Project Number 4: Direct Numerical Integration of Schödenger Equation

1. Test Data

To check my simulation was correct I needed to see how it compares to a analytical solution. For this I used the gaussian wave packet with no potential, which we know the solution. This solution is written in the hand out and in Griffiths. The key features of the solutions are that the solution should spread out and it should propagate forward with a given velocity.

Like in all the other projects I set $\hbar = m = 1$. I was able to produce this easily and set a=1 and $k_0 = 1$. My solution will be shown below.

2. Finite Difference Method

To carry out this numerical solution the finite different method was used. To use this we need $\frac{\partial \psi}{\partial t}$ and $\frac{\partial \psi^2}{\partial x^2}$ because these are the derivative we will need for the Schödenger Equation.

First we will need $\frac{\partial \psi}{\partial t}$ which is

$$\frac{\partial \psi}{\partial t} = \frac{\psi_{j,k+1} - \psi_{j,k}}{\Delta t} \tag{1}$$

where j is the position step and k is the time step.

This equation can be derived by just using the definition of a derivative. We just use the value of ψ at some x step and at some t step and then ψ at the same x step and at the t+Δt. Then we just use our definition of a derivate to find equation(1).

Next we need $\frac{\partial^2 \psi}{\partial x^2}$ which is

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\psi_{j+1,k} + \psi_{j-1,k} - 2\psi_{j,k}}{(\Delta x)^2} \tag{2}$$

where j is the position step and k is the time step.

To Derive this equation we again go back to the definition of a derivative but apply it twice and this time we are using x as changing variable. So we find the difference in ψ going from the j-1 position to the j position over the difference in the position of j and j-1. Then you repeat this but for the j+1 and j position. This gives you an estimate on the first derivative about the j point. But we need the second derivative about j which is the rate of change of these first derivatives. So we apply the definition of the derivative to these two first derivatives and then we will find equation (2).

Now that we have all the parts of the Schödenger Equation we can plug equation (1) and (2) into the Schödenger Equation, with $\hbar = m = 1$. The by doing a little bit of algebra and noticing that $\frac{\partial \psi}{\partial t} * \Delta t = \Delta \psi$ we get equation (3) which tells us how to find the future wave function.

$$\psi_{j,k+1} = \psi_{j,k} + \frac{i\Delta t}{2(\Delta x)^2}(\psi_{j+1,k} + \psi_{j-1,k} - 2\psi_{j,k}) - i(\Delta t)V_j\psi_{j,k} \tag{3}$$

3. Results with Finite Difference Method

I tried many different values of p, a, and the number of time and position points. What I found was that this method of finite different is extremely unstable. The only simulation I could really produce was when p=1 (Fig. 1), the number of x points was 100, and the number of t points was 1,000. If I increase p I found that my solution's amplitude would get larger and larger as time went on (see below). I set $t_i = 0 \quad t_f = 5\pi$, Fig. 2.Then I saw that my solution started to rip apart near x=0 and then this ripping moved to the right slowly until my whole solution was at infinity. Nevertheless I found I could produce this one situation.

The way that my program works is that I produce an animation that shows the analytic solution of the left and the numerical on the right, so I will just show pictures for that.

As you can see the numerical solution on the right matches the analytical on the left until the very end. I then attempted to increase p=4 and found that my solution was extremely inaccurate. I am puzzled by this but interested. These results at the end.

3.1. **Leap From Method.**

I then wanted to try the leap frog integration method because this instability was really disappointing. The leap frog method is not difficult to understand but the coding process was tricky but I learned a lot. The results from this method were enormously improved and I never found and all my results were at least stable (never went to infinity).

For this method we use the fact that the derivative of the real and imaginary parts of our wave function are only dependent on each other but not on themselves. To show this we write the complex wave function as the sum of its real and imaginary parts, that being

$$\psi(x,t) = R(x,t) + iI(x,t) \tag{4}$$

then putting this into the Schödenger equationwe can get and equation that has one real and one complex quantity on the left and two real and two complex quantities on the right. We then know that the real part on the left must equal the real on the right, and the same for the complex. From this we can find two

equations

$$\frac{\partial R}{\partial t} = -\frac{1}{2}\frac{\partial^2 I}{\partial^2 x^2} + VI \tag{5}$$

/Users/owenmannion/Documents/Physics 424 H/Numerical Solutions to Schrodenger Equation/Write Up/Project 3 Write Up.tex

$$\frac{\partial I}{\partial t} = \frac{1}{2}\frac{\partial^2 R}{\partial^2 x^2} - VR \tag{6}$$

where R is the real part of ψ and I is the imaginary part. With this we can find a future real value from an imaginary value, and vice versa. So if we do our usual method of integration, but that would not help us much. What we do for this method though is we evaluate R and I at different t values center about the a given T value, in which we want to know the wave function. This allows us to make a much more accurate determination of the wave function. We are evaluating the derivative at a smaller difference in time.

But this runs into some issues. First e are using two grids of points, one off set in the time direction by half a time step from the other. So how do you write your initial wave function?

What I did was that I set the initial wave function to be equal to what the analytic solution was, and I plot this at $t = 0$. Then while I do that I set the Imaginary part equal to the imaginary part of the analytic solution at the time equal to one time step, so this initializes my imaginary part at a time that is one time step off from my real part. Then I made my initial Real part equal to the real part of the analytic solution at $t = 0$. So this shifted my real and imaginary parts by one time step and then I could begin

Then to plot the ψ you run into an issue. The time points for when the real and imaginary parts are defined, are not the same. These points are shifted by half a time step, so how do you plot $\psi(x, t)$? I could not find an answer online so I ignored this. I still got very good results are you will see below.

4. Results of Leap Frog Method

I tried the same simulation that was stable for the finite difference method. The plots are shown in Fig. 3. It is exactly what we see in the analytic solution and never becomes unstable. Then I increase p to 15, which would be immediately unstable for the finite difference. The plots are shown in Fig. 4. As you can see the numeric solution travels much slower and is somewhat messy in the middle, but it still moves and is stable. I tried this for p=5 swell and found a very accurate result compared to the analytic.

It is very interesting how much more stability this method allows and the increased accuracy in the results. Another interesting feature is that even with the leap frog method I found that as p increase the height of my solution alway rose.

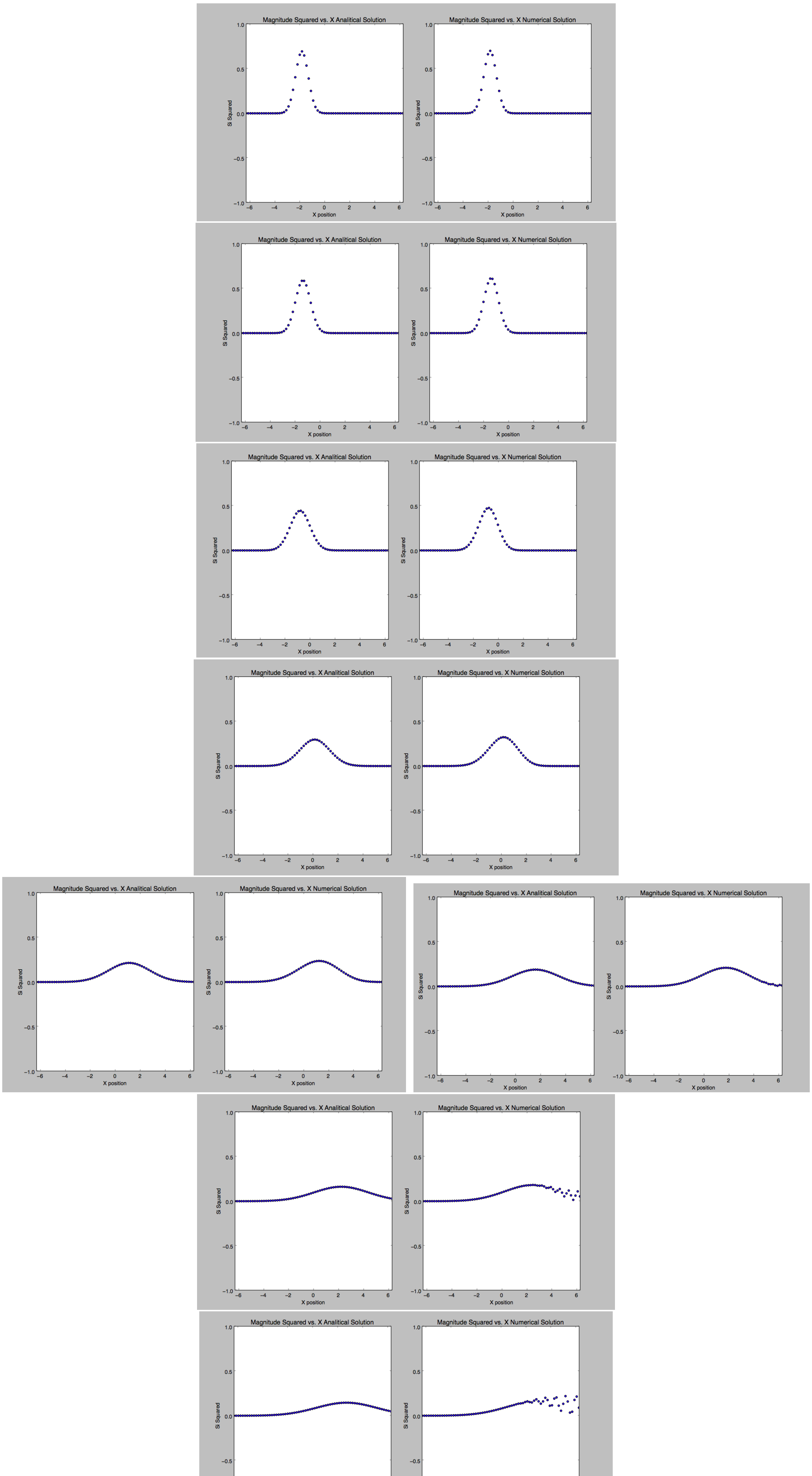
5. Harmonic Oscillator Potential

Trying to add the potential when using the finite difference method was impossible, I got unstable solutions extremely fast. But With the leap frog method I found beautiful results. I used values such that the maximum my particle would go was $\sqrt{8} = 2.828....$ Fig. 6 shows the results and it is clear the particle stops roughly at 2.8 and turns around. Also in the center of the potential is was moving very fast. I never found instability, meaning I let my simulation run for a few minutes and it kept going back and forth without any error.

6. Step Potential and Tunneling

Then once I had my program up and running for the harmonic oscillator potential I could extend this to any potential I wanted. So I tried the infinite step potential and the finite step potential.

When I did the infinite step potential I set the potential equal to 100 for x greater than zero and equal to zero for negative x. This resulted in the classical case where the particle reflects backwards. This is shown in Fig. 6. Then I used the finite step well because I wanted to see tunneling. When I did this I found that I needed my potential to be equal to roughly 10 and the momentum to be 6 to see any tunneling the pictures for this are in Fig. 7.


Magnitude Squared vs. X Analitical Solution
Magnitude Squared vs. X Numerical Solution
Si Squared
X position

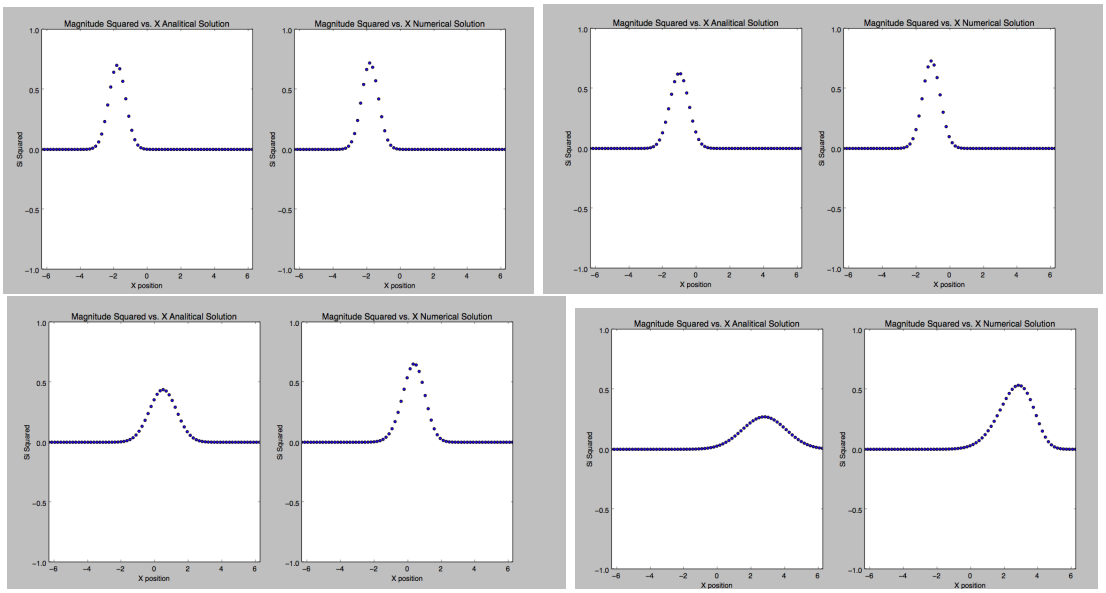


FIGURE 2. Forward Method p=4 as you can see the height increases as time increases

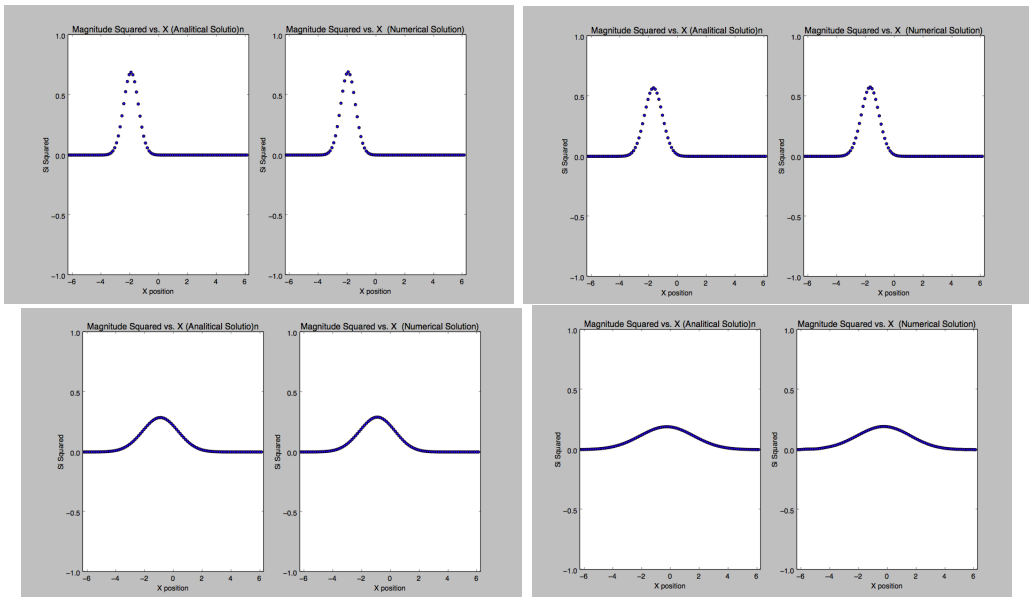


FIGURE 3. Leap Frog Method p=1

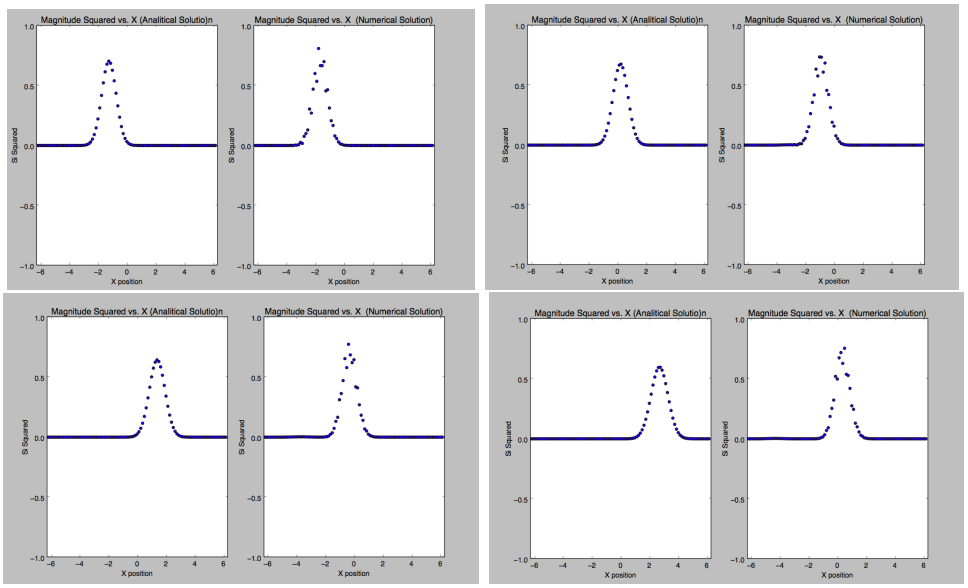


FIGURE 4. Leap Frog Method p=15

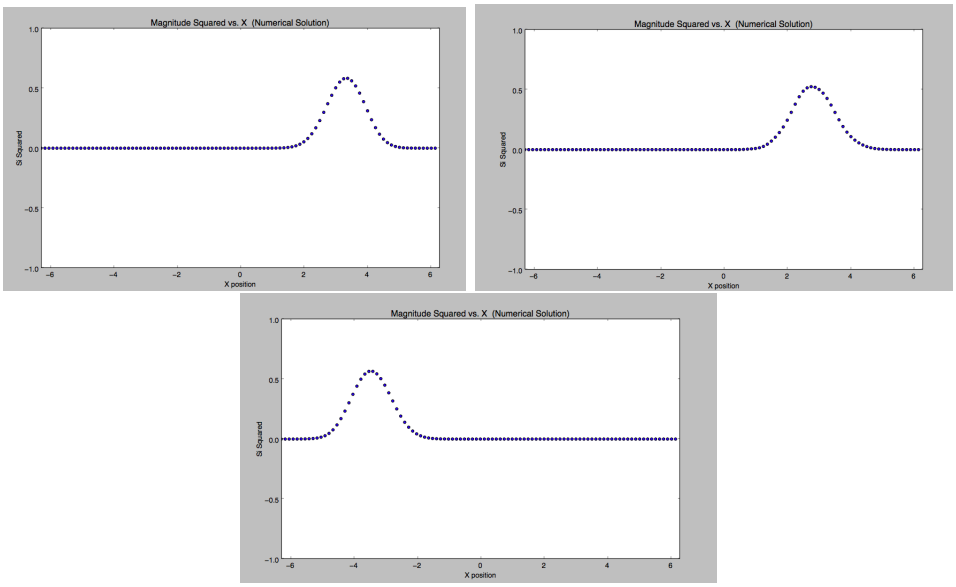


FIGURE 5. Leap Frog Method Harmonic Potential with p=4 , k=1

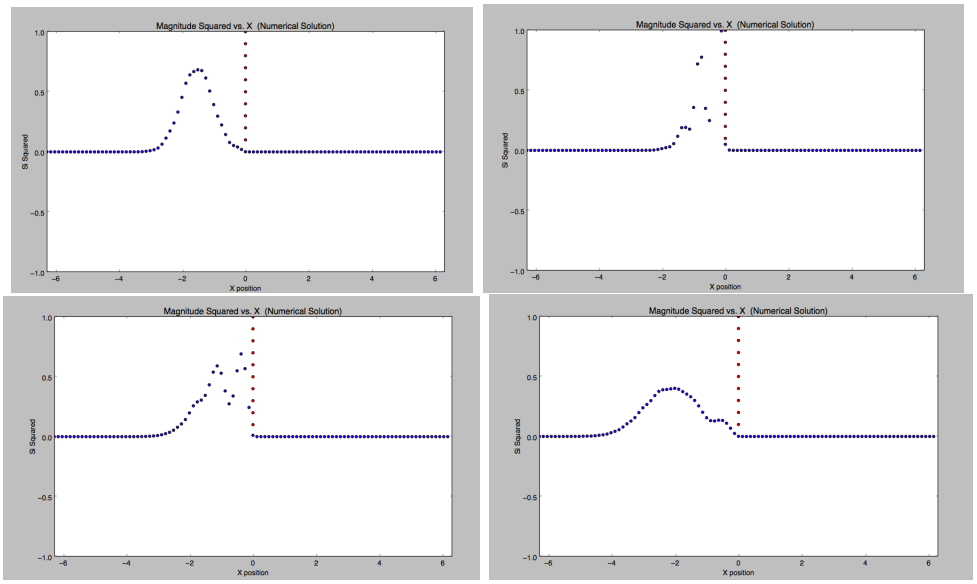


FIGURE 6. Leap Frog Method for infinite step potential, the location of the potent is in red.

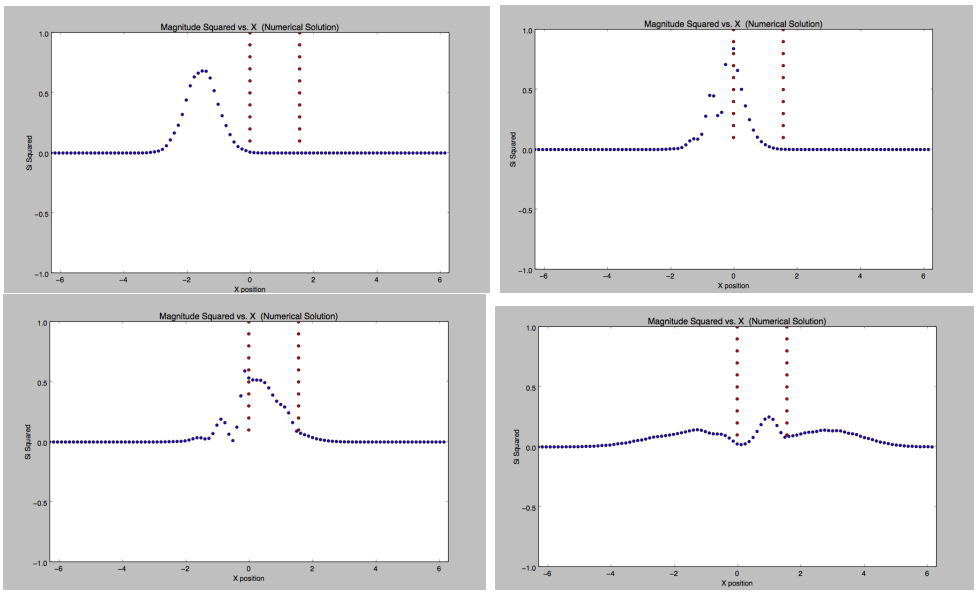


FIGURE 7. Leap Frog Method for finite step potential, the location of the potent is in red.