Quantum Stat Mech

Last time introduced basic idea:

1) Count up all the many body states in your system,
2) Organize by configuration = list of occupied energy levels
3) Determine probabilities by assuming all states equally likely

Today, do this in general

Suppose N particles, total energy E

In potential with single-particle energies (= levels)
$E_1, E_2, E_3, \ldots$

Also allow each energy to be degenerate
d_1, d_2, d_3
states per level (includes spin)

Example, spin $\frac{1}{2}$ electrons in 3D cubical box:
ground state $d_1 = 2$ (spin)
1st excited state $d_2 = 6$ (excitation in $x, y,$ or z)$\times$(spin)

Label configurations with occupation numbers
$(N_1, N_2, \ldots)$

$N_n =$ # of particles in level n

Need to count how many many-body states corresponds
to a given configuration.

Define number $= Q(N_1, N_2, \ldots)$

Of course Q depends on exchange symmetry ...

<u>Distinguishable particles</u>

Start with $n=1$, have N_1 particles

How many ways to pick N_1 particles from the total N?

N	choices for	first
$N-1$	"	second
$N-2$	"	third
$\vdots$		
$N-N_1+1$	"	N_1^{th}

So $N \cdot (N-1) \cdot \ldots (N-N_1+1) = \dfrac{N!}{(N-N_1)!}$ possibilites

However, it doesn't matter what order I pick
those N_1 particles in
ie, particle B could come first or last, no difference.

We counted those possibilities separately...
need to divide out different permutations of N_1

How many permutations?

N_1	choices for	first
N_1-1	"	second
$\vdots$		
1	"	last

So $N_1!$ permutations

Thus really $\frac{N!}{N_1!(N-N_1)!}$ distinct ways to select N_1 particles out of N

$$= \binom{N}{N_1} \text{, binomial coefficient}$$

Now each of these could go into any of d_1 different states

So $d_1^{N_1}$ more choices

Total possibilities $= \frac{N! \, d_1^{N_1}}{N_1!(N-N_1)!}$

Now for $n=2$, everything is the same, except only $N-N_1$ particles left to choose from

So we have $\frac{(N-N_1)! \, d_2^{N_2}}{N_2!(N-N_1-N_2)!}$ possibilities

and so forth.

Finally, multiply everything to get Q:

$$Q = \frac{N! \, d_1^{N_1}}{N_1!(N-N_1)!} \cdot \frac{(N-N_1)! \, d_2^{N_2}}{N_2!(N-N_1-N_2)!} \times \frac{(N-N_1-N_2)! \, d_3^{N_3}}{N_3! \ldots} \times \ldots$$

$$= N! \frac{d_1^{N_1} d_2^{N_2} \ldots}{N_1! \, N_2! \ldots} = \boxed{N! \prod_{n=1}^{\infty} \frac{d_n^{N_n}}{N_n!}}$$

Thats for distinguishable particles.

Bosons:

Now don't need to worry about how to pick N_1 particles from N:
- particles identical, so just one way

Quantum state will be superposition of all $\binom{N}{N_1}$ choices anyway

But harder to decide how many ways to distribute N_1 particles over d_1 states

Book shows one way, I'll sketch another (Problem 5.25)

For given d_1, consider various N_1s:

$N_1 = 1 \Rightarrow d$ ways

$N_1 = 2 \Rightarrow$ put both in same state: d ways
<u>or</u> in different states $\frac{1}{2} d(d-1)$ way

Total $d + \frac{1}{2} d(d-1) = \frac{1}{2} d(d+1)$ ways

$N_1 = 3 \Rightarrow$ all three in same state: d ways
two in one, one in another $d(d-1)$ ways
all three separate $d \cdot (d-1)(d-2) \frac{1}{3!}$

total $d + d(d-1) + \frac{1}{6} d(d-1)(d-2)$

$$= \frac{1}{6} d(d^2 + 3d + 2)$$

$$= \frac{d(d+1)(d+2)}{6}$$

$N_1 = 4$: all in one state: d way

3 in one, 1 in another: $d(d-1)$

2 in one, 2 in another: $\frac{1}{2} d(d-1)$

2 in one, 1 in two others:

$$d \cdot \left[(d-1)(d-2) \frac{1}{2} \right]$$

all different: $d(d-1)(d-2)(d-3) \frac{1}{4!}$

$$\text{Total} = \frac{d(d+1)(d+2)(d+3)}{24}$$

Generalize, have $\dfrac{(d_1+N_1-1)!}{(d_1-1)!\,N_1!} = \binom{d+N-1}{N}$

So for bosons, $\boxed{Q = \prod_{n=1}^{\infty} \dfrac{(N_n+d_n-1)!}{N_n!\,(d_n-1)!}}$

Finally fermions pretty easy

Only one way to pick N_1 particles

Distribute over d_1 states, only one particle per state

d_1 choices for first

$d_1 - 1$ for 2^{nd}

$\vdots$

$d_1 - N_1 + 1$ for N_1^{th}

$= \dfrac{d_1!}{(d_1-N_1)!}$ But different permutations the same, divide by $N_1!$

Get $\frac{d_1!}{(d_1-N_1)!\,N_1!} = \binom{d_1}{N_1}$ ways

So $Q = \prod_n \frac{d_n!}{N_n!\,(d_n-N_n)!}$

Note if $N_n > d_n$, not a possible configuration

OK: interpret $k! = \infty$ for $k < 0$