

# Solving Time Independent Schrödinger Equation with Airy's Function and Numerov Method

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## I. INTRODUCTION

With Newton's three laws of motion, we can relate quantities such as position, momentum and potential of a particle to understand its behavior. However, laws of Newtonian mechanics break down at the microscopic level, as suggested by many experimental phenomena in the past century: for example, black-body radiation, quantum tunneling, and photo-electric effect. Quantum mechanics offers an alternative model that accounts for these experimental findings. In quantum mechanics, particles are described by their wave equations, which are normalized solutions to the Schrödinger Equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi. \quad (1)$$

Here,  $\Psi$  is wave equation,  $\hbar$  is the reduced Planck's constant,  $m$  is the mass of the particle, and  $V(x,t)$  is the potential function of the particle.

Therefore, to study the behavior of a particle in certain potential field, it is very important to solve the Schrödinger equation. In particular, this project will focus on the solutions to equation (1) when  $V$  is time-invariant.

In this case, we can assume that the solution is separable. Suppose that  $\Psi(x,t) = \psi(x)\phi(t)$ . Then equation (1) can be rewritten as:

$$i\hbar \frac{1}{\phi} \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{\partial^2 \psi}{\partial x^2} + V. \quad (2)$$

We set equation (2) equal to a separation constant  $E$ ,<sup>1</sup> we can solve for  $\phi$  with the left hand side (LHS) of the equation:

$$\phi(t) = Ce^{-i\frac{E}{\hbar}t},$$

and the right hand side (RHS) of (2) turns into:

$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \right) \psi = E\psi. \quad (3)$$

Equation (3) is commonly known as the Time-Independent Schrödinger Equation (TISE). The operator in the LHS,  $-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V$ , is called the Hamiltonian operator. [1]

The first part of this project will focus on solving the TISE with a linear potential, analytically, by means of Airy functions, and numerically, via Numerov Method. We will compare the energy eigenvalues and the results of both methods. The Airy functions are then used to approximate solutions to the TISE with a more complicated potential well,

<sup>1</sup>In physics, the value of  $E$  is the energy of particle described by the wave function that solves this equation. For this reason,  $E$  is often called the energy eigenvalue.

by solving the TISE on a piece-wise linear function. Finally, results of this process will be compared to the Numerov Method.

## II. AIRY FUNCTIONS

Airy Function, named after the British astronomer and physicist George Biddell Airy, refers to solutions to the partial differential equation (PDE) of the following form:

$$\frac{d^2y}{dx^2} - xy = 0. \quad (4)$$

The two independent Airy functions take forms of:

$$\text{Ai}(x) = \frac{1}{\pi} \int_0^{\infty} \cos\left(xt + \frac{t^3}{3}\right) dt$$

$$\text{Bi}(x) = \frac{1}{\pi} \int_0^{\infty} e^{xt - \frac{t^3}{3}} + \sin\left(xt + \frac{t^3}{3}\right) dt.$$

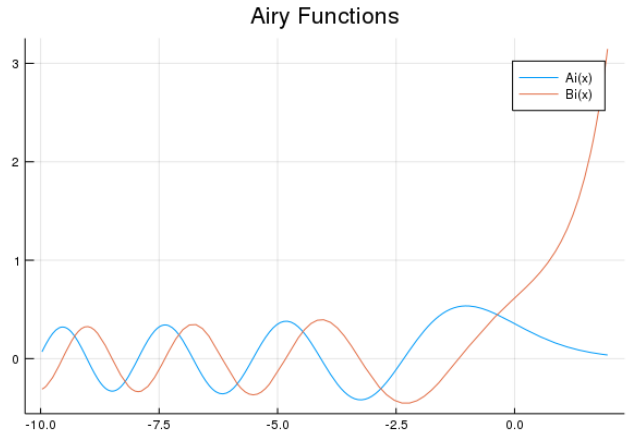


Fig. 1. Graph of Airy Functions

The package SpecialFuntions.jl includes the Airy Functions, which makes it easy to work with on Julia. Figure 1 is a graph of the Airy Functions using Julia

One important property of the Airy Functions is that at  $x = 0$ , character of the Airy functions changes from oscillatory to exponential.  $\text{Ai}(x)$  vanishes to 0 at infinity whereas  $\text{Bi}(x)$  is unbounded.

The Airy equations appear quite frequently in quantum mechanics. Imagine that a particle with charge  $q$  and mass  $m$  is placed in a constant electric field  $\mathcal{E}$ , and suppose there is an infinite potential barrier at  $x = 0$ . Expressed

mathematically, when we have a time-invariant potential well:

$$\begin{cases} V(x) = \infty & x < 0 \\ V(x) = q\mathcal{E}x & x \geq 0. \end{cases}$$

Which, for  $x > 0$ , gives the TISE:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + (q\mathcal{E}x - E)\psi = 0. \quad (5)$$

We can see that equation (5) is very similar to the Airy equation (4). In fact, it is not difficult to see that, with the following changes of variables:

$$\begin{aligned} \xi &= \tilde{x} - \tilde{E} \\ \tilde{x} &= \left(\frac{2mq\mathcal{E}}{\hbar^2}\right)^{\frac{1}{3}}x \\ \tilde{E} &= \left(\frac{2m}{q^2\mathcal{E}^2\hbar^2}\right)^{\frac{1}{3}}E, \end{aligned}$$

one can rewrite equation (3) as:

$$\frac{d^2\Psi}{d\xi^2} - \xi\Psi = 0.$$

The solutions to this equation is precisely the Airy functions:

$$\Psi = C_1 \text{Ai}(\xi) + C_2 \text{Bi}(\xi).$$

Since we require a physical wave function to be normalizable, it must be true  $C_2 = 0$ . Therefore:

$$\Psi(x, t) = \sum_n C_n \text{Ai}\left(\left(\frac{2mq\mathcal{E}}{\hbar^2}\right)^{\frac{1}{3}}\left(x - \frac{E}{q\mathcal{E}}\right)\right) e^{-i\frac{E_n}{\hbar}t}.$$

Because of the infinite potential barrier, we restrict  $\Psi(x, t) = 0$  for all  $x \leq 0$  to find each normal mode:

$$E_n = -\left(\frac{q^2\mathcal{E}^2\hbar^2}{2m}\right)^{\frac{1}{3}}a_n,$$

where  $a_n$  is the  $n^{\text{th}}$  zero of  $\text{Ai}(x)$ . To keep computation simple, we shall assume that all physical constants  $q = \mathcal{E} = m = \hbar = 1$ . Thus:

$$E_n = -2^{-1/3}a_n$$

### III. NUMERICAL SOLUTION

#### A. Numerov Method

For a second order PDE, in the absence of first order terms, (as in equation (3)) the Numerov method can be applied to find the numerical solution. The Numerov Method is a frequently used integration scheme for PDEs of the form:

$$\Psi'' = f(x)\Psi. \quad (6)$$

If we denote:  $x_i = i\Delta x$ ,  $\Psi_i := \Psi(x_i)$  and  $f_i := f(x_i)$ ; the Numerov method gives the following formula[2]:

$$\Psi_{i+1} = \frac{\Psi_{i-1}(12 - \Delta x^2 f_{i-1}) - 2\Psi_i(5\Delta x^2 f_i + 12)}{\Delta x^2 f_{i+1} - 12} + \mathcal{O}(\Delta x^6). \quad (7)$$

In this case, as shown in equation (5),  $f_i = 2(V_i - E)$ . To see this, we can begin by applying

$$1 + \frac{\Delta x^2}{12} \frac{d^2}{dx^2}$$

to equation (6). This gives that

$$\Psi'' + \frac{\Delta x^2}{12} \Psi^{(4)} = f\Psi + \frac{\Delta x^2}{12} \frac{d^2}{dx^2}(f\Psi). \quad (8)$$

We may wish to rewrite  $\Psi''$  to get rid of  $\Psi^{(4)}$  on the LHS. Considering the Taylor expansion of  $\Psi$  around  $x_i$ , we see that:

$$\begin{aligned} \Psi_{i+1} &= \Psi_i + \Delta x \Psi'_i + \frac{\Delta x^2 \Psi''_i}{2} + \frac{\Delta x^3 \Psi'''_i}{6} + \frac{\Delta x^4 \Psi^{(4)}_i}{24} + \dots \\ \Psi_{i-1} &= \Psi_i - \Delta x \Psi'_i + \frac{\Delta x^2 \Psi''_i}{2} - \frac{\Delta x^3 \Psi'''_i}{6} + \frac{\Delta x^4 \Psi^{(4)}_i}{24} + \dots \end{aligned}$$

Summing these two equations, we have:

$$\Psi_{i+1} + \Psi_{i-1} = 2\Psi_i + \Delta x^2 \Psi''_i + 2\frac{\Delta x^4 \Psi^{(4)}_i}{12} + \mathcal{O}(\Delta x^6).$$

Rearranging, it follows that  $\Psi''_i$  can be rewritten as:

$$\Psi''_i = \frac{\Psi_{i+1} - 2\Psi_i + \Psi_{i-1}}{\Delta x^2} - \frac{\Delta x^4 \Psi^{(4)}_i}{12} + \mathcal{O}(\Delta x^6). \quad (9)$$

To find  $\frac{d^2}{dx^2}(f\Psi)$  on the RHS, we let  $g(x) := f(x)\Psi(x)$ . Recall, using Euler's method, we have that:

$$\begin{aligned} g''_i &= \frac{g_{i+1} - 2g_i + g_{i-1}}{\Delta x^2} + \mathcal{O}(\Delta x^4) \\ \implies \frac{d^2}{dx^2}(f\Psi) &= \frac{f_{i+1}\Psi_{i+1} - 2f_i\Psi_i + f_{i-1}\Psi_{i-1}}{\Delta x^2} + \mathcal{O}(\Delta x^4) \end{aligned} \quad (10)$$

Now, substitute the expression for  $\Psi''$  from equation (9) into the LHS of (8), and substitute the expression for  $\frac{d^2}{dx^2}(f\Psi)$  in (10) into the RHS of (8), giving us:

$$\begin{aligned} &\frac{\Psi_{i+1} - 2\Psi_i + \Psi_{i-1}}{\Delta x^2} \\ &= f_i\Psi_i + \frac{f_{i+1}\Psi_{i+1} - 2f_i\Psi_i + f_{i-1}\Psi_{i-1}}{12} + \mathcal{O}(\Delta x^6) \\ &= \frac{f_{i+1}\Psi_{i+1} + 10f_i\Psi_i + f_{i-1}\Psi_{i-1}}{12} + \mathcal{O}(\Delta x^6). \end{aligned} \quad (11)$$

The integration scheme given by equation (7) comes from rearranging the above equation.[3]

#### B. Matrix Numerov Discretization

Naively, we can take  $\Psi_0 = 0$  and  $\Psi_1$  to be a sufficiently small number (or 0) to carry out the numerical scheme, similar to the Up-winding scheme. However, a problem emerges as one tries to apply it: not all choices of  $E$  yield an accurate numerical solution. We must realize that solutions to the TISE are eigenfunctions of the Hamiltonian operator, which are normal modes of the full solution; therefore, before we can implement this method, we first need to numerically solve for the energy eigenstates. There are many methods serving this purpose. We can take advantage of the

Numerov method to discretize the Hamiltonian operator to find the eigenvalues in question. This is known as the Matrix Numerov method.

Since  $\Psi$  converges to 0, for all positive  $\varepsilon$ , there exist a  $N$  sufficiently large such that  $|\Psi_M| < \varepsilon$  for all  $M \geq N$ . Therefore, on the interval  $[0, N\Delta x]$ , if we choose an appropriately small  $\varepsilon$ , we have, approximately, the Dirichlet Boundary condition  $\Psi_0 = \Psi_{N+1} = 0$ .

Then based on equation (11), we can rewrite (5) as:

$$\begin{aligned} & -\frac{1}{2} \left( \frac{\Psi_{i-1} - 2\Psi_i + \Psi_{i+1}}{\Delta x^2} \right) \\ & + \frac{V_{i-1}\Psi_{i-1} + 10V_i\Psi_i + V_{i+1}\Psi_{i+1}}{12} \\ & = E \frac{\Psi_{i-1} + 10\Psi_i + \Psi_{i+1}}{12}. \end{aligned}$$

Define  $\tilde{\Psi}$  to be the column vector  $\tilde{\Psi} = [\Psi_1, \Psi_2, \dots, \Psi_N]^T$ ;  $\tilde{V}$  to be the diagonal matrix  $\tilde{V} = \text{diag}\{V_1, V_2, \dots, V_N\} = q\mathcal{E}\text{diag}\{\Delta x, 2\Delta x, \dots, N\Delta x\}$ ;  $A$  and  $B$  to be the matrices:

$$\begin{aligned} A &= \frac{1}{\Delta x^2} \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & & \ddots & \ddots & \\ & & & 1 & -2 \\ & & & & 1 & -2 \end{bmatrix} \\ B &= \frac{1}{12} \begin{bmatrix} 10 & 1 & & & \\ 1 & 10 & 1 & & \\ & & \ddots & \ddots & \\ & & & 1 & 10 \end{bmatrix}. \\ \left(-\frac{1}{2}B^{-1}A + X\right)\tilde{\Psi} &= E\tilde{\Psi}. \end{aligned} \quad (12)$$

To determine  $N$  and  $\Delta x$ , we consider the physical meaning of these quantities.  $E$ , an eigenvalue of the Hamiltonian operator, is the energy of the energy eigenstate the solution represents. It is associated with de Broglie wavelength of  $\lambda_b = \frac{h}{p} = \frac{h}{\sqrt{2mE_n}}$ , where  $h$  is Planck's constant and  $p$  is the momentum. Suppose that we want to find the first  $m$  energy eigenstates, then our choice of  $\Delta x$  has to be comparable to its minimum de Broglie wavelength, which is given by  $\lambda_{min} = \frac{h}{\sqrt{2mE_m}}$ . To keep the units consistent, we will choose  $\Delta x = \frac{\lambda_{min}}{2\pi}$ . We can find  $N$  by restricting  $\Psi_N$  to be small. Notice, when  $\tilde{x} > \tilde{E}_m$ ,  $\Psi$  decays exponentially; hence, we can choose the end of our range to be  $\lambda$  greater than where the potential is equivalent to the energy.

Once we obtain the discrete representation of the Hamiltonian operator, we can easily find its eigenvalues using eigvals. (Notice the Hamiltonian operator is positive definite and symmetric.) Choosing the maximum desired energy state to be  $E_m = 30$ , the eigenvalue problem takes about 0.06 seconds, and the result is recorded in table 1 (I), where it is also compared with the actual values given by Airy Functions. The code in Julia can be found in appendix VI-A.

<sup>2</sup>The factor of  $2\pi$  comes from the fact that  $h = 2\pi\hbar = 2\pi$ , assuming  $\hbar = 1$

After we solve the eigenvalue problem, each corresponding eigenvector is a discretized solution to the TISE. Alternatively, if we had implemented other methods to find the eigenvalues, we can proceed to use equation (6) to integrate the TISE without having to find the eigenvectors. We can use  $\Psi_0 = 0$ ,  $\Psi_1 = 0.001$ ,  $f_i = \frac{2m}{\hbar^2}(V_i - E) = 2(x - 21.4129)$  and  $\Delta x = 0.1291$ ,  $n = 238$  (These quantities are determined using the process mentioned above).

### C. Results

TABLE I  
ENERGY EIGENVALUES: MATRIX NUMEROV METHOD (MNM)

Energy State	1	2	5	10	30
MNM (e)	1.8558	3.2446	6.3051	10.1815	21.4129
Actual (an)	1.8858	3.2446	6.3053	10.1822	21.4196
Difference (d)	0.0000	0.0000	0.0002	0.0007	0.0067

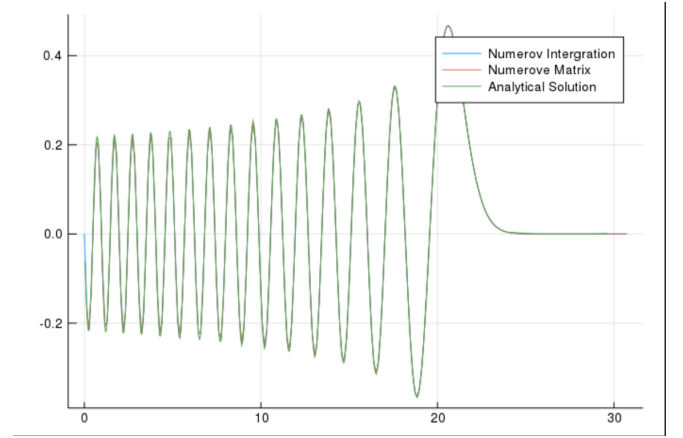


Fig. 2. Graph Numerical Solutions with Numerov Method

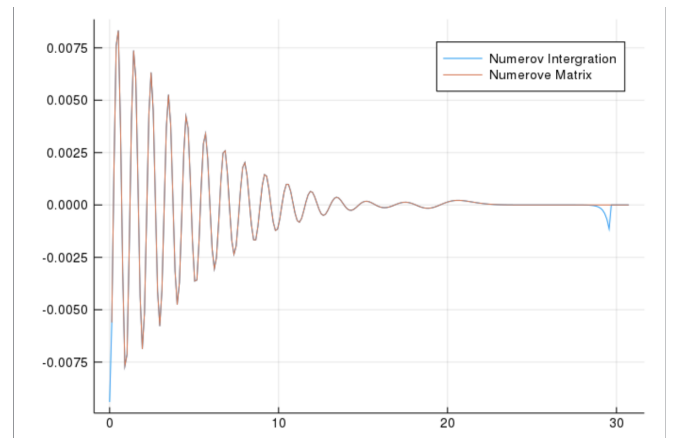


Fig. 3. Difference between the NM and analytic solution

Table I shows the comparison between the energy eigenvalues obtained with Numerov method and actual values. Figure 2 is the plot of numerical solution and the analytic error, and figure 3 is the graph of the numerical solution's error.

As shown, for lower energy levels, the discretization of the TISE with Numerov method is a simple yet quite accurate. For especially lower energy states, eigenvalues obtained are precise with at least five significant digit, and for higher energy states such as  $E_{30}$ , the error in the numerical solution is within 0.01.

In the following section, the Numerov Method solution will be used to verify the accuracy of numerical solutions to TISEs without an analytic solution.

#### IV. THE AIRY FUNCTION METHOD

The model mentioned in section 1 is one of very few cases where an analytic solution could be found. Most real life particles are messy, and they're subjected to multiple forms of potentials such as the strong force and the gravitational force. Rarely do we have a simple linear potential well. However, the fact that Airy Functions solve the TISE with linear potentials can be exploited to approximate the TISE with more complicated potential functions. For the rest of this project, the focus will move to solving the TISE with more complicated potentials using the Airy Functions, and results are verified using the Numerov Method.

##### A. Formulation

Suppose we have a continuous function  $V(x)$  and we wish to solve the TISE on the interval  $[a, b]$ . We can choose the partition  $P = \{x_0 = a, x_1, \dots, x_N = b\}$  and define  $g$ :

$$g(x) = \frac{x - x_{i-1}}{x_i - x_{i-1}} V(x_i) + \frac{x_i - x}{x_i - x_{i-1}} V(x_{i-1}),$$

for  $x \in [x_{i-1}, x_i]$ . Suppose  $\Delta x = x_{i+1} - x_i$  for all  $i$ . (Figure 4 shows an example of  $g$ ) It can be shown that  $g$  is continuous,  $g(x_i) = V(x_i)$  for  $x_i \in P$  and for all  $\varepsilon > 0$ ,  $\exists P$  s.t.  $\int_a^b |g - V| dx < \varepsilon$ . This follows from the fact that for  $x \in [x_i, x_{i+1}]$

$$\inf f(x) \leq g(x) \leq \sup f(x),$$

and (by continuity)

$$\lim_{x_{i+1} - x_i \rightarrow 0} \sup f(x) - \inf f(x) = 0$$

$$\implies |f(x) - g(x)| \leq \sup f(x) - \inf f(x) \leq \frac{\varepsilon}{N(b-a)}$$

for some choice of  $\Delta x$ .

It follows that  $g$  can be an arbitrarily good approximation for any continuous functions, and for each interval in the partition, we see that  $g$  is linear. With appropriate restrictions, the TISE is solvable with the change of variables defined in section 1.

Thus, we limit the potential to be strictly increasing for  $x \geq 0$ , and infinite for  $x < 0$ . Suppose the solutions for the TISE on the interval  $[x_i, x_{i+1}]$  is  $\Psi_i$ , then we have

$$\Psi_i = A_i \text{Ai}(\xi_i(x)) + B_i \text{Bi}(\xi_i(x))$$

where

$$\xi_i(x) = \left( \frac{V_i x_{i+1} - V_{i+1} x_i}{x_{i+1} - x_i} + \frac{V_{i+1} - V_i}{x_{i+1} - x_i} x - E \right) \left( \frac{V_{i+1} - V_i}{x_{i+1} - x_i} \right)^{-\frac{2}{3}}$$

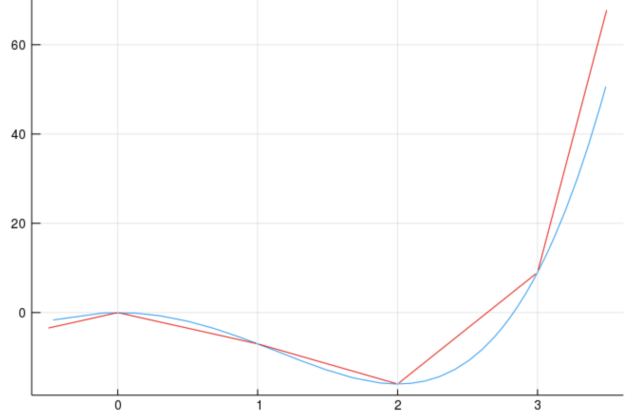


Fig. 4.  $g(x)$  and  $V(x) = x^4 - 8x^2$ ,  $\Delta x = 1$

and  $A_i, B_i$  are constants that can be solved for by imposing the boundary conditions  $\Psi_i(x_{i+1}^-) = \Psi_{i+1}(x_{i+1}^+)$  and  $\Psi'_i(x_{i+1}^-) = \Psi'_{i+1}(x_{i+1}^+)$ . We also know that for the equation to be normalizable,  $B_N = 0$ . Once we have these, we can express the solution as a piece-wise defined function:

$$\Psi = \Psi_i, (x \in [x_i, x_{i+1}))$$

Again, the first difficulty in implementing this method comes from finding the eigenvalues  $E$ . Unlike the the constant electric field potential, we can't find  $E$  by restricting it's value at 0 and  $\infty$ , since each  $\Psi_i$  lives only in the interval  $[x_i, x_{i+1})$ . However, the Matrix Numerov method from part 1 still holds.

To get the coefficients we would need to solve the system of equations given by the boundary conditions, given that  $B_N = 0$ .

$$A_{n-1} a_{n-1}^n + B_{n-1} b_{n-1}^n = A_n a_n^n$$

$$A_{n-1} \delta a_{n-1}^n + B_{n-1} \delta b_{n-1}^n = A_n \delta a_n^n$$

Where  $\text{Ai}_m^n = \text{Ai}(\xi_m(x_n))$ ,  $b_m^n = \text{Bi}(\xi_m(x_n))$ , and  $\delta \text{Ai}_m^n = \text{Ai}(\xi_m(x_n)) \frac{d\xi_m(x)}{dx} \Big|_{x=x_n}$ ,  $\delta b_m^n = \text{Bi}(\xi_m(x_n)) \frac{d\xi_m(x)}{dx} \Big|_{x=x_n}$ . Starting from the back, we can rewrite  $A_{n-1}$  and  $B_{n-1}$  in terms of  $A_n$ :

$$A_{n-1} = A_n \frac{a_n^n - \delta a_n^n \frac{b_{n-1}^n}{\delta b_{n-1}^n}}{a_{n-1}^n - \delta a_{n-1}^n \frac{b_{n-1}^n}{\delta b_{n-1}^n}}$$

$$B_{n-1} = A_n \frac{a_n^n - \delta a_n^n \frac{a_{n-1}^n}{\delta a_{n-1}^n}}{b_{n-1}^n - \delta b_{n-1}^n \frac{a_{n-1}^n}{\delta a_{n-1}^n}}$$

Then assume we know  $A_i$  and  $B_i$ ,

$$A_{i-1} = A_n \frac{c - \delta c \frac{b_{i-1}^i}{\delta b_{i-1}^i}}{a_{i-1}^i - \delta a_{i-1}^i \frac{b_{i-1}^i}{\delta b_{i-1}^i}}$$

$$B_{i-1} = A_n \frac{c - \delta c \frac{a_{i-1}^i}{\delta a_{i-1}^i}}{b_{i-1}^i - \delta b_{i-1}^i \frac{a_{i-1}^i}{\delta a_{i-1}^i}}$$

where

$$c = A_i a_i^j + B_i b_i^j$$

$$\delta c = A_i \delta a_i^j + B_i \delta b_i^j$$

After this process is complete, we rewrote all the coefficients in terms of  $A_n$ . Finally, the magnitude of  $A_n$  can be determined with normalization.

### B. Results

To test the validity of this method, we will use  $V(x) = q\mathcal{E}x = x$  to see if it yield the same result.

When we set  $V(x) = x$ ,  $g(x) = V(x) = x$ . Therefore, we

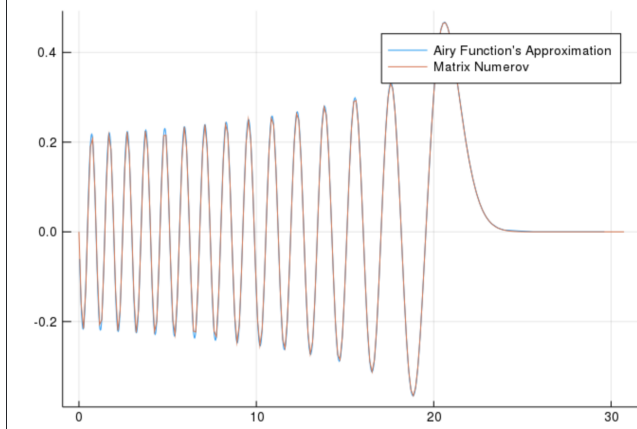


Fig. 5. Solution using Airy's approximation for  $V(x) = q\mathcal{E}x$

should expect to get the same result as the analytic solution in section 1 using the Airy functions approximation. The result is graphed in figure 5. Numerical result obtained using Matrix Numerov method, which is shown to be very close to the actual solution, is also graphed for comparison.

Then, we can take this method and apply it to a more complicated potential well:  $V(x) = 0.6x^{1.3} + \sqrt{x}$ . Using the same energy state, we obtain the following result:

The solution for  $V(x) = 0.6x^{1.3} + \sqrt{x}$  is graphed in figure

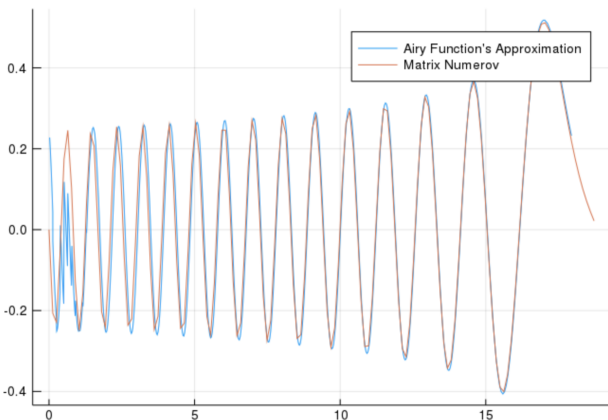


Fig. 6. Airy's approximation for  $V(x) = 0.6x^{1.3} + \sqrt{x}$

6, and figure 7 shows the relative error. As we see, the behavior of the approximation is very coarse for  $0 < x < 1$ ,

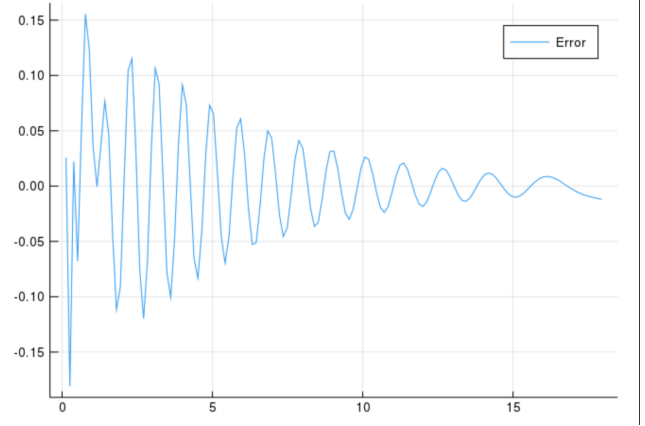


Fig. 7. Errors for  $V(x) = 0.6x^{1.3} + \sqrt{x}$

and the period of the approximation is slightly off. The error seems very large due to the mis-matching period. Overall, this method gives a reasonable estimation. The Julia code for this process can be found in appendix VI-B

### V. CONCLUSION

In this project, the Numerov integration scheme and the Numerov method is used to discretize the time-independent Schrödinger equation, as well as to find eigenvalues and eigenfunctions of the Hamiltonian operator. The eigenfunctions represent the energy eigenstates, and the corresponding eigenvalues represent the energy of that state. The eigenvalues and the eigenfunctions can be used to construct full solutions to the Schrödinger Equation. Then, utilizing Airy functions, the TISE is solved analytically for a linear potential well, and results are compared with the numerical results given by the Numerov method. For lower energy states, Numerov method has been shown to be highly precise. Then, the solutions to TISE with more complicated potential well were approximated using a piece-wise linear function close to the potential. The TISE was solved piece-wisely using Airy functions, and is "stitched" together, producing a continuous and differentiable approximation. This was then compared with the results produced by Numerov Method. We have shown that in some regions, the error is large and the behavior of the approximation is coarse, but overall it is reasonable.

The Airy functions approach is often used to solve for eigenvalues[4][5], but we have shown that it can also be used to approximate the energy eigenfunctions rather well. One advantage of this approach over other numerical solutions is that this approximation is differentiable at end points, and smooth elsewhere. Though this approach produces precise eigenvalues for complicated potential wells, one may wish to refine the process of finding energy eigenfunctions (such as varying the length of the intervals). Furthermore, one may wish to study the solution to the TISE with a negatively-sloped linear potential well ( $V(x) = -|x|$ ), so that the Airy function approach may be generalized to TISEs with arbitrary continuous potentials.

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## VI. APPENDIX

### A. Code part 1

```
using SpecialFunctions, Roots
using LinearAlgebra

#Determine dx and n:
V(x)=x; Em=30;
dx=1/sqrt(2*Em)
n=floor(Em/dx+2*pi)

#Finding En in e:
dv=[1 for i in 1:n];
du=[1 for i in 1:n-1];
A=Tridiagonal(du, dv*(-2), du)/dx^2;
B=Tridiagonal(du, 10*dv, du)/12;
X=Diagonal([dx*i for i in 1:n]);
@time H=-1/2*inv(B)*A+X;
@time e=sort(eigvals(Array(H)))

#Compare with analytical result:
an=find_zeros(airyai, -50, 0)/(-2^(1/3));
an=sort(an)
d=[an[i]-e[i] for i in 1:30]
```

### B. Code part 2

```
#Determine dx and n:
using LinearAlgebra
V(x)=x; Em=30;
#V(x)=0.6*x^1.3+sqrt(x)
dx=1/sqrt(2*Em)
xr=find_zeros(x->V(x)-Em, 0, 100)[1]
n=convert(Int64, floor(xr/dx+2*pi))

#Finding En in e:
dv=[1 for i in 1:n];
du=[1 for i in 1:n-1];
A=Tridiagonal(du, dv*(-2), du)/dx^2;
B=Tridiagonal(du, 10*dv, du)/12;
Vx=Diagonal(V.((1:n)*dx))
@time H=-1/2*inv(B)*A+Vx;
eigs=eigen(Array(H))
e=sort(eigs.values)
ei=copy.(e)
```

```
vi=V.((0:n)*dx)

#Matrix Numerov
idm=findall(x->x==e[Em], eigs.values);
tpm=zeros(n+1);
for i in 1:n
    tpm[i+1]=eigs.vectors[i, idm][1]
end;

#Define the general solution
function xi(x, y)
    x+=y*sqrt(eps())
    i=convert(Int64, floor(x/dx))+1
    return ((vi[i]*(i)-vi[i+1]*(i-1))+vi[i+1]-
    vi[i])/dx*(x-y*sqrt(eps()))-ei[Em]
    *2^(1/3)/((vi[i+1]-vi[i])/dx)^(2/3)
end
aiz(x, y)=airyai(xi(x, y))
biz(x, y)=airybi(xi(x, y))
using Plots
plot(x->aiz(x, 0), 0, 10)
plot!(x->biz(x, 1), 0, 10)
function aizp(x, y)
    x+=y*sqrt(eps())
    i=convert(Int64, floor(x/dx))
    return ((vi[i+2]-vi[i+1])/dx)^(1/3)*
    airyaiprime(xi(x-y*sqrt(eps()), y))
end
function bizp(x, y)
    x+=y*sqrt(eps())
    i=convert(Int64, floor(x/dx))
    return ((vi[i+2]-vi[i+1])/dx)^(1/3)*
    airybiprime(xi(x-y*sqrt(eps()), y))
end

#Finding coefficients
An=zeros(n-1); Bn=zeros(n-1); An[n-1]=1
An[n-2]=An[n-1]*(aiz((n-2)*dx, 1)-biz((n-2)*dx, -1)
/bizp((n-2)*dx, -1)*aizp((n-2)*dx, 1)
/(aiz((n-2)*dx, -1)-biz((n-2)*dx, -1)
/bizp((n-1)*dx, -1)*aizp((n-1)*dx, -1))
Bn[n-2]=An[n-1]*(aiz((n-2)*dx, 1)-aiz((n-2)*dx, -1)
/aizp((n-2)*dx, -1)*aizp((n-2)*dx, 1)
/(biz((n-2)*dx, -1)-aiz((n-2)*dx, -1)
/aizp((n-1)*dx, -1)*bizp((n-1)*dx, -1))
for i in 2:n-1
    tpa=An[n-i+1]*aiz((n-i+1)*dx, 1)+
    Bn[n-i+1]*biz((n-i+1)*dx, 1) tpb
    =An[n-i+1]*aizp((n-i+1)*dx, 1)
    +Bn[n-i+1]*bizp((n-i+1)*dx, 1)
    An[n-i]=(tpa-tpb*(biz((n-i+1)*dx, -1))
    /bizp((n-i+1)*dx, -1))/(aiz((n-i+1)*dx, -1)
    -aizp((n-i+1)*dx, -1)*(biz((n-i+1)*dx, -1))
    /bizp((n-i+1)*dx, -1))
    Bn[n-i]=(tpa-tpb*(aiz((n-i+1)*dx, -1))
    /aizp((n-i+1)*dx, -1))/(biz((n-i+1)*dx, -1)
    -bizp((n-i+1)*dx, -1)*(aiz((n-i+1)*dx, -1))
```

```

    / aizp((n-i+1)*dx, -1))
end
function p(x)
    i=convert(Int64, floor(x/dx))
    return An[i+1]*aiz(x,0)+Bn[i+1]*biz(x,0)
end

#Airy's Approximation
using QuadGK
tna=1/sqrt(quadgk(x->p(x)^2,0,Em)[1]);
#Matrix Numerov
tnm=1/sqrt(sum(tpm.^2)*dx);
#Difference
tr=convert(Int64, floor(Em/dx))
tx=zeros(tr)
for i in 1:tr-1
    global tr
    tx[i+1]=tpm[i+1]*tnm-tna*p(dx*i)
end

plot(x->p(x)*tna,0,Em, label="Airy Function's Approximation")
plot!((0:n)*dx, tpm*tnm, label="Matrix Numerov")
plot((1:tr)*dx, tx, label="Error")

```