Example: The harmonic oscillator

Suppose we have a single harmonic oscillator.
The energy eigenstates are $E_n = \hbar\omega(n + 1/2)$

The canonical partition function will be

$$Q = \sum_n e^{-\beta E_n} = \sum_n e^{-\beta\hbar\omega(n+1/2)} = e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} (e^{-\beta\hbar\omega})^n$$

$$Q = \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}}$$

$$\langle E \rangle = -\frac{\partial}{\partial\beta} \ln Q = -\frac{\partial}{\partial\beta}\left[-\beta\frac{\hbar\omega}{2} - \ln(1-e^{-\beta\hbar\omega})\right]$$

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

We could write

$\langle E \rangle = \hbar\omega(\langle n \rangle + 1/2)$ where $\langle n \rangle$ is the average level of occupation of the h.o.

$$\Rightarrow \langle n \rangle = \frac{1}{e^{\beta\hbar\omega}-1}$$

Quantum Many particle systems

N identical particles described by a wavefunction

$$\psi(\vec{r}_1 s_1, \vec{r}_2 s_2, \ldots, \vec{r}_N s_N) \qquad \vec{r}_i = \text{position particle } i$$
$$= \psi(1, 2, \ldots, N) \qquad s_i = \text{spin of particle } i$$

Indentical particles $\Rightarrow$ prob distribution $|\psi|^2$ should be symmetric under interchange of any pair of coordinates: $|\psi(1, \ldots i, \ldots, j, \ldots N)|^2 = |\psi(1, \ldots, j, \ldots, i, \ldots N)|^2$

$\Rightarrow$ two possible symmetries for ψ

1) ψ is symmetric under pair interchanges
$$\psi(1, \ldots, i, \ldots, j, \ldots, N) = \psi(1, \ldots, j, \ldots, i, \ldots N)$$
2) ψ is antisymmetric under pair interchanges
$$\psi(1, \ldots, i, \ldots, j, \ldots N) = -\psi(1, \ldots, j, \ldots i, \ldots N)$$

(1) = Bose-Einstein statistics - particle called "bosons"
(2) = Fermi-Dirac statistics - particles called "fermions"

For a general permutation $\mathbb{P}$ that interchanges any number of pairs of particles

(1) BE $\Rightarrow$ $\mathbb{P}\psi = \psi$

(2) FD $\Rightarrow$ $\mathbb{P}\psi = (-1)^p \psi$ where p = # pair interchanges
$$= \begin{cases} +\psi & \text{for even permutation} \\ -\psi & \text{for odd permutation} \end{cases}$$

BE statistics are for particles with integer spin, $S = 0, 1, 2, \dots$
FD statistics are for particles with half integer spin, $S = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$
(proved by quantum field theory)

Consider <u>non-interacting</u> particles

$$\mathcal{H}(1,2,3,\dots N) = \mathcal{H}^{(1)}(1) + \mathcal{H}^{(1)}(2) + \cdots \mathcal{H}^{(1)}(N)$$

sum of single particle Hamiltonians

$$\Rightarrow \psi(1,2,\dots,N) = \phi_1(1)\phi_2(2)\cdots\phi_N(N)$$

where ϕ_i is an eigenstate of single particle $\mathcal{H}^{(1)}$ with energy ϵ_i.

But ψ above does not have proper symmetry.

for BE $\quad \psi_{BE} = \frac{1}{\sqrt{N_P}} \sum_{\mathbb{P}} \mathbb{P}\psi \leftarrow \psi = \phi_1 \phi_2 \cdots \phi_N$ as above

normalization

$\leftarrow$ sum over all permutations $\mathbb{P}$

N_p = # possible permutations of N particles $= N!$

for FD $\quad \psi_{FD} = \frac{1}{\sqrt{N_P}} \sum_{\mathbb{P}} (-1)^P \mathbb{P}\psi$

You can verify that the above symmetrizing operations give

$$\left\{ \begin{aligned} \mathbb{P}_0 \psi_{BE} &= \psi_{BE} \\ \mathbb{P}_0 \psi_{FD} &= (-1)^{P_0} \psi_{FD} \end{aligned} \right\} \text{ as desired}$$

For ψ described by the N single particle eigenstates $\phi_{i_1}, \phi_{i_2}, \cdots \phi_{i_N}$, the total energy is

$$E = \epsilon_{i_1} + \epsilon_{i_2} + \cdots + \epsilon_{i_N} = \sum_j n_j \epsilon_j$$

where n_j is the number of particles in state ϕ_j.

For FD statistics, $n_j = 0$ or 1 only possibilities.

This is because if $\psi(1, 2, \cdots, N) = \phi_1(1)\phi_1(2)\phi_{i_3}(3)\cdots\phi_{i_N}(N)$

particles 1 and 2 in same state ϕ_1

then when we construct

$$\psi_{FD} = \frac{1}{\sqrt{N_p}} \sum_{\mathbb{P}} (-1)^p \mathbb{P}\psi$$

then for every term in the sum $\phi_1(i)\phi_1(j)\phi_{i_3}(k)\cdots\phi_{i_N}(l)$
there must also be a term $(-1)\phi_1(j)\phi_1(i)\phi_{i_3}(k)\cdots\phi_{i_N}(l)$
so these cancel pair by pair
and we find $\psi_{FD} = 0$

$\Rightarrow$ <u>Pauli Exclusion Principle</u> — no two ~~particles~~ fermions can occupy the same state, or no two fermions can have the same "quantum numbers".

For BE statistics there is no such restriction and $n_j = 0, 1, 2, 3, \ldots$ any integer.

The specification of any <u>non-interacting</u> N particle quantum state is given by the occupation numbers $\{n_i\}$. Each set of $\{n_i\}$ corresponds to <u>one</u> N particle state.