Exercise 4

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1 Slater Determinant Transforms

The objective here is to show that taking a slater determinant into a new orthonormal basis will still allow it to be written as a Slater determinant.

To begin, we assume we have some wavefunctions and particles ψ_n and x_n, which can be put into the standard format as:

$$\boldsymbol{\Psi} = \begin{pmatrix} \psi_1(x_1) & \dots & \psi_1(x_n) \\ \vdots & \ddots & \vdots \\ \psi_n(x_1) & \dots & \psi_n(x_n) \end{pmatrix} \tag{1}$$

Where trivially we have that the wavefunction is the determinant of this matrix $\boldsymbol{\Psi}$.

Now let us consider a conversion to another orthonormal basis. We then know that this means that there is a relationship

$$\phi_a = \Sigma_i C_{a,i} \psi_i \tag{2}$$

We then realize that this can itself be represented as a matrix of the form

$$\vec{\phi} = \boldsymbol{C}\vec{\psi} \tag{3}$$

Where each of the vectors $\vec{\phi}$ and $\vec{\psi}$ are the orthnormal bases.

So with this we can then note that if we wish to write out a particular ψ_a in terms of ϕ, it follows that

$$\boldsymbol{C^{-1}}\vec{\phi} = \vec{\psi} \tag{4}$$

We then recognize that each column of the matrix $\boldsymbol{\Psi}$ is just the basis vector with a different x_i in it.

We thus see that $\boldsymbol{C^{-1}\Psi}$ creates a new matrix $\boldsymbol{\Phi}$ in the $\vec{\phi}$ basis.

Finally we note that

$$\Phi = det(\boldsymbol{\Psi}) \tag{5}$$

At this point we note that, taking advantage of the unitarity of $\boldsymbol{C}$

$$det(\boldsymbol{\Phi}) = det(\boldsymbol{C^{-1}\Psi}) = det(\boldsymbol{C^{-1}})\Phi \tag{6}$$

Now we then note that

$$det(\boldsymbol{C^{-1}}) = det(\boldsymbol{C}^T) = |det(\boldsymbol{C})| \tag{7}$$

From this it follows that

$$det(\boldsymbol{C^{-1}}) = e^{i\theta} \tag{8}$$

And so we have from here

$$det(\boldsymbol{\Phi}) = det(\boldsymbol{C^{-1}\Phi}) = e^{i\theta}det(\boldsymbol{\Psi}) = e^{i\theta}\Phi \tag{9}$$

And so we see that we can continue to write the slater determinant as a determinant in another basis.

2 Variation Of Energy

We now consider how energy might vary as a function of $\langle\Phi|$.

We then have that

$$\delta\Phi = \sum_i \frac{\partial}{\partial\psi_i}\Phi\partial\psi_i = \sum_{j=1}^{A}\frac{1}{\sqrt{A!}}\sum_p(-1)^p P\prod_{i\neq j}^{A}\psi_i\delta\psi_j \tag{10}$$

Now we can then find the following, recognizing that the change in ψ or ψ^* are equivalent:

$$\delta\left\langle E\right\rangle = \sum_j \frac{\delta}{\delta\psi_j^*}\delta\psi_j^*\left\langle\Phi\right|\hat{H}\left|\Phi\right\rangle \tag{11}$$

Which we see , recognizing the form of $\delta\Phi$ that this is simply the same as:

$$\delta \langle E \rangle = \langle \delta\psi | H | \psi \rangle \tag{12}$$

Now, knowing

$$H = \sum_{i=1}^{A} (t(x_i) + u(x_i)) + \frac{1}{2} \sum_{i \neq j}^{A} v(x_i, x_j) \tag{13}$$

Hence we have that

$$\delta \langle E \rangle = \langle \delta\psi | \left(\sum_{i=1}^{A} (t(x_i) + u(x_i)) + \frac{1}{2} \sum_{i \neq j}^{A} v(x_i, x_j) \right) | \psi \rangle \tag{14}$$

We can then note that in the one body term the expectation value of the off diagonal matrix elements is 0, which means in our case that:

$$\delta \langle E_1 \rangle = \sum_j \langle \Phi \frac{\delta\psi_j}{\psi_j} | \left(\sum_{i=1}^{A} (t(x_i) + u(x_i))) | \Phi \rangle \right) \tag{15}$$

Now we can further note that for the one body term, if we do not match $\langle \delta\psi_i | , | \psi_i \rangle$ we will be left with an expectation value that includes some term $\langle \delta\psi_j | | \psi_j \rangle$, which must be zero if no operator is considered to be acting between, trivially.

We can then see that the one body term is just

$$\delta \langle E \rangle = \sum_i \langle \delta\psi_i | (t(x_i) + u(x_i)) | \psi_i \rangle \tag{16}$$

We note then that a nearly identical argument suffices for the two body operator, which we have derived previously ought to have a form like

$$\sum_{i \neq j}^{N} \langle \frac{\delta\Phi}{\psi_i\psi_j} | (\langle \delta\psi_i\psi_j | v | \psi_i\psi_j \rangle - \langle \psi_i\psi_j | v | \psi_j\psi_i \rangle) | \frac{\Phi}{\psi_i\psi_j} \rangle + \langle \frac{\delta\Phi}{\psi_i\psi_j} | (\langle \delta\psi_i\psi_j | v | \psi_i\psi_j \rangle - \langle \delta\psi_i\psi_j | v | \psi_j\psi_i \rangle) | \frac{\Phi}{\psi_i\psi_j} \rangle \tag{17}$$

Because here we must again remove all terms where our varied wavefunction is not acted on by an operator, i.e. they evaluate to 0, we can remove most terms as we did before, leaving the expected answer as:

$$\delta \langle E \rangle = \sum_i \langle \delta\psi_i | (t(x_i) + u(x_i)) | \psi_i \rangle + \sum_{i \neq j}^{N} (\langle \delta\psi_i\psi_j | v | \psi_i\psi_j \rangle - \langle \delta\psi_i\psi_j | v | \psi_j\psi_i \rangle) \tag{18}$$