import matplotlib.pyplot as plt import numpy as np import matplotlib.pyplot as plt from scipy.integrate import solve ivp

Consider a particle of mass m=1 moving in a 2D double-well potential $V(x,y)=-x^2+0.25x^4+3y^2$

Some of the assumptions for this system are as follows:

• The particle is moving in a frictionless environment • The varying of x and y are independent of each other

from IPython.display import Image from IPython.core.display import HTML

Motivation/Background This problem is inspired by Example 6.5.2 and 6.5.3 from Nonlinear Dynamics and Chaos by Steven Strogatz. Additionally, we discussed a similar problem in class. I choose to expand the problem by another dimension for extra credit to explore higher complexity. The problem is as follows:

Define potential function V = lambda x, y: -x**2 + 0.25*x**4 + 3*y**2# Visualize the problem on 3D plot

In []: # Import packages

x = np.linspace(-2, 2, 100)y = np.linspace(-1, 1, 100)X, Y = np.meshgrid(x, y)# Plotting functions

fig = plt.figure(figsize=(8, 8)) ax = fig.add subplot(111, projection='3d')

ax.plot_surface(X, Y, V(X, Y), cmap='viridis')

ax.set xlabel('x') ax.set ylabel('y') ax.set_zlabel('V(x,y)')

ax.view_init(30, 30)

plt.show()

3.0 2.5 2.0

1.5 0.0 -0.5-1.00 -0.75 -0.50 -0.25 0.00 0.25 0.75 1.0 2.0 **Analytical Investigation**

-1.0

 $-rac{\partial V}{\partial x}=\ddot{x}=2x-x^3$

 $-\frac{\partial V}{\partial y} = \ddot{y} = -6y$

 $\dot{x}=v_x$

 $\dot{v_x}=2x-x^3$

 $\dot{y}=v_y$

 $\dot{v_y} = -6y$

 $E = rac{1}{2}(\dot{x}^2 + \dot{y}^2) + V(x,y)$

 $rac{dE}{dt} = \dot{x}\ddot{x} + \dot{y}\ddot{y} + rac{\partial V}{\partial x}\dot{x} + rac{\partial V}{\partial y}\dot{y}$

 $rac{dE}{dt} = \dot{x}(2x-x^3) + \dot{y}(-6y) + (-2x+x^3)\dot{x} + (6y^2)\dot{y}$

 $\frac{dE}{dt} = 0$

 $\ddot{x} = -\delta \dot{x} - \alpha x - \beta x^3 + \gamma \cos(\omega t)$

 $y(t) = y_0 \cos(\sqrt{6}t)$

Phase Diagram for y

Numerical vs Analytical for y

Numerical Solution Analytical Solution

>

-2 ·

-6

-1

-2

-3

-0.5

0.0

Change perspective -> NOTE: Feel free to vary the angles to explore

We can easily take this potential and find the equations of motion for the system. Note that the equations of motion are as follows: Additionally, we can use our standard procedure to write in terms of first order ODEs:

This will be helpful for our numerical investigation. Going back to looking at the 2nd order ODEs, we make multiple claims about how the system behaves.

1. The system conserves energy. We can show this to be by seeing that the total energy's derivative with respect to time is 0: 1. Looking at the x EOM, we can compare it to the Duffing oscillator equation: oscillation between the two wells.

We can see that the x EOM is the same as the Duffing oscillator equation with $\delta=0$, $\alpha=-2$, $\beta=1$, and $\gamma=0$. This means that it is a undamp and unforced Duffing oscillator. Looking at the Wikipedia page it points out the relation of "Jacobi elliptic function" for this special condition allowing for an analyitical solution. I tried to solve this analytically using this method but I was limited by my lack of knowledge of this method. Nevertheless, by looking at the graph of the potential we can still draw conclusions of expected behaviors. At initial condition of x = 0 v_x = 0 we get no movement in the x direction. At -2 < x < 2 v_x = 0 we get an oscillation in the well it starts in. At x < -2 and x > 2 v_x = 0 we get an 1. Looking at the y EOM, we can see that it is a simple harmonic oscillator with a spring constant of 6. Looking at the graph above this makes sense since in the y direction we get a parabola that a particle would roll back and forth in. This gives us an analytical solution when vy = 0 of: Computational Investigation # Phase diagram and trajectories # Define ODEs def xODE(x, vx): xdot, vxdot = vx, 2*x - x**3return xdot, vxdot def yODE(y, vy): ydot, vydot = vy, -6*yreturn ydot, vydot # Define phase diagram functions (copied from ICAs) def xPhase(X, VX): xdot, vxdot = np.zeros(X.shape), np.zeros(VX.shape) Xlim, Ylim = X.shape

for i in range(Xlim): for j in range(Ylim): xloc = X[i, j]vxloc = VX[i, j]xdot[i,j], vxdot[i,j] = xODE(xloc, vxloc) return xdot, vxdot def yPhase(Y, VY): ydot, vydot = np.zeros(Y.shape), np.zeros(VY.shape) Xlim, Ylim = Y.shapefor i in range(Xlim): for j in range(Ylim): yloc = Y[i, j]vyloc = VY[i, j]ydot[i,j], vydot[i,j] = yODE(yloc, vyloc) return ydot, vydot # Put into format for solve_ivp to find trajectories def x IVP(t, curr val): xdot, vxdot = xODE(curr_val[0], curr_val[1]) return [xdot, vxdot] def y_IVP(t, curr_val): ydot, vydot = yODE(curr_val[0], curr_val[1]) return [ydot, vydot] # Initialize variables x = np.linspace(-8, 8, 20)vx = np.linspace(-8, 8, 20)y = np.linspace(-8, 8, 20)vy = np.linspace(-8, 8, 20)X, VX = np.meshgrid(x, vx)Y, VY = np.meshgrid(y, vy) tmax = 10t = np.linspace(0, tmax, 100)tspan = (0, tmax)# Set initial conditions -> NOTE: Feel free to vary the initial conditions to explore init condX = [1.9, 0] $init_condY = [3, 0]$

solX = solve ivp(x IVP, tspan, init condX, t eval=t, method='RK45') solY = solve_ivp(y_IVP, tspan, init_condY, t_eval=t, method='RK45')

plt.streamplot(X, VX, xPhase(X, VX)[0], xPhase(X, VX)[1])

Solve for trajectories

plt.figure(figsize=(18, 6))

Plot numerical solutions plt.figure(figsize=(18, 6))

plt.plot(solX.t, solX.y[0], c='red') plt.title('Numerical Solution for x')

plt.subplot(1, 2, 1)

plt.xlabel('\$t\$') plt.ylabel('\$x\$')

plt.plot(solX.y[0], solX.y[1], c='red')

plt.title('Phase Diagram for x')

Plot phase diagram

plt.subplot(1, 2, 1)

plt.xlabel('\$x\$')

plt.ylabel('\$v x\$') plt.grid() plt.subplot(1, 2, 2) plt.streamplot(Y, VY, yPhase(Y, VY)[0], yPhase(Y, VY)[1]) plt.plot(solY.y[0], solY.y[1], c='red') plt.title('Phase Diagram for y') plt.xlabel('\$y\$') plt.ylabel('\$v_y\$') plt.grid() plt.show() Phase Diagram for x 2 · š -2 · -6 Comments on phase diagrams: The phase diagrams are shown to be what we expected. The x phase diagram shows multiple different behaviors. At -2 < x < 2 v_x=0 we get the double oscillation. The y phase diagram shows that for any y at v_y=0 we simply go to -y and then back to y. An interesting result that I neglected to discuss in the analytical investigation are situations where the initial velocities are infact not 0. # Inspecting numerical solutions

plt.grid() plt.subplot(1, 2, 2) plt.plot(solY.t, solY.y[0], c='red', label='Numerical Solution') plt.plot(solY.t, init_condY[0]*np.cos(np.sqrt(6)*solY.t), c='blue', label='Analytical Solution') plt.title('Numerical vs Analytical for y') plt.xlabel('\$t\$') plt.ylabel('\$y\$') plt.grid() plt.legend() plt.show() Numerical Solution for x 1.8 1.6 1.4 1.2 1.0 0.8 t In []: # Inspecting energy # Define energy function def energy(x, vx, y, vy): return 0.5*(vx**2 + vy**2) + V(x, y) # Plot energy plt.figure(figsize=(18, 6)) plt.subplot(1, 2, 1) plt.plot(solX.t, energy(solX.y[0], solX.y[1], solY.y[0], solY.y[1]), c='red') plt.title('Total Energy over Time') plt.xlabel('\$t\$') plt.ylabel('\$E\$') plt.grid() Total Energy over Time

26.665 26.660 26.655 26.650 26.645 26.640 10 Comments on total energy plot The energy plot shows that the system does indeed conserve energy as it only varies marginally. This is expected since we showed analytically that the system conserves energy. Visualizing different initial conditions init1 = [0, 0, 0, 0] # No energyinit2 = [1.9, 0, 0, 0] # Oscillation stuck in potential well init3 = [3, 2, 1, 0] # Oscillation going between potential wells init4 = [0, 0, 5, 0] # Oscillation in y init5 = [0, 0, 3, 2] # Oscillation in y with vxinit6 = [4, 0, 2, 0] # Oscillation in x and y def IVP(t, curr_val): xdot, vxdot = xODE(curr_val[0], curr_val[1]) ydot, vydot = yODE(curr_val[2], curr_val[3]) return [xdot, vxdot, ydot, vydot] # Initialize variables tmax = 5t = np.linspace(0, tmax, 40)tspan = (0, tmax)

Solve for trajectories sol1 = solve ivp(IVP, tspan, init1, t eval=t, method='RK45') sol2 = solve_ivp(IVP, tspan, init2, t_eval=t, method='RK45') sol3 = solve_ivp(IVP, tspan, init3, t_eval=t, method='RK45') sol4 = solve_ivp(IVP, tspan, init4, t_eval=t, method='RK45') sol5 = solve_ivp(IVP, tspan, init5, t_eval=t, method='RK45') sol6 = solve_ivp(IVP, tspan, init6, t_eval=t, method='RK45') # Plot trajectories on potential # Plot potential x = np.linspace(-4, 4, 100)y = np.linspace(-4, 1, 100)X, Y = np.meshgrid(x, y)fig = plt.figure(figsize=(8, 8)) ax = fig.add_subplot(111, projection='3d') ax.plot_surface(X, Y, V(X, Y), cmap='viridis', alpha=0.5) ax.set_xlabel('x') ax.set_ylabel('y') ax.set_zlabel('V(x,y)') # Plot trajectories plt.plot(sol1.y[0], sol1.y[2], V(sol1.y[0], sol1.y[2]), c='red', label='[0, 0, 0, 0]') plt.plot(sol2.y[0], sol2.y[2], V(sol2.y[0], sol2.y[2]), c='blue', label='[1.9, 0, 0, 0]') plt.plot(sol3.y[0], sol3.y[2], V(sol3.y[0], sol3.y[2]), c='green', label='[3, 2, 1, 0]') plt.plot(sol4.y[0], sol4.y[2], V(sol4.y[0], sol4.y[2]), c='orange', label='[0, 0, 5, 0]') plt.plot(sol5.y[0], sol5.y[2], V(sol5.y[0], sol5.y[2]), c='purple', label='[0, 0, 3, 2]') plt.plot(sol6.y[0], sol6.y[2], V(sol6.y[0], sol6.y[2]), c='black', label='[4, 0, 2, 0]') plt.legend() # Change perspective -> NOTE: Feel free to vary the angles to explore ax.view_init(30, 60) plt.show() **—** [0, 0, 0, 0] [1.9, 0, 0, 0] **—** [3, 2, 1, 0] **—** [0, 0, 5, 0] **—** [0, 0, 3, 2] [4, 0, 2, 0] 40 20 0

-2 -3 -1

ax.plot(sol2.y[0][:frame], sol2.y[2][:frame], V(sol2.y[0][:frame], sol2.y[2][:frame]), c='blue', label='[1.9, 0, 0, 0]') ax.plot(sol3.y[0][:frame], sol3.y[2][:frame], V(sol3.y[0][:frame], sol3.y[2][:frame]), c='green', label='[3, 2, 1, 0]') ax.plot(sol4.y[0][:frame], sol4.y[2][:frame], V(sol4.y[0][:frame], sol4.y[2][:frame]), c='orange', label='[0, 0, 5, 0]') ax.plot(sol5.y[0][:frame], sol5.y[2][:frame], V(sol5.y[0][:frame], sol5.y[2][:frame]), c='purple', label='[0, 0, 3, 2]') ax.plot(sol6.y[0][:frame], sol6.y[2][:frame], V(sol6.y[0][:frame], sol6.y[2][:frame]), c='black', label='[4, 0, 2, 0]')

ax.scatter(sol2.y[0][frame], sol2.y[2][frame], V(sol2.y[0][frame], sol2.y[2][frame]), c='blue') ax.scatter(sol3.y[0][frame], sol3.y[2][frame], V(sol3.y[0][frame], sol3.y[2][frame]), c='green') ax.scatter(sol4.y[0][frame], sol4.y[2][frame], V(sol4.y[0][frame], sol4.y[2][frame]), c="orange")ax.scatter(sol5.y[0][frame], sol5.y[2][frame], V(sol5.y[0][frame], sol5.y[2][frame]), c="purple")ax.scatter(sol6.y[0][frame], sol6.y[2][frame], V(sol6.y[0][frame], sol6.y[2][frame]), c='black')

ani = FuncAnimation(fig, update, frames=num_frames, init_func=init, blit=False, interval=150);

-4 -2 2 3

import matplotlib.pyplot as plt

fig, ax = plt.subplots()

if frame % 20 === 0: print(frame) # Plot potential

ax.set_xlabel('x') ax.set ylabel('y') ax.set zlabel('V(x,y)') ax.set xlim(-4, 4)ax.set ylim(-4, 4)ax.view_init(30, 60) # # Plot trajectories

#Plot current point

num_frames = len(t)

HTML(ani.to_jshtml())

plt.close()

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x = np.linspace(-4, 4, 100)y = np.linspace(-4, 4, 100)X, Y = np.meshgrid(x, y)

print("init")

def update(frame):

def init():

from matplotlib.animation import FuncAnimation

ax = fig.add_subplot(111, projection='3d')

ani.save('project1.gif', writer='imagemagick', fps=60)

MovieWriter imagemagick unavailable; using Pillow instead.

ax.plot surface(X, Y, V(X, Y), cmap='viridis', alpha=0.5)

In []: # Plot as animation (because I'm addicted to them because they're cool)

In []: # from IPython.display import HTML

In []: # # Save as gif