Lecture 7

Last time, introduced idea of band structure in solids

= Effect of crystal on single particle states

States ~ plane waves, but allowed values of E
are restricted to certain bands
# of states in each band = 2 × # of atoms in crystal

If electrons fill top band, get insulator
if not, get conductor.

Semiconductor: insulator with small gap to next band

So far, talked mostly about how exchange symmetry
determines ground state of systems

Also important for systems not in ground state...
say at non-zero temperature.

Subject of statistical mechanics.

Main idea: don't want to keep track of exact
quantum state of macroscopic system, $\sim 10^{23}$ particles

Worry about macroscopic qualities instead

For instance: suppose total energy is E

Assume system equally likely to be in any
many-body quantum state with that E

Typically many states within dE of E

To characterize system, need to count them

Convenient to define three terms:

"state" = many-body quantum state, energy E

"level" = set of single particle states, all with energy E_n

"configuration" = list of how many particles are in each level

Example, problem 5.23

System = three particles in 1D harmonic oscillator, freq ω. Total energy $E = \frac{9}{2}\hbar\omega$

Questions:

a) What are possible configurations?

b) How many distinct states for each?

c) What is most probable configuration?

d) What is prob. for a given particle to have various energies?

Think about distinguishable particles first: Label as A, B, C

Have $E_n = \hbar\omega(n+\frac{1}{2})$ $n = 0, 1, 2, \ldots$

Three particles, so zero point energy = $\frac{3}{2}\hbar\omega$

Leaves $3\hbar\omega$ available.

a) Three possible configurations:

I. One with $n=3$, two with $n=0$

II. One with $n=2$, one with $n=1$, one with $n=0$

III. Three with $n=1$

Could list configurations as

$$\begin{array}{c} n= \;\; 0 \quad 1 \quad 2 \quad 3 \\ [2,\ 0,\ 0,\ 1,\ \ldots] \\ [1,\ 1,\ 1,\ 0,\ \ldots] \\ [0,\ 3,\ 0,\ 0,\ \ldots] \end{array}$$

b) For I, any one of three could be in $n=3$ level

So three states

Could write as

$$\begin{array}{ccc} n_A & n_B & n_C \\ (3 & 0 & 0) \\ (0 & 3 & 0) \\ (0 & 0 & 3) \end{array}$$

For II, have states $(0,1,2)$ $(0,2,1)$ $(1,2,0)$ $(1,0,2)$ $(2,1,0)$ $(2,0,1)$

Six states

For III, have only $(1\,1\,1)$: one state

So total of $3+6+1=10$ states possible

c) Assume all states equally likely.

Then most prob. configuration is one with most states : II. $\text{Prob} = 6/10 = 60\%$

d) If pick particle at random, what is chance to have $n=3$?

Need to be in configuration I ($\frac{3}{10}$ chance)
and pick right particle ($\frac{1}{3}$ chance)

Total prob $\equiv P_3 = \frac{3}{10} \times \frac{1}{3} = \boxed{\frac{1}{10}}$

For $n=2$, need config II:

$$P_2 = \frac{6}{10} \times \frac{1}{3} = \boxed{\frac{2}{10}}$$

For $n=1$, could have configs II or III:

$$P_1 = \underbrace{\frac{6}{10}}_{\text{configs II}} \times \underbrace{\frac{1}{3}}_{\text{right particle}} + \underbrace{\frac{1}{10}}_{\text{config III}} \times \underbrace{\frac{3}{3}}_{\text{any particle works}} = \boxed{\frac{3}{10}}$$

For $n=0$, have

$$P_0 = \underbrace{\frac{3}{10} \times \frac{2}{3}}_{\text{configs I}} + \underbrace{\frac{6}{10} \times \frac{1}{3}}_{\text{configs II}} = \boxed{\frac{4}{10}}$$

Note probs add to 1, as they should.

Now answer same questions for bosons & fermions

Bosons

a) Same configurations as before

b) Boson indistinguishable, so only <u>one</u> state per config

ψ = superposition of previous states

For instance, $\psi_I = \frac{1}{\sqrt{3}}\left[|300\rangle + |030\rangle + |003\rangle \right]$

So total # of states = 3

c) Since each state equally likely, each config is equally likely, so prob = 1/3 each

d) Need to work out

$$P_3 = \underset{\text{config}}{\frac{1}{3}} \times \underset{\text{right particle}}{\frac{1}{3}} = \frac{1}{9}$$

$$P_2 = \frac{1}{3} \times \frac{1}{3} = \frac{1}{9}$$

$$P_1 = \frac{1}{3} \times \frac{1}{3} + \frac{1}{3} \times \frac{3}{3} = \frac{4}{9}$$

$$P_0 = \frac{1}{3} \times \frac{2}{3} + \frac{1}{3} \times \frac{1}{3} = \frac{3}{9}$$

(check, they sum to one ✓)

For fermion (ignoring spin)

a) Can't have more than one particle per single-particle state

So configs I and III aren't allowed
$\Rightarrow$ only II is possible, $P = \underline{1}$

b) Only one state, antisymmetric superposition

c) $\underline{\text{II}}$

d) Just question of picking right particle. So

$$P_3 = 0 \qquad P_2 = P_1 = P_0 = \frac{1}{3}$$

(not possible in config II)

One note, how would we write down antisymmetric state?

Use Slater determinant. If particles A to N, states 1 to n, have

$$\psi(r_A, r_B, \ldots r_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(r_A) & \psi_2(r_A) & \ldots & \psi_n(r_A) \\ \psi_1(r_B) & \psi_2(r_B) & \ldots & \psi_n(r_B) \\ \vdots & & & \\ \psi_1(r_N) & \psi_2(r_N) & \ldots & \psi_n(r_N) \end{vmatrix}$$

Evaluate like regular determinant

Here have

$$\psi(A,B,C) = \frac{1}{\sqrt{6}} \begin{vmatrix} \psi_1(A) & \psi_2(A) & \psi_3(A) \\ \psi_1(B) & \psi_2(B) & \psi_3(B) \\ \psi_1(C) & \psi_2(C) & \psi_3(C) \end{vmatrix}$$

$$= \frac{1}{\sqrt{6}} \Big[\psi_1(A)\psi_2(B)\psi_3(C) + \psi_2(A)\psi_3(B)\psi_1(C) + \psi_3(A)\psi_1(B)\psi_2(C) - \psi_1(A)\psi_3(B)\psi_2(C) - \psi_2(A)\psi_1(B)\psi_3(C) - \psi_3(A)\psi_2(B)\psi_1(C) \Big]$$

Next time, do counting for general system