Computational Physics
Set 1

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Introduction

In this report, I will present all of the plots from the codes for each of the problems. The assignment was just to translate the codes from "Matlab" to "Python", and I add some explanation to each of them. My explanation to the "codes" and how I've written each part of it are present as comments in the code.

Problem 1

In this problem, we want to solve this equation with the following initial condition:

$$\frac{df}{dt} = cos(t) \qquad ; \qquad f(0) = 1 \tag{1}$$

The analytical solution is $f(t) = 1 + \sin(t)$ .By using Python code, the following result would be obtained:

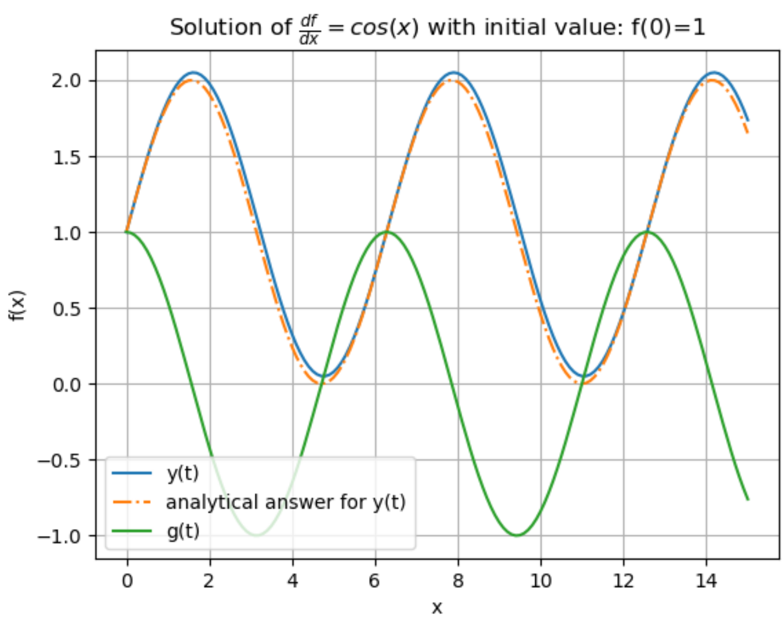

Figure 1: Numerical solution of equation (1), with analytical solution, and also g(t)=cos(t) function

Problem 2

In this problem, we have to solve five differential equations numerically. I've constructed a differentiation operator $D = \frac{d}{dx}$ operator specifically for first order differential equations, and $D_1 = \frac{d}{dx}$ and $D_2 = \frac{d^2}{dx^2}$ for second order differential equations.

Here are the equations, their initial conditions, and their solutions:

$$\frac{df}{dx} = -2x \qquad ; \qquad f(0) = 0 \tag{2}$$

The analytical solution for equation (2) is $f(x) = -x^2$.

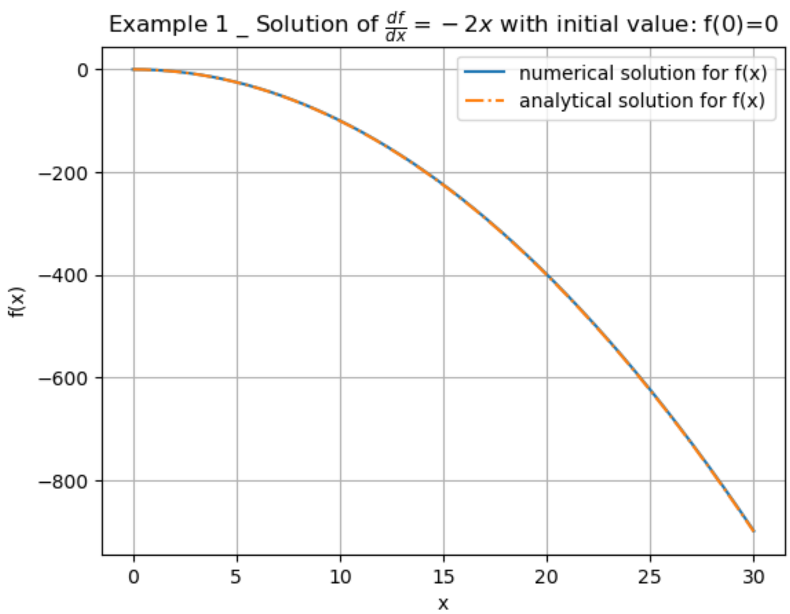

Figure 2: Numerical and analytical solutions of equation (2)

$$\frac{df}{dx} = \frac{f}{4} \qquad ; \qquad f(0) = 1 \tag{3}$$

The analytical solution for equation (3) is $f(x) = \exp(\frac{x}{4})$.

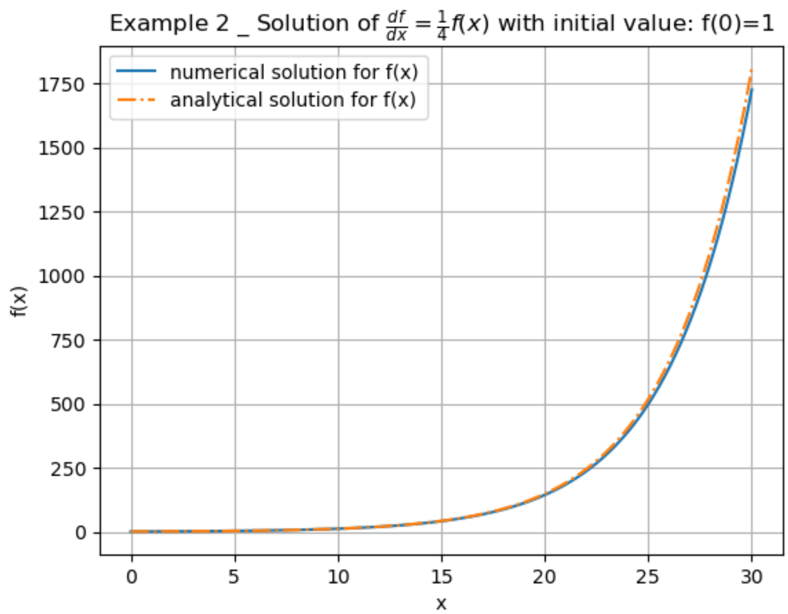

Figure 3: Numerical and analytical solutions of equation (3)

$$\frac{d^2 f}{dx^2} + f = 0 \qquad ; \qquad f(0) = 1, \;\; f'(0) = 0 \tag{4}$$

Equation (4) is in fact equation of simple harmonic oscillator. Its analytical solution is $f(x) = \cos(x)$.

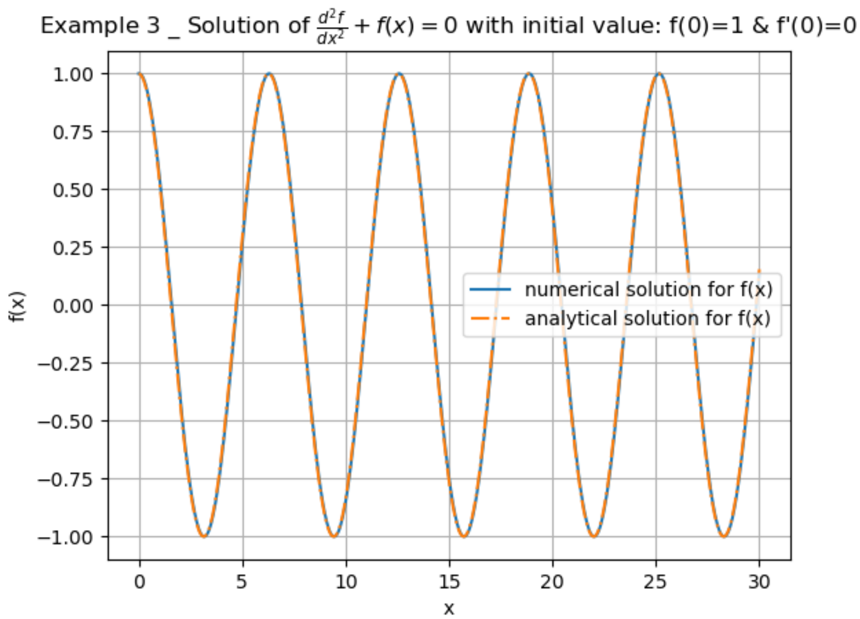

Figure 4: Numerical and analytical solutions of equation (4), this equation is representative of simple harmonic oscillation

For the last two equations, instead of comparing the numerical solution with analytical solution and plotting both, I use "scipy.integrate.odeint" to solve the equation numerically again and compare this two numerical solutions with each other.

$$\frac{d^2f}{dx^2} + 0.4\frac{df}{dx} + f = 0 \qquad ; \qquad f(0) = 1, \;\; f'(0) = 0 \tag{5}$$

Equation (5) is the equation of damped harmonic oscillator.

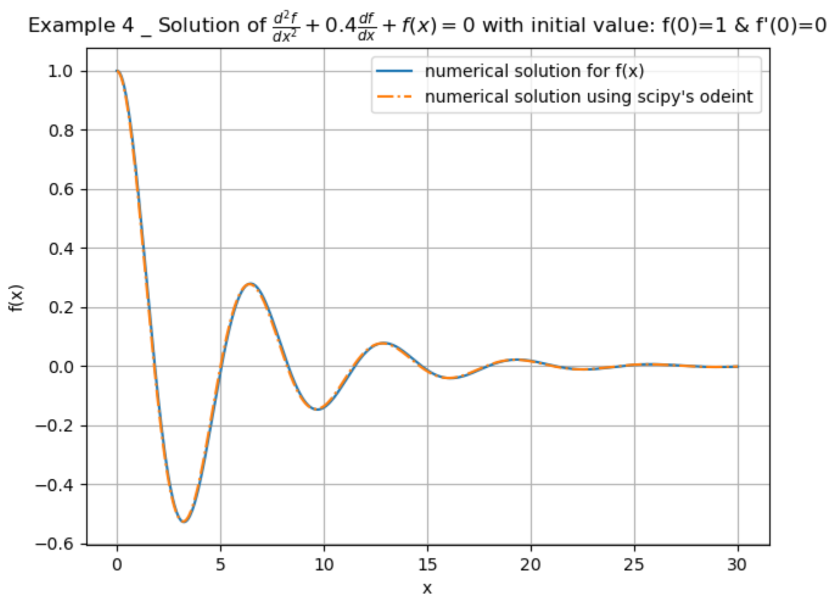

Figure 5: Numerical solutions of equation (5), this equation is representative of damped harmonic oscillation

$$\frac{d^2 f}{dx^2} + 0.5\frac{df}{dx} + f = \sin(x) \qquad ; \qquad f(0) = 1, \;\; f'(0) = 0 \tag{6}$$

Equation (6) is the equation of driven harmonic oscillator.

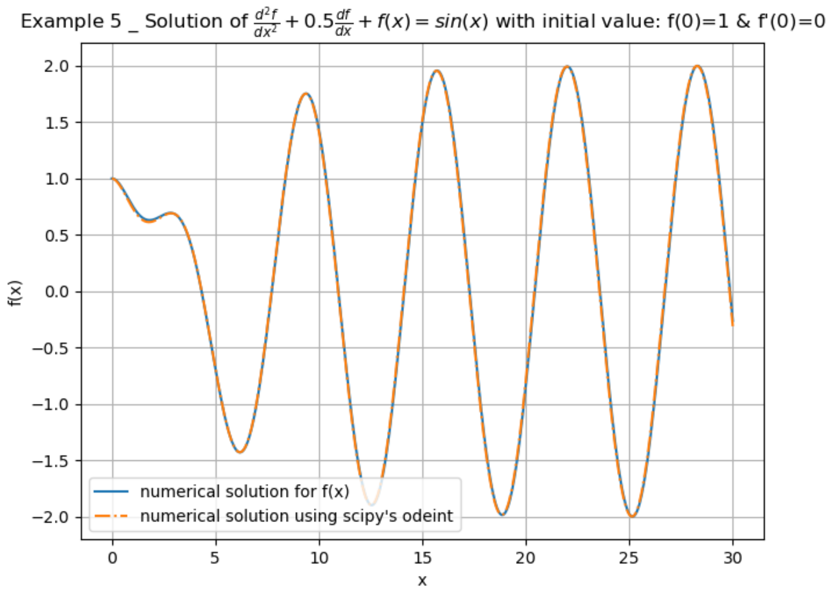

Figure 6: Numerical solutions of equation (6), this equation is representative of driven harmonic oscillation

Problem 3

In this problem we are dealing with 4 eigenvalue problems. We have to solve Schrödinger equation for 4 potentials. Then I plot the potential, its ground state and first excited state wave function and probability distribution function. Ultimately, I use a bar chart for illustrating energy levels and compare them with each other. At the end of the problem, there are sanity checks that are in the code, I just show the mathematical expressions that I've used in my code. Note that in the code, I've used $\hbar = 1, m = 1, \omega = 1$.

One dimensional time-independent Schrödinger equation would be:

$$[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)]\psi(x) = E\psi(x) \tag{7}$$

First, we have simple harmonic oscillator potential:

$$V(x) = \frac{1}{2}m\omega^2 x^2 \tag{8}$$

The following plots are obtained by solving Schrödinger equation (equation (7)) for this potential.

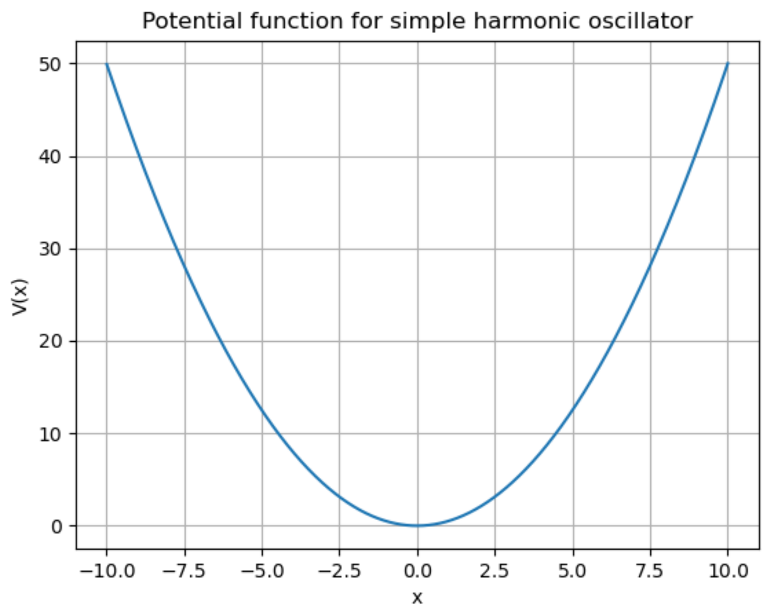

Figure 7: Potential function of equation (8), simple harmonic oscillator

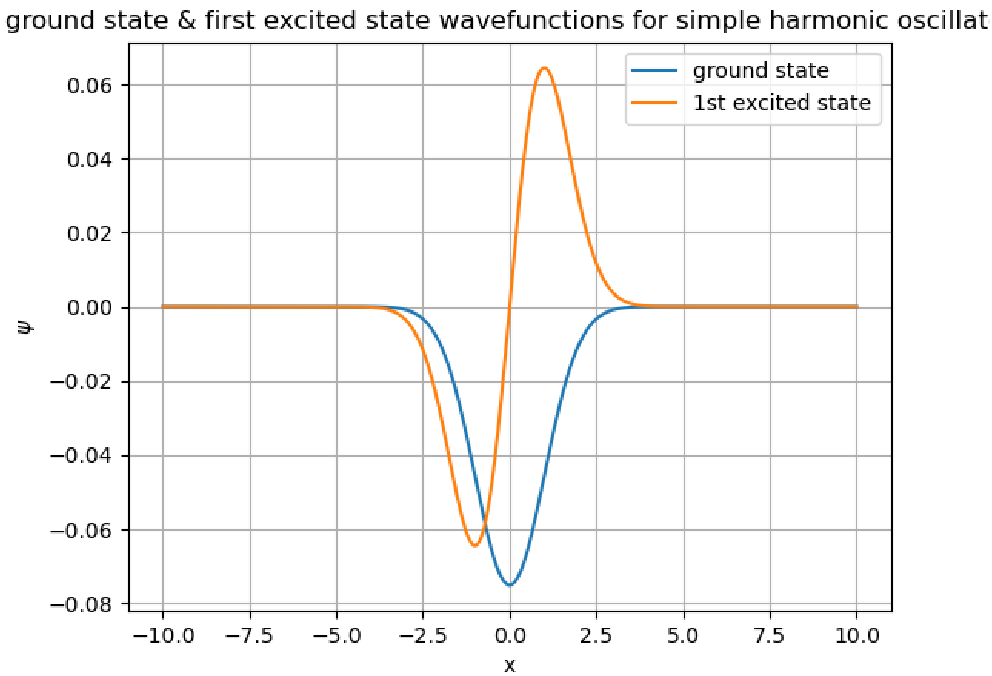

Figure 8: Wave functions for equation (8), simple harmonic oscillator

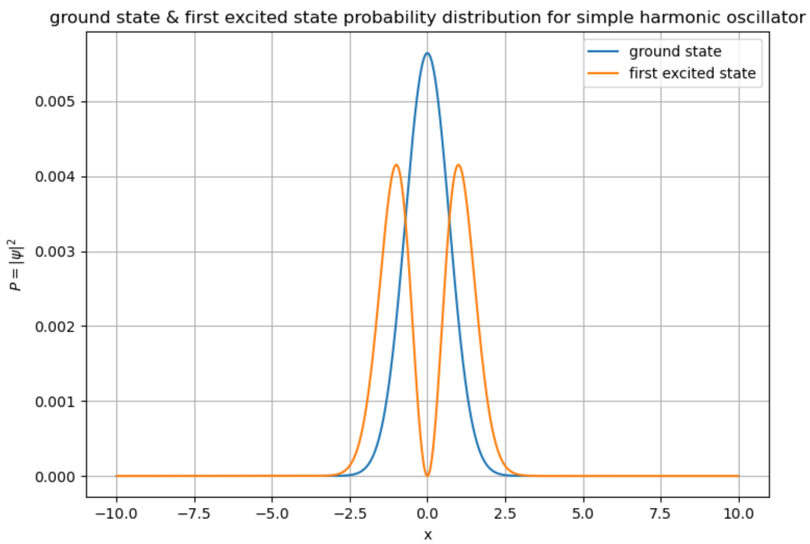

Figure 9: Probability distribution functions for equation (8), simple harmonic oscillator

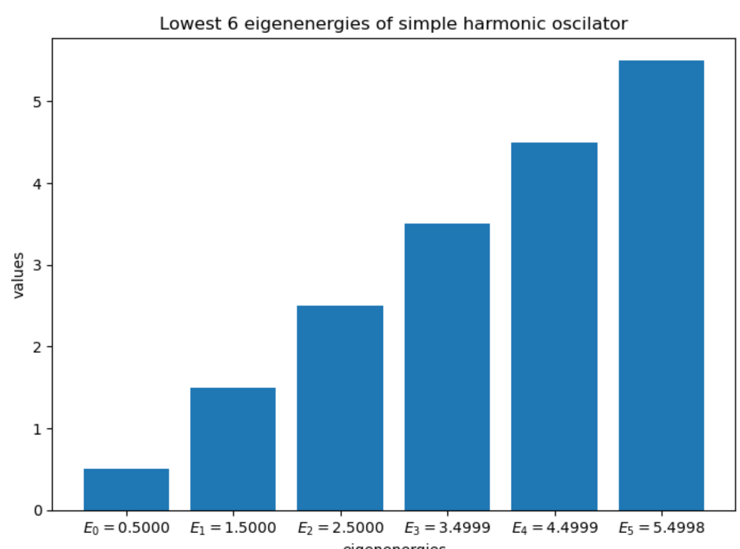

Figure 10: Energy eigenvalues for equation (8), simple harmonic oscillator

Note that energy eigenvalues are consistent with theoretical formula $E_n = \hbar\omega(b + \frac{1}{2})$.

The next potential is for infinite square well:

$$V(x) = \begin{cases} 0 & \text{if } |x| < 3 \\ \infty & \text{if } |x| \geq 0 \end{cases} \tag{9}$$

The following plots are obtained by solving Schrödinger equation (equation (7)) for this potential.

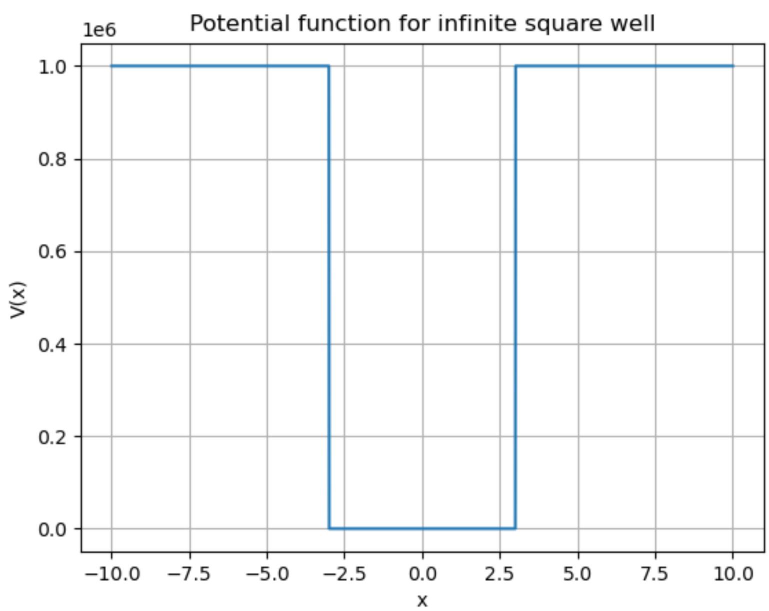

Figure 11: Potential function of equation (9), infinite square well

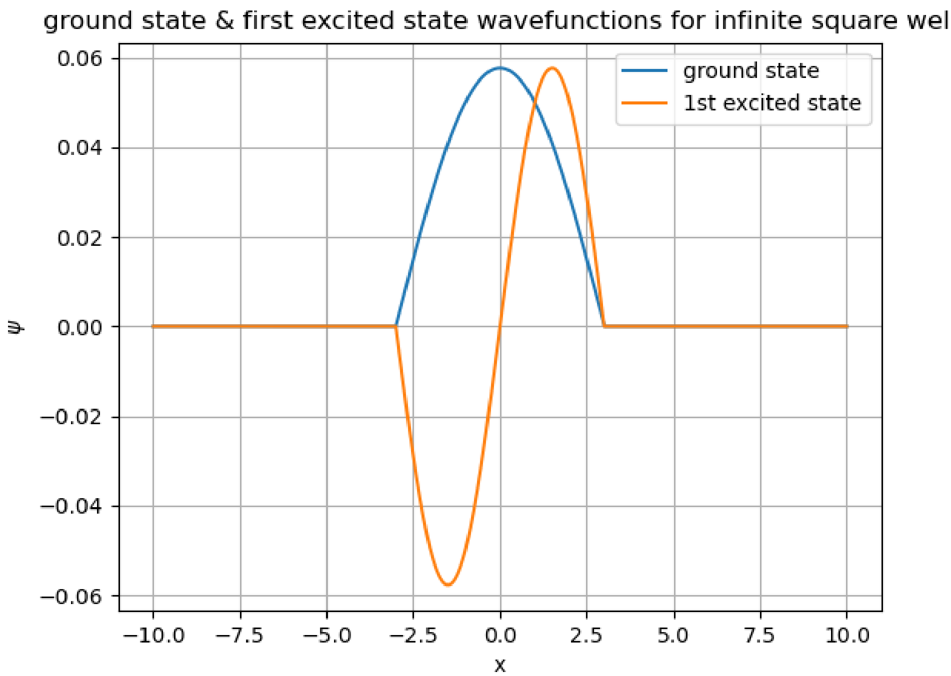

Figure 12: Wave functions for equation (9), infinite square well

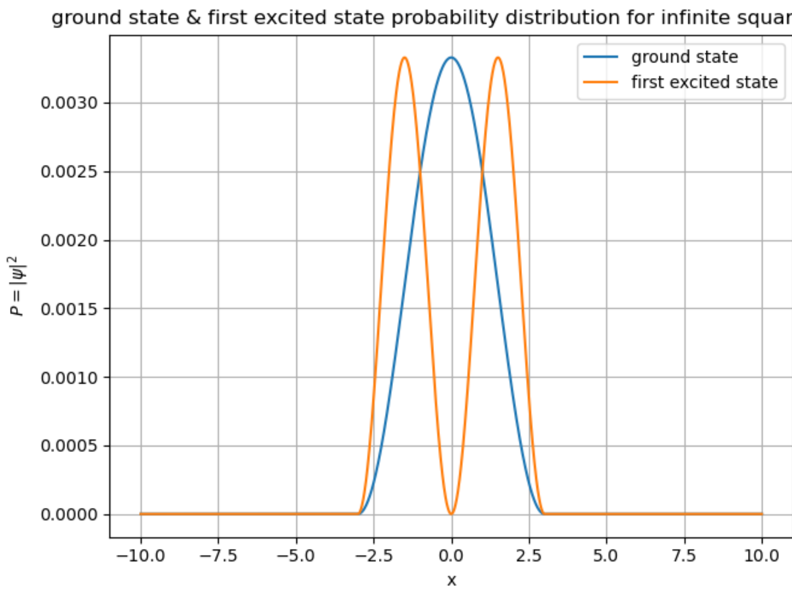

Figure 13: Probability distribution functions for equation (9), infinite square well

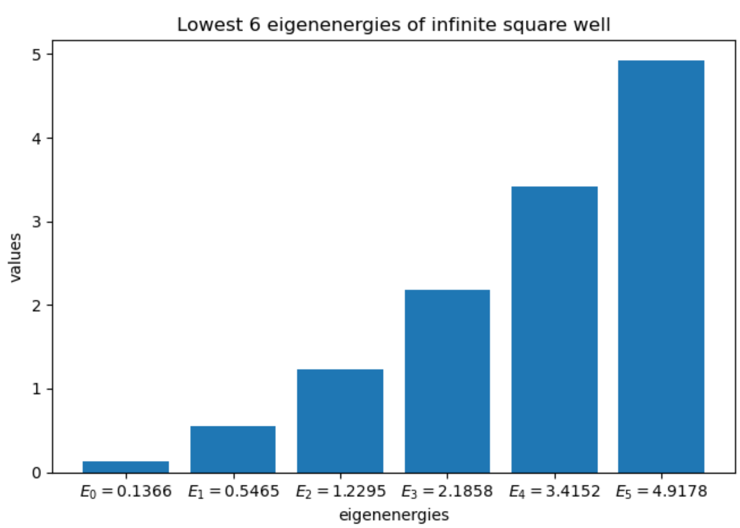

Figure 14: Energy eigenvalues for equation (9), infinite square well

The third potential we are dealing with is a cosine potential function:

$$V(x) = 1 - \cos(\frac{x}{10}) \tag{10}$$

The following plots are obtained by solving Schrödinger equation (equation (7)) for this potential.

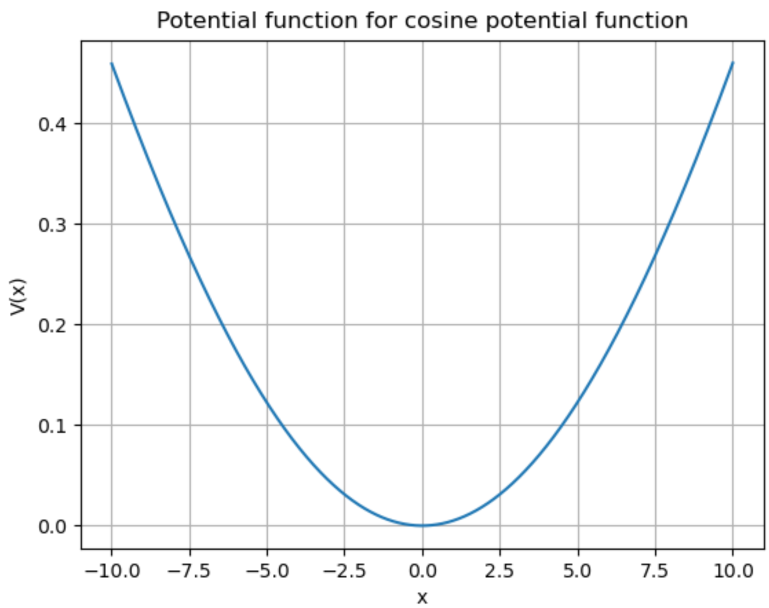

Figure 15: Potential function of equation (10), cosine potential function

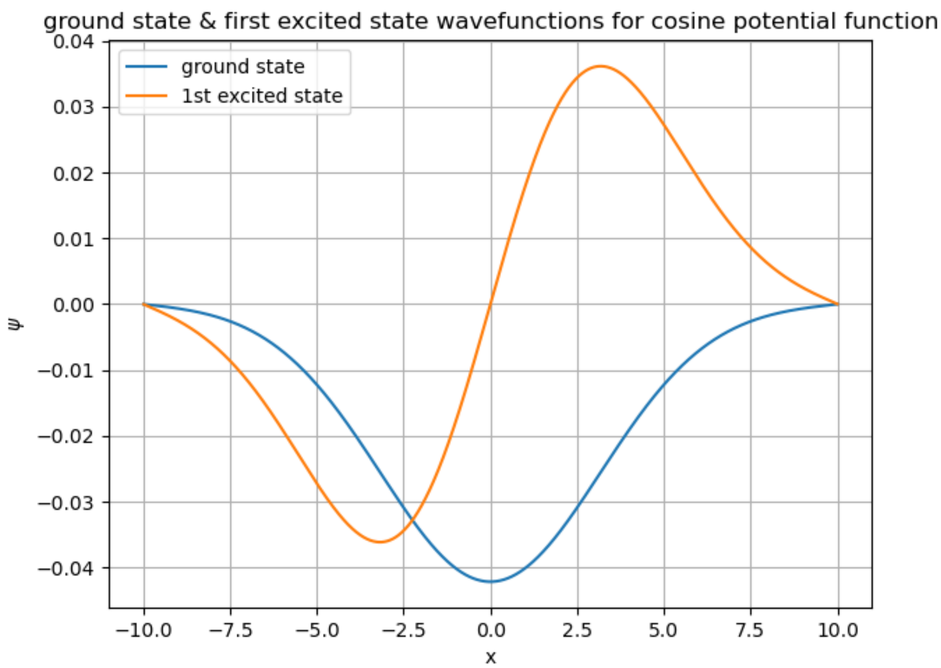

Figure 16: Wave functions for equation (10), cosine potential function

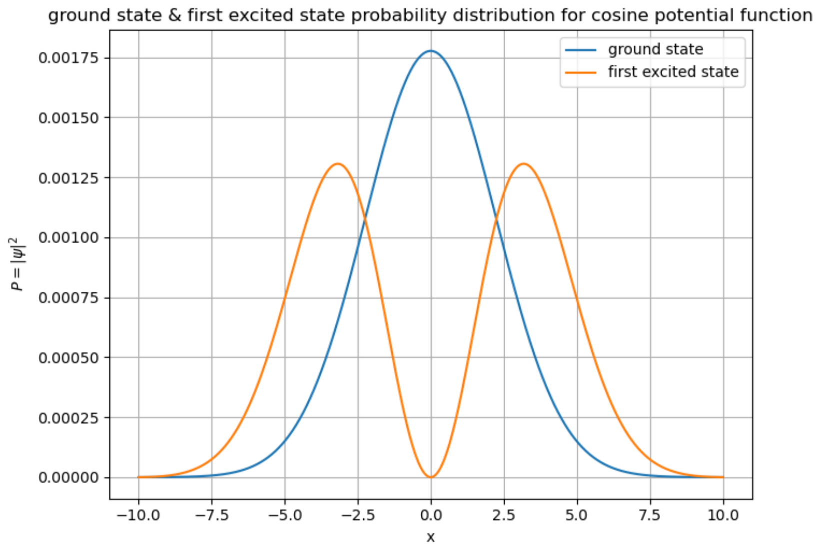

Figure 17: Probability distribution functions for equation (10), cosine potential function

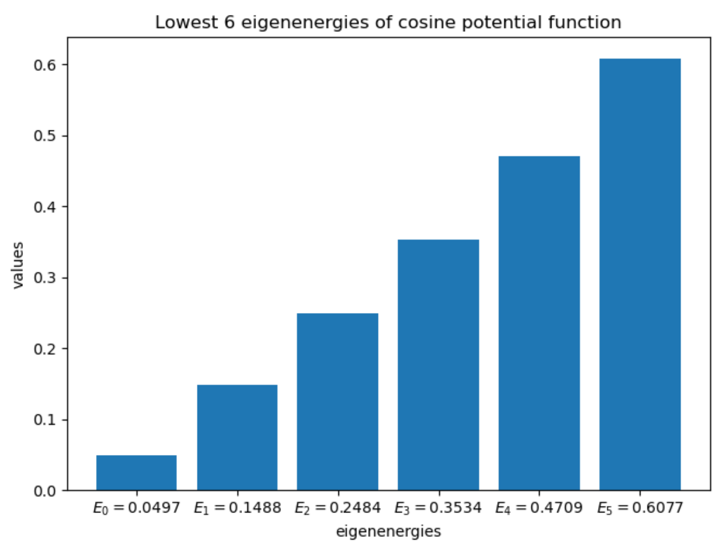

Figure 18: Energy eigenvalues for equation (10), cosine potential function

The fourth and last potential function is linear distance potential:

$$V(x) = |x| \tag{11}$$

The following plots are obtained by solving Schrödinger equation (equation (7)) for this potential.

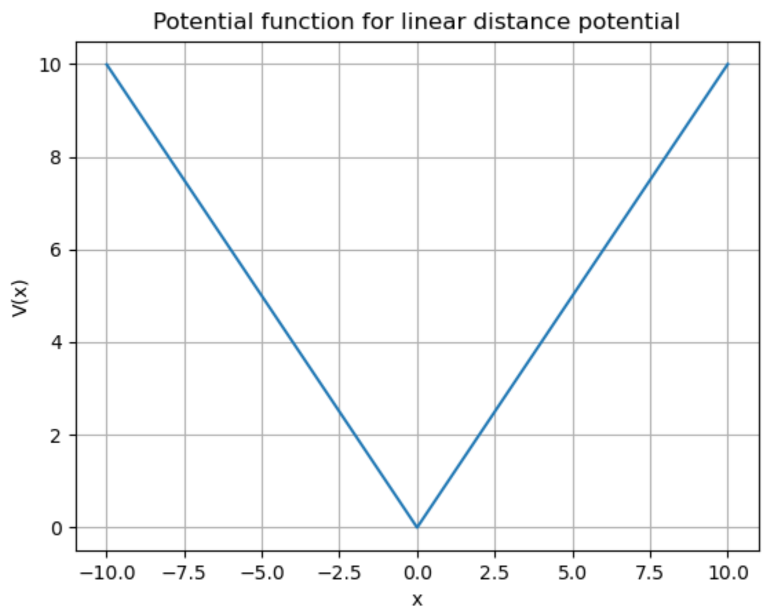

Figure 19: Potential function of equation (11), linear distance potential

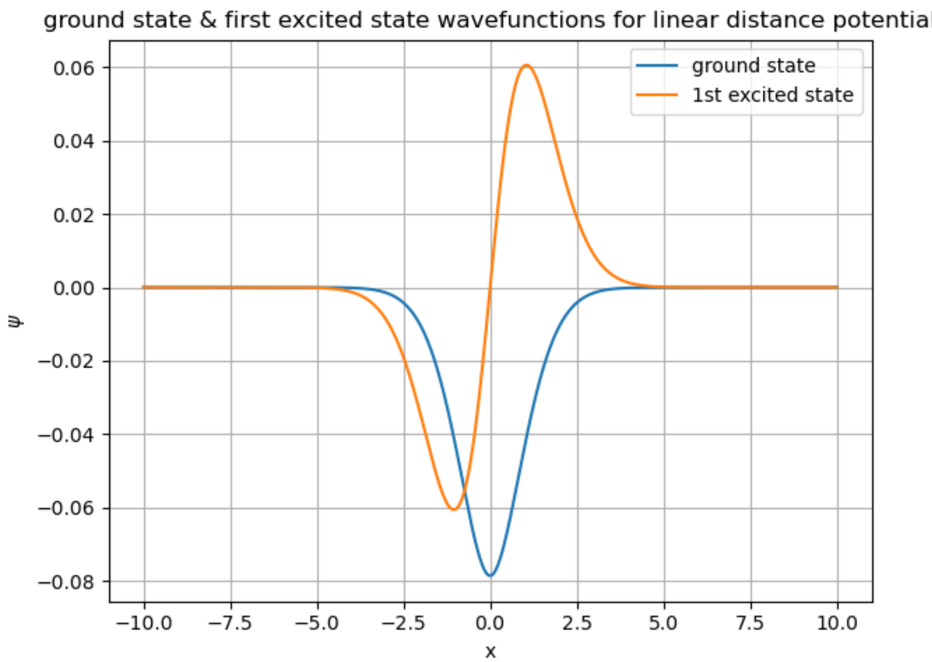

Figure 20: Wave functions for equation (11), linear distance potential

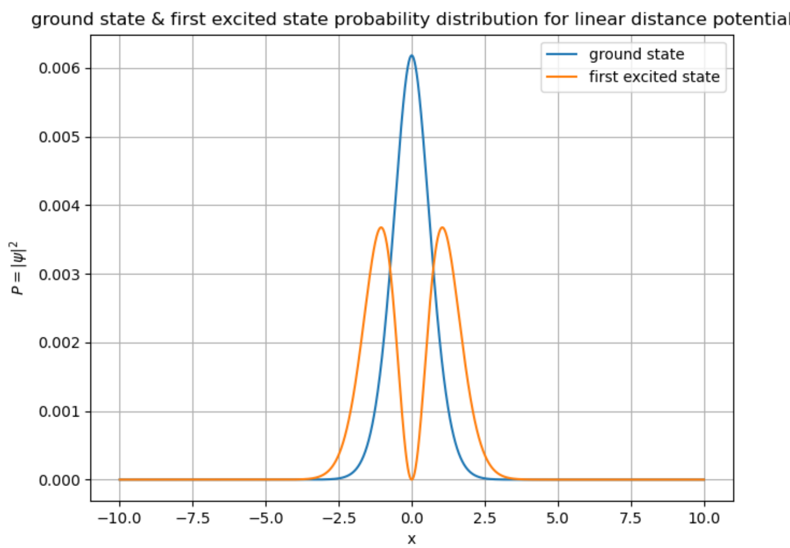

Figure 21: Probability distribution functions for equation (11), linear distance potential

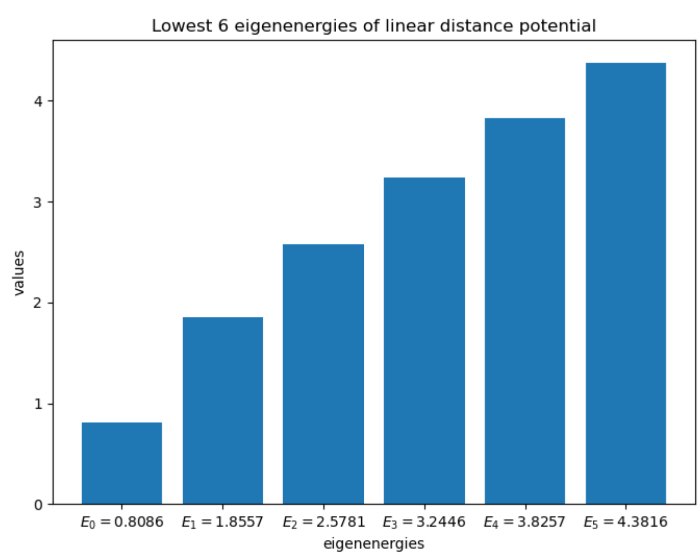

Figure 22: Energy eigenvalues for equation (11), linear distance potential

At the end of this problem, I test some identities in my code and observe that the are true (approximately, because of the inevitable error in numerical work).

First, we can obtain a hermitian operator by simply doing this:

$$M_H = \frac{1}{2}(M + M^\dagger) \tag{12}$$

Orthonormality of eigenvectors of a hermitian operator means:

$$\hat{H}|v_i\rangle = \lambda_i|v_i\rangle \quad \& \quad \hat{H}^\dagger = \hat{H} \quad then \quad \langle v_i|v_j\rangle = \delta_{ij} \tag{13}$$

Definition of a unitary operator U:

$$if \quad \hat{U} \quad is \quad Unitary \qquad then \qquad \hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{1} \tag{14}$$

And the last one is resolution of identity:

$$\sum_j |v_j\rangle\langle v_j| = \hat{1} \tag{15}$$

Problem 4

In this problem we are dealing with a 2-dimensional Schrödinger equation. In this case, the Schrödinger equation takes the form:

$$[-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}) + V(x,y)]\psi(x,y) = E\psi(x,y) \tag{16}$$

And the potential is a 2-dimensional harmonic oscillator:

$$V(x,y) = \frac{1}{2}m\omega^2(x^2 + y^2) \tag{17}$$

Similar to problem 3, I assume that for the numerical solution we have $\hbar = 1, m = 1, \omega = 1$. By solving the Schrödinger equation (16) for potential (17), following results would be obtained:

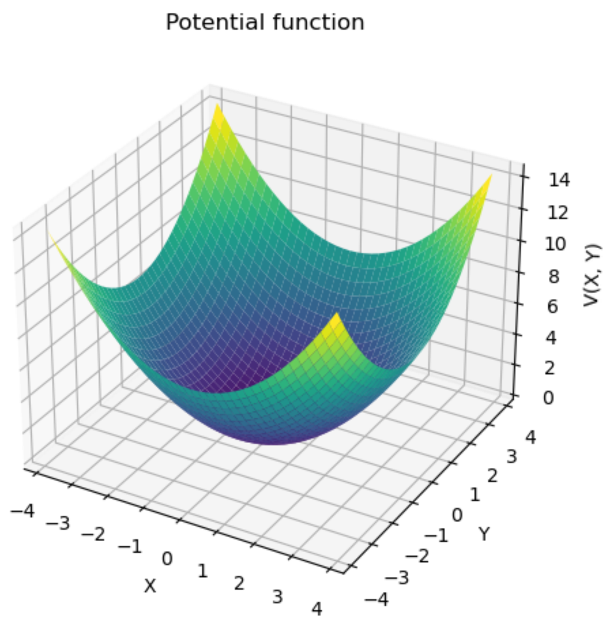

Figure 23: Potential function of 2-dimensional harmonic oscillator (equation (17))

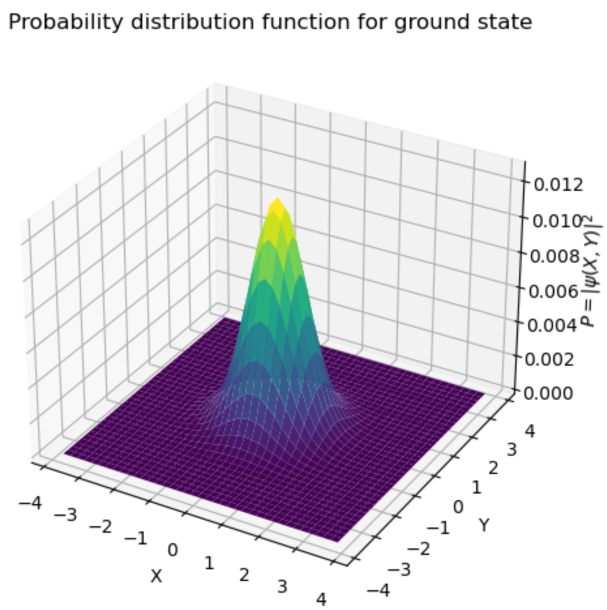

Figure 24: Probability distribution function for ground state of 2-dimensional harmonic oscillator (equation (17))

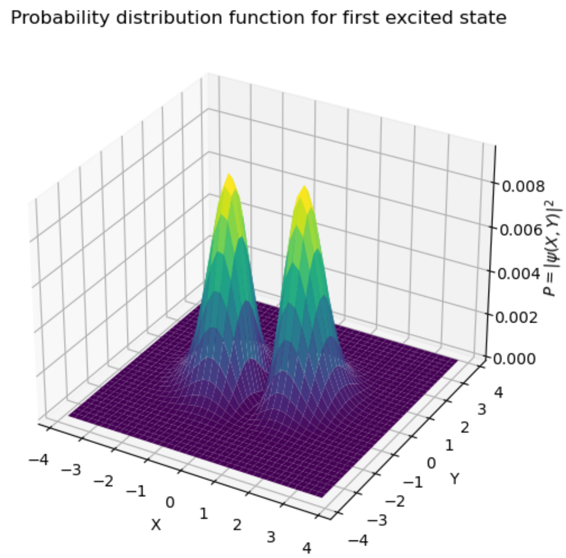

Figure 25: Probability distribution function for first excited state of 2-dimensional harmonic oscillator (equation (17))

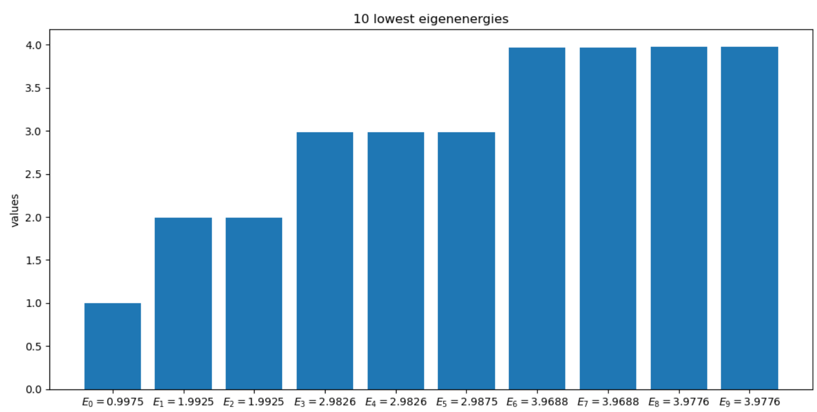

Figure 26: Energy eigenvalues for 2-dimensional harmonic oscillator (equation (17))

Note that from figure 26 it is easily seen that the ground state is non-degenerate, the first excited state is doubly degenerate, the second excited state is triply degenerate, the third excited state is quadruply degenerate and ... . The eigenenergies are in complete consistence with theoretical formula $E_{n_x,n_y} = \hbar\omega(n_x + n_y + \frac{1}{2})$.