Phy 981 Assignment 3

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Exercise 5

(a) (TO DO)

(b) The normalization integral is:

$$
\begin{aligned}
\langle \Phi_0 | \Phi_0 \rangle &= \prod_{i=1}^{n} \prod_{j=1}^{n} \left\langle 0 \middle| a_{\alpha_i} a^\dagger_{\alpha_j} \middle| 0 \right\rangle \\
&= \prod_{i=1}^{n} \prod_{j=1}^{n} \left[\cancelto{0}{\left\langle 0 \middle| \left\{ a_{\alpha_i} a^\dagger_{\alpha_j} \right\} \middle| 0 \right\rangle} + \left\langle 0 \middle| \left\{ a_{\alpha_i} a^\dagger_{\alpha_j} \right\} \middle| 0 \right\rangle \right] \\
&= \prod_{i=1}^{n} \prod_{j=1}^{n} \delta_{ij} = \delta_{ij}
\end{aligned}
$$

Exercise 6

For the one-body matrix element, use Wick's theorem:

$$
\left\langle \alpha_1 \alpha_2 \middle| \hat{F} \middle| \alpha_1 \alpha_2 \right\rangle = \sum_{\alpha\beta} \langle \alpha | f | \beta \rangle \left\langle 0 \middle| a_{\alpha_2} a_{\alpha_1} a^\dagger_{\alpha} a_\beta a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \middle| 0 \right\rangle .
$$

To keep things simple, I'll organize the contractions in a table:

$a_{\alpha_2} a_{\alpha_1} a^\dagger_{\alpha} a_\beta a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}$	$-\delta_{\alpha_1\alpha_2}\delta_{\alpha\alpha_1}\delta_{\beta\alpha_2}$
$a_{\alpha_2} a_{\alpha_1} a^\dagger_{\alpha} a_\beta a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}$	$\delta_{\alpha\alpha_2}\delta_{\beta\alpha_2}$
$a_{\alpha_2} a_{\alpha_1} a^\dagger_{\alpha} a_\beta a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}$	$\delta_{\alpha\alpha_1}\delta_{\beta\alpha_1}$
$a_{\alpha_2} a_{\alpha_1} a^\dagger_{\alpha} a_\beta a^\dagger_{\alpha_1} a^\dagger_{\alpha_2}$	$-\delta_{\alpha_1\alpha_2}\delta_{\alpha\alpha_2}\delta_{\beta\alpha_1}$

Since $\alpha_1 \neq \alpha_2$, only the second and third terms are nonzero. Thus,

$$
\boxed{\left\langle \alpha_1 \alpha_2 \middle| \hat{F} \middle| \alpha_1 \alpha_2 \right\rangle = \left\langle \alpha_1 \middle| \hat{f} \middle| \alpha_2 \right\rangle + \left\langle \alpha_2 \middle| \hat{f} \middle| \alpha_2 \right\rangle} \tag{1}
$$

just as in the previous exercises.

For the two-body operator,

$$\left\langle \alpha_1\alpha_2 \middle| \hat{G} \middle| \alpha_1\alpha_2 \right\rangle = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta|g|\gamma\delta\rangle \left\langle 0 \middle| a_{\alpha_2} a_{\alpha_1} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \middle| 0 \right\rangle .$$

The nonzero contractions are:

$$\begin{array}{c|c}
a_{\alpha_2} a_{\alpha_1} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger & \delta_{\alpha\alpha_2}\delta_{\beta\alpha_1}\delta_{\gamma\alpha_2}\delta_{\delta\alpha_1} \\
a_{\alpha_2} a_{\alpha_1} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger & -\delta_{\alpha\alpha_2}\delta_{\beta\alpha_1}\delta_{\gamma\alpha_1}\delta_{\delta\alpha_2} \\
a_{\alpha_2} a_{\alpha_1} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger & -\delta_{\alpha\alpha_1}\delta_{\beta\alpha_2}\delta_{\gamma\alpha_2}\delta_{\delta\alpha_1} \\
a_{\alpha_2} a_{\alpha_1} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger & \delta_{\alpha\alpha_1}\delta_{\beta\alpha_2}\delta_{\gamma\alpha_1}\delta_{\delta\alpha_2}
\end{array}$$

This means that

$$\begin{aligned}\left\langle \alpha_1\alpha_2 \middle| \hat{G} \middle| \alpha_1\alpha_2 \right\rangle = \frac{1}{4} \{ &\langle \alpha_2\alpha_1|g|\alpha_2\alpha_1\rangle - \langle \alpha_2\alpha_1|g|\alpha_1\alpha_2\rangle \\ &- \langle \alpha_1\alpha_2|g|\alpha_2\alpha_1\rangle + \langle \alpha_1\alpha_2|g|\alpha_1\alpha_2\rangle \}\end{aligned}$$

Using the symmetries of the antisymmetrized matrix elements, this reduces to

$$\boxed{\left\langle \alpha_1\alpha_2 \middle| \hat{G} \middle| \alpha_1\alpha_2 \right\rangle = \langle \alpha_1\alpha_2|g|\alpha_1\alpha_2\rangle_{\mathrm{AS}}} \tag{2}$$

which is the same result as we found last week.

Exercise 7

This form of the one-body part of the Hamiltonian can be found using Wick's theorem.

$$\begin{aligned}
\hat{H}_0 &= \sum_{pq} \langle p|h_0|q\rangle\, a_p^\dagger a_q \\
&= \sum_{pq} \langle p|h_0|q\rangle \left[\left\{ a_p^\dagger a_q \right\} + \left\{ a_p^\dagger a_q \right\} \right] \\
&= \sum_{pq} \langle p|h_0|q\rangle \left[\left\{ a_p^\dagger a_q \right\} + \delta_{pq\in i} \right] \\
&= \sum_{pq} \langle p|h_0|q\rangle \left\{ a_p^\dagger a_q \right\} + \sum_i \langle i|h_0|i\rangle
\end{aligned}$$

Here, p and q represent general one-particle states, and i represents a hole state inside the closed shell. The symbol $\delta_{pq\in i}$ is defined as follows:

$$\delta_{pq\in i} = \begin{cases} 1 & \text{if } p = q \text{ and } p, q \le F \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

In this situation, the reference vacuum is a some closed-core shell that is relevant to the problem at hand.

Exercise 8

We can use the same method as above for the two-body operator, but the calculation is a bit more complicated.

$$\hat{H}_I = \frac{1}{4} \sum_{pqrs} \langle pq|v|rs\rangle \, a_p^\dagger a_q^\dagger a_s a_r$$

To use Wick's theorem, we'll need all of the possible contractions. I'll list them in the table below along with their associated terms (neglecting the 1/4).

$a_p^\dagger a_q^\dagger a_s a_r$	$\delta_{qs\in i}$	$+ \langle pi|v|ri\rangle \, a_p^\dagger a_r$
$a_p^\dagger a_q^\dagger a_s a_r$	$\delta_{pr\in i}$	$+ \langle iq|v|is\rangle \, a_q^\dagger a_s$
$a_p^\dagger a_q^\dagger a_s a_r$	$-\delta_{qr\in i}$	$- \langle pi|v|is\rangle \, a_p^\dagger a_s$
$a_p^\dagger a_q^\dagger a_s a_r$	$-\delta_{ps\in i}$	$- \langle iq|v|ri\rangle \, a_q^\dagger a_r$
$a_p^\dagger a_q^\dagger a_s a_r$	$\delta_{pr\in i}\delta_{qs\in j}$	$+ \langle ij|v|ij\rangle$
$a_p^\dagger a_q^\dagger a_s a_r$	$-\delta_{ps\in i}\delta_{qr\in j}$	$- \langle ij|v|ji\rangle$

The first four terms in the table can be combined by using the symmetry of the antisymmetric matrix element and the fact that the labels p, q, r, s are arbitrary. The last two terms can also be combined using symmetry. These combine with the uncontracted term to give the final answer:

$$\boxed{\hat{H}_I = \frac{1}{4} \sum_{pqrs} \langle pq|v|rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \sum_{pqi} \langle pi|v|qi\rangle \left\{a_p^\dagger a_q\right\} + \frac{1}{2} \sum_{ij} \langle ij|v|ij\rangle} \tag{4}$$

Here, p, q, r, s are general one-particle states, i, j represent hole states below the Fermi level, and $\delta_{pq\in i}$ is defined as above in (3).