Exercises Week 36

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Exercise 1

a)

$$\langle SD|\,\hat{F}\,|SD\rangle$$

The onebody operator $\hat{F}$ can be written as:

$$\hat{F} = \sum_{i}^{N} \hat{f}(x_i) = \sum_{\mu\nu} \langle\mu|\,\hat{h}\,|\nu\rangle\, a_\mu^\dagger a_\nu$$

In this case, we have two particles, with states ψ_i and ψ_j.

$$\langle SD|\,\hat{F}\,|SD\rangle = \sum_{\mu\nu} \underbrace{\langle\mu|\,\hat{f}\,|\nu\rangle}_{\text{scalar}} \langle SD|\, a_\mu^\dagger \alpha_\nu\,|SD\rangle$$

We are summing over all states, but the product is only non-zero if $\mu = \nu$. We are left with:

$$\sum_{\mu} \langle\mu|\,\hat{f}\,|\mu\rangle\,\langle SD|\, a_\mu^\dagger a_\mu\,|SD\rangle = \sum_{\mu} \langle\mu|\,\hat{f}\,|\mu\rangle$$

The twobody operator $\hat{G}$ can be written as:

$$\hat{G} = \sum_{i>j}^{N} \hat{g}(x_i, x_j) = \frac{1}{2}\sum_{\mu\nu\delta\gamma} \langle\mu\nu|\,\hat{g}\,|\delta\gamma\rangle\, a_\mu^\dagger a_\nu^\dagger a_\delta a_\gamma$$

$$\langle SD|\,\hat{G}\,|SD\rangle = \frac{1}{2}\sum_{\mu\nu\delta\gamma} \langle\mu\nu|\,\hat{g}\,|\delta\gamma\rangle\,\langle SD|\, a_\mu^\dagger a_\nu^\dagger a_\delta a_\gamma\,|SD\rangle$$

If $\mu = \nu$ or $\delta = \gamma$, as a_μ, we get zero as $a_\mu^\dagger a_\mu^\dagger\,|SD\rangle = 0$, or $a_\mu a_\mu\,|SD\rangle$. We also need to have $\mu = \delta$ or $\nu = \gamma$, to add back the particles we removed.

$$\langle SD|\,\hat{G}\,|SD\rangle = \frac{1}{2}\sum_{\mu\nu}\Big(\langle\mu\nu|\,\hat{g}\,|\mu\nu\rangle\,\langle SD|\, a_\mu^\dagger a_\nu^\dagger a_\mu a_\nu\,|SD\rangle + \langle\mu\nu|\,\hat{g}\,|\nu\mu\rangle\,\langle SD|\, a_\mu^\dagger a_\nu^\dagger a_\mu a_\nu\,|SD\rangle\Big)$$

As the creation and annihilation operators for different particles work independently, we know that $a_\mu^\dagger a_\nu^\dagger a_\mu a_\nu = a_\mu^\dagger a_\mu a_\nu^\dagger a_\nu$. We also have the anticommutation relations:

$$a_\mu^\dagger a_\nu^\dagger = -a_\nu^\dagger a_\mu^\dagger \quad , \quad a_\mu a_\nu = -a_\nu a_\mu \quad , \quad a_\mu^\dagger a_\nu = \delta_{\mu\nu} - a_\nu^\dagger a_\mu$$

The number operator is defined as:

$$\hat{n}_\mu = a_\mu^\dagger a_\mu$$

With this we can simplify the above:

$$\langle SD|\, a_\mu^\dagger a_\nu^\dagger a_\nu a_\mu\,|SD\rangle = \langle SD|\, a_\mu^\dagger a_\mu a_\nu^\dagger a_\nu\,|SD\rangle = \langle SD|\, n_\mu n_\nu\,|SD\rangle = 1$$

$$\langle SD|\, a_\mu^\dagger a_\nu^\dagger a_\mu a_\nu\,|SD\rangle = -\langle SD|\, a_\mu^\dagger a_\mu a_\nu^\dagger a_\nu\,|SD\rangle = -\langle SD|\, n_\mu n_\nu\,|SD\rangle = -1$$

With this we get:

$$\langle SD|\,\hat{G}\,|SD\rangle = \frac{1}{2}\sum_{\mu\nu}\left(\langle\mu\nu|\,\hat{g}\,|\mu\nu\rangle - \langle\mu\nu|\,\hat{g}\,|\nu\mu\rangle\right)$$

We see that this is the Hartree and Fock terms.

b)

Onebody

$$\langle SD|\,\hat{F}\,\left|SD_i^j\right\rangle .$$

For this, we must take into account that $\left\langle SD\middle|SD_i^j\right\rangle = 0$. Using the creation and annihilation operators we can get the original slater determinant back:

$$a_i^\dagger a_j\left|SD_i^j\right\rangle = |SD\rangle$$

The integral vanishes for combinations other than μ and ν.

$$\langle SD|\,\hat{F}\,\left|SD_i^j\right\rangle = \langle i|\,\hat{f}\,|j\rangle$$

Twobody

$$\langle SD|\,\hat{G}\,\left|SD_i^j\right\rangle \frac{1}{2}\sum_{\mu\nu}\langle\mu\nu|\,\hat{g}\,|\delta\gamma\rangle\,\langle SD|\,a_\mu^\dagger a_\nu^\dagger a_\delta a_\gamma\left|SD_i^j\right\rangle$$

To add to the sum, the product must be non-zero. This can't happen when the indices are the same, as we make a permutation to $|SD\rangle$. We sum over a single indices instead:

$$\begin{aligned}\langle SD|\,\hat{G}\,\left|SD_i^j\right\rangle = \frac{1}{2}\sum_{\mu}\Big[&\langle\mu i|\,\hat{g}\,|\mu j\rangle\,\langle SD|\,a_\mu^\dagger a_i^\dagger a_j a_\mu\left|SD_i^j\right\rangle\\ &+\langle\mu i|\,\hat{g}\,|j\mu\rangle\,\langle SD|\,a_\mu^\dagger a_i^\dagger a_\mu a_j\left|SD_i^j\right\rangle\\ &+\langle i\mu|\,\hat{g}\,|\mu j\rangle\,\langle SD|\,a_i^\dagger a_\mu^\dagger a_\mu a_j\left|SD_i^j\right\rangle\\ &+\langle i\mu|\,\hat{g}\,|j\mu\rangle\,\langle SD|\,a_i^\dagger a_\mu^\dagger a_\mu a_j\left|SD_i^j\right\rangle\Big]\end{aligned}$$

This can be simplified by the fact that generally $\langle\mu\nu|\,\hat{q}\,|\delta\gamma\rangle = \langle\nu\mu|\,\hat{q}\,|\gamma\delta\rangle$ and using the anticommutation relations.

$$\sum_{\mu}\Big[\langle\mu i|\,\hat{g}\,|\mu j\rangle - \langle\mu i|\,\hat{g}\,|j\mu\rangle\Big]$$

c)

Onebody

$$\langle SD|\,\hat{F}\,\left|SD_{ij}^{kl}\right\rangle = \sum_{\mu\nu}\langle\mu|\,\hat{f}\,|\nu\rangle\,\langle SD|\,a_\mu^\dagger a_\nu\left|SD_{ij}^{kl}\right\rangle$$

As we switch out tow particles, we have no equal indices between the two slater determinants. This gives:

$$\langle SD|\,\hat{F}\,\left|SD_{ij}^{kl}\right\rangle = 0$$

Twobody

$$\langle SD|\,\hat{G}\,\left|SD_{ij}^{kl}\right\rangle = \frac{1}{2}\sum_{\mu\nu}\langle\mu\nu|\,\hat{g}\,|\delta\gamma\rangle\,\langle SD|\,a_\mu^\dagger a_\nu^\dagger a_\delta a_\gamma\left|SD_{ij}^{kl}\right\rangle$$

As the permutation of the slater determinant switches state ϕ_i and ϕ_j with ϕ_k and ϕ_l respectively, we only see a non-zero contribution when the ϕ_k and ϕ_l are annihilated, and ϕ_i and ϕ_j are created. This gives:

$$\langle SD|\, \hat{G} \left|SD_{ij}^{kl}\right\rangle = \frac{1}{2}\Big[\langle ij|\, \hat{g} \,|kl\rangle \langle SD|\, a_i^\dagger a_j^\dagger a_k a_l \left|SD_{ij}^{kl}\right\rangle$$
$$+ \langle ij|\, \hat{g} \,|lk\rangle \langle SD|\, a_i^\dagger a_j^\dagger a_l a_k \left|SD_{ij}^{kl}\right\rangle$$
$$+ \langle ji|\, \hat{g} \,|kl\rangle \langle SD|\, a_j^\dagger a_i^\dagger a_k a_l \left|SD_{ij}^{kl}\right\rangle$$
$$+ \langle ji|\, \hat{g} \,|lk\rangle \langle SD|\, a_j^\dagger a_i^\dagger a_l a_k \left|SD_{ij}^{kl}\right\rangle \Big]$$

Using the same simplifications as before, we get:

$$\langle SD|\, \hat{G} \left|SD_{ij}^{kl}\right\rangle = \langle ij|\, \hat{g} \,|kl\rangle - \langle ij|\, \hat{g} \,|lk\rangle$$

With no permutation, the onebody operator has N terms, and the twobody had $N^2/2$. With two permutations, we have 0 terms for the onebody operator, and the twobody havinging N terms. With three permutations, both the onebody and twobody operator have 0 terms. A three body operator would have a single term.

Exercise 2

a)

We examine the case when $N = 2$:

$$\Psi_{\text{AS}} = \frac{1}{\sqrt{2}} \left(\psi_1(\mathbf{x_1})\psi_2(\mathbf{x_2}) - \psi_1(\mathbf{x_2})\psi_2(\mathbf{x_1})\right)$$

$$n(\mathbf{x}) = 2 \int \,\mathrm{d}x_1 \,\mathrm{d}x_2 \left|\Psi_{\text{AS}}\right|^2$$

$$n(\mathbf{x}) = 2 \int \,\mathrm{d}x_1 \,\mathrm{d}x_2 \frac{1}{\sqrt{2}}\Big(\psi_1(\mathbf{x_1})\psi_2(\mathbf{x_2}) - \psi_1(\mathbf{x_2})\psi_2(\mathbf{x_1})\Big)^* \frac{1}{\sqrt{2}}\Big(\psi_1(\mathbf{x_1})\psi_2(\mathbf{x_2}) - \psi_1(\mathbf{x_2})\psi_2(\mathbf{x_1})\Big)$$

Only the parallel products are non-zero.

$$n(\mathbf{x}) = \psi_1^*\psi_1 + \psi_2^*\psi_2 = \left|\psi_1\right|^2 + \left|\psi_2\right|^2 = \sum_k \left|\psi_k\right|^2$$

b)

We already know that:

$$\langle SD|\, \hat{F} \,|SD\rangle = \sum_\alpha \langle \alpha|\, \hat{f} \,|\alpha\rangle$$

Which in this case is:

$$\langle \alpha_1\alpha_2|\, \hat{F} \,|\alpha_1\alpha_2\rangle = \langle \alpha_1|\, \hat{f} \,|\alpha_1\rangle + \langle \alpha_2|\, \hat{f} \,|\alpha_2\rangle$$

Same goes for twobody operator:

$$\langle SD|\, \hat{G} \,|SD\rangle = \frac{1}{2}\Big(\langle \alpha_1\alpha_2|\, \hat{g} \,|\alpha_1\alpha_2\rangle - \langle \alpha_1\alpha_2|\, \hat{g} \,|\alpha_2\alpha_1\rangle + \langle \alpha_2\alpha_1|\, \hat{g} \,|\alpha_1\alpha_2\rangle - \langle \alpha_2\alpha_1|\, \hat{g} \,|\alpha_2\alpha_1\rangle \Big)$$

Again, using the fact that $\langle \mu\nu|\, \hat{g} \,|\delta\gamma\rangle = \langle \nu\mu|\, \hat{g} \,|\gamma\delta\rangle$, as we made to permutations, we can simplify to:

$$\langle \alpha_1\alpha_2|\, \hat{G} \,|\alpha_1\alpha_2\rangle = \langle \alpha_1\alpha_2|\, \hat{g} \,|\alpha_1\alpha_2\rangle - \langle \alpha_1\alpha_2|\, \hat{g} \,|\alpha_2\alpha_1\rangle = \langle \alpha_1\alpha_2|\, \hat{g} \,|\alpha_1\alpha_2\rangle_{\text{AS}}$$