PH881 Computational Physics

Mini - Project

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Topics

- Qualitative Proof of Heisenberg Principle
- Solving Schrödinger Equation in One-dimension for:
  1. Infinite Potential Well
  2. Quantum Harmonic Oscillator
  3. Hydrogen Atom

1. Heisenberg Uncertainty Principle

Statement

The more precisely the position of some particle is determined, the less precisely its momentum can be known and vice-versa.

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

How can we depict it?

By choosing any wave-function, we can calculate its fourier transform and plot the probability functions in both cases. From there we can understand the uncertainty in x(position) and k(momentum = $\hbar$k).

Problem statement

Take two examples of wave-functions:

1. Exp(ikx): Sinusoidal wave
2. Delta function

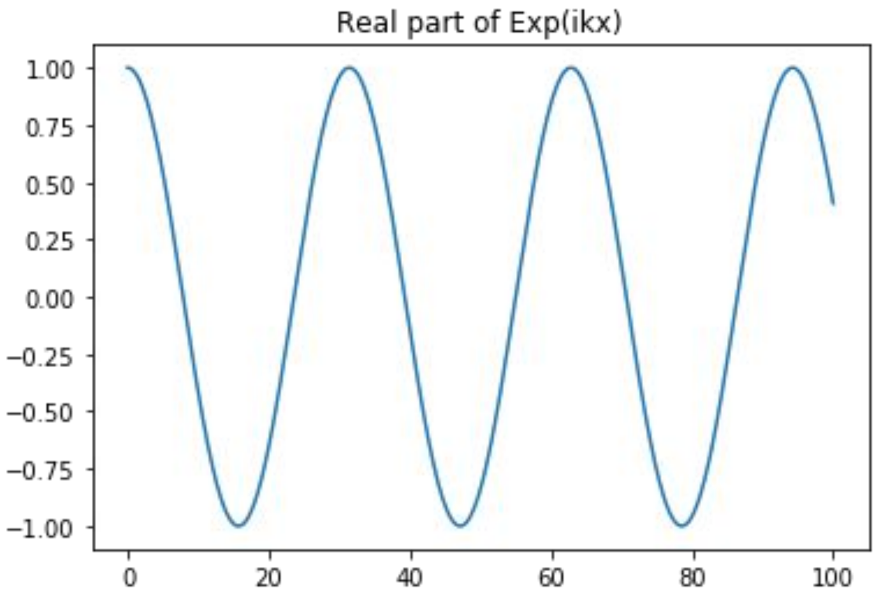
Depict Heisenberg Uncertainty Principle using fourier transforms.

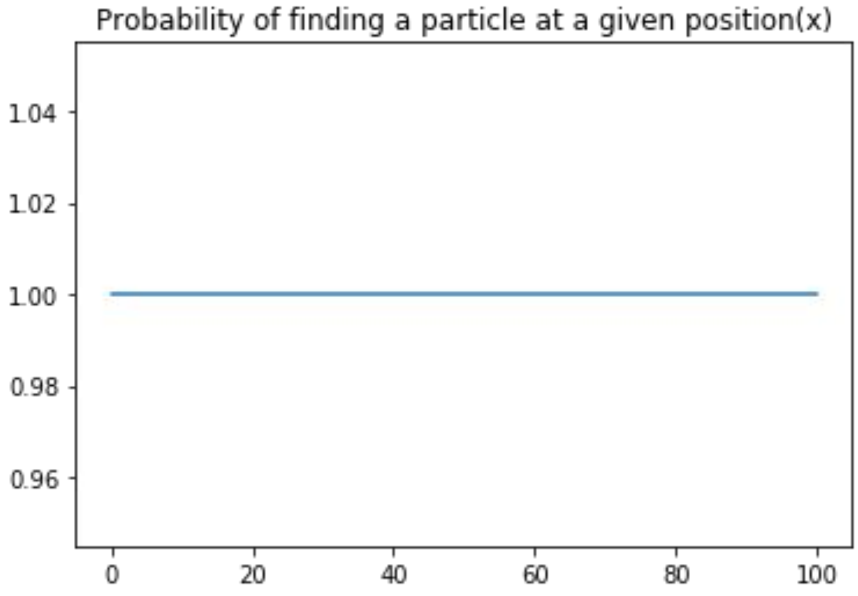
Implementation

Exponential Wave-Function

Real part of Exp(ikx)

Probability of finding a particle at a given position(x)



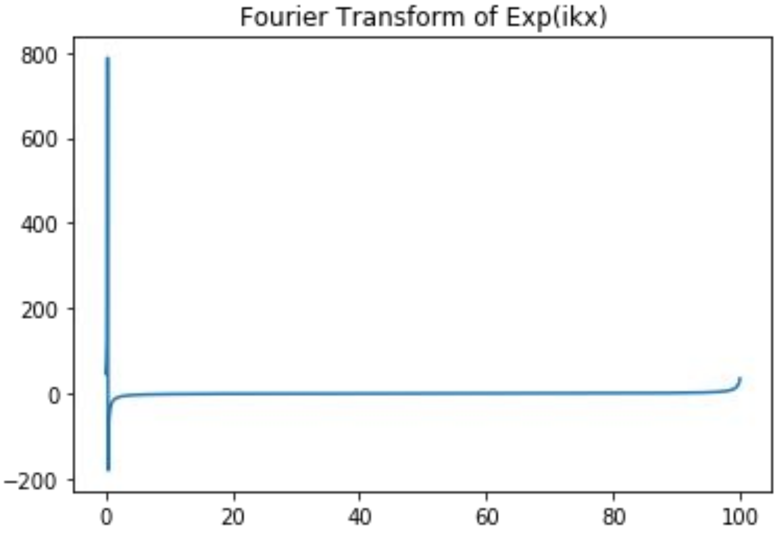


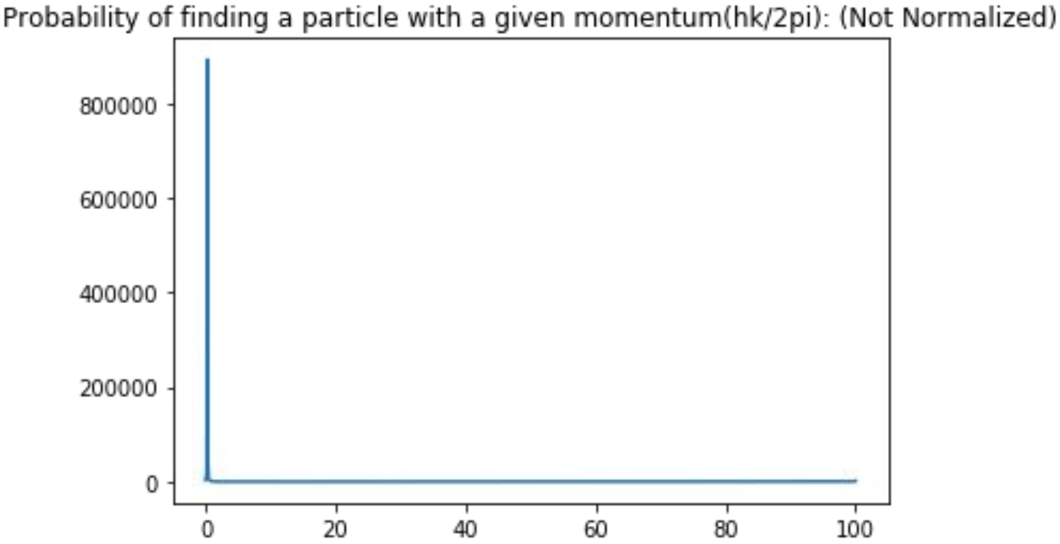
Large uncertainty in position.

Exponential Wave-Function

Fourier Transform of Exp(ikx)

Probability of finding a particle with a given momentum($\hbar k$)



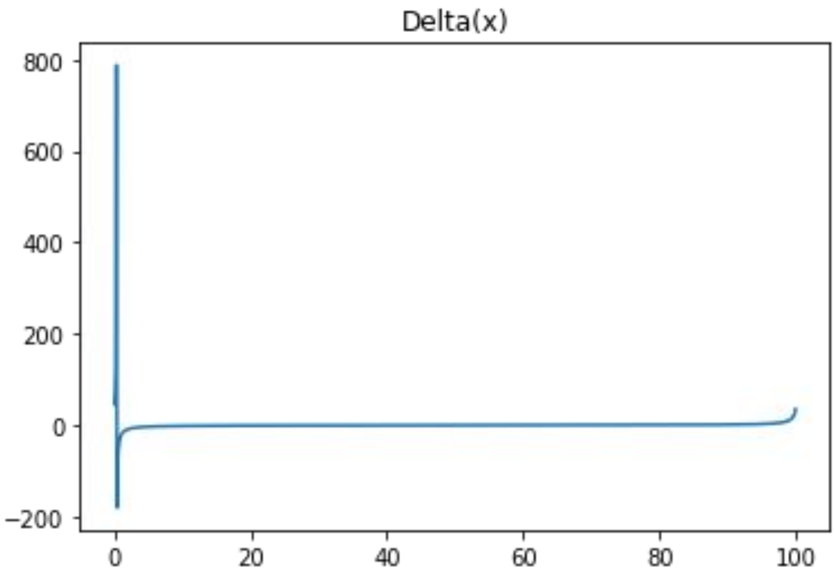


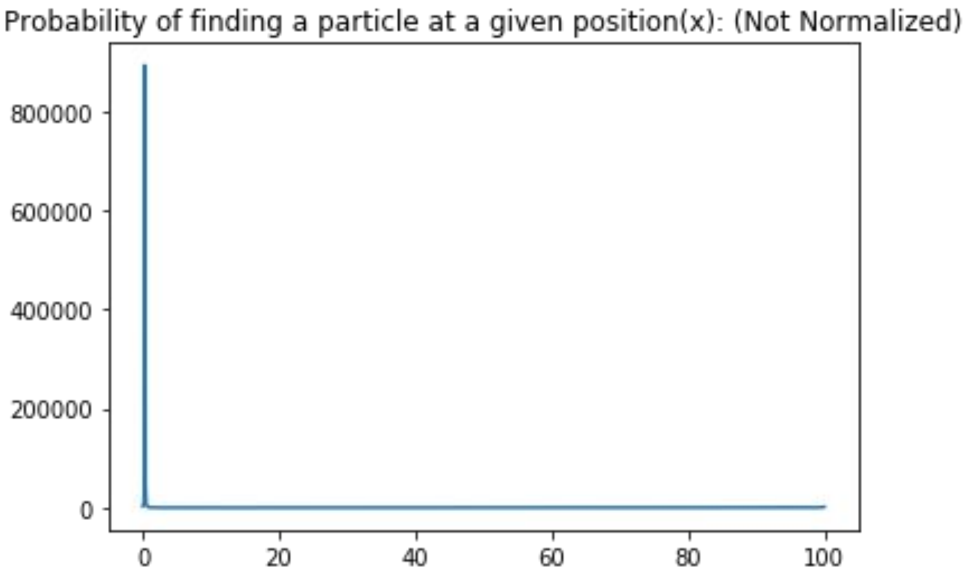
Small uncertainty in momentum.

Delta Wave-Function

Delta(x)

Probability of finding a particle at a given position(x)



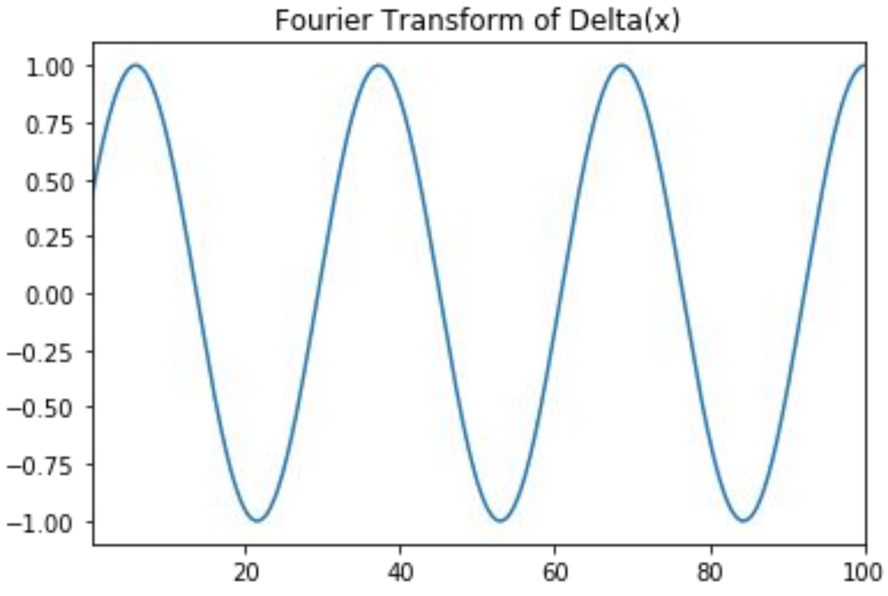


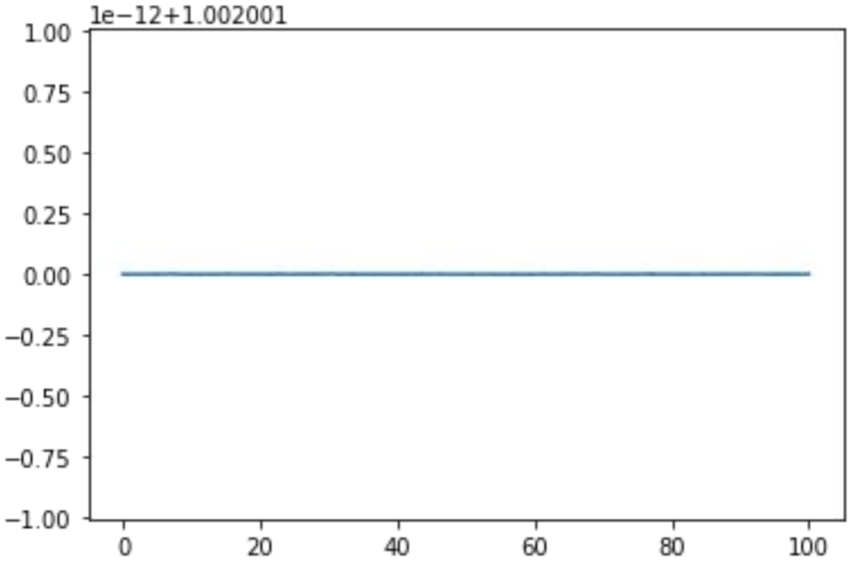
Small uncertainty in position.

Delta Wave-Function

Fourier Transform of Delta(x)

Probability of finding a particle with a given momentum($\hbar$k)





Large uncertainty in momentum.

Result:

With both kinds of wave-functions, we see that the accuracy of both position and momentum do not go hand in hand. If we know position very accurately then uncertainty in k(momentum) is large and vice-versa.

2. Solving Schrödinger Equation in One-dimension

Need to solve

The Schrödinger equation is used to find the allowed energy levels of quantum mechanical systems (such as atoms or transistors). The associated wave-function gives the probability of finding the particle at a certain position.

Problem Statement

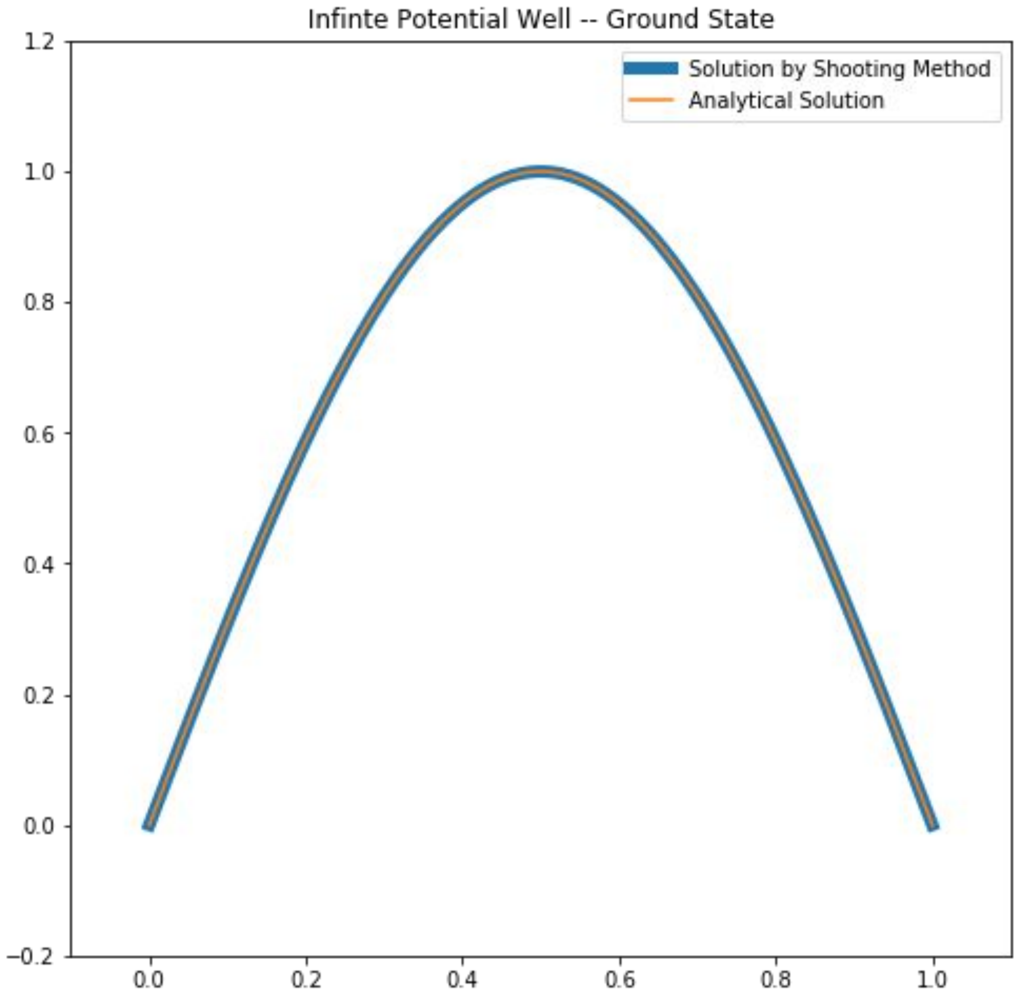
Solve the Schrodinger equation by shooting and analytical method for:

1. Infinite Potential Well (Ground, First excited and Second excited State)
2. Quantum Harmonic Oscillator (Ground, First excited and Second excited State)
3. Hydrogen atom (1s, 2s, 2p, 3s states)

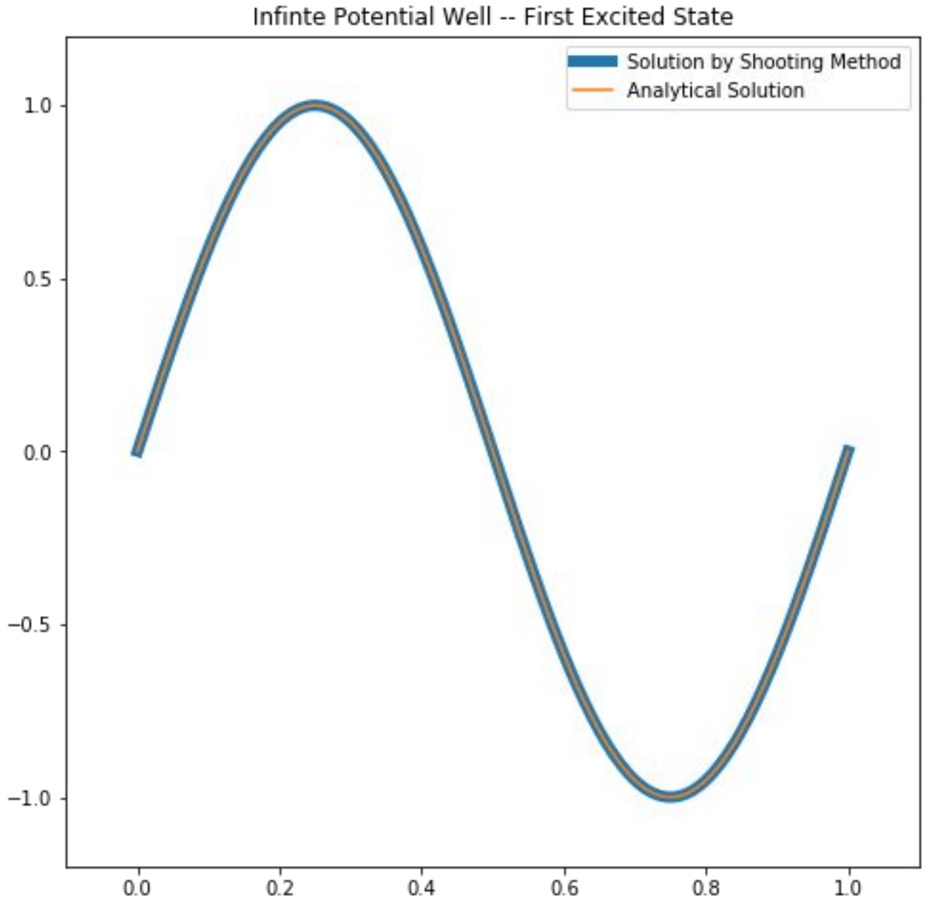
Solution:

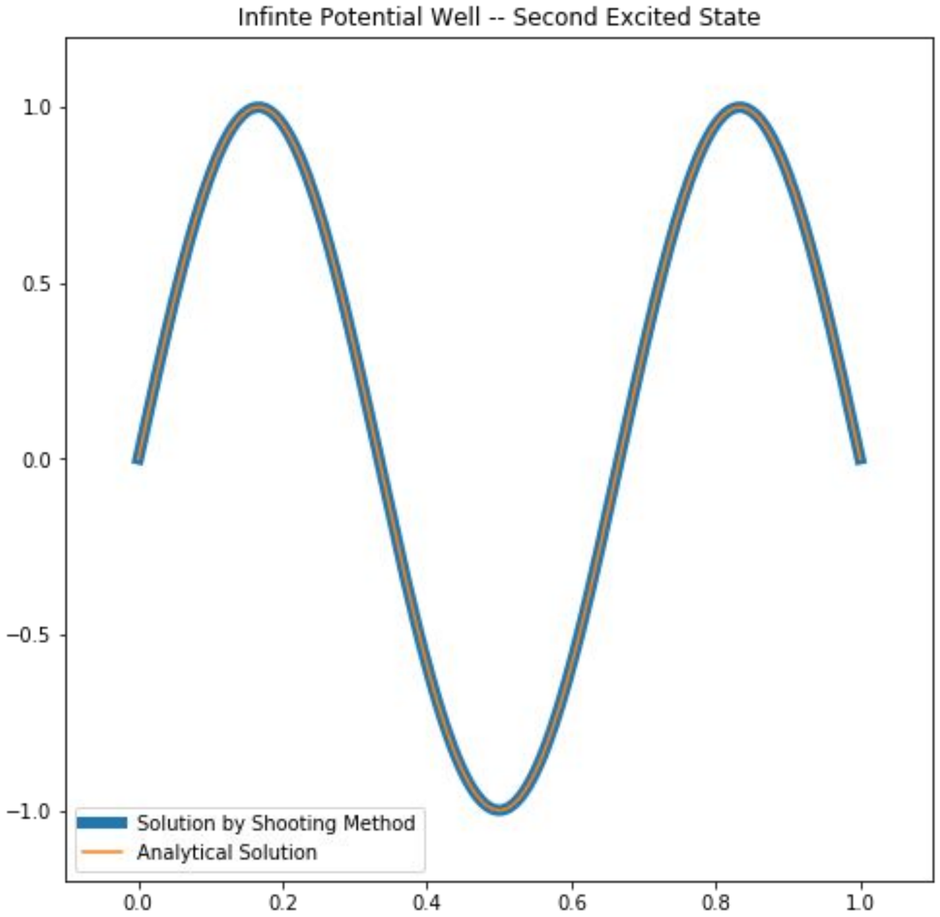
- Numerical Integration method used is the Fourth Order Runge Kutta Method.
- The harmonic is determined by counting the nodes of the wave-function.
- The energy is then refined by a number of functions in the code like OptimizeEnergy, Normalize etc.
- Potentials are as follows:
    - Infinite Potential Well: $V(x<0)$ = infinite; $V(x = (0,1)) = 0$; $V(x>1)$ = infinite.
    - Quantum Harmonic Oscillator: $V(x) = x^2$
    - Hydrogen Atom: Different Potential for different states.
- Initial conditions on the left side of the graph are given.
- Normalization is done just by dividing all the values of the wave-function by the maximum value of the wave-function.

Infinite Potential Well

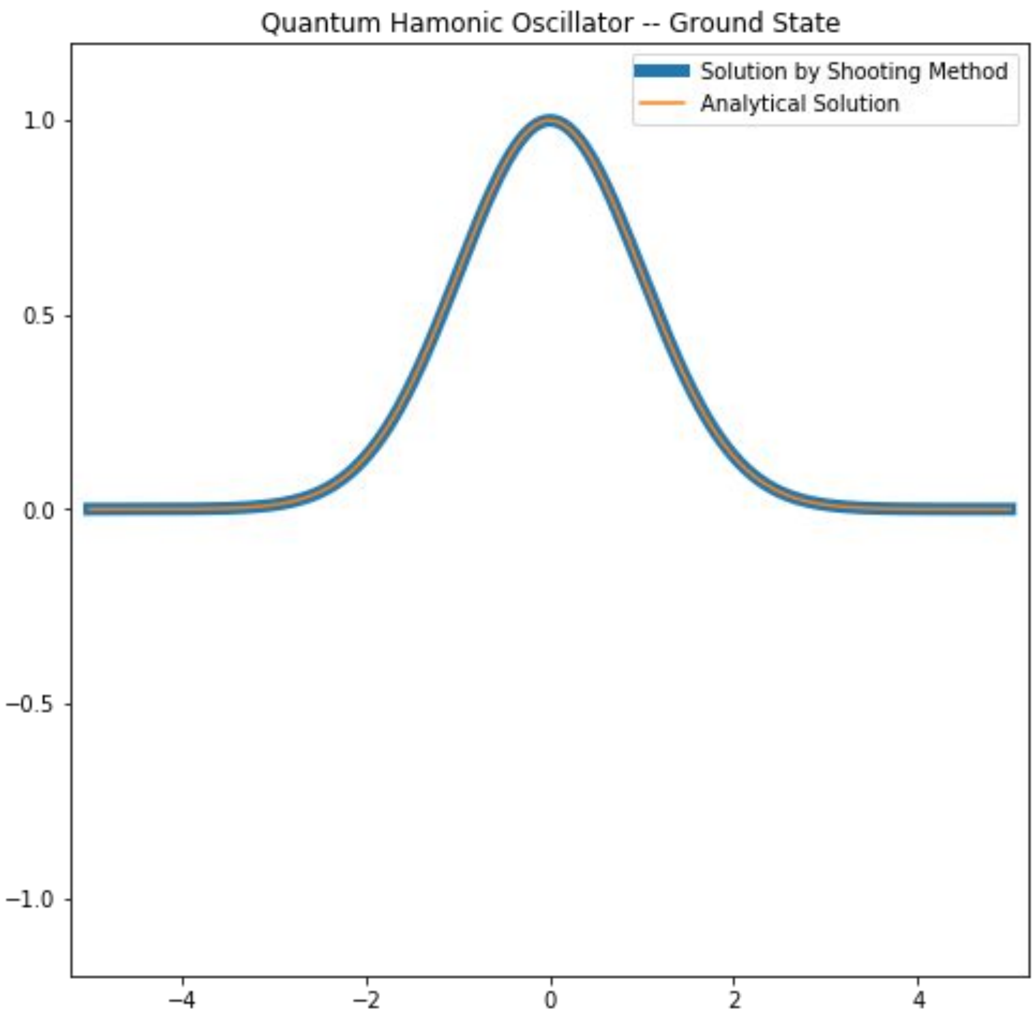


Infinite Potential Well





Quantum Harmonic Oscillator



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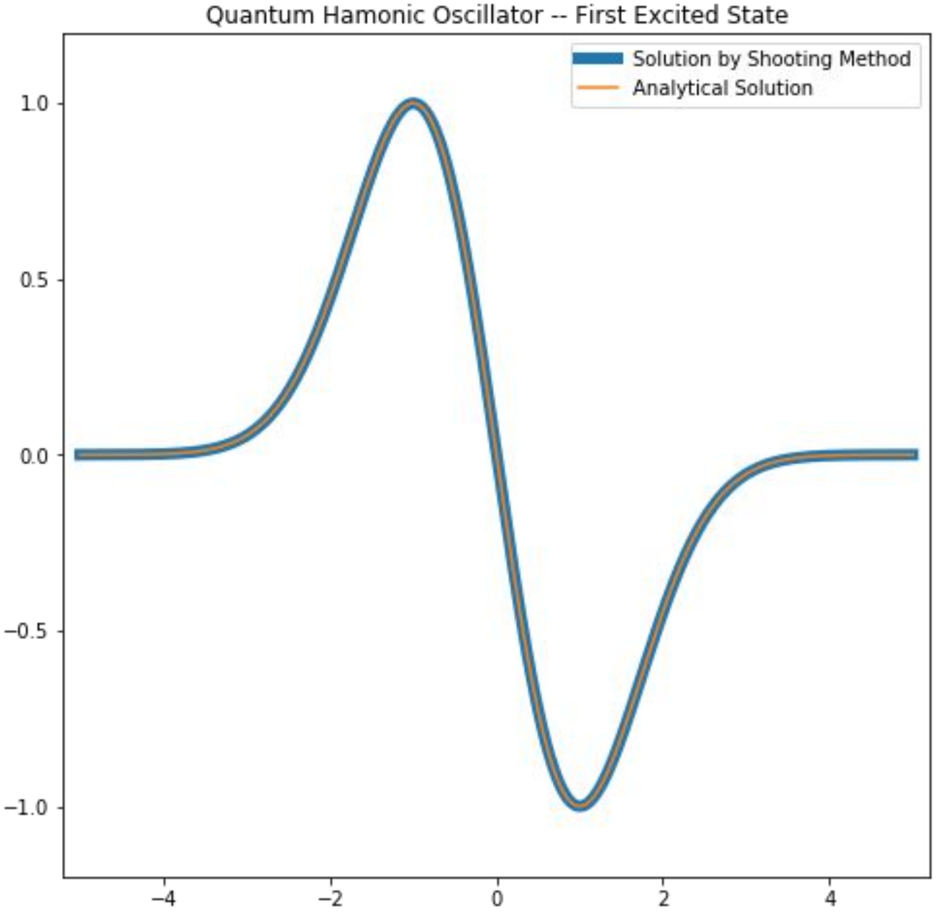
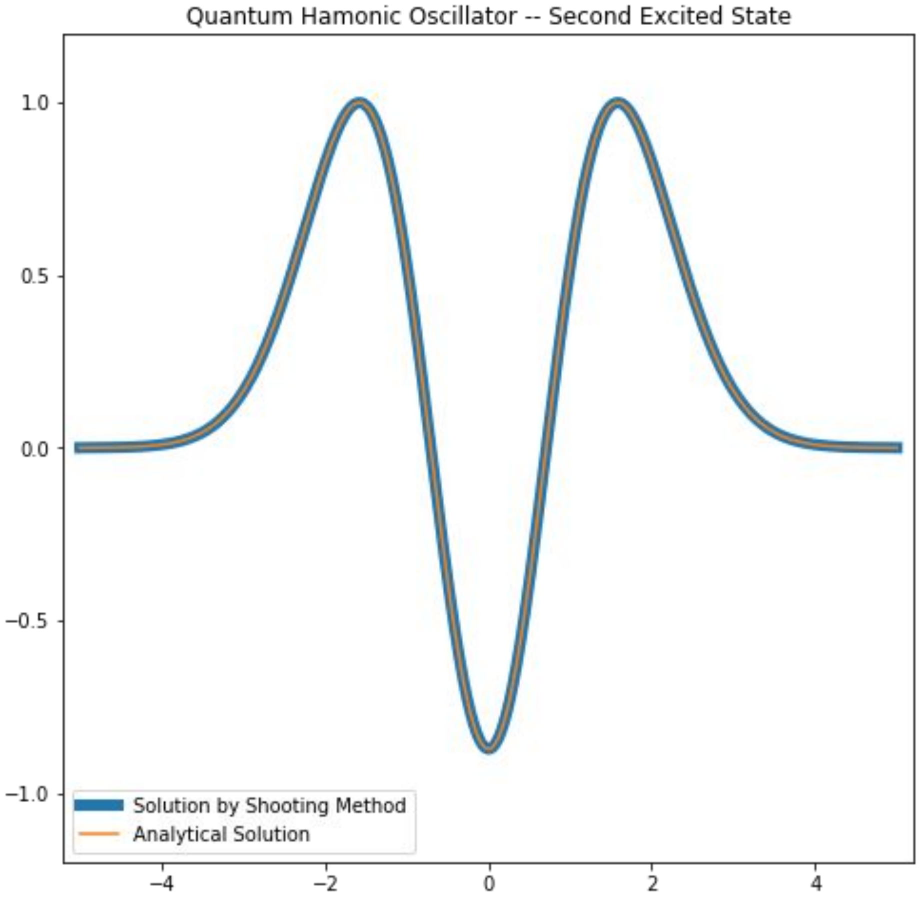
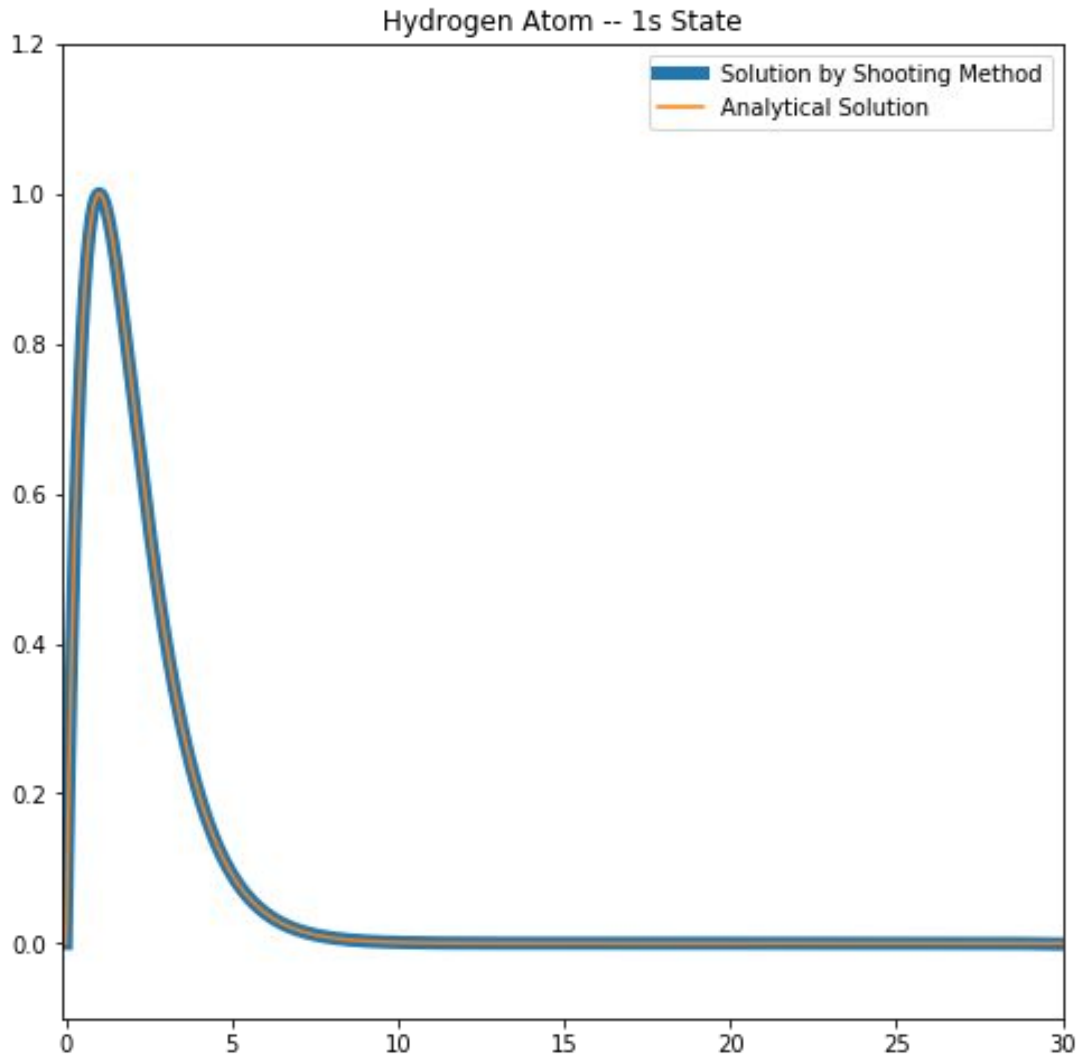




Hydrogen Atom



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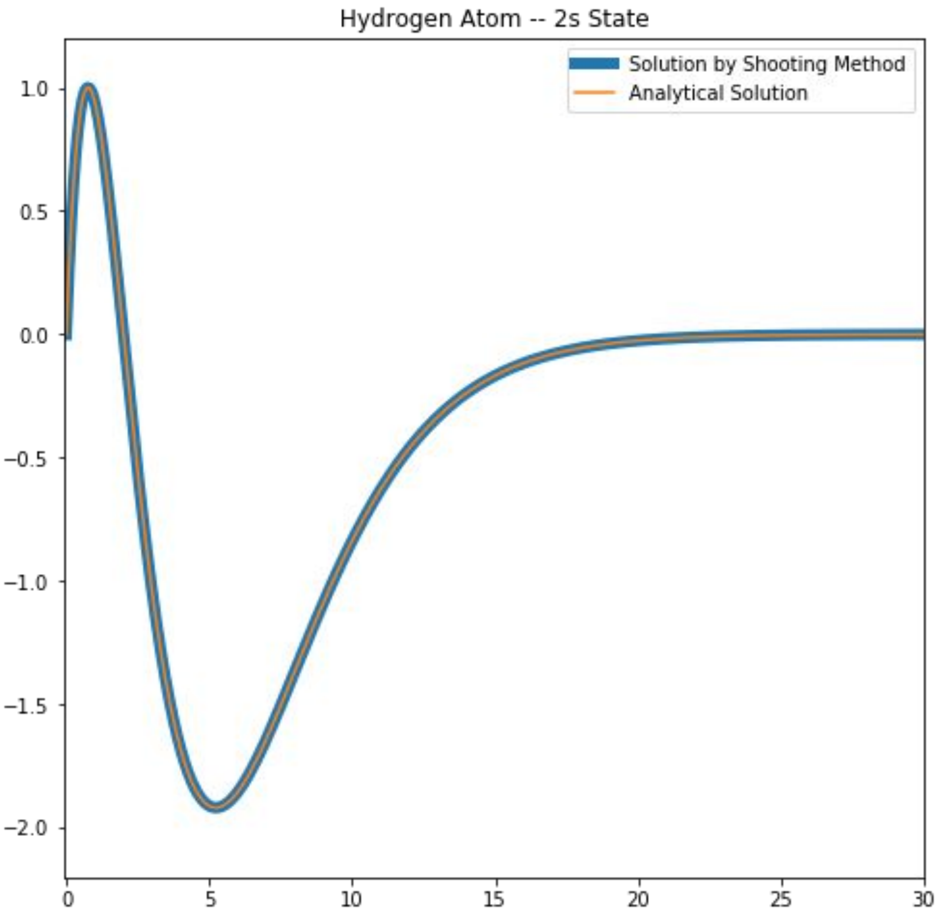
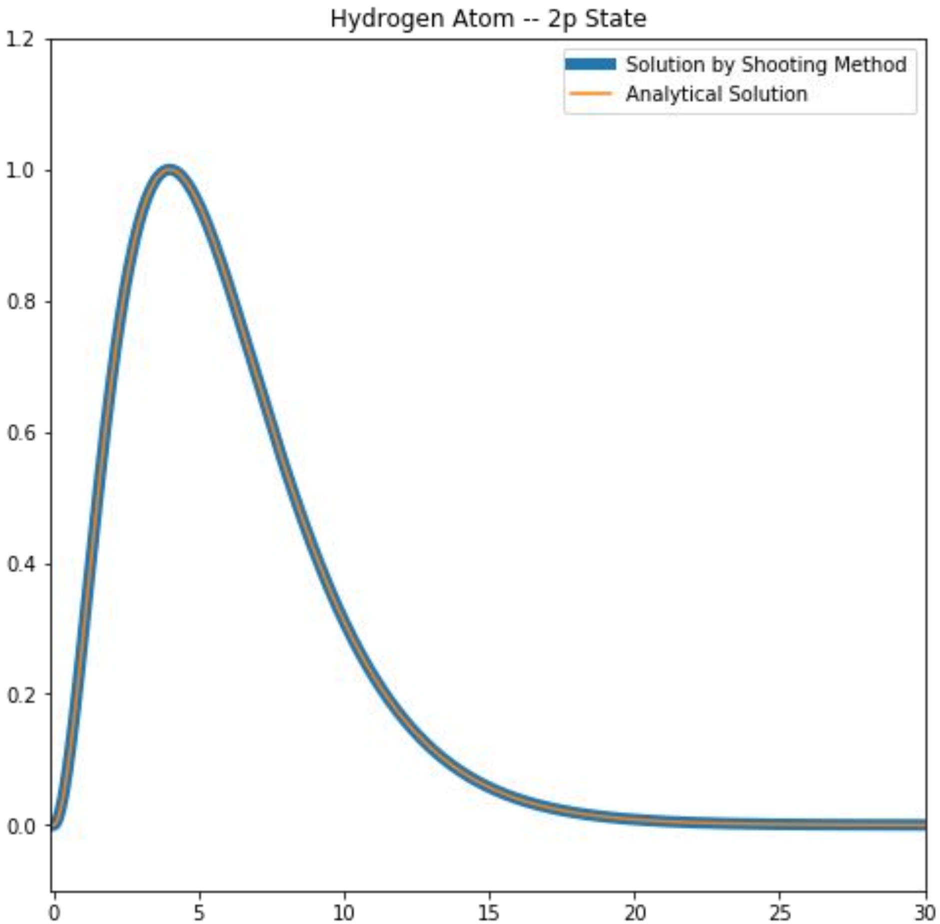
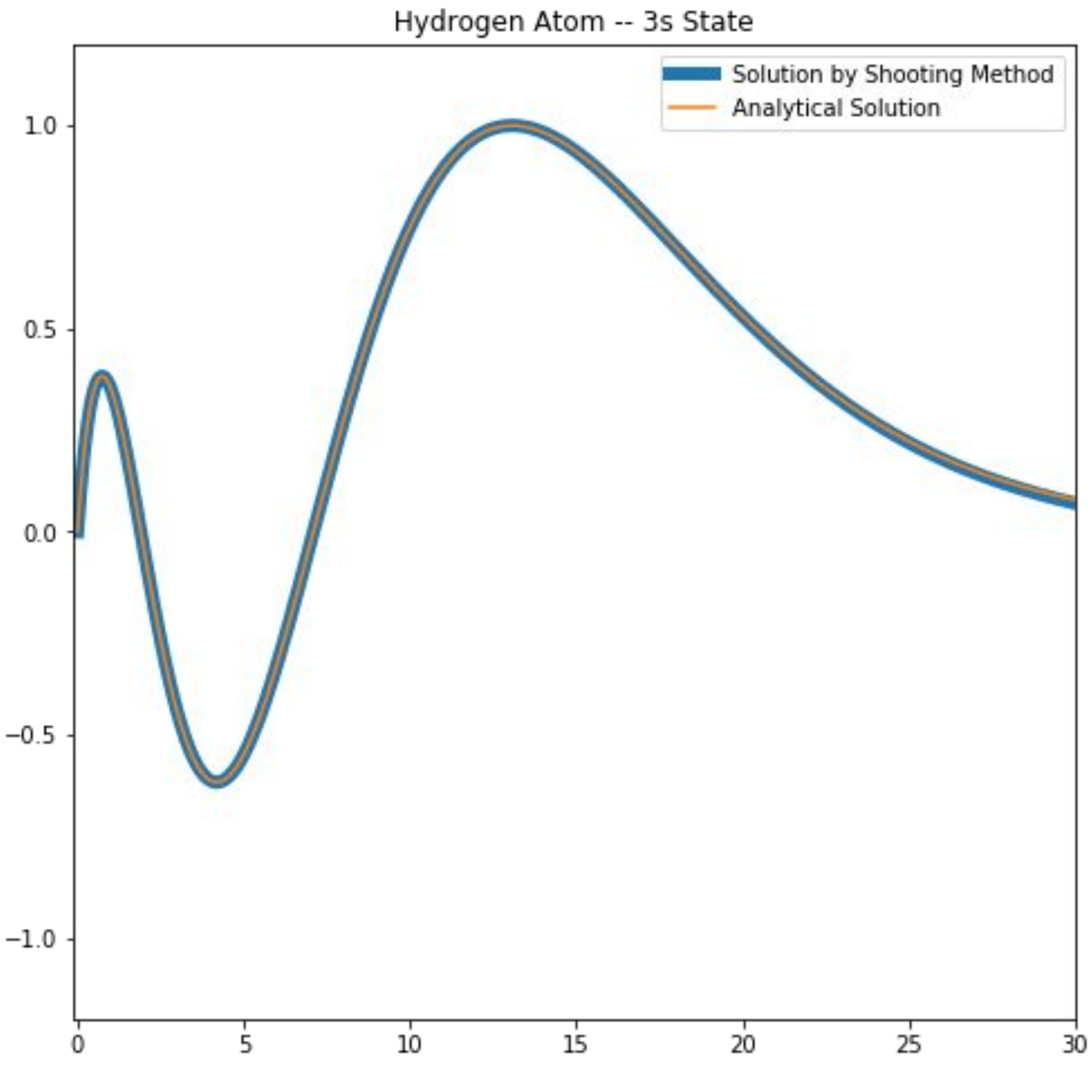




Hydrogen Atom



References:

- A First Course in Computational Physics - Paul L. DeVries and Javier E. Hasbun
- Numerical Solutions of Schrödinger Equation - Neill Lambert