1 Definition of creation and annihilation operators

Suppose we have a complete set of states $\psi_n(\vec{r})\}$ or $\{|n\rangle\}$. Then an n-particle fermionic state can be written as a Slater determinant. Note that $(\vec{r}_i)$ here denotes space and spin coordinates:

$$\Psi(\vec{r}_1, \dots, \vec{r}_N) = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \psi_{n_1}(P\vec{r}_1)\psi_{n_2}(P\vec{r}_2)\cdots\psi_{n_N}(P\vec{r}_N),$$

with the sum over all $N!$ permutations P of N objects. This wave function is obviously anti-symmetric under the interchange of any two particles. Notationally, it is painful to deal with Slater determinants. So a new formalism was developed called the **occupation number representation**, where we denote each of the wave functions to be included in the Slater determinant (as a shorthand):

$$|1, 0, 0, \dots\rangle = \psi_1(\vec{r}_1),$$

$$|0, 1, 1, 0, \dots\rangle = \frac{1}{\sqrt{2}}\big(\psi_2(\vec{r}_1)\psi_3(\vec{r}_2) - \psi_3(\vec{r}_1)\psi_2(\vec{r}_2)\big).$$

We introduce abstract operators in this space in the spirit of Dirac:

$$\hat{c}_k^\dagger |n_1, n_2, \dots, n_k, \dots\rangle = |n_1, n_2, \dots, n_k + 1, \dots\rangle$$

where $c_k^\dagger$ creates the state k, and

$$\hat{c}_k |n_1, n_2, \dots, n_k, \dots\rangle = |n_1, n_2, \dots, n_k - 1, \dots\rangle$$

where $\hat{c}_k$ destroys the state k. The Pauli exclusion principle says $n_k = 0$ or 1 only, so

$$(\hat{c}_k^\dagger)^2 = (\hat{c}_k)^2 = 0.$$

Now, we can define the vacuum state as:

$$|0\rangle = |0, 0, 0, \dots\rangle.$$

Acting on this vacuum state gives us:

$$\hat{c}_k^\dagger |0\rangle = \psi_k(\vec{r}_1)$$

and:

$$\hat{c}_{k'}^\dagger \hat{c}_k^\dagger |0\rangle = \frac{1}{\sqrt{2}}\left(\psi_{k'}(\vec{r}_1)\psi_k(\vec{r}_2) - \psi_k(\vec{r}_1)\psi_{k'}(\vec{r}_2)\right),$$

but

$$\hat{c}_k^\dagger \hat{c}_{k'}^\dagger |0\rangle = \frac{1}{\sqrt{2}}\left(\psi_k(\vec{r}_1)\psi_{k'}(\vec{r}_2) - \psi_{k'}(\vec{r}_1)\psi_k(\vec{r}_2)\right),$$

which shows us that $\hat{c}_{k'}^\dagger \hat{c}_k^\dagger \neq \hat{c}_k^\dagger \hat{c}_{k'}^\dagger$, meaning the operators don't commute and we get the anticommutation relation:

$$(\hat{c}_{k'}^\dagger, \hat{c}_k^\dagger)_+ = 0$$

In general, we get the following anticommutation relations:

$$(\hat{c}_k^\dagger, \hat{c}_{k'}^\dagger)_+ = 0, \quad (\hat{c}_k, \hat{c}_{k'})_+ = 0, \quad (\hat{c}_k^\dagger, \hat{c}_{k'})_+ = \delta_{kk'}.$$

From the definitions above of the creation and annhiliation operators, it follows further that:

$$\begin{cases} \hat{c}_k^\dagger|0_k\rangle = |1_k\rangle \\ \hat{c}_k^\dagger|1_k\rangle = 0 \\ \hat{c}_k|0_k\rangle = 0 \\ \hat{c}_k|1_k\rangle = |0_k\rangle \end{cases}$$

so $\hat{c}_k^\dagger\hat{c}_k|0_k\rangle = 0$ and $\hat{c}_k^\dagger\hat{c}_k|1_k\rangle = 1 \cdot |1_k\rangle$. As a result, we can think of $\hat{c}_k^\dagger\hat{c}_k$ as counting the occupation number at state k. We can thus define the so-called **number operator** $\hat{n}_k = \hat{c}_k^\dagger\hat{c}_k$ which has the following commutation relations:

$$\begin{cases} [\hat{n}_k, \hat{c}_k^\dagger] = \hat{c}_k^\dagger\hat{c}_k\hat{c}_k^\dagger - \hat{c}_k^\dagger\hat{c}_k^\dagger\hat{c}_k = \hat{c}_k^\dagger(\hat{c}_k, \hat{c}_k^\dagger)_+ = \hat{c}_k^\dagger \\ [\hat{n}_k, \hat{c}_k^\dagger] = \hat{c}_k^\dagger \\ [\hat{n}_k, \hat{c}_k] = \hat{c}_k^\dagger\hat{c}_k\hat{c}_k - \hat{c}_k\hat{c}_k^\dagger\hat{c}_k = -\hat{c}_k(\hat{c}_k^\dagger, \hat{c}_k)_+ = -\hat{c}_k \\ [\hat{n}_k, \hat{c}_k] = -\hat{c}_k \end{cases}$$

Notice that these operators are thus very similar to raising and lowering operators for the simple harmonic oscillator.

Furthermore, we can define the operator $\hat{N} = \sum_k \hat{n}_k$ which is called the **total number operator**. It acts as:

$$\hat{N}|n_1, n_2, \dots\rangle = \sum_{k=1}^{\infty} n_k|n_1, n_2, \dots\rangle.$$

So $\hat{N}$ counts the number of occupied states.

2 Representation of Operators

2.1 One-Electron Operators

Consider the one electron operators $\hat{O}_1$ given by:

$$\langle l\sigma|\hat{O}|l'\sigma'\rangle = \int dr_1\, \psi_l(\vec{r}_1)\chi_\sigma^\dagger\hat{O}(\vec{r})_{\sigma\sigma'}\chi_{\sigma'}\psi_{l'}(\vec{r}_1)$$

where l labels spatial wave functions, σ labels spin wave functions. We thus see that:

$$\hat{O} \iff \sum_{l\sigma l'\sigma'} \langle l\sigma|\hat{O}|l'\sigma'\rangle \hat{c}_{l\sigma}^\dagger\hat{c}_{l'\sigma'}$$

Let us consider an example.

Example: Consider the momentum operator $\hat{\vec{p}} = -i\hbar\vec{\nabla}$ and suppose that the states are plane waves $\frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{r}}\chi_\sigma = \phi_{k\sigma}$. Then we have:

$$\langle\phi_{k\sigma}|\hat{\vec{p}}|\phi_{k'\sigma'}\rangle = \frac{1}{V}\int dr\, e^{-i\vec{k}\cdot\vec{r}}\chi^\dagger_\sigma\left(-i\hbar\vec{\nabla}\right)\chi_{\sigma'}e^{i\vec{k}'\cdot\vec{r}} = \delta_{\sigma\sigma'}\hbar\vec{k}\delta(\vec{k}-\vec{k}')$$

As a result, we have:

$$\hat{\vec{p}} \iff \sum_{k\sigma k'\sigma'}\delta_{\sigma\sigma'}\delta_{kk'}\hbar\vec{k}\hat{c}^\dagger_{k\sigma}\hat{c}_{k'\sigma'} = \sum_{k\sigma}\hbar\vec{k}\hat{c}^\dagger_{k\sigma}\hat{c}_{k'\sigma'} = \sum_{k\sigma}\hbar\vec{k}\hat{n}_{k\sigma}$$

2.2 Spin Operators

Recall our familiar spin operators in matrix form. We can equivalently represent them as in our second quantization notation. As a example, take $\hat{S}_z$, $\hat{S}_+$, and $\hat{S}_-$:

$$\hat{S}_z = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \iff \frac{1}{2}\sum_\ell\left(\hat{c}^\dagger_{\ell\uparrow}\hat{c}_{\ell\uparrow} - \hat{c}^\dagger_{\ell\downarrow}\hat{c}_{\ell\downarrow}\right) = \frac{1}{2}\sum_\ell\left(\hat{n}_{\ell\uparrow} - \hat{n}_{\ell\downarrow}\right)$$

$$\hat{S}_+ = \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix} \iff \sum_\ell \hat{c}^\dagger_{\ell\uparrow}\hat{c}_{\ell\downarrow}$$

$$\hat{S}_- = \begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix} \iff \sum_\ell \hat{c}^\dagger_{\ell\downarrow}\hat{c}_{\ell\uparrow}$$

2.3 Two-Particle Operators

Above we consider one-particle operators, but what about two particle operators of the form:

$$\hat{O}_2 = \frac{e^2}{r_{ij}} = \frac{e^2}{|\vec{r}_i - \vec{r}_j|}.$$

We can express them as:

$$\sum_{l_1l_2l_3l_4}\sum_{\sigma_1\sigma_2\sigma_3\sigma_4}\langle l_1\sigma_1, l_2\sigma_2|\hat{O}_2|l_3\sigma_3, l_4\sigma_4\rangle\hat{c}^\dagger_{l_1\sigma_1}\hat{c}^\dagger_{l_2\sigma_2}\hat{c}_{l_3\sigma_3}\hat{c}_{l_4\sigma_4}$$

where 1 and 4 correspond to $\vec{r}_1$, 2 and 3 to $\vec{r}_2$. Furthermore:

$$\langle l_1\sigma_1, l_2\sigma_2|\hat{O}_2|l_3\sigma_3, l_4\sigma_4\rangle = \int d\vec{r}_1\int d\vec{r}_2\,\phi^*_{l_1\sigma_1}(\vec{r}_1)\phi^*_{l_2\sigma_2}(\vec{r}_2)\hat{O}_2(\vec{r}_1,\vec{r}_2)\phi_{l_3\sigma_3}(\vec{r}_2)\phi_{l_4\sigma_4}(\vec{r}_1)$$

Again, let us consider an example for clarity.
Example: Consider the two particle isotropic interaction given by the operator $\hat{O}_2 = V(|\vec{r}_1 - \vec{r}_2|)$. We can evaluate in a plane-wave basis by:

$$\begin{aligned}\langle\phi_{k_1\sigma_1}\phi_{k_2\sigma_2}|V(|\vec{r}_1-\vec{r}_2|)|\phi_{k_3\sigma_3}\phi_{k_4\sigma_4}\rangle &= \frac{1}{V^2}\langle\sigma_1\sigma_4|\sigma_2\sigma_3\rangle\int e^{-i(\vec{k}_1\cdot\vec{r}_1+\vec{k}_2\cdot\vec{r}_2)}V(|\vec{r}_1-\vec{r}_2|)e^{i(\vec{k}_3\cdot\vec{r}_2+\vec{k}_4\cdot\vec{r}_1)}d^3r_1d^3r_2\\ &= \frac{1}{V^2}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}\int e^{-i(\vec{k}_1-\vec{k}_4)\cdot\vec{r}_1}e^{-i(\vec{k}_2-\vec{k}_3)\cdot\vec{r}_2}V(|\vec{r}_1-\vec{r}_2|)d^3r_1d^3r_2\end{aligned}$$

Now let $\vec{R} = \frac{\vec{r}_1 + \vec{r}_2}{2}$ and $\vec{r} = \vec{r}_1 - \vec{r}_2$. We get:

$$
\begin{aligned}
&= \frac{1}{V^2}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}\int e^{-i(\vec{k}_1+\vec{k}_2-\vec{k}_3-\vec{k}_4)\cdot\vec{R}}e^{-i(\vec{k}_1-\vec{k}_3)\cdot\vec{r}/2}e^{i(\vec{k}_2-\vec{k}_4)\cdot\vec{r}/2}U(r)\,dR\,dr \\
&= \frac{1}{V}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}\int e^{-i(\vec{k}_1-\vec{k}_4)\cdot\vec{r}}U(r)\,dr\,\delta(\vec{k}_1+\vec{k}_2-\vec{k}_3-\vec{k}_4) \\
&= \frac{1}{V}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}\delta(\vec{k}_1+\vec{k}_2-\vec{k}_3-\vec{k}_4)V_{FT}(\vec{k}_1-\vec{k}_4)
\end{aligned}
$$

where we set $U(r) = \frac{e^2}{r}$ and $V_{FT}(\vec{k}_1 - \vec{k}_4) = \frac{4\pi e^2}{|\vec{k}_1-\vec{k}_4|^2}\frac{1}{V}$. As a result, we find the **Coulomb operator** to be:

$$
\frac{1}{2}\sum_{kk'}\sum_{\sigma\sigma'}\frac{4\pi e^2}{q^2 V}\hat{c}^\dagger_{k+q\sigma}\hat{c}^\dagger_{k'-q\sigma'}\hat{c}_{k'\sigma'}\hat{c}_{k\sigma}
$$

where the $\frac{1}{2}$ avoids double counting.

This method of dealing with creation and annihilation operators is called **second quantization**. As before, we will find working with this operator formalism will make life easier than working with wave functions.