Homework H18 Solution

1. Show that if $|a\rangle$and $|b\rangle$and orthogonal and normalized (this is called "orthonormal" for short), then

$$\frac{1}{\sqrt{2}}(|a_1\rangle|b_2\rangle - |a_2\rangle|b_1\rangle)$$

is normalized.

Solution:
Note that the subscripts 1 & 2 denote the electron labels.

So, $\psi(1,2) = \frac{1}{\sqrt{2}}(|a_1\rangle|b_2\rangle - |a_2\rangle|b_1\rangle)$

$$P = \langle\psi|\psi\rangle = \frac{1}{2}(\langle a_1|\langle b_2| - \langle a_2|\langle b_1|)(|a_1\rangle|b_2\rangle - |a_2\rangle|b_1\rangle)$$

$$= \frac{1}{2}(\langle a_1|a_1\rangle\langle b_2|b_2\rangle - \langle a_1|b_1\rangle\langle b_2|a_2\rangle - \langle a_2|b_2\rangle\langle b_1|a_1\rangle + \langle a_2\,|a_2\rangle\langle b_1|b_1\rangle)$$

$$= \frac{1}{2}(1+1) = 1$$

Be careful to note that the integral is carried by the "bra" ($\langle\ |$). Hence the integration variable is the co-ordinates of the electron in the bra. Hence, the integral $\langle a_1|a_2\rangle$ is meaningless since you cannot integrate the wavefunction of one electron over the integration variable of another.

2. Worked Problem 7.1.

Solution: See the solution in the book. Recollect that this is similar to what you did with the 3D rigidly rotating molecule, where you separated the Hamiltonian into two parts. Here, similarly, $\hat{H}_1$ acts only on electron "1", and $\hat{H}_2$ acts only on electron "2".

3. Problem 7.1.

Solution:
Consider the two H nuclei designated A & B, and the two electrons 1 & 2. Electron 1 is in atom A, and electron 2 is in atom B. Since the two atoms are non-interacting, there is no repulsion or attraction between electrons and/or nuclei of the two different atoms. Hence, the Hamiltonians for the two atoms can be written separately as,

$$\hat{H}_A = -\frac{\hbar^2}{2m}{\nabla_1}^2 - \frac{e^2}{4\pi\varepsilon_0 r_{1A}}$$

$$\hat{H}_B = -\frac{\hbar^2}{2m}\nabla_2{}^2 - \frac{e^2}{4\pi\varepsilon_0 r_{2B}}$$

and the total Hamiltonian for the system is $\hat{H} = \hat{H}_A + \hat{H}_B$.

Since the Hamiltonian is additively separable, the wavefunction should be product separable.

$$\therefore \psi = \psi_{1s}^{A}(1).\psi_{1s}^{B}(2)$$

4. Problem 7.3.

Solution:

$$\psi(1,2) = \begin{vmatrix} \psi_a(1) & \psi_a(2) \\ \psi_b(1) & \psi_b(2) \end{vmatrix}$$

Lets write the wavefunction for interchanged electrons as,

$$\psi(2,1) = \begin{vmatrix} \psi_a(2) & \psi_a(1) \\ \psi_b(2) & \psi_b(1) \end{vmatrix}$$

$$= \psi_a(2)\psi_b(1) - \psi_b(2)\psi_a(1)$$

$$= -[\psi_a(1)\psi_b(2) - \psi_b(1)\psi_a(2)$$

$$= -\begin{vmatrix} \psi_a(1) & \psi_a(2) \\ \psi_b(1) & \psi_b(2) \end{vmatrix}$$

$$= -\psi(1,2)$$

This shows that the wavefunction represented by Slater determinant is anti-symmetric with respect to electron interchange.