SOLVING ODES NUMERICALLY FOR VARIOUS PHYSICS PROBLEMS

HOMEWORK #3

DUE DATE: 03/22/2013

QUESTION 1

1. Consider the problem of planetary motion around the Sun, as discussed during lecture 8.

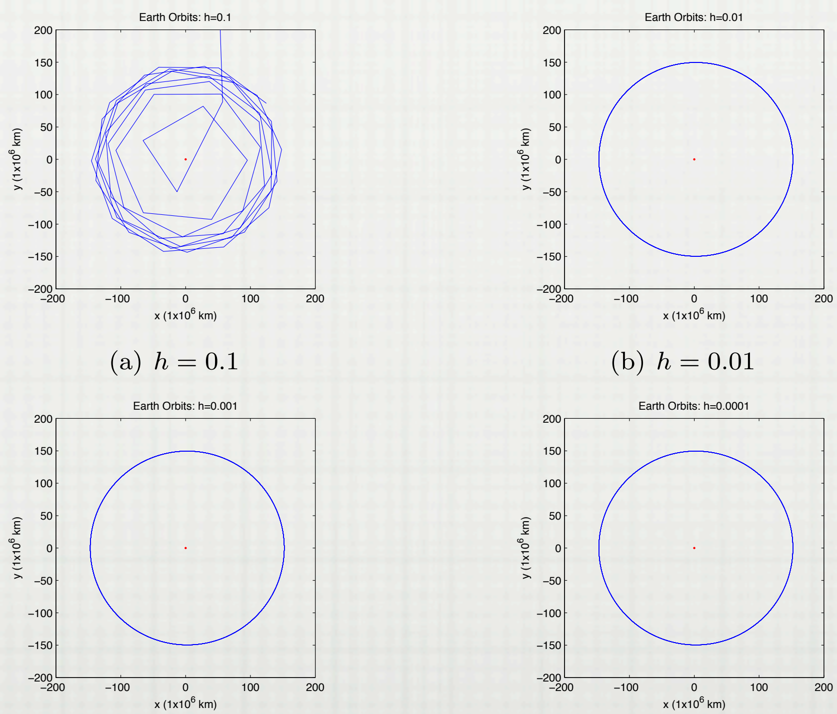
   (a) Write a C++ code, using Runge-Kutta at fourth order (RK4) to describe the motion of Earth and Jupiter around the Sun. You will use the RK4 library provided in class.

   - First discuss the trajectories when Jupiter and Earth do not interact. (Hint: you will have 2 bodies, 2 spatial variables per body and no cross-terms)
   - Then, turn on the Jupiter-Earth gravitational interaction. (Hint: same as before but with a cross-term between Jupiter and Earth)
   - In both cases, use realistic numbers for the orbits (size of the orbit, velocity at aphelion or perihelion, etc...). Verify Kepler's laws and compute periodicity.
   - Repeat your calculations, by artificially increasing the mass of Jupiter by a factor of 1,000. Discuss the effect on the orbits. Make sure you make clear plots of the orbits.

   Note: it is a good idea to use astronomical units.

Q1: IDEA OF THE SOLUTION

$$\vec{F_G} = m(\ddot{x}, \ddot{y}) = -\frac{GMm}{r^3}(x, y)$$



(a) $h = 0.1$ (b) $h = 0.01$

(c) $h = 0.001$ (d) $h = 0.0001$

Figure 1: Plots of the orbit of Earth around the Sun using different values of h. Each axis has the same scale.

NON-INTERACTING JUPITER AND EARTH

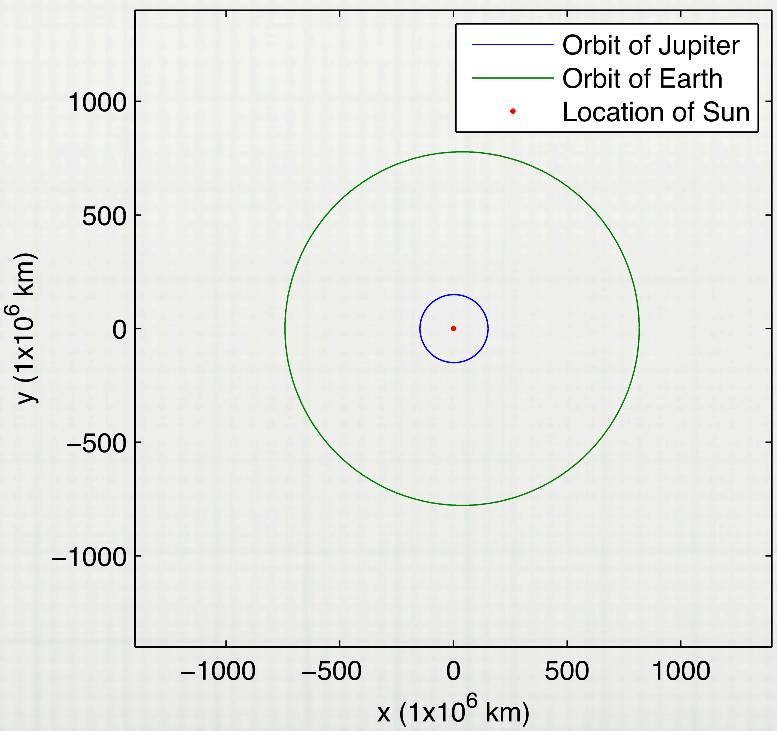
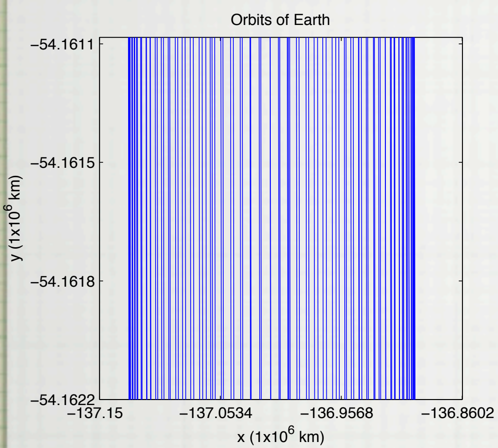
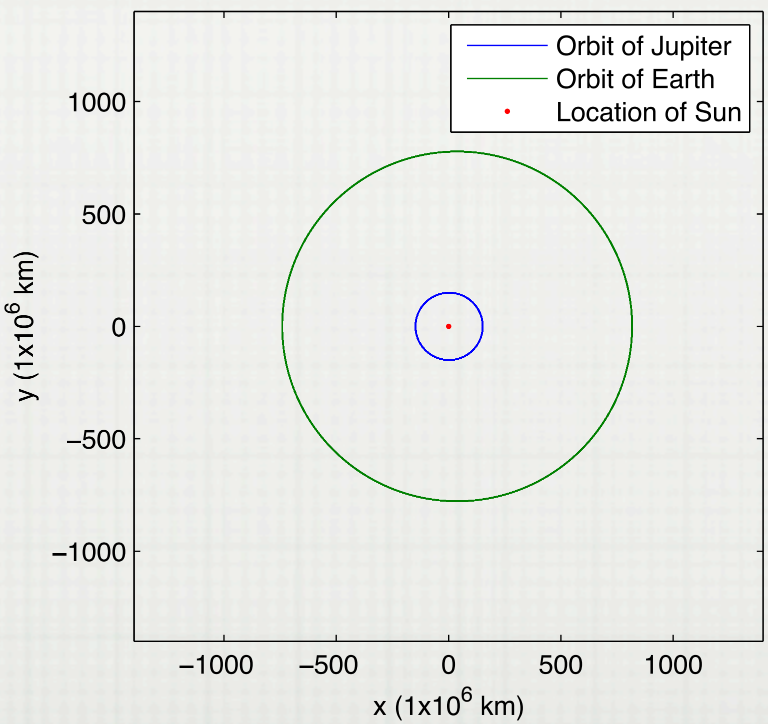


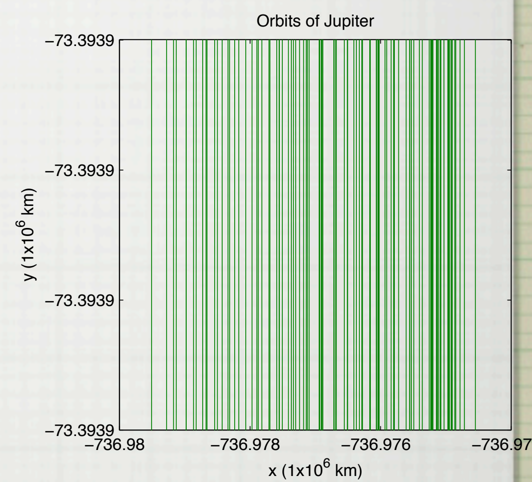
Figure 2: 1 period of the orbits of Earth and Jupiter around the Sun, ignoring Earth-Jupiter gravitational interactions. Each axis has the same scale.

INTERACTING JUPITER AND EARTH



(a) Earth's Orbits





(b) Jupiter's Orbits

Figure 3: 100 orbits of Earth and Jupiter around the Sun, including Earth-Jupiter gravitational interactions. Each axis has the same scale.

FAT JUPITER

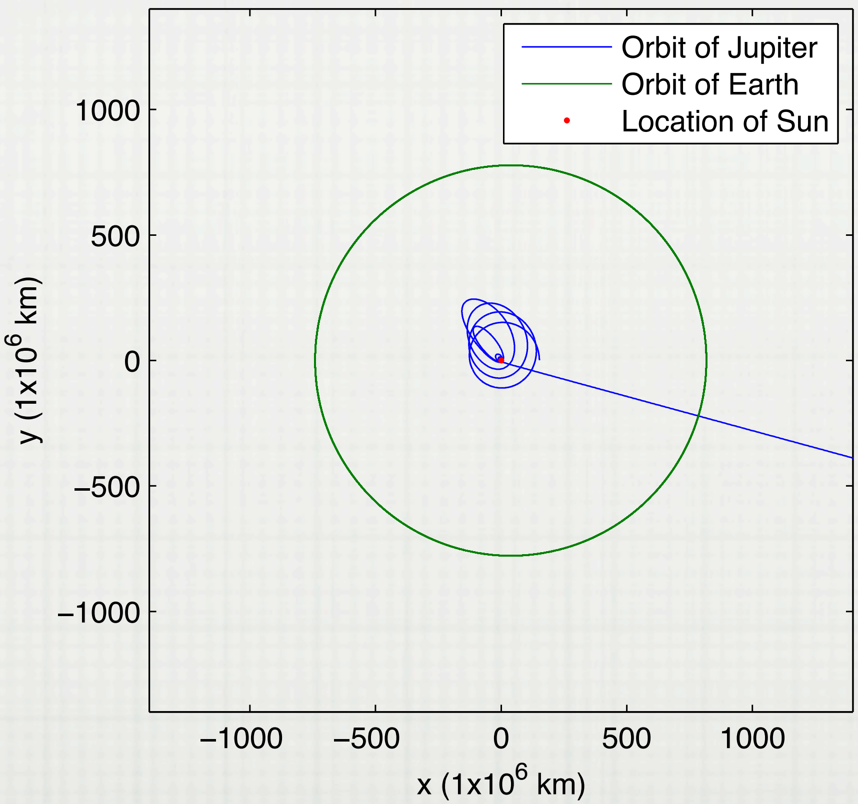


Figure 5: Orbits of Earth and Jupiter around the Sun, including Earth-Jupiter gravitational interactions with Jupiter's mass increased by a factor of 1000. Each axis has the same scale.

QUESTION 2

(b) Study the precession of the perihelion of Mercury due to general relativity corrections to the $1/r^2$ classical gravitational law. Use the following equation of the modified force:

$$F_G = \frac{GM_S M_M}{r^2}(1 + \frac{\alpha}{r^2})$$

where M_M and M_S correspond to the mass of Mercury and the Sun, respectively. Use $\alpha \sim 10^{-8}$ as a small coefficient accounting to relativity corrections.

- Plot the trajectory of Mercury for a given $\alpha = 0.01 AU^2$. Draw the line between the Sun and the closest approach of Mercury for a few trajectories. The change in direction indicates the change of orientation of the perihelion.
- Plot the orbit's orientation change with time for $\alpha = 0.0008 AU^2$.

In all these calculations, do not consider the effect of the planets on the Sun (Sun is static); choose initial conditions properly, test your step size h carefully.

MERCURY: G.R. CORRECTION

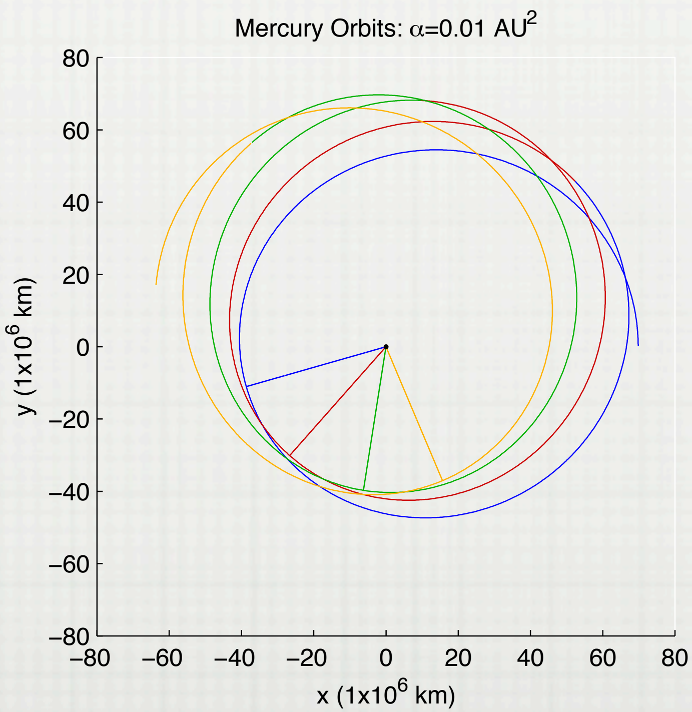
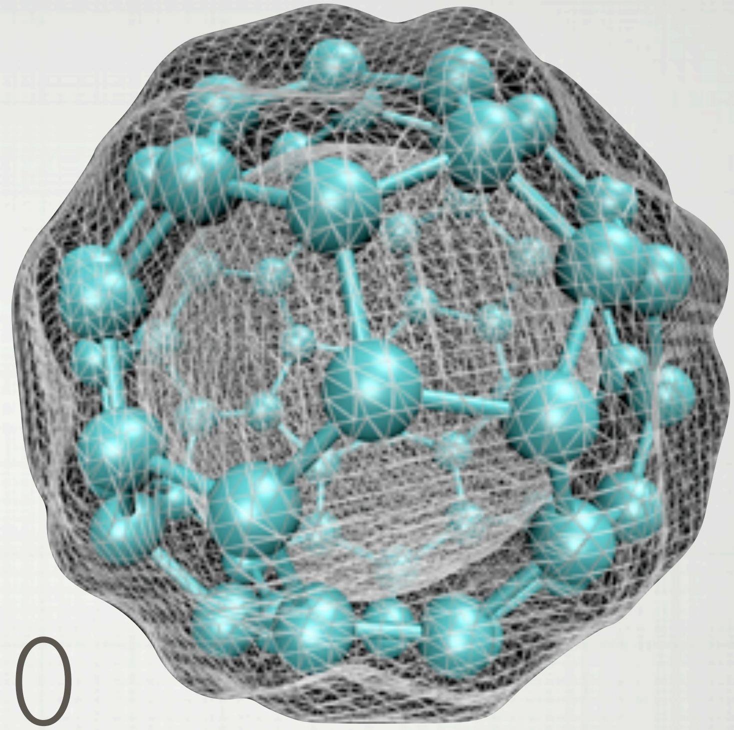


Figure 6: Plots of the orbits of Mercury around the Sun at different times with $\alpha = 0.01 AU^2$. The orbits plotted are consecutive. Each axis has the same scale.

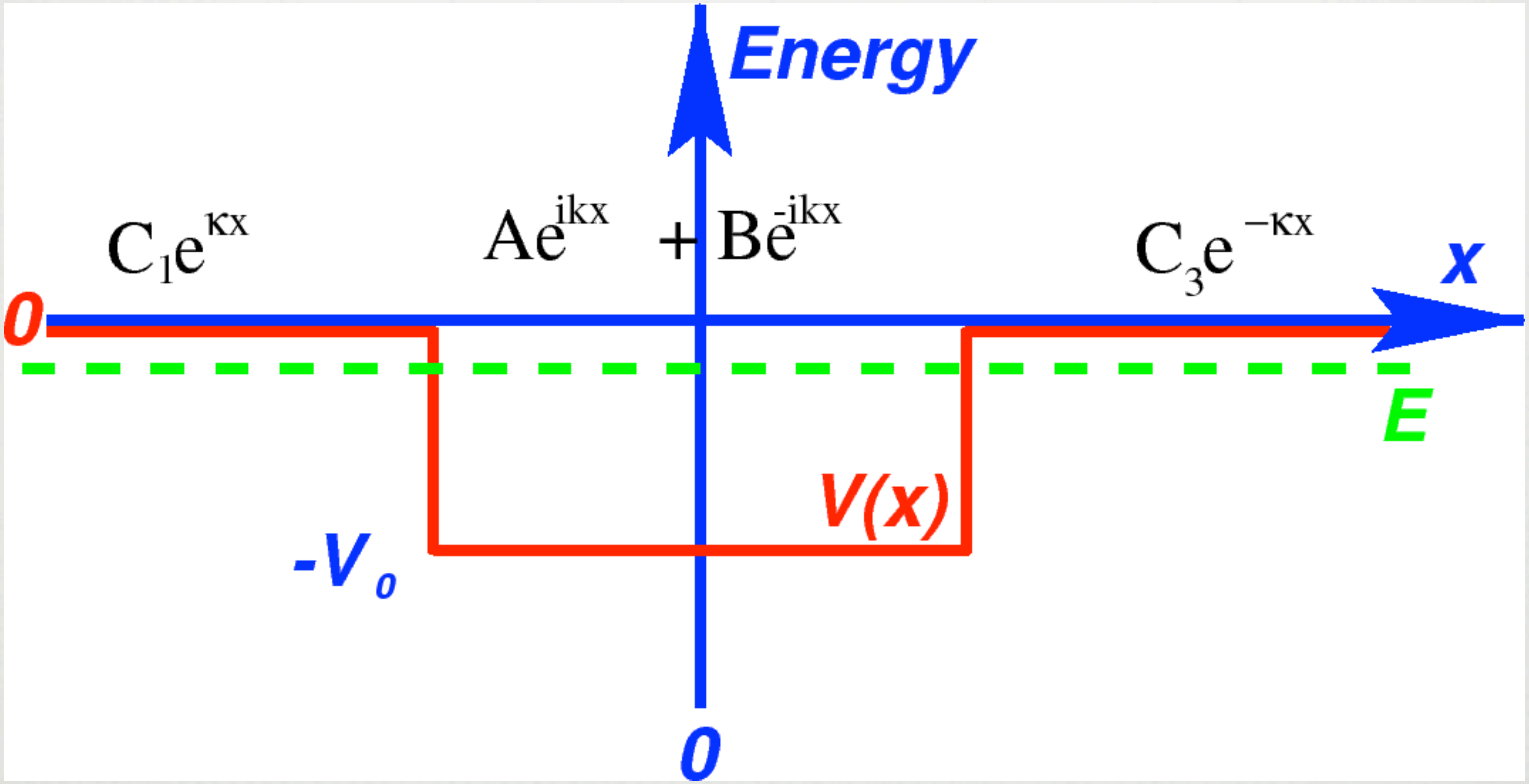
QUESTION 3

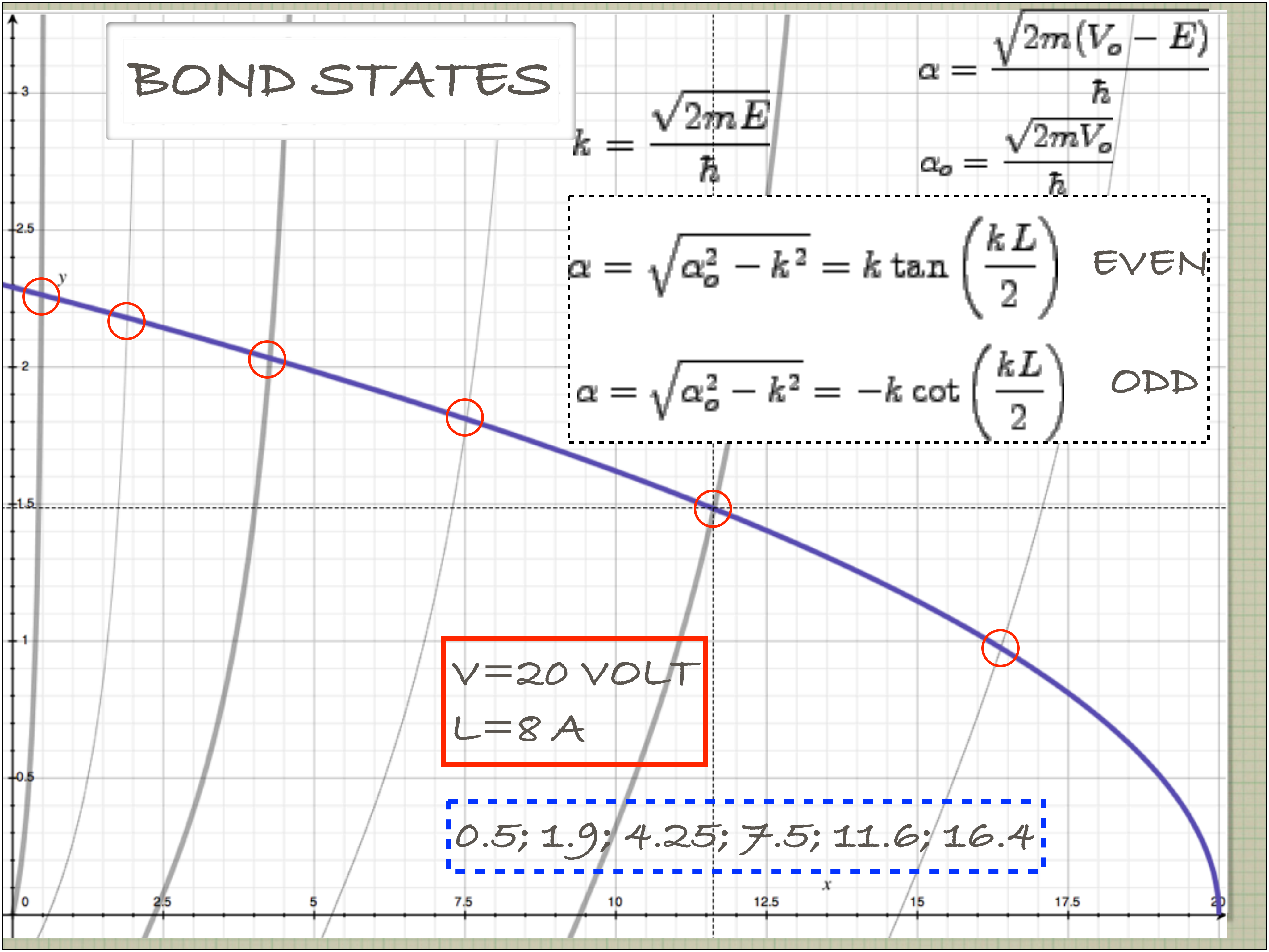
2. Select a problem of your choice from any physics class (or book) where ODEs cannot be solved analytically. Present the physics of the problem carefully and make a case for the solution you obtained, in light of the conditions you selected.



PHY-4810
COMPUTATIONAL PHYSICS

LECTURE 9: ODE AND 1D QUANTUM MECHANICS


Energy
$C_1 e^{\kappa x}$
$Ae^{ikx} + Be^{-ikx}$
$C_3 e^{-\kappa x}$
x
0
E
V(x)
-V0
0


BOND STATES
$k = \frac{\sqrt{2mE}}{\hbar}$
$\alpha = \frac{\sqrt{2m(V_o - E)}}{\hbar}$
$\alpha_o = \frac{\sqrt{2mV_o}}{\hbar}$
$\alpha = \sqrt{\alpha_o^2 - k^2} = k \tan\left(\frac{kL}{2}\right)$ EVEN
$\alpha = \sqrt{\alpha_o^2 - k^2} = -k \cot\left(\frac{kL}{2}\right)$ ODD
V=20 VOLT
L=8 A
0.5; 1.9; 4.25; 7.5; 11.6; 16.4
y
x
0
2.5
5
7.5
10
12.5
15
17.5
20
0.5
1
1.5
2
2.5
3

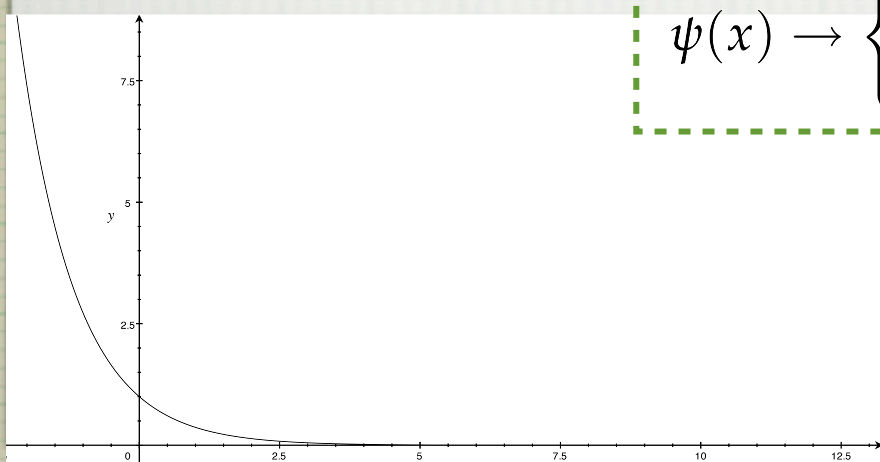
QUANTUM MECHANICS, BOND STATES

- Schroedinger equation

$$\boxed{\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x).}$$

- With boundary conditions

$$\boxed{\psi(x) \to \begin{cases} e^{-x} & \text{for } x \to +\infty \\ e^{+x} & \text{for } x \to -\infty \end{cases}}$$



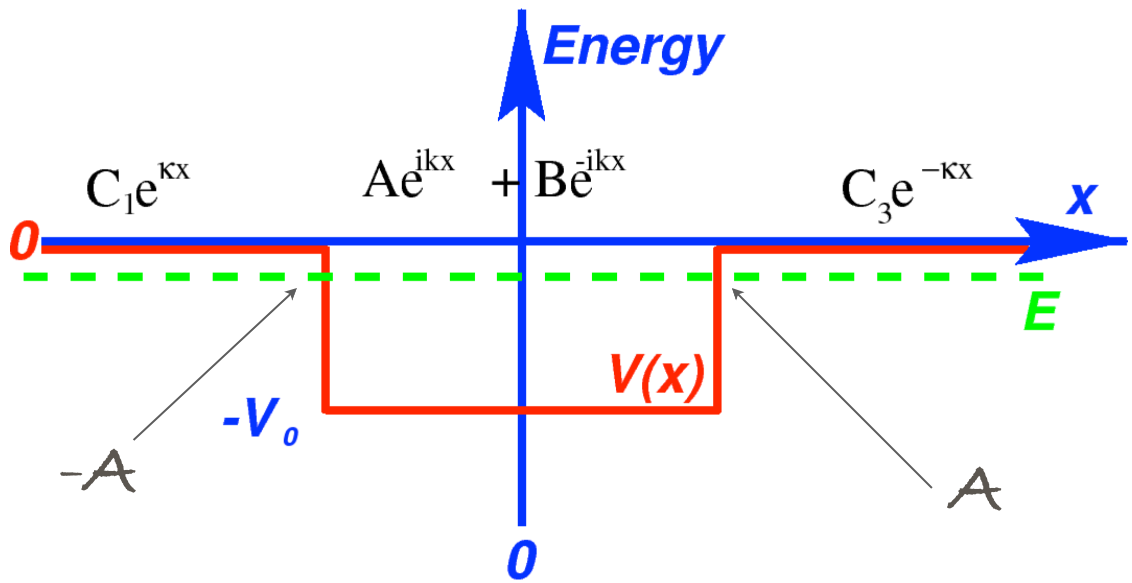
SCHROEDINGER EQUATION FOR A SIMPLE SQUARE WELL

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E + V_0)\psi(x) = 0 \quad \text{for } |x| \leq a$$

$V = V_0$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = 0 \quad \text{for } |x| > a$$

$V = 0$



QUANTUM WELL: CANONICAL FORM

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E + V_0)\psi(x) = 0 \quad \text{for } |x| \leq a$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = 0 \quad \text{for } |x| > a$$

PROBLEM TO SOLVE

$$f^{(0)}(x) = \psi(x)$$

$$f^{(1)}(x) = \frac{d\psi(x)}{dx}$$

RK VARIABLES

$$\frac{df^{(0)}(x)}{dx} = f^{(1)}(x) \qquad \frac{df^{(1)}(x)}{dx} = -(E + V)f^{(0)}(x)$$

CANONICAL FORM

BOUNDARY CONDITIONS

- Far on the left:

$$f^{(0)}(x \to -\infty) \sim e^{kx}$$

- Derivative:

$$f^{(1)}(x \to -\infty) \sim -ke^{kx} = -kf^{(0)}$$

$$k = \sqrt{E - V(-\infty)}$$

- Far on the right?

UNITS: EV AND ANGSTROMS

- **Here, we solve S.E. for electrons in realistic, nanometer size wells, for this reason, we choose the units such that energies are expressed in eV, voltage in Volts, and distance in angstroms.**
- **In practice, this boils down to using the following value**

$$\left(\frac{\hbar^2}{2m}\right)^{-1} = 0.2624$$

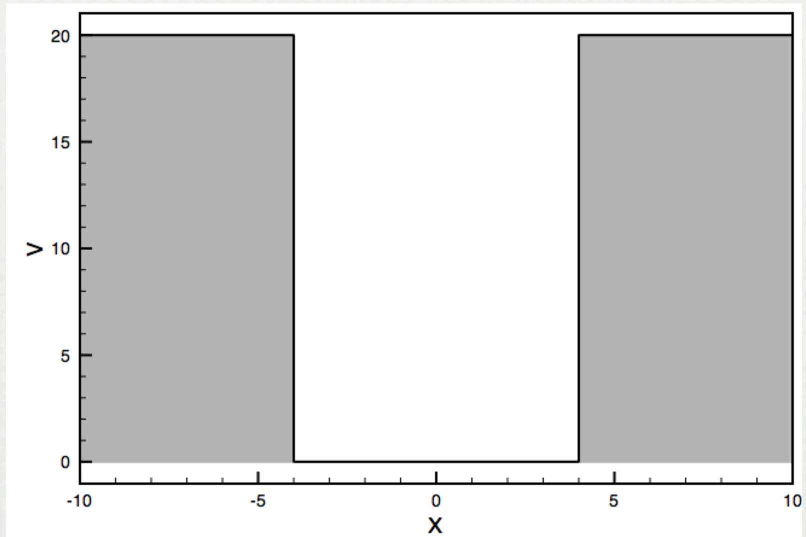
- **Question: what units do we have?**

HOW TO SOLVE IN PRACTICE?

- We know the WF is very small on the left of the well
- We know we can propagate or step the WF using SE.
- However, we need to make sure the propagated WF obeys boundary conditions far at the right as well
- Soon, we see that not every value of the energy will work!
- Think of it as throwing a ball far away, the place where it will land will depend on the initial velocity (its energy)

C++ CODE FOR S.E.

```
Doub pot(Doub x)
{
  if(x<-a){
      return V1;
  }
  else if (x > a){
      return V3;
  }
  else
      return V2;
}
void bondstates(const Doub x, VecDoub_I & y, VecDoub_O & dydx)
{
  dydx[0]=y[1];
  dydx[1]=-0.2624*(energy-pot(x))*y[0];
}
```

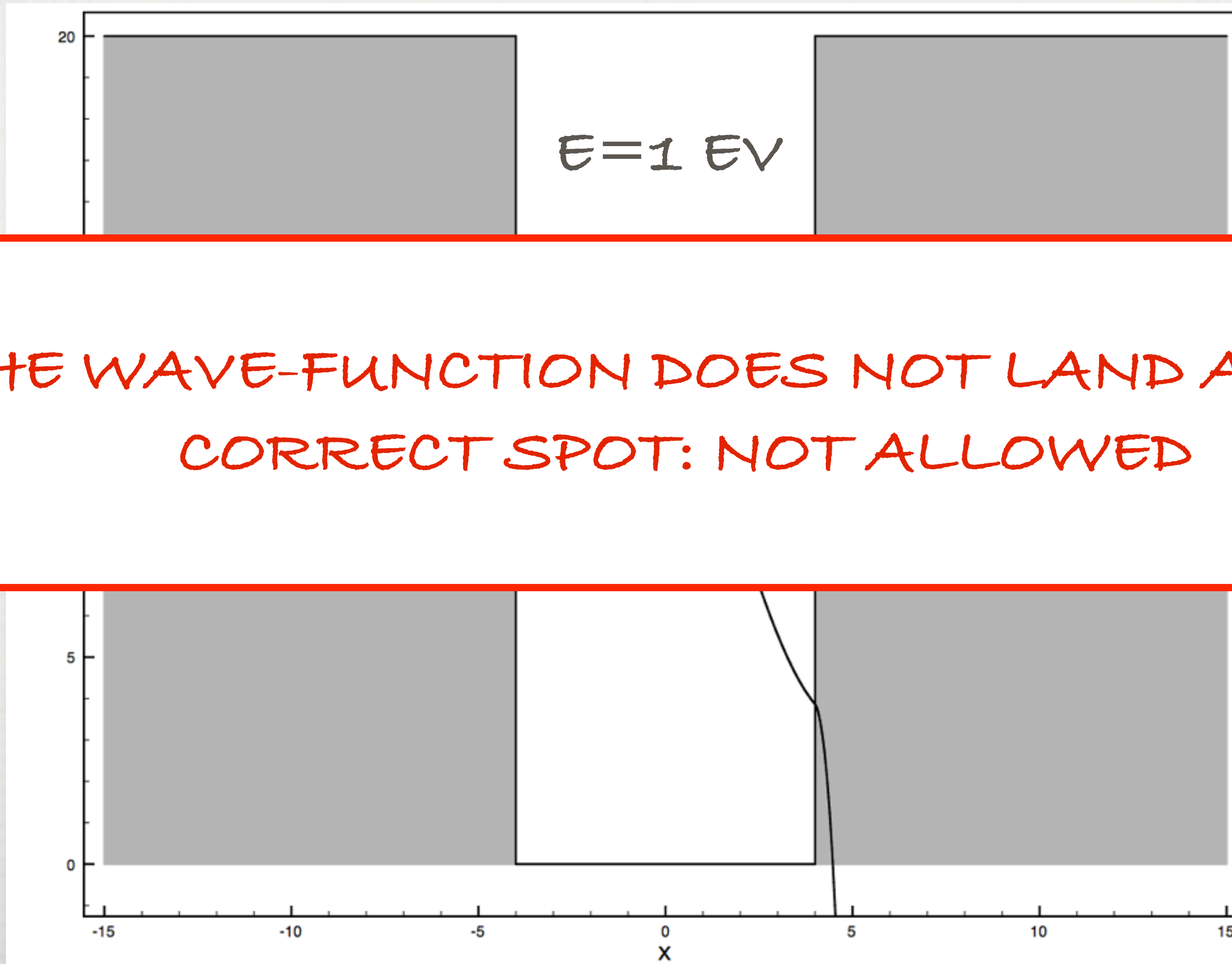


$V_1=V_2=20$

V

$V_3=0$

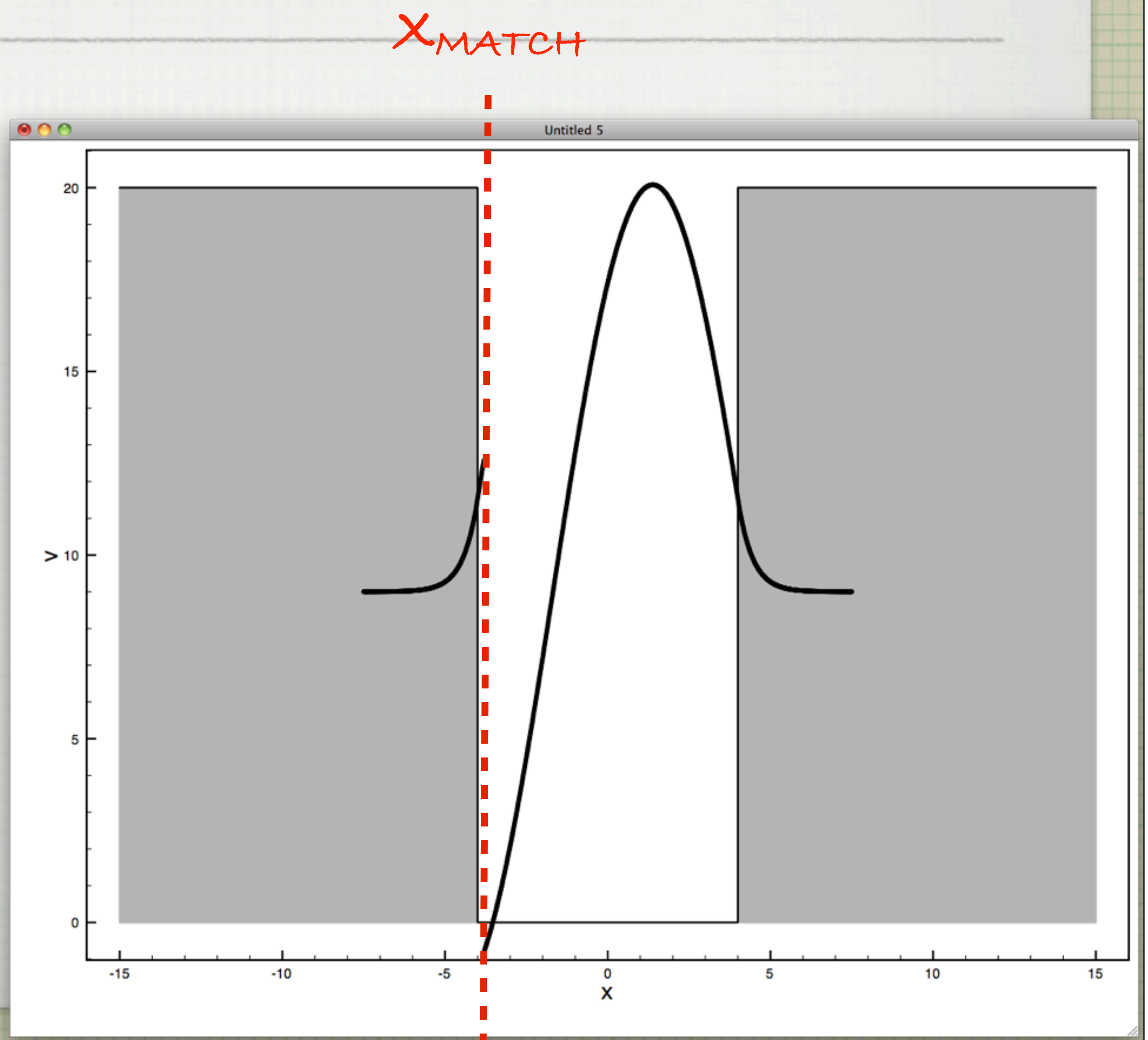
EXAMPLE: NOT ALLOWED VALUE OF E



THE WAVE-FUNCTION DOES NOT LAND AT THE CORRECT SPOT: NOT ALLOWED

MATCHING WAVE-FUNCTION

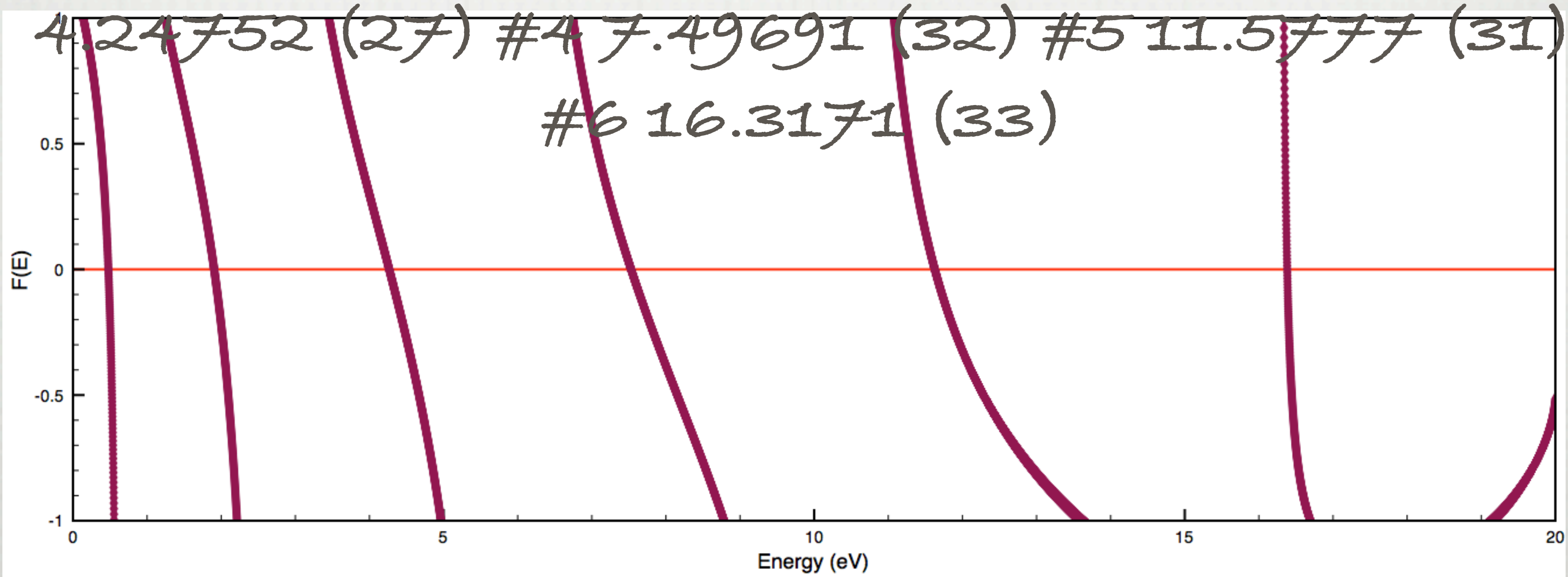
- Pick a x_{match} somewhere in the well
- Propagate the wf from the left and from the right
- Check if the function and its derivative are continuous.
- If they are not, choose another energy until they are.



NUMERICAL CRITERIA: LOGARITHMIC DERIVATIVE

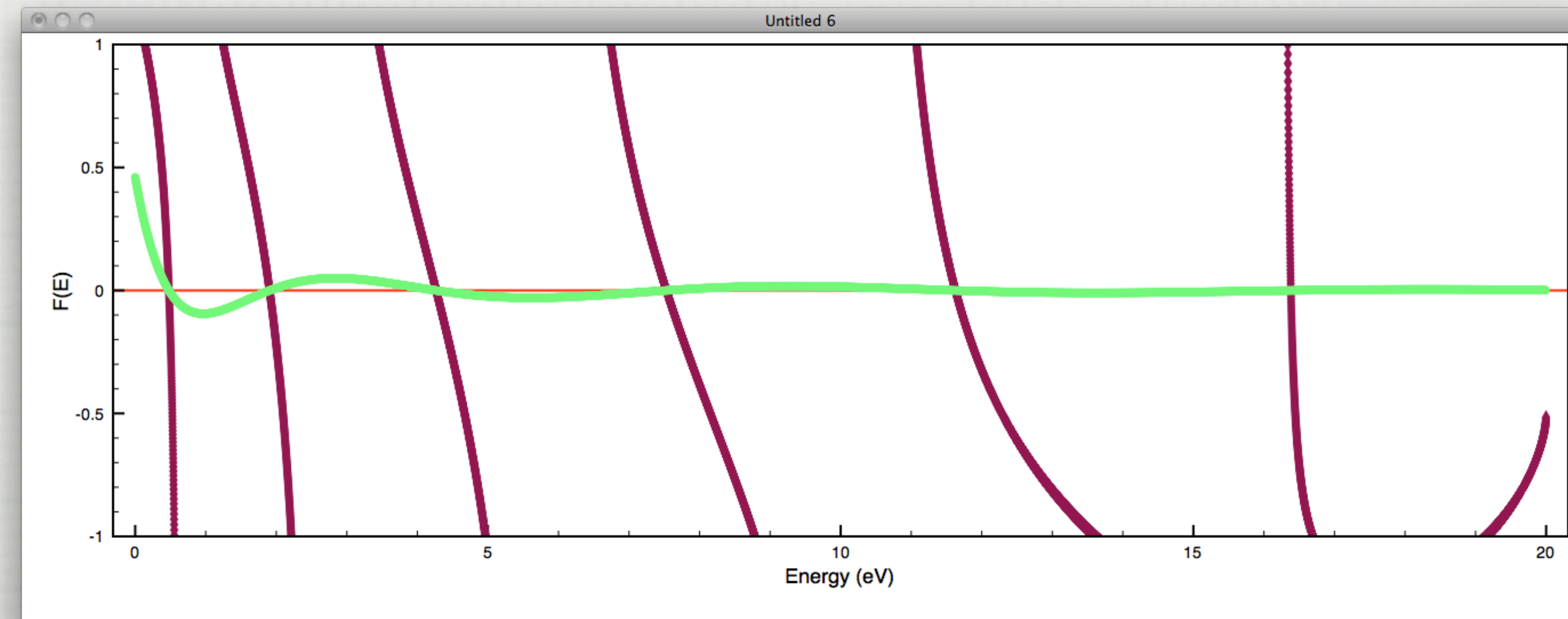
- **matching y_L'/y_L and y_R'/y_R will ensure matching wf and derivative**
- **finding zeros of : $F(E)= (y_L'/y_L - y_R'/y_R)/(y_L'/y_L + y_R'/y_R)$ at the matching point**

ZEROS AT: # 0.47522 (29) 2# 1.89622 (30) #3 4.24752 (27) #4 7.49691 (32) #5 11.5777 (31) #6 16.3171 (33)



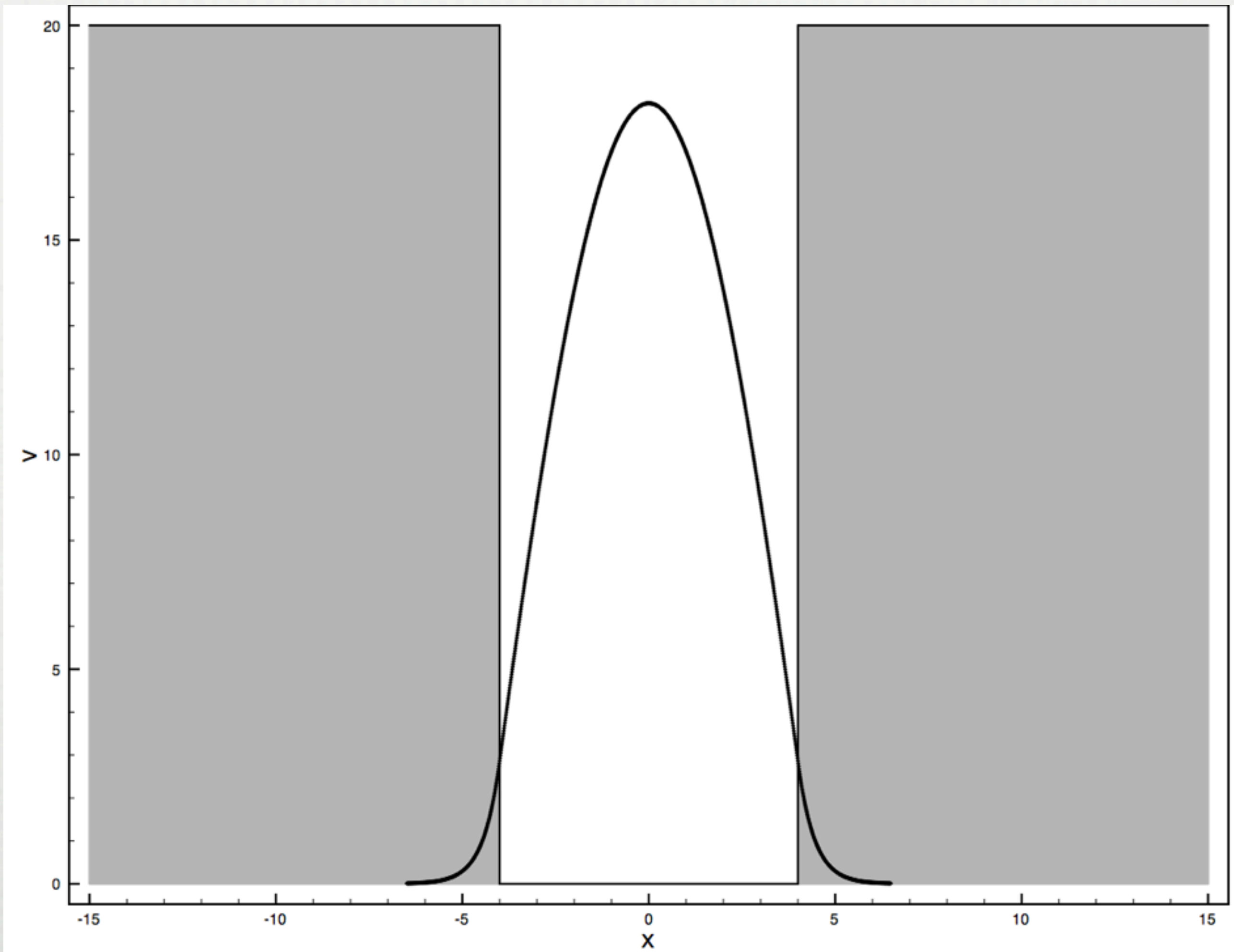
NOTE ABOUT F

- finding zeros of : $F(E) = (y_L'/y_L - y_R'/y_R)/(y_L'/y_L + y_R'/y_R)$ at the matching point
- or $F'(E) = y_L'y_R - y_R'y_L$ should be equivalent

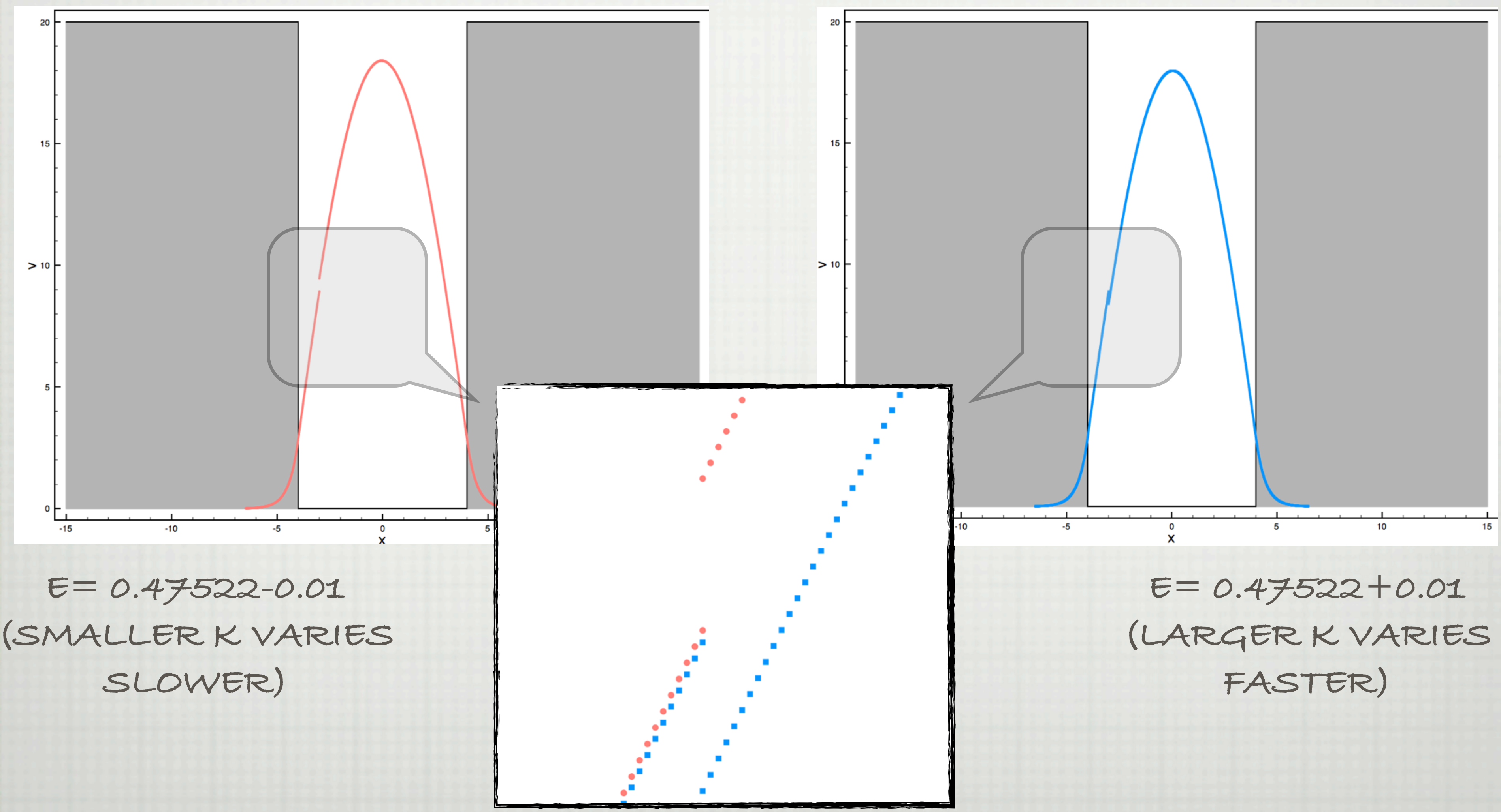


LOWEST STATE

E= 0.47522



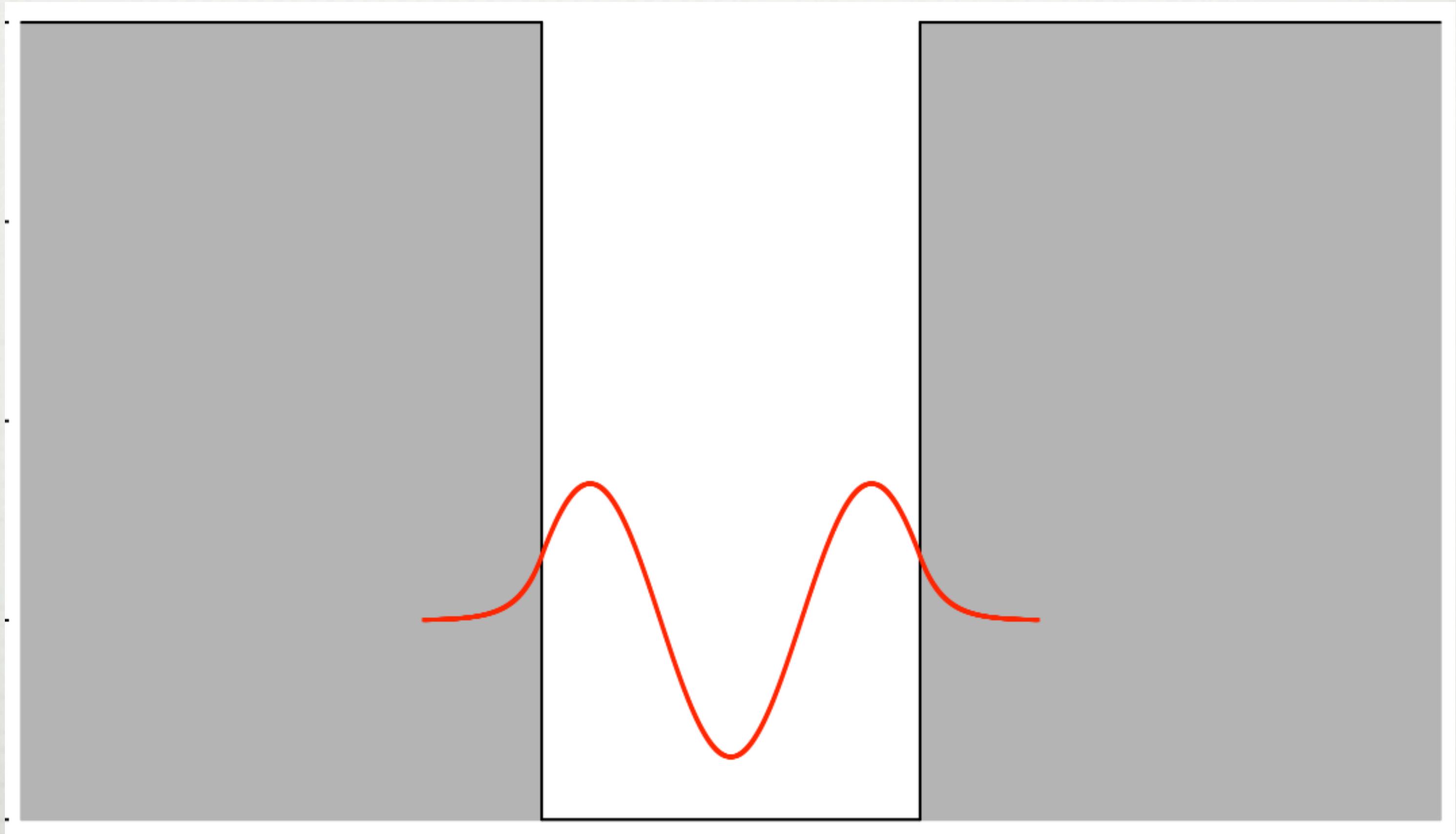
LOWEST STATE: MISMATCH



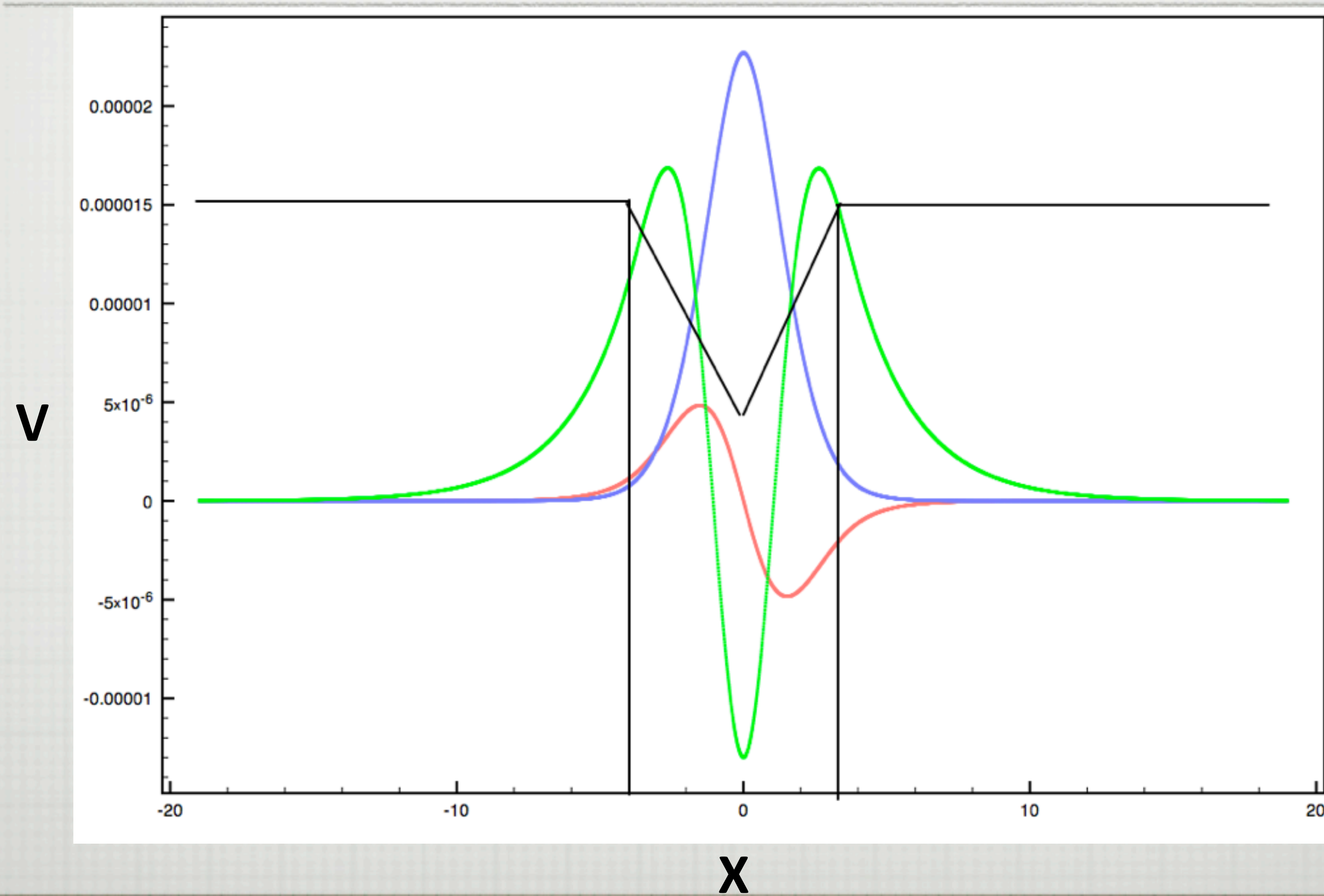
E= 0.47522-0.01
(SMALLER K VARIES SLOWER)

E= 0.47522+0.01
(LARGER K VARIES FASTER)

THIRD STATE: N=3



ANOTHER WELL...



SUMMARY

- Numerical ODE techniques can be used to solve any problem with derivatives
- Sometimes applying the initial conditions is not straightforward
- Eigenvalue problem is an example where "Shooting" needs to be done

BEYOND RK4