Comparison of the 1-D Quantum Harmonic Oscillator and the 1-D Infinite Square well

100794934

December 2015

Contents

1 Background on project

1.1 What my project is about

This semester I found PH2210: Quantum Mechanics to be by far the most interesting module so when I discovered that I had to make a python project about something I have studied this term, I already knew it would involve quantum physics. After some careful thought I decided to focus on the 1-D quantum harmonic oscillator and the 1-D infinite square well as I found problem sheet 6 the most enjoyable to code. After researching the two quantum systems on the internet I found valuable resources for both however, I was unable to find a web-page or application that compared the two and so I decided to create my application as a visual aid that allowed the user to compared various properties of both the 1-D quantum harmonic

1.2 How I went about creating my code

After spending many hours attempting to plot the wave-function of the 1-D infinite square well (along with a user interface), I was finally able to and within half an hour I created a second programme plotting the probability distribution of the wave function. My next task was to merge the two programmes onto a single tkInter window. After this, I created all the classes that would various functions (see section 1.3) in different windows and home page class which had buttons opened each new windows as I found this the best way to prevent my programme from crashing. I then improved the graphs (adding titles, changing the axis, spine and also adding a legend), added help buttons for all the user interfaces and various pieces of information to the right hand side of each graph explaining to the user what the graph demonstrates.

1.3 Physics demonstrated by the code

1.3.1 The 1-D Infinite Square Well

The infinite square well describes a particle free to move in a space surrounded by impenetrable barriers. The model is used as a hypothetical example to illustrate the differences between classical and quantum systems.To solve the Infinite Square Well problem, we must first recall the 1-D time independent Schrödinger equation[1]:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi \tag{1}$$

Where the boundary conditions of the infinite square well is defined by:

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

This boundary condition implies that the first derivative does not need to be continuous at the boundary [2]. The solution to this problem after normalisation is:

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \tag{3}$$

The probability distribution is given by the square of the wave-function which is:

$$\mid \Psi_n(x) \mid^2 = \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right) \tag{4}$$

And the energy levels is given by:

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \tag{5}$$

1.3.2 The 1-D quantum harmonic oscillator

The 1-D quantum harmonic oscillator is one of the foundation problems of quantum mechanics as many potentials look like a harmonic oscillator near their minimum so many other systems can be approximated to it. Some of these systems include understanding of complex modes of vibration in larger molecules, the motion of atoms in a solid lattice and the theory of heat capacity. The harmonic oscillator Hamiltonian is given by:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 \tag{6}$$

Leading to the Schrödinger equation becoming:

$$\frac{-\hbar^2}{2m}\frac{d^2\Psi_n}{dx^2} + \frac{1}{2}m\omega^2x^2\Psi_n = E\Psi_n \tag{7}$$

The wave-functions for the quantum harmonic oscillator contain the Gaussian form which allows them to satisfy the necessary boundary conditions at infinity. In the wave-function associated with a given value of the quantum number n, the Gaussian is multiplied by a polynomial of order n called a Hermite polynomial. The wave-function is then:

$$\Psi_n(y) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \sqrt{\frac{1}{2^n n}} H_n(y) e^{\frac{-y^2}{2}}, where H_n(y) = Hermitepolynomial \tag{8}$$

The classical probability distribution is given by:

$$P_c l(x) = \frac{1}{\pi\sqrt{2n+1}} \tag{9}$$

Which will be compared to the quantum probability distribution in my code. To calculate the probability distribution you square this wave-function and the energy of this system is given by:

$$E_n = (n + 1/2)\hbar\omega \tag{10}$$

2 The Code

2.1 What my code can plot

On the main page I designed my code to compare:

- The wave-function of the 1-D infinite Potential Well and the 1-D Quantum Harmonic Oscillator
- The probability distribution of the 1-D infinite Potential Well and the 1-D Quantum Harmonic Oscillator
- The wave-function and probability distribution of the 1-D infinite Potential Well
- The wave-function and probability distribution of the the 1-D Quantum Harmonic Oscillator
- The classical and Quantum probability distribution of the the 1-D Quantum Harmonic Oscillator
- The energy levels of the 1-D infinite Potential Well and the 1-D Quantum Harmonic Oscillator

2.2 What my second window looks like

Each of the bullet points above correspond to a button on the main page of the GUI which when clicked, a second page appears which allows the user to plot a graph whilst also having the option to change a few variables and access to a help button. All the other corresponding buttons open up windows similar to the one seen in Figure 1 that correspond to various properties of the quantum systems along with some basic description of what each graph is showing.

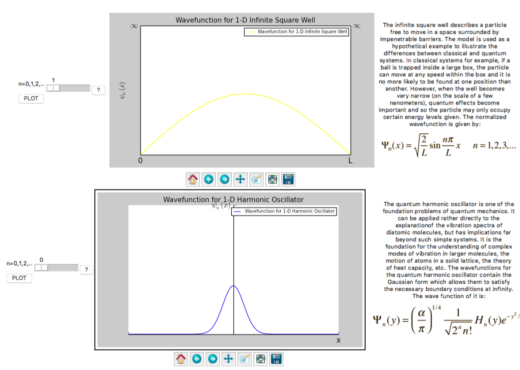

Figure 1: Scree shot of my second window which can allow the user to plot 2 graphs

To allow my code to plot two graphs on a new window, I used the following two lines of code:

```
def InfiniteSqWellandHarmonic(self):
    self.newWindow = Toplevel(self.master)
    self.app = InfiniteSqWell(self.newWindow), Harmonic(self.newWindow)
```

Figure 2: How I was able to plot 2 graphs in a new window

3 Problems Encountered with the code

Some problems I found were for some reason when I attempted to plot the energy levels nothing happened and so the best way I found to solve this was to make both energy equations a function of x by multiplying the energies by x^0 and this somehow made it work. I also wanted to plot 2 different energy values for n so I attempted to create 2 more functions for the energy but when I attempted to plot them on the same graph it wouldn't work so I decided not to include it in my code however, the functions can be seen near the top of the code but I haven't used them. Also for some reason the help buttons for the energy levels aren't in the correct position which I will be attempting to fix up until I had in my project

4 Conclusion

To conclude I feel that my project was successful in demonstrating various aspects of quantum mechanics by creating a visual aid however, if I had more time, I would have also liked to demonstrate various other properties of the system for example that the wave-functions are orthogonal and also create a code that would have been in a new window that could calculate the expected value squared and uncertainty.

5 Bibliography

References

[1] Particle in a box http://www.physicspages.com/2011/01/26/the-infinite-square-well-particle-in-a-box/

[2] Harmonic Osccilator http://quantummechanics.ucsd.edu/ph130a /130$_n otes/node153.html$