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. Quantum mechanics in a box

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 possibilities 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 $\psi = A_n\sin\left(\sqrt{\lambda_n}x'\right) + B_n\cos\left(\sqrt{\lambda_n}x'\right)$. 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.

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

and we have the analytic solution as announced in [1].

The implementation of a finite-difference-scheme is done using sparse matrix formatting for the cases when the discretization step is very small. Otherwise a dense matrix format is sufficient.

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The implementation of

$$\alpha_n = \langle \psi_n | \Psi_0 \rangle = \int \mathrm{d}x' \, \psi_n^*(x')\Psi_0(x') \tag{9}$$

can be done in a simple fashion by taking optimized inner-product implementations for general vectors, so calculating the actual integral is actually not needed.

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To compute the error of a numerical solution, we must have a metric of some sort. Let us use

$$E[\bar{\psi}_n(x')] = \int \mathrm{d}x' \, |\bar{\psi}_n(x') - \psi_n(x')|^2 \tag{10}$$

of

as an example, where the bar denotes the numerical approximation to the analytic function. Using the reduced units previously discussed, we can express the full state

$$\Psi(x,t) = \sum_n \alpha_n \exp\left(-\frac{iE_n t}{\hbar}\right)\psi_n(x) \tag{11}$$

as

$$\begin{aligned}
\sum_n \alpha_n \exp\left(-\frac{iE_n t}{\hbar}\right)\psi_n(x) &= \sum_n \alpha_n \exp\left(-\frac{iE_n t}{\hbar}\right)\psi_n(x) \\
&= \sum_n \exp\left(-\frac{i\frac{\hbar^2\lambda_n}{2mL^2}\frac{2mL^2t'}{\hbar}}{\hbar}\right)\psi_n(x') \\
&= \sum_n \alpha_n \exp(-i\lambda_n t')\psi_n(x').
\end{aligned}$$

3. Adding a barrier to the boc-potential

Let us now consider a potential barrier in the box, modeled by the dimensionless potential $\nu(x') = t_0 V_0/\hbar$, where $t_0 = \frac{2mL^2}{\hbar}$ as in Equation (4), and is given by

$$\nu(x') = \begin{cases} 0, & 0 < x' < \frac{1}{3} \\ \frac{2mL^2V_0}{\hbar^2}, & \frac{1}{3} < x' < \frac{2}{3} \\ 0, & \frac{2}{3} < x' < 1 \\ \infty, & \text{otherwise} \end{cases} \tag{12}$$

References

[1] J. T. Kjellstadli, A. Sala, and I. Simonsen. Assignment 3: The world of quantum mechanics. `http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/Assignments/TFY4235_Assignment_03.pdf`, 2020.