Proceedings of the National Conference
On Undergraduate Research NCUR (2006)
University of North Carolina Asheville
Asheville, North Carolina
April 6-8, 2006

Numerical Analysis of the Inverse Trapezoidal Potential

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Abstract

Analysis of one-dimensional potential wells in quantum mechanics is a classic research area, and new methods and problems are still being developed. While all purely analytic solutions have long been discovered, many unexplored approaches exist, such as those discussed by Gilmore[1]. One interesting potential is the inverse trapezoidal potential. A well known limiting case of this potential, the finite square well, can be used to verify the behaviour of the system. The energy levels of this potential can be approximated by applying an eighth-order Runge-Kutta[2] algorithm to the Schrödinger equation over the whole range of slopes of the trapezoid. This algorithm is used to generate a large amount of data about the system. This data is then used to derive and confirm a model that approximates the bound state energies very accurately.
Keywords: Schrödinger Equation, Runge-Kutta, Finite Square Well

1. Introduction

One-dimensional potentials have provided a great deal of insight and understanding into quantum mechanics in the history of modern physics. Systems with analytic solutions are very useful for teaching[3], but most systems do not have elegant solutions. Transfer matrices[1] currently offer an interesting new approach to one-dimensional systems, but the results still depend on numerical analysis. The trapezoidal potential is simply constructed, but is not solvable analytically. However, in a well-understood special case, it reduces to a system that does have an analytical solution. This is the finite square well, which can be used to verify the results of the numerical analysis, and which also offers interesting theoretical information about the behaviour of particles in this potential.

2. Theory

The one-dimensional Schrödinger equation is a second-order linear differential equation. Numerical approaches are therefore more time-consuming, since algorithms such as Runge-Kutta are derived for use with first order systems. However, a basic technique can be used to apply these methods. By separating the Schrödinger equation into two first-order differential equations (1), the algorithms can be applied in two steps, and a numerical result can be obtained.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

$$\sqrt{\frac{2m}{\hbar^2}(V-E)}\psi = \frac{d\psi}{dx} \quad \sqrt{\frac{2m}{\hbar^2}(V-E)}\psi' = \frac{d\psi'}{dx} \tag{1}$$

The wavefunction in this case is ψ, and ψ' is the first space derivative. Initially, a fourth-order Runge-Kutta algorithm was used, but a desire for higher accuracy led to the adoption of Shanks's 1966 eighth-order coefficients[2]. In addition to breaking down the Schrödinger equation into two first order differential equations, several unit substitutions (2) were made in order to decrease calculation time and make the results easier to interpret.

$$\frac{2m}{\hbar^2}(V-E) = -k^2 = 1m^{-1} \tag{2}$$

Two commonly used units in quantum mechanics are the electron-volt and the electron mass. Both of these units are of an appropriate magnitude for this analysis. Choosing units of energy and mass defines the unit length of this system:

$$eV = 1.602177 \cdot 10^{-19} J \qquad\qquad m_e = 9.109383 \cdot 10^{-31} kg$$

$$\sqrt{\frac{\hbar^2}{2m(V-E)}} = \frac{1}{k} = 1.951919 \cdot 10^{-10} m \approx 2\mathring{A} \tag{3}$$

The unit of length for this analysis is approximately two Angstroms, the mass is that of the electron, and the unit of energy is the electron-volt. The actual values of the physical constants are not used in calculation, but can be easily replaced in the final results.

3. Constructing the Approximation

Given these simplifications, it becomes convenient to refer to a specific trapezoidal potential by its slope, s. After much experimentation, parameters for the well were chosen based on simplicity and the number of supported energy levels in the finite well case. The well was given the following dimensions, where V' is the potential outside the well, and l is the distance taken to reach this potential:

$$V(x) = \left\{ \begin{array}{ll} 0 & |x| < 2 \\ 20 & \frac{20}{s} + 2 < x \\ s(x-2) & 2 \leq x \leq \frac{20}{s} + 2 \end{array} \right\} \qquad s = \frac{V'}{l} \tag{4}$$

In order to find the energy levels of the above function while using the two step numerical approximation, a brute force method must be used, and some quantum mechanics theory must be employed in interpreting the results. For a given E, the wavefunction must evaluated at some point which represents a distance that is approximately infinitely far from the center of the well. (A distance of about thirty Angstroms was used, which was a sufficient substitute for infinity in these calculations. By tracing the evolution of the energy states from the larger slopes, it was possible to trace individual bound states even at very small slopes. Furthermore, most of the analysis occurs where s tends to infinity, so this was never an issue in analysis). Starting at $E = 0$, E is evaluated at the approximate infinity and then increased by a fixed amount each iteration. This yields the expectation values at infinity of a large range of energies. Any energy that has a nonzero expectation value at infinity is not normalizable, and is therefore not a possible solution. The energies that did return normalizable energies at infinity did correspond to physically possible energy states. This fact is corroborated by examining the evolution of the energy states in the finite square well as the sides of the well fall.

Evaluating the wavefunctions at infinity for a given E has two parts. In order to find the wavefunction at a given distance, it must start at the center of the well and move incrementally away. The size of the increment is the step size of the numerical method. Since this a second order differential equation, information about ψ and its first derivative at zero are necessary in order to solve it numerically. This information is different for odd and even energy states (5), so the evaluation must be done twice. For even states, ψ is one and the derivative is zero. For odd states, ψ is zero and the derivative is one[5].

$$\begin{bmatrix} \psi(0) = 1 \\ \psi'(0) = 0 \end{bmatrix} Even \qquad \begin{bmatrix} \psi(0) = 0 \\ \psi'(0) = 1 \end{bmatrix} Odd \tag{5}$$

By incrementally increasing both E and x, the wavefunctions of many energies can be computed at an approximately infinite distance.

This configuration will return the value of the wavefunction at infinity for either parity for a specific input energy. By specifying a large enough range of energies and initial conditions, the normalizable and therefore possible energy states can be identified[6].

3.1 numerical results

After writing and revising the code, all of the analysis was done in Java, and Maple was used to check some results. An eighth-order Runge-Kutta algorithm derived by Shanks[2] was used. Maple has a Dverk[4] seventh-eighth order algorithm built-in, and that was used to check specific or limiting results. Dverk is a modified Runge-Kutta algorithm that was developed as a general differential equation solver for use in computer software. On a 2.4 Ghz 256 MB RAM computer, using the Maple algorithm over the wide range of energies was considerably more time consuming than running the specialized Java code, and therefore there are not redundant sets of data for every s. However, the level of agreement between the two programs was high enough for the all of results checked (around three decimal places) that achieving complete redundancy was unnecessary. Near the end of the project, a second set of data was taken, this time accurate to five decimal places instead of two, which matched up exactly with the original data for the shared points.

If the physical constants are reassigned to the resulting data, it is possible to examine the properties of the system in detail. The height of the potential well is 20 eV, and the width in the case of the finite square well is 7.80767 $\mathring{A}$. The six energy values for this finite square well are approximately 0.50 eV, 1.99 eV, 4.45 eV, 7.86 eV, 12.12 eV, and 17.02 eV. Other slope values start with the same base width, but have an increasing width as the energy increases, and changing energy spectra as the slope changes. As the well tends toward $V = 0$ everywhere, all the energy states decrease more quickly towards zero, as expected.

4. Analysis

As intended by the choice of well dimensions, there were six bound states in the special case of the finite square well. Analysis of the evolution of these six states as the well approaches the free particle state comprises the majority of the data analysis. Initially, the energy data was interpreted as functions of two different variables, s and θ. After some preliminary examination, it was apparent that the functions offered different perspectives on the behaviour of the well.

The first set of data taken was the evolution of the energy levels as a function of θ, in five degree increments. As the graph of this data demonstrates (see Figure 1), there are inflection points near the middle of each series. This means that the energy levels experience the slowest rate of increase when the well is far from both the limiting cases. Since no explicit function exists for this data, numerical techniques are necessary to analyze it. The method of using a difference operator[7] was used to take the second space derivatives of each series, in order to approximate the value of each inflection point. The author's guess that the inflection points were not all at 45^o proved to be correct, as only the ground state has an inflection point here. As the energy level rises, the location of the inflection point moves closer to zero. In terms of the behaviour of the well, this means that the higher energy states increase faster than the lower ones, making room for them to evolve simultaneously. This data was interesting, but difficult to analyze due to the steep curve at $\theta = 90$.

The graph of the energy levels as a function of s became more important for understanding the long term behaviour of the well. The data for this variable is very smooth, which makes it easier to apply numerical techniques. The difference operator method was again used here to approximate numerical derivatives of the data functions. As s approaches zero, the energy levels all drop to zero very quickly. However, as s increases to infinity, the evolution slows down, and the bound state energies approach the corresponding finite square well energies (see Figure 2). This is a very strong confirmation of the accuracy of the data.

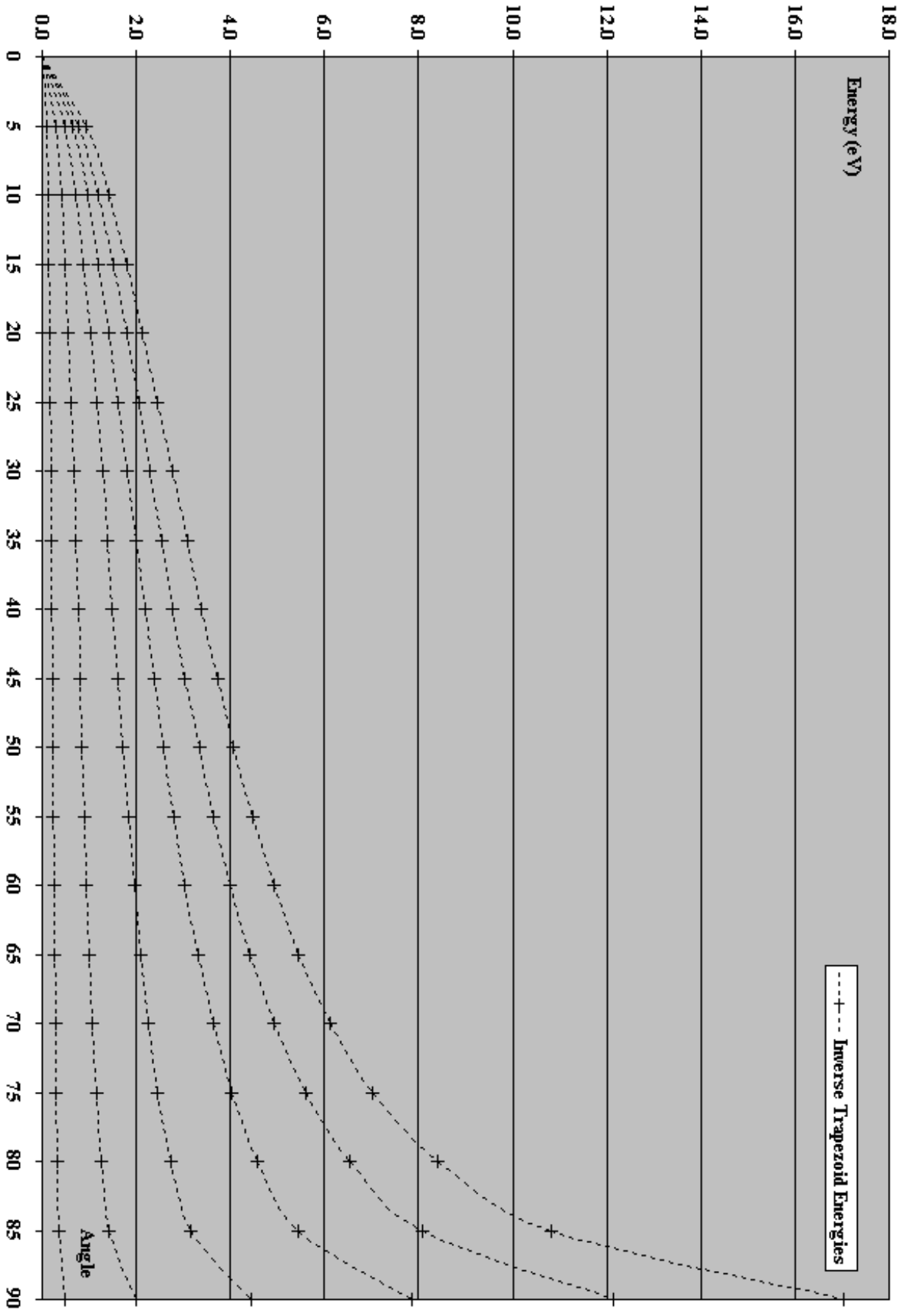

Figure 1: Evolution of the bound state energies as a function of angle.

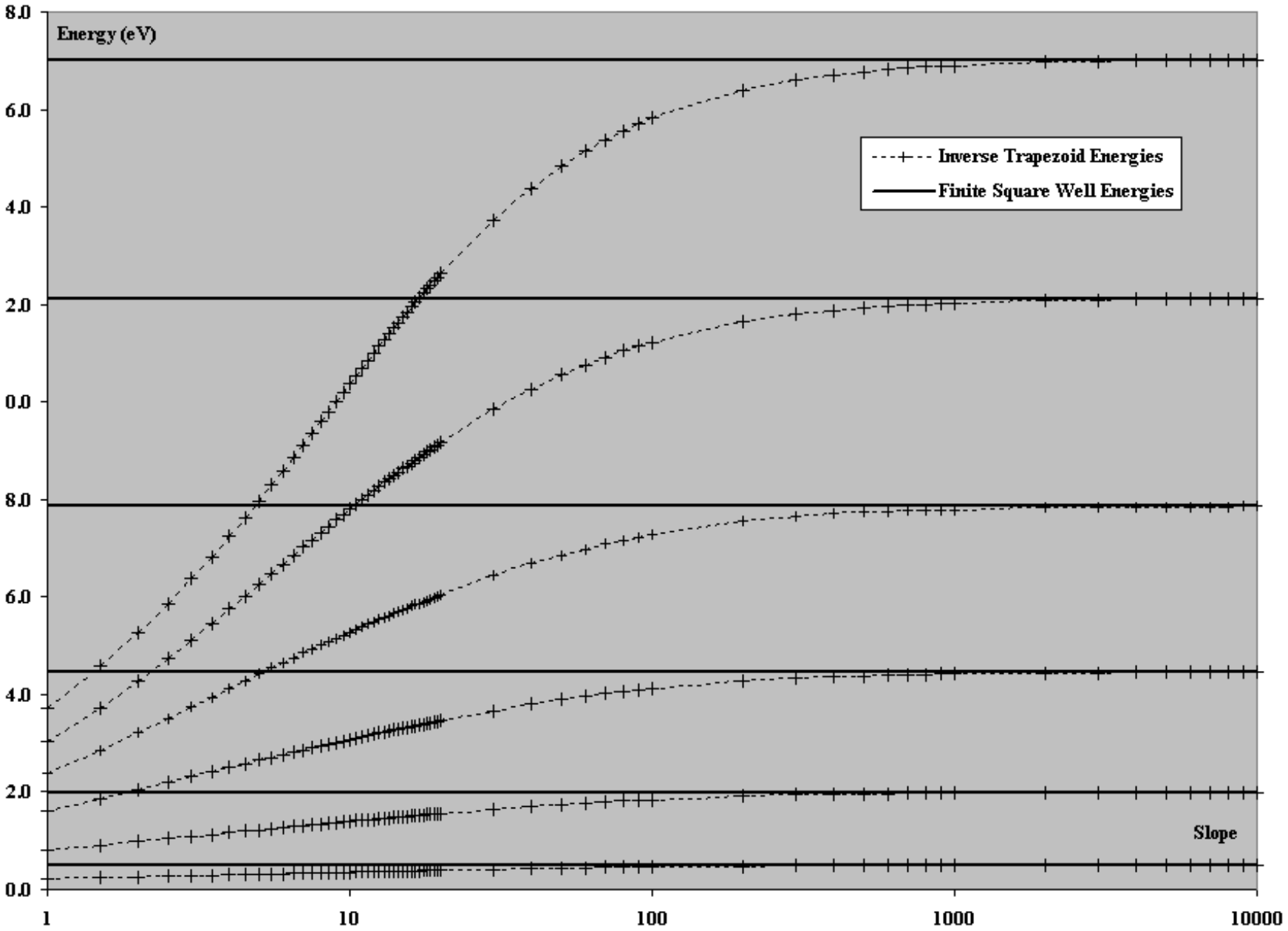

Figure 2: Evolution of the bound state energies as a function of slope, plotted logarithmically.

The slow evolution of the energy states combined with the strict asymptotic behaviour made this system initially difficult to model for all slopes. However, imposing boundary conditions on these functions, and determining some additional properties through differential analysis allowed an accurate model to be derived. The boundary conditions are as follows:

$$E_n(0) = 0 \qquad\qquad E_n(\infty) = F_n \tag{6}$$

Here, E_n is the energy of the nth bound state in a trapezoid of slope s. F_n is the energy of the nth bound state in a finite square well with the same dimensions. In between the two extremes of $s = 0$ and $s = \infty$ lie the data produced by the numerical techniques.

After much experimentation, a method was developed to model this data accurately using differential equations and numerical derivatives. Taking numerical derivatives in this case involves the simple difference operator mentioned above. Dividing the original function E_n by its numerical derivative E_n' produces a third function, f, that is very accurately modeled by a quadratic (7). This approximation is supported by the analysis of f', which is in fact linear. Both functions have roots at $s = 0$, which makes the differential analysis much simpler.

$$\frac{d}{ds}f(s) = 2\alpha s \qquad\qquad f(s) = \alpha s^2 \tag{7}$$

The term $2\alpha s$ is used here to make the final result easier to interpret. Since the relationship of E_n to E_n' is defined, it is possible to begin solving the differential equation for E_n:

$$\frac{E_n(s)}{E_n'(s)} = \alpha s^2 \qquad\qquad \frac{1}{E}\frac{dE}{ds} = \frac{1}{\alpha s^2}$$

After integrating the left side to obtain the natural log of E_n, the right side can be integrated to obtain a function of s:

$$\int \frac{dE}{E} = \int \frac{ds}{\alpha s^2} \qquad\qquad ln(E) = -\frac{1}{\alpha s}$$

Then, raising e to the power of the right side and multiplying by a constant yields the energies of the bound states as a function of slope:

$$E_n(s) = F_n e^{-\frac{1}{\alpha s}} \tag{8}$$

The constant in front is just the nth bound state of the finite square well of matching dimensions. This function describes the evolution of the nth bound state as the slope of the trapezoid changes. As expected, it satisfies the initial boundary conditions as well as the intermediate differential equations:

$$E_n(0) = F_n e^{-\infty} = 0 \qquad\qquad E_n(\infty) = F_n e^{-0} = F_n$$

$$\frac{E_n(s)}{E_n'(s)} = \frac{F_n e^{-\frac{1}{\alpha s}} \cdot \alpha s^2}{F_n e^{-\frac{1}{\alpha s}}} = \alpha s^2$$

The accuracy of this approximation can be judged by examining Figure 3. The units of slope are given here:

$$5.12316 \cdot 10^9 \frac{eV}{m}$$

The quantity alpha varies as a function of s and of n, and also likely depends on the well dimensions. The formulation of this value from these initial parameters has not yet been discovered:

$$\alpha = \alpha(s, n, V', s) \tag{9}$$

The α used to model the data is a constant, and was chosen to optimize the least-squares value of the approximation, which is 0.31. For Figure 3,

$$\alpha \approx 0.13$$

5. Conclusion

The behaviour of the inverse trapezoidal potential can be understood using numerical analysis. By simplifying the problem, applying the Runge-Kutta technique, and utilizing Java to carry out the detailed calculations, it is possible to obtain numerical results for a problem that cannot be solved analytically. Additionally, this particular potential has limiting cases that verify the results, and also provide a theoretical framework in which to make sense of the data. The approximating function is sufficiently accurate, especially given the simplicity of the derivation. This function should apply to all trapezoids of a similar construction. However, the function that determines α remains unexplained. Through further analysis of trapezoidal wells, it may be possible to express α in terms of the initial parameters.

6. Acknowledgements

The author wishes to express his sincere thanks to Dr. Michael Ruiz for his valuable guidance.

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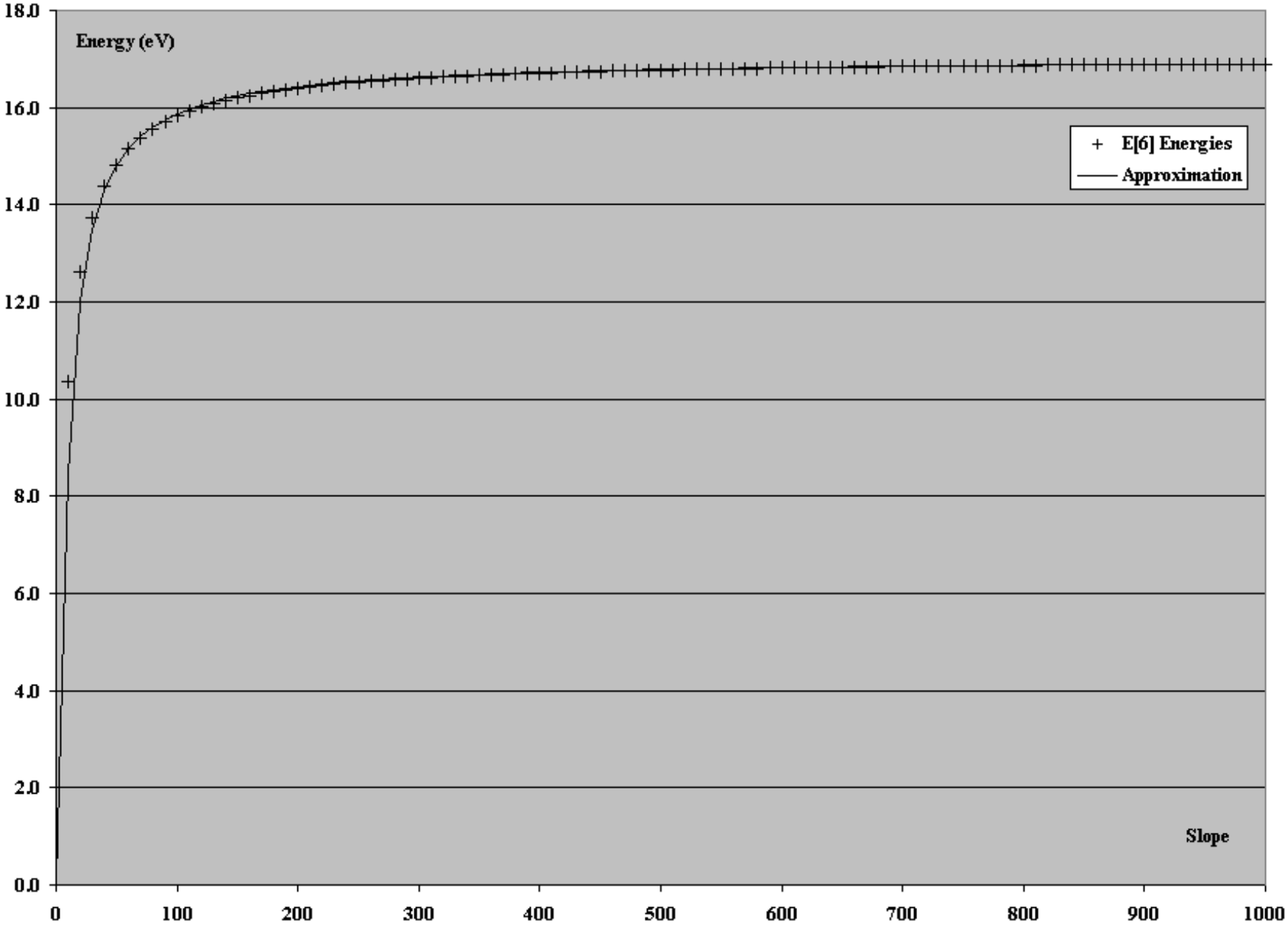

Figure 3: Approximating function plotted with true data points.