- Declaration: Oct 4,2024
- Project supervisor: Krzysztof Pawłowski, `pawlowski@cft.edu.pl`
- Consultation: Oct 10, 2024 (Thursday!)
  If needed – another meeting in the week Oct, 14-18
- Presentation: Oct. 25, 2024

Tips & tricks – clever derivations of hydrogen spectrum

Many scientists independently introduced the foundations of quantum mechanics, using different frameworks. Among them were Erwin Schrödinger (wave mechanics), Wolfgang Pauli (group theory), and Werner Heisenberg (operator algebra). Remarkably, such different descriptions lead to the same result!!

In this project, you will learn their mathematical tricks to derive the spectrum of the hydrogen atom. Your task is to find the spectrum using three different methods:

a) Solving differential equation (standard, a'la Schrödinger)

b) Using "ladder" operators – clever analogy to harmonic oscillator

c) Using symmetries and analogy to the angular momentum operator.

A'la Schrödinger

This is the most popular derivation, presented in many quantum mechanics courses, based on the brute-force solution of the differential equation:

$$\left(\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{2}{\rho} - \epsilon\right) u_l = 0 \tag{1}$$

In this standard derivation one finds the form of the solution in the limits $\rho \to \infty$, and $\rho \to 0$, propose a form of the solution and proves, that it is correct.

You can use any textbook to remind yourself of the derivation based on the solution of the differential equation.

A'la Heisenberg

Let's define two families of operators:

$$\hat{A}_{l,+} := \frac{d}{d\rho} - \frac{l+1}{\rho} + \frac{1}{l+1} \tag{2}$$

$$\hat{A}_{l,-} := \frac{d}{d\rho} + \frac{l+1}{\rho} - \frac{1}{l+1} \tag{3}$$

Use them to derive the spectrum of hydrogen, by following the steps:

1. Express the relation
$$\hat{A}_{l,-}\hat{A}_{l,+}u_l = ? \tag{4}$$
in terms of u_l, l and ϵ (without operators).

2. Compute the difference:
$$\hat{A}_{l,+}\hat{A}_{l,-} - \hat{A}_{l+1,-}\hat{A}_{l+1,+} = ? \tag{5}$$

3. Use the result from the preceding point to prove that if u_l is a solution, then $\hat{A}_{l,+} u_l$ is also a solution.

4. Prove, that
$$\int u_l^* \hat{A}_{l,-} \hat{A}_{l,+} u_l = -\int |\hat{A}_{l,+} u_l|^2 \tag{6}$$
Deduce from this result, that $\epsilon \leq \frac{1}{(l+1)^2}$
5. Find the whole spectrum, using analogy to the derivation of the spectrum of a harmonic oscillator.

A'la Pauli

The conserved quantities during the motion of a planet around the Sun are energy, orbital momentum, but also the Runge-Lenz vector:
$$\mathbf{A} := \frac{1}{m}\mathbf{p} \times \mathbf{L} - k\frac{\mathbf{r}}{r}. \tag{7}$$
One can use its quantized version
$$\hat{\mathbf{A}} = \frac{1}{2m}\left(\hat{\mathbf{p}} \times \hat{\mathbf{L}} + \hat{\mathbf{L}} \times \hat{\mathbf{p}}\right) - k\frac{\hat{\mathbf{r}}}{r} \qquad k = 1/(4\pi\epsilon_0) \tag{8}$$
to derive the spectrum of the hydrogen, following the steps

1. Show that the Runge-Lenz vector is conserved, namely
$$\left[\hat{H}, \hat{A}\right] = 0. \tag{9}$$
2. Define yet another vectorial operator:
$$\hat{\boldsymbol{T}} = \frac{1}{2}\left(\hat{\mathbf{L}} + \sqrt{\frac{m}{2\epsilon}}\,\hat{\mathbf{A}}\right) \tag{10}$$
Show that:
$$\hat{\boldsymbol{T}} \times \hat{\boldsymbol{T}} = i\hbar\hat{\boldsymbol{T}} \tag{11}$$
What you can say about the spectrum of $\hat{\boldsymbol{T}}$?
Does $\hat{\boldsymbol{T}}$ commutes with the Hamiltonian $\hat{H}$?
3. Prove the relation
$$4\hat{\boldsymbol{T}}^2 = -\hbar^2 - \frac{k^2 m}{2\epsilon} \tag{12}$$
Deduce from it the spectrum of hydrogen.