WS 2021/22

[Oral] (3 pts.)

Problem 9.1: Hydrogen atom – Lowest states

 $\hookrightarrow \texttt{ID: ex_hydrogen_atom_lowest_states:qm2122}$

Learning objective

In this exercise, we will derive the wave functions of the Hydrogen atom for the ground state and first excited states, verify some basic properties, and determine some expectation values. An important aspect is to show that the typical velocity of the electron in the Hydrogen atoms is αc with α the fine structure constant and c the speed of light. Therefore the electrons have not to be treated fully relativistically, but nevertheless are fast enough such that relativistic correction are important.

Consider the wave functions $\psi_{n,\ell,m}$ of the Hydrogen atom as derived in the lecture.

- a) Write explicitly the 1s, 2s, and $2p_z$ wave functions which correspond to the set of quantum numbers $\{n, \ell, m\} = \{1, 0, 0\}, \{2, 0, 0\}, \text{ and } \{2, 1, 0\}$, respectively.
- b) Using the previously derived expressions, show explicitly that the wave functions are orthonormal.
- c) Determine the expectation value of the radial components r, r^2, p_r and p_r^2 in the ground state (i.e. the 1s state). Determine the velocity and show that it scales as the fine structure constant α .

Problem 9.2: Hydrogen atom - Coherent states

[Written] (4 pts.)

 \hookrightarrow ID: ex_hydrogen_atom_coherent_states:qm2122

Learning objective

In this exercise, we show how to construct wave packets which resemble the classical motion of a particle in the Coulomb potential. In analogy to the harmonic oscillator, these wave states are also called *coherent states*.

Let us consider states of the Hydrogen atom with quantum numbers $\ell = n - 1$ and $m = \pm \ell$. In the limit $n \to \infty$ they correspond to circular orbitals.

- a) Write explicitly the wave function $\psi_{n,\ell,m}(r,\theta,\varphi)$ for $\ell = m = n 1$.
- b) How does $\langle r \rangle$ scale with the principal quantum number *n* for the wave function $\psi_{n,n-1,n-1}(r,\theta,\varphi)$?
- c) Calculate the standard deviation $\Delta r/\langle r \rangle$ as a function of the principal quantum number n with $\psi_{n,n-1,n-1}(r,\theta,\varphi)$.
- d) Plot the probability density $|\psi_{n,n-1,n-1}|^2$ in the plane of motion (plane of the trajectory) and its orthogonal direction when the principal quantum number takes the values n = 5, 20, 50, and 100.

Problem 9.3: Hydrogen Atom - An algebraic approach

 $\hookrightarrow \texttt{ID: ex_hydrogen_atom_an_algebraic_approach:qm2122}$

Learning objective

In this exercise, we show that it is possible to derive the energy spectrum of the bound states for the Hydrogen atom using an algebraic approach. Historically, this was first achieved by WOLFGANG PAULI even *before* ERWIN SCHRÖDINGER published his famous equation.

a) Let $N := M/\sqrt{\lambda}$ with $\lambda \in \mathbb{R}_+$, where M is the Runge-Lenz vector as defined in problem 8.3. Determine λ such that the following algebra is satisfied:

$$[L_i, L_j] = i\hbar \varepsilon_{ijk} L_k \tag{1a}$$

$$[L_i, N_j] = i\hbar \varepsilon_{ijk} N_k \tag{1b}$$

$$[N_i, N_j] = i\hbar \varepsilon_{ijk} L_k \tag{1c}$$

Hint: Use Eq. (13) of problem 8.3 and that H commutes with all operators N_i and L_i and therefore can be replaced by its eigenvalue.

b) Define the new operators

$$\boldsymbol{A} := \frac{1}{2} \left(\boldsymbol{L} + \boldsymbol{N} \right)$$
 and $\boldsymbol{B} := \frac{1}{2} \left(\boldsymbol{L} - \boldsymbol{N} \right)$ (2)

and derive their commutator algebra.

- c) Derive the eigenvalues¹ of A^2 and B^2 by comparison with the known angular momentum algebra.
- d) Define the new operators²

$$C_1 := A^2 + B^2$$
 and $C_2 := A^2 - B^2$ (3)

and show that $C_1 = \frac{1}{2} (L^2 + N^2)$ and $C_2 = 0$. Conclude that the eigenvalues of A^2 and B^2 coincide.

e) Use Eq. (11) of problem 8.3 to derive a relation between H and L^2 , N^2 and solve it for H. Finally, derive the eigenvalues of H from the eigenvalues of $L^2 + N^2$ and compare them with the results from the lecture. Be happy.

¹... for irreducible representations.

²In the theory of Lie algebras, those are known as *Casimir operators*. The Casimir operator of the angular momentum algebra is L^2 and characterized by $[L_i, L^2] = 0$ for all *i*.