Hartree Fock HW

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June 25, 2015

1. Approximate the many-body wavefunctions of different systems in which the single electrons are under the harmonic oscillator potential. Recall we do this via the Slater determinant:

$$\Psi(\{\boldsymbol{\gamma_i}\}) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(\boldsymbol{\gamma}_1) & \psi_1(\boldsymbol{\gamma}_2) & ... & \psi_1(\boldsymbol{\gamma}_N) \\ \psi_2(\boldsymbol{\gamma}_1) & \psi_2(\boldsymbol{\gamma}_2) & ... & \psi_2(\boldsymbol{\gamma}_N) \\ ... & ... & & ... \\ \psi_N(\boldsymbol{\gamma}_1) & \psi_N(\boldsymbol{\gamma}_2) & ... & \psi_N(\boldsymbol{\gamma}_N) \end{vmatrix} \tag{1}$$

We will assume the space and spin components of the single-body wavefunctions are separable:

$$\psi(\boldsymbol{\gamma}) = \phi(\mathbf{r})\chi(\boldsymbol{\sigma}) \tag{2}$$

(a) Electrons a and b are spin-up and spin-down respectively, both in ground state:

$$\begin{aligned} \Psi(\boldsymbol{\gamma}_a, \boldsymbol{\gamma}_b) &= \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_a(\boldsymbol{\gamma}_a) & \psi_a(\boldsymbol{\gamma}_b) \\ \psi_b(\boldsymbol{\gamma}_a) & \psi_b(\boldsymbol{\gamma}_b) \end{vmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_0(\mathbf{r}_a)\chi_+(\boldsymbol{\sigma}_a) & \phi_0(\mathbf{r}_b)\chi_+(\boldsymbol{\sigma}_b) \\ \phi_0(\mathbf{r}_a)\chi_-(\boldsymbol{\sigma}_a) & \phi_0(\mathbf{r}_b)\chi_-(\boldsymbol{\sigma}_b) \end{vmatrix} \\ &= \frac{1}{\sqrt{2}}\phi_0(\mathbf{r}_a)\phi_0(\mathbf{r}_b)\left[\chi_+(\boldsymbol{\sigma}_a)\chi_-(\boldsymbol{\sigma}_b) - \chi_+(\boldsymbol{\sigma}_b)\chi_-(\boldsymbol{\sigma}_a)\right] \end{aligned} \tag{3}$$

(b) Electrons a and b are in the ground state and first excited state respectively, both spin-up:

$$\begin{aligned} \Psi(\boldsymbol{\gamma}_a, \boldsymbol{\gamma}_b) &= \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_a(\boldsymbol{\gamma}_a) & \psi_a(\boldsymbol{\gamma}_b) \\ \psi_b(\boldsymbol{\gamma}_a) & \psi_b(\boldsymbol{\gamma}_b) \end{vmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_0(\mathbf{r}_a)\chi_+(\boldsymbol{\sigma}_a) & \phi_0(\mathbf{r}_b)\chi_+(\boldsymbol{\sigma}_b) \\ \phi_1(\mathbf{r}_a)\chi_+(\boldsymbol{\sigma}_a) & \phi_1(\mathbf{r}_b)\chi_+(\boldsymbol{\sigma}_b) \end{vmatrix} \\ &= \frac{1}{\sqrt{2}}\chi_+(\boldsymbol{\sigma}_a)\chi_+(\boldsymbol{\sigma}_b)\left[\phi_0(\mathbf{r}_a)\phi_1(\mathbf{r}_b) - \phi_0(\mathbf{r}_b)\phi_1(\mathbf{r}_a)\right] \end{aligned} \tag{4}$$

(c) Electron a is spin-up in the ground state. Electrons b and c are spin-up and spin-down respectively in the first excited state:

$$\begin{aligned} \Psi(\boldsymbol{\gamma}_a, \boldsymbol{\gamma}_b, \boldsymbol{\gamma}_c) &= \frac{1}{\sqrt{6}} \begin{vmatrix} \psi_a(\boldsymbol{\gamma}_a) & \psi_a(\boldsymbol{\gamma}_b) & \psi_a(\boldsymbol{\gamma}_c) \\ \psi_b(\boldsymbol{\gamma}_a) & \psi_b(\boldsymbol{\gamma}_b) & \psi_b(\boldsymbol{\gamma}_c) \\ \psi_c(\boldsymbol{\gamma}_a) & \psi_c(\boldsymbol{\gamma}_b) & \psi_c(\boldsymbol{\gamma}_c) \end{vmatrix} \\ &= \frac{1}{\sqrt{6}} \left[\psi_a(\boldsymbol{\gamma}_a) \begin{vmatrix} \psi_b(\boldsymbol{\gamma}_b) & \psi_b(\boldsymbol{\gamma}_c) \\ \psi_c(\boldsymbol{\gamma}_b) & \psi_c(\boldsymbol{\gamma}_c) \end{vmatrix} - \psi_a(\boldsymbol{\gamma}_b) \begin{vmatrix} \psi_b(\boldsymbol{\gamma}_a) & \psi_b(\boldsymbol{\gamma}_c) \\ \psi_c(\boldsymbol{\gamma}_a) & \psi_c(\boldsymbol{\gamma}_c) \end{vmatrix} + \psi_a(\boldsymbol{\gamma}_c) \begin{vmatrix} \psi_b(\boldsymbol{\gamma}_a) & \psi_b(\boldsymbol{\gamma}_b) \\ \psi_c(\boldsymbol{\gamma}_a) & \psi_c(\boldsymbol{\gamma}_b) \end{vmatrix}\right] \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{\sqrt{6}} \left\{ \phi_0(\mathbf{r}_a)\chi_+(\boldsymbol{\sigma}_a) \begin{vmatrix} \phi_1(\mathbf{r}_b)\chi_+(\boldsymbol{\sigma}_b) & \phi_1(\mathbf{r}_c)\chi_+(\boldsymbol{\sigma}_c) \\ \phi_1(\mathbf{r}_b)\chi_-(\boldsymbol{\sigma}_b) & \phi_1(\mathbf{r}_c)\chi_-(\boldsymbol{\sigma}_c) \end{vmatrix} \right. \\
&\qquad - \phi_0(\mathbf{r}_b)\chi_+(\boldsymbol{\sigma}_b) \begin{vmatrix} \phi_1(\mathbf{r}_a)\chi_+(\boldsymbol{\sigma}_a) & \phi_1(\mathbf{r}_c)\chi_+(\boldsymbol{\sigma}_c) \\ \phi_1(\mathbf{r}_a)\chi_-(\boldsymbol{\sigma}_a) & \phi_1(\mathbf{r}_c)\chi_-(\boldsymbol{\sigma}_c) \end{vmatrix} \\
&\qquad \left. - \phi_0(\mathbf{r}_c)\chi_+(\boldsymbol{\sigma}_c) \begin{vmatrix} \phi_1(\mathbf{r}_a)\chi_+(\boldsymbol{\sigma}_a) & \phi_1(\mathbf{r}_b)\chi_+(\boldsymbol{\sigma}_b) \\ \phi_1(\mathbf{r}_a)\chi_-(\boldsymbol{\sigma}_a) & \phi_1(\mathbf{r}_b)\chi_-(\boldsymbol{\sigma}_b) \end{vmatrix} \right\} \\
&= \frac{1}{\sqrt{6}} \{ \phi_0(\mathbf{r}_a)\phi_1(\mathbf{r}_b)\phi_1(\mathbf{r}_c)\chi_+(\boldsymbol{\sigma}_a) \left[\chi_+(\boldsymbol{\sigma}_b)\chi_-(\boldsymbol{\sigma}_c) - \chi_+(\boldsymbol{\sigma}_c)\chi_-(\boldsymbol{\sigma}_b) \right] \\
&\qquad - \phi_0(\mathbf{r}_b)\phi_1(\mathbf{r}_a)\phi_1(\mathbf{r}_c)\chi_+(\boldsymbol{\sigma}_b) \left[\chi_+(\boldsymbol{\sigma}_a)\chi_-(\boldsymbol{\sigma}_c) - \chi_+(\boldsymbol{\sigma}_c)\chi_-(\boldsymbol{\sigma}_a) \right] \\
&\qquad - \phi_0(\mathbf{r}_c)\phi_1(\mathbf{r}_a)\phi_1(\mathbf{r}_b)\chi_+(\boldsymbol{\sigma}_c) \left[\chi_+(\boldsymbol{\sigma}_a)\chi_-(\boldsymbol{\sigma}_b) - \chi_+(\boldsymbol{\sigma}_a)\chi_-(\boldsymbol{\sigma}_b) \right] \}
\end{aligned} \tag{5}
$$

2. Recall:

$$
\Psi(\{\boldsymbol{\gamma_i}\}) = \frac{1}{\sqrt{N!}} \sum_{k \in \mathbb{K}} \epsilon_k \prod_{j=1}^{N} \psi_{k_j}(\gamma_j) \tag{6}
$$

$$
\begin{aligned}
\langle \Psi(\{\boldsymbol{\gamma_i}\}) | \Psi(\{\boldsymbol{\gamma_i}\}) \rangle &= \frac{1}{N!} \sum_{k \in \mathbb{K}} \sum_{k' \in \mathbb{K}} \int d\boldsymbol{\gamma}_1 ... d\boldsymbol{\gamma}_N \epsilon_k \epsilon_{k'} \prod_{j=1}^{N} \left[\psi^*_{k_j}(\boldsymbol{\gamma}_j) \right] \prod_{j=1}^{N} \left[\psi_{k'_j}(\boldsymbol{\gamma}_j) \right] \\
&= \frac{1}{N!} \sum_{k \in \mathbb{K}} \sum_{k' \in \mathbb{K}} \prod_{i=1}^{N} \left[\int d\boldsymbol{\gamma}_i \psi^*_{k_j}(\boldsymbol{\gamma}_i) \psi_{k'_j}(\boldsymbol{\gamma}_i) \right] \epsilon_k \epsilon_{k'} \\
&= \frac{1}{N!} \sum_{k \in \mathbb{K}} \sum_{k' \in \mathbb{K}} \prod_{i=1}^{N} \left[\delta_{k_i, k'_i} \right] \epsilon_k \epsilon_{k'} \\
&= \frac{1}{N!} \sum_{k \in \mathbb{K}} \epsilon_k \epsilon_k \\
&= \frac{1}{N!} \sum_{k \in \mathbb{K}} 1 \\
&= \frac{1}{N!} N! \\
&= 1
\end{aligned} \tag{7}
$$