Physics 461

Quantum Mechanics

Computational Project

Nate Schulz

Spring 2009
Uiterwaal

Square Well

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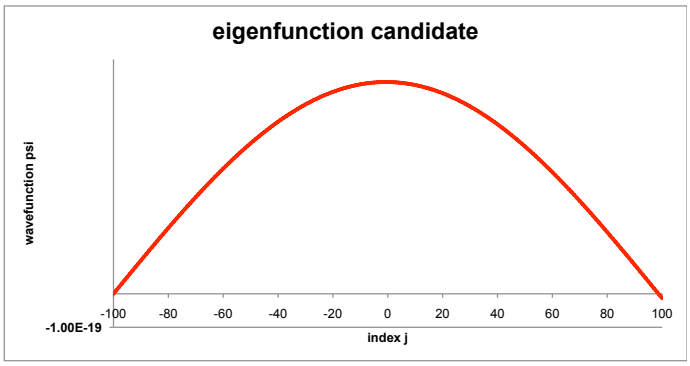

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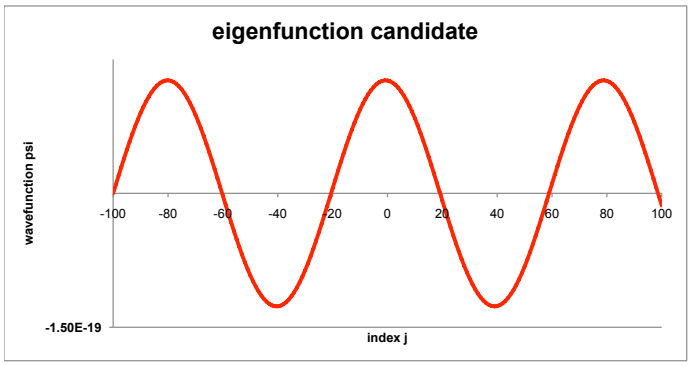

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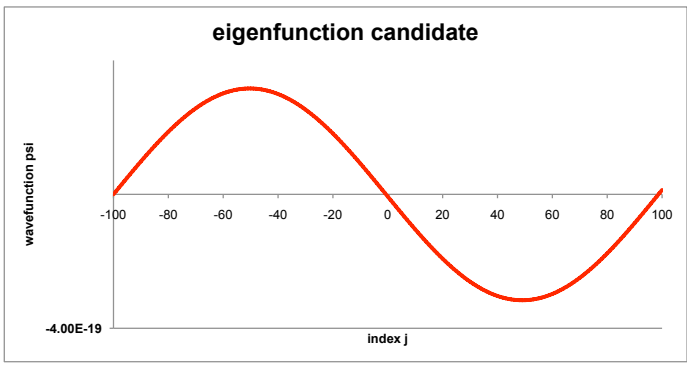

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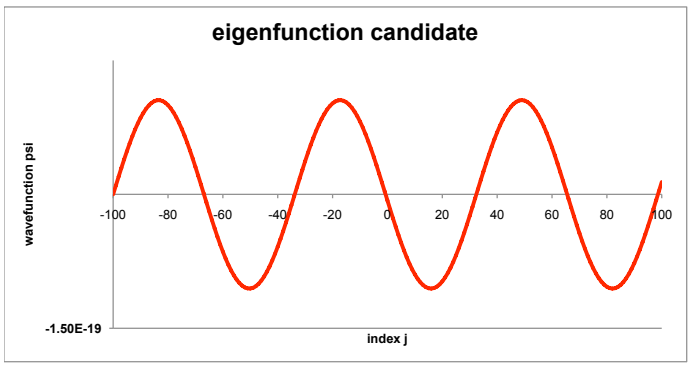

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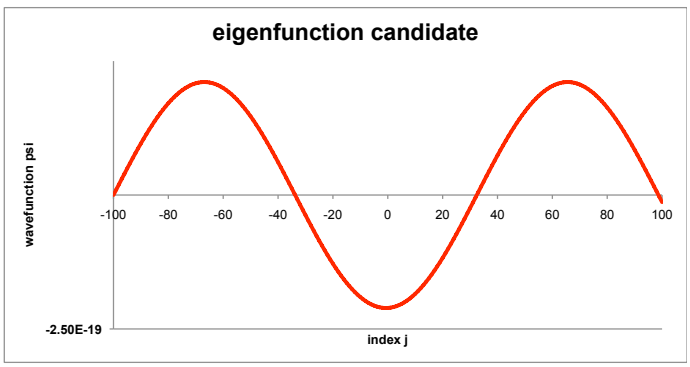

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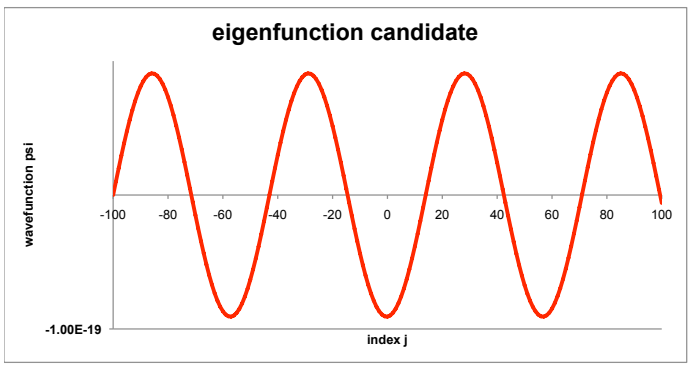

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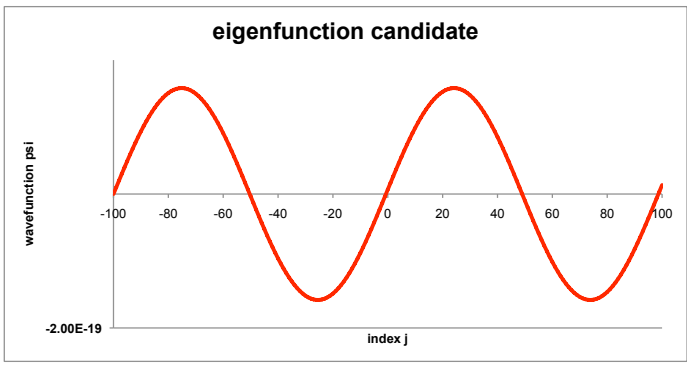

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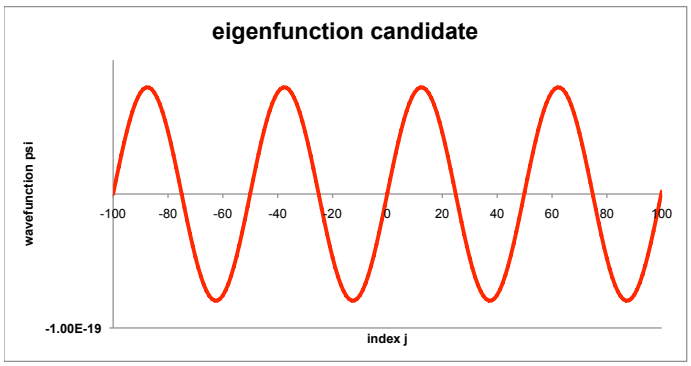
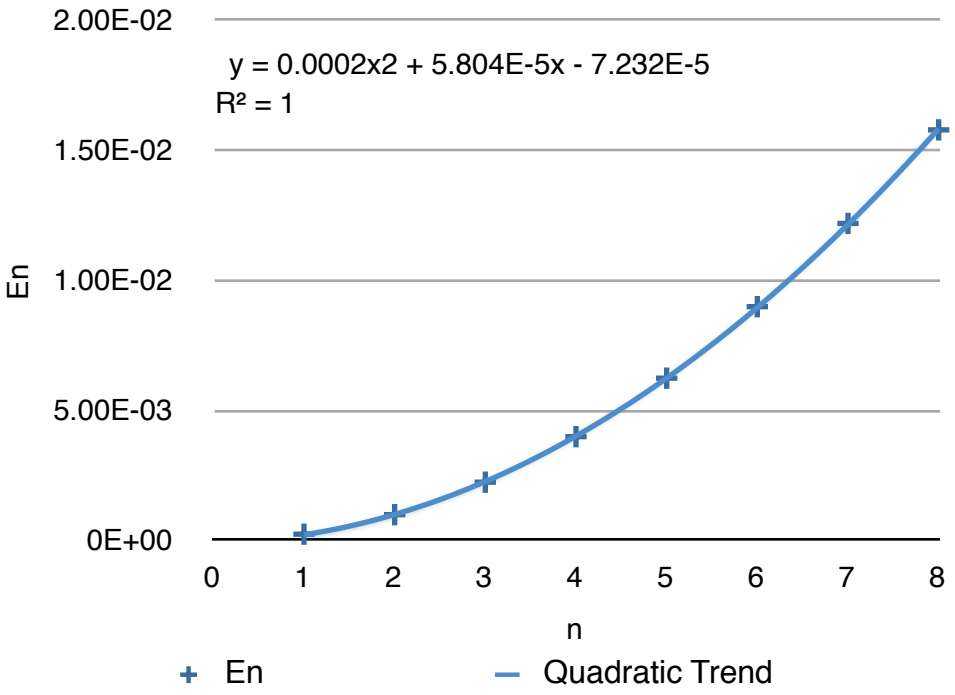
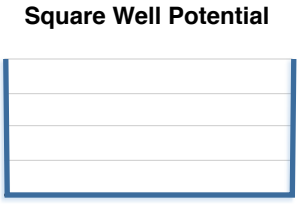






n	En
1	2.500E-04
2	1.000E-03
3	2.250E-03
4	4.000E-03
5	6.250E-03
6	9.000E-03
7	1.220E-02
8	1.580E-02

Infinite Square Well Potential
C = N/A

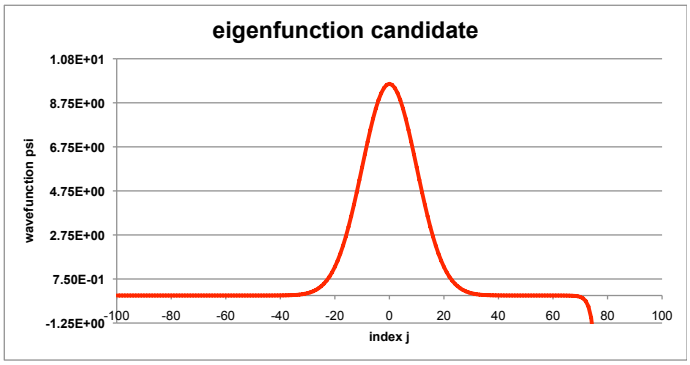
To simulate an infinite square well in excel, all potential energy values were set equal to zero and then the formulae recalculated the values of ψ. These values were displayed on a graph and began to depict a sinusoidal function that is the wavefunction. To determine a good starting energy value, the second eigenstate was determined first since it is represented as one full sinusoidal motion on the graph. Once the second eigenstate energy was determined, the next step was to estimate the value of the first and remaining eigenvalues. To do this, the following relationship was used.

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} \Rightarrow \varepsilon_n = \frac{E_n}{U_0} = n^2 \pi^2 \left(\frac{\Delta x}{L}\right)^2 \qquad (2)$$

After the rough estimates bring the basic shape of the eigenfunction to the numerical graph, Excel's "goal-seek" function was used to more precisely determine the value of the eigenenergies.

Harmonic Oscillator

n=1



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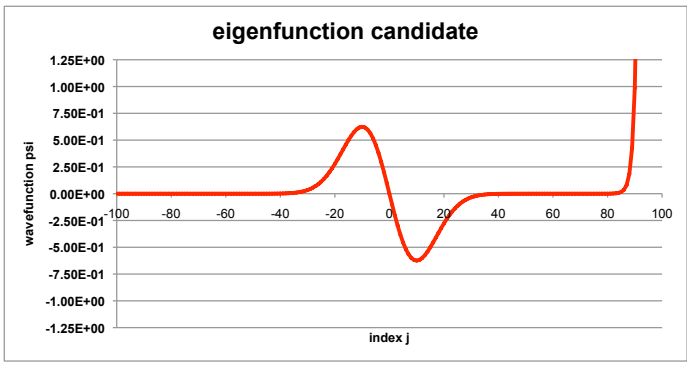

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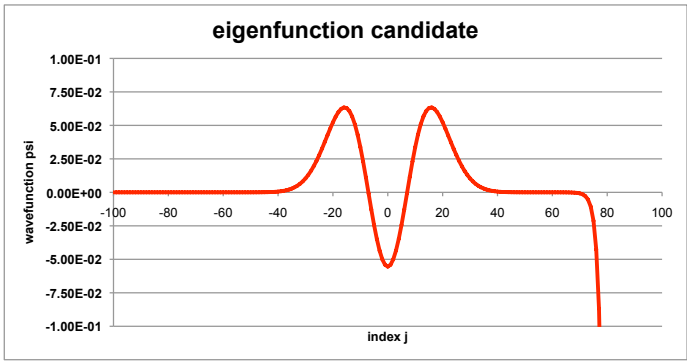

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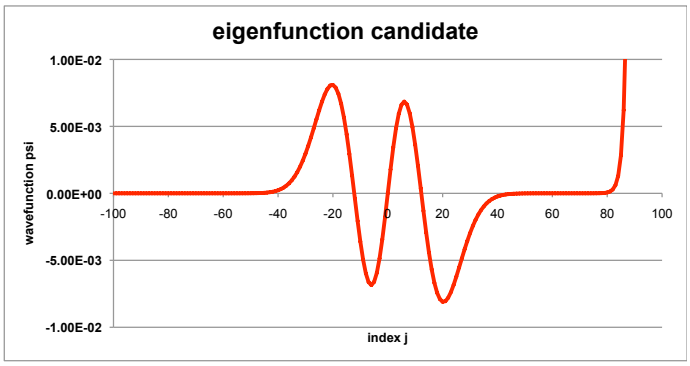

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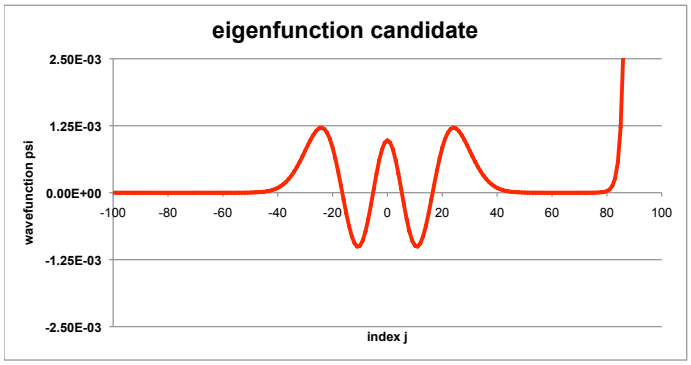

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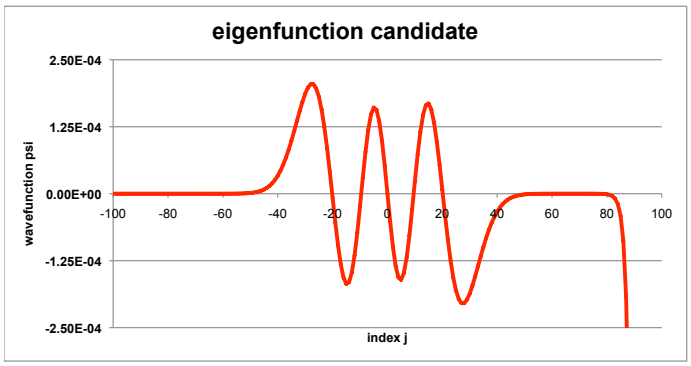

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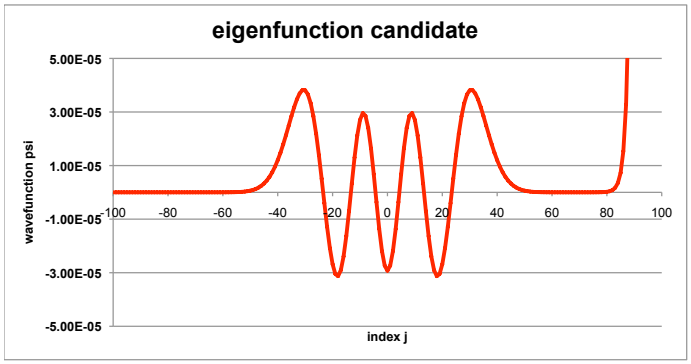

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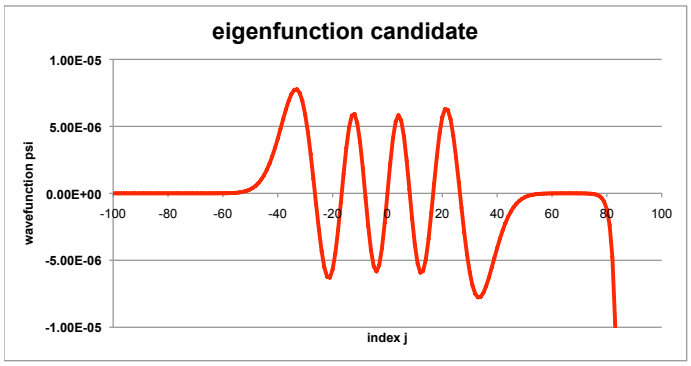
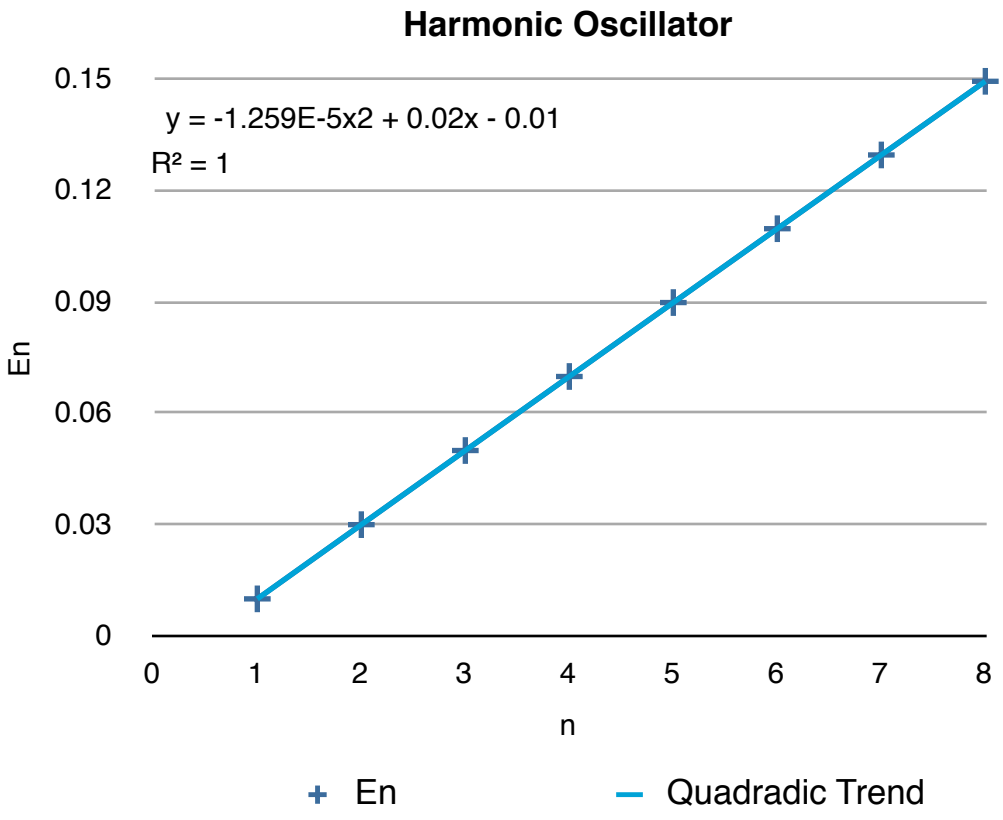
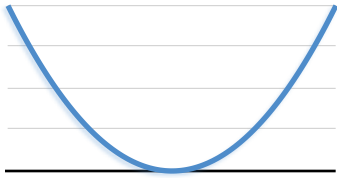




Harmonic Oscillator Potential



n	En
1	9.994E-03
2	2.997E-02
3	4.992E-02
4	6.984E-02
5	8.974E-02
6	1.096E-01
7	1.295E-01
8	1.493E-01

Harmonic Oscillator
C = 1.0 x 10^{-4}

This numerical model of a quantum mechanical harmonic oscillator, follows the same model as the infinite square well model using a different potential. Here, the potential was a calculated parabolic function to simulate the potential of a harmonic oscillator. The eight standing-wave eigenfunctions were calculated using the same formulae used in the square well model, but the new numerical potentials gave rise to a different set of eigenfunctions.

The Hamiltonian for the harmonic oscillator system is

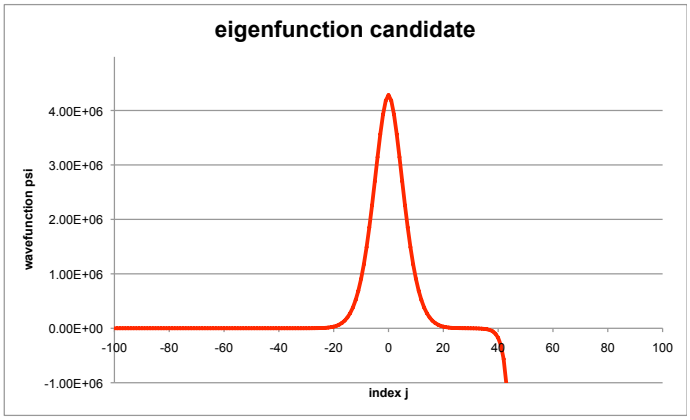
$$H = \frac{p^2}{2m} + \frac{K}{2}x^2,$$

which means the the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi}{\partial x^2} + \frac{K}{2}x^2\varphi = E\varphi.$$

The numerical spreadsheet method is used to solve for the eigen-energies of this equation by viewing the output of the first eight eigenfunctions on the graph.

V-Well Potential n=1



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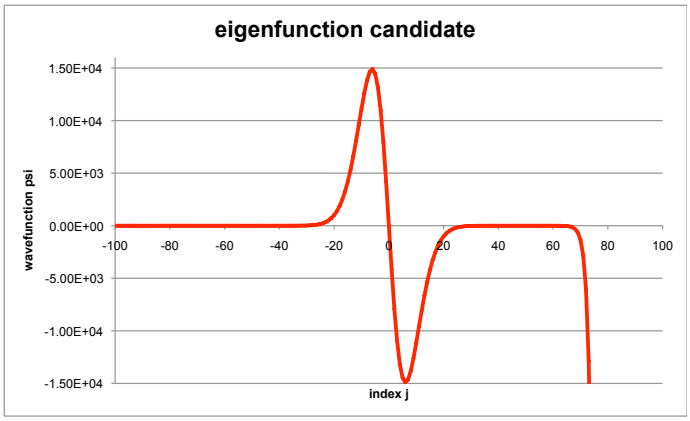

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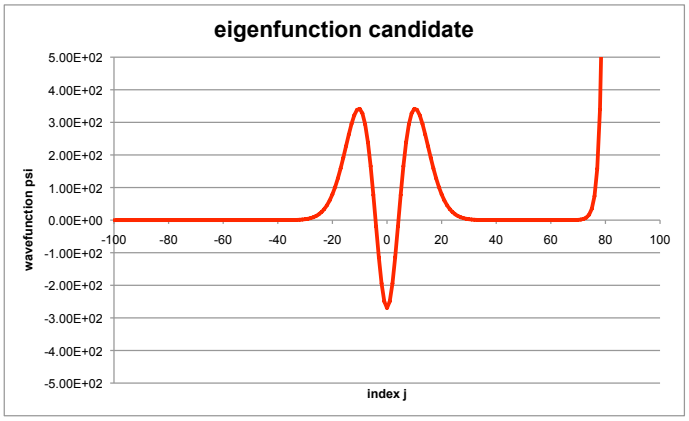

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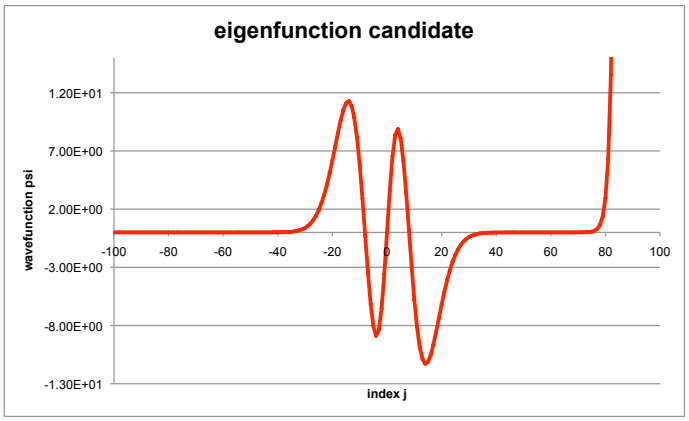

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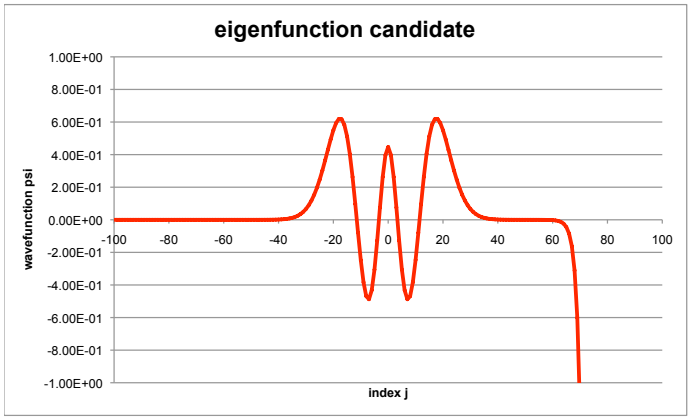

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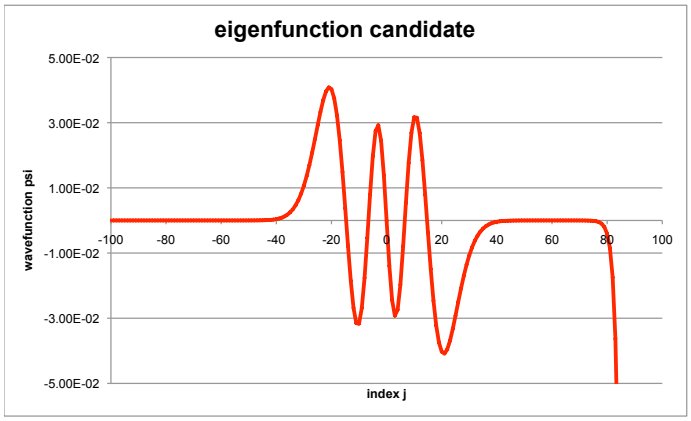

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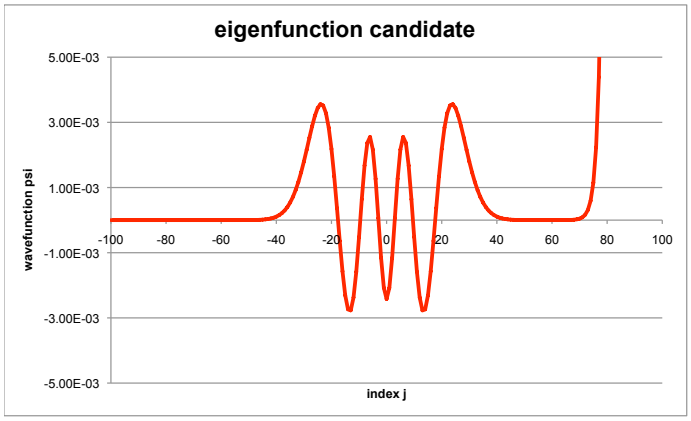

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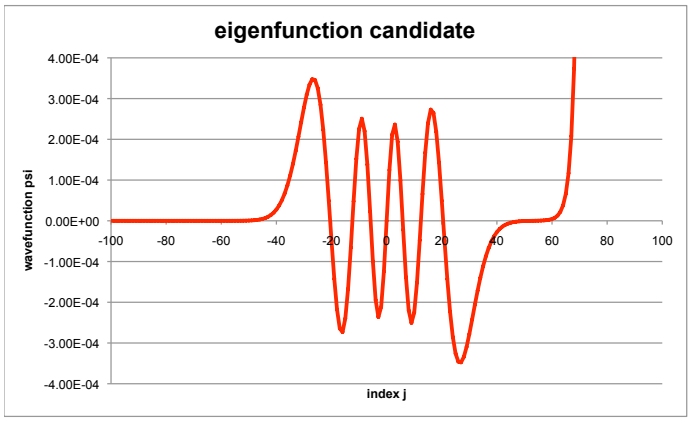

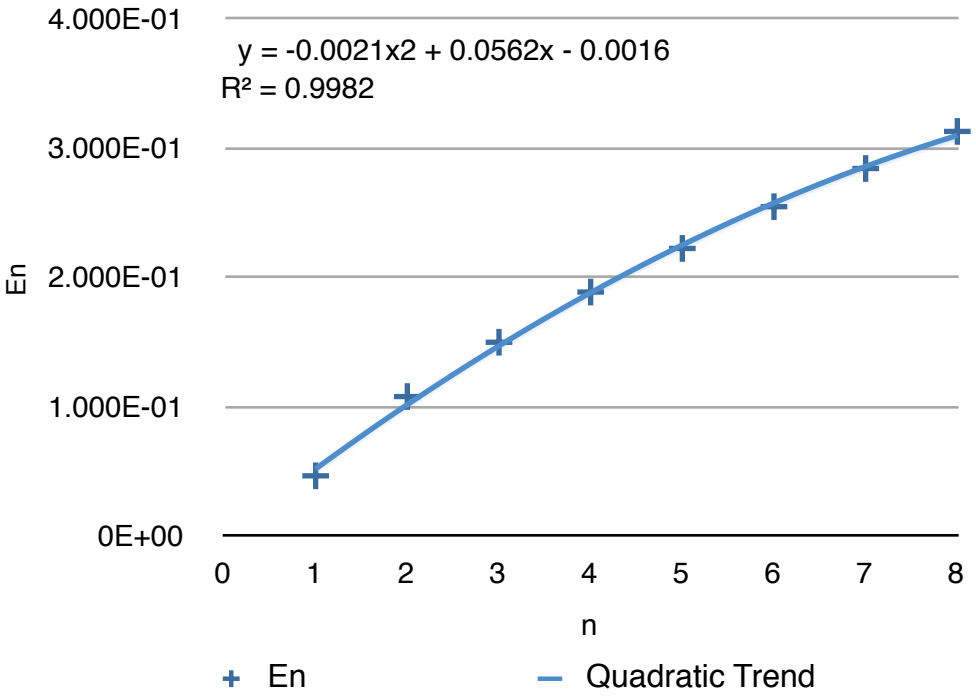

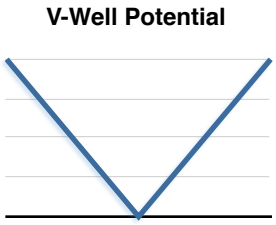

n	E_n
1	4.704E-02
2	1.083E-01
3	1.503E-01
4	1.891E-01
5	2.228E-01
6	2.551E-01
7	2.847E-01
8	3.133E-01

V-Well
C = 1.0 x 10^{-2}

The V-Well, or triangular well, is a potential that remains without exact analytical solutions. This means that eigen-energies of this potential can only be calculated numerically. This potential was simulated with a positive absolute value function running between -100 and 100 normalized to 1. The eigenfunction values were then calculated using the same formulae used in the first two simulations. The different potential values were multiplied by a constant C, which was used to control the magnitude of wavefunction (ψ). The eigen-energies were found using the same technique as the last two simulations. Excel's goal-seek was again used to determine the values to greater accuracy once the basic shape was created on the numerical graph.

This project utilized the time-independent Schrödinger equation which when combined with the Hamiltonian operator creates eigenvalue equations that can be solved to obtain eigenvalues. Below is the eigenvalue equation these numerical calculations solved.

$$H\psi(x) = E\psi(x)$$

The eigenvalues describe physical energy characteristics of quantum mechanical standing waves. This project focused on obtaining the eigenvalue energies of three different potentials.

Using Microsoft Excel, we were able to numerically solve for the first eight eigenenergies for the three different potentials using the difference equation. Which can be scaled with dimensionless values of ε and v_j

$$\Psi_{j+1} = \left[2 - \frac{2m(\Delta x)^2}{\hbar^2}\left(E - V_j\right)\right]\Psi_j - \Psi_{j-1}$$

$$\varepsilon \equiv \frac{E}{U_0} \qquad v_j \equiv \frac{V_j}{U_0}$$

$$\Rightarrow \Psi_{j+1} = \left[2 - (\varepsilon - v_j)\right]\Psi_j - \Psi_{j-1}$$

The difference equation allows for numerical approximation of the second derivative of the three wavefunctions ψ. Using this equation entered into an Excel spreadsheet along with each of the three numerical potentials in a range from -100 to +100, the numerical values of the eigenfunctions were obtained. The graphs were created by simply graphing these calculated values against the -100 to 100 index values.

These three simulations helped me to better understand the physical relationships behind the math that we do in lecture and homework. I find that I learn best by doing, and making these graphs and writing some simple explanations forced me to do some work beyond what some homework problems require, so it was most helpful.