Problem set 1
FYS-KJM4480

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Exercise 1

In this problem we consider the Slater determinant

$$\Phi_\lambda^{AS}(x_1, x_2, \ldots, x_N; \alpha_1, \ldots, \alpha_N) = \frac{1}{\sqrt{N!}} \sum_p (-)^p \hat{P} \prod_{i=1}^N \psi_{\alpha_i}(x_i).$$

Where α_i are quantum numbers and N is the number of particles. The sum over p is a summation over all possible permutations.

a)

If we let $N = 3$, the Slater determinant becomes:

$$\begin{aligned}\Phi_\lambda^{AS}(\boldsymbol{x}; \boldsymbol{\alpha}) = \frac{1}{\sqrt{6}}\Big(&\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\psi_{\alpha_3}(x_3) - \psi_{\alpha_1}(x_2)\psi_{\alpha_2}(x_1)\psi_{\alpha_3}(x_3) \\ &+ \psi_{\alpha_1}(x_2)\psi_{\alpha_2}(x_3)\psi_{\alpha_3}(x_1) - \psi_{\alpha_1}(x_3)\psi_{\alpha_2}(x_2)\psi_{\alpha_3}(x_1) \\ &+ \psi_{\alpha_1}(x_3)\psi_{\alpha_2}(x_1)\psi_{\alpha_3}(x_2) - \psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_3)\psi_{\alpha_3}(x_2)\Big)\end{aligned}$$

b)

We will no show that the slater determinant is normalized, in the sense that

$$\langle \Phi_\lambda^{AS} | \Phi_\lambda^{AS} \rangle = \int |\Phi_\lambda^{AS}(x_1, \ldots, x_N, \alpha_1, \ldots, \alpha_N)|^2 = 1.$$

To do this we will assume that the single-particle states forms an orthonormal set, i.e.,

$$\langle \psi_{\alpha_i} | \psi_{\alpha_j} \rangle = \int \psi_{\alpha_i}^*(x) \psi_{\alpha_j}(x) \, \mathrm{d}x = \delta_{ij},$$

where δ_{ij} is the Kronecker-delta.

To easily see that the slater determinant is normalized, we write it using the antisymmetrizer operator

$$\Phi_\lambda^{AS} = \sqrt{N!}\mathcal{A}\prod_{i=1}^{N}\phi_H.$$

Where we have used the *Hartree-function*:

$$\phi_H \equiv \prod_{i=1}^{N}\psi_{\alpha_i}(x_i).$$

We can then write the inner-product as

$$\langle\Phi_\lambda^{AS}|\Phi_\lambda^{AS}\rangle = N!\int \mathcal{A}^*\phi_H^*\mathcal{A}\phi_H \ \mathrm{d}\boldsymbol{x}.$$

We can simplify this as follows

$$\langle\Phi_\lambda^{AS}|\Phi_\lambda^{AS}\rangle = N!\int \phi_H^*\mathcal{A}^2\phi_H \ \mathrm{d}\boldsymbol{x} = N!\int \phi_H^*\mathcal{A}\phi_H \ \mathrm{d}\boldsymbol{x}.$$

Where we have used the fact that the antisymmetrizer is unitary, $\mathcal{A}^\dagger = \mathcal{A}$ and that it is a projection operator, meaning $\mathcal{A}^2 = \mathcal{A}$. We now write out the definition of the antisymmetrizer, giving

$$\langle\Phi_\lambda^{AS}|\Phi_\lambda^{AS}\rangle = \sum_p(-)^p\int \phi_H^*\hat{P}\phi_H \ \mathrm{d}\boldsymbol{x}.$$

As the permutation operator only acts on one of the Hartree-functions, the two functions will never be similar and the orthogonality of the single-particle states makes these cross-products cancel out. We are left only with the contribution when the permuation operator is identity, giving

$$\langle\Phi_\lambda^{AS}|\Phi_\lambda^{AS}\rangle = \int \phi_H^*\phi_H \ \mathrm{d}\boldsymbol{x} = 1.$$

Where we again used our assumption about the normality of the single-particle states.

c)

We now define a general onebody operator and a general twobody operator:

$$\hat{F} = \sum_{i=1}^{N}\hat{f}(x_i), \qquad \hat{G} = \sum_{i<j}\hat{g}(x_i, x_j).$$

And we will now calculate the expectation value of these operators for a two-particle Slater determinant.

$$\langle\Phi_{\alpha_1\alpha_2}^{AS}|\hat{F}|\Phi_{\alpha_1\alpha_2}^{AS}\rangle, \qquad \langle\Phi_{\alpha_1\alpha_2}^{AS}|\hat{G}|\Phi_{\alpha_1\alpha_2}^{AS}\rangle.$$

We start with the onebody operator, using the same technique as above using the antisymmetrizer, we can write out the integral as follows

$$\langle\Phi_{\alpha_1\alpha_2}^{AS}|\hat{F}|\Phi_{\alpha_1\alpha_2}^{AS}\rangle = N!\int \phi_H^*\hat{F}\mathcal{A}\phi_H \ \mathrm{d}\boldsymbol{x}.$$

We now insert the definitions of the two operators

$$\langle \Phi^{AS}_{\alpha_1\alpha_2} | \hat{F} | \Phi^{AS}_{\alpha_1\alpha_2} \rangle = \sum_{i=1}^{N} \sum_{p} (-)^p \int \phi_H^* \hat{f} \hat{P} \phi_H \, \mathrm{d}\boldsymbol{x}.$$

As earlier, if one of the Hartree-functions is permutated, the integral vanishes, so we are left with

$$\langle \Phi^{AS}_{\alpha_1\alpha_2} | \hat{F} | \Phi^{AS}_{\alpha_1\alpha_2} \rangle = \sum_{i=1}^{N} \int \phi_H^* \hat{f} \phi_H \, \mathrm{d}\boldsymbol{x}.$$