TFY4235 - The World of Quantum Mechanics

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Abstract

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1. Introduction

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \tag{1}$$

$$H\psi_n = E_n\psi_n \tag{2}$$

2. The Hamiltonian

The Schrödinger equation tells us the time-evolution of the wave function, which, according to the Copenhagen interpretation of quantum mechanics, has the physical interpretation of a probability amplitude when squaring the absolute value. In our current setup, where we have

$$V = \begin{cases} 0, & 0 < x < L \\ \infty, & \text{otherwise} \end{cases}, \tag{3}$$

there is 0% chance of finding the particle inside the "walls" (at $x < 0$ or $x > L$). Thus, the wave function must go to zero at these points. Defining $x' = x/L$ and $t' = t/t_0$, and inserting in Equation (1).

$$\begin{aligned} i\hbar\frac{\partial\psi}{\partial t} &= i\hbar\frac{\partial\psi}{\partial t'}\frac{\partial t'}{\partial t} = \frac{-\hbar^2}{2mL^2}\frac{\partial^2\psi}{\partial x'^2} \\ \implies i\frac{\partial\psi}{\partial t'} &= \frac{-\hbar}{2mL^2\frac{\partial t'}{\partial t}}\frac{\partial\psi}{\partial x'^2} \end{aligned}$$

Thus, setting

$$t' = \frac{\hbar}{2mL^2}t, \quad x' = \frac{x}{L} \tag{4}$$

gives the wanted dimensionless equation

$$i\frac{\partial\psi}{\partial t'} = -\frac{\partial^2\psi}{\partial x'^2} \tag{5}$$

Inserting our new variables in Equation (2) with

$$H = \frac{\hat{p}^2}{2m} + V(x) = -\frac{-\hbar}{2mL^2}\frac{\partial^2}{\partial x'^2} + \tilde{V}(x')$$

, we get

$$\begin{aligned} \frac{-\hbar^2}{2mL^2}\frac{\partial^2\psi_n}{\partial x'^2} &= E_n\psi_n \implies \\ -\frac{\partial^2\psi_n}{\partial x'^2} &= \lambda_n\psi_n, \end{aligned} \tag{6}$$

with the relation

$$\lambda_n = \frac{2mL^2E_n}{\hbar^2} \tag{7}$$

between the energy levels and the dimensionless eigenvalues. The boundary conditions that the wave function disappears in the walls, but the walls are now at $x' = 0$ and $x' = 1$. It is now clear that choosing $x_0 = L$ is suitable, as it makes us able to work on the simple domain $[0, 1]$. Any other proportionality constant $\alpha \in \mathbb{R}$ such that $x' = \alpha x/L$ should work as well, scaling both the time and energies by a factor α^2, as long as x' is dimensionless. Other scaling possibilites are also possible, and have consequences for the analytic expressions for ψ. For example scaling the interval to be mirrored about $x = 0$ would only pick out the even terms in a Fourier series expansion.

Solving Equation (6) with the imposed boundary conditions can be done analytically in the following manner. Since we are looking for solutions that have self-similar second derivatives with an extra minussign, we guess a solution on the form $\psi = A_n\sin(\sqrt{\lambda_n}x') + B_n\cos(\sqrt{\lambda_n}x')$. The boundary condition $\psi(x' = 0) = 0$ gives $B_n = 0$, while the boundary condition $\psi(x' = 1) = 0$ gives the restriction to λ_n that $\sqrt{\lambda_n} = n\pi$, hence the labels n are also justified. Our analytic solution is therefore

$$\psi_n(x') = \mathcal{N}\sin(\pi n x'), \tag{8}$$

where $\mathcal{N}$ is a normalization constant to be decided.

$$\begin{aligned} 1 = \langle\psi_n|\psi_n\rangle &= \mathcal{N}^2\int_0^1 \mathrm{d}x'\sin^2(n\pi x') \\ &= \mathcal{N}^2\int_0^1 \mathrm{d}x'\,\frac{1-\cos(2\pi n x')}{2} = \frac{\mathcal{N}^2}{2} \\ &\implies \mathcal{N} = \sqrt{2}. \end{aligned}$$

References