Identical Fermions

The concepts here are very similar to the case of identical bosons except that the wave-f^n now must be anti-symmetric under the exchange of any pair of particles.

That is, $\psi(x_1, x_2, x_3, \ldots x_N)$ (1)

$$= -\psi(x_2, x_1, x_3, \ldots, x_N)$$

$$= -\psi(x_1, x_3, x_2, \ldots, x_N)$$

$$= +\psi(x_N, x_3, x_2, \ldots, x_1)$$

etc.

For separable Hamiltonians, this implies that the wave-f^n vanishes when two particles are in the same single-particle eigenstate.

This is because one simultaneously also has the condition, $\psi(x_1, x_2, x_3, \ldots x_N)$ (2)

$$= \psi(x_2, x_1, x_3, \ldots x_N).$$

Clearly (1) and (2) imply that $\psi = 0$

Constructing anti-symmetric wave-f^{n}s using single-particle eigenstates

The idea is very similar to the case of identical bosons. Instead of symmetrizing, we now anti-symmetrize:

Consider a two-particle system:

$$\psi^{\text{anti-sym}} = \left[u^{\alpha_1}(x_1)\, u^{\alpha_2}(x_2) - u^{\alpha_2}(x_1)\, u^{\alpha_1}(x_1) \right]$$

This is a valid wave-f^n for fermions.

Clearly, $\psi^{\text{anti-sym}}$ vanishes when $\alpha_1 = \alpha_2$.

Consider the case of three particles now.

In parallel to our discussion for the bosons, the wave-f^n is now $\psi(x_1, x_2, x_3) =$

$$\det \begin{bmatrix} u^{\alpha_1}(x_1) & u^{\alpha_1}(x_2) & u^{\alpha_1}(x_3) \\ u^{\alpha_2}(x_2) & u^{\alpha_2}(x_2) & u^{\alpha_2}(x_3) \\ u^{\alpha_3}(x_1) & u^{\alpha_3}(x_2) & u^{\alpha_3}(x_3) \end{bmatrix}$$

where 'det' denotes determinant of a matrix. Explicitly,

$$\psi(x_1, x_2, x_3) =$$

$$
\begin{aligned}
& u^{\alpha_1}(x_1)\, u^{\alpha_2}(x_2)\, u^{\alpha_3}(x_3) \\
& - u^{\alpha_1}(x_1)\, u^{\alpha_2}(x_3)\, u^{\alpha_3}(x_2) \\
& + u^{\alpha_1}(x_2)\, u^{\alpha_2}(x_3)\, u^{\alpha_3}(x_1) \\
& - u^{\alpha_1}(x_2)\, u^{\alpha_2}(x_2)\, u^{\alpha_3}(x_3) \\
& + u^{\alpha_1}(x_3)\, u^{\alpha_2}(x_2)\, u^{\alpha_3}(x_2) \\
& - u^{\alpha_1}(x_3)\, u^{\alpha_2}(x_2)\, u^{\alpha_3}(x_1)
\end{aligned}
$$

Check that $\psi(x_1, x_2, x_3)$ changes sign under the operation of exchange of any pair of particles.

Example: Two indistinguishable fermions in a harmonic potential

$$\hat{H} = \frac{P_1^2}{2} + \frac{1}{2} m\omega^2 \hat{x}_1^2 + \frac{P_2^2}{2} + \frac{1}{2} m\omega^2 \hat{x}_2^2$$

What is the partition f^n?

Again, the single particle eigenstates are unchanged. In the sum,

$$Z_{fermion} = \sum_{n_1, n_2} e^{-\beta\hbar\omega(n_1 + \frac{1}{2} + n_2 + \frac{1}{2})}$$

one needs to put the restriction that $n_1 \neq n_2$ and that $(n_1, n_2) \equiv (n_2, n_1)$

Thus, $Z_{fermion} = \frac{1}{2} \sum_{n_1 \neq n_2} e^{-\beta\hbar\omega(n_1 + \frac{1}{2} + n_2 + \frac{1}{2})}$

$$= \frac{1}{2} \Big[\sum_{n_1, n_2} e^{-\beta\hbar\omega(n_1 + \frac{1}{2} + n_2 + \frac{1}{2})} - \sum_{n_1 = n_2} e^{-\beta\hbar\omega(n_1 + \frac{1}{2} + n_2 + \frac{1}{2})}$$

$$= \frac{1}{2} Z_{distinguishable} - \frac{1}{2} \sum_{n} e^{-\beta\hbar\omega(2n+1)}$$

$$= \frac{1}{2} \frac{e^{-\beta\hbar\omega}}{[1 - e^{-\beta\hbar\omega}]^2} - \frac{1}{2} \frac{e^{-\beta\hbar\omega}}{1 - e^{-2\beta\hbar\omega}}$$

Note that,

$$Z_{fermion} + Z_{boson} = Z_{distinguishable}$$

for this problem.

It is obvious that by definition, identical fermions 'repel' each other since no two can be in the same state. It requires a bit more thought to see that in stark contrast, identical bosons tend to clump together. To see this, consider a separable Hamiltonian which has just three single-particle states. Given two particles, we ask what is the value of the ratio ξ:

$$\xi = \frac{\text{probability that the two particles are in the same state}}{\text{probability that the two particles are in different states.}}$$

Fermions : $\xi = 0$

Bosons : $\xi = 1$

Distinguishable : $\xi = \frac{1}{2}$

Thus, bosons tend to stay together relative to distinguishable particles.

Discussion generalizes to the case of N particles in g levels.

$$\xi = \frac{\text{prob. that all particles in the same level}}{\text{prob. that } \underline{\text{all}} \text{ particles in different levels.}}$$

Fermions : $\xi = 0$

Bosons : $\xi = \dfrac{g}{[g \cdot (g-1) \cdot (g-2) \ldots (g-N+1)] / N!}$

Distinguishable: $\xi = \dfrac{g}{g \cdot (g-1) \ldots (g-N+1)}$

Indistinguish-ability

$$\Rightarrow \boxed{\frac{\xi_{\text{Bosons}}}{\xi_{\text{Distinguishable}}} = N!}$$

Partition Functions of Identical Bosons and Fermions for Separable Hamiltonians

As discussed above, for a separable Hamiltonian of identical particles, the eigenstates can be labeled fully by specifying which of the single particle levels are occupied. i.e.

$$\hat{H} \, | E^\alpha \rangle = E^\alpha \, | n_1^\alpha, n_2^\alpha, \ldots, n_L^\alpha \rangle$$

(L = number of single particle levels — could be infinite)

with $E^\alpha = \sum_{i=1}^{L} \varepsilon_i \, n_i^\alpha$

As one may observe from the example of two particles in a harmonic potential, the partition f^n is rather challenging to calculate in the canonical ensemble i.e. when $\sum_i n_i^\alpha = N$ is fixed. The calculation is simplified dramatically in the Grand canonical ensemble. Let us see how this works:

Identical bosons at temperature β^{-1} and chemical potential μ :

$$Z_{Boson} = \mathrm{Tr}\, e^{-\beta(\hat{H} - \mu \hat{N})}$$

$$= \sum_{\alpha} \langle E^{\alpha} | e^{-\beta(\hat{H} - \mu \hat{N})} | E^{\alpha} \rangle$$

$$= \sum_{n_i^{\alpha}} e^{-\beta \sum_i (\varepsilon_i - \mu) n_i^{\alpha}}$$

Note that since we are in GCE, the sum over α has been replaced by sum over $\{n_i^{\alpha}\}$, the occupancies of single-particle eigenstates $|u_i\rangle$ in the many-body eigenstate $|E^{\alpha}\rangle$.

For bosons, there is no restriction on n_i^{α} - except that it must be a non-negative integer. Thus,

$$Z_{Boson} = \sum_{n_i^{\alpha}=0}^{\infty} \prod_i e^{-\beta(\varepsilon_i - \mu) n_i^{\alpha}}$$

Interchanging the order of summation and product :

$$\boxed{Z_{Boson} = \prod_i \frac{1}{1 - e^{-\beta(\varepsilon_i - \mu)}}}$$

Average occupation of levels for free bosons:

$$\langle \hat{n}_i \rangle = \frac{\mathrm{Tr}\, \hat{n}_i\, e^{-\beta(\hat{H}-\mu\hat{N})}}{\mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}}$$

$$= \frac{\sum_\alpha \langle E^\alpha | \hat{n}_i\, e^{-\beta[\sum_i \hat{n}_i \varepsilon_i - \mu \sum_i \hat{n}_i]} | E^\alpha \rangle}{\sum_\alpha \langle E^\alpha | e^{-\beta[\sum_i \hat{n}_i \varepsilon_i - \mu]} | E^\alpha \rangle}$$

Since $|E^\alpha\rangle = |n_1^\alpha, n_2^\alpha, \ldots n_N^\alpha\rangle$

$$\Rightarrow \quad \hat{n}_i |E^\alpha\rangle = n_i^\alpha |E^\alpha\rangle$$

Thus,
$$\langle \hat{n}_i \rangle = \frac{\sum_{n_i^\alpha=0}^{\infty} n_i^\alpha\, e^{-\beta(\varepsilon_i-\mu)n_i^\alpha}}{\sum_{n_i^\alpha=0}^{\infty} e^{-\beta(\varepsilon_i-\mu)n_i^\alpha}}$$

(note that the sums over levels $j \neq i$ cancel out from the denominator and the numerator)

$$\Rightarrow \quad \langle \hat{n}_i \rangle = \frac{-1}{Z_i}\frac{\partial Z_i}{\partial \beta(\varepsilon_i-\mu)}$$

where $Z_i = \sum_{n_i^\alpha=0}^{\infty} e^{-\beta(\varepsilon_i-\mu)n_i^\alpha}$

$$= \frac{1}{1-e^{-\beta(\varepsilon_i-\mu)}}$$

$$= \frac{e^{-\beta(\varepsilon_i-\mu)}}{1-e^{-\beta(\varepsilon_i-\mu)}}$$

$$= \frac{1}{e^{\beta(\varepsilon_i-\mu)}-1} \quad \leftarrow \text{“Bose-Einstein distribution”}$$

Identical fermions at temperature β^{-1} and chemical potential μ:

For fermions, the formal expression for Z is same as that for bosons (since it only depended on separability of H and identical particles). However, $n_i^\alpha = 0$ or 1 only

Thus, $Z_{fermion} =$

$$\sum_{n_i^\alpha = 0,1} \prod_i e^{-\beta(\varepsilon_i - \mu) n_i^\alpha}$$

$$\Rightarrow \quad Z_{fermion} = \prod_i \left[1 + e^{-\beta(\varepsilon_i - \mu)}\right]$$

Average occupation of levels:

$$\langle \hat{n}_i \rangle = \frac{\sum_{n_i^\alpha = 0,1} n_i^\alpha \, e^{-\beta(\varepsilon_i - \mu) n_i^\alpha}}{\sum_{n_i^\alpha = 0,1} e^{-\beta(\varepsilon_i - \mu) n_i^\alpha}}$$

note: $(\langle \hat{n}_i \rangle \leq 1)$

$$\Rightarrow \quad \boxed{\langle \hat{n}_i \rangle = \frac{e^{-\beta(\varepsilon_i - \mu)}}{1 + e^{-\beta(\varepsilon_i - \mu)}} = \frac{1}{1 + e^{\beta(\varepsilon_i - \mu)}}}$$

"Fermi-Dirac Distribution"

Alternative Derivation to obtain occupation numbers via Minimizing Grand free Energy

Recall how we derived the canonical ensemble by minimizing the free energy (Eqns. 32 - 35). Here we follow a similar approach to derive Bose and Fermi distributions for separable/free Hamiltonians.

We want to minimize:

$$\Omega = E - TS - \mu N$$

for as yet unknown distribution $\{n_i\}$ of single particle levels $|u_i\rangle$.

Let's calculate the three terms E, N and S in terms of $\{n_i\}$ and then minimize Ω.

Bosons :

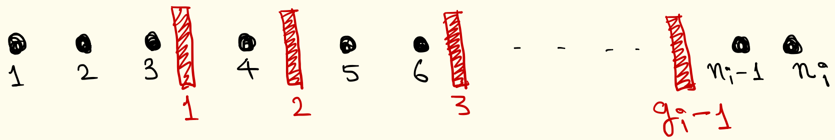
It is easier to do the calculation if we group the single-particle levels in groups so that the i'th group has g_i number of single-particle levels at mean energy ε_i and the variation $d\varepsilon_i$ of energy across levels within the same group is small : $d\varepsilon_i \ll \varepsilon_i$. We denote the number of particles within i'th group by $n_i \gg 1$.

The total entropy S is the sum of entropy contribution from individual groups.

The entropy contribution of i'th group is given by :

$$S_i = \log W_i$$

where W_i is the number of ways of distributing n_i bosons in g_i single particle levels. To solve this counting problem, consider the following construction



Above we have introduced $g_i - 1$ dividers to separate n_i particles into g_i groups. The number of distinct ways to do so is :

$$W_i = \frac{(n_i + g_i - 1)!}{(g_i - 1)!\; n_i!}$$

total no. of permutations of particles + dividers.

Identical particles

Dividers are identical too!

Thus, $S_i = \log W_i$

$$\simeq (n_i + g_i - 1)\log(n_i + g_i - 1) - (g_i - 1)\log(g_i - 1) - n_i \log(n_i)$$

As mentioned already, the total entropy S is the sum of individual contributions S_i.

$$\Rightarrow \quad S = \sum_i \Big[(n_i + g_i - 1)\log(n_i + g_i - 1) - (g_i - 1)\log(g_i - 1) - n_i \log(n_i) \Big]$$

The total energy E and particle number N are easier to express:

$$E = \langle \hat{H} \rangle = \sum_i \varepsilon_i n_i$$

Recall that the i-th group has energy ε_i for all g_i levels within it.

$$N = \langle \hat{N} \rangle = \sum_i n_i$$

Thus, $\Omega = E - TS - \mu N$

$$= \sum_i \Big[(\varepsilon_i - \mu) n_i - T \big\{ (n_i + g_i - 1)\log(n_i + g_i - 1) - (g_i - 1)\log(g_i - 1) - n_i \log(n_i) \big\} \Big]$$

Minimizing Ω w.r.t. to individual n_i's $\Rightarrow$

$$\Rightarrow \quad (\varepsilon_i - \mu) - T \log\left[\frac{n_i + g_i - 1}{n_i} \right] = 0$$

The occupation of group i is $\dfrac{n_i}{g_i} = f_i$

and since $n_i \gg 1$, the above Eqn. becomes

$$1 + f_i^{-1} = e^{(\varepsilon_i - \mu)\beta}$$

$$\Rightarrow \quad \boxed{f_i = \frac{1}{e^{\beta(\varepsilon_i - \mu)} - 1}}$$

which is indeed the Bose distribution.

Fermions :

We follow a similar approach for the fermions. The counting involved in calculating S_i, the entropy contribution of the i-th group, is indeed different. Each level can be occupied by at most one fermion $\Rightarrow$ W_i = number of ways to choose n_i levels out of g_i levels (which are then filled).

$$\Rightarrow \quad W_i = \frac{g_i!}{n_i!\,(g_i - n_i)!}$$

Using this and recalling that $S = \sum_i S_i = \sum_i \log W_i$

$$\partial \mathcal{R}(\{n_i\}) / \partial n_i$$

$$= \sum_i \left\{ (\varepsilon_i - \mu) - T \log\left[\frac{g_i - n_i}{n_i}\right] \right\} = 0$$

$$\Rightarrow \quad \log\left[\frac{g_i}{n_i} - 1\right] = \beta(\varepsilon_i - \mu)$$

$\Rightarrow$ Occupation of i'th group

$$= \frac{n_i}{g_i} \equiv f_i$$

$$\boxed{= \frac{1}{e^{\beta(\varepsilon_i - \mu)} + 1}}$$