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

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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.

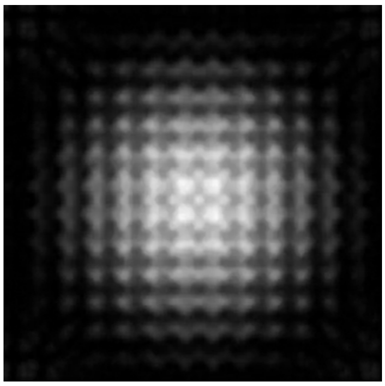

Figure 1: A screenshot of a "particle in a box" simulation found on Youtube

[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 Memory Management

4.2 Optimizations

4.3 Implementations Details

5 Results

6 Code

6.1 Code

6.2 License: GNU General Public License