$\{1,0,1\}$
γ	2		1	$\psi_0(2)\psi_2(1)$	$\{1,0,1\}$

$p_\alpha = p_\beta = p_\gamma = \frac{1}{3}$; $\overline{n_0} = \overline{n_1} = \overline{n_2} = \frac{2}{3}$, $\sum_{m=0}^{2} \overline{n_m} = N = 2$

b) identical bosons

α		(2)		$\psi_1(1)\psi_1(2)$	$\{0,2,0\}$
β	(1)		(1)	$\frac{1}{\sqrt{2}}[\psi_0(1)\psi_2(2) + \psi_0(2)\psi_2(1)]$	$\{1,0,1\}$

$p_\alpha = p_\beta = \frac{1}{2}$; $\overline{n_0} = \overline{n_2} = \frac{1}{2}$, $\overline{n_1} = 1$

c) identical fermions

α	(1)		(1)	$\frac{1}{2}[\psi_0(1)\psi_2(2) - \psi_2(1)\psi_0(2)]$	$\{1,0,1\}$

$p_\alpha = 1$; $\overline{n_0} = \overline{n_2} = 1$, $\overline{n_1} = 0$

What if $N \gg 1$? What is the energy stored in each mode?

main result from stat. mech. :

probability to find a system in a state with energy E_s is $\propto e^{-E_s/kT}$ if in thermal equilibrium.

k – Boltzmann const , $k_B = 1.38 \times 10^{-23} \frac{J}{K}$

T – absolute temp. [K]

② $N \gg 1$ identical bosons (weakly interacting)
probability to find n bosons in m state

$$p_m(n) \propto e^{-\frac{nE_m}{kT}} \quad \leftarrow E_s$$

now any quant. system with energy spectrum $\{E_m\}$

avg. number of bosons in state m:

$$\overline{n_m} = \sum_{n=0}^{N} n\, p_m(n) \overset{N\to\infty}{=} \frac{\sum_{n=0}^{\infty} n e^{-nE_m/kT}}{\sum_{n=0}^{\infty} e^{-nE_m/kT}}$$

$$\left[\begin{array}{l} \sum_{n=0}^{\infty} e^{-na} = \frac{1}{1-e^{-a}}\ ; \\ \sum_{n=0}^{\infty} n e^{-na} = -\frac{\partial}{\partial a}\left(\sum_{n=0}^{\infty} e^{-na}\right) = \frac{e^{-a}}{(1-e^{-a})^2} \end{array}\right] \Rightarrow$$

$$\boxed{\overline{n_m} = \frac{1}{e^{E_m/kT}-1}}$$

describes photons / phonons

③ Compute total # of particles

$$N = \sum_m \frac{1}{e^{E_m/kT}-1}\ ,$$ depends on T !

unphysical if particles are conserved.

Solution: add a const to all single-part. energies
(i.e. apply a uniform potential energy)
This does not change the quant. mechanics,
it shifts all E_m by the same amount

$$E_m \to E_m - \mu$$

$$\Rightarrow p_m(n) \propto e^{-n(E_m-\mu)/kT}$$

$$\boxed{\overline{n_m} = \frac{1}{e^{(E_m-\mu)/kT}-1}}$$

← Bose-Einstein distribution fcn.

$$N = \sum_m \overline{n_m}$$ ← an implicit equation that can be used to calculate energy shift μ

$\mu = \mu(T)$ ← "chemical potential"

④ Look at fermions

$p_m(n) \propto e^{-nE_m/kT}$

but only $n=0,1$ possible

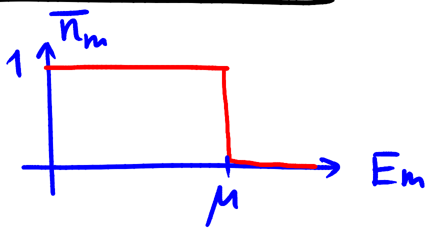
$$\overline{n_m} = \frac{\sum_{n=0}^{1} n e^{-nE_m/kT}}{\sum_{n=0}^{1} e^{-nE_m/kT}} = \frac{1}{e^{E_m/kT}+1}$$

Again: $N = \sum_m \frac{1}{e^{E_m/kT}+1}$ depends on T.

to fix replace $E_m \to E_m - \mu$, $\Rightarrow$

$$\boxed{\overline{n_m} = \frac{1}{e^{(E_m-\mu)/kT}+1}} \leftarrow \text{Fermi–Dirac}$$

@ $T \to 0$



all states $E_m < \mu$ filled

— " — $E_m > \mu$ empty

$\mu(T=0) \leftarrow$ Fermi energy

* Fermi gas (gas of fermions) with $kT \ll \mu$
  (i.e. $n=1$ for $E \ll \mu$) is called degenerate

* Fermi gas with $n \ll 1$ for all states $\leftarrow$ nondegenerate

⑤ Transition to classical statistics

@ high E, both FD and BE become

$$n(E) \propto \frac{1}{e^{E/kT}} = e^{-E/kT} \leftarrow \text{Maxwell–Boltzmann}$$

(FD, BE) $\to$ MB if particles can be distinguished
(= no overlap in wavefcns)

avg. part. distance $\gg$ quant. uncertainty in position
$d \gg \Delta x$

estimate Δx: $\Delta x \Delta p_x \sim \frac{\hbar}{2}$, $\Delta p_x^2 \sim m^2 v_x^2 \sim mkT$

$$\Delta x \sim \frac{\hbar}{2\sqrt{mkT}}$$

estimate d: $(V/N)^{1/3}$

$\Rightarrow$ if $\left.\begin{array}{l} \left(\frac{N}{V}\right)\frac{\hbar^3}{8(mkT)^{3/2}} \ll 1 \\ * \text{ heavy particles} \\ * \text{ high temp.} \\ * \text{ dilute} \end{array}\right\} \Rightarrow$ use MB

Some examples:

H_2 gas STP : $\Delta x/d \sim 10^{-7}$, $\Rightarrow$ MB

electrons in silver : $\Delta x/d \sim 5$, $\Rightarrow$ FD

⑥ Applications

* degenerate Fermi gas $\rightarrow$ electrons in a metal
* BE predicts the possibility of $n_0 \rightarrow N$ in ground state with <u>same</u> $\psi_0(\vec{r})$ at sufficiently low T.
  $\Rightarrow$ "Bose-Einstein Condensate" (BEC)
  This wavefcn becomes a characteristic of a BEC
  Examples: atomic cooling
  superfluid
  superconducter