Computational Physics Assignment 2

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Contents

1 Important Information Before Starting

1. Programming language used: Python3 (tested on version 3.8.10)
2. Python packages (can be installed using: pip3 install ¡package name¿)::
   (a) numpy
   (b) matplotlib
   (c) scipy (fsolve, solve_ivp, linalg)
3. Use the file uploaded in moodle and save them under the same folder. Execute the files named below using command
   python3 <filename with extension> if using terminal on linux based system:
   - Debsubhra_Assignment2_Prob1.py
   - Debsubhra_Assignment2_Prob2_1.py
   - Debsubhra_Assignment2_Prob2_2.py
   - Debsubhra_Assignment2_Prob2_3.py
   - Debsubhra_Assignment_Prob3.py
4. If any issues regarding execution of the files come up, please DM me via moodle.

2 Problem 1

2.1 Underlying theory

We have a boundary value problem in our hand to solve. The differential equation governing the motion of the football is given by,

$$\frac{d^2\mathbf{r}}{dt^2} = \mathbf{g} - \frac{D}{m}v^2 \tag{1}$$

Here $v = \left|\frac{d\mathbf{r}}{dt}\right|$. $\mathbf{g} = -g\hat{k}$. Now to solve the problem we have used the shooting method. The steps are as following,

1. First we have chosen an initial guess for the three components of the initial velocity of the football and solved the differential equation of find the final y and z coordinates of the football when $x = 22$m.

2. We have expressed the final y and z coordinates of the foorball when $x = 22$m as two function of $\{v_x, v_y, v_z\}$, where these 3 are the cartesian components of the initial velocity. Along with this as we also know the magnitude of the initial velocity we have also another constraint. So, we have three equations and three unknowns.

3. After that we simply used the Newton-Raphson method to find out the roots of the system of equations, such that all the boundary conditions are satisfied. $'RK45'$ has been used to solve the differential equation.

2.2 Output

If the magnitude of the initial velocity is 70km/hr. Then the angle with the horizontal would be,26.39°.
If the magnitude of the initial velocity is 85km/hr. Then the angle with the horizontal would be, 18.679°.
In the both case the angle with the perpendicular to the net drawn from the point of shooting, is 8.68°.
The graph shown below says how the angle with horizontal(θ) should change with the magnitude

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When the magnitude of starting velocity is 70 km/hr, the angle with the horizontal (in degrees) would be:  26.39157884302364
When the magnitude of starting velocity is 85 km/hr, the angle with the horizontal (in degrees) would be:  18.67867965476605
```

of the initial velocity.

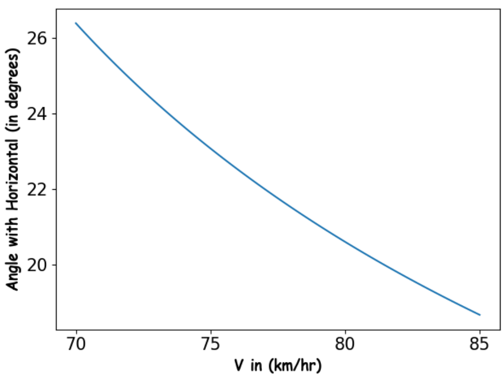

Figure 1: The variation of the angle with the horizontal with the magnitude of the Initial Velocity

3 Problem 2

3.1 Underlying Theory

We would like to calculate the low-lying energy eigenvalues and eigenstates of a particle in the ne dimensional potential

$$V(x) = \frac{1}{2}kx^2 + \frac{\lambda}{4!}x^4 \tag{2}$$

We want to solve the two cases corresponding to $k = \pm 1$ and $\lambda = 1$. Now to solve the problem we have used the relaxation method with periodic boundary condition. We have scaled $\hbar$ and m (mass of the particle) to unity.
After putting the system in a finite box, $x \in \left[-\frac{L}{2}, \frac{L}{2}\right)$ we have discretized the box in sum N points. Now the problem turns into a linear algebra problem of eigenvalue finding. The equation is given by,

$$\begin{bmatrix} \frac{2}{h^2}+2V & -\frac{1}{h^2} & 0 & 0 & 0 & \cdots & 0 & -\frac{1}{h^2} \\ -\frac{1}{h^2} & \frac{2}{h^2}+2V & -\frac{1}{h^2} & 0 & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{h^2} & \frac{2}{h^2}+2V & -\frac{1}{h^2} & 0 & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{h^2} & \frac{2}{h^2}+2V & -\frac{1}{h^2} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -\frac{1}{h^2} & 0 & \cdots & \cdots & \cdots & \cdots & -\frac{1}{h^2} & \frac{2}{h^2}+2V \end{bmatrix} \Psi = 2E\Psi \tag{3}$$

Using linear algebra routine we have calculated the energy eigenvalue and eigenvectors of this system.

3.2 Output

In the figure (2) below we have plotted the energy eigenstates with calculated energy eigenvalues for the case $k = 1$ and $\lambda = 1$. The box size has been used is $x \in [-5, 5)$. We have discretized the intervals using 4000 point with grid size of 0.0025. We have plotted the lowest 6 wavefunction for $k = 1$ and $\lambda = 1$ case. The lowest lying 6 eigenvalues found are 0.5277352, 1.63129536, 2.82217473, 4.0859978, 5.41339245 and 6.79761563 respectively.

For the case of $k = -1$ and $\lambda = 1$ we have used the same box size and grid length to compute

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The energy eigenvalues are:  [ 0.5277352   1.63129536  2.82217473  4.0859978   5.41339245  6.79761563
  8.23352152  9.71702204 11.24477244 12.81397356 14.42224054 16.06751158
 17.74798253 19.46205839 21.20831673 22.98547932 24.79238991 26.62799642
 28.4913366  30.38152622 32.29774937 34.2392503  36.20532657 38.19532324
 40.2086279  42.24466635 44.30289894 46.3828173  48.48394153 50.60581772]
```

the lowest lying eigenvalues and the eigenvectors. The plots of the eigenfunctions are shown in the figure (3). The energy eigenvalues of the lowest lying 6 eigenstates are −0.82988992, −0.85562476, 0.07159974, 0.45156963, 1.16718499 and 1.93839799 respectively.

```
Enter the value of k: -1
The energy eigenvalues are:  [-0.85562476 -0.82988992  0.07159974  0.45156963  1.16718499  1.93839799
  2.80885902  3.75485642  4.76885821  5.84410521  6.97542126  8.15858608
  9.39008583 10.6669383  11.98657443 13.34675372 14.74550184 16.18106364
 17.6518668  19.15649332 20.69365681 22.26218405 23.86100005 25.48911554
 27.14561665 28.82965617 30.54044616 32.27725164 34.03938512 35.82620195]
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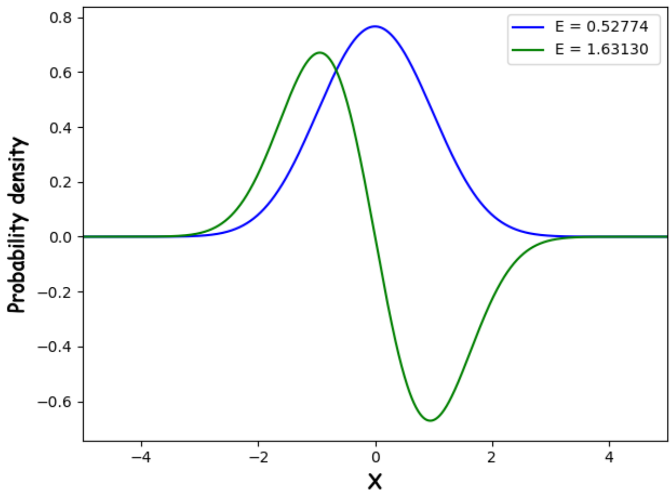
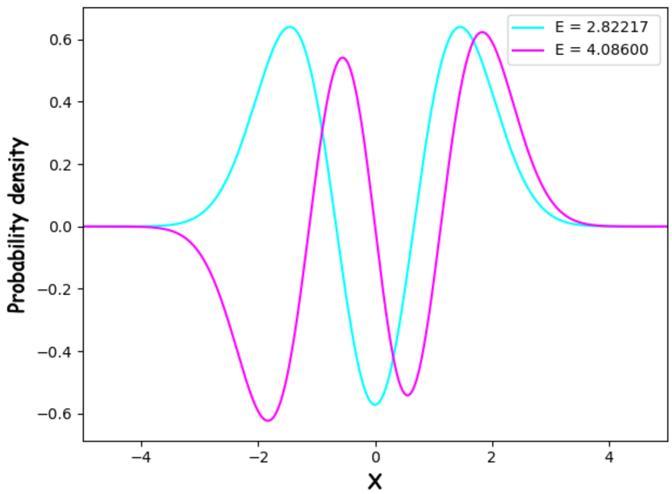
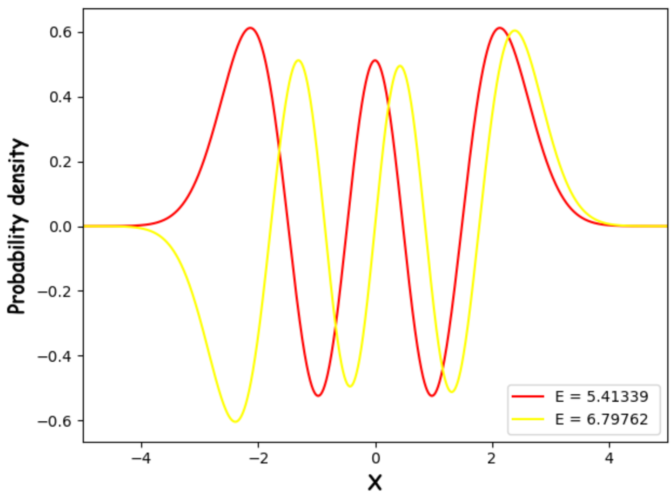


(a) Normalized Eigenfunction for Ground state and $1st$ Excited State

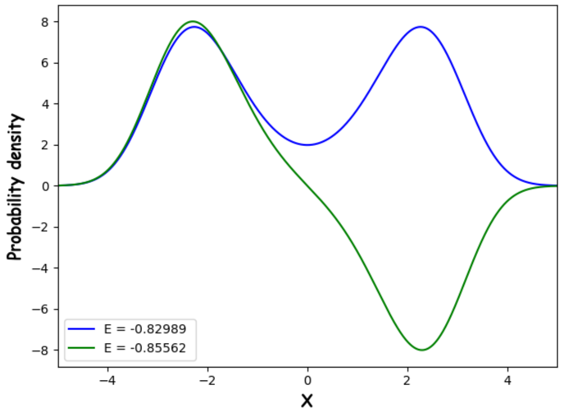


(b) Normalized Eigenfunction for $2nd$ and $3rd$ Excited State

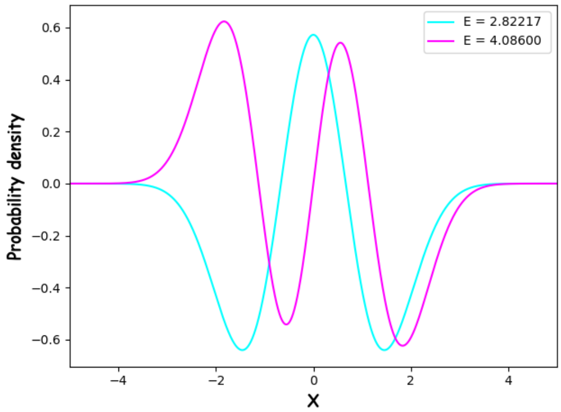


(c) Normalized Eigenfunction for $4th$ and $5th$ Excited State

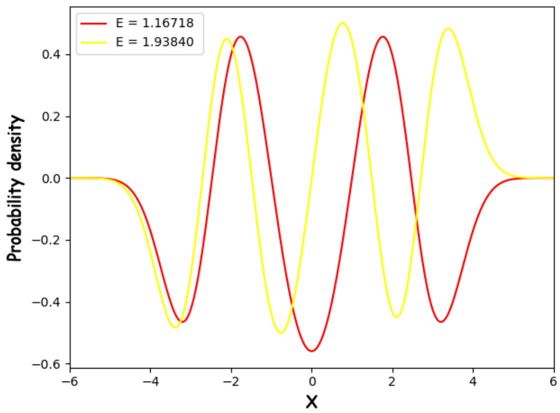
Figure 2: 6 Lowest Energy Eigenstate of the Quartic Potential with$k = 1$ and $\lambda = 1$



(a) Normalized Eigenfunction for Ground state and $1st$ Excited State



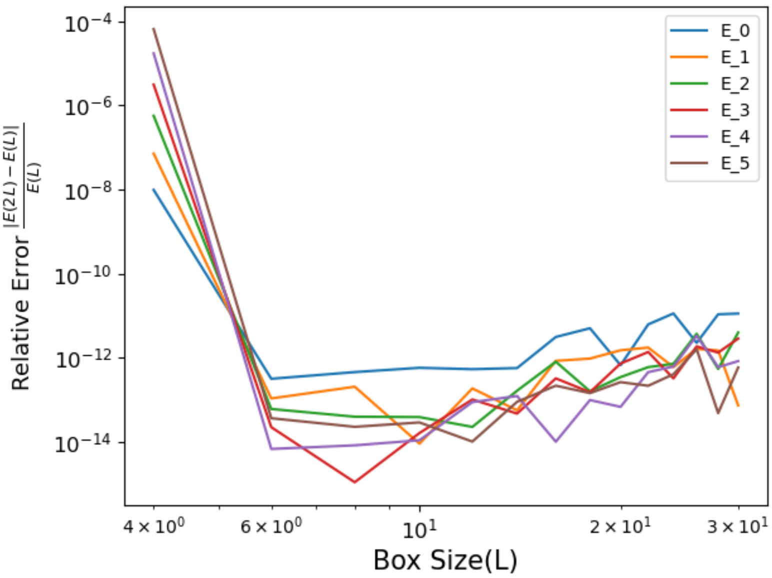
(b) Normalized Eigenfunction for $2nd$ and $3rd$ Excited State



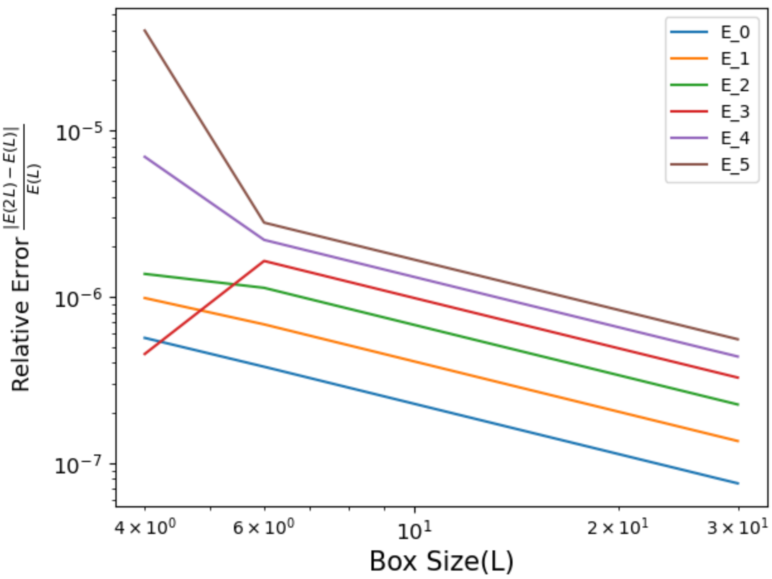
(c) Normalized Eigenfunction for $4th$ and $5th$ Excited State

Figure 3: 6 Lowest Energy Eigenstate of the Quartic Potential with$k = -1$ and $\lambda = 1$

Now we would like to look into how the finite L-correction evolves with L in the periodic boundary condition and Dirichlet boundary condition. For this we have chosen some box size like $\{L_1, L_2, L_3, \cdots\}$. We have plotted the relative error against the box size. The relative error is defined to be $\epsilon = \frac{|E(2L)-E(L)|}{E(L)}$. We have plotted this quantity against L. For this particular case we have chosed the L values to be, $\{4, 6, 8, \cdots, 30\}$. The grid size is fixed in all the cases to 0.04. Figure (4) shows the variation of finite L-correction in periodic boundary condition and the Dirichlet boundary condition. As from the graphs we can clearly see for the periodic boundary conditions the finite L corrections reduce very quickly than that of the Dirichlet boundary condition.



(a) The Finite L correction for The Periodic Boundary Condition



(b) The Finite L correction for The Dirichlet Boundary Condition

Figure 4: The Variation of the finite L-correction with L for the case $k = 1$ and $\lambda = 1$

4 Problem 3

4.1 Underlying Theory

We would like to calculate the average and the rms error of the correlation function for each time slice. The rms error is given by,

$$\epsilon(t) = \sqrt{\frac{\sigma^2(t)}{N-1}} \tag{4}$$

We can calculate the variance in two mathematical equivalent ways.

$$\sigma^2(t) = \frac{1}{N}\sum_{m=1}^{N}\left(C_m(t) - \bar{C}(t)\right)^2 \tag{5}$$

$$\sigma^2(t) = \frac{1}{N}\sum_{m=1}^{N} C_m(t)^2 - \bar{C}(t)^2 \tag{6}$$

The round-off error in the second definition is more than that found from the first definition.
For calculating the mean and variance in a single loop and without increasing the round-off error, we have used the Welford's online algorithm. In this algorithm, we use a recursion relation of mean and variance. Let's say we have $\bar{x}_{N-1}$ and σ^2_{N-1} is the mean and variance of $(N-1)$ data points. If we add an data points x_N, then the new mean and the variance will depend on the old mean and the variance in the following way,

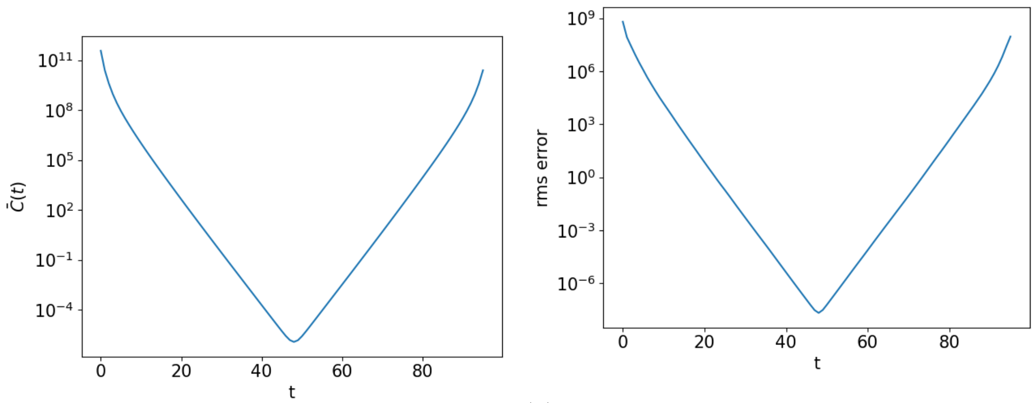
$$\bar{x}_N = \bar{x}_{N-1} + \frac{x_N - \bar{x}_{N-1}}{N} \tag{7}$$

$$C_N = C_{N-1} + (x_N - \bar{x}_{N-1})(x_N - \bar{x}_N) \tag{8}$$

Here $C_N = N\sigma^2_N$. Using this recursion relation we can calculate the mean and variance of the data set using only one loop.
After that we have used the same method to calculate the covariance matrix and calculated the eigenvalues using numpy.linalg.eigval library function.

4.2 Output

The average value of the correlation function and the rms error is plotted against time in the figure (5)



(a) Average Correlation Function Vs Time

(b) RMS Error of the Correlation Function Vs Time

Figure 5: Plots for Correlation Function

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The eigenvalues of the covariance matrix are:  [2.39635068e-05 5.98642334e-06 1.49738244e-08 4.48828724e-09
 1.37758587e-09 3.76455255e-10 2.68247588e-10 5.28375394e-11
 3.92635312e-11 8.99876828e-12 9.39427742e-12 2.46053277e-12
 1.79193658e-12 6.90566710e-13 2.67010049e-13 9.40166672e-14
 8.58761073e-14 1.70833961e-14 1.18804550e-14 5.81282599e-15
 3.74651271e-15 1.37598634e-15 6.77247513e-16 2.96433954e-16
 1.44212651e-16 4.78572911e-17 2.67982610e-17 6.10890452e-18
 2.59796563e-18 6.01721111e-19]
```

The eigenvalues of the covariance matrix is shown above.