EEE434/591: Quantum Mechanics

1. The potential energy of an electron in a hydrogen atom (in MKS units) is

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r},$$

where e is the electron charge and r is the distance of the electron from the proton. The hydrogen atom is, of course, a three-dimensional system, and r is the radial coordinate of a spherical coordinate system with the origin at the proton. However, we can model this system by a simple, continuous one-dimensional potential energy whose TISE we can solve. For this purpose, we can assume that the potential energy term in the 1D TISE is of the form:

$$V(x) = \begin{cases} -\dfrac{e^2}{4\pi\varepsilon_0 x}, & x > 0 \\ \infty, & x \le 0 \end{cases}$$

The bound state energies of an electron in this potential can be determined using the method of power series that was explained on the example of a simple harmonic oscillator (SHO). Let's find the solution step-by-step:

(a) Simplify the TISE for the total energy E by changing the variable of differentiation from x to one that is dimensionless. Define this new variable ξ in terms of the constant:

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2},$$

which represents the Bohr radius of the hydrogen atom. Introduce a dimensionless energy parameter ε defined by:

$$\varepsilon^{-2} = -\frac{2mEa_0^2}{\hbar^2},$$

and the dimensionless length variable ξ

$$\xi = \frac{2x}{\varepsilon a_0}.$$

(b) The equation that you have obtained can not be immediately solved by, for example, inserting into a power series expansion. You need to calculate the asymptotic limit, i.e. the solution $g(\xi)$ for $\xi \to \infty$.

(c) Once you have calculated the asymptotic solution $g(\xi)$, express the wavefunction as $\psi(\xi) = Ag(\xi)f(\xi)$, and find the differential equation for $f(\xi)$.

(d) Solve the differential equation for $f(\xi)$ using a power series expansion, i.e.

$$f(\xi) = \sum_{j=0}^{\infty} c_j \xi^j \ ,$$

in which one must set $c_0 = 0$ (Why?). Derive a recurrence relation for the coefficients c_j in this series.

(e) Give an argument to show that the infinite series for $f(\xi)$ must be truncated at some finite order, and show that doing so leads to the restriction that ε must equal a positive integer number.

(f) From the results from part (*e*), obtain an expression for the allowed bound state energies of this model hydrogen atom. Look up the equation for the bound-state energies of an actual, three-dimensional hydrogen atom and compare your result to this answer. Is the result you obtained accurately describing the energies of this system? Can you think of any important physical effects that have been totally ignored in this model?

(g) Using the recurrence relation of part (*e*), write down the un-normalized spatial functions for the first three bound states of this model potential energy. Plot these functions and discuss their behavior.

2. Consider an electromagnetic resonator with a resonant frequency of 10^{10} Hz. What is the energy separation of the oscillator levels? How does this compare to the thermal energy fluctuations?

3. Determine the expectation values for the kinetic and potential energies in a harmonic oscillator. What can you say about $\langle T \rangle$ and $\langle V \rangle$?

4. By methods similar to those we used for the evaluation of $\langle x^2 \rangle$, evaluate $\langle x^4 \rangle$ and $\langle p^4 \rangle$ for the case that $\psi = \psi_n(x)$, where n represents arbitrary eigenvalue of the microscopic simple harmonic oscillator.