ASSESSMENT
Atomic physics

Assignment 1: Quantum basics and performing calculations

Compiled: July 2, 2026

Learning outcomes and objectives

This assignment will give you practice in

- Executing the fundamental linear algebra techniques that are required to do atomic physics
- Perform quantitative calculations using the quantum mechanical theory of hydrogen-like atoms
- Undertaking stationary perturbation theory and variational method calculations
- Predicting the hyperfine structure of an (exotic) atom

Exercise 1 *You will need this* (12 points)

We are going to have a brief refresher of linear algebra, or explicitly, the changing of our basis and the effects of this has on a rotation operator. This is a question you might find on a maths exam; however, being able to perform this task by hand is critical for quantum mechanics - indeed look at past tests and exams for this subject.
Consider the matrix

$$A = \begin{pmatrix} 4 & 0 & -3 \\ 0 & 5 & 0 \\ -3 & 0 & 4 \end{pmatrix}.$$

a. (1 mark) What is a Hermitian matrix? Is the matix A Hermitian?

b. (2 marks) Find the eigenvalues for the matrix A

c. (3 marks) Find the eigenvectors for the matrix A

d. (4 marks) Write down the diagonalising matrix P which satisfies the relation

$$P^{-1}AP = D$$

where D is the diagonal matrix constructed from each eigenvalue. Verify explicitly that this relation holds.

HINT: You shouldn't have to calculate anything to write down P. You may also use the relation that for a Hermitian Matrix A, P will be unitary, that is $P^{-1} = P^{\dagger}$ (provided things are normalised).

e. (2 marks) The namesake of Hermitian matrices, Charles Hermite, demonstrated that such matrices have the property that their eigenvalues are always real. Why is this relevant to quantum mechanics?

Exercise 2 *Like Hydrogen* (15 points)

a. (4 marks) Tritium is an isotope of hydrogen, with a nucleus comprising one proton and two neutrons. The tritium nucleus (triton) is radioactive, decaying via β emission to a helium-3 nucleus which comprises two protons and one neutron. An electron is initially in the ground state of a tritium atom. After the (instantaneous) β decay, what is the probability that the electron is in the ground state of the new atom?

b. Muons are effectively heavy electrons. They rapidly decay into electrons with a lifetime of approximately 2.2 μs - see the *lifetime of the muon experiment* in third year labs - but through some technical wizardry, it is possible to produce muonic hydrogen and perform precision spectroscopy on these atoms before they decay. Indeed, said spectroscopy has led to a still-unanswered problem, the so-called *proton radius problem*.

As muons are much heavier than electrons, muonic hydrogen is a much smaller atom than vanilla hydrogen. As such, the finite size of the nucleus plays an more significant role in the energy-level structure of the system. The effective Coulomb potential can be approximated as

$$V(r) = \begin{cases} -\frac{Ze^2}{r} & r \geq R \\ -\frac{Ze^2}{R}\left(\frac{3}{2} - \frac{1}{2}\frac{r^2}{R^2}\right) & r \leq R \end{cases}$$

where R is the region over which the nuclear charge is distributed.

i) (1 mark) Express the Hamiltonian for muonic hydrogen as a perturbation of a hydrogenic system.

ii) (3 marks) Posit how the energies for all the states with $n = 1, 2$, and 3 will be shifted. How will the levels be shifted relative to absolutely, and relatively? Draw an energy-level diagram, indicating the unperturbed states, the perturbed states, and discuss the physical origins of any differences between states.

iii) (2 marks) Calculate the first-order change in energy for the ground state of muonic hydrogen. You can make the approximation that $R \ll a_\mu$, where a_μ is the Bohr radius for the muon.
HINT: make this approximation (*very*) early!

iv) (3 marks) The charge radius R is often measured by probing the $2s \to 2p$ transition. Find an expression for the (angular) frequency of this transition, thus showing one can indeed measure R from measurement of this transition.

v) (2 marks) Can you suggest reasons that the $2s \to 2p$ transition is used to measure R instead of directly measuring the ground state energy?

Exercise 3 *Perturbation theory* (11 points)

Consider a perturbed infinite square well with the potential

$$V(x) = \begin{cases} 0 & 0 \leq x < L/2 \\ V_0 & L/2 \leq x < L \\ \infty & \text{otherwise} \end{cases}$$

a. (3 marks) Calculate the first-order energy correction for this potential

b. (6 marks) Obtain an expression for the second-order energy correction for this potential, and evaluate explicitly the correction for the ground state

HINT: The following result may be useful:

$$\sum_{n=1}^{\infty} \frac{n^2}{(4n^2-1)^3} = \frac{\pi^2}{256}$$

c. (2 marks) Sketch both the unperturbed and perturbed wavefunction, and comment on what is physics of what is occurring.

NOTE: You needn't actually evaluate the wavefunctions, a qualitative sketch will suffice.

Exercise 4 *Variational method* (15 points)

Electrons in many-electron atoms generally experience a *screened* potential, that is, a potential that is smaller in magnitude than that due solely to its interaction with the nucleus due to other electrons shielding the nuclear charge.

In atomic units, we can model this screened potential using

$$V(r) = -\frac{Z}{r} + \frac{1 - e^{-\mu r}}{r} \equiv V_0 + V'$$

where μ is a constant determined by atomic properties[a]. We are going to use our intuition and propose a trial wave function for the ground state of the form

$$|\psi_{trial}\rangle \propto e^{-\lambda Z r} Y_0^0(\theta, \phi)$$

You are going to use the variational method to find a bound on the ground-state energy.

a. (1 mark) Determined the normalisation constant for the trail wave function $|\psi_{trial}\rangle$

b. (4 marks) Calculate the expectation value $\langle\psi_{trial}|T|\psi_{trial}\rangle$, where T is the kinetic energy operator

c. (2 marks) Calculate the expectation value $\langle\psi_{trial}|V_0|\psi_{trial}\rangle$, where V_0 is the normal Coulomb potential

d. (2 marks) Calculate the expectation value $\langle\psi_{trial}|V'|\psi_{trial}\rangle$, where V' is the perturbation to the screening potential

e. (6 marks) Using the above, calculate a bound on the ground state energy of the system, assuming a screening potential of $\mu = 0.1\,\text{a.u.}^{-1}$. You may solve non-trivial polynomials computationally (indeed, it is encouraged) but ensure to include executable code in your response.

[a] The symbol μ here is convention, and is unfortunate given the question above, but the two μ are very much unrelated!

Exercise 5 *Positronium* (12 points)

In February 2024, positronium was laser cooled, heralding the era for precision measurements involving antimatter. Positronium atom is a hydrogen-like atom with a positron ($m = m_e$, $q = +e$, spin 1/2) as the nucleus and a bound electron. The hyperfine structure in the ground state of positronium is described by a perturbation Hamiltonian $H' = A\mathbf{S}_1 \cdot \mathbf{S}_2/\hbar^2$ where $\mathbf{S}_i$ are the spins of the electron and positron.

a. (2 marks) What is the Bohr energy of the ground state of positronium (that is, you can ignore the hyperfine structure)?

b. (3 marks) The electron and positron spins can be coupled to form the total spin $\mathbf{S}$ of the atom. Write down the spin states of the coupled and uncoupled bases and how they relate to each other.

c. (5 marks) Express the hyperfine Hamiltonian in the ground state as a matrix in both the coupled and uncoupled spin bases, explicitly showing how one arrives at these results.

d. (2 marks) Determine the effect of the hyperfine perturbation interaction on the ground state of positronium. Draw an energy level diagram to illustrate your results.