

Tutorial 1 - Introduction to quantum mechanics

Reminder on universal constants :

$$h = 6.64 \times 10^{-34} \text{ J.s}, \hbar = h/2\pi, k_B = 10^{-23} \text{ J.kg}^{-1}, c = 3 \times 10^8 \text{ m.s}^{-1}, m_e = 9 \times 10^{-31} \text{ kg}, m_p = 1.6 \times 10^{-27} \text{ kg}, e = 1.6 \times 10^{-19} \text{ C}$$

1 Flat potential well

A quantum well is a potential landscape strongly confining particles in a narrow region of space. Such potential wells are not only the most standard example of quantum mechanics - they also successfully account for practical situations. From an applied perspective, potential wells are well suited to describe quantum dots, where brutal changes in the structure of the material result in a tight confinement (\sim nm) of the electrons. From a more fundamental perspective, potential wells provide a good model for atomic nuclei, where nucleons (protons and neutrons) are confined in a $\sim 10^{-15}$ m radius by the strong interaction.

Let us consider a particle of mass m in a potential well

$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ V_0 & x < 0 \text{ or } x > L \end{cases} \quad (1)$$

where the Hamiltonian is given by

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad (2)$$

For simplicity, we will restrict the problem to 1D and will assume the well to be infinitely deep ($V_0 = +\infty$), such that

$$\psi(x) = 0 \text{ if } x \leq 0 \text{ or } x \geq L \quad (3)$$

1. Show that the eigenstates of the Hamiltonian are the wave functions $|\phi_n\rangle$ such that

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \quad (4)$$

with energies

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} = n^2 E_0 \quad (5)$$

2. Scratch your head a bit to try and find how this result can be interesting from an energy perspective.
Hint: you can use it to estimate orders of magnitudes.
3. To prepare the next lecture, generalize these results to an infinitely deep well in 3D, and to an infinitely deep 1D well with size $L \rightarrow \infty$.

2 Quantum rules

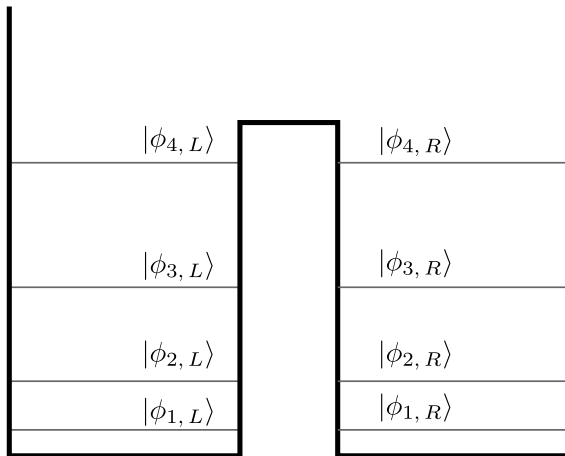
The aim of the exercise is to have you play with basic quantum mechanics postulates.

1. Let's consider that the particle is in the state $|\psi\rangle = \frac{1}{\sqrt{2}} |\phi_2\rangle - \frac{1}{\sqrt{3}} |\phi_3\rangle + \frac{e^{i\pi/4}}{\sqrt{6}} |\phi_5\rangle$.
 - (a) If we measure the energy of the particle, what is the probability of finding the value E_0 ? $2 E_0$? $4 E_0$? $16 E_0$? $25 E_0$?
 - (b) Let's assume we have a large number of systems all prepared in the state $|\psi\rangle$. We measure the energy of each of them. What's the average value ?

2. If the particle is in the eigenstate $|\phi_2\rangle$, what is the density of probability of finding the particle at any position x_0 ? What is the average position of the particle? How does the average position evolve over time?
3. We prepare the system in the initial state $\psi_0(x) = \sqrt{\frac{1}{L}} \sin\left(\frac{\pi x}{L}\right) + \sqrt{\frac{1}{L}} \sin\left(\frac{2\pi x}{L}\right)$. Express the time evolution of this state.
 - (a) What is the average position of the particle as a function of time?
 - (b) What is the average energy of the particle as a function of time?

3 Double well

We now consider a double well structure (see fig. below).



- We first assume that the two wells are isolated (ie the middle barrier is very high) and note H_0 the corresponding Hamiltonian - the expression of which will not be calculate. In each well, as studied above, the eigenstates of the Hamiltonian have discrete energy values and we label them $\{|\phi_{n,L}\rangle\}$ in the left well and $\{|\phi_{n,R}\rangle\}$ in the right well respectively. Each value E_n of the energy spectrum thus corresponds to two states (namely $|\phi_{n,L}\rangle$ and $|\phi_{n,R}\rangle$) - ie each energy is twice degenerated.

- We now take into account the tunnel transition through the separation wall by considering an additional coupling term V such that

$$\hat{V} |\phi_{n,L}\rangle = -J |\phi_{n,R}\rangle \quad (6)$$

$$\hat{V} |\phi_{n,R}\rangle = -J |\phi_{n,L}\rangle \quad (7)$$

1. Write the total Hamiltonian $H = H_0 + V$ in the basis of $\{|\phi_{n,L}\rangle, |\phi_{n,R}\rangle\}$
2. Find the eigenstates of the total Hamiltonian, and the corresponding energies.