Solving the Eigenvalue Problem for the Discrete Schrödinger Equation

Samuel Altier
Department of Physics & Engineering Physics, Fordham University, Bronx, NY 10458

The Schrödinger Equation is fundamental to the study of the world from a quantum mechanical standpoint. An important aspect of the study of the equation is extracting the physical eigenenergies from the equation, as they are the physical quantities that are most readily accessible and meaningful to us. One approach to extracting these data from the equation is to reframe the problem as a discrete matrix system, which allows us to use conventional eigenvalue finding methods from linear algebra. I will cover one such method, its results for a pair of potentials, and its limitations in the context of the problem.

I. INTRODUCTION

The eigenvalue problem is all too common when it comes to solving physical problems, so it should be unsurprising that it appears when trying to solve the Schrödinger equation, the cornerstone of quantum mechanics. The Schrödinger equation is the central equation for describing the quantum state of a non-relativistic particle; understanding the states permitted by the equation under the influence of a potentials is very important to developing more advanced theories in particle physics and beyond. While there are many ways to justify the equation itself, be it by "deriving" it via a variety of mechanical methods (stochastic, hydrodynamic, etc.) [1] or simply taking it as a postulate, there is no denying its fundamental importance to modern physical understanding and interpretation.

Because the equation is centrally important to the subject of modern physics, I will be solving the aforementioned eigenvalue problem for a pair of potentials (quadratic and quartic) so that the properties of their eigenvalues and associated energies might be better understood. In Sec. II, I will discuss and explain the theoretical underpinnings of the Schrödinger equation, the quantum harmonic oscillator, and the anharmonic oscillator, as well as demonstrate a method for discretizing the equation. In Sec. III, I will provide a description of the algorithm which I use to solve the discretized eigenvalue problem. In Sec. IV, I will outline pertinent results from the computations, followed by an analysis of errors and limitations of the Jacobi method in Sec. V. Finally, in Sec. VI I will discuss corrections to the results using the findings of the previous section.

II. THEORY

A. Schrödinger Equation and the Quantum SHO

The Schrödinger equation is the major postulate and hallmark of non-relativistic quantum mechanics, governing the behavior of a vast multitude of microscopic phenomena. It is assumed as result of various mathematical identities from statistical and classical mechanics [2]. It takes on two forms: one that depends on time and one that does not. The general, time dependent equation from Ref. [2] goes as follows

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t) + V(\vec{r},t)\Psi(\vec{r},t) \quad (1)$$

As explained in Ref. [3], finding solutions to the equation is made much easier by assuming a separable solution, which allows us to solve the time independent form, which can be formulated with the Hamiltonian ($\hat{H}$) as follows:

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

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) \quad (3)$$

$$\hat{H}\psi(\vec{r}) = E\psi(\vec{r}) \quad (4)$$

The overall solution to this time independent equation is found by multiplying in the separable time solution $e^{-iEt/\hbar}$, which can then have boundary conditions applied to find the coefficients for the general separable solution. An important observation is that Eqn. 4 is an eigenvalue problem with the energy quanta as the eigenvalues, allowing for some interesting numerical methods for solving the problem as will be discussed in the next two sections.

An important potential for real world applications is the quadratic potential, which arises in all manner of physical problems, and forms the basis for the quantum version of the harmonic oscillator [4].

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega_0^2x^2 \quad (5)$$

The time-independent oscillator can be described in one dimension by substituting Eqn. 5 into the 1-dimensional Hamiltonian for Eqn. 4. Using the method of ladder operators [4], it is easy to analytically determine the eigen-energies for the oscillator, which are given by:

$$E_n = \hbar\omega_0(n + \frac{1}{2}) \tag{6}$$

A quick observation of the above is that the energy levels are evenly spaced, which should be expected given the manner in which the ladder operators are applied to find the solution. Because the analytic solution to this problem is known, I will be using it as a baseline to analyze the results for other potentials.

The anharmonic quartic potential is another potential of interest, due to its applications in various effective quantum theories. The pure quartic eigenvalues (Potential $V(x) = \frac{1}{4}\lambda x^4$ are given in [5] and go as follows:

$$E_n = 0.867145(n + \frac{1}{2})^{\frac{4}{3}}\lambda^{\frac{1}{3}} = 0.344127, 1.48895, ... \tag{7}$$

I will be simply adding the anharmonic quartic term with $\lambda = 1$ to the harmonic potential in order to do my simulation. This formulation will expect lower eigenvalues in the orders that I will be studying due to the lowering of the potential around the origin [5].

B. Discretizing the Schrödinger Equation

Having discussed the continuous form of the Schrödinger equation, I will now develop a discrete form that I will be able to use in my numerical solution. This form will give rise to a matrix representation of the problem allowing for application of the Jacobi algorithm. The method of discretization involves the forward centered second derivative with spacing a to replace the differential operator, and a discrete potential to replace the potential function.

$$\frac{-\hbar^2}{2m}\frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{a^2} + V_i\psi_i = E\psi_i \tag{8}$$

We can further improve this by factoring a negative from the numerator of the discrete derivative, flipping the signs and giving and making the substitution:

$$t_0 = \frac{\hbar^2}{2ma^2} \tag{9}$$

Allowing us to rewrite it as:

$$-t_0\psi_{i+1} + 2t_0\psi_i - t_0\psi_{i-1} + V_i\psi_i = E\psi_i \tag{10}$$

A form which is easily lent to matrix form. The particular form of the matrix depends on the choice of boundary conditions, whether Dirichlet, periodic, or otherwise. Eqn. 11 shows the form of the matrix for periodic boundary conditions. The equivalent Dirichlet matrix can be obtained by replacing the upper-rightmost and lower-leftmost elements with 0.

$$\begin{bmatrix} 2t_0 + V_1 & -t_0 & \dots & -t_0 \\ -t_0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -t_0 \\ -t_0 & \dots & -t_0 & 2t_0 + V_n \end{bmatrix} \vec{\psi_n} = E\vec{\psi_n}$$

(11)

Where all of the elements not on the first off-diagonals and not in the anti-diagonal corners are all 0; Dirichlet boundary conditions are achieved by replacing the anti-diagonal corners with 0.

This setup is explicitly a matrix eigenvalue problem, for which there are numerous methods to compute a solution.

III. JACOBI EIGENVALUE ALGORITHM

Now that I have established the problem at hand as a matrix eigenvalue problem, I will present the method that I used to perform the computations. Developed by Carl Gustav Jacob Jacobi in the mid-1800s, the Jacobi Eigenvalue Algorithm (JEA) did not see popular use until the advent of modern computers, due to its slow convergence and computationally intensive structure. The basic method of the JEA arises from the concept of matrix similarity transformations, which can be seen below:

$$J^T A J = B \tag{12}$$

Two matrices are called similar if the operation on the left in Eqn. 12 results in a diagonal matrix. The most important property of such a similarity transformation is that the resulting diagonal matrix contains the eigenvalues of the matrix A along its main diagonal. The problem with determining a similar matrix to perform the similarity transformation is that it is often quite difficult to find its exact form. To circumvent this problem, Jacobi proposed the use of an iterative method for determining a similar matrix, writing the similarity matrix as a product of a series of plane rotational matrices which slowly make the matrix "more diagonal." The appropriate similar matrix can then be approximated as the product of these various rotations without us ever having to generate or consider the eventual form of the similar matrix.

We define a Givens rotation matrix J:

$$J_{ij}(\theta,p,q) = \begin{cases} 0 & i \neq j, i, j \neq p, q \\ 1 & i = j, i, j \neq p, q \\ \cos\theta & i = j = p \; OR \; i = j = q \\ \sin\theta & i = q, \; j = p \\ -\sin\theta & i = p, \; j = q \end{cases} \quad (13)$$

Such that whenever J is multiplied by some matrix A, it performs a plane rotation of θ in the pth and qth columns. Jacobi's algorithm proceeds by intelligent choice of the angle θ such that the similarity transformation using J is able to zero the largest (by magnitude) off-diagonal elements a_{pq}, a_{qp} of A. Only values falling on a square whose corners are at A_{pp}, A_{qq}, A_{pq}, and A_{qp} are affected by the rotation. The goal of this rotation is to zero the off-diagonal corners, thus making the matrix more diagonal.

Convergence of the algorithm is measured based on the sum of the squares of the off-diagonal elements, as a means to test the approximate "diagonality" of the matrix after each iteration. We define this diagonality function as:

$$Off(A) = \sum_{i \neq j} a_{ij}^2 \quad (14)$$

Targeting the elements with the largest magnitudes allows later rotations to be more effective, as each one will decrease the value from Eqn. 14 more rapidly and maximize the increase in overall diagonality of the resulting matrix, while (importantly) maintaining the symmetry of the matrix.

I have mentioned that an "intelligent" choice of angle is important to maximize the efficacy of the algorithm, making the determination of the angle a key step pre-rotation. Using a clever simplification to the 2-by-2 case that specifically zeroes the chosen off-diagonal entries, Refs. [6] and [7] show that the angle can be determined using a simple quadratic system that, for the desired angle θ with matrix A whose maximum element falls in row p, column q, yields:

$$\tau = \frac{A_{qq} - A_{pp}}{2A_{pq}} \quad (15)$$

$$\tan\theta = \frac{sign(\tau)}{|\tau| + \sqrt{1+\tau^2}} \quad (16)$$

Eqns. 15 and 16 allow us to write the cosine and sine elements of the rotation matrix in terms of tangent, allowing us to avoid using further trig or inverse trig functions to extract or use θ and minimize round-off errors.

There is one major advantage of the Jacobi algorithm, which, unfortunately, I was not able to exploit for this project. The advantage is that it is parallelizable [6], due to the fact that the iterative rotations only affect parts of the rows and columns containing the off-diagonal maxima. As such, multiple rotations can be performed in parallel so long as the corresponding parts of the rows and columns do not overlap, which can be ensured by decomposing the matrix into a series of smaller regions.

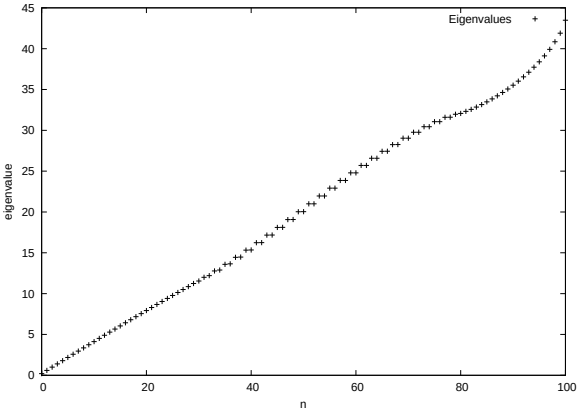

FIG. 1: Trends in generated eigenvalues for harmonic potential from Jacobi code; linear trend is visible but imperfect, following the error trend in Fig. 6

IV. RESULTS

For all simulations, I set $\hbar = 1$ and $k = 1$, resulting in a value $\omega_0 = 4a$ for the harmonic oscillator, where a is the discretization (this fact comes from Eqns. 9 and 5). So the expected progression was a linear trend of half integer multiples of 0.4, which fits the data produced for the harmonic oscillator quite well, as seen in Fig. 1. There was some deviation, as expected, but this deviation was predictable, a fact which I will further explain in Sec. V. The quartic results, with no error corrections applied, experience apparent degeneracy (pairs of repeated eigenvalues) after about halfway through the data set, as can be seen in Fig. 2.

Similar degenerate eigenpairs were visible for the sextic order potential, showing that this is a fundamental problem with or property of the Jacobi method in this case.

V. ALGORITHMIC LIMITATIONS AND ERROR ANALYSIS

A discussion of the limitations of the JEA with respect to each potential and to its performance is necessary before covering the specific results for the potentials, so that the errors and constraints can be properly under-

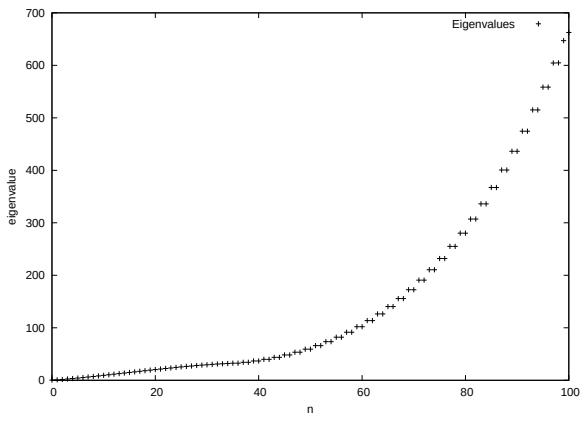

FIG. 2: Trends in generated eigenvalues for quartic potential; degenerate pairs are visible after about halfway through the data set

stood. The quadratic potential served as my baseline for testing and error analysis, as it has analytically known energy levels.

The first major problem for the computations was that small discretizations for the potential would cause large errors in the resulting eigenvalues for the quadratic potential, on the order of 200 times the spacing even at the lowest energy level (zeroth eigenvalue) for $dx = 0.01$ and lower powers of 10. This result forced me into using a discretization of 0.1 in every case, because quantifying the errors for the higher order potentials would be next to impossible if the errors in the baseline quadratic potential were hard to track. Similar blowing up of results occurred for the other potentials at other spacings.

An interesting behavior came from the compute times, which varied wildly between potentials, with the quartic and sextic potentials experiencing far superior compute times at higher matrix sizes while the quadratic suffered a severe drop off in speed between rank 200 and rank 500. At the scale that the potential was distributed over (25 units to either side of the origin at rank 500), the quartic and sextic degree potentials were much larger at the boundaries and smaller around the origin, making the diagonal comparatively much larger in magnitude than the off-diagonal elements (and thus the matrix "more diagonal"), giving a plausible explanation for the trend of shorter compute times. This trend can be seen in Table I, with the sixth order potential outperforming the quartic, and vastly outperforming the quadratic in terms of compute time. This effect can be seen in Fig. 4, which excludes the sixth order potential because it would be indistinguishable from the quartic, but it is still obvious that the trend of increased compute performance comes with higher order potentials. This performance in time was not matched in performance with generating plausible, distinct higher order eigenvalues, as the values started to appear in degenerate identical pairs past a certain point.

A good result from the quadratic potential was an apparent uniformity of error growth, up to a point about 16% through the whole set of points. With increasing matrix size, I found that the the error growth became sporadic around a fifth of the way through all eigenvalues. As such, corrections were possible by fitting the error growth to a polynomial for points below the threshold of a fifth (really 16%) of the generated data points and then adding the error to the data to the data. The error was able to be added because the eigenvalues before this point were bounded above by the actual values in the case of the harmonic oscillator. The equation of fit for error growth can be seen in Fig. 6, and is given by:

$$f(x) = 0.000002x^3 + 0.000527x^2 + 0.0026x - 0.0079 \quad (17)$$

Because of the long time associated with the quadratic potential using large matrices, and the correspondingly higher number of rotations required to reach the desired accuracy, it is reasonable to guess that the errors for the quadratic potential overestimate the errors for the higher order potentials. As such, we can guess on the overestimation of energies for the quartic potential and be able to determine with good accuracy the general trend on the eigen-energies for that potential once proper corrections have been carried out.

Different boundary conditions might have also affected results, so I tested both Dirichlet and periodic boundary conditions and the difference in the resulting eigenvalues. Fig. 3 shows that the boundary conditions were approximately the same in the region of interest mentioned above, meaning that choice of boundary conditions was unimportant for the region where the error increased uniformly with n. Additionally, there was a negligible difference in compute time between the two types of boundary conditions.

The last key observation is that higher rank matrices do not increase accuracy of eigenvalues that converge in lower rank matrices, meaning that increasing matrix size is not a suitable means of decreasing errors on the lower order energies. However, it is a good way of increasing the suitability of the fit approximating our errors, because it does increase the region in which the error grows uniformly.

VI. CORRECTIONS TO THE DATA

Applying the correction scheme from Sec. V of using the uniform error trend to correct higher order potentials yields much better trends for the quartic potential. The corrected trend was also linear, much like the harmonic result, but with a growth spacing of 2.5 times the fundamental frequency, given by:

$$f(x) = 1.061792x^1 + -0.757395 \quad (18)$$

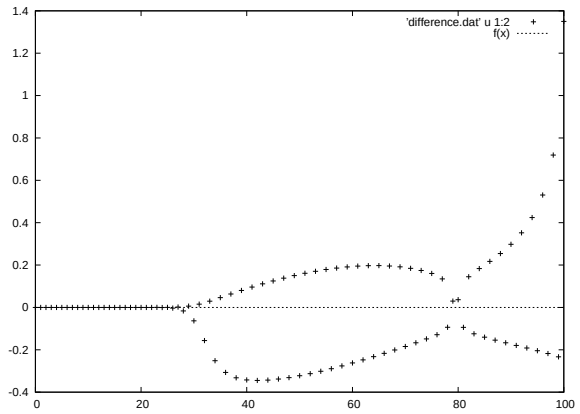

FIG. 3: A plot of the difference in results between dirichlet and periodic boundary conditions. Positive means the periodic result was larger, negative means the dirichlet result was larger. Zero means they were the same.

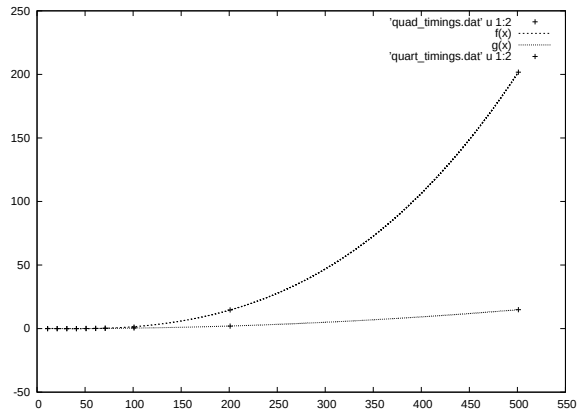

FIG. 4: Trends in timing for quadratic ($f(x)$), quartic ($g(x)$) potentials.
$f(x) = 0.000001 * x^3 + 0.000219 * x^2 + -0.024 * x^1 + 0.435$
$g(x) = 0.000066 * x^2 + -0.003415 * x^1 + 0.071989 * x^0$

Size	31	41	51	61	71	101	201	501
x^2	0.015	0.031	0.093	0.156	0.312	1.171	14.719	201.75
x^4	0.015	0.031	0.078	0.140	0.218	0.468	1.968	14.890
x^6	0.015	0.031	0.046	0.078	0.109	0.218	0.968	7.062

TABLE I: Timings, in seconds, for the an array of matrix sizes for several potentials. Each displays growth with matrix size, as expected, however, the algorithm experiences extreme jumps in duration for large matrices for the quadratic potential, and comparatively much smaller for the higher order potentials

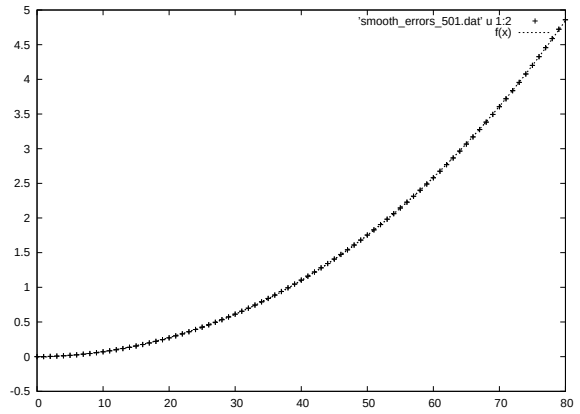

FIG. 5: The polynomial fit to data set containing the errors for a selection of points for which the error growth was smooth (about the 1st 25% of the data points). $f(x) = 0.000002 * x^3 + 0.000527 * x^2 + 0.002616 * x^1 + -0.007903 * x^0$

Because of the timing considerations discussed in the previous section, I believe that the errors from the harmonic solution should overestimate the errors on further potentials. Because of the uniformity of the trend resulting from the corrections to the quartic potential, the correction seems valid, though from Ref. [5] it is clear that the expected trend is not explicitly linear for a pure quartic oscillator, so it is likely that this anharmonic term on the potential will not change that fact. Additionally, the computed values are smaller than the expectation values for the pure quartic oscillator [5], which is what was expected given the additional harmonic term which will decrease the energy in the low eigenvalue regime.

VII. CONCLUSION

Overall, the Jacobi algorithm is an effective method for finding approximate low order eigenvalues for potentials. It breaks down after a certain threshold value, but it also provides a uniform growth in error that can be fit to and extrapolated to minimize uncertainty in the resulting eigen-energies. As expected from reducing an "infinite" eigenvalue problem to a finite one, there are several problems with it, including long compute times, poor conditioning for high order eigenvalues, and degeneracy for the highest order values computed. It works well for the well known quadratic potential, converging well for relatively small (rank 100, 200) matrices for the first 25 or so eigen-energies. The error fitting methods used in this paper are imperfect, especially because of compute

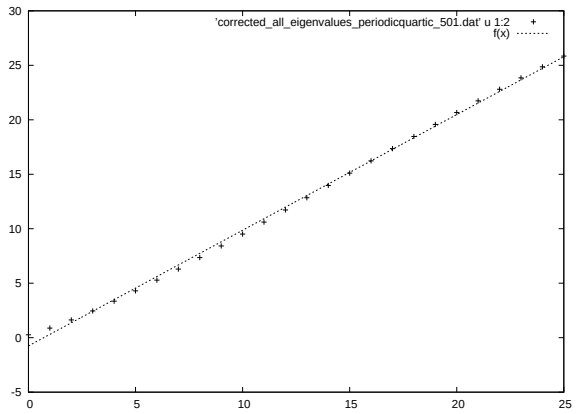

FIG. 6: The linear fit for the corrected quartic data, as given in Eqn. 18

time restrictions which prevented me from checking the validity of the error fit for much higher order matrix configurations. Finally, I discovered that, in regions where the errors could be corrected for (with a uniform, predictable error), choice of boundary conditions for matric construction was unimportant for the purposes of getting "good" values.

The harmonic oscillator was a good test of the algorithm, and, because of its known results, I was able to determine a reasonable approximation for errors on the eigenvalues. The quartic term oscillator behaved as expected, with eigenvalues smaller than the pure quartic oscillator in the region that I was able to probe. For those interested, plots for the pure quartic eigenvalues have been included in the directory containing this pdf.

[1] A. M. Cetto, L. d. la Peña, and A. Valdés-Hernández, Quantum Studies: Mathematics and Foundations **2**, 275 (2015), ISSN 2196-5617, URL https://doi.org/10.1007/s40509-015-0047-5.

[2] W. P. Schleich, D. M. Greenberger, D. H. Kobe, and M. O. Scully, *Schrödinger equation revisited* (2013), URL https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3619330/.

[3] W.-H. Wang, H.-X. Cao, Z.-H. Guo, and B.-M. Yu, Communications in Theoretical Physics **62**, 205 (2014), URL https://doi.org/10.1088%2F0253-6102%2F62%2F2%2F06.

[4] R. L. Liboff, *Introductory Quantum Mechanics* (Pearson Education, 2015).

[5] S. M. Blinder, *Wolfram foundation* (2019), URL https://notebookarchive.org/eigenvalues-for-a-pure-quartic-oscillator--2019-03-9q5kl

[6] J. Lambers (2011), URL https://web.stanford.edu/class/cme335/lecture7.pdf.

[7] E. A. Carlen (2003), URL http://people.math.gatech.edu/~aleykin3/math2605fall10/CARLEN/chap3.pdf.