L62-Quantum Statistics

Friday, February 19, 2016 08:23

* Reminder: Strategy for multiparticle systems: $\mathcal{H} = \sum_i \mathcal{H}_i(x_i)$

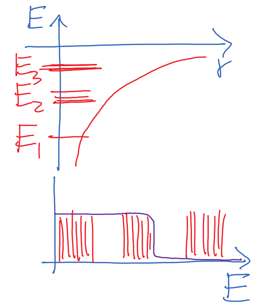
  a) determine single-particle states (spectrum) $\mathcal{H}_1 \phi_n(x) = E_n \phi_n(x)$

  b) distribute N particles into single-particle states $\psi(x_1, x_2 \ldots x_n) = \phi_1(x_1)\phi_2(x_2)\ldots\phi_n(x_n)$

  c) [anti]symmetrize identical {fermions} bosons $P_{ij}\psi = \pm\psi$
  to determine and count states – Pauli Exclusion Principle

* Examples: a) atom: slater determinant; H-like spectrum

  b) solids: i) Fermi gas model ii) Bloch theorem
  - give different spectra & degeneracies.
  - in ground state, all lowest levels are occupied to E_F



* Excitations should be treated statistically ....

  – we cannot follow the state of each particle, instead let us consider the probability $n(\varepsilon)$ of finding a single-particle state in the symmetrized wave function of energy ε

  – Recall the Maxwell-Boltzman distribution discussed during the first week in PHY 520.
  – We also derived the Planck (Bose-Einstein) distribution of Black Body radiation (γ bosons).
  – Now we will also derive the Fermi-Dirac distribution of fermions, like electrons, n stars...

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Plot[{1/(Exp[x]), 1/(Exp[x]-1), 1/(Exp[x]+1)},
 {x, -3, 3}, PlotRange → {0, 3}]
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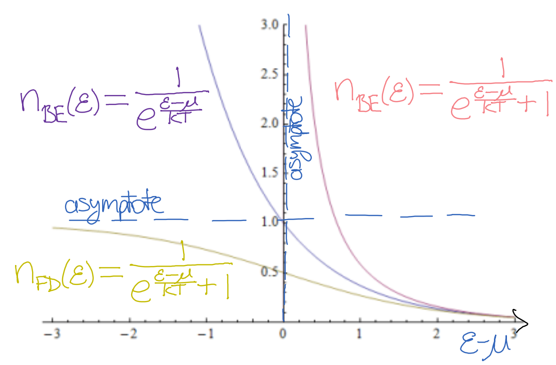

  – we will derive each of these statistical distributions.
  – all we know is the total energy of the system
  – there can be many configurations of each particle in individual states.
  – Thermal equalibrium: each configaration is equally likely (thermal fluctuations constantly randomly shift configurations.)

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* Example: 3 particles in an infinite square well x_A, x_B, x_C.

$$E = E_A + E_B + E_C = \frac{\pi^2\hbar^2}{2m}\left(n_A^2 + n_B^2 + n_C^2\right) \qquad \text{let } E = \frac{\pi^2\hbar^2}{2m}\cdot 363$$

$$363 = \underbrace{\overset{n_A^2 + n_B^2 + n_C^2}{11^2 + 11^2 + 11^2}}_{1 \text{ perm.}} = \underbrace{13^2 + 13^2 + 5^2}_{3 \text{ perm.}} = \underbrace{19^2 + 1^2 + 1^2}_{3 \text{ perm.}} = \underbrace{17^2 + 7^2 + 5^2}_{6 \text{ perm.}}$$

- configurations:

	n=	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	....
1x	(11,11,11) =	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	...
3x	(13,13,5) =	0	0	0	0	1	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	...
3x	(19,1,1) =	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	...
6x	(17,7,5) =	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	....

- distinguishable particles:

$$P(E_n) = \sum_{\text{config.}} \frac{(\text{degeneracy of config})}{(\text{total \# of states})} \times \frac{(\text{\# particles in state } E_n)}{(\text{total \# of particles})}$$

$n =$	1	5	7	11	13	17	19		
$P_{MB}(E_n) =$	(2	3	2	1	2	2	1)	/13	$\sum_n P_{MB}(E_n) = 1$

- fermions: only one state: (17, 7, 5) antisymmetrized

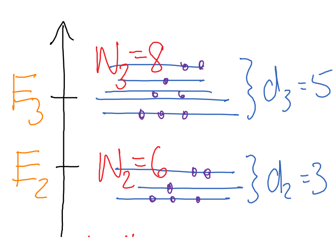
$$P_{FD}(E_n) = (0 \quad 1 \quad 1 \quad 0 \quad 0 \quad 1 \quad 0)/3 \qquad \sum_n P_{FD}(E_n) = 1$$

- bosons: one state in each configuration

$$P_{BE}(E_n) = (2 \quad 2 \quad 1 \quad 3 \quad 2 \quad 1 \quad 1)/12 \qquad \sum_n P_{BE}(E_n) = 1$$

* General case of counting states:

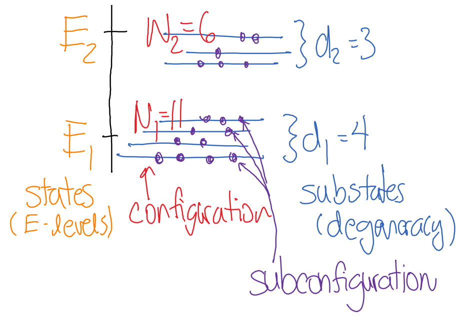
- single particle states:
  energy E_1, E_2, E_3 w/ degeneracy d_1, d_2, d_3



- for the N-particle wave function,

- for the N-particle wave function, how many states are there in the configuration $N_1, N_2, N_3 \ldots$, where $\sum N_i = N$?

$= Q(N_1, N_2, N_3, \ldots)$ "degeneracy" of configuration.



a) Distinguishable particles: Maxwell-Boltzman statistics.

\# ways to select N_1 particles for E_1 $= \binom{N}{N_1} \equiv \dfrac{N!}{N_1!\,(N-N_1)!}$ binomial coefficient

$$= \frac{N(N-1)\cdots(N-N_1+1)}{1\cdot 2 \cdots N_1} = \frac{N\,(\text{first choices}) \times [N-1]\,(\text{left overs}) \times \ldots}{\#\text{ permutations of selections}}$$

$\times\ d_1^{N_1}$ = d_1 choices for each particle

\# ways to select N_2 particles from $N-N_1$ into d_2 substates

$$= \binom{N-N_1}{N_2} d_2^{N_2} = \frac{(N-N_1)!\, d_2^{N_2}}{(N_2)!\,(N-N_1-N_2)!} \quad \text{and so on.}$$

The total # of microstates of $(N_1, N_2, N_3 \ldots)$ is the product

$$Q_{MB}(N_1, N_2, N_3 \ldots) = \frac{N!\, d_1^{N_1}}{N_1!\,\cancel{(N-N_1)!}} \cdot \frac{\cancel{(N-N_1)!}\, d_2^{N_2}}{N_2!\,\cancel{(N-N_1-N_2)!}} \cdot \frac{\cancel{(N-N_1-N_2)!}\, d_3^{N_3}}{N_3!\,\cancel{(N-N_1-N_2-N_3)!}} \cdots \frac{\cancel{N_n!}\, d_n^{N_n}}{N_n!\,\cancel{(0!)}}$$

$$= \frac{N!\, d_1^{N_1} d_2^{N_2} \cdots d_n^{N_n}}{N_1!\, N_2!\, N_3! \cdots N_n!} = N! \prod_{i=1}^{n} \frac{d_i^{N_i}}{N_i!} \equiv \binom{N}{N_1, N_2, \ldots N_n} \prod_{i=1}^{n} d_i^{N_i}$$

note: $(x_1 + x_2 + \ldots x_n)^N = \sum_{N_1+N_2+\ldots=N} \underbrace{\binom{N}{N_1, N_2, \ldots N_n}} x_1^{N_1} x_2^{N_2} \cdots x_n^{N_n}$

multinomial coeff. = # of ways of splitting N into $N_1, N_2, N_3 \ldots$

b) Identical fermions: Fermi-Dirac statistics

Easiest: each substate can have 0 or 1 particles in it. The antisymmetric wavefunction is unique for each subconfiguration of substates.

\# ways of distributing N_i particles into d_i substates

$= \binom{N_i}{\ }$ = # ways to pick N_i ... $\{0, 1\}$

ways of distributing N_i particles into d_i substates

$$= \binom{N_i}{d_i} = \#\text{ ways to split } N_i \text{ into } \{0,1\}$$

$$Q_{FD}(N_1, N_2, N_3 \ldots) = \prod_{i=1}^{n} \binom{N_i}{d_i} = \prod_{i=1}^{n} \frac{N_i!}{d_i!\,(N_i-d_i)!}$$

c) Identical bosons: Bose-Einstein statistics.

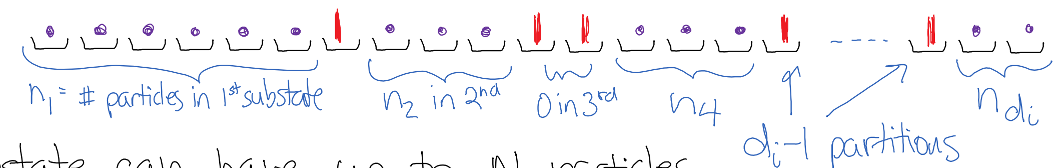
Hardest conceptually: each substate fits unlimited particles
Symmetric wave function unique for each subconfiguration.

ways of distributing N_i particles into d_i substates

$$= \binom{N_i+d_i-1}{d_i-1} = \frac{(N_i+d_i-1)!}{N_i!\,(d_i-1)!}$$

ways of putting d_i-1 partitions "|" into N_i+d_i-1 slots, leaving N_i particles "•"

counting trick:



each substate can have up to N_i particles

$$Q_{BE} = \prod_{i=1}^{n} \binom{N_i+d_i-1}{N_i} = \prod_{i=1}^{N} \frac{(N_i+d_i-1)!}{N_i!\,(d_i-1)!}$$

Next step: use conservation of energy & principle of indifference to determine $n(\varepsilon)$ = probability of being in single-particle state ε