Exercises Week 35

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Exercise 1

a)

$$\Phi^{AS} = \frac{1}{\sqrt{3!}} \sum_{p=0}^{3!} (-1)^p \prod_{i=1}^{3} \psi_{a_i}(x_i)$$

$$\frac{1}{\sqrt{6}} \Big(\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\psi_{\alpha_3}(x_3) - \psi_{\alpha_1}(x_2)\psi_{\alpha_1}(x_1)\psi_{\alpha_3}(x_3) + \psi_{\alpha_1}(x_2)\psi_{\alpha_2}(x_3)\psi_{\alpha_3}(x_1)$$
$$- \psi_{\alpha_1}(x_3)\psi_{\alpha_2}(x_2)\psi_{\alpha_3}(x_1) + \psi_{\alpha_1}(x_3)\psi_{\alpha_2}(x_1)\psi_{\alpha_3}(x_2) - \psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_3)\psi_{\alpha_3}(x_2) \Big)$$

b)

$$\left\langle \Phi_\lambda^{AS} \middle| \Phi_\lambda^{AS} \right\rangle = \int \left| \Phi_\lambda^{AS}(x_1, \dots, x_N, \alpha_1, \dots, \alpha_N) \right|^2 \mathrm{d}\tau = 1$$

We assume the particles-states to be orthonormal.

$$\left\langle \psi_{\alpha_i} \middle| \psi_{\alpha_j} \right\rangle = \int \psi_{\alpha_i}^*(\mathbf{r}) \psi_{\alpha_j}(\mathbf{r}) \mathrm{d}\mathbf{r} = \delta_{ij}$$

Using the antisymmetrizer operator $\mathcal{A}$ and Hartree-function ϕ_H:

$$\mathcal{A} = \frac{1}{N!} \sum_p (-)^p \hat{P} \quad , \quad \phi_H = \prod_{i=1}^{N} \psi_{\alpha_i}(x_i)$$

We can rewrite the Slater determinant to be the following:

$$\Phi_\lambda^{AS} = \sqrt{N!} \mathcal{A} \phi_H$$

We now have a new expression for the original inner product:

$$\left\langle \Phi_\lambda^{AS} \middle| \Phi_\lambda^{AS} \right\rangle = N! \int \mathcal{A}^* \phi_H^* \mathcal{A} \phi_H \mathrm{d}\tau$$

Using that $\mathcal{A}^2 = \mathcal{A}$, as $\mathcal{A}$ is Hermitian, and that it is a projection operator we can simplify:

$$N! \int \phi_H^* \mathcal{A} \phi_H \mathrm{d}\tau = \sum_p (-)^p \int \phi_H^* \hat{P} \phi_H \mathrm{d}\tau$$

The permutation operator acts on the Hartree-function, which makes all it's states different. The only contribution comes when the permutation is identity.

$$\left\langle \Phi_\lambda^{AS} \middle| \Phi_\lambda^{AS} \right\rangle = \int \phi_H^* \phi_H \mathrm{d}\tau = 1$$

c)

Onebody Operator:

$$\left\langle \Phi^{AS}_{\alpha_1\alpha_2} \middle| \hat{F} \middle| \Phi^{AS}_{\alpha_1\alpha_2} \right\rangle = 2 \int \psi^*_{\alpha_1}(x_1)\psi^*_{\alpha_2}(x_2)\hat{F}\mathcal{A}\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\mathrm{d}\tau$$

Inserting its the operators definition:

$$\left\langle \Phi^{AS}_{\alpha_1\alpha_2} \middle| \hat{F} \middle| \Phi^{AS}_{\alpha_1\alpha_2} \right\rangle = \sum_p (-)^p \int \psi^*_{\alpha_1}(x_1)\psi^*_{\alpha_2}(x_2)\hat{f}(x_1)\hat{P}\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\mathrm{d}\tau + \sum_p (-)^p \int \psi^*_{\alpha_1}(x_1)\psi^*_{\alpha_2}(x_2)\hat{f}(x_2)\hat{P}\psi_{\alpha_1}(x_1$$

The Hartree-function, when permuted, will make the integral vanish. There is only one term of each sum left.

$$\left\langle \Phi^{AS}_{\alpha_1\alpha_2} \middle| \hat{F} \middle| \Phi^{AS}_{\alpha_1\alpha_2} \right\rangle = \int \psi^*_{\alpha_1}(x_1)\psi^*_{\alpha_2}(x_2)\hat{f}(x_1)\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\mathrm{d}\tau + \int \psi^*_{\alpha_1}(x_1)\psi^*_{\alpha_2}(x_2)\hat{f}(x_2)\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\mathrm{d}\tau$$

As the onebody operator only acts on a single particle, we can integrate over the other coordinate. The single-particle states are orthonormal, giving a unitary integral.

$$\left\langle \Phi^{AS}_{\alpha_1\alpha_2} \middle| \hat{F} \middle| \Phi^{AS}_{\alpha_1\alpha_2} \right\rangle = \int \psi^*_{\alpha_1}(\mathbf{r})\hat{f}(\mathbf{r})\psi_{\alpha_1}(\mathbf{r})\mathrm{d}\mathbf{r} + \int \psi^*_{\alpha_2}(\mathbf{r})\hat{f}(\mathbf{r})\psi_{\alpha_2}(\mathbf{r})\mathrm{d}\mathbf{r}$$

With this we get a general expression for a onebody operator:

$$\langle \alpha_i | \, \hat{q} \, | \alpha_j \rangle \equiv \int \psi^*_{\alpha_i}(\mathbf{r})\hat{q}(\mathbf{r})\psi_{\alpha_j}(\mathbf{r})\mathrm{d}\mathbf{r}$$

This gives:

$$\left\langle \Phi^{AS}_{\alpha_1\alpha_2} \middle| \hat{f} \middle| \Phi^{AS}_{\alpha_1\alpha_2} \right\rangle \equiv \langle \alpha_1 | \, \hat{f} \, | \alpha_1 \rangle + \langle \alpha_2 | \, \hat{f} \, | \alpha_2 \rangle$$

Twobody Operator:

$$\left\langle \Phi^{AS}_{\alpha_1\alpha_2} \middle| \hat{G} \middle| \Phi^{AS}_{\alpha_1\alpha_2} \right\rangle = 2 \int \psi^*_{\alpha_1}(x_1)\psi^*_{\alpha_2}(x_2)\hat{G}\mathcal{A}\psi_{\alpha_1}(x_2)\psi_{\alpha_2}(x_2)\mathrm{d}\tau$$

Given that there generally only are two particles, we insert the definition of $\hat{G}$.

$$\left\langle \Phi^{AS}_{\alpha_1\alpha_2} \middle| \hat{G} \middle| \Phi^{AS}_{\alpha_1\alpha_2} \right\rangle 2 \int \psi^*_{\alpha_1}(x_1)\psi^*_{\alpha_2}(x_2)\hat{G}\mathcal{A}\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\mathrm{d}\tau$$

$$\left\langle \Phi^{AS}_{\alpha_1\alpha_2} \middle| \hat{G} \middle| \Phi^{AS}_{\alpha_1\alpha_2} \right\rangle = \sum_p (-)^p \int \psi^*_{\alpha_1}(x_1)\psi^*_{\alpha_2}(x_2)\hat{P}\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\mathrm{d}\tau$$

Writing out the permutations:

$$\begin{aligned}\left\langle \Phi^{AS}_{\alpha_1\alpha_2} \middle| \hat{G} \middle| \Phi^{AS}_{\alpha_1\alpha_2} \right\rangle &= \int \psi^*_{\alpha_1}(x_1)\psi^*_{\alpha_2}(x_2)\hat{g}(x_1,x_2)\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\mathrm{d}\tau \\ &\quad - \int \psi^*_{\alpha_1}(x_1)\psi^*_{\alpha_2}(x_2)\hat{g}(x_1,x_2)\underbrace{\psi_{\alpha_1}(x_2)\psi_{\alpha_2}(x_1)}_{\text{switched pos.}}\mathrm{d}\tau\end{aligned}$$

The first term is the Hartree-term, the second is the Fock-term. We can use a shorthand notation:

$$\langle\alpha\beta|\,\hat{q}\,|\gamma\delta\rangle \equiv \int \psi^*_{\alpha_1}(x_1)\psi^*_{\beta}(x_2)\hat{q}(x_1,x_2)\psi_{\gamma}(x_1)\psi_{\delta}(x_2)\mathrm{d}x_1\mathrm{d}x_2$$

With:

$$\langle\alpha\beta|\,\hat{q}\,|\gamma\delta\rangle_{AS} = \langle\alpha\beta|\,\hat{q}\,|\gamma\delta\rangle + \langle\alpha\beta|\,\hat{q}\,|\delta\gamma\rangle$$

This finally gives:

$$\left\langle\Phi^{AS}_{\alpha_1\alpha_2}\right|\hat{G}\left|\Phi^{AS}_{\alpha_1\alpha_2}\right\rangle = \langle\alpha_1\alpha_2|\,\hat{g}\,|\alpha_1\alpha_2\rangle_{AS}$$

As the particles are indistinguishable, the operators must have permutation symmetry, making them commute with the permutation operator. They should also be Hermitian, as they correspond to physical observables.

$$\left[\mathcal{A},\hat{F}\right] = \left[\mathcal{A},\hat{G}\right] = 0$$

Exercise 2

a)

There are three states. One particle with spin up and one with spin down. As the particles are indistinguishable, we do not care which particle is which. We therefore have a total of six slater determinants:

11 12 13 23 33 22

If the particles must be in the same state, we have only three slater determinants

11 22 33

b)

Each element of the matrix representation of the Hamiltonian in the basis of $\{\Phi_0,\Phi_1\}$ is defined as following:

$$\begin{pmatrix} \langle\Phi_0|\,\hat{H}\,|\Phi_0\rangle & \langle\Phi_0|\,\hat{H}\,|\Phi_1\rangle \\ \langle\Phi_1|\,\hat{H}\,|\Phi_0\rangle & \langle\Phi_1|\,\hat{H}\,|\Phi_1\rangle \end{pmatrix}$$

The off-diagonal elements have energie values from the particle interactions, which we know have a value of $-g$. Using the definition of $\hat{H}_0$, we clearly see that the energie from this part of the total Hamiltonian, is $2d$ and $4d$.

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

To find the eigenvalues we solve the following:

$$\left(\hat{H}-\lambda I\right)|\Psi\rangle = 0 \Rightarrow \det\left(\hat{H}-\lambda I\right) = 0$$

$$\lambda^2 + (2g-6d)\lambda + 8d^2 - 24dg$$

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

Adding it back in to the equation and diagonalizing we get:

$$\begin{pmatrix} \frac{d \pm \sqrt{d^2+g^2}}{g} & 0 \\ 0 & 1 \end{pmatrix}$$

Now we define our eigenstates from our basis:

$$|\Psi_0\rangle = \frac{d + \sqrt{d^2+g^2}}{g} |\Phi_0\rangle |\Phi_1\rangle$$

$$|\Psi_1\rangle = \frac{d - \sqrt{d^2+g^2}}{g} |\Phi_0\rangle |\Phi_1\rangle$$

For simplification we add the new variable $\gamma \equiv d/g$. It represents the ratio between the energy from the interaction and the energy level. Using this on the eigenstates:

$$|\Psi_0\rangle = \left(\gamma + \sqrt{1+\gamma^2}\right) |\Phi_0\rangle + |\Phi\rangle$$

$$|\Psi_1\rangle = \left(\gamma - \sqrt{1+\gamma^2}\right) |\Phi_0\rangle + |\Phi_1\rangle$$

c)

With $p = 3$, we only get a new element on the diagonal for the Hamiltonian

$$\begin{pmatrix} 2d-g & -g & -g \\ -g & 4d-g & -g \\ -g & -g & 6d-g \end{pmatrix} = \begin{pmatrix} 2\gamma-1 & -1 & -1 \\ -1 & 4\gamma-1 & -1 \\ -1 & -1 & 6\gamma-1 \end{pmatrix}$$