# Phy 981 Assignment 2

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## Exercise 3

(a) For $N = 3$, $\Phi^{\mathrm{AS}}$ is

$$\Phi_\lambda^{\mathrm{AS}} = \frac{1}{\sqrt{3!}} \sum_p (-)^p \hat{P}\, \psi_{\alpha_1}(x_1)\, \psi_{\alpha_2}(x_2)\, \psi_{\alpha_3}(x_3)$$

$$\begin{aligned}\Phi_\lambda^{\mathrm{AS}} = \frac{1}{\sqrt{6}} [&\psi_{\alpha_1}(x_1)\, \psi_{\alpha_2}(x_2)\, \psi_{\alpha_3}(x_3) - \psi_{\alpha_1}(x_2)\, \psi_{\alpha_2}(x_1)\, \psi_{\alpha_3}(x_3) \\ &- \psi_{\alpha_1}(x_3)\, \psi_{\alpha_2}(x_2)\, \psi_{\alpha_3}(x_1) - \psi_{\alpha_1}(x_1)\, \psi_{\alpha_2}(x_3)\, \psi_{\alpha_3}(x_2) \\ &+ \psi_{\alpha_1}(x_3)\, \psi_{\alpha_2}(x_1)\, \psi_{\alpha_3}(x_2) + \psi_{\alpha_1}(x_2)\, \psi_{\alpha_2}(x_3)\, \psi_{\alpha_3}(x_1)]\end{aligned}$$

(b) The integral can be written out as

$$\int dx_1 \dots dx_N \frac{1}{N!} \left[ \sum_p (-)^p \hat{P} \prod_{i=1}^N \psi^*_{\alpha_i}(x_i) \right] \left[ \sum_p (-)^p \hat{P} \prod_{i=1}^N \psi_{\alpha_i}(x_i) \right].$$

However, since the basis functions $\psi_{\alpha_i}(x_i)$ are orthogonal, the only terms that will survive the integration are those with corresponding permutations from each sum. In other words, the integral can be written as

$$\frac{1}{N!} \int dx_1 \dots dx_N \sum_p (-)^{2p} \hat{P} \prod_{i=1}^N \psi^*_{\alpha_i}(x_i)\, \psi_{\alpha_i}(x_i)\,.$$

Now, using the normality of the basis functions, this can be rewritten as follows:

$$\begin{aligned}&\frac{1}{N!} \sum_p \int dx_1 \dots dx_N\, \hat{P} \prod_{i=1}^N \psi^*_{\alpha_i}(x_i)\, \psi_{\alpha_i}(x_i) \\ &\quad = \frac{1}{N!} \sum_p \prod_{i=1}^N \int dx_i\, \psi^*_{\alpha_i}(x_i)\, \psi_{\alpha_i}(x_i) \\ &\quad\quad = \frac{1}{N!} \sum_p (1) = \frac{N!}{N!} = 1\end{aligned}$$

(c) For the one-body operator $\hat{F} = \hat{f}(x_1) + \hat{f}(x_2)$,

$$\begin{aligned}
&\left\langle \Phi^{AS}_{\alpha_1\alpha_2} \middle| \hat{f}(x_1) + \hat{f}(x_2) \middle| \Phi^{AS}_{\alpha_1\alpha_2} \right\rangle \\
&= \frac{1}{2} \int dx_1\, dx_2\ \left[\psi^*_{\alpha_1}(x_1)\,\psi^*_{\alpha_2}(x_2) - \psi^*_{\alpha_2}(x_1)\,\psi^*_{\alpha_1}(x_2)\right] \left(\hat{f}(x_1) + \hat{f}(x_2)\right) \\
&\qquad \times \left[\psi_{\alpha_1}(x_1)\,\psi_{\alpha_2}(x_2) - \psi_{\alpha_2}(x_1)\,\psi_{\alpha_1}(x_2)\right].
\end{aligned}$$

Since the functions $\psi_{\alpha_i}$ are orthogonal, the cross terms drop out. Thus, the above becomes

$$\begin{aligned}
&\frac{1}{2}\left\{ \int dx_1\, dx_2\ \left[\psi^*_{\alpha_1}(x_1)\,\psi^*_{\alpha_2}(x_2)\right] \left(\hat{f}(x_1) + \hat{f}(x_2)\right) \left[\psi_{\alpha_1}(x_1)\,\psi_{\alpha_2}(x_2)\right] \right. \\
&\quad \left. + \int dx_1\, dx_2\ \left[\psi^*_{\alpha_2}(x_1)\,\psi^*_{\alpha_1}(x_2)\right] \left(\hat{f}(x_1) + \hat{f}(x_2)\right) \left[\psi_{\alpha_2}(x_1)\,\psi_{\alpha_1}(x_2)\right] \right\}.
\end{aligned}$$

However, since $x_1$ and $x_2$ are arbitrary bound variables, we can just switch them in the second term and find

$$\begin{aligned}
&\frac{1}{2}\left\{ 2 \int dx_1\, dx_2\ \left[\psi^*_{\alpha_1}(x_1)\,\psi^*_{\alpha_2}(x_2)\right] \left(\hat{f}(x_1) + \hat{f}(x_2)\right) \left[\psi_{\alpha_1}(x_1)\,\psi_{\alpha_2}(x_2)\right] \right\} \\
&\qquad = \boxed{\left\langle \alpha_1\alpha_2 \middle| \hat{f}(x_1) \middle| \alpha_1\alpha_2 \right\rangle + \left\langle \alpha_1\alpha_2 \middle| \hat{f}(x_2) \middle| \alpha_1\alpha_2 \right\rangle}
\end{aligned}$$

The calculation is similar for the two-body operator. This time,

$$\hat{G} = \sum_{i>j}^{N} \hat{g}(x_i, x_j) = \hat{g}(x_1, x_2)$$

since $\hat{g}$ is invariant under an exchange of $x_1$ and $x_2$. Then,

$$\begin{aligned}
&\left\langle \Phi^{AS}_{\alpha_1\alpha_2} \middle| \hat{g}(x_1, x_2) \middle| \Phi^{AS}_{\alpha_1\alpha_2} \right\rangle \\
&= \frac{1}{2} \int dx_1\, dx_2\ \left[\psi^*_{\alpha_1}(x_1)\,\psi^*_{\alpha_2}(x_2) - \psi^*_{\alpha_2}(x_1)\,\psi^*_{\alpha_1}(x_2)\right] \hat{g}(x_1, x_2) \\
&\qquad \times \left[\psi_{\alpha_1}(x_1)\,\psi_{\alpha_2}(x_2) - \psi_{\alpha_2}(x_1)\,\psi_{\alpha_1}(x_2)\right] \\
&= \frac{1}{2} \int dx_1\, dx_2\ \psi^*_{\alpha_1}(x_1)\,\psi^*_{\alpha_2}(x_2)\,\hat{g}(x_1, x_2)\psi_{\alpha_1}(x_1)\,\psi_{\alpha_2}(x_2) \\
&\quad + \frac{1}{2} \int dx_1\, dx_2\ \psi^*_{\alpha_2}(x_1)\,\psi^*_{\alpha_1}(x_2)\,\hat{g}(x_1, x_2)\psi_{\alpha_2}(x_1)\,\psi_{\alpha_1}(x_2) \\
&\quad - \frac{1}{2} \int dx_1\, dx_2\ \psi^*_{\alpha_1}(x_1)\,\psi^*_{\alpha_2}(x_2)\,\hat{g}(x_1, x_2)\psi_{\alpha_2}(x_1)\,\psi_{\alpha_1}(x_2) \\
&\quad - \frac{1}{2} \int dx_1\, dx_2\ \psi^*_{\alpha_2}(x_1)\,\psi^*_{\alpha_1}(x_2)\,\hat{g}(x_1, x_2)\psi_{\alpha_1}(x_1)\,\psi_{\alpha_2}(x_2).
\end{aligned}$$

Using the same trick of swapping the indices as above, this becomes

$$\begin{aligned}
&\int dx_1\, dx_2\, \psi^*_{\alpha_1}(x_1)\, \psi^*_{\alpha_2}(x_2)\, \hat{g}(x_1, x_2)\psi_{\alpha_1}(x_1)\, \psi_{\alpha_2}(x_2) \\
&- \int dx_1\, dx_2\, \psi^*_{\alpha_1}(x_1)\, \psi^*_{\alpha_2}(x_2)\, \hat{g}(x_1, x_2)\psi_{\alpha_2}(x_1)\, \psi_{\alpha_1}(x_2) \\
&= \langle \alpha_1\alpha_2|\hat{g}(x_1, x_2)|\alpha_1\alpha_2\rangle - \langle \alpha_1\alpha_2|\hat{g}(x_1, x_2)|\alpha_2\alpha_1\rangle \\
&= \boxed{\langle \alpha_1\alpha_2|\hat{g}(x_1, x_2)|\alpha_1\alpha_2\rangle_{\text{AS}}}
\end{aligned}$$

The shorthand notation for the Slater determinant, $\Phi^{AS}_{\alpha_1\alpha_2}$, indicates that the determinant is antisymmetric and is taken over two particles with quantum numbers $\alpha_1$ and $\alpha_2$.

In addition to permutation symmetry, I would expect that the one-body operator will be diagonal in the basis of single-particle states, and the two-body operator will be symmetric to reflect the permutation symmetry.

# Exercise 4

(a) This is a problem of combinatorics. Since the Pauli principle forbids putting more than one particle into a state with a particular $p$ and spin, the number of possible Slater determinants is

$$\binom{6}{2} = \frac{6!}{2!(6-2)!} = \boxed{15.}$$

If we limit ourselves to only states with paired particles, as below, then there would be three possible Slater determinants.

(b) Based on the assumption that the one-body part of the Hamiltonian has the form

$$\hat{h}_0\psi_{p\sigma} = pd\ \psi_{p\sigma}, \tag{1}$$

the matrix elements it produces should be

$$\left\langle \Phi_0 \middle| \hat{H}_0 \middle| \Phi_0 \right\rangle = \sum_i \langle p_i\sigma_i|h_0|p_i\sigma_i\rangle\,. \tag{2}$$

If we assume that both particles must be in the same state $p$, then this can only take values of $2d$ or $4d$, so

$$\hat{H}_0 = \begin{pmatrix} 2d & 0 \\ 0 & 4d \end{pmatrix} \tag{3}$$

The problem states that the two-body part of the Hamiltonian has matrix elements uniformly equal to $-g$. Therefore, the overall Hamiltonian is

$$\hat{H} = \hat{H}_0 + \hat{H}_I = \boxed{\begin{pmatrix} 2d-g & -g \\ -g & 4d-g \end{pmatrix}} \tag{4}$$

Using Mathematica, one can show that this matrix has eigenvalues

$$\lambda_\pm = 3d - g \pm \sqrt{d^2 + g^2} \tag{5}$$

and eigenvectors

$$v_\pm = \begin{pmatrix} \dfrac{d \mp \sqrt{d^2+g^2}}{g} & 1 \end{pmatrix}^T. \tag{6}$$

The state with two particles in $p = 2$ mixes with the state with two particles in $p = 1$ through the off-diagonal elements of the Hamiltonian matrix. Thus,

$$\boxed{\langle 22|H|11\rangle = -g} \tag{7}$$

The eigenvectors of the Hamilton can be interpreted as a linear combination of the Slater determinants for two particles in each of the states $p = 1$ and $p = 2$. Since there is some mixing between these two states (the interaction part of the Hamiltonian), the "true" eigenvectors of the system are a linear combination of the basis states of the non-interacting particles.

(c) Based on the math above, we can write, by inspection,

$$\hat{H} = \begin{pmatrix} 2d-g & -g & -g \\ -g & 4d-g & -g \\ -g & -g & 6d-g \end{pmatrix} \tag{8}$$

for the case with the $p = 3$ state available. There is no closed-form analytic solution to the eigenvalue problem for this matrix, but it can be diagonalized numerically if we choose values for $d$ and $g$. I'll set $d = 1$ and look at two values of $g$:

**Small g:** The case of small $g$ corresponds to weak interactions between the particles. If we set $g = 0.001$, then the matrix is approximately diagonal. The eigenvalues in this case are, to three figures, 2.00, 4.00, and 6.00 (the diagonal of the matrix), and the eigenvectors are

$$\begin{pmatrix} 1.00 \\ 0.00 \\ 0.00 \end{pmatrix}, \begin{pmatrix} 0.00 \\ 1.00 \\ 0.00 \end{pmatrix}, \text{ and } \begin{pmatrix} 0.00 \\ 0.00 \\ 1.00 \end{pmatrix}$$

when taken to the same precision. This is expected since if the particles barely interact, then the single-particle states are a good basis.

**Large g:** If we set $g = 10$, then things are much less clean. This produces eigenvalues of $-26.09$, 5.20, and 2.89, and eigenvectors

$$\begin{pmatrix} -0.616 \\ -0.575 \\ -0.539 \end{pmatrix}, \begin{pmatrix} -0.204 \\ -0.544 \\ 0.814 \end{pmatrix}, \text{ and } \begin{pmatrix} 0.761 \\ -0.611 \\ -0.218 \end{pmatrix}.$$

Unsurprisingly, a strong interaction term produces a strong mixing of the single-particle states.