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Project: Project 9 Numerical Simulation of Quantum Mechanics

Week 1 Goals: To program enough to solve for the lowest energy, and then move to higher energies and plot graphs similar to 10.4 in *Computational Physics*, N.J. Giordano and H. Nakanishi, 2nd edition.

Actually achieved: Solved for the lowest allowed energy.

Referenced materials:
Computational Physics, N.J. Giordano and H. Nakanishi, 2nd edition
Numerical Analysis, R.L. Burden, J.D.Faires
Introduction to Quantum Mechanics, D.J. Griffiths
Stack Overflow: Stack Overflow

Summary:
Computational Physics was referred to for the original idea as well as the project goals and some of the formulae, initial conditions and pseudo code.

The numerical algorithm is as follows:
$\psi(n+1) = 2 * \psi(n) - \psi(n-1) - 2 * (\Delta x)^2 (E - V(n)) * \psi(n)$
$\psi(n+1)$ is the next point, $\psi(n)$ is the previous point, $\psi(n-1)$ is the two previous point, $V(n)$ is the potential at the point n, Δx is the spacial step, and E is the energy we are varying.

Some success on the lowest energy level solution where we get characteristic behaviour, ½ wave between ±L for the amplitude of wave function and remains at 0 for a bit outside ±L, where potential step occurs, after staying at 0 for a while the wave function then diverges to ±∞. Cap set such that as it diverges beyond a “Point of No Return” the algorithm sets the value to ± 2.5.

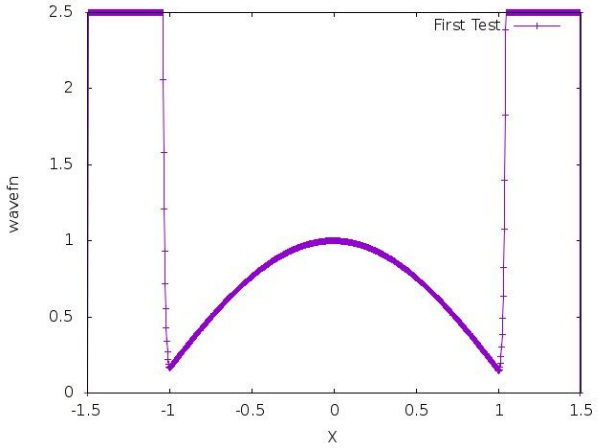
Introduction to Quantum Mechanics was referred to for a more general idea of QM and didn’t help a whole lot towards the project.

Numerical Analysis was referred to but not used at this stage, due to the complexity of some of the algorithm, but will ultimately be used for some of the methods of numerical integration (*Chap. 4*), and *Chaps. 9, 10, 11* seem as though they will be useful at some point.

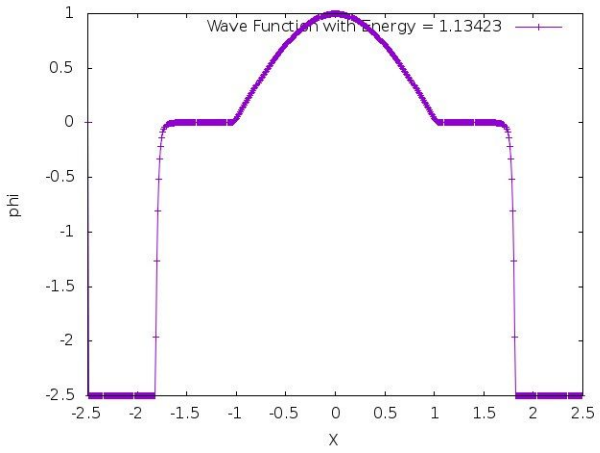
Stack Overflow was referred to for some programming techniques, such as use of pointers for returning arrays and values.

Problem arose when moving to higher energies and more complete waves. Instead of getting a full wave it is as if the wave was flipped up to the positive value, i.e. $\left|e^{ikx}\right|$.

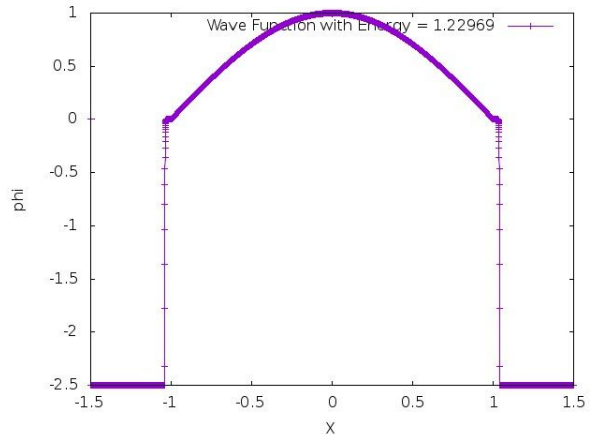
To Implement: Normalise the wave function such that the probability of finding an electron, by the usual method, between ± L is 1, and 0 outside, and to fix the higher energy problems.



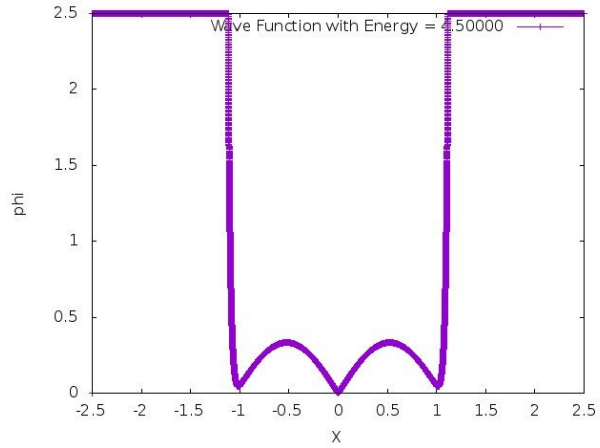
First Successful Test



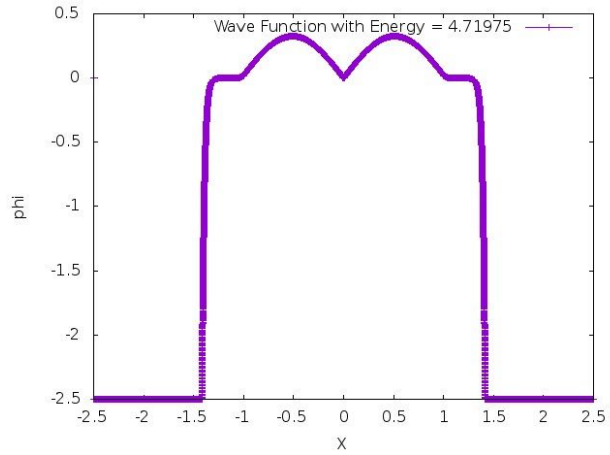
Energy of 1.13423 2nd successful graph



Energy of 1.22969 3rd successful graph



Semi Unsuccessful Test



Another Unsuccessful Test