Exercises 3

Exercise 3.1

A particle is confined in a linear box of length L surrounded by walls of infinite potential. The ground state of this system is described by the following wave function:

$$\Psi_1(x) = \sqrt{\frac{2}{L}} \times \sin\left(\frac{\pi x}{L}\right)$$

a) What is the probability of finding the particle at a given position x?
b) At which position is the maximum probability density?
c) What is the total probability of finding the particle in the box?
d) If L = 10 nm, what is the probability that the particle is between 4:95 and 5:05 nm?

Note: Exercise 3.1 will be solved on the board during the exercise session this Friday, September 27, 2024.

a) As we saw, the probability density of finding the particle at a given position x is given by the square of the wavefunction :

$$\Psi_1(x)^2 = \left(\sqrt{\frac{2}{L}}\sin\left(\pi\frac{x}{L}\right)\right)^2 = \frac{2}{L}\sin^2\left(\pi\frac{x}{L}\right)$$

And the probability itself is calculated by integrating the probability density between two points. Therefore, if we calculate the probability of finding the particle at a single specific position x, the bornes of the integral are the same :

$$\int_x^x \Psi_1(x)^2 dx$$

and consequently the integral yields 0. The probability of finding the particle at a particular position x iequals zero.

b) The position with the highest probability corresponds to the maximum of the probability density functions $\Psi_1(x)^2$. A look at the graphical representation of the wavefunction shows a peak at the middle of the box ($x = \frac{L}{2}$), otherwise it can be calculated. When $\Psi^2{}_1$ is at its maximum, its first derivative must be equal to zero :

$$\begin{aligned} 0 = \Psi_1^2(x)' &= \left[\tfrac{2}{L}\sin^2\left(\tfrac{\pi x}{L}\right)\right]' \\ &= \left[\tfrac{1}{L} - \tfrac{1}{L}\cos\left(\tfrac{2\pi x}{L}\right)\right]' \\ &= \tfrac{1}{L}\sin\left(\tfrac{2\pi x}{L}\right)\cdot\tfrac{2\pi}{L} \end{aligned} \quad \text{using, } \sin^2\alpha = \tfrac{1-\cos(2\alpha)}{2}$$

Since $\sin\left(\frac{2\pi x}{L}\right) = 0$, then $\frac{2\pi x}{L} = 0 + k\pi$ with k a positive integer. Moreover since $x \in [0, L]$, $x = \frac{L}{2}$
.

$x = 0$ and $x = L$ also yield first derivative euqal to zero, however they correspond to mimima and not maxima. This can be easily verified by calculated the second derivative of $\Psi_1^2(x)$:

$$\Psi_1^2(x)'' = \left(\frac{2\pi}{L^2}\sin\left(\frac{2\pi x}{L}\right)\right)' = \frac{4\pi^2}{L^3}\cos\left(\frac{2\pi x}{L}\right)$$

Therefore when $x = 0$ ou $x = L$ the second derivative is positive whereas it's negative for $x = L/2$. A second derivative yielding negative values matches a maximum.

c) The particle is confined wihtin the box so the totale probability of finding the particule inside the box must be 1, this can be verified by integrating Ψ_1^2 from 0 to L :

$$\begin{aligned}\int_0^L \Psi_1^2(x)dx &= \int_0^L \tfrac{2}{L}\sin^2\left(\pi\tfrac{x}{L}\right)dx \\ &= \tfrac{2}{L}\int_0^L \tfrac{1-\cos\left(2\pi\frac{x}{L}\right)}{2}dx \\ &= \tfrac{1}{L}\int_0^L dx - \tfrac{1}{L}\int_0^L \cos\left(2\pi\tfrac{x}{L}\right)dx \\ &= \tfrac{1}{L}(L-0) - \tfrac{1}{L}\tfrac{L}{2\pi}\left[\sin\left(2\pi\tfrac{x}{L}\right)\right]_0^L \\ &= 1 - \tfrac{1}{2\pi}\cdot(0-0) = 1\end{aligned}$$

en utilisant $\sin^2\alpha = \frac{1-\cos(2\alpha)}{2}$

d) Following the same procedure, with $L = 10$, we find:

$$\begin{aligned}P(4.95 \le x \le 5.05) &= \int_{4.95}^{5.05}\Psi^2(x)dx = \ldots \\ &= \tfrac{1}{10}(5.05-4.95) - \tfrac{1}{2\pi}\left\{\sin\left(2\pi\tfrac{5.05}{10}\right) - \sin\left(2\pi\tfrac{4.95}{10}\right)\right\} \cong 0.02\end{aligned}$$

The particle has therefore a probability of approx. 2% of being found between 4.95 and 5.05 nm.

Exercise 3.2

The total energy of the particle in the box can be calculated as

$$E_{\text{tot}} = E_{\text{kin}} + E_{\text{pot}},$$

where the kinetic energy is given by

$$E_{\text{kin}} = \frac{1}{2}mv^2.$$

Write down an expression for the total energy of the particle in the box, using the de Broglie relationship ($p = mv = \frac{h}{\lambda}$) and the fact that the wavelength must satisfy $\lambda = \frac{2L}{n}$.
What is the main implication of this equation?

Following the expression for the total energy and substituting, we get:

$$E_{\text{tot}} = \frac{1}{2}mv^2 + 0,$$

since $E_{\text{pot}} = 0$ inside the box.

Finally substituting the momentum, we obtain:

$$E_{\text{tot}} = \frac{1}{2}\frac{(mv)^2}{m}$$

$$\text{E}_{\text{tot}} = \frac{1}{2m}p^2 = \frac{1}{2m}\frac{h^2}{\lambda^2} = \frac{1}{2m}\frac{h^2n^2}{(2\text{L})^2} = \frac{n^2h^2}{8mL^2}.$$

Exercise 3.3

True or False?

a) The ground state energy of a particle in a box (PDB) is zero.
b) The energy levels of the PDB are equidistant.
c) Increasing the steady-state energy of the PDB is equivalent to increasing the number of nodes in the wave function.
d) All solutions of the time-independent Schrödinger equation for the PDB are allowed steady-state wave functions.
e) The transition of the PDB that absorbs the longest wavelength photon is from the n = 1 level to the n = 2 level.

(a) False: the energy of a particle in a one-dimensional box is described by $\text{E}\ (n) = \frac{h^2n^2}{8mL^2}$. The fundamental state corresponds to n = 1 and its energy is greater than zero. n = 0 is not a solution for the particle in a box.

(b) False. They become further and further apart as energy increases, as they are proportional to n^2.

(c) True. The wave function $\Psi_n(x) = \sqrt{\frac{2}{L}} \times \sin\left(\frac{n\pi x}{L}\right)$ has n - 1 nodes.

(d) True. The time-independent Schrödinger equation ($\hat{H}\Psi = E\Psi$) describes all eprmis stationary states characterized by an eigenvalue (E) and an eigenfunction (Ψ).

(e) True. $\Delta E \propto n_2^2 - n_1^2$ so the smallest possible energy (corresponding to the longest possible wavelength) for a transition from n_1 to n_2 corresponds to the first transition (n_1 = 1 and n_2= 2).

Exercise 3.4

The concept of quantization of energy is foundational in quantum mechanics. In atomic systems, electrons can only occupy specific, quantized energy levels. ~~However, when a photon with energy greater than the difference between two energy levels interacts with an atom, the electron can transition to a higher energy level, and the excess energy becomes kinetic energy of the electron~~.

Given: The energy levels of the hydrogen atom are described by the formula:

$$E_n = -\frac{13.6\ eV}{n^2}$$

a) Calculate the energy of the first two energy levels (n=1 and n=2) of the hydrogen atom.

b) ~~If the electron in the hydrogen atom absorbs a photon with an energy of 12 eV while in the ground state (n=1), to which energy level, if any, will the electron transition? Calculate the kinetic energy acquired by the electron due to the excess energy from the photon.~~

c) ~~Based on your results, discuss the implications for atomic systems when they interact with high-energy photons.~~

Solution:

a) Using the provided formula:

For n=1: E_1=−13.6 eV
For n=2: E_2=−3.4 eV

b) ~~Energy needed for the transition from n=1 to n=2:~~ $\cancel{\Delta E = E_2 - E_1 = 10.2\ \text{eV}}$

~~Given photon energy = 12 eV~~

~~Excess energy which will become kinetic energy (KE):~~

$\cancel{\text{KE}=12\ eV-10.2\ eV=1.8\ eV}$

~~Thus, after absorbing the photon, the electron transitions to the n=2 level and also acquires a kinetic energy of 1.8 eV due to the excess energy of the photon.~~

We removed this exercise because the photon's energy, 12 eV, does not correspond to any of the possible transition from $n = 1$ to $n > 1$ the photon will not be absorbed. According to the energy quantization principle, only photons/radiation with energy matching exactly the difference between two energy levels, n_i and n_j (with $\mathrm{E}(\mathrm{n}_i) < \mathrm{E}(\mathrm{n}_j)$) can be absorbed by the system to promote an electron to the n_j level.

b) ~~When atomic systems interact with high-energy photons that provide more energy than required for a transition between quantized levels, the excess energy isn't wasted. Instead, it becomes kinetic energy of the electron. This can lead to the electron moving faster within the atom or potentially being ejected from the atom entirely, a phenomenon known in atomic physics as the photoelectric effect.~~

We also removed this exercise because we did not talk about high-energy photons in class. If you are interested in learning more, feel free to read onwards. the interaction between atomic systems and photons can lead to three distinct processes, categorized by the energy range of the incident photons:

1. **Low-Energy Regime (Visible to Early UV)**: In this range, interactions are governed by quantum mechanical principles, particularly energy quantization.

This results in discrete spectral lines in absorption and emission spectra, where transitions between energy levels are either allowed or forbidden based on quantum rules (as seen in class!)-

2. **Moderate-Energy Regime (UV)**: In this range, photoionization becomes the dominant process. When a photon's energy exceeds the electron's binding energy, the photon ejects the electron, producing a free electron. The kinetic energy of the electron will correspond to the excess energy beyond the ionization potential, following the photoelectric effect (as seen in class!).
3. **High-Energy Regime (X-rays to Gamma Rays)**: At photon energies beyond the electron rest energy (~511 keV), scattering processes like Thomson and Compton scattering dominate. As photon energies increase further into the MeV range (gamma rays), more complex interactions occur, including pair production, photodisintegration, and photofission. These high-energy processes involve interactions with both atomic nuclei and electrons (not seen in class!).