PHYS 410-Computational Physics- Homework 4

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Date: Nov 2016

Part I

In this part, we would like to use from Shooting method to apply the boundary condition that we discussed about and find the six lowest energy eigenvalue and eigenstates.

As we have seen in Quantum mechanic course, potential that behaves like double well potential have odd and even eigen energies and they are splited form each other. As we know the deference between each two paire increase by level of energy.

the following code show the finding energy for odd case and the even one has the similar strucutre

Part II

Now we use the fourth-order explicit Runge-Kutta solver RK4 to solve the Schroodinger equation on the domain $[x0, x0]$, where we take $x0 = 0.6nm$ we set $E = 1eV$. we use the initial conditions $\psi(x_0) = 0$ and $\psi(x_0) = \epsilon$, with $\epsilon = 10^{-5}$ so that $\psi(x) \neq 0$ on the entire domain. We observe that the solution $\psi(x)$ blows up when x increases. The is as a following:

```
function test

f = @(t,v) [v(2), +1*(2/0.076)*v(1)*(-500*t^2+3500*t^4+((500*500)/(4*3500))-1)]; % BVP we are solving
[vShooting,tShooting] = RK4(f,[-0.6,0.6],[0,10^(-5)]); % solution

plot(tShooting,vShooting(:,1),'-',tShooting,vShooting(:,2),'-.')
title('Solution of Schroodnger equation for E=1 eV and and D[\psi,x]=10^-5   ')
xlabel('nm')
ylabel('\psi and D[\psi,x]')
%plot(tShooting,vShooting(:,1),'-')

end
```

The reason is that In the classically forbidden regions, Schrodinger equation admits two linearly independent solutions, one of which increases while the other decreases. therefore if have $\psi' > 0$ in some point it guaranties the ψ increases continuously. thus there are just specific energies provide 'physical' solution. Physics means for example the sum of probability should be one over whole space time.

Now in order to find the solutions of Schroodinger which we call them eigenfunctions, we need to work on boundary value problem. hopefully according to our potential, we have symmetry under changing of parity, thus we deduce that the eigenstates $\psi(x)$ are either even or odd functions of x. This tells us that we only need to numerically integrate the equation on the interval $[x0, 0]$, with appropriate boundary conditions at $x = 0$.

According to Fig2, the odd function should vanishes at center thus :

$$\psi(x = 0) = 0, \qquad \text{Odd} \tag{1}$$

and for even wave functions the first derivite of wave function should vanishes at center:

$$\psi'(x = 0) = 0, \qquad \text{Even} \tag{2}$$

We can use this advantage to solve the differential equation with Shooting method.

in shooting method instead of solving boundary value problems :

$$D[f, x] = 0, \qquad x(0) = a, x(1) = b \tag{3}$$

we try to find the solution of

$$D[f, x] = 0, \qquad x(0) = a, x(a) = c \tag{4}$$

such that this solution gives value of b at $x = 1$. the method has been exploit in the following code. we substitute the Even and parity condition is Shooting method and looking for energy that provides the solution consistent. It's useful to recall that in general $\psi \sim e^{ikx}$ thus $\psi'(x = 0) \sim k$, this helps us to start out initial guess with reasonable value.

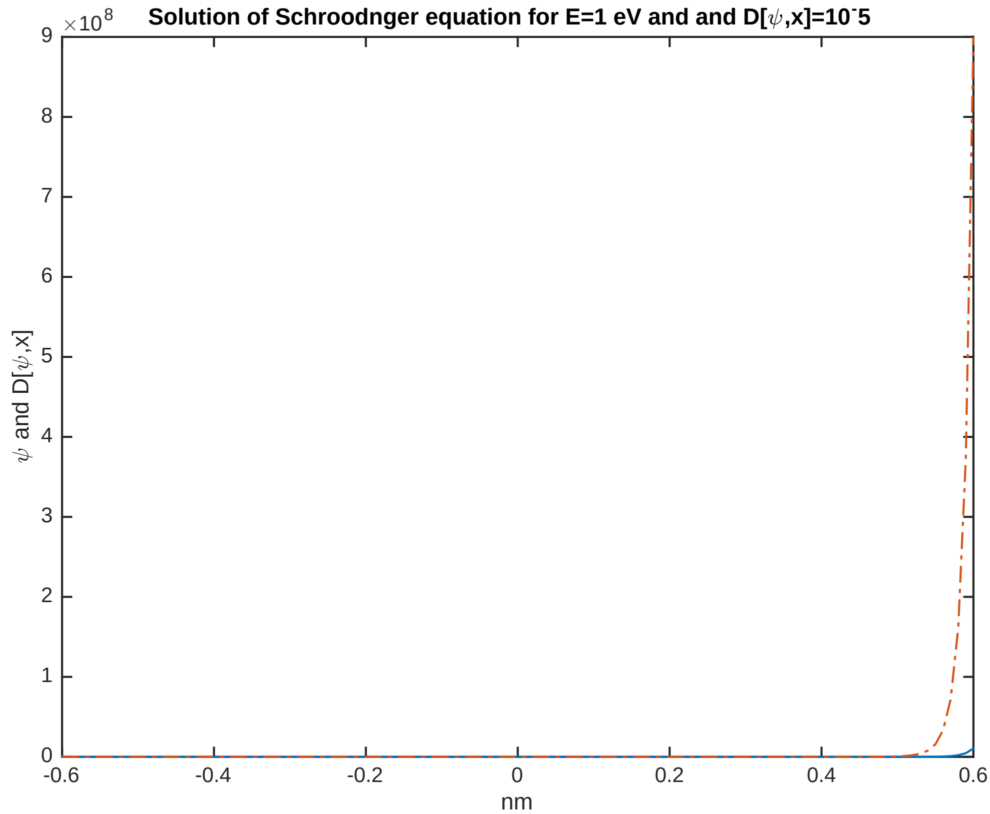

Figure 1: Solutions of Schroodinger equation with E=1ev

Matlab Code

```
function Odd
%% First method: Shooting method

```

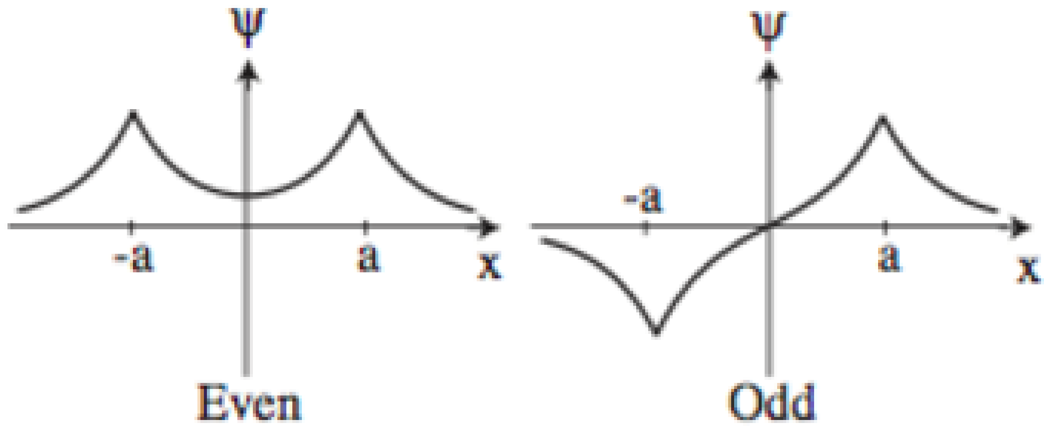

Figure 2: Even and Odd wave functions

```
% Finding v'(0) = C such that v(1) = 0

C0 = 26;            % initial guess (try C0=10 for second solution)
C = fzero(@endpoint,C0);

f = @(t,v) [v(2), +1*(2/0.076)*v(1)*(-500*t^2+3500*t^4+((500*500)/(4*3500))-C
    ^2*(0.076/2))];        % BVP we are solving- Schroodinger Equation
[vShooting,tShooting] = RK4(f,[0,0.6],[0,C]); % solution

function v1 = endpoint(C)

f = @(t,v) [v(2), +1*(2/0.076)*v(1)*(-500*t^2+3500*t^4+((500*500)/(4*3500))-C
    ^2*(0.076/2))];
v = RK4(f,[0,0.6],[0,C]);

v1 = v(end,1); % corresponds to v(1)
v1p= v(end,2);

end

[V1,T1] = RK4(f,[-0.6,0.6],[0,C]); % solution

plot(T1,V1(:,1),'-',T1,V1(:,2),'-.')

end
```

```
function Even
%% Shooting method

% Finding v'(0) = C such that v(1) = 0

C0 = 24.34;            % initial guess (try C0=10 for second solution)
C = fzero(@endpoint,C0);

f = @(t,v) [v(2), +1*(2/0.076)*v(1)*(-500*t^2+3500*t^4+((500*500)/(4*3500))-C
    ^2*(0.076/2))];        % BVP we are solving
[vShooting,tShooting] = RK4(f,[0,0.6],[C,0]); % solution

function v1 = endpoint(C)
```

```
f = @(t,v) [v(2), +1*(2/0.076)*v(1)*(-500*t^2+3500*t^4+((500*500)/(4*3500))-C^2*(0.076/2))];
v = RK4(f,[0,0.6],[C,0]);

v1 = v(end,1); % corresponds to v(1)
v1p= v(end,2);


[vv,tt] = RK4(f,[0,0.6],[C,0]); % solution

plot(tt,vv(:,1),'-',tt,vv(:,2),'-.')

end
```

We need to try many C_0 as a initial guess to find specific C that provides consistent equation that obeys from Schrodinger equation and represent the eigenstates of our system which is the anharmonic oscillator.

Our trials provides the following table for six lowest enrgies:

$$\begin{aligned} E_{1,E} &= 5.8463eV \\ E_{1,O} &= 5.8822eV \\ E_{2,E} &= 15.3463eV \\ E_{2,O} &= 16.6473eV \\ E_{3,E} &= 22.5586eV \\ E_{3,O} &= 27.6146eV \end{aligned} \tag{5}$$

Now we can plot the eigenes states in one plot in one figure. We plot the potential in the background to see how is the relation between potential and probability of wave function at that point. We normalize the wave function by using the trapz function in MATLAB:

$$\int |\psi|^2 dx = C, \qquad \psi \to \frac{1}{\sqrt{C}}\psi \tag{6}$$

We also shift the base line of wave function with its associated energy to observe the behavior of wave function better. As we expect the odd eigen states are zeor at center and Even ones are flat the center which is consistent with what we expect from even and odd functions . The final plot is as a following

As we can see the two lowest energy are very near to each other.

According to WKB method we can say something by theory about the eigen values approximately. If we define:

$$\phi = \frac{1}{\hbar}\int_{-x_1}^{x_1}\sqrt{\frac{2mE}{\hbar^2}} \tag{7}$$

then

$$E_n^{\pm} \simeq (n+\frac{1}{2})\hbar\omega \mp \frac{\hbar\omega}{2\pi}e^{-\phi} \tag{8}$$

as we can see the Even modes have less energy compare to Odd ones.

In general if the barrier were impenetrable, $\phi \to \infty$, we would simply have two detached harmonic oscillators, and the energies $E_n = (n+1/2)\hbar\omega$ would be doubly degenerate, since the particle could be in the left well or in the right one. When the barrier becomes finite, putting the two wells into "communication", the degeneracy is lifted. The even states, ψ_+ have slightly lower energy, and the odd ones, ψ_- have slightly higher energy.

```

C1=20.9305;
f = @(t,v) [v(2), +1*(2/0.076)*v(1)*(-500*t^2+3500*t^4+((500*500)/(4*3500))-C1^2*(0.076/2))];
[V1,T1] = RK4(f,[-0.6,0.6],[0,C1]); % solution

plot(TTT1,VVV1)
Q1 = trapz(T1,V1(:,1).*V1(:,1))
%VV1=(V1+C1^2*(0.076/2))./(sqrt(Q1));
VV1=(V1)./(sqrt(Q1));
%VV1=V1./(100);
```

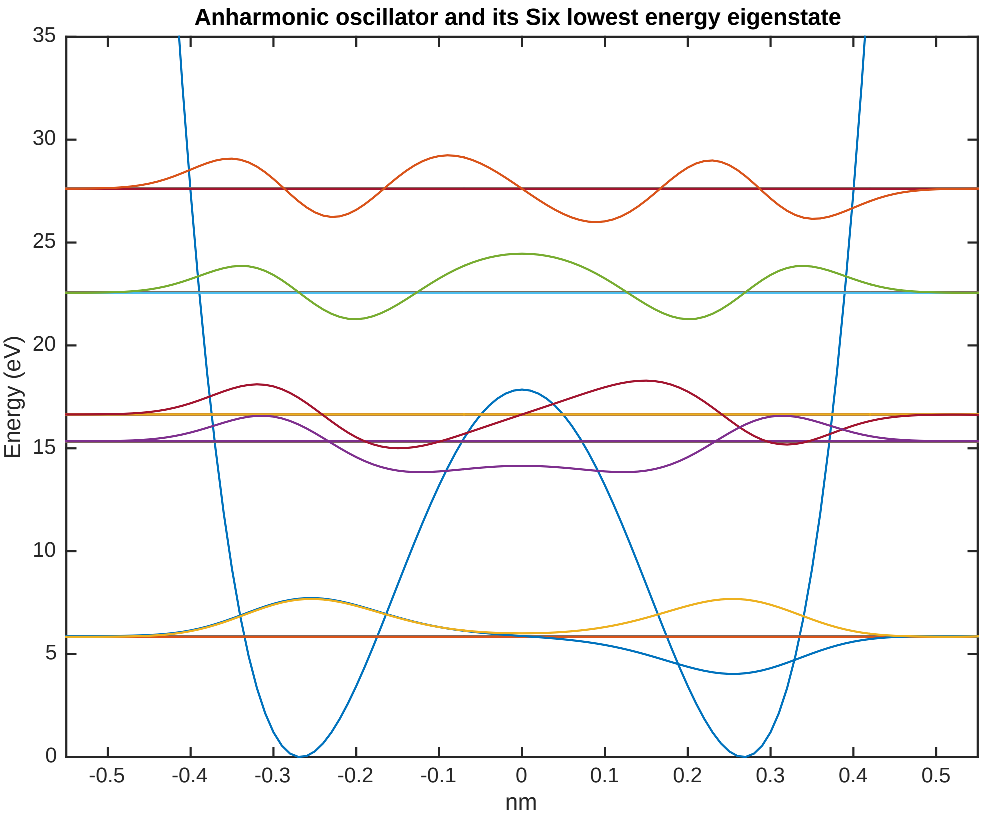

Figure 3: Six lowest EigenEnergies

```
%plot(T1,V1(:,1),'-',T1,V1(:,2),'-.')
%plot(T1,V1(:,1),'-')
C2=12.4416;
f = @(t,v) [v(2), +1*(2/0.076)*v(1)*(-500*t^2+3500*t^4+((500*500)/(4*3500))-C2
    ^2*(0.076/2))];
```

```
[V2,T2] = RK4(f,[-0.6,0.6],[0,C2]); % solution
[VVV2,TTT2] = RK4(f,[-10,10],[0,C2]); % solution
Q2 = trapz(T2,V2(:,1).*V2(:,1))
VV2=V2./(sqrt(Q2));
%plot(T2,VV2(:,1),'-',T1,VV1(:,1),'-')

C3=26.9574;
f = @(t,v) [v(2), +1*(2/0.076)*v(1)*(-500*t^2+3500*t^4+((500*500)/(4*3500))-C3^2*(0.076/2))];
[V3,T3] = RK4(f,[-0.6,0.6],[0,C3]); % solution
[VVV3,TTT3] = RK4(f,[-100,100],[0,C3]); % solution
Q3 = trapz(T3,V3(:,1).*V3(:,1))
VV3=V3./(sqrt(Q3));
%plot(T2,V2(:,1),T1,V1(:,1),T3,V3(:,1))
%legend('T2','T1','T3')
E1=(C1^2*(0.076/2)).*ones(length(T1));
E2=(C2^2*(0.076/2)).*ones(length(T1));
E3=(C3^2*(0.076/2)).*ones(length(T1));
EE1=C1^2*(0.076/2)
EE2=C2^2*(0.076/2)
EE3=C3^2*(0.076/2)


D1=12.4036;
f = @(t,v) [v(2), +1*(2/0.076)*v(1)*(-500*t^2+3500*t^4+((500*500)/(4*3500))-D1^2*(0.076/2))];
[V4,T4] = RK4(f,[-0.6,0.6],[D1,0]); % solution
Q4 = trapz(T4,V4(:,1).*V4(:,1));
VV4=V4./(sqrt(Q4));




D2=20.0960;
f = @(t,v) [v(2), +1*(2/0.076)*v(1)*(-500*t^2+3500*t^4+((500*500)/(4*3500))-D2^2*(0.076/2))];
[V5,T5] = RK4(f,[-0.6,0.6],[D2,0]); % solution
Q5 = trapz(T5,V5(:,1).*V5(:,1));
VV5=V5./(sqrt(Q5));

D3=24.3649;
f = @(t,v) [v(2), +1*(2/0.076)*v(1)*(-500*t^2+3500*t^4+((500*500)/(4*3500))-D3^2*(0.076/2))];
[V6,T6] = RK4(f,[-0.6,0.6],[D3,0]); % solution
Q6 = trapz(T6,V6(:,1).*V6(:,1));
VV6=V6./(sqrt(Q6));

E4=(D1^2*(0.076/2)).*ones(length(T1));
EE4=D1^2*(0.076/2)
E5=(D2^2*(0.076/2)).*ones(length(T1));
EE5=D2^2*(0.076/2)
E6=(D3^2*(0.076/2)).*ones(length(T1));
EE6=D3^2*(0.076/2)

V=@(x) -500*x.^2+3500*x.^4+(500*500)/(4*3500);
pot=feval(V,T1);
%plot(T1,pot,T1,V1(:,1),T1,E1,T2,V2(:,1),T3,V3(:,1))
plot(T1,pot,T1,E1,T1,E2,T1,E3,T1,E4,T1,E5,T1,E6,T1,VV1(:,1)+EE1,T1,VV2(:,1)+EE2,T1,VV3(:,1)+EE3,T1,VV4(:,1)+EE4,T1,VV5(:,1)+EE5,T1,VV6(:,1)+EE6)
ylim([0 35])
xlim([-0.55 0.55])
```

```
title('Anharmonic oscillator and its Six lowest energy eigenstate ')
xlabel('nm')
ylabel('Energy (eV)')
```