4/30/2013  Lecture 20  Ideal quantum systems

I. Different types of statistical systems
   A. Fixed # particles, fixed energy (thermally isolated)
      All states equally probable \( P(E_i) = \frac{1}{Z} \)
      \( \Rightarrow \) Microcanonical ensemble
   B. Fixed # particles, energy exchange with reservoir (constant \( T \))
      \( T \) determines state occupation (Boltzmann factor)
      \( \Rightarrow \) Canonical ensemble \( P(E_i) = \frac{1}{Z} \exp(-\beta E_i) \)
   C. Particles and energy are exchanged with reservoir (Gibbs factor)
      \( \Rightarrow \) Grand Canonical Ensemble \( P(E_i) = ? \)

II. Grand Canonical Ensemble

<table>
<thead>
<tr>
<th>Energy ( U_s )</th>
<th>Energy ( U_r )</th>
<th>Conservation:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particles ( N_s )</td>
<td>Particles ( N_r )</td>
<td>( V = U_r + U_s )</td>
</tr>
<tr>
<td>System: ( N_s )</td>
<td>Reservoir: ( N_r )</td>
<td>( N = N_r + N_s )</td>
</tr>
</tbody>
</table>
in eq. The mean number of particles is fixed

- Reservoir control a system $I_r$ (Im equilibrium)

A. Calculate probabilities for system states for given $\mu, T$

1. System state $\alpha_i$: Energy $E_i \Rightarrow$ spectrum

- $n_i$ particles with energy $E_i \Rightarrow$ energy level

if we specify $\alpha_i$ (a microstate of the system) we
have reduced

$Z_\alpha (\alpha_i) = 1 \Rightarrow S_\alpha (\alpha_i) = 0$

$\Omega (\alpha_i) = Z_\alpha (\alpha_i) \Omega_R (\alpha_i) = Z_R (\alpha_i) \Rightarrow$ Ergodic principle

applies to all states of the combined system.

2. If we have 2 different microstates for the system $\alpha_1, \alpha_2$

$P (\alpha_2) = \frac{\Omega_R (\alpha_2)}{\Omega_R (\alpha_1)} \Rightarrow$ relative probability of 2 system states

3. Use the Therm. Identity (neglect)

$S = S (V, V, N) \Rightarrow dS_R = \frac{1}{T} (dU_R + P dV_R - \mu dN_R)$

Concieve $V \Rightarrow \Delta U_R = - \Delta S_R$

$N \Rightarrow \Delta U_R = - \Delta N_S$
\[ \Delta S_r = -\frac{1}{T} \Delta U_s + \frac{k}{T} \Delta N_s \]

\[ S_r(\alpha_2) - S_r(\alpha_1) = -\frac{1}{T} \left( E(\alpha_2) - E(\alpha_1) \right) + \frac{k}{T} \left( N_2 - N_1 \right) \]

\[ P(\alpha_2) = \frac{\exp \left( \frac{\mu N_s(\alpha_2) - E(\alpha_2)}{kT} \right)}{P(\alpha_1)} \]

4. Gibbs factor = \( \exp \left( \frac{\mu N(\alpha) - E(\alpha)}{kT} \right) \) \( \Rightarrow \) analog to Boltzmann factor

5. \( P(\alpha) = \text{prob. that system is in state } \alpha \) \( \text{[Energy } E, \text{ # particles } N] \)

\[ P(\alpha) = \frac{1}{Z} \exp \left( \frac{\mu N(\alpha) - E(\alpha)}{kT} \right) \]

6. \( Z = \text{grand partition function} = \sum_\alpha \exp \left( \frac{\mu N(\alpha) - E(\alpha)}{kT} \right) \]

\( \alpha \Rightarrow \text{index that refers to a particular state of the system} \)

\( \text{which is specified by occupation numbers } N \), \( \Rightarrow \{N_1, N_2,...\} \)

\( Z = \sum_\text{all possible } \{N\} \text{ for all microscopic states of a system with total # of particles } \alpha \)
III. Summary of system properties

<table>
<thead>
<tr>
<th>Macro (system) state</th>
<th>Microstates</th>
<th>Canonical</th>
<th>Grand Canonical</th>
</tr>
</thead>
<tbody>
<tr>
<td>U, V, N</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(T, fluctuate)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>State Prob.</td>
<td>P(Ω)</td>
<td>1/Ω</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(\frac{1}{\Omega} \exp \left(-\frac{E(\Omega)}{k_B T}\right))</td>
<td>(\frac{1}{\Omega} \exp \left(-\frac{E(\Omega) + \mu N_N}{k_B T}\right))</td>
</tr>
</tbody>
</table>

Thermodynamic potentials:
\[ S(U, V, N) = k_B \ln \Omega \]
\[ F = -k_B T \ln \Omega \]
\[ \Phi = k_B T \ln \Omega \]

\(\Phi\) = "Landau Free Energy"

\[ d\Phi = -\beta dT - pdV - N d\mu \]
\[ \left( \frac{\partial \Phi}{\partial N} \right)_{U, V} = -N \]

Note: This is computationally convenient but not natural. Natural variables are \( N, V \).

- Total Energy of GCE \( \Rightarrow U_S \)

\[ U_S = \sum_i E_i + \sum_i E_2 + \ldots = \sum_i E_i \]

all states \( \Rightarrow \) state energy

- Each Picl must be in some state

\[ N = \sum_i n_i \]

all states, (some might have \( n_i = 0 \))
\[ \Theta = \sum_{n_i} \exp \left( -\frac{n_i (E_i - \mu)}{kT} \right) \]

\[ N = \sum_{n_i} \text{states} \]

Sum over all possible occupancies and all states (energy state) for each occupancy

Gibbs sum depends on single level spectrum (E_i)

chemical potential (\mu) \n
\[ n_i \rightarrow \text{occupancy } i \text{ depends on system being Fermions or Bosons.} \]

\[ \Rightarrow \text{To calculate } \Theta \text{ we need to know how many particles/state } N(E_i) \]

\[ \Rightarrow N(E_i) \text{ depends on particle type} \]

IV Bosons + Fermions: Two primary classes.

a) "All" particles are either bosons or fermions

(true for composite particles)

Bosons: Zero or integer spin (units of h)

\[ j \] 

\[ \text{e.g. } \text{photons, even } Z \text{ nuclei} \]
b) Bosons: Wfn is unchanged if you interchange field labels.

\[ \psi(1, 2, 3) = \psi(2, 1, 3) \] (3 bosons)

3) How many bosons can fit in a state? \( \rightarrow \) Unlimited

3. Fermions: half integer spin

a) ex: electrons, protons, neutrons, odd Z nuclei

b) Fermion Wfn changes sign if interchange field labels.

\[ \psi(1, 2, 3) = -\psi(2, 1, 3) \]

c) How many fermions in state i? \( \leq 1 \) only

Fermi exclusion principle

4. Composite objects: made of bosons + fermions

ex \( ^3\text{He} = 2e^- + 2p^+ + 1n^o = 5 \) fermions

\( \implies ^3\text{He} \) obeys Fermi statistics

5. Occupation Numbers:

a) Fermions: \( n_i = 0, 1 \) (only)

b) Bosons: \( n_i = \) any integer \( (0, 1, 2 \cdots) \)
Example: 1-d Box (Length $L$); 2 non-interacting particles

$$E_1 = \frac{\hbar^2}{8mL^2} \text{ } n_1^2 \text{ } \uparrow \text{ } \text{inc } E$$

$$E_2 = E_{n_1} \uparrow + E_{n_2} = \left( \frac{\hbar^2}{8mL^2} \right) \left( n_1^2 + n_2^2 \right)$$

- $n_1, n_2 \equiv \text{quantum number for particle 1, particle 2}$
- State for particle 1
- State for particle 2

To compare states for classical (indistinguishable) particles, bosons, and fermions

<table>
<thead>
<tr>
<th>State (n)</th>
<th>Classical (Indistinguishable)</th>
<th>Bosons</th>
<th>Fermions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy</td>
<td>#1</td>
<td>#2</td>
<td>#1</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>8</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>10</td>
<td>3</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>$\frac{1}{3}$</td>
<td>3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>3</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>18</td>
<td>3</td>
<td>3</td>
<td>3</td>
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