

Quantentheorie II Übung 6

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1. Questions

- (a) Which of the following operators are possible in a system of two identical particles?

$$\vec{x}_1 - \vec{x}_2, \quad \vec{x}_1 + \vec{x}_2, \quad (\vec{x}_1 - \vec{x}_2)^2, \quad \vec{p}_1 \cdot \vec{p}_2$$

- (b) Repeat the 1-dimensional potential well problem. What are the energy eigenstates and eigenvalues?
- (c) What is the hydrogen molecule Hamiltonian only with the Coulomb interaction and without spins?
- (d) Which Hamiltonian eigenstates are used to describe the hydrogen molecules in the Heitler-London theory?

2. **Two identical particles in potential well:** two identical particles are in a one-dimensional potential well

$$V(r) = \begin{cases} 0, & \text{for } |r| < r_0, \\ \infty, & \text{for } |r| \geq r_0. \end{cases}$$

The two particles do not interact with each other and are in parallel spin states: the magnetic quantum numbers of both particles are the same, m_s .

- (a) Write down the Hamiltonian of this two-particle system and show that the energy eigenstates can be factorized into space and spin parts.
- (b) What are the allowed space wave functions for bosons and fermions respectively when we consider the spin state assumption above?
- (c) Write down the energy eigenstates and eigenvalues for bosons and fermions and specify the groundstate energies.

3. **Hydrogen molecule without spin:** the approximate groundstate energy of hydrogen molecules can be calculated using the Rayleigh–Ritz method (Variationsverfahren). We take a trial state $|g\rangle$,

$$|g\rangle = c_1 |\phi_a^{(1)}\rangle |\phi_b^{(2)}\rangle + c_2 |\phi_b^{(1)}\rangle |\phi_a^{(2)}\rangle,$$

where c_1 and c_2 are real numbers and should be determined appropriately. $|\phi_{a,b}^{(i)}\rangle$ are the eigenstates of

$$\left(\frac{\vec{p}_i^2}{2m} - \frac{\alpha}{r_{iA}} \right) |\phi_A^{(i)}\rangle = E_A |\phi_A^{(i)}\rangle,$$

with $A \in \{a, b\}$ and $i \in \{1, 2\}$ as introduced from the lecture.

- (a) Write the Hamiltonian of the hydrogen molecule H and compute

$$\langle H \rangle_g = \frac{\langle g | H | g \rangle}{\langle g | g \rangle}.$$

- (b) What condition should be satisfied if $|g\rangle$ is a groundstate and what is the relation of c_1 and c_2 obtained from the condition?
- (c) Write down the symmetric and antisymmetric groundstates $|g\rangle^{(\pm)}$ and the eigenvalues E_{\pm} . Compare the results from the lecture.

4. **Hydrogen molecule with spin:** we now consider the spins of the electrons.

- (a) Write down the symmetric (+) and antisymmetric (−) spin states $|S m_S\rangle^{(\pm)}$ using the total spin quantum numbers $\vec{S} = \vec{S}_1 + \vec{S}_2$ and $m_S = m_{S_1} + m_{S_2}$.
- (b) The space part of the wave function (see lecture or previous exercise) satisfies

$$\frac{{}^{(\pm)}\langle g | H | g \rangle^{(\pm)}}{{}^{(\pm)}\langle g | g \rangle^{(\pm)}} = E_{\pm}.$$

Now we search for an equivalent Hamiltonian \hat{H}_{spin} which applies only to the spin part, i.e. depends only on the spin operators \vec{S}_1 and \vec{S}_2 . Construct the operator \hat{H}_{spin} which produces eigenvalues

$$\hat{H}_{\text{spin}} |S m_S\rangle^{(\mp)} = E_{\pm} |S m_S\rangle^{(\mp)}.$$

- (c) Discuss the preferred spin state for the energy groundstate.