Please read through the entire set of problems before starting to work on them!

Problem 1: Scattering against a potential barrier

In this problem we study a particle of mass m and energy $E < V_0$ in one dimension, meeting a potential barrier given by

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & x \geq 0 \end{cases} \tag{1}$$

a) Draw a sketch of this potential and write down the mathematical boundary conditions the particle's wave function has to obey at the point $x = 0$.

b) Write down the time-independent Schrödinger equation and determine its solutions (with unknown coefficients) in the intervals I ($x < 0$) and II ($x \geq 0$). Express the solution in interval I as a superposition of a right-going and a left-going plane wave, naming the coefficients in front of these terms A and B, respectively.

c) Use the boundary conditions found in **a)** to show that

$$A\left(1 + \frac{ik}{\kappa}\right) = -B\left(1 - \frac{ik}{\kappa}\right) \tag{2}$$

where $k = \sqrt{2mE}/\hbar$ and $\kappa = \sqrt{2m(V_0 - E)}/\hbar$.
Finally, compute the reflection coefficient $R = |B/A|^2$. Comment on the result!

Problem 2: Hydrogen and helium

In the first part of this problem we shall completely neglect any effects due to the spin of the electron. Thus, the eigenvalue equation for the energy of an electron in a hydrogen atom takes the form

$$\hat{H}_0 \psi_{nlm_l} = -\frac{E_0}{n^2}\psi_{nlm_l} \tag{3}$$

where E_0 is a constant.

a) Write down the Hamiltonian $\hat{H}_0$ and what conditions the quantum numbers n, l and m_l have to obey. What is the physical interpretation of the quantum numbers l and m_l? What is the degeneracy of a level with given n?

The lowest energy eigenstate is given by

$$\psi_{100}(r, \theta, \phi) = A \exp\left(-\frac{r}{a_0}\right)$$

where A is a normalization constant, and $a_0 = 4\pi\epsilon_0\hbar^2/m_e e^2$. It the following it may be of use that, expressed in spherical coordinates, we may write

$$\nabla^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2} r - \frac{1}{\hbar^2 r^2}\hat{\mathbf{L}}^2$$

with

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] . \tag{4}$$

Moreover, we remind you that the radial probability density is given by $P(r) = r^2 |R(r)|^2$ where $R(r)$ is the radial part of the wave function. Another useful expression is the integral $\int_0^\infty \rho^k \exp(-\rho) d\rho = k!$, where k is an integer.

b) Explain (without doing any calculation!) that the eigenvalue of $\hat{\mathbf{L}}^2$ in the state ψ_{100} is zero. By inserting ψ_{100} into the eigenvalue equation, show that it is an eigenstate of $\hat{H}_0$, and determine the eigenvalue E_0 expressed in terms of natural constants. (To check your result, you may want to verify that $E_0 = 13.6$ eV.)

c) Show that the normalization constant A equals $A = 1/\sqrt{\pi} a_0^{3/2}$.

d) Calculate the expectation value $\langle r_{100} \rangle$ in this state, as well as the most probable radius (i.e. distance from the nucleus) of the electron. Briefly explain why these two results differ from each other.

Assume now that the atom is placed in an external magnetic field of strength B, directed along the z-axis. We still neglect effects due to the spin of the electron. Due to this magnetic field, the Hamiltonian thus changes from $\hat{H}_0$ to $\hat{H}_0 + \hat{H}_1$, where

$$\hat{H}_1 = \frac{eB}{2m_e} \hat{L}_z \tag{5}$$

e) Are the states ψ_{nlm_l} in equation (3) still eigenstates of this modified Hamiltonian? Explain the reasoning behind your answer. Explain why $\hat{H}_1$ splits the degeneracy you found in **a)** . Calculate the corresponding shift in energy for the various states of the $1s$ and $2p$ levels.

For the remainder of this problem, we shall return to the case of no external magnetic field and, instead, study the helium atom. For this, we shall use the simplest possible approximation where the electron-electron interaction is neglected completely. In other words, we use the simplified Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m_e} \left(\nabla_1^2 + \nabla_2^2 \right) - \frac{1}{4\pi\epsilon_0} \left(\frac{2e}{r_1} + \frac{2e}{r_2} \right) , \tag{6}$$

where the indices 1 and 2 refer to the coordinates of the two electrons. In this approximation, one assumes that the electrons occupy single-particle orbitals ϕ_{nlm_l} of the same type as in the hydrogen atom, with energies

$$E_n = -\frac{Z^2 E_0}{n^2} \tag{7}$$

where $Z = 2$ in the case of helium.

f) Write down the time independent ground state wave function (expressed in terms of the single-particle wave functions ϕ_{nlm_l}) for the two electrons in the helium atom; remember to include both the spatial part and the spin part. Calculate the ground state energy of the helium atom in this approximation.

g) Finally, let us examine the first excited state of the helium atom, with one of the electrons excited to the $2s$ orbital. Write down the allowed (time independent) wave functions for this state, again expressed in terms of ϕ_{nlm_l}. Argue qualitatively (i.e. in words) which of these configurations is expected to have the lowest energy in the real helium atom. (Hint: Exchange)