Numerical Methods in Physics
Wave Packet Dynamics

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1 Free Evolution

1.1 Selection of Time Step

In order to find the biggest possible time steps we could use we simply started with reducing increasing the timestep until it we saw significant error. But we went so far that the the time step got so large that it went through the solution space ($x = [0, 1]$) after just a few steps. Thus the smallest time step we used was $3.45 \cdot 10^{-4}$. The smallest spacial step we used before the solution started to get jaggy was 0.01. Since the solution took such a small time to solve for we will use significantly smaller time steps and spacial time steps for the rest of the exercises, such a solution is given as an example in figure **??**. In order to look at what k_0 to use wee looked at
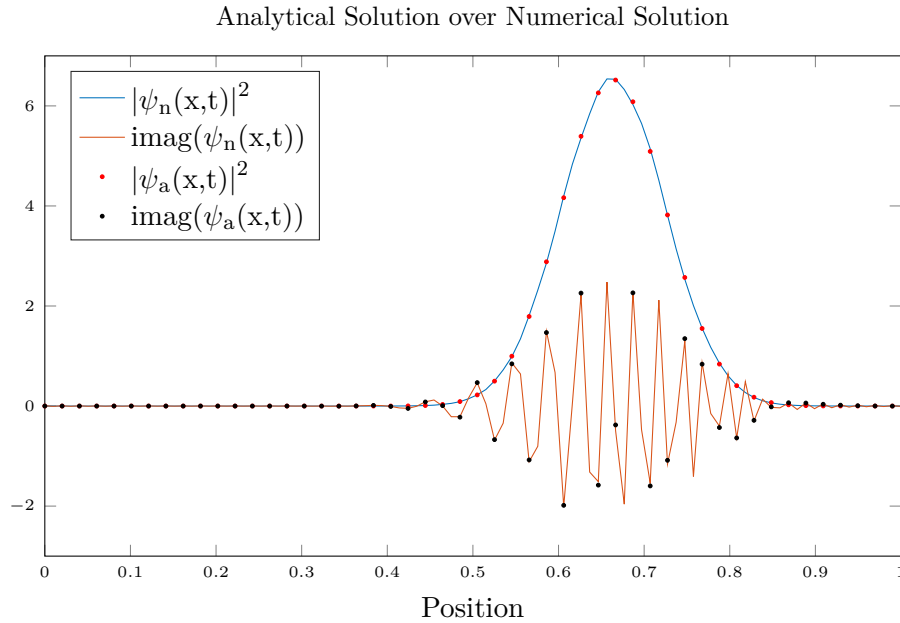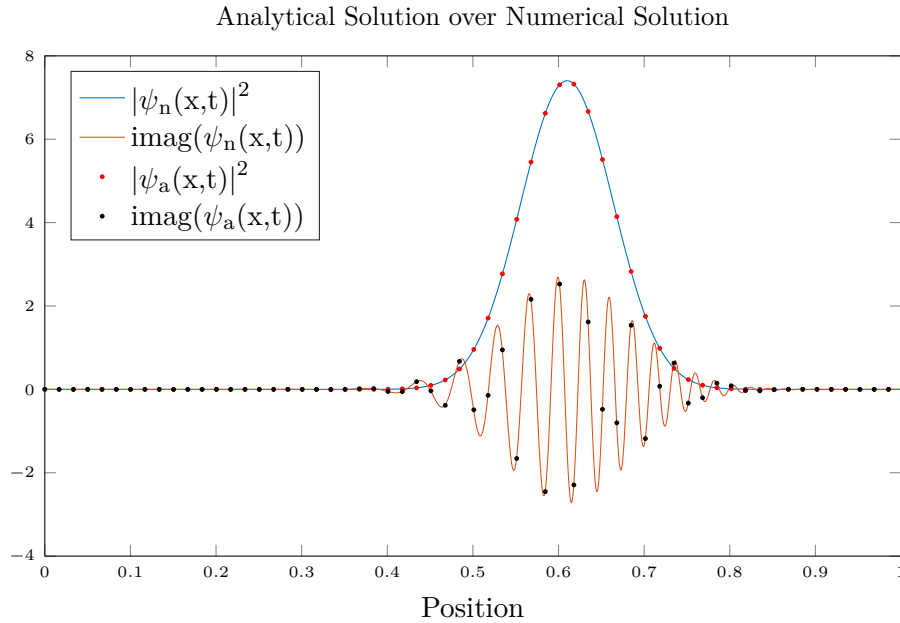
Analytical Solution over Numerical Solution
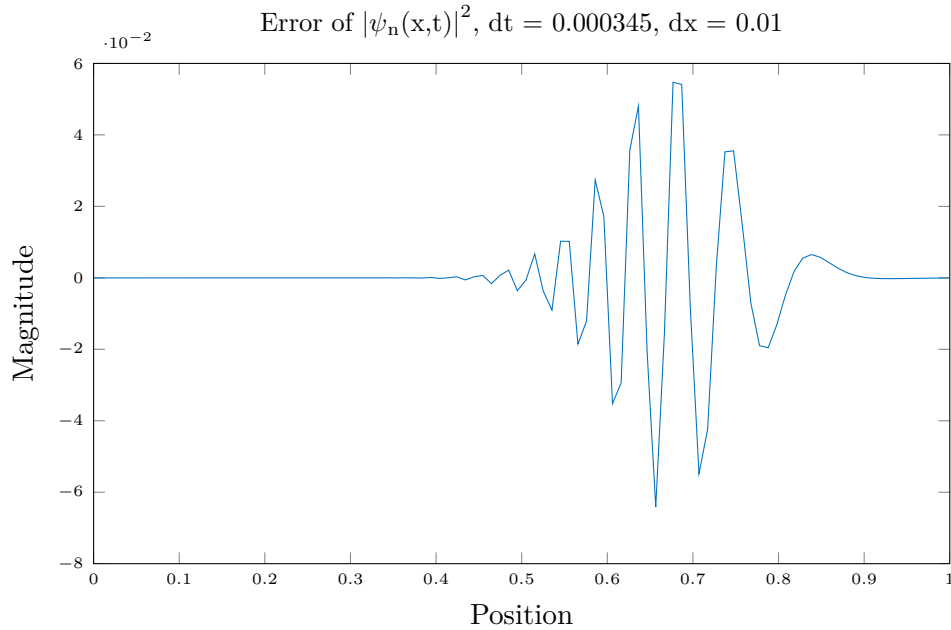
(a) The numerical solution (ψ_n) plotted against the analytical solution (ψ_a).

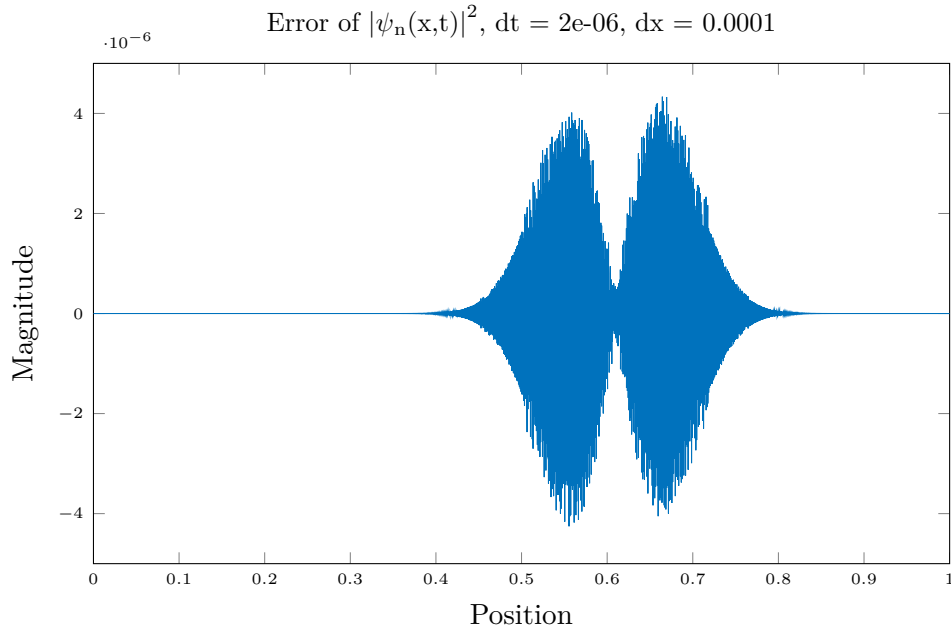Error of $|\psi_n(x,t)|^2$, dt = 0.000345, dx = 0.01

(b) The error is defined as the difference between the analytical solution and numerical solution.

Figure 1 – The numerical solution at the largest tested time and spacial step. One can clearly see in figure 1b that the solution is starting to get jaggy from the spacial step. The larger time step never gets to the point where the solution seem to go bad before just running off our solution space $x = [0, 1]$ in just a few steps. The error is not particularly large compared to the solution values, as seen in figure 1b

Analytical Solution over Numerical Solution

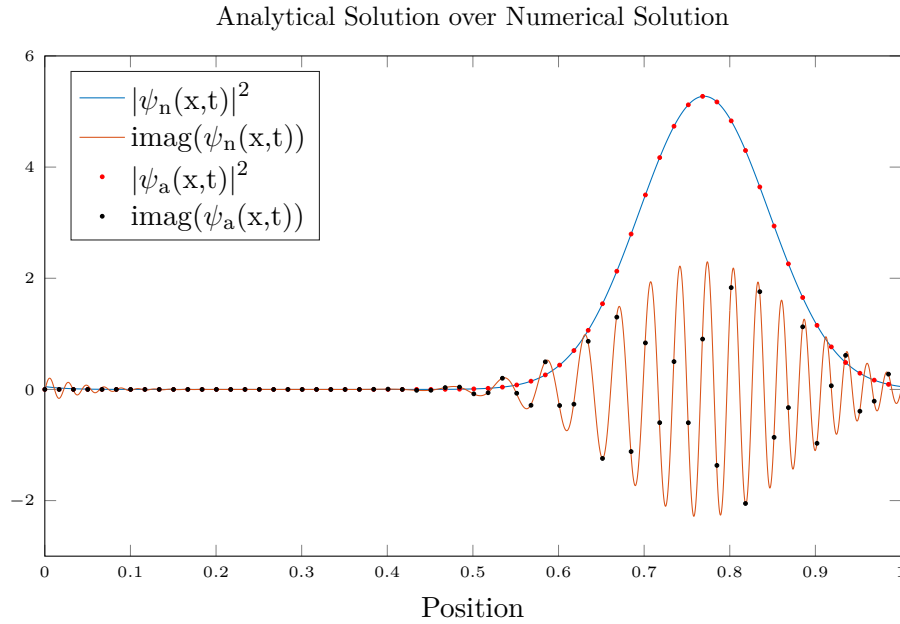**(a)** The numerical solution (ψ_n) plotted against the analytical solution (ψ_a).

(b) The error is defined as the difference between the analytical solution and numerical solution.

Figure 2 – Here we see the error using smaller timesteps and spacial steps to get good resolution and precision on how the function will look in the end.

1.2   Behavior at the end of the Solution Space

looking at figure **??** we can clearly see the periodic behavior of the numerical solution. This is in a stark contrast against the numerical solution. This probably lies in the fast fourier transform package used. This because the discrete fourier transform can only be done on periodic problems. Thus as soon we are outside of our spacial solutions space of

$x = [0, 1]$ we will get significant error. This is highlighted in figure 3b.

**(a)** The numerical solution (ψ_n) plotted against the analytical solution (ψ_a).
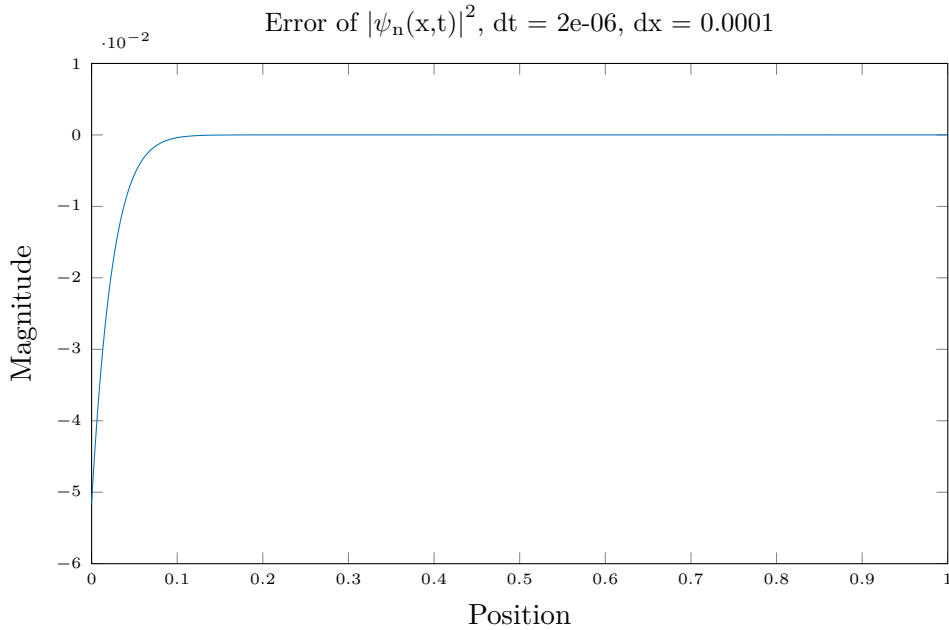
**(b)** The error is defined as the difference between the analytical solution and numerical solution.

Figure 3 – The numerical and analytical solution as it passes its solution space of $x = [0, 1]$. One can clearly see in figure 3a that the numerical solution is periodic. The error caused by this is highlighted in figure 3b

2   Potential Well

We can see in figure **??** the effect of a potential barrier. Part of the wavefunction is reflected by it, while a large part goes trough it. Here we had to change the time step to $1 \cdot 10^{-7}$ in order to get a smooth plot.
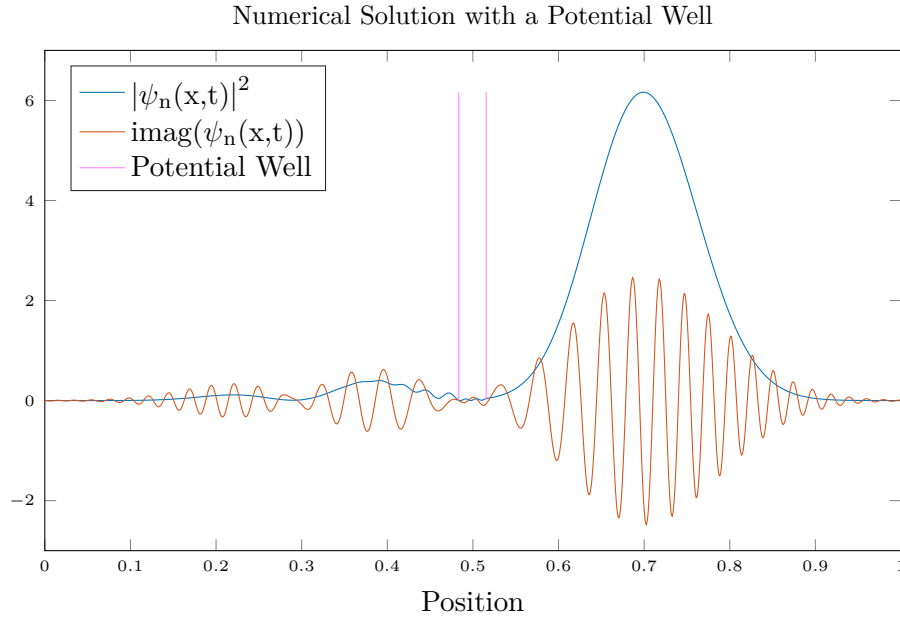
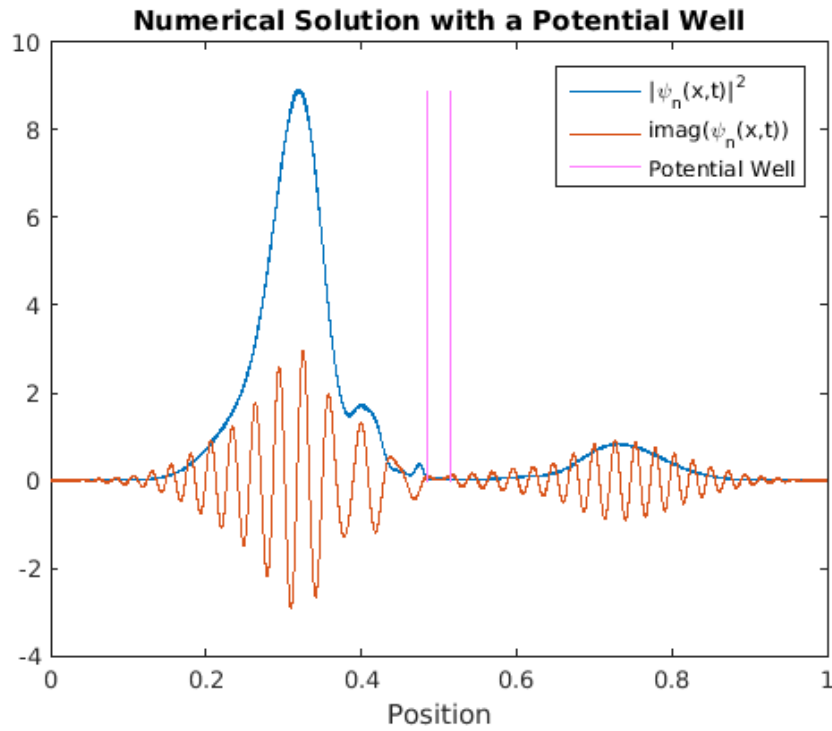**(a)** The numerical solution of $|\psi_n(x,t)|^2$ after it has hit the potential well.
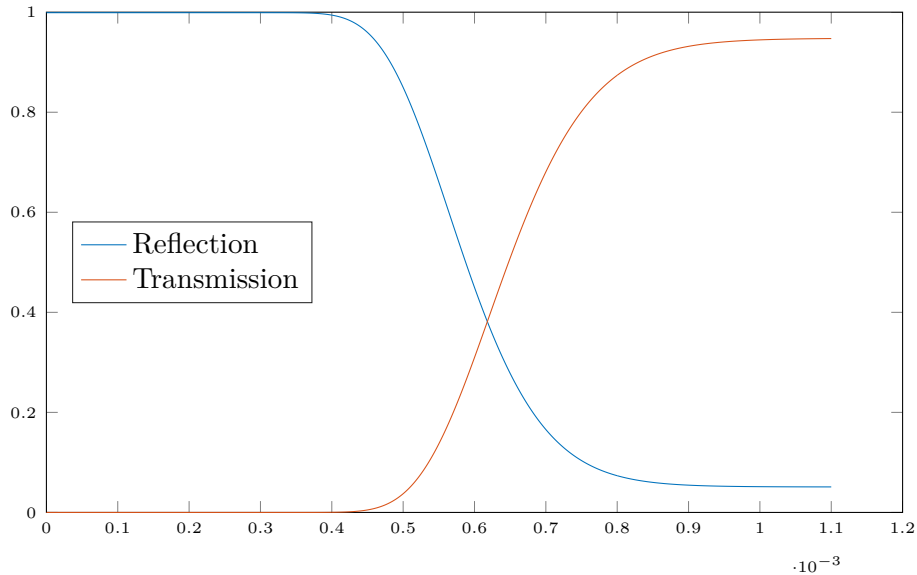
(b) Here we clearly see the transmission and reflection before and after the wave function hits the potential well.
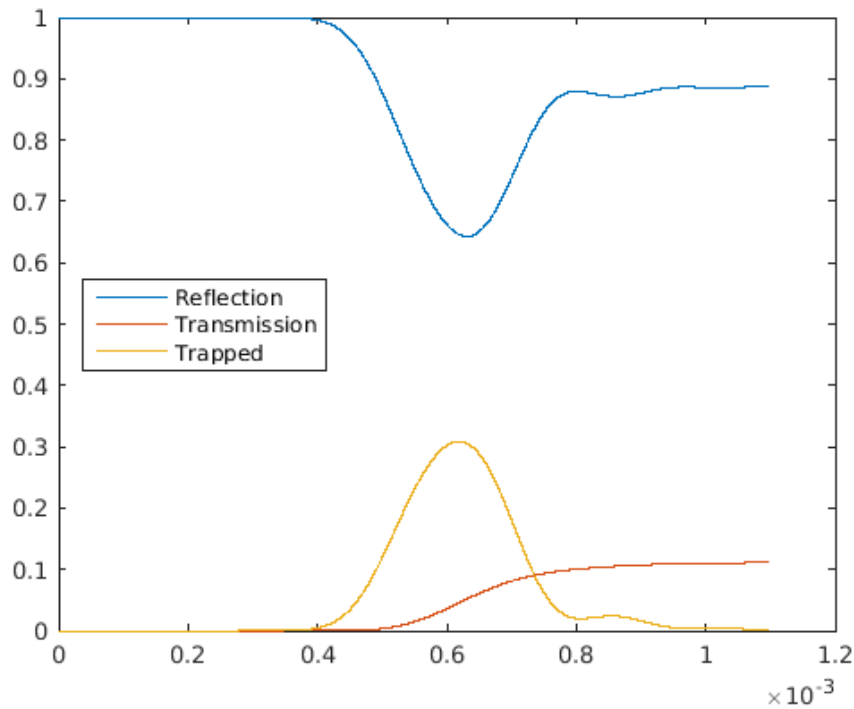
Figure 4 – Here we depict the effect of the wave function hitting the potential well.

3   Square Barrier

In figure 5b we can see the effect of the square barrier on the wave function. After the wave function hits the square barrier part of it is trapped a while before a large part is reflected and a small part tunnels trough. Here we also had the timestep on $1 \cdot 10^{-7}$

(a) The numerical solution of $|\psi_n(x,t)|^2$ after it has hit the square barrier.

(b) Here we clearly see the transmission and reflection before and after the wave function hits the square barrier.

Figure 5 – Here we depict the effect of the wave function hitting the square barrier. Note in figure 5b how a certain part of the wave function is trapped inside for while before a large part is reflected and a small part tunnels through.