Simulating a two dimensional particle in a square quantum box with CUDA

George Zakhour

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Contents

1 Background, Motive and Experiment

The particle in box problem is one of the first problems given to undergraduate students in a course about quantum mechanics. It showcases how the energy of particles is quantized and it highlights the probabilistic nature of quantum mechanics, especially with the idea that the particle is not located in a fixed position but it has a likelihood of existing at any point in space.

The particle in a box is an experiment in which a particle is stuck inside a box and cannot escape. The energy outside this box is ∞ while inside it is 0. The particle thus moves inside the box of dimensions LxL.

Trying to imagine how these probabilities are scattered in the box is hard and one can't do without a simulation of the physical properties of the particle (position, energy and momentum).

In this simulation I try and simulate the "particle in a box" problem to display the probabilities of the position and the energy of the particle at each state.

2 Expected Output

Searching online, I have found a Youtube video that simulates the particle in a box[1], but lacks essential information on the state of the system, for example the dimensions of the box and the energy levels of the particle at each frame. Although lacking these essential variables I will base my results on the video.

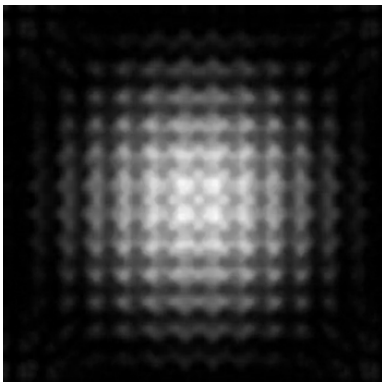

Figure 1: A screenshot of a "particle in a box" simulation found on Youtube

[1] Particle in a Box - Youtube $h$ttp://www.youtube.com/watch?v=jevKmFfcaxE

3 The mathematics of a particle in a box

3.1 In one dimension

3.1.1 Finding the Wave Function from Schrodinger's Equation

The time dependent Schrodinger equation is given as:

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V\right)\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) \tag{1}$$

The time independent Schrodinger equation is given as:

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V\right)\Phi(x) = E\Phi(x) \tag{2}$$

Where Ψ is the wave equation. In terms of Φ, Ψ is denoted as:

$$\Psi(x,t) = e^{-i(E/\hbar)t}\Phi(x) \tag{3}$$

Assuming the following is a solution to (2):

$$\Phi(x) = A\cos(kx) + B\sin(kx) \tag{4}$$

And given these two conditions that arise from the experiment:

$$\Phi(0) = \Phi(L) = 0$$

We plug them in the (4) and find the following:

$$\begin{cases} A &= 0 \\ k &= \frac{n}{L}\pi \quad \text{(n is the energy level)} \end{cases} \tag{5}$$

To find the value of B we need to normalize the equation.
The probability of finding the particle inside $[0; L]$ is 1 because it cannot escape.

$$\int_0^L |\Phi|^2 dx = 1 \tag{6}$$

$$B^2\int_0^L \sin^2\left(\frac{n}{L}\pi x\right)dx = 1 \tag{7}$$

And thus $B = \sqrt{\frac{2}{L}}$.
Finally we get the solution to the time independent Schrodinger equation

$$\Phi(x) = \sqrt{\frac{2}{L}}\sin(\frac{n}{L}\pi x) \tag{8}$$

3.1.2 Energy at each quantum level n

We note the following

$$\frac{\partial^2}{\partial x^2}\Phi = -\left(\frac{n\pi}{L}\right)^2\Phi \tag{9}$$

If we replace the results in (2) we find:

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

Or simply:

$$E_n = n^2 E_1$$
$$E_1 = \frac{\hbar^2 \pi^2}{2mL^2}$$

3.1.3 Probability function of the position

The probability of finding the particle between a and b is the following:

$$\begin{cases} \int_a^b |\Phi|^2 dx & \text{if } a, b \in [0, L] \\ 0 & \text{otherwise} \end{cases} \tag{10}$$

If we wish to find the position inside a box of width ϵ and center a we would integrate between $a - \epsilon/2$ and $a + \epsilon/2$ where both ends are between 0 and L The integration will lead to the following:

$$P(x) = \frac{\epsilon}{L} + \frac{1}{2n\pi}\left[\sin\left(\frac{2n\pi}{L}(a - \epsilon/2)\right) - \sin\left(\frac{2n\pi}{L}(a + \epsilon/2)\right)\right]$$

Which can be reduced more to the following form:

$$P(x) = \frac{\epsilon}{L} - \frac{1}{n\pi}\sin\left(\frac{n\pi}{L}\epsilon\right)\cos\left(\frac{2n\pi}{L}x\right)$$

3.2 In two dimensions

3.2.1 The time-independent solution

This time we suppose the solution is

$$\Phi(x, y) = X(x)Y(y) \tag{11}$$

$$X(x) = A\cos(k_x x) + B\sin(k_x x)$$
$$Y(y) = C\cos(k_y y) + D\sin(k_y y)$$

Plugging (11) in (2) and doing similar operations as *3.1.1* we get the following solution:

$$\Phi(x, y) = \frac{2}{L}\sin\left(\frac{n_x \pi}{L}x\right)\sin\left(\frac{n_y \pi}{L}y\right) \tag{12}$$

3.2.2 Energy in two dimensions

Doing the same steps as *3.1.2* we find that the energy has become:

$$E_{n_x, n_y} = \frac{\hbar^2 \pi^2}{2mL^2}(n_x^2 + n_y^2) \tag{13}$$

Or simply:

$$E_{n_x, n_y} = (n_x^2 + n_y^2)\; E_{1,1}$$
$$E_{1,1} = \frac{\hbar^2 \pi^2}{2mL^2}$$

3.2.3 Probability function of the position

Similar to section *3.1.3* to find the probability of finding the particle inside the box of size ϵxϵ we integrate the wave function inside a box of center (x, y) and width ϵ.

$$P(x, y) = \int_{y-\epsilon/2}^{y+\epsilon/2} \int_{x-\epsilon/2}^{x+\epsilon/2} |\Phi(x, y)|^2 dxdy$$

After evaluating the integral we get the following function:

$$P(x, y) = \frac{1}{L^2}\, p(x)\, p(y) \tag{14}$$

$$p(\alpha) = \epsilon - \frac{L}{n_\alpha \pi} \cos\left(\frac{2n_\alpha \pi}{L}\alpha\right) \sin\left(\frac{n_\alpha \pi}{L}\epsilon\right)$$

3.3 Generalizing the time-independent solution

The equation that we have found so far depends on two quantum numbers n_x and n_y and describes the particle for these energy levels only. However the final time-dependant equation is a combination of many of these equations. The final time-independent equation is:

$$\Phi(x, y) = \sum_n c_n \Phi_{n_x,n_y}(x, y) \tag{15}$$

Where the constant c_n is the square root of the probability of getting the equation Φ_{n_x,n_y} that describes the particle in the box.

3.4 Generalizing the probability function

Since we have a more general wave function we need to have a more general probability function for the position. The new definition is generated from integrating Φ between $a - \epsilon/2$ and $a + \epsilon/2$. The result is:

$$P(x, y) = \sum_n c_n^2\, P_n(x, y)$$

4 Implementation

4.1 Synopsis

This simulation will display the probability of finding the particle in sub-boxes in the box as well as display the energy in the sub-box of width ϵ. Each frame displays the particle with a new set of probabilities for each energy level.

The probability of the position will be visualized by the intensity of the color. The brighter the color, the higher the probability.

The energy however will be visualized using the standard colors assigned to energies; lower energies have blue-shades while high energies have red-shades.

4.2 Conventions

Some of the conventions adopted throughout the code are

- words in functions, structs and variable names are separated by an _ (underscore)
- CUDA kernels start with the keyword `cuda_`.
  For example `cuda_probability`
- CUDA device functions start with `cuda_` and end with `_device`.
  For example `cuda_probability_1d_device`
- Tiny mathematical and physical constants, such as $\hbar$ are expressed as float numbers without their orders.
  For example $\hbar = 1.054 \cdot 10^{-34}$ is defined as `#define HBAR 1.054`

4.3 Brightness and Color mapping

4.3.1 Brightness

The intensity of the colors denote the probability of finding the particle. Since probabilities are always between 0 and 1, converting them to intensities is just a matter of mapping the probabilities from $[0, 1]$ to $[0, 255]$.

However ϵ is a small number, so the probability is always small; usually less than 0.1%. Therefore we need to find the highest probability in the space and remap from $[0, \max]$ to $[0, 255]$. At first I have tried to brute force the problem exploiting my GPU using functions to find maximums using reduction. But the process of finding the highest probability of a particle with 10 energy levels inside a box divided into 262,144 boxes took around 28ms. Allowing me to get only 35fps in the animation.
A new solution needed to be adopted and I went over the equations again to try and find that maximum analytically. My results are:

For $p(\alpha)$ to be maximal

$$\frac{\epsilon}{L} - \frac{1}{n_\alpha \pi} \sin\left(\frac{n_\alpha \pi}{L}\epsilon\right) \cos\left(2\frac{n_\alpha \pi}{L}\alpha\right)$$

needs to be maximal. And this is achieved when $\cos x = -1$ which is possible since $0 \leq x \leq 2\pi$. Therefore the highest probability for one energy level is:

$$\frac{\epsilon}{L} + \frac{1}{n_\alpha \pi} \sin(\frac{n_\alpha \pi}{L}\epsilon)$$

Following similar analysis we can deduce that the highest probability (denoted by m) is close to, but not exactly:

$$m = m_x.m_y$$

$$m_\alpha = \frac{\epsilon}{L} + \sum_i \left(c_i^2 \frac{1}{n_{\alpha_i}\pi} \sin\left(\frac{n_{\alpha_i}\pi}{L}\epsilon\right)\right)$$

4.3.2 Tint and Color

The tint in the color represents the energy of the particle. Red is the highest energy and blue is the lowest. If we can map the energy in an interval between 0 and 1 we can easily get the RGB values. The following equation can be applied

$$\begin{bmatrix} R_{xy} \\ G_{xy} \\ B_{xy} \end{bmatrix} = P(x,y) \begin{bmatrix} 255E \\ 20 \\ 255(1-E) \end{bmatrix}$$

Where $P(x, y)$ is the probability of finding the particle at (x, y) and between 0 and 1. And E is the energy remapped between 0 and 1.

To problem of remapping the energy is easy to solve. Through mathematical analysis we can show that the highest energy we can find is

$$E_{max} = (n_{max_x}^2 + n_{max_y}^2)\frac{\hbar^2\pi^2}{2mL^2}$$

And therefore we can remap any energy we find to a value in the interval $[0, 1]$ and find the corresponding RGB values.

5 API

6 Results

7 Code License: GNU General Public License