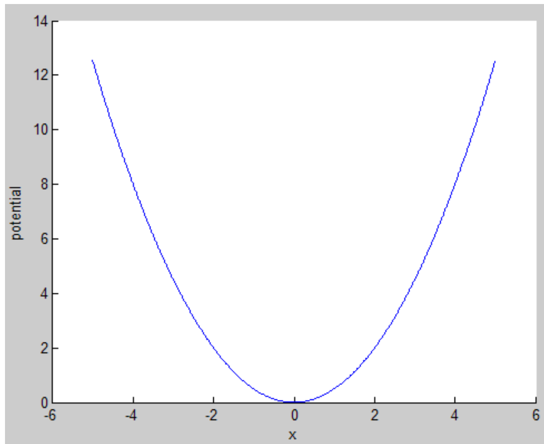
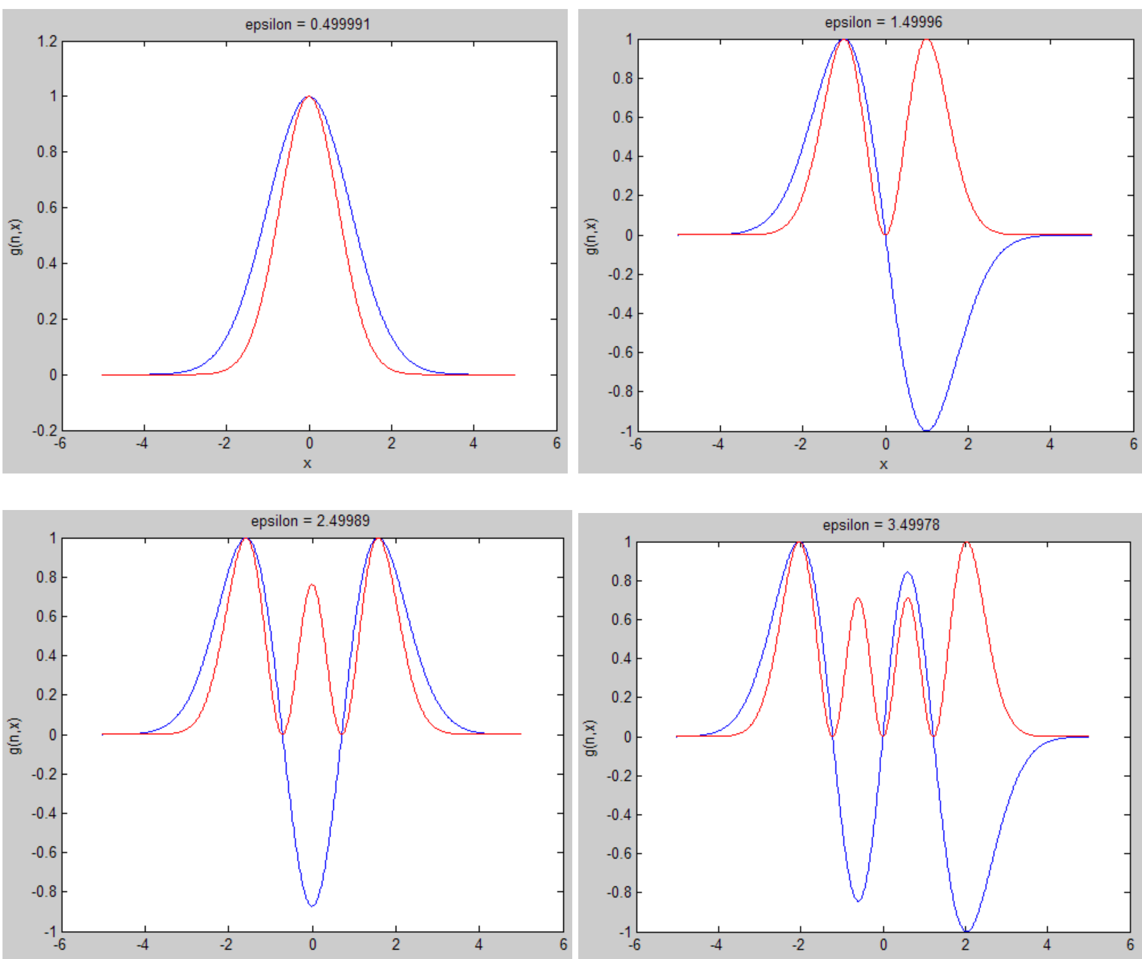
Schroedinger Equation Examples:

Numerical solutions of the time-independent Schroedinger equation for various potentials

by Dr. Colton, Physics 581 (last updated: Fall 2020)

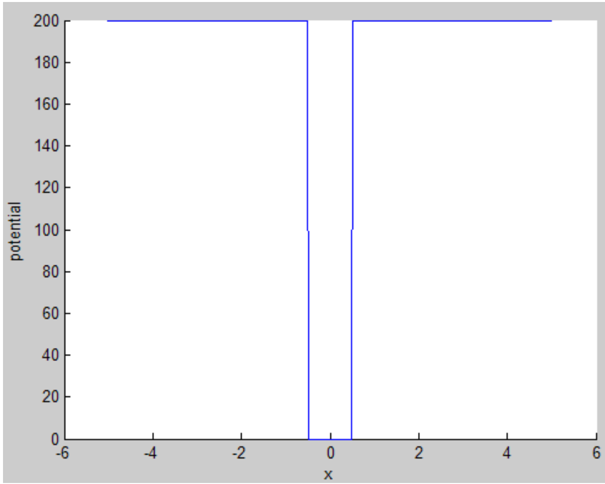
1. Harmonic oscillator potential

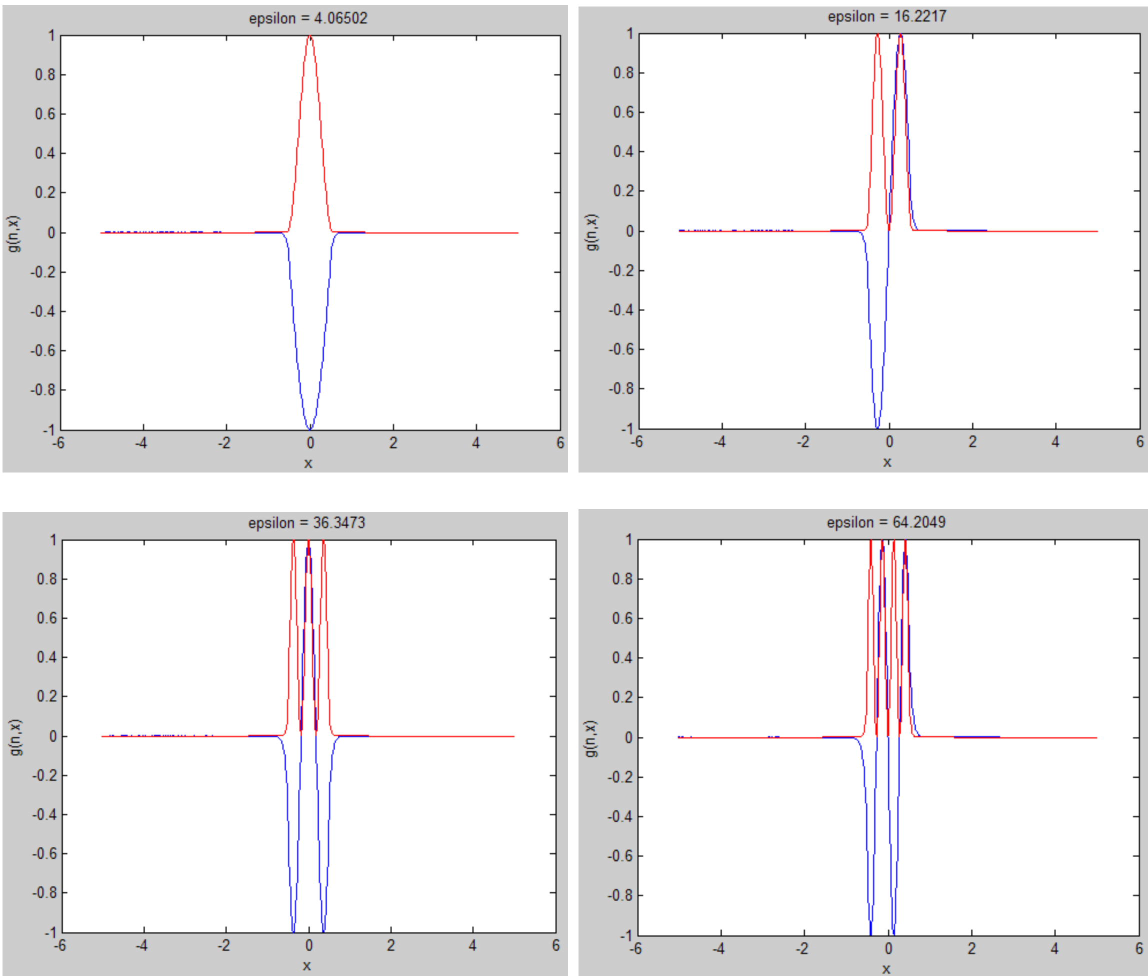




Notice the energies: 0.5, 1.5, 2.5, 3.5, ... $E \sim n + ½$

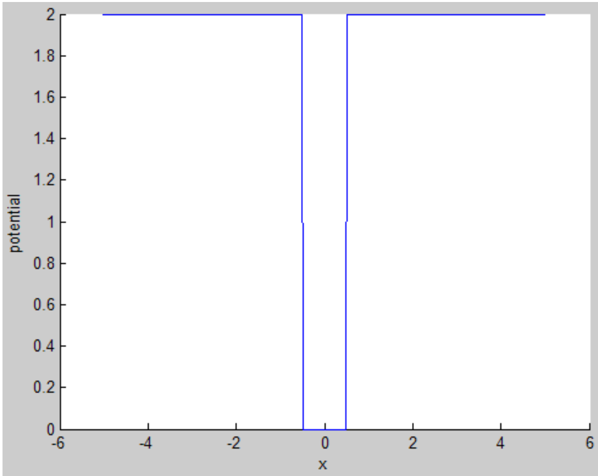
2. Infinite square well potential (huge finite well, actually)

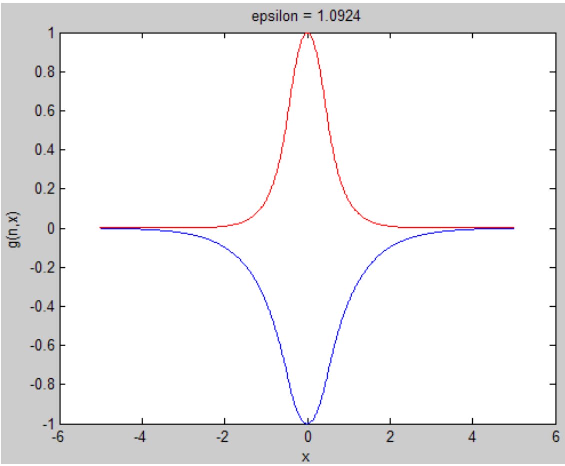


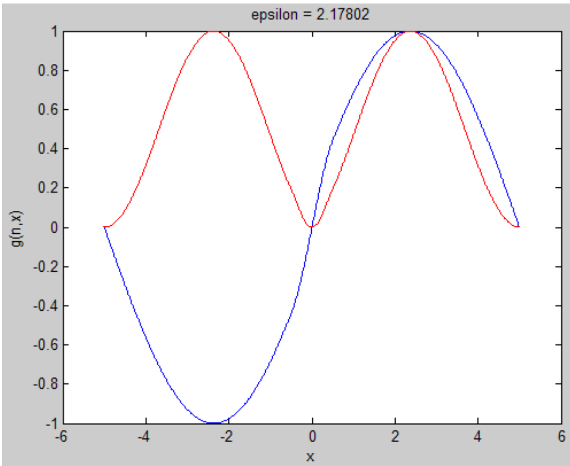


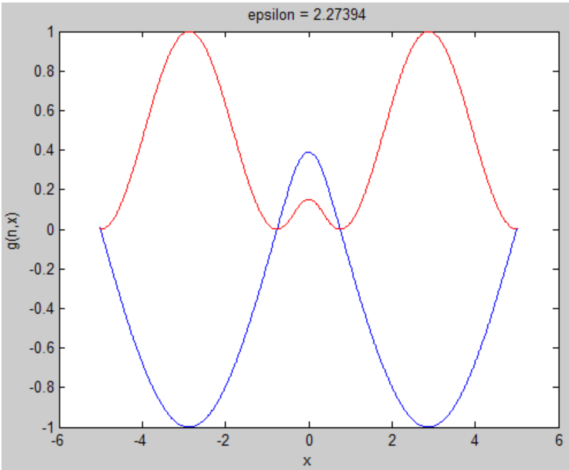
Notice that the energies increase as n^2: $4\times1^2, 4\times2^2, 4\times3^2, 4\times4^2, \ldots$ $E \sim n^2$

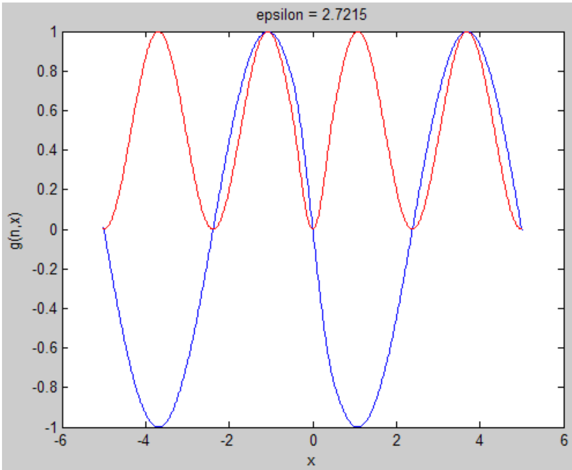
Square well potential (shallow well)





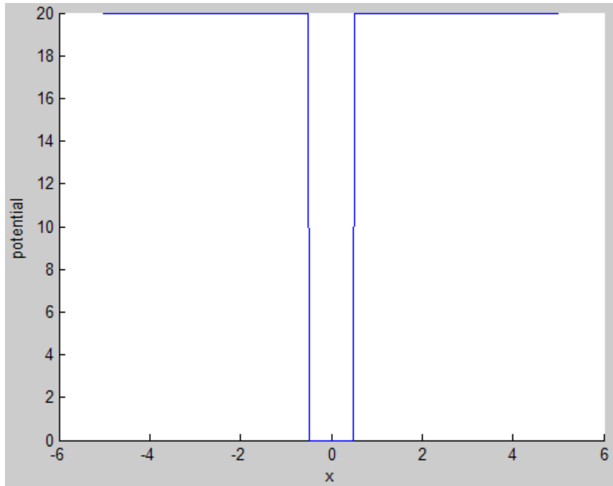


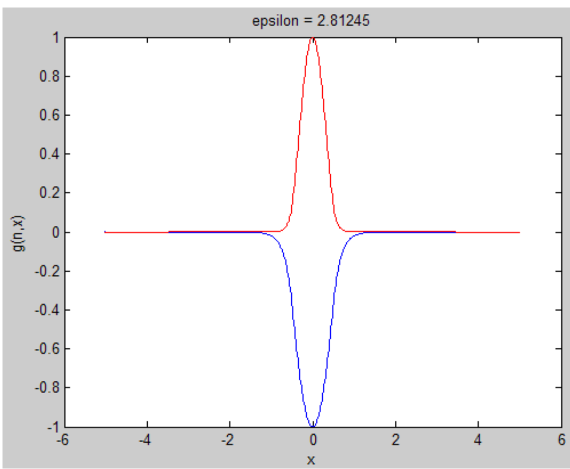


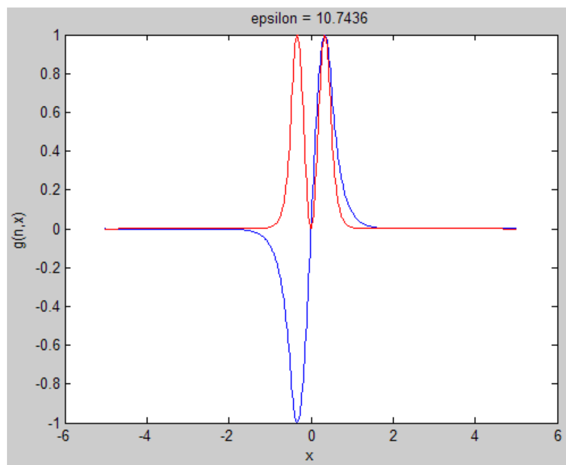


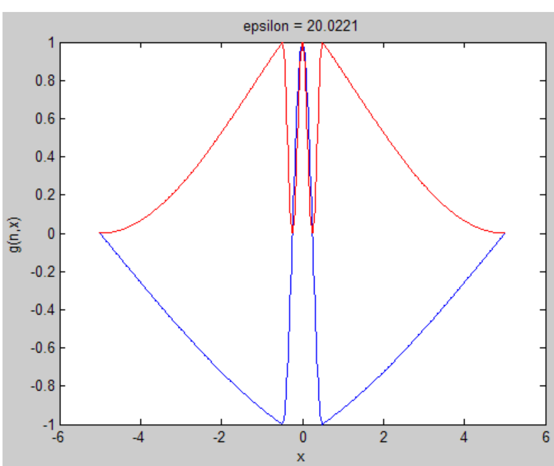
Note: energies above 2 should technically be unbound states, but I'm forcing the endpoints to go to zero so this acts as a finite well inside an infinite well, so they are still bound states.

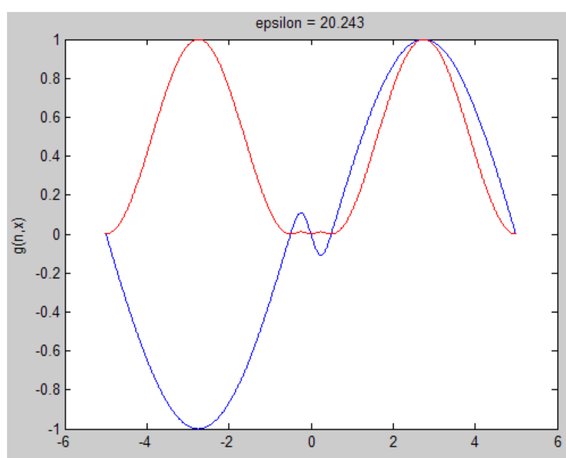
3. Square well potential (medium well)





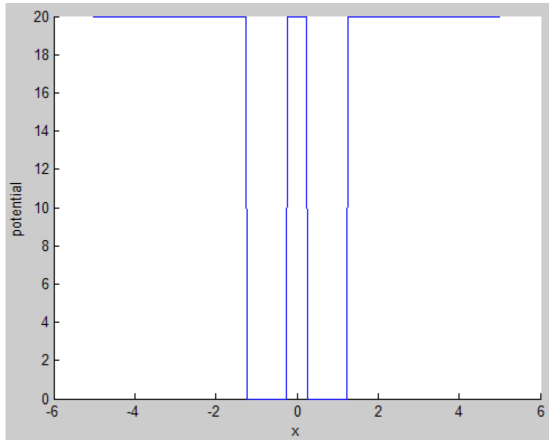


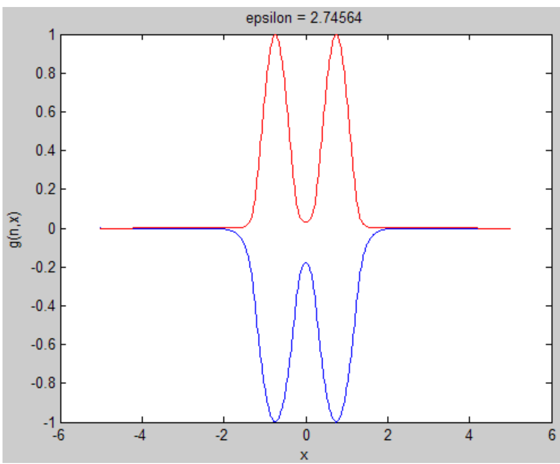




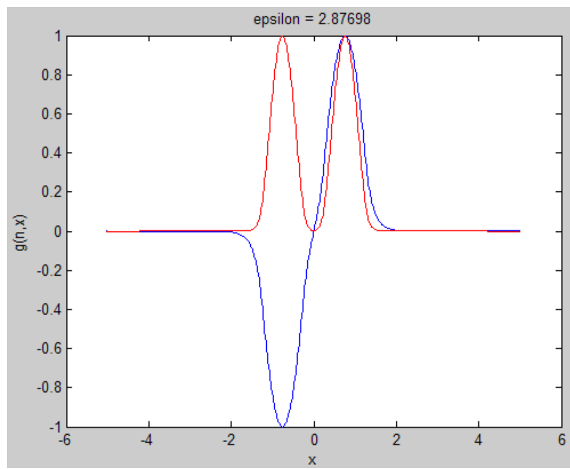
Note: energies above 20 should technically be unbound states.

4. Double square well potential (two medium wells)

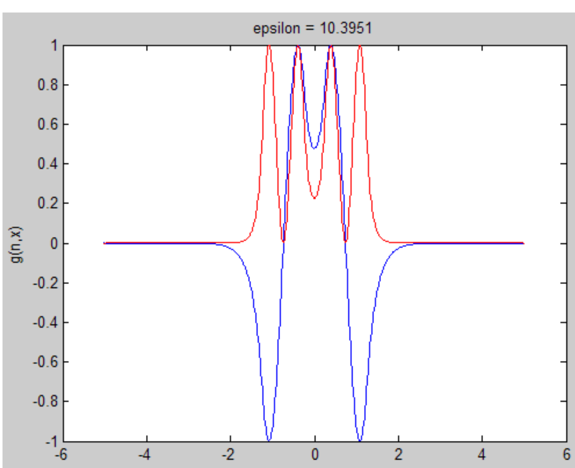




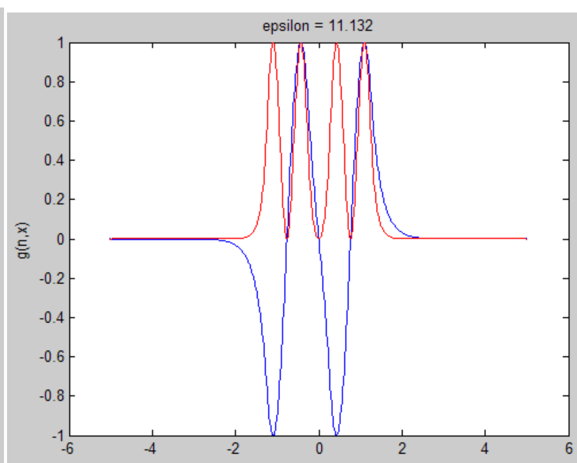
A little below the single medium well ground state energy of 2.81245



A little above the single medium well ground state energy of 2.81245

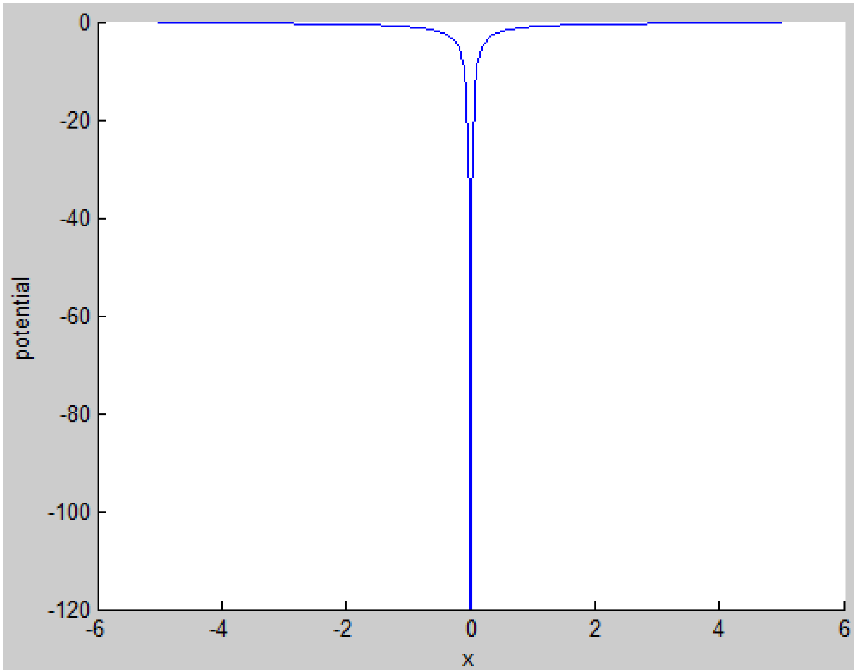


A little below the single medium well first excited state energy of 10.7436



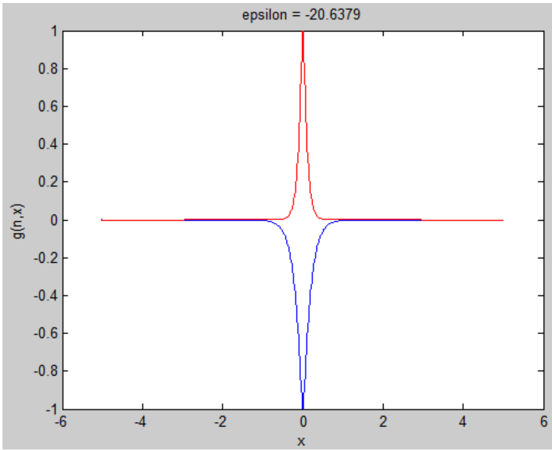
A little above the single medium well ground state energy of 10.7436

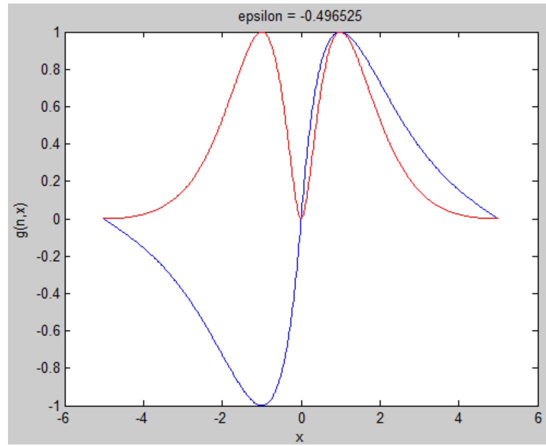
5. Coulomb potential (1D)

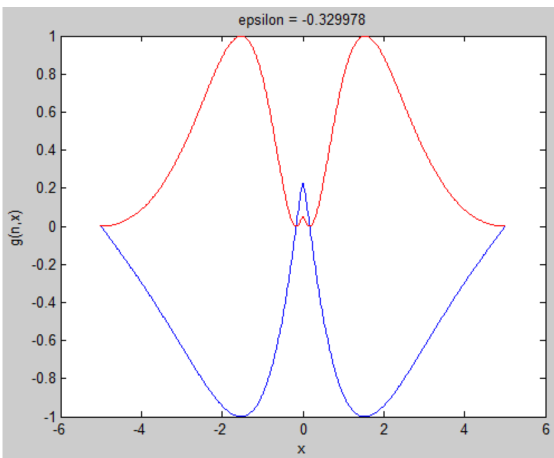


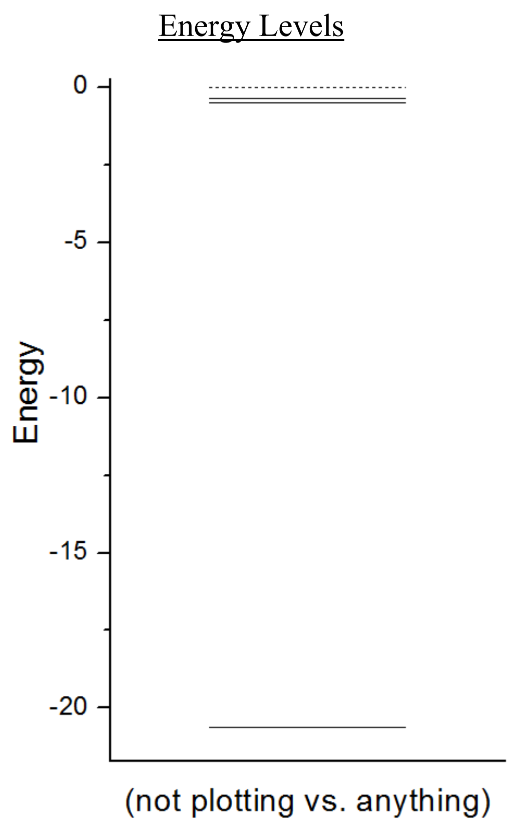
Domain from -5 to 5; 1 well, potential =1/|*x*|

There are only three bound states



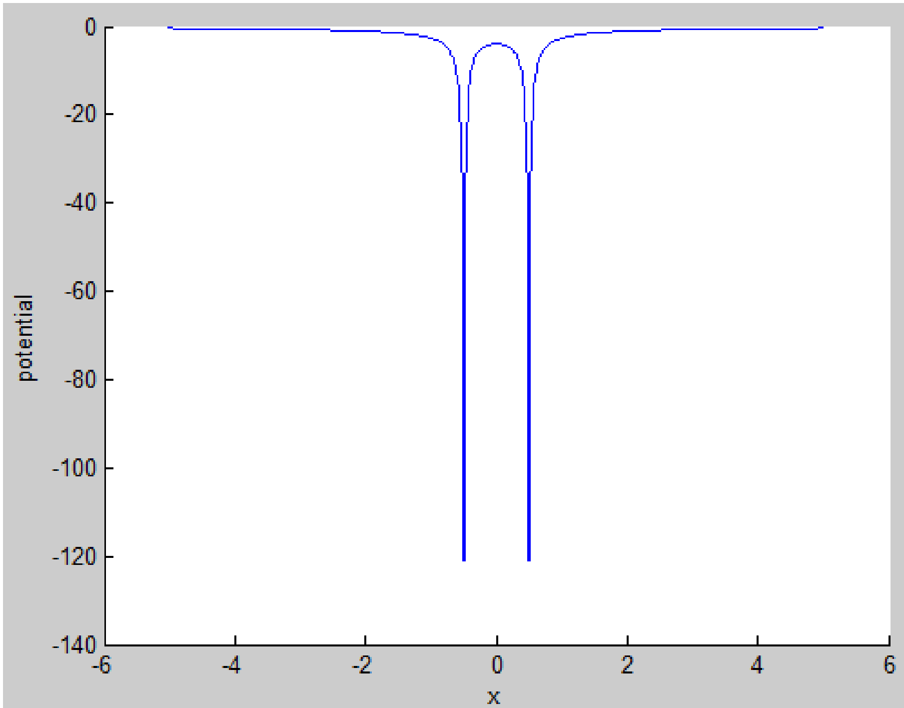






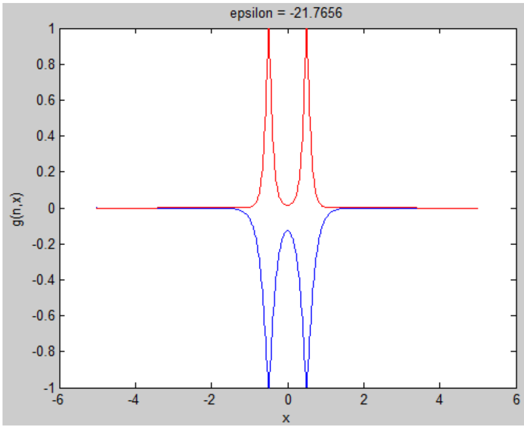
(For 3D Coulomb potential, there are an infinite number of bound state energies: 1s, 2s, 2p, 3s, …)

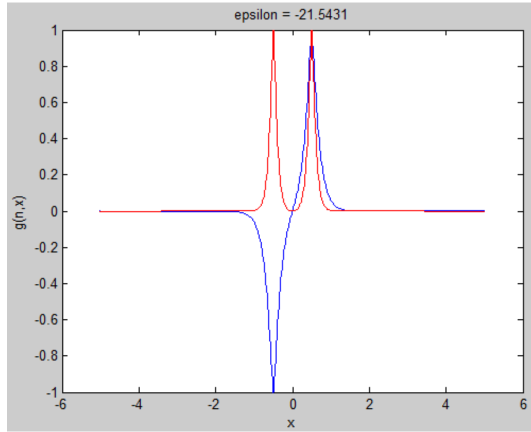
6. Two neighboring "Coulomb wells" (in 1D)

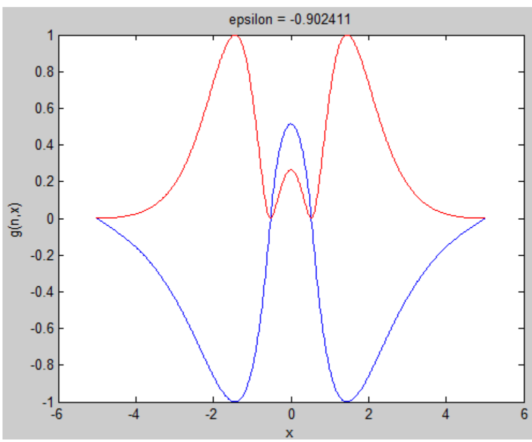


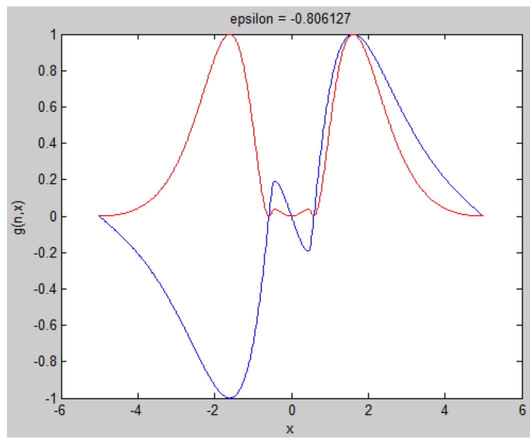
Domain from -5 to 5; 2 wells, centered at -0.5 and 0.5
potential = $-1/|x+0.5| - 1/|x-0.5|$

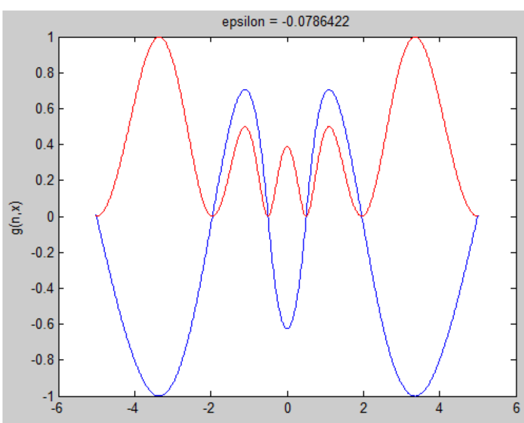
Five bound states:

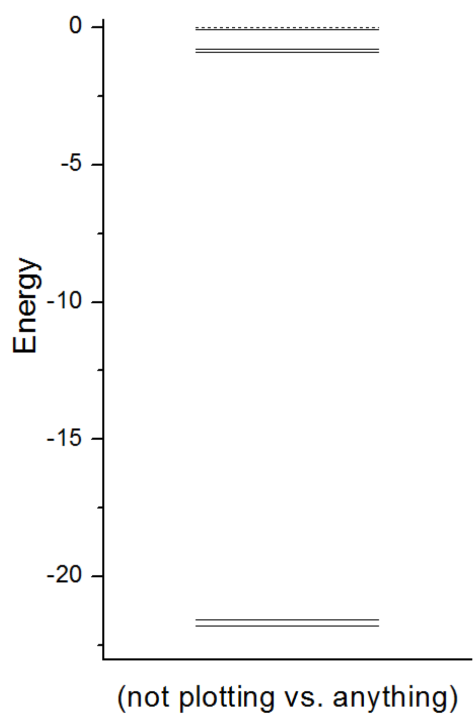








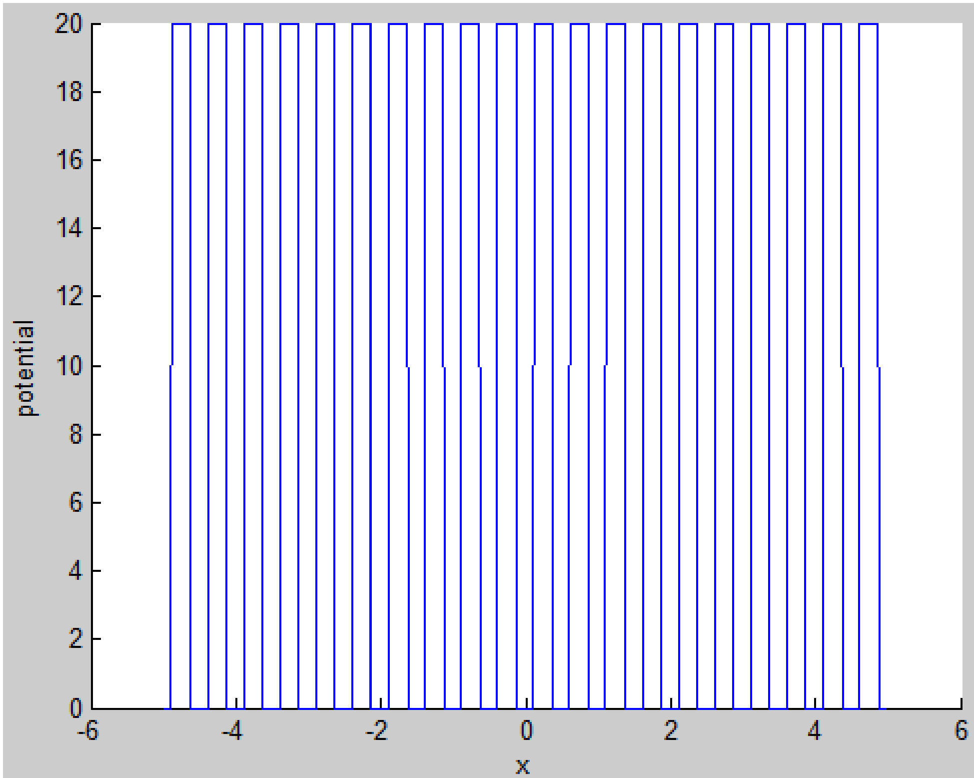




<u>Notice:</u>

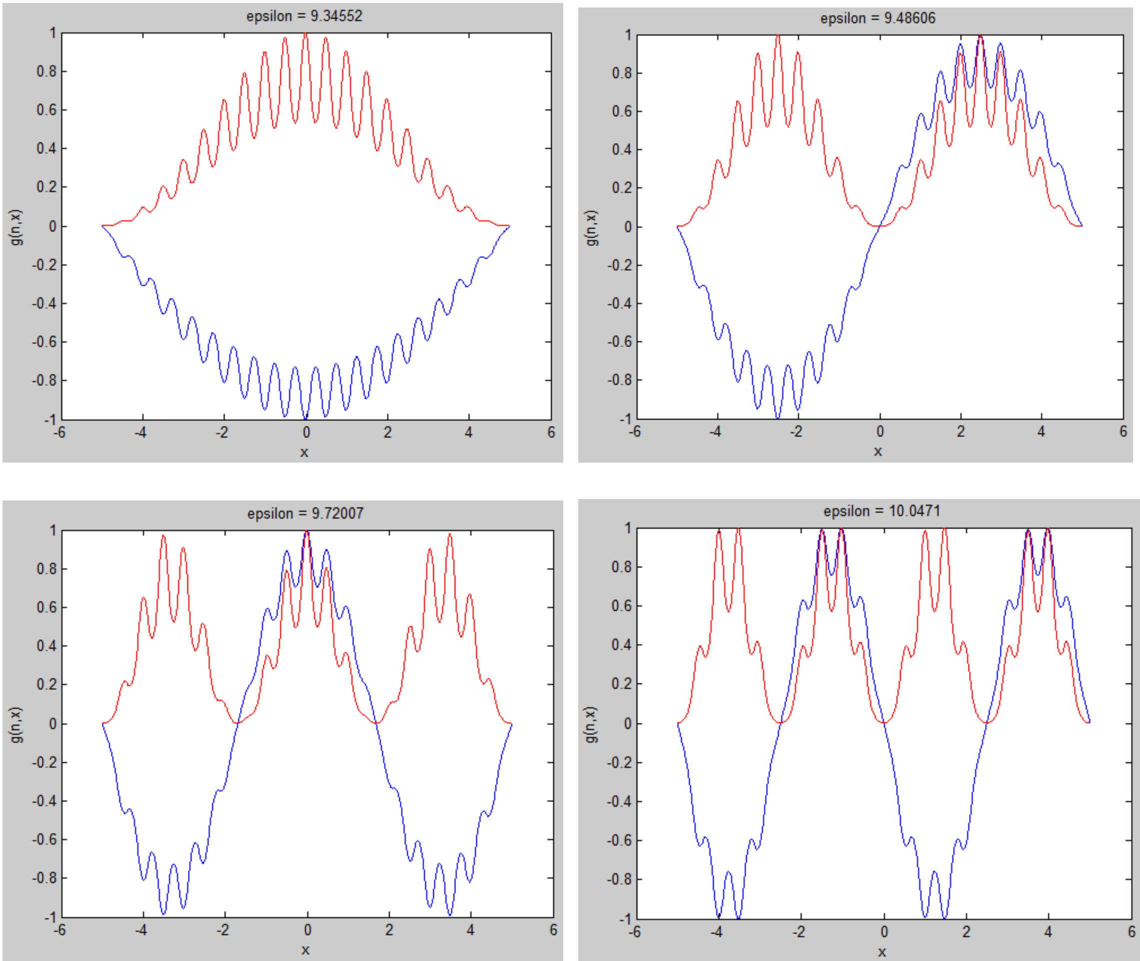
1. The first two wavefunctions are very close to $\psi_{\text{leftwell}} + \psi_{\text{rightwell}}$ and $\psi_{\text{leftwell}} - \psi_{\text{rightwell}}$, respectively.
2. The 3rd and 4th wavefunctions are "antibonding".

7. 19 Shallow Wells

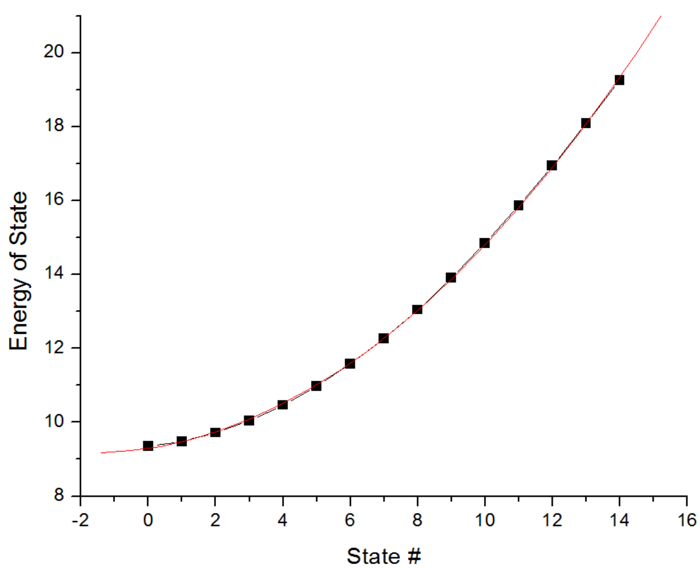


Domain from -5 to 5; 19 wells across domain
Each barrier = 20 high; Each well & barrier = 0.5 wide
(An extra fraction of a well on each side.)

First four wavefunctions (and their corresponding energies)

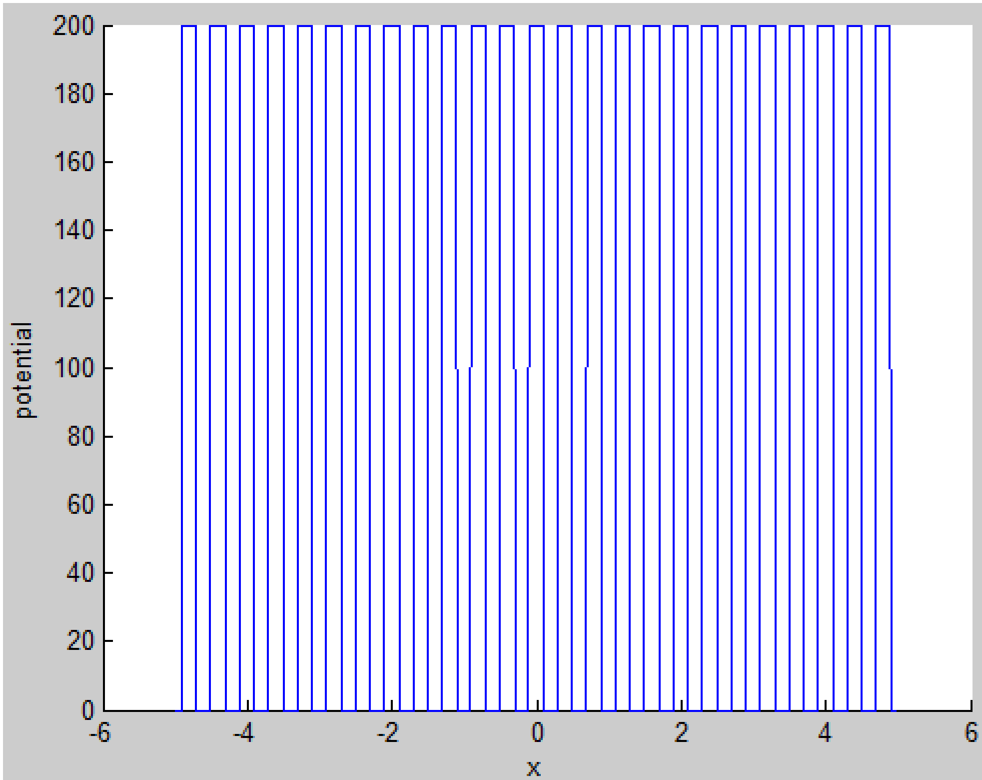


All 15 bound states (fitted to a parabola):



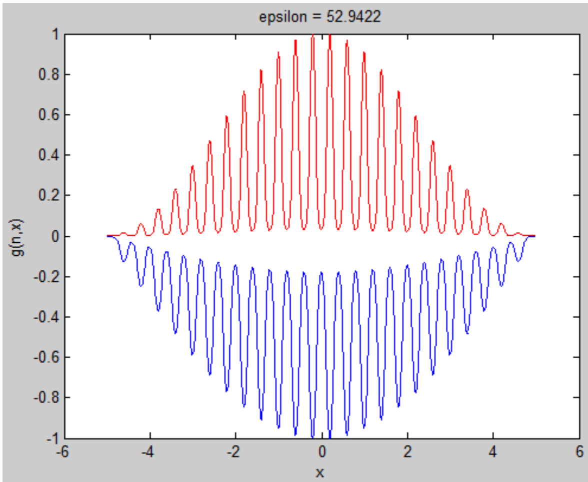
Notice: The energies fit on the parabola nearly exactly! You can therefore say that $E \sim (\text{something})^2$. The "something" turns out to be the wavevector, *k*.

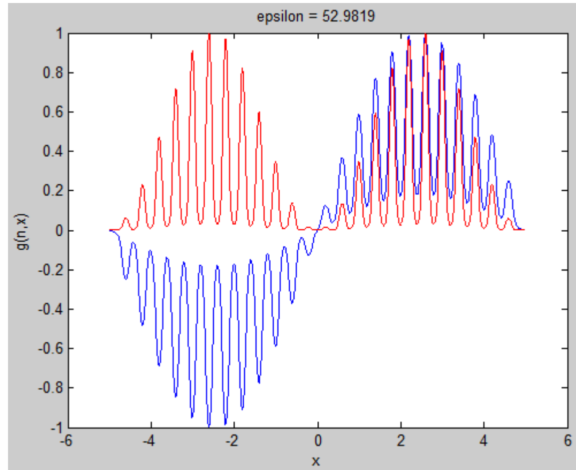
8. 24 Deep Wells

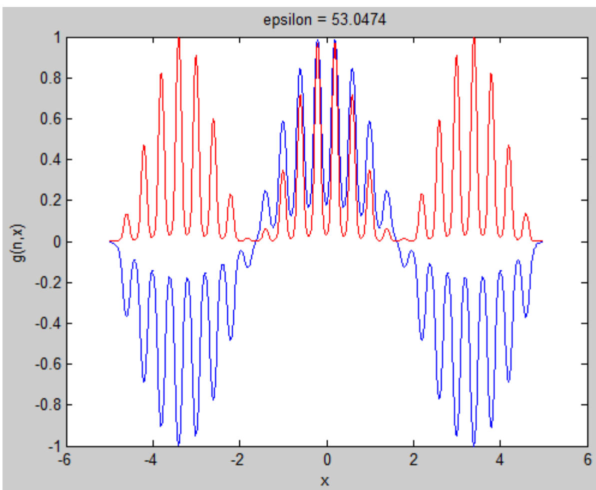


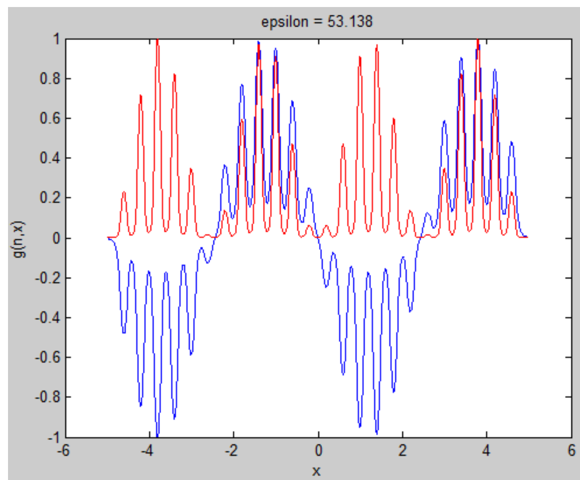
Domain from -5 to 5; 24 wells across domain
Each barrier = 200 high; Each well & barrier = 0.4 wide
(An extra fraction of a well on each side.)

First four wavefunctions (and their corresponding energies)

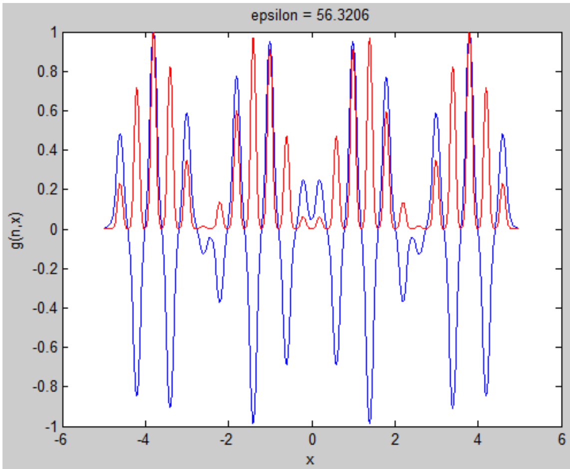


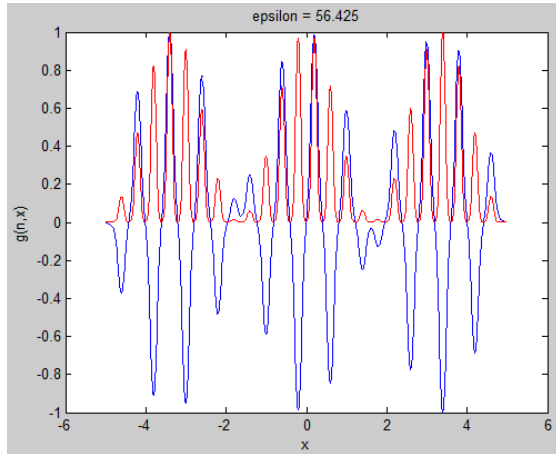


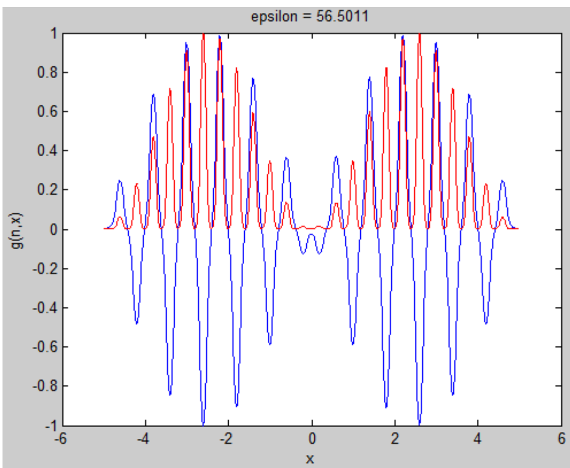


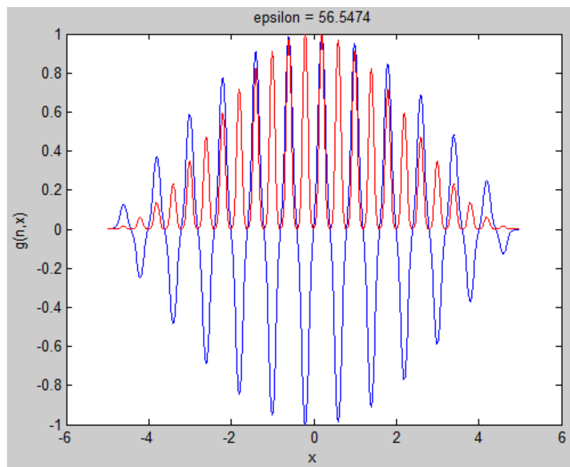


Wavefunctions #21, 22, 23, and 24

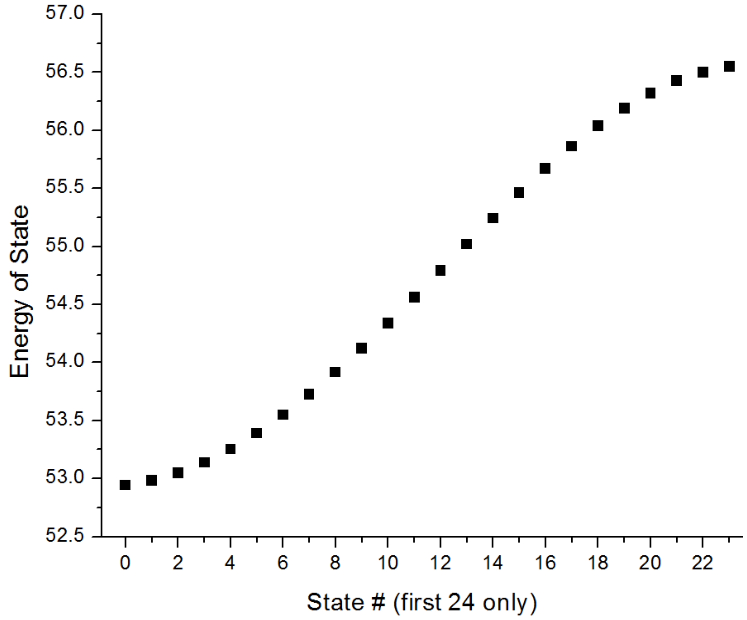






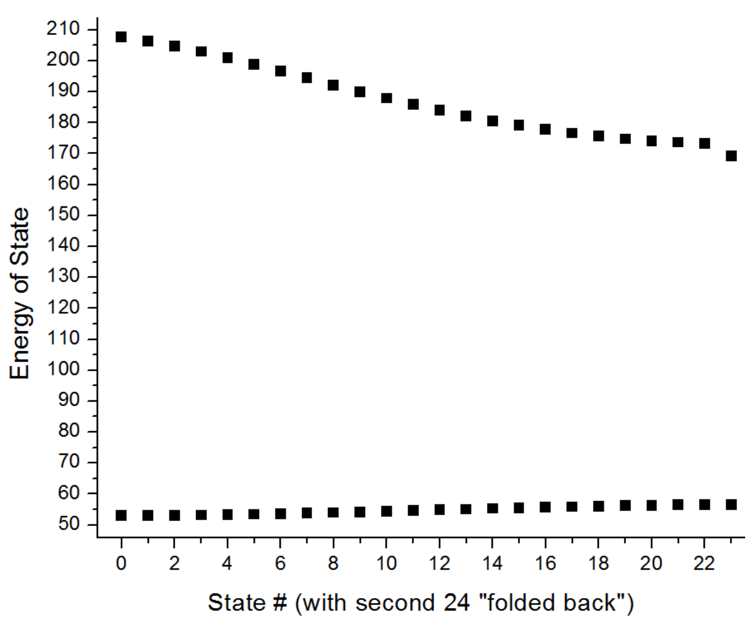


First 24 states: all with energies less than 60



Notice: Not a parabola!

First 48 states, with higher energy state numbers "folded back"
(count state numbers as 0, 1, 2, 3, …, 20, 21, 22, 23, 23, 22, 21, 20, …, 3, 2, 1, 0)



Notice: The presence of the states at the upper energies somehow "repels" the energies of the lower states on the right. They clearly deviate from a perfect parabola.

(Also, technically some of the states I've plotted in upper curve would be unbound because their energy went over 200… we'll not worry about that.)