Creation and annihilation operators

Suppose we have a complete set of states
$\{\psi_n(r)\}$ or $\{|n\rangle\}$

Then an n-particle fermionic state can be written as a slater determinant ($\vec{r}_i$ denotes space and spin coordinates)

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

with the sum over all N! permutations P of N objects

This wave function is obviously antisymmetric under the interchange of any two particles.

Notationally, it is painful to deal with Slater determinants. So a new formalism was developed called the <u>occupation number representation</u> where we denote each of the wave functions to be included in the Slater determinant (as a short hand).

$$|1,0,0,\ldots\rangle = \psi_1(\vec{r}_1)$$
$$|0,1,1,0,\ldots\rangle = \frac{1}{\sqrt{2}}\left(\psi_2(\vec{r}_1)\,\psi_3(\vec{r}_2) - \psi_3(\vec{r}_1)\,\psi_2(\vec{r}_2)\right)$$

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

$$c_k^\dagger |n_1, n_2, \ldots, n_k, \ldots\rangle = |n_1, n_2, \ldots, n_k+1, \ldots\rangle$$
creates the state k

$$c_k |n_1, n_2, \ldots, n_k, \ldots\rangle = |n_1, n_2, \ldots, n_k-1, \ldots\rangle$$
destroys the state k

The Pauli exclusion principle says $n_k = 0$ or 1 only so

$$(c_k^\dagger)^2 = (c_k)^2 = 0$$

Define the vacuum state as $|0\rangle = |0, 0, 0, \ldots\rangle$

$$c_k^\dagger |0\rangle = \psi_k(\vec{r}_1)$$
$$c_{k'}^\dagger c_k^\dagger |0\rangle = \tfrac{1}{\sqrt{2}}\left(\psi_k(\vec{r}_1)\psi_{k'}(\vec{r}_2) - \psi_{k'}(\vec{r}_1)\psi_k(\vec{r}_2)\right)$$

but

$$c_k^\dagger c_{k'}^\dagger |0\rangle = \tfrac{1}{\sqrt{2}}\left(\psi_{k'}(\vec{r}_1)\psi_k(\vec{r}_2) - \psi_k(\vec{r}_1)\psi_{k'}(\vec{r}_2)\right)$$

$$\Rightarrow \quad c_{k'}^\dagger c_k^\dagger + c_k^\dagger c_{k'}^\dagger = 0 \qquad (c_{k'}^\dagger, c_k^\dagger)_+ = 0$$

In general we get the following anticommutation relations

$$(c_k^\dagger, c_{k'}^\dagger)_+ = 0 \quad (c_k, c_{k'})_+ = 0 \quad (c_k^\dagger, c_{k'})_+ = \delta_{kk'}$$

$$c_k^\dagger |0_k\rangle = |1_k\rangle \qquad c_k^\dagger |1_k\rangle = 0$$
$$c_k |0_k\rangle = 0 \qquad c_k |1_k\rangle = |0_k\rangle$$

so $c_k^\dagger c_k |0_k\rangle = 0 \qquad c_k^\dagger c_k |1_k\rangle = 1 \cdot |1_k\rangle$

$c_k^\dagger c_k$ counts the occupation number of state k

Define $\hat{n}_k = c_k^\dagger c_k$, Then

$$[\hat{n}_k, c_k^\dagger]_- = c_k^\dagger c_k c_k^\dagger - c_k^\dagger \cancel{c_k^\dagger} c_k$$
$$= c_k^\dagger (c_k, c_k^\dagger)_+ = c_k^\dagger$$

$$\boxed{[\hat{n}_k, c_k^\dagger]_- = c_k^\dagger}$$

$$[n_k, c_k]_- = c_k^\dagger \cancel{c_k} c_k - c_k c_k^\dagger c_k$$
$$= -c_k (c_k^\dagger, c_k)_+ = -c_k$$

$$\boxed{[\hat{n}_k, c_k]_- = -c_k}$$

Very similar to raising and lowering operators for the simple-harmonic oscillator.

The operator $\hat{N} = \sum_k \hat{n}_k$ = total number operator

$$\hat{N} |n_1, n_2, \cdots\rangle = \sum_{k=1}^{\infty} n_k |n_1, n_2, n_3, \cdots\rangle$$

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

Representation of operators

one electron operators $\hat{O}_1$

$$\langle l\sigma | \hat{O} | l'\sigma' \rangle = \int dr_1\, \psi_l(\vec{r}_1)\, \chi_\sigma^+\, \hat{O}(r_1)_{\sigma\sigma'}\, \chi_{\sigma'}\, \psi_{l'}(\vec{r}_1)$$

$$\hat{O} \Leftrightarrow \sum_{l\sigma l'\sigma'} \langle l\sigma | \hat{O} | l'\sigma' \rangle\, c^+_{l\sigma}\, c_{l'\sigma'}$$

l labels spatial wave function

σ labels spin wave function

example: momentum operator

$\vec{p} = -i\hbar\vec{\nabla}$ suppose states are plane waves

$$\frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} \chi_\sigma = \phi_{k\sigma}$$

$$(\phi_{k\sigma} | \hat{\vec{p}} | \phi_{k'\sigma'}) = \frac{1}{V} \int dr\, e^{-ik\cdot r}\, \chi_\sigma^+ (-i\hbar\nabla)\, \chi_{\sigma'} e^{ik'\cdot r}$$

$$= \delta_{\sigma\sigma'}\, \hbar k\, \delta(k-k')$$

$$\vec{p} \Leftrightarrow \sum_{\substack{kk'\\ \sigma\sigma'}} \delta_{\sigma\sigma'}\, \delta_{kk'}\, \hbar\vec{k}\, c^+_{k\sigma} c_{k'\sigma'} = \sum_{k\sigma} \hbar\vec{k}\, c^+_{k\sigma} c_{k\sigma}$$

$$= \sum_{k\sigma} \hbar\vec{k}\, \hat{n}_{k\sigma}$$

spin operators

$$S_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \Leftrightarrow \sum_l \frac{1}{2}\left(c^+_{l\uparrow} c_{l\uparrow} - c^+_{l\downarrow} c_{l\downarrow}\right) = \frac{1}{2}\sum_l \left(\hat{n}_{l\uparrow} - \hat{n}_{l\downarrow}\right)$$

$$S_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \Leftrightarrow \sum_l c^+_{l\uparrow} c_{l\downarrow} \qquad S_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \Leftrightarrow \sum_l c^+_{l\downarrow} c_{l\uparrow}$$

~~On the homework~~

two particle operators

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

$$\Rightarrow \sum_{\substack{l_1 l_2 l_3 l_4 \\ \sigma_1\sigma_2\sigma_3\sigma_4}} \langle l_1\sigma_1\, l_2\sigma_2 | \hat{O}_2 | l_3\sigma_3\, l_4\sigma_4 \rangle$$

$$* \; c^\dagger_{l_1\sigma_1} c^\dagger_{l_2\sigma_2} c_{l_3\sigma_3} c_{l_4\sigma_4}$$

1 and 4 correspond to $\vec{r}_1$ 2 and 3 to $\vec{r}_2$

$$\langle l_1\sigma_1\, l_2\sigma_2 | \hat{O}_2 | l_3\sigma_3\, l_4\sigma_4 \rangle = \int dr_1 \int dr_2$$

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

example $\hat{O}_2 = V(|r_1 - r_2|)$ = two particle isotropic interaction

evaluate in a plane-wave basis

$$\langle \phi_{k_1\sigma_1}\, \phi_{k_2\sigma_2} | V(|r_1-r_2|) | \phi_{k_3\sigma_3}\, \phi_{k_4\sigma_4} \rangle$$

$$= \frac{1}{V^2} \langle\sigma_1|\sigma_4\rangle \langle\sigma_2|\sigma_3\rangle \int e^{-ik_1\cdot r_1 - ik_2\cdot r_2 + ik_3\cdot r_3 + ik_4\cdot r_4}\, V(|r_1-r_2|)\, dr_1 d$$

$$= \frac{1}{V^2} \delta_{\sigma_1\sigma_4} \delta_{\sigma_2\sigma_3} \int e^{-i(k_1-k_4)\cdot r_1 - i(k_3-k_4)\cdot r_2}\, V(|r_1-r_2|)\, d^3r_1\, d^3r_2$$

let $\vec{r}_1 = \vec{R} + \frac{\vec{r}}{2}$ $\quad \vec{r}_2 = \vec{R} - \frac{\vec{r}}{2}$

$$= \frac{1}{V^2}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}\int e^{-i(k_1+k_2-k_3-k_4)\cdot\vec{R}}\, e^{-i\frac{1}{2}(k_1-k_2+k_3-k_4)\cdot\vec{r}}\, v(r)\, dR\, dr$$

$$= \frac{1}{V}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}\int e^{-i(k_1-k_4)\cdot\vec{r}}\, v(r)\, dr \quad \delta(k_1+k_2-k_3-k_4)$$

$$= \frac{1}{V}\delta_{\sigma_1\sigma_4}\delta_{\sigma_2\sigma_3}\,\delta(k_1+k_2-k_3-k_4)\; V_{FT}(\vec{k}_1-\vec{k}_4)$$

$$v(r) = \frac{e^2}{r} \qquad V_{FT}(k_1-k_4) = \frac{4\pi e^2}{|k_1-k_4|^2}\frac{1}{V}$$

So we find the Coulomb operator is

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

avoids double counting

This method of dealing with creation and annihilation operators is called

<u>second quantization</u>

As before, we will find working with this operator formalism will make life easier than working with wave functions.