

Quantum Chemistry

Seminar 4

Many-particle systems

Exercise 1 (Anila)

Show that the state vectors of the two-electron spin, $|\uparrow\rangle|\uparrow\rangle$, $|\uparrow\rangle|\downarrow\rangle$, $|\downarrow\rangle|\uparrow\rangle$ and $|\downarrow\rangle|\downarrow\rangle$, are eigenvectors of the z-component of the total spin of the system, $\hat{S}_z = \hat{S}_{1z} \otimes \hat{1} + \hat{1} \otimes \hat{S}_{2z}$, where $\hat{1}$ is the unity operator on the one-electron spin space. (Hint: $(\hat{S}_{1z} \otimes \hat{1})|x\rangle|y\rangle = \hat{S}_{1z}|x\rangle\hat{1}|y\rangle$ and $(\hat{1} \otimes \hat{S}_{2z})|x\rangle|y\rangle = \hat{1}|x\rangle\hat{S}_{2z}|y\rangle$.)

Exercise 2 (unassigned)

Using the symmetrization / antisymmetrization operators (lesson 4, page 10), symmetrize / antisymmetrize vectors of the following basis set on the spin Hilbert space of two electrons: $|\uparrow\rangle|\uparrow\rangle$, $|\uparrow\rangle|\downarrow\rangle$, $|\downarrow\rangle|\uparrow\rangle$ and $|\downarrow\rangle|\downarrow\rangle$. Find normalization constants of the resulting wave functions supposing that $\langle\uparrow|\uparrow\rangle = \langle\downarrow|\downarrow\rangle = 1$ and $\langle\uparrow|\downarrow\rangle = 0$.

Exercise 3 (Shaho)

Show that the Slater determinant of two particles is normalized if the one-particle wave functions it consists of are orthonormal.