Phy 981 Assignment 3

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Exercise 5

(a) Using bra-ket notation, the transformation can be written as follows:

$$|\psi_a\rangle = \sum_\lambda C_{a\lambda} |\phi_\lambda\rangle \tag{1}$$

This makes the orthogonality integral easy to compute.

$$\begin{aligned}
\langle\psi_b|\psi_a\rangle &= \sum_{\lambda\nu} C_{a\lambda} C^*_{\nu b} \langle\phi_\nu|\phi_\lambda\rangle \\
&= \sum_{\lambda\nu} C_{a\lambda} C^*_{\nu b} \delta_{\lambda\nu} \\
&= \sum_{\lambda} C_{a\lambda} C^*_{\lambda b} \\
&= (\mathbf{C}\mathbf{C}^*)_{ab} = \delta_{ab}
\end{aligned}$$

The last step follows from the unitarity of the matrix $\mathbf{C}$. This proves that the new basis is orthonormal.

Equation (1) shows the transformation for one basis wavefunction. This can be extended intuitively to a one-dimensional vector of wavefunctions,

$$\begin{pmatrix} \psi_a \\ \psi_b \\ \vdots \\ \psi_A \end{pmatrix} = \begin{pmatrix} C_{a\lambda} & C_{a\mu} & \dots & C_{aA} \\ C_{b\lambda} & C_{b\mu} & \dots & C_{bA} \\ \vdots & \vdots & \ddots & \vdots \\ C_{A\lambda} & C_{A\mu} & \dots & C_{AA} \end{pmatrix} \begin{pmatrix} \phi_\lambda \\ \phi_\mu \\ \vdots \\ \phi_A \end{pmatrix}. \tag{2}$$

Importantly, note that the wavefunctions $\{\phi_a, \phi_b, \dots\}$ above really mean $\{\phi_a(x_1), \phi_b(x_1), \dots\}$. This implies that if we vary the argument x_i to the wavefunctions, we can extend (2) to two dimensions:

$$\begin{pmatrix} \psi_a(x_1) & \psi_a(x_2) & \dots & \psi_a(x_A) \\ \psi_b(x_1) & \psi_b(x_2) & \dots & \psi_b(x_A) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_A(x_1) & \psi_A(x_2) & \dots & \psi_A(x_A) \end{pmatrix} = \begin{pmatrix} C_{a\lambda} & C_{a\mu} & \dots & C_{aA} \\ C_{b\lambda} & C_{b\mu} & \dots & C_{bA} \\ \vdots & \vdots & \ddots & \vdots \\ C_{A\lambda} & C_{A\mu} & \dots & C_{AA} \end{pmatrix} \begin{pmatrix} \phi_\lambda(x_1) & \phi_\lambda(x_2) & \dots & \phi_\lambda(x_A) \\ \phi_\mu(x_1) & \phi_\mu(x_2) & \dots & \phi_\mu(x_A) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_A(x_1) & \phi_A(x_2) & \dots & \phi_A(x_A) \end{pmatrix} \tag{3}$$

The rules of matrix multiplication ensure that we will get the same result for each of the column vectors as we would in (2).

Now, for brevity, let (3) be written as

$$\mathbf{\Psi} = \mathbf{C}\mathbf{\Phi}. \tag{4}$$

The matrices $\mathbf{\Psi}$ and $\mathbf{\Phi}$ are exactly the same as the matrices we would use to find the Slater determinants in the new and old bases, respectively. Thus,

$$|\Psi\rangle = \det(\mathbf{\Psi}) = \det(\mathbf{C}\mathbf{\Phi}) = \det(\mathbf{C})\det(\mathbf{\Phi}) = \det(\mathbf{C})\,|\Phi\rangle$$

The second-to-last step above is valid because $\mathbf{C}$ and $\mathbf{\Phi}$ are square matrices. Therefore, the Slater determinant in the new basis is equal to the determinant in the old basis times the determinant of the transformation matrix.

Finally, since $\mathbf{C}$ is a unitary matrix, $|\det(\mathbf{C})| = 1$ by definition. Therefore, the two Slater determinants are equal up to a phase.

(b) The normalization integral is:

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

Exercise 6

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

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

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

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

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

$$
\boxed{\langle \alpha_1 \alpha_2 | \hat{F} | \alpha_1 \alpha_2 \rangle = \langle \alpha_1 | \hat{f} | \alpha_2 \rangle + \langle \alpha_2 | \hat{f} | \alpha_2 \rangle} \tag{5}
$$

just as in the previous exercises.

For the two-body operator,

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

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

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

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

$$
\boxed{\langle \alpha_1 \alpha_2 | \hat{G} | \alpha_1 \alpha_2 \rangle = \langle \alpha_1 \alpha_2 | g | \alpha_1 \alpha_2 \rangle_{\mathrm{AS}}} \tag{6}
$$

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:

$$\delta_{pq\in i} = \begin{cases} 1 & \text{if } p = q \text{ and } p, q \leq F \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

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:

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

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 (7).