50.117 Graphics and Visualization

Final Project Report

Cheryl Goh Qian Ping (1002421)
Tan Ting Yu (1002169)
Reuben Wang Rong Wen (1001519)

§ Introduction §

Non-relativistic quantum mechanics presents itself as a rich field of study which, despite its success, remains strange and unintuitive even to its greatest proponents. The governing equation of quantum mechanical systems is the famed Schrödinger's equation:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\Psi(x,t) &= \hat{H}\Psi(x,t) \\ \hat{H} &= \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right] \end{aligned} \tag{1}$$

for which this is relevant in the context of 1D systems. Even when constrained to exit along 1D, quantum particles (as represented by the wavefunction $\Psi(x,t)$) exhibit interesting and non-trivial dynamics. Furthermore, the wavefunctions exist over a complex field ($\Psi(x,t) \in \mathbb{C}$), making its visualization in spatial dimensions higher than 1 impossible (1 spatial dimension and 2 Argand plane axes already constitute 3 dimensions for visualization).

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§1 Project Overview

In this work, we have implemented a dynamic visualization of the time-evolution of a quantum wavefunction in 1D, subjected to an infinite-square well potential. A visualization of the infinite-square well potential and its lowest order ($n = 1, 2, 3$) *stationary* solutions are given in figure 1 below.

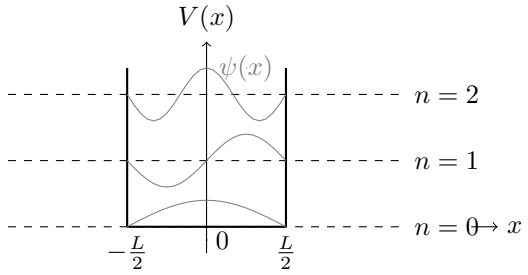

Figure 1: $n = 1, 2, 3$ Infinite-Square Well Wave Functions

In our visualization, we have made the fictitious surface that connects the wavefunction to the coordinate axis flow like a cloth system purely for graphical output visualization purposes. We have also implemented normal mappings and coloring for added aesthetic appeal. In the next section, we describe the mathematical model we employ to simulate our quantum system.

§2 The Quantum Model

The infinte-square well potential can be effectively modelled as using a piece-wise function. This system is also often referred to as a *particle in a box*. Mathematically, we write the potential as:

$$V(x) = \begin{cases} 0, & -\frac{L}{2} < x < \frac{L}{2} \\ \infty, & \text{otherwise} \end{cases} \tag{2}$$

Because the particle is trapped within the region $x \in \left[-\frac{L}{2}, \frac{L}{2}\right]$ region, the wave function **must** vanish at $x = -L/2$ and $x = L/2$. The first step in obtaining solutions to the Schrödinger equation is to look for separable solutions. These solutions are also known as *stationary states* (time-independent states).

§2.1 Stationary States

To solve for stationary states, we first assert that the solutions we look for are separable:

$$\Psi(x,t) = \psi(x)f(t) \tag{3}$$

plugging this into Schrdinger's equation, we get

$$\begin{aligned} & i\hbar\frac{df(t)}{dt}\psi(x) = \Big(\hat{H}\psi(x)\Big)f(t) \\ \Rightarrow\ & i\hbar\frac{1}{f(t)}\frac{df(t)}{dt} = \frac{1}{\psi(x)}\hat{H}\psi(x) \end{aligned} \tag{4}$$

Because the left-hand side is solely dependent on t whereas the right-hand side is solely dependent on x, the only way these 2 sides could be equal is if they were both equal to a constant. Dimensional analysis dictates that this constant has units of energy, making it convenient to label the separation constant as E. As such, we arrive at the following 2 equations:

$$\begin{cases} i\hbar\frac{df(t)}{dt} = Ef(t) \\ \hat{H}\psi(x) = E\psi(x) \end{cases} \tag{5}$$

Looking first at the time dependent equation:

$$\begin{aligned} & \frac{df(t)}{dt} = -\frac{iE}{\hbar}f(t) \\ \Rightarrow\ & f(t) = f(0)e^{-\frac{iE}{\hbar}t} \end{aligned} \tag{6}$$

With this result, we can write our stationary state as:

$$\Psi(x,t) = \psi(x)e^{-\frac{iE}{\hbar}t} \tag{7}$$

The stationary states $\psi(x)$ actually solves the eigenvalue problem:

$$\hat{H}\psi(x) = E\psi(x) \tag{8}$$

and are hence also known as *energy eigenstates*. The *spectral theorem* states that any arbitrary quantum state can be constructed from a superposition (linear combination) of eigenstates. Hence, we can always construct quantum state from a superposition of stationary states:

$$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} \alpha_n \psi_n(x) e^{-\frac{iE_n}{\hbar}t}} \tag{9}$$

§2.2 ISW Energy Eigenstates

In order to find the closed-form solutions to the energy eigenstates $\psi(x)$ of the infinite-square well (ISW) potential, we set-up our problem with knowledge of differential equations as follows:

$$\begin{aligned} & -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x), \quad x \in \left[-\frac{L}{2}, \frac{L}{2}\right] \\ \Rightarrow\ & \psi(x) = Ae^{ikx} + Be^{-ikx} \end{aligned}$$

Applying the boundary conditions.

$$\begin{aligned} \psi(-\frac{L}{2}) = 0 \quad &\Rightarrow \quad Ae^{-ik\frac{L}{2}} + Be^{ik\frac{L}{2}} = 0 \\ \psi(\frac{L}{2}) = 0 \quad &\Rightarrow \quad Ae^{ik\frac{L}{2}} + Be^{-ik\frac{L}{2}} = 0 \\ \Rightarrow \quad & 2iB\sin(kL) = 0 \\ \Rightarrow \quad & k_n = \frac{n\pi}{L}, \quad n \in \mathbb{N}\backslash\{0\} \end{aligned} \tag{10}$$

where n is called the *quantization* index and dictates the energy state of the particle. The associate energy eigenstate is then:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{R}(x + \frac{L}{2})\right) \tag{11}$$

Which means any wavefunction of the infinite-square well can be written as:

$$\Psi(x,t) = \sum_{n=1}^{\infty} \alpha_n \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{R}(x + \frac{L}{2})\right) e^{-\frac{iE_n}{\hbar}t} \tag{12}$$

This is the basis of how we build our wavefunctions in our implemented simulation. For our simulation, we are using a linear combination of 5 energy eigenstates with equal coefficients:

$$\boxed{\Psi(x,t) = \mathcal{N} \sum_{n=n_{min}}^{n_{min}+5} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{R}(x + \frac{L}{2})\right) e^{-\frac{iE_n}{\hbar}t}} \tag{13}$$

where $\mathcal{N}$ is the overall normalization constant.

§3 The Cloth System

Cloth systems are well covered in this course, for which we have made use of this to add to the visual appeal of our final output. We have implemented a particle system cloth model via the 2D lattice technique employed in assignment 3. In order to solve the equations of motion for lattice node (particle), our default numerical solver uses the *Runge-Kutta 4th order (RK4) method*. However, we have also implemented the forward Euler method, trapezoidal method and Runge–Kutta–Fehlberg (RKF45) methods as optional arguments to the user.

§3.1 Cloth and Quantum System

We integrate our cloth system with our quantum wavefunction by superimposing the 2 different spaces. The 2 spaces we need to integrate are:

1. Cloth System: 3-dimensional real-coordinate space ($\mathbb{R}^3$), having the standard Cartesian (x, y, z) axes.
2. Quantum System: $1+2$-dimensional real-space, with axes representing $(x, \text{Re}\{\Psi(x,t)\}, \text{Im}\{\Psi(x,t)\})$. Note that $\Psi(x,t)$ lives in a Hilbert space (complex vector space with an inner-product).

The convention we use to map the axes of the quantum system to the cloth system is as follows:

$$\begin{aligned} x \quad &\rightarrow \quad x \\ \text{Re}\{\Psi\} \quad &\rightarrow \quad y \\ \text{Im}\{\Psi\} \quad &\rightarrow \quad z \end{aligned} \tag{14}$$

To this end, the values of the wavefunction at every value of x, $\Psi(x,t)$ will form a boundary/rope that guides the cloth along. The other edge of the cloth will be fixed to the x-axis. A visualization of this is given in figure 2 below.

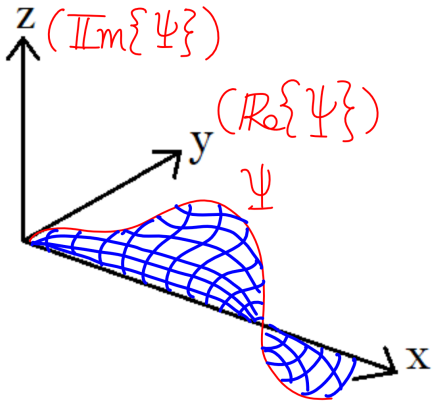

Figure 2: Red indicates the quantum wavefunction, blue indicates the cloth system.

We have implemented a vertex normal mapping along with the cloth system which allows users to toggle between the wire frame and smooth cloth modes. However, since the cloth system works on iterative force addition while wavefunction evolution specifies values of the wavefunction itself during unitary time-evolution, we need to manually compute the effective force that would act on the initialized wavefunction 'rope'. To do so, we did a naive forward (finite) difference derivative approximation twice to attain the 'acceleration' of the rope:

$$\begin{aligned} \mathcal{X}(t) &= \begin{bmatrix} \text{Re}\{\Psi(x,t)\} \\ \text{Im}\{\Psi(x,t)\} \end{bmatrix} \\ \Rightarrow \quad \mathcal{V}(t) &\approx \begin{bmatrix} \frac{\text{Re}\{\Psi(x,t)\} - \text{Re}\{\Psi(x,t-dt)\}}{dt} \\ \frac{\text{Im}\{\Psi(x,t)\} - \text{Im}\{\Psi(x,t-dt)\}}{dt} \end{bmatrix} \\ \Rightarrow \quad \mathcal{A}(t) &\approx \begin{bmatrix} \frac{\mathcal{V}_y(t) - \mathcal{V}_y(t-dt)}{dt} \\ \frac{\mathcal{V}_z(t) - \mathcal{V}_z(t-dt)}{dt} \end{bmatrix} \end{aligned} \tag{15}$$

This approximation however, causes an accumulation of errors if the simulation is left running for too long and future works should implement a more numerically stable derivative approximation method.

§3.2 Cloth Coloring

To provide some colors for the cloth wire mesh, we used OpenGL's default glColor3f function which take in 3 floating point values for red, green and blue respectively. We decided to pass randomised floating point values into this function to make the wire mesh have this "trippy" effect where the colors seem to change continuously. A visualization of this is given in figure 3 below.

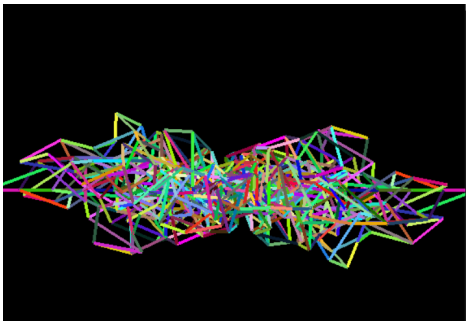

Figure 3: Colored wire mesh rendered.

Similarly, for the cloth surface, we decided to use similar approach to render a multi-coloured surface as well. We then used OpenGL's glMaterialfv function which takes in 3 arguments, namely: GLenum face, GLenum pname and GLfloat array of the color values. The GLfloat array consists of the randomised RGB values similar to what was done in the wire mesh rendering. A visualization of this is given in figure 4 below.

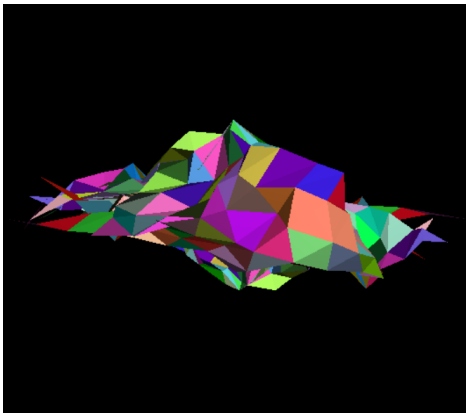

Figure 4: Colored cloth surface rendered.