

**Exercise 3.1 Wave packet in one dimension**

The Schrödinger equation is a fundamental and extremely useful element of quantum mechanics. It allows us to calculate the dynamics and properties of a legion of quantum systems.

In this exercise you will get acquainted with the equation by applying it to the simplest system possible: a single particle moving in one dimension.

Let us first recapitulate some basics. The time dependent Schrödinger equation of a quantum system represented by the wave function  $\Psi(t, \vec{x})$  and ruled by the Hamiltonian  $H$  is, as you know,

$$i\hbar \frac{\partial}{\partial t} \Psi(t, \vec{x}) = H\Psi(t, \vec{x}).$$

When the Hamiltonian is time independent, the evolution of the wave function can be obtained by

$$\Psi(t, \vec{x}) = e^{-\frac{i(t-t_0)}{\hbar} H} \Psi(t_0, \vec{x}).$$

Finally, the Hamiltonian of a single particle moving in a time independent potential is given by

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}).$$

- a) Consider the wave function of a single particle. You might have heard that the square of the wave function may be interpreted as the probability that the particle can be found in a given region of space,

$$\text{Prob}[\text{particle is somewhere in region } V \text{ at instant } t] = \int_V \Psi^*(t, \vec{x}) \Psi(t, \vec{x}) d\vec{x}.$$

This interpretation makes sense only if the probability of finding the particle *anywhere in the universe* is constant over time.

Prove that this is true for the case of a particle in a time independent, one-dimensional potential:

$$\frac{d}{dt} \int_{-\infty}^{+\infty} \Psi^*(t, x) \Psi(t, x) dx = 0.$$

- b) We shall now observe a phenomenon known as the spreading of the wave packet. Consider a free particle in one dimension ( $V = 0$ ) with the initial wave function of Gaussian shape

$$\Psi(0, x) = (\pi\Delta_0^2)^{-\frac{1}{4}} \exp\left(\frac{ip_0x}{\hbar}\right) \exp\left(\frac{-x^2}{2\Delta_0^2}\right).$$

Show that, at generic instant  $t$ , the wave is still a Gaussian, of width

$$\Delta(t) = \Delta_0 \sqrt{1 + \frac{\hbar^2 t^2}{m^2 \Delta_0^4}}.$$

What happens to the mean position and mean momentum of the particle over time? And to the uncertainty on these quantities?

- c) Suppose now that the particle feels the influence of a slowly varying potential  $V(x)$ . How does that affect the previous result?

**Exercise 3.2 Hydrogen atom and Rydberg constant**

In this exercise you will see how to determine the value of the Rydberg constant  $R$  using only results from classical and old quantum theory about the structure of the atoms.

- a) Consider an atom formed by an electron orbiting a single proton. Use the fact that the electron is in a Coulomb potential of the form  $U = -ke^2/r$  and Kepler's laws for the motion of classical rigid bodies in such potentials to derive the relation

$$\nu(E) = \frac{1}{\pi e^2} \sqrt{\frac{2|E|^3}{m}},$$

where  $\nu$  is the frequency of a given orbital and  $E$  the energy associated with that orbital. Recall now Bohr's prediction for the energy of each energy level of the discrete hydrogen spectrum,

$$E_n = -\hbar R \frac{1}{n^2}.$$

If we further consider Einstein's relation  $E = \hbar\nu$ , what is the expression for the frequency of the photons emitted when the electrons jumps from the energy level  $n$  to the  $n - k$  one, in the limit  $n \gg 1$ ? Relate these results to obtain the value of the Rydberg constant,

$$R = \frac{2\pi^2 m e^4}{h^3}.$$

- b) Imagine now that you are a PhD student in the beginning of the twentieth century, before Heisenberg's uncertainty principle was known. Your supervisor tells you that he would like to observe the trajectory of an electron orbiting the nucleus of a hydrogen atom and urges you to design and assemble an experiment that would allow one to do so. Before getting your hands dirty, you decide to make some simple calculations. Explain why such experiment would not be realisable.

**Tip:** Suppose you want to detect the electron by scattering with another particle (eg. a photon). Which conditions would you have to impose on this particle in order to achieve resolution of the order of the radius of the atom? What would happen to an electron hit by a particle fulfilling those conditions? Can you think of another way of following the trajectory of the electron?

### Exercise 3.3 Spatial quantisation: the Stern-Gerlach experiment

The Stern-Gerlach experiment was massively important – it led to the notion of quantisation of space, among others. Imagine a small magnetic dipole passing through a magnetic field that is perpendicular to the initial velocity of the centre of mass of the dipole. If the field is not uniform, the trajectory of the dipole will be deflected by an angle that depends on the angle between the dipole and the magnetic field. Classically this angle may vary continuously, so if several dipoles were shot through the field, they would form a continuous spectrum as they hit a screen. However, when electrons were used in the experiment, a discrete spectrum was observed, which motivated the assumption that electrons have a quantized intrinsic angular momentum – the spin.

- a) First we consider an uniform magnetic field  $\vec{B}$  and the classical Hamiltonian

$$H = -\vec{\mu} \cdot \vec{B},$$

with the magnetic moment of the electron given by  $\vec{\mu} = \mu_B \vec{L}$ , where  $\mu_B$  is a constant.

Use the classical Poisson bracket formalism to derive the result

$$\dot{\vec{L}} = \mu_B \vec{L} \times \vec{B}.$$

Note that this implies a precession of the dipole in the magnetic field, with the component of  $\vec{L}$  that is parallel to the field remaining constant and the perpendicular components varying.

- b) Consider now that the electron has to travel through a segment of length  $l$  along the  $\hat{x}$  direction where there is a perpendicular magnetic field that varies along this direction,  $\vec{B} = B(x)\hat{z}$ .

Using the relation  $\vec{F} = -\nabla H$ , derive an expression for the angle between the velocity of the electron as it entered the field and its velocity after being deflected through by the magnetic field.

What does the fact that a discrete spectrum of final deflection angles was observed tell you about the nature of  $\vec{\mu}$ ?