Lecture 37: Fock Space

Friday, April 24, 2020

At the end of the last lecture, we noticed that if we made the ladder operators commute, we automatically get Boson statistics, whereas anti-commutation (a Poisson bracket or alternatively, we can subscript the commutator with a + sign) gives Fermion statistics:

$$\left[[a_i, a_j]_\pm\right]^\dagger = \left[a_j^\dagger, a_i^\dagger\right]_\pm = 0$$

$$\left[a_i, a_j^\dagger\right] = \delta_{ij}$$

$$N_i = a_i^\dagger a_i$$

is the number of particles in the energy eigenstate enumerated by i.

Let's now consider hydrogen:

$$|\psi_0\rangle = \int \mathrm{d}^3x\, \psi_{nlm}(x) a_x^\dagger |0\rangle$$

We need to normalize it:

$$\langle\psi_0|\psi_0\rangle = \int \mathrm{d}^3x\, \mathrm{d}^3x'\, \langle 0| a_{x'} \psi^*(x')\psi(x) a_x^\dagger |0\rangle = \int \mathrm{d}^3x\, \mathrm{d}^3x'\, \psi^*(x')\psi^*(x)\delta^3(x-x') = \int \mathrm{d}^3x\, |\psi(x)|^2 = 1$$

$$|k\rangle = \sum_x |x\rangle \langle x|k\rangle$$

$$a_k = \sum_x \langle x|k\rangle a_x$$

$$|\psi\rangle = \int \mathrm{d}^3k\, \psi(k) a_k^\dagger |0\rangle$$

If the system is in a box, k is discrete:

$$\left[a_k, a_p^\dagger\right] = \delta_{p,k}$$

What is the probability of of being in the x_0 state?

$$\begin{aligned}
\Pr(x_0) &= |\langle 0|a_{x_0}|\psi\rangle|^2 \\
&= \left|\langle 0|a_{x_0} \int \mathrm{d}^3x\, \psi(x) a_x^\dagger|0\rangle\right|^2 \\
&= \left|\langle 0|\delta^3(x_0 - x)|0\rangle\right| = |\psi(x_0)|^2
\end{aligned}$$

This checks out with what we would expect.

Lets look at the Helium ground state (ignoring the Coulomb repulsion):

$$\int \mathrm{d}^3x\, \mathrm{d}^3y\, \psi_{100}(x)\psi_{100}(y) a_{x\uparrow}^\dagger a_{y\downarrow}^\dagger |0\rangle$$

What is the probability of finding one particle at x_0^1 and S_1 and one at x_2^2 and S_2?

$$\begin{aligned}
\left\langle x_{0,S_1}^1, x_{0,S_2}^2 \middle|\psi\right\rangle &= \int \mathrm{d}^3x, y\, \langle 0| a_{x_{0,S_1}^1} a_{x_{0,S_2}^2} a_{x\uparrow}^\dagger a_{y\downarrow}^\dagger |0\rangle\, \psi_{100}(x)\psi_{100}(y) \\
&= \int \left[\langle 0| a_{x_{0,S_1}^1} \delta^3(x_0^2 - x)\delta_{S_2,\uparrow} a_{y\downarrow}^\dagger |0\rangle - \langle 0| a_{x_{0,S_1}^1} a_{x\uparrow}^\dagger a_{x_{0,S_1}^2} a_{y\downarrow}^\dagger |0\rangle\right] \mathrm{d}^3x, y\, \psi_{100}(x)\psi_{100}(y) \\
&= \int \mathrm{d}^3x, y\, \{[\delta^3(x_0^1 - y)\delta(x_0^2 - x)\delta_{S_2,\uparrow}\delta_{\downarrow,S_1}] - [\delta^3(x_0^2 - y)\delta_{S_2,\downarrow}\delta^3(x_0^1 - x)\delta_{S_1,\uparrow}]\}\psi_{100}(x)\psi_{100}(y) \\
&= \psi_{100}(x_0^2)\psi_{100}(x_0^1)\delta_{S_2,\uparrow}\delta_{S_1,\downarrow} - \psi_{100}(x_0^1)\psi_{100}(x_0^2)\delta_{S_2,\downarrow}\delta_{S_1,\uparrow}
\end{aligned}$$

By choosing the proper commutation relation for the statistics of electrons, we get an anticommuting wave function as expected.

0.1 Operations on Fock Space

$$H_{\text{free}} = \sum_{\vec{\mathbf{k}}} \frac{\hbar^2 \vec{\mathbf{k}}^2}{2m} a^\dagger_{\vec{\mathbf{k}}} a_{\vec{\mathbf{k}}}$$
$$\vec{\mathbf{p}} = \sum_k \hbar \vec{\mathbf{k}} a^\dagger_k a_k$$

Some interesting properties of Bosons and Fermions are that Bosons fall into ground-state condensates while Fermions build a "sea" of states. How do we include interactions between the particles, which are obviously crucial? Suppose we have pairwise interactions:

$$H = \sum_{ij} \frac{1}{2} V_{ij} N_i N_j$$

where the 1/2 avoids double-counting. For electromagnetism, we have interactions of the form

$$\frac{e^2}{\vec{\mathbf{x}}_1 - \vec{\mathbf{x}}_2} \rho(x_1)\rho(x_2)$$

where our N_i's are the charge density and V_{ij} is the fraction term. Let's consider Fermions:

$$\begin{aligned} H &= \sum_{ij} \frac{1}{2} V_{ij} a^\dagger_i a_i a^\dagger_j a_j \\ &= \sum_{ij} \frac{1}{2} V_{ij} \left[-a^\dagger_i a^\dagger_j a_i a_j + a^\dagger_i a^\dagger_j \delta_{ij} \right] \\ &= \frac{1}{2} \sum_{i \neq j} V_{ij} N_i N_j + \frac{1}{2} \sum_i V_{ii} N_i (N_i - 1) \\ &= \frac{1}{2} \sum_{ij} N_i N_j - \frac{1}{2} \sum_i V_{ii} N_i \end{aligned}$$

This operator has a name:

$$\Pi_{ij} = N_i N_j - N_i \delta_{ij}$$

is called the pair distribution operator. Let's apply this to the Coulomb interaction.

$$H = \sum \frac{p_i^2}{2m} + \frac{e^2}{2} \sum_{i \neq j} \frac{e^{-\mu(x_i - x_j)}}{x_i - x_j} + \frac{e^2}{2} \int \mathrm{d}^3 x, x' \, \frac{\rho(x)\rho(x') e^{-\mu(x - x')}}{|x - x'|} - e^2 \int \mathrm{d}^3 x \sum_i \frac{\rho(x)}{|x - x_i|} e^{-\mu(x - x_i)}$$

where the final term is an additional positive charge density (since a lot of electrons together won't make for an interesting particle, the system will blow apart).

We will eventually take $\mu \to 0$. This is called a regulator. In the intermediate parts of this calculation, we will find some rather annoying divergences without it.