Nuclear Structure

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1 Wavefunction for N=3

We can easily calculate the explicit form of our Slater determinant as such:

$$\Phi_\lambda^{AS} = \frac{1}{\sqrt{N!}}\Sigma_p(-1)^p P \Pi_{i=1}^{3}\psi_{\alpha_i}(x_i) \tag{1}$$

This can be found via an actual determinant as such:

$$\Phi_\lambda^{AS} = \frac{1}{\sqrt{3!}}\begin{vmatrix} \psi_1(x_1) & \psi_1(x_2) & \psi_1(x_3) \\ \psi_2(x_1) & \psi_2(x_2) & \psi_2(x_3) \\ \psi_3(x_1) & \psi_3(x_2) & \psi_3(x_3) \end{vmatrix} \tag{2}$$

We then merely take this determenant to find that

$$\begin{gathered}\Phi_\lambda^{AS} = \frac{1}{\sqrt{3!}}(\psi_1(x_1)(\psi_2(x_2)\psi_3(x_3) - \psi_3(x_2)\psi_2(x_3)) + \\ \psi_1(x_2)(\psi_3(x_1)\psi_1(x_3) - \psi_1(x_1)\psi_3(x_3)) + \psi_1(x_3)(\psi_2(x_1)\psi_3(x_2) - \psi_3(x_1)\psi_2(x_2)))\end{gathered} \tag{3}$$

2 Normalization

In order to prove normalization we argue from induction. We note that the case where $N = 1$ is trivial, as it is merely then that $\Phi = \psi$, as $\frac{1}{N!} = 1$ in this case, and so is trivially normalized.

Let us now assume that the previous $N - 1$ Slater deteriminants were normalized properly. We prove that the Nth Slater determinant is also normalized.

So we consider this determinant and show that:

$$\Phi_N = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_N(x_1) & \cdots & \psi_N(x_N) \\ \vdots & \ddots & \vdots \\ \psi_1(x_1) & \cdots & \psi_1(x_N) \end{vmatrix} \tag{4}$$

Now taking this determinant we can sum over the elements of the top row times the determinant of the matrix formed by removing the top row and the ith column, where i is the index of the item of the top row being multiplied. We can then note that this forms a Slater-esque determinant which I denote as χ_i, where we are taking a slater determinant of the matrix of size $N-1$ with the wavefunction $\psi_i(x_i)$ replaced by $\psi_i(x_N)$, and where there is no normalization constant.

We then have that

$$\Phi_N = \frac{1}{\sqrt{N!}}\Sigma_i(-1)^i\psi_N(x_i)\chi_i \tag{5}$$

Now we thus have that in the expansion of $\Phi_N^*\Phi_N$, only those terms involving $\psi_N(x_i)^*\chi_i^*\psi_N(x_i)\chi_i$ will survive, because any other term will involve $\psi_N(x_i)^*\chi_j$ or $\psi_N(x_i)\chi_j^*$. But those terms must therefore contain $\psi_N(x_i)$ and $\psi_k(x_i)$ for $k \neq N$. This is then 0 because each ψ_i is orthonormalized.

We then just have the sum:

$$\Phi_N^*\Phi_N = \Sigma_i\frac{1}{N!}(\psi_N(x_i)^*\chi_i^*\psi_N(x_i)\chi_i) \tag{6}$$

We then note that the $\psi_N(x_i)^*\psi_N(x_i)$ will integrate out to 1 by orthonormality. We then have that

$$\int d\vec{x\Phi}_N^*\Phi_N = \Sigma\frac{1}{N!}\int d\vec{x\chi}_i^*\chi_i \tag{7}$$

We then have that from the assumption that the normalization condition holds, that as the indicies i are arbitrary, it follows that

$$\int d\vec{x\chi}_i^*\chi_i = \int d\vec{x(}N-1)!\Phi_(N-1)^*\Phi_(N-1) = (N-1)! \tag{8}$$

We then have that, noting that there are N indicies being summed over:

$$\int d\vec{x\Phi}_N^*\Phi_N = \Sigma\frac{1}{N!}\int d\vec{x\chi}_i^*\chi_i = \frac{N}{N!}(N-1)! = 1 \tag{9}$$

We then have via induction that the normalization condition holds for all Slater determinants.

3 Matrix Elements

We define two operators

$$F \hat{=} \Sigma_i^N f\hat{(}x_i) \tag{10}$$

$$G\hat{=}\Sigma_{i>j}^{N}\hat{g(x_i, x_j)} \tag{11}$$

We then note that for a two particle system the slater determinant must be:

$$\Phi = \frac{1}{\sqrt{2}}(\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)) \tag{12}$$

We furthermore note that this means in the two particle case:

$$F\hat{=}\hat{f(x_1)} + \hat{f(x_2)} \tag{13}$$

$$G\hat{=}\hat{g(x_i, x_j)} \tag{14}$$

We then define $< \psi_i(x_i)| < \psi_j(x_j)|$ as $< \psi_i\psi_j|$

From this it follows that

$$\begin{aligned} < \Phi|\hat{F|}\Phi >= \frac{1}{2}(< \psi_1\psi_2|(\hat{f(x_1)} + \hat{f(x_2)})|\psi_1\psi_2 > - < \psi_1\psi_2|(\hat{f(x_1)} + \hat{f(x_2)})|\psi_2\psi_1 > - \\ < \psi_2\psi_1|(\hat{f(x_1)} + \hat{f(x_2)})|\psi_1\psi_2 > + < \psi_2\psi_1|(\hat{f(x_1)} + \hat{f(x_2)})|\psi_2\psi_1 >) \end{aligned} \tag{15}$$

Now since the f terms don't interact between the two variables x_1, x_2, it follows that

$$\begin{aligned} < \Phi|\hat{F|}\Phi >= \frac{1}{2}(< \psi_1(x_1)|\hat{f(x_1)}|\psi_1(x_1) > + < \psi_1(x_2)|(\hat{f(x_2)}|\psi_1(x_2) > \\ + < \psi_2(x_1)|\hat{f(x_1)}|\psi_2(x_1) > + < \psi_2(x_2)|\hat{f(x_2)}|\psi_2(x_2) >) \end{aligned} \tag{16}$$

In the case that the f operators are the same for both particles(as would again be the same for identical particles) it follows that

$$< \Phi|\hat{F|}\Phi >=< \psi_1(x_1)|\hat{f(x_1)}|\psi_1(x_1) > + < \psi_2(x_1)|\hat{f(x_1)}|\psi_2(x_1) > \tag{17}$$

We can do the same now with the g term, as:

$$\begin{aligned} < \Phi|\hat{G|}\Phi >= \frac{1}{2}(< \psi_1\psi_2|(\hat{g(x_1, x_2)})|\psi_1\psi_2 > - < \psi_1\psi_2|(\hat{g(x_1, x_2)})|\psi_2\psi_1 > - \\ < \psi_2\psi_1|(\hat{g(x_1, x_2)})|\psi_1\psi_2 > + < \psi_2\psi_1|(\hat{g(x_1, x_2)})|\psi_2\psi_1 >) \end{aligned} \tag{18}$$

Noting that in the g case there is no distinction between x_1 and x_2 it follows that if they are indistinguishable particles(as they must be for the slater determinant to be a reasonable choice)

$$< \Phi|\hat{G|}\Phi >= (< \psi_1\psi_2|(\hat{g(x_1, x_2)})|\psi_1\psi_2 > - < \psi_1\psi_2|(\hat{g(x_1, x_2)})|\psi_2\psi_1 > \tag{19}$$

3.1 An Explication of the Shorthand

We represent the slater determinant of wavefunctions, for example in the two dimensional case, as:

$$\Phi = |\nu\mu >= \frac{1}{\sqrt{2}}(\nu(x_1)\mu(x_2) - \mu(x_2)\nu(x_2)) \tag{20}$$

Hence when taking these expectation values we have:

$$< \nu\mu|\hat{O}|\nu\mu > \tag{21}$$

From this I think we can anticipate that there will be a symmetry in operators being considered based on a change in index, as would be expected. Which is to say that the Slater Determinant at some level will interact in a standard way with the operators so that we ight "ignore" the fact that the system is in fact composed of them.