Homework 7

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1 One-dimensional Kronig-Penney problem

1.1 Question

Numerically solves the motion of a simple pendulum using Euler's method, midpoint method, RK4, Euler-trapezoidal method .

1.2 Solution

When the angle is small, we can make the approximation: sin( ) = , so the problem of simple pendulum can be turned into a harmonic oscillator problem.

$$\left\{\begin{array}{lll} \frac{dv}{dt} & = & -\frac{k}{m}x = -\omega^2 x \\ \frac{dx}{dt} & = & v \end{array}\right. \tag{1}$$

We can implement the four algorithms to solve the ODEs according to the slides.

1.3 Psudocode

Algorithm 1 Euler's Method

Input: time array t ,initial position and speed x_0 and v_0,ω^2

Output: position and speed series x and v.

h=t[1]-t[0]
for i in range len(t do
    xtemp=x[i]+v[i]h
    vtemp=v[i]-ω^2x[i]h
    x=append(x,xtemp)
    v=append(v,vtemp)
end for
return x,v

Algorithm 2 Midpoint Method

Input: time array t ,initial position and speed x_0 and v_0,ω^2

Output: position and speed series x and v.

h=t[1]-t[0]
for i in range len(t **do**
    xmid=x[i]+v[i]h/2
    vmid=v[i]-ω^2x[i]h/2
    xtemp=x[i]+vmid*h
    vtemp=v[i]-ω^2xmid*h
    x=append(x,xtemp)
    v=append(v,vtemp)
end for
return x,v

Algorithm 3 Euler Trapezoidal Method

Input: time array t ,initial position and speed x_0 and v_0,ω^2,error

Output: position and speed series x and v.

h=t[1]-t[0]
for i in range len(t) **do**
    xc_1=x[i]+v[i]h
    vc_1=v[i]-ω^2x[i]h
    while |xc_1-xc_2|>error or |vc_1-vc_2|>error **do**
        xc_2=x[i]+h/2*(v[i]+vc_1)
        vc_2=v[i]-ω^2h/2*(x[i]+xc_1)
    end while
end for
return x,v

Algorithm 4 4th order R-K Method

Input: time array t ,func,initial y_0

Output: y array

```
h=t[1]-t[0]
for i in range len(t) do
    k1 = func(y[i])
    k2 = func(y[i] + 0.5 * h * k1)
    k3 = func(y[i] + 0.5 * h * k2)
    k4 = func(y[i] + h * k3)
    y[i+1]=y[i]+1 / 6 * (k1 + 2 * k2 + 2 * k3 + k4) * h
end for
return y
```

1.4 Results

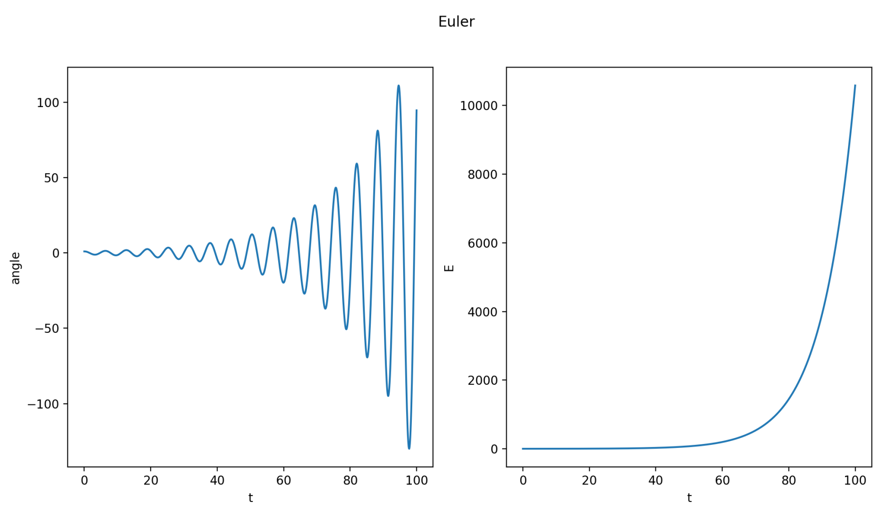

Figure 1: Euler

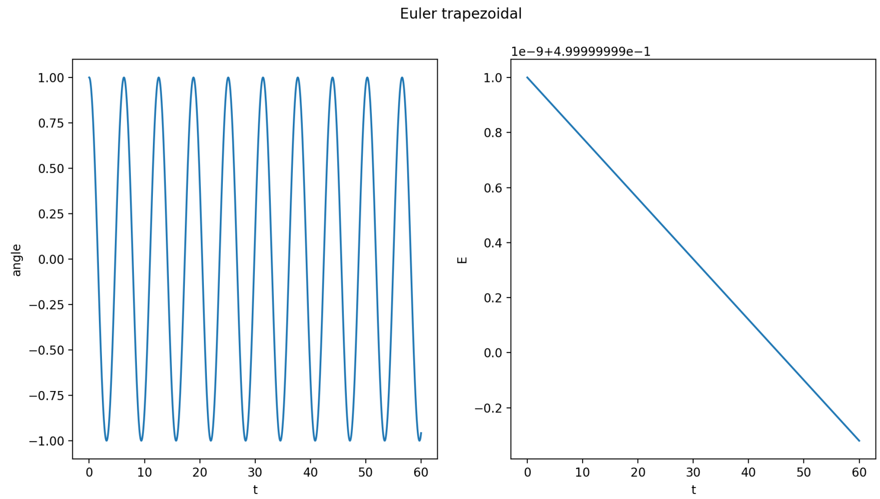

Figure 2: Euler Trapezoidal

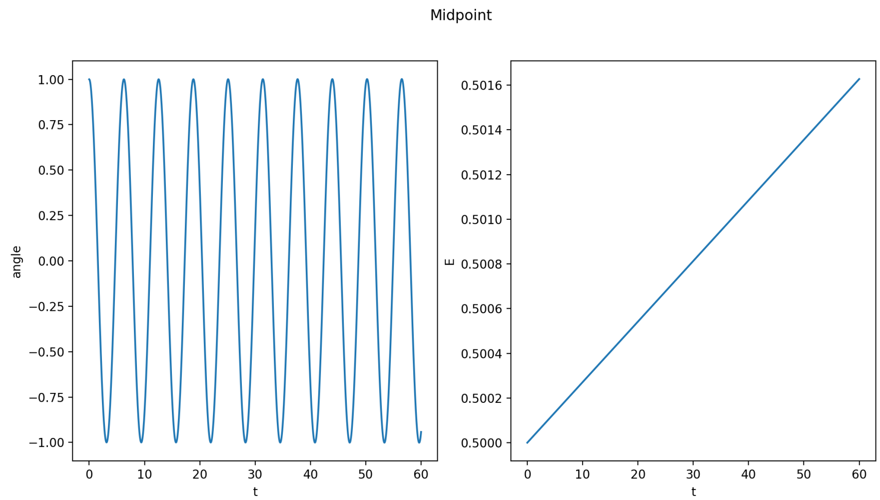

Figure 3: Midpoint

We can see from Figure 1-4 that the divergence of energy in all of the four methods while Euler method has an exponential trend and the rest have linear trends. There is a decrease in divergence speed of the four methods.

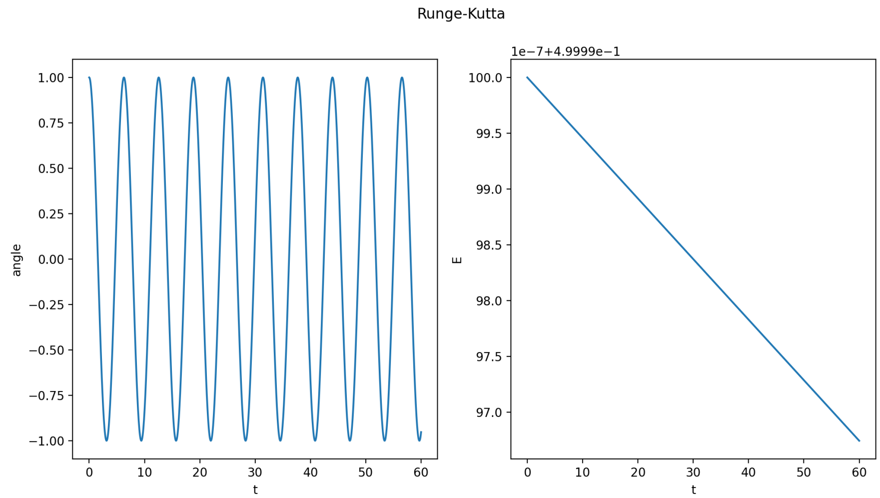

Figure 4: Runge-Kutta

2 Detecting periodicity

2.1 Question

Write a code to numerically solves radial Schrödinger equation for

$$[-\frac{1}{2}\nabla^2 + V(\mathbf{r})]\psi(\mathbf{r}) = E\psi(\mathbf{r}), V(\mathbf{r}) = V(r) \tag{2}$$

where $V(r) = -1/r$ or $V(r) = -1/r^4$

2.2 Solution

We can use the shooting method combined with the secant method to solve radial Schrödinger equation.For convenience,we set $m = h/2\pi = 1$.

$$\psi(\mathbf{r}) = R_l(r)Y_l^m(\theta,\phi) = (u_l(r)/r)Y_l^m(\theta,\phi) \tag{3}$$

$$\frac{d^2}{dr^2}u_l(r) = -2[E - V(r) - \frac{l(l+1)}{2r^2}]u_l(r) \tag{4}$$

To apply the shooting method,we rewrite the eq.(4):

$$\begin{cases} \frac{dU1}{dr} &= U2 \\ \frac{dU2}{dr} &= -2[E - V(r) - \frac{l(l+1)}{2r^2}]U1 \end{cases} \tag{5}$$

2.3 Psudocode

Algorithm 5 The shooting method

Input: newton(),initial U,diff2(),r,E,Elist,odeint(),l

Output: Eigen Energy

```
for E in Elist do
    u[i]=odeint(diff2,initial U,r,args=(E[i],l))
end for
find the zero point of u,return the index
for index in Elist do
    Eigen Energy=newton(shoot,Elist[index],args=(diff2,initial U,r,l))
end for
return Eigen Energy
```

2.4 Results

If the potential function is $V(r) = \frac{1}{r}$,the lowest three eigen-values are -0.499,-0.125(l=0),-0.125(l=1),and the wave functions in figure 6 and 7.

```
[ 999 1749 1887 1936 1959 1980]
[-0.49980039443778973, -0.1249750421922013, -0.05554815855748794, -0.03124491930965184,
7506358781278]
```

```
[1749 1887 1936 1959 1979]
[-0.12499999855781534, -0.05555555548380342, -0.031248629853302623,
```

Figure 5: Eigen-Energy

As for the situation when $V(r) = \frac{1}{r^4}$,the shooting method failed because the wave function oscillates rapidly.And thus we can't optimize the best Enenrgy by newton method or others,which will fall into the local minimal value or just can't converge.Even we applied the non-uniform grid to avoid this,it failed.The Schrödinger's equation is essentially a second-order equation, both the derivative and the second-order derivative in the vicinity of zero will repeatedly change signs. Moreover, according to Shi-Hai Dong's work(https://arxiv.org/pdf/quant-ph/9902081.pdf),$V(r) = \frac{1}{r^4}$doesn't have a bound state,so the question is wrong.

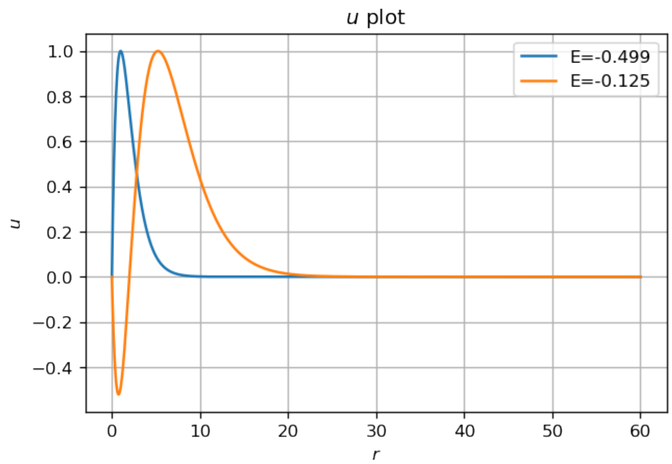

Figure 6: wave function,l=0

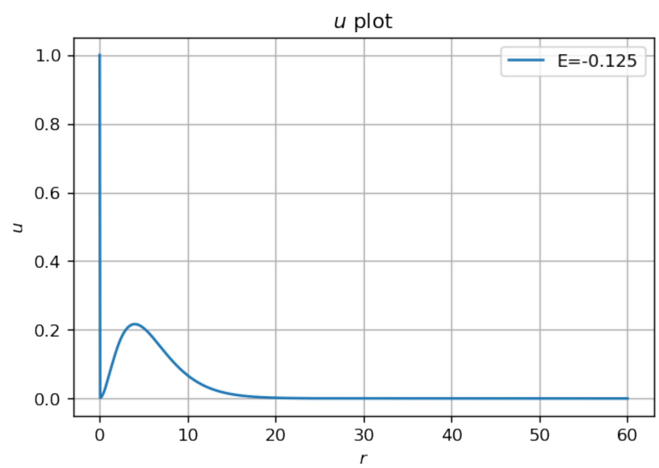

Figure 7: wave function,l=1

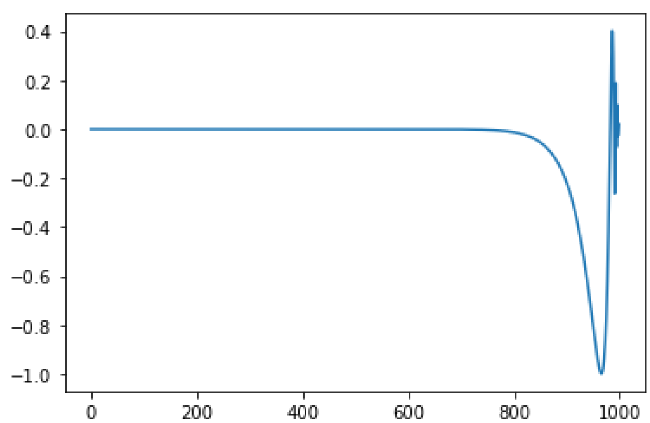

Figure 8: oscillating rapidly