Attempting to Model a Particle in a Box Using Newton-Cotes Method

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1 Abstract

This paper discusses the fundamental scientific background of and the attempt to model a particle's position inside a box at varying energy states. Another model provided by Dr. Oelgoetz shows the expected graph with a correctly calculated graph. This is used as the basis of how our model was incomplete, and we attempt to hypothesize reasons for why the computational method did not represent a particle accurately.

2 Introduction and Background

In the Quantum Mechanical field of science, a particle in a box describes the free movement allowed for that particle to move surrounded by potential barriers. This model is also referred to, more accurately, as an infinite potential well. When the length of the well becomes very small classical systems cannot be applied to a particle. Therefore Quantum Mechanical effects have to taken into consideration. To put the size of the well into perspective their length is commonly measured analytically as angstroms. The conversion of angstrom to meter is, 1 to 1e-10 scale. At these small units of distance a particle may occupy specific energy states. An electron will always occupy the lowest energy state possible for the potential energy of that electron. Also electrons can never occupy a state with zero potential energy. This state would imply the electron is stationary. This would only be hypothetically possible at absolute zero, which science has not yet achieved. It continues to remain a lower limit of heat.

In a one-dimensional model of a particle in a box, the wells contain space of zero potential. This means the particle or electron is free to move inside the well and no force can act upon it. In contrast, the barriers contain infinite potential. Meaning the particle is repelled by infinitely large forces whence the particle touches a barrier; thus preventing escape.

3 Methods and Modeling

The position function of a particle is defined by Schrodinger's equation:

$$i\hbar\frac{\delta}{\delta t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\delta^2}{\delta x^2}\Psi(x,t) + V(x)\Psi(x,t) \tag{1}$$

, which is a wavefunction. $\hbar$ is Planck's constant, m refers to the m of the particle (in our model the particle is an electron), i is an imaginary unit, and t is time.

For our purposes the expectation value of the positon for a particle at a given time is more useful. The general form for this is:

$$< x >= \int_{-\inf}^{\inf} xP_n(x)dx \tag{2}$$

or

$$< x|P_n|x > \tag{3}$$

This equation defines the rate at which we can expect an electron to be contained at a certain position inside the box. The integral was solve numerically using Boole's Rule. Boole's Rule is a fifth-order Newton-Cotes formula, which has the structure:

$$\int_{x_1}^{x_5} f(x)dx = \frac{2}{45}h(7f_1 + 32f_2 + 12f_3 + 32f_4 + 7f_5) - \frac{8}{945}h^7 f^{(6)}(\epsilon) \tag{4}$$

, f is some function, where the average along some distance along a curve is taken using intervals x_1 through x_5.

4 Results

The below four figures, depict the output for the data produced from our computational method. They are in pairs: the first two are electrons at the lowest energy state, the first figure defines the Hamiltonian for sine and cosine values superimposed over the hypothetical well structures. Figure 2 does not contain the well structure. Figure 3 and Figure 4 are similar to the first two, but for a higher energy level.

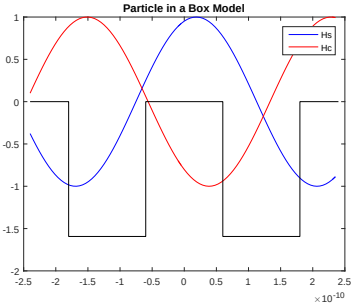

Figure 1:
This is suppose to model the position across the wells for an electron at the lowest energy state superimposed over the structure of the wells.

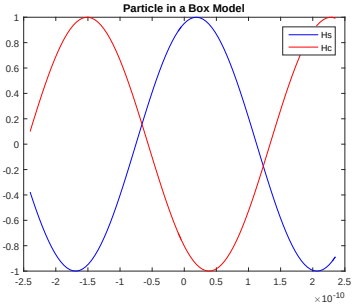

Figure 2:
This is suppose to model the position across the wells for an electron at the same energy state as Figure 2 without being superimposed over the structure of the wells.

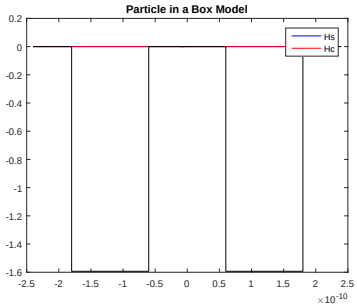

Figure 3:
This is suppose to model the position across the wells for an electron at an energy state superimposed over the structure of the wells.

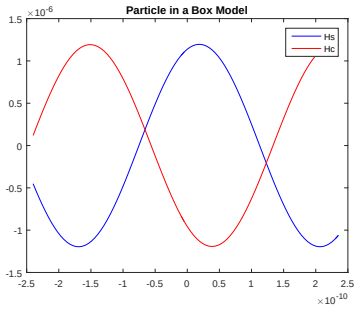

Figure 4:
This is suppose to model the position across the wells for an electron at the same energy state as Figure 3 without being superimposed over the structure of the wells.

The following figure shows the output from the Matlab code proved by Dr. Oelgeotz allowing a comparison of accuracy between methods. Figure 5 is what Figure 1 is suppose to appear as. Clearly the two are very dissimilar. We will try to note some reasons for the difference in output. The first is that when we calculated my Ψ values I did not add the potential energy values times the sine function to my Hamiltonian. The sine value was multiplied the Hamiltonian. This error was not found after submission of the source code. Another may be from incorrect input into the Lapack library function, dysev. The source code was written in C++, and Lapack is written in Fortran. Writing out from C++ to Fortran requires the A-matrix to be condensed to

a one dimensional array rather than a two dimensional. The documentation was not written for C++, which caused difficulty in translating to fit C++ form.

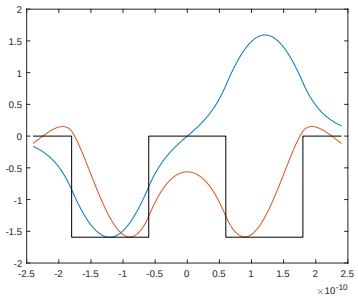

Figure 5:
This shows the correct position of an electron at the lowest energy state superimposed over the structure of the wells, provided by Dr. Oelgoetz.

5 Conclusion

In conclusion, we discussed the fundamental scientific background of the particle in a box scenario, and the modeling of a particle's position inside a box at varying energy states using Boole's rule, a Newton-Cotes method. Using the model provided by Dr. Oelgoetz, we saw the expected graph with a correctly calculated graph which was used as the basis of how our model was incomplete, and we hypothesized reasons for why the computational method, based on the submission source code, did not represent a particle accurately.

References

[1] E. Anderson, Z. Bai, J. Dongarra, A. Greenbaum, A McKenney, J. Du Croz, S. Hammerling, J. Demmel, C. Bischof, D. Sorensen *LAPACK: a portable linear algebra library for high-performance computers* 1990. University of Tennessee, New York University, NAG Ltd., University of California, Berkeley, Argonne National Laboratory, Rice University.

[2] J. Oelgeotz, Dr. *Physics 4000 - Computational Lecture* 2016. Austin Peay State University, Department of Physics and Astronomy.

[3] n.a. *Particle in a Box* 10 December 2016. Wikimedia Foundation, Inc.