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Project: Project 9 Numerical Simulation of Quantum Mechanics

Week 2 Goals: To continue on last week's work, solve the symmetrical potential for multiple values for energy for both even and odd parity, write a function to normalize the wave function using integration and move on to solving the wave equation by the matching method, and test it using the Lennard Jones Potential function.

Note: Goals not reached, function for the lennard jones potential made but matching method not implemented. Solved for the symmetrical potential for multiple energies and both parities.

Referenced materials:
Computational Physics, N.J. Giordano and H. Nakanishi, 2nd edition

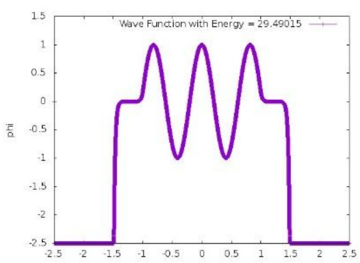
Summary:
Values for the initial conditions adjusted until desired graphs achieved.

Function used to integrate between the boundary conditions of the wave function squared to get the area, and then multiply by the constant factor of $\frac{1}{\sqrt{area}}$ so that when it is next integrated that the area is 1.

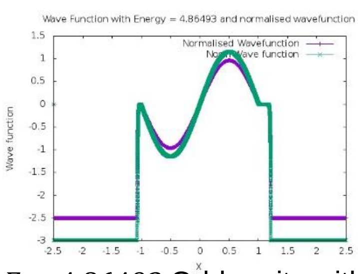
Lennard Jones Potential plotted as per the formula below.

$$V(x) = 4\epsilon\left(\left(\frac{\sigma}{x}\right)^{12} - \left(\frac{\sigma}{x}\right)^{6}\right)$$

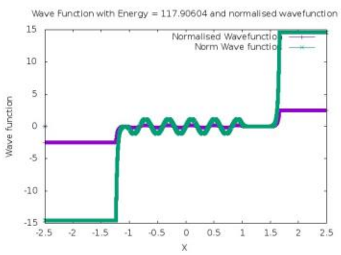
No further was gotten.



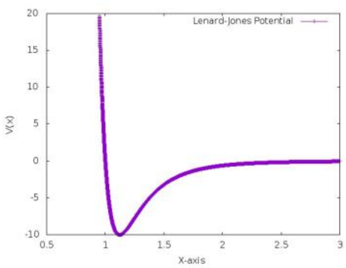
$E = 29.49015$ Even parity



$E = 4.86493$ Odd parity with the normalized function overlay



$E = 117.90604$ Odd parity with normalized function overlay



Lennard Jones potential $\epsilon = 10$, $\sigma = 1$

Goals for next week: Implement the matching method and solve for the LJ potential as well as the case where the potential has a slight potential step around $x = 0$