Quantum Sandbox:
General Solutions to the Schrödinger Equations in 1D Piece-wise Continues Potentials

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1 Abstract

The introduction of quantum mechanics at the undergraduate level poses one of the greatest leaps for students in physics education. Despite this, there is sparse practice and exposure to anything but the proverbial analytical solutions to the Schrödinger equation. This paper proposes a more flexible and available web-hosted approach to computational solutions of the Schrödinger equations. This quantum sandbox provides user-determined well-size, potential functions, and particle type. By implementing a LAPACK algorithm for solving eigenvalue problems in conjunction with approximating the Hamiltonian using a finite difference method, the program delivers the energy eigenvalues and converging wave functions to custom potentials. With energy eigenvalues accurate to the third decimal point, this algorithm is an accurate and efficient approach to solving and visualizing bound state wave function behavior.

2 Introduction

It is exceedingly difficult to learn a challenging subject with limited practice material. This should come as no surprise. The idiom learning-by-doing is a well-cemented pedagogical truth([**MR10**]). Something difficult is foreign, abstract, and unintuitive. Quantum mechanics is all of these things. At an undergraduate level, quantum physics is a paradigm shift from the years of classical interpretations and experiences. The practice material is limited to only a small handful of undergraduate quantum physics problems that can be solved by hand. For example the quantum harmonic oscillator, Dirac potentials, and variations of particle in a box. Fogged by an accompanying influx of new math needed to describe quantum models how can we expect students to gain any intuition for the wave function abstraction. It follows that "Teachers were challenged to enthuse their students for quantum physics as they struggled to convey the relevance of the subject to their students"([**Bou+21**]). Those in STEM might chuckle at the function abstraction $y = mx + b$. This formula borders on the mundane and self-evident to many. We have the tools, visualizations, and practice to feel

comfortable with such an abstraction. This is exactly what quantum physics education is missing ([**SG21**]).

The lack of educational resources for quantum mechanics is not the only problem that this research tackles. In the pursuit of creating a flexible framework that allows students to experiment with wave functions, it became clear that there was a problem. Most papers cite specific algorithms or strategies for modeling specific problems. For example Quantum mechanical modeling of Zn-based spinel oxides. The paper proposes that "using calculations in the framework of the density functional theory (DFT) were carried out using four B3LYP HSE06, PBE0, and PBESol hybrid (DFT/HF, HF = Hartree-Fock) functionals implemented in the CRYSTAL17 code" ([**Oli+20**]). The world of research solves ever more niche problems with solutions tailored toward the best results. What this project needed was in some ways the opposite: A generalized computational method that did pretty well at solving a wide range of problems. The research, development, and restrictions of this kind of code are the discussion in this paper. A flexible algorithm will open the doors for a physics sandbox of sorts. A place for undergraduate students to tinker and fill their tool belts with the different basic features of quantum mechanics.

3 Methods and Development

Developing a suitable tool for students requires a fast and accurate algorithm, combined with a robust user experience. Although the presentation of the web-hosted tool born from this research is not the topic of this paper the restrictions that a website puts on computation are a core factor in picking the right code for the job. The constraints and features are as follows. The code must be accurate so students can work with useful numerical results. The code should execute relatively quickly so students are not left to wait on results. Finally, the code needs to be flexible enough to handle an extremely wide range of input parameters. The goal was to give students total control of the potential, the well size, and the particle mass. To ensure the project was feasible, the desired algorithm would be solving for wave functions and energy eigenstates of one-dimensional piece-wise continuous step potentials.

There are two major paradigms when it comes to the description of wave function behavior. The more well known formulation of the Schrodinger equation (Equation 1) and its foil in the language of linear algebra (Equation 2). Although both figures describe the same phenomena, algorithmic solutions usually fall into one of these two categories: A differential equation or an eigenvalue equation.

Equation 1:

$$-\frac{\hbar}{2m}\nabla^2\psi(x) + V(x)\psi(x) = E\psi(x)$$

Equation 2:

$$\hat{H}\psi = E\psi$$

3.1 Algorithms: Integration

A comprehensive literature search will give you plenty of confidence in using integration methods to solve the Schrodinger equation. Unfortunately the popular options like Monte Carlo methods for evaluating path integrals ([**Kra+18**], [**Wes+18**], [**AZL12**]) are out of the picture. Relaxation methods that were tested were simply too slow and noisy for our constraints. The shooting technique using Fourth Order Runge-Kutta integration was both a well-established ([**Kha+18**]) and a much faster alternative. Despite the accuracy of the energy states produced using this technique, the corresponding wave functions displayed significant numerical instability (fig 2). It was clear that an alternative approach was needed.

3.2 Algorithms: Eigenvalues

Eigenvalue routines have moderate speeds but offer benefits in other areas. Using this paradigm was the obvious choice for this project. Before we can begin any sort of calculation we can use the finite difference method to estimate the differentials in the operator H ([**92**], [**KSB21**]). Once we have constructed the matrix we can look at its tridiagonal structure to confirm that the matrix is hermitian. This would be the logical outcome as the observable, energy, should have a corresponding Hermitian operator called the Hamiltonian. The Hermitian matrix is convenient as eigenvalues can be extracted from equation 1 with a simple bisection algorithm in $O(n^2)$ time. The specific LAPACK routine used was xSTEBZ to calculate the energy eigenvalues (Appendix 1). The eigenvectors are subsequently solved using Rayleigh Quotients which are twice as fast as regular power methods ([**Hal96**]). Unlike integration-based shooting methods, the eigenvectors produced are all orthogonal. This confronts the problem of numerical instability and assures that wave functions always have the right shape. It is worth pointing out that the Monte Carlo approach mentioned above generates more accurate wave functions. For this project, however, this is irrelevant because our focus is only on wave shape and eigenvalue accuracy. These are the parameters desired to make for an effective teaching tool.

3.3 Implementation Considerations

Now that a suitable collection of algorithms have been selected, there are implementation details that need to be kept in mind. Despite the fast and iterative nature of xSTEBZ choosing a sample rate $1/n$ will greatly impact the accuracy and the speed of the algorithm. The time that the algorithm takes to execute is

far more important than just user experience. A major concern in the implementation is HTTP request timeouts. The cloud provider used to host the website only allows the TCP connection to stay open for thirty seconds. This means the resolution n must provide accurate results to systems with many energy levels and numerous potential subdivisions while staying below the thirty-second threshold. Another related implementation detail that can be adjusted is the extension. This refers to the extension of the domain beyond the bounds of the well. It is important to capture these regions first and foremost because the higher energy level wave functions bleed out from the bounds of the potential well. In addition, extension plays a crucial role in the accuracy of the algorithm. Larger extensions decrease the local resolution around the potential well. However larger extensions also help enforce the normalization behavior of the wave function at its limits. To meet all constraints, $n = 1000$ and an extension factor of 2 were selected.

4 Error

To impart any confidence in computational solutions understanding possible sources of error is essential. The error analysis is chiefly concerned with the eigenvalues. Eigenvalues are the only numerical quantity measured by this algorithm whose accuracy matters to the website's users. There are two main contenders for sources of error in the design of this routine. These two errors correspond to two equations that are discussed below.

4.1 Hamiltonian Construction Error :

Before xSTEBZ can be implemented, the Hamiltonian (H) needs to be constructed (Appendix 1). To estimate the differential operators that makeup H we utilize the finite difference method (KSB21). The truncation error associated with this approximation is dependent on the step size Δx(equation 3). The factor of C is an arbitrary scaling factor. This truncation error is representative of the input error or accuracy of H.

Equation 3:

$$|\hat{y}'' - y''| \simeq C\Delta x$$

4.2 Eigenvalue Error:

The xSTEBZ eigenvalue accuracy (equation 4) is accessible through some dilapidated LAPACK documentation([**NET**]). The function $p(n)$ is described as a moderately increasing function of n. The documentation reveals nothing more about its description ([**NET**]). A conservative option is to assume that $p(n)$ is linear. The next relevant element associated with this error is the $||H||_2$. The two norm is important because the square root of the result is equal to

the magnitude of the largest eigenvalue of H ([**LJL14**]). The final component ϵ is simply the machine precision. Eigenvalue error is intimately related to the depth of your well. Deeper wells mean greater maximum eigenvalues and larger eigenvalues mean more error. Resolution is also critical. As n increases the accuracy of our eigenvalues decreases. However, choosing a small resolution is not an option because as n decreases Δx increases. As mentioned above in the previous section an increase in step size would degrade our Hamiltonian. This give-and-take relationship between resolution and step size made perfectly tracking and quantifying the net effects of input parameters on eigenvalue accuracy beyond the scope of this project.

Equation 4:

$$|\hat{\lambda}_i - \lambda_i| = p(n)\epsilon||H||_2$$

5 Results

The research above was synthesized into a web-hosted quantum sandbox that provides a myriad of customization. The algorithm supports drastic changes in well size, potentials, and particles while maintaining its performance. In a vacuum, the algorithm accuracy is unmatched with maximum eigenvalues error of 0.006877% for the first 100 eigenvalues. Attached to a website we see a fall in performance with maximum eigenvalues error of 5.65011% for the first 100 states (figure 1).

5.1 Discussion

Although the project was a resounding success, there are still many avenues left unexplored. For example, as mentioned in the methods section, axis extension vs resolution has not been completely resolved. There likely exists an optimal ratio like $\frac{extension}{resolution}$ that maximizes the local resolution while enforcing wave function normalization. Another future area of interest would be a better understanding of error propagation. If n is responsible for both an increase and decrease in accuracy there is likely a sweet spot where we keep step size small while maximizing resolution. The last area that has not been mentioned at all is the appearance of degenerate states in symmetric wells. Currently, there is no way to quantify their appearance so the website user is left to identify them. This might cause some confusion and should be attended to in the future. In conclusion this algorithm not only provided optimal flexibility in solving the simple generic 1D potentials, but the project has real application as a teaching tool. Despite some unanswered questions, the algorithm is functional and performs quickly and accurately.

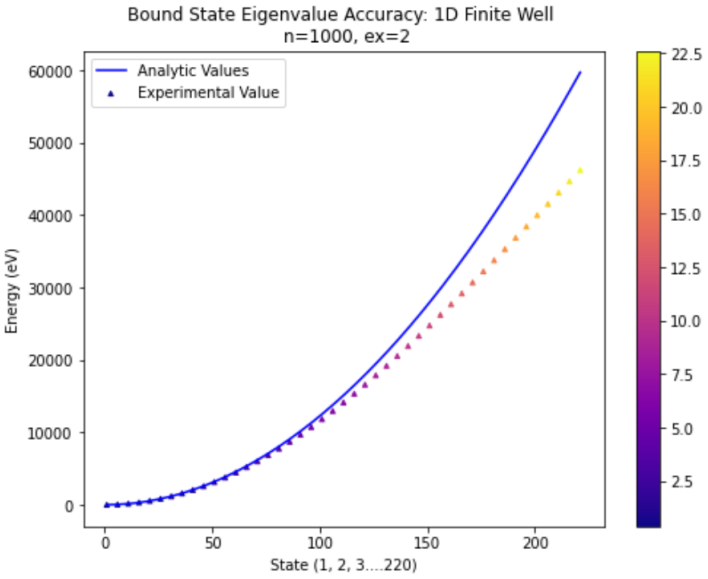

Figure 1: The graph above compares the analytical solutions of a very deep square well to computed energies. The color is representative of the percent error associated with each energy. The algorithms input parameters match those deployed on the website.

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6 Appendix

1. **Bisection Method For Hermitian Matrices:**
This eigenvalue problem includes a tridiagonal Matrix. As mentioned above this drastically increases the simplicity and speed of finding a solution. A brief description of how we leverage the Hamiltonian (H) is included below:

$$p(\lambda) = det(H - I\lambda) = \begin{vmatrix} \delta_1 - \lambda & \gamma_2 & 0 & \dots & 0 \\ \gamma_2 & \delta_2 - \lambda & \gamma_3 & & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \gamma_n \\ 0 & \dots & 0 & \gamma_n & \delta_n - \lambda \end{vmatrix}$$

$p_0(\lambda) = 1$
$p_1(\lambda) = \delta_1 - \lambda$
$p_2(\lambda) = (\delta_2 - \lambda)p_1(\lambda) - \gamma_2^2 p_0(\lambda)$
$p_n(\lambda) = (\delta_n - \lambda)p_{n-1}(\lambda) - \gamma_n^2 p_{n-2}(\lambda)$

This characteristic polynomial forms a Strum chain (article) where each p_n has one zero that corresponds to the eigenvalue λ_n. The zeroes can we determined with either newtons method ([[**92**]]) or bisection ([[**92**]]).

2. **Numerical Instability:**
Numerical instability causes the calculated solution to diverge quickly from the true solution. This "blowing up" effect towards $\pm\infty$ is often the cause of truncation errors and/or sensitive input parameters ([**20**]). While both integration and eigenvalue models suffer from some instability (fig 2). It appears to be much more evident in integration models ([**Nur04**]). This is no major surprise as integration algorithms like RK4 require either none zero initial x_i or $\psi'(x_i)$. State-dependent wave function exponential decay at the good boundaries makes reasonable guesses for these initial conditions very difficult. Ambiguity in the initial condition is only amplified by truncation errors that scale based on step size. To understand how these factors complement each other, imagine you want to play it safe with your initial conditions. You pick a point far away from the well because you know this will be close to zero. Unfortunately, as in all numerical integration problems, you are resolution constrained. The more careful you are with initial conditions the larger your step size and the greater the truncation error.

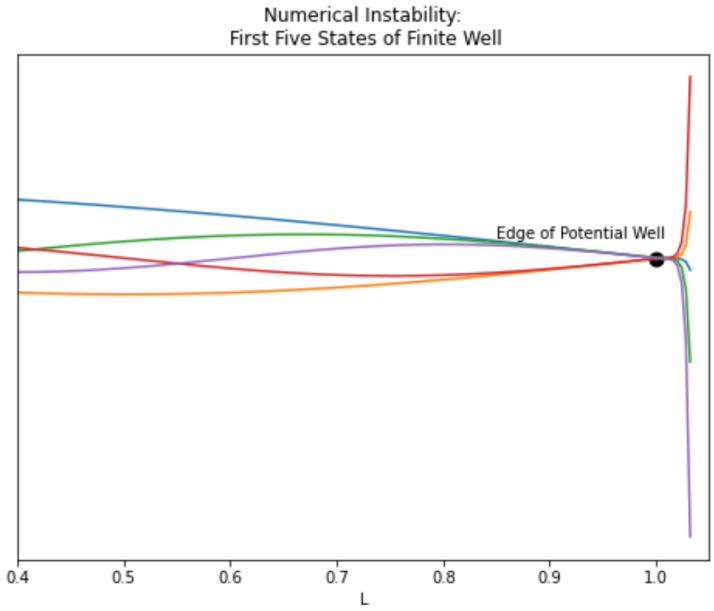

Figure 2: Displayed above are the first five wave functions in a finite well. The integration was done with RK4 using analytical energy values for the corresponding states. Normally with accurate energy state values, we would expect the wave functions to begin to converge at the edge of the well. Instead, the behavior is far more erratic Defying normalization conditions, the resulting waves "blow up".