

# Centered-Difference Applications for Schrödinger's Equation

A Senior Project

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### **Abstract**

This project enumerates methods utilizing discretized centered-difference approximations on the second order differential equation for quantum particles known as Schrödinger's Equation. An eigenvalue-eigenfunction scheme is developed to sieve for valid solutions to The Time Independent Schrödinger Equation. Additionally the Crank-Nicolson method is applied to the Time Dependent Schrödinger Equation to describe wavefunction (eigenfunction) time evolution. The validity of these methods is discussed with applications to several fundamental pedagogical introductory quantum mechanic systems.

# Contents

<b>1</b>	<b>Introduction</b>	<b>5</b>
1.1	Background . . . . .	6
1.2	Postulates of Quantum Mechanics . . . . .	6
1.3	Numerical Method . . . . .	10
<b>2</b>	<b>Applications</b>	<b>13</b>
2.1	Time Independent Energy Eigenvalue Sieve . . . . .	13
2.1.1	Particle in a Box . . . . .	15
2.1.2	Quantum Harmonic Oscillator . . . . .	17
2.1.3	Nonanalytic solutions . . . . .	20
2.2	Crank-Nicolson on Schrödinger's Equation . . . . .	25
2.2.1	Stationary States . . . . .	25
2.2.2	Tunneling . . . . .	28
<b>3</b>	<b>Concluding Remarks</b>	<b>29</b>
<b>4</b>	<b>Appendix</b>	<b>30</b>
4.1	More on Time Independent Wavefunctions $\psi$ . . . . .	30
4.2	More on Time Dependent Wavefunctions $\Psi$ . . . . .	31
4.2.1	Relax Transition . . . . .	32
4.2.2	Tunneling . . . . .	33
<b>5</b>	<b>Glossary</b>	<b>34</b>

# 1 Introduction

When investigating the world of small particles it is useful to solve The Schrödinger Equation. Solutions to The Schrödinger Equation describe the probability distribution of independent particles and how likely they are found in either a basis of position or momentum.

Investigations described in this report utilize Schrödinger Equation to solve for motion states and uses a position basis. Schrödingers Equation contains information about a particles environment  $V(\hat{r}, t)$  and yields a solution of its distribution called a wavefunction  $\Psi(\hat{r}, t)$ . Solutions in a position basis yield an expression of a quantum particle's probable location. A non-zero wavefunction at any location  $(x, y, z)$  will have non-zero probability of the particle being located at such position. Wavefunction with a momentum  $\Phi(p, t)$  basis similarly describe the particles plausible distribution of momentum ( $p = mv$ ). If the wavefunction of a momentum value is zero there will never exist a particle with the given momentum. Schrödingers equation can describe numerous phenomenon; applicable in fields from medical imaging to chemical engineering to astronomy. Unfortunately, the number of solutions with an analytic "nice" solution are rare compared to the entire universe of conceivable potentials.

Consequently, real world problems are examined using a variety of mathematical tools. The first mathematical tool in the quantum mechanical tool box utilizes approximations to simplify a problem. One well studied method quantum mechanics is perturbation theory. By starting from a known solvable system one may add a perturbation to a solvable potential and find consequent changes to the unperturbed eigenfunction. Perturbation schemes are incredibly versatile and famous for its highly accurate calculations for multibody interactions including predictions of fine and hyperfine splitting for atomic emissions. These corrections to a Bohr model atom are consequence of coupling between protons and bound electrons. Toolless such interactions complicate the mathematical expression for the particles environment ( $V$ ) which begets insurmountable differential equations.

Another handy tool, which encompasses the majority of subsequent sections, useful for any differential equations involves discretization both space and time differentiation and computing a finite difference. By exchanging a relation over infinitesimal differences (calculus) for finite separations many unsolvable problems become solvable in the discrete case by simple and direct numerical calculations.

## 1.1 Background

Until the development of modern formulation of quantum mechanics, several late 19<sup>th</sup> century experimental peculiarities reported by Rutherford, Millikan, and Bragg befuddled classical physics and each inspired separate ad hoc models. Before these challenges, the well formulated dynamic system of fields founded by the 1750s mathematicians Leonhard Euler and Joseph Louis Lagrange experienced huge success establishing the foundation for mechanical engineering. Together they constructed the Euler-Lagrange system of equations which is well suited to describing many physical phenomena. Hamilton extended these systems expressing the same mechanics as an expression of energy conservation. A century later James Clark Maxwell developed a new system of field equations for all electromagnetic phenomena, yet all of these successes fell short to describe nature's "lumpiness" found by aforementioned physical science pioneers.

Inspired by Albert Einstein's discretization of light waves as a photon, Louis de Broglie postulated a dual wave and particle nature of all matter. Matter waves arise from an uncertainty of any measurable quantity because the particle is energetic a concept first argued by Werner Heisenberg. Schrödinger's contribution extended the wave equation to include massive particles with de Broglie's wavelength. Quantum mechanics proved capable unifying Niels Bohr's quantized angular momentum, the massive localized positive charge identified in Rutherford's gold foil experiment, and paved way for developments in atomic spectroscopy and modern chemistry.

## 1.2 Postulates of Quantum Mechanics

The Schrödinger Equation may be interpreted as a quantum description of conservation of energy consistent with de Broglie's relations for matter waves and the associated energy and momentum of electromagnetic waves Planck formulated. Below I demonstrate an informal proof unifying these quantities. Beginning from the expression of total energy called the Hamiltonian, the sum of kinetic energy  $T$ , and the potential energy  $V$

$$E_{total} = \hat{H} = T + V \quad (1)$$

where kinetic energy is expressible using mass  $m$  and velocity  $v$ . By exchanging momentum  $p = mv$  and velocity we may write two alternative form of kinetic energy.

$$T = \frac{mv^2}{2} = \frac{p^2}{2m} \quad (2)$$

Recall the following relationships between wavenumber  $k$  and wavelength  $\lambda$  and similar relations for frequency  $f$  and angular frequency  $\omega$

$$k = \frac{2\pi}{\lambda}$$

$$\omega = 2\pi f$$

Note the importance of Planck constant and its reduced form relating wave values to energy and momentum (called h-bar).  $\hbar = \frac{h}{2\pi}$  Planck's relations for momentum and energy of a wave state

$$k = \frac{p}{\hbar} \quad (3)$$

and

$$E = hf = \hbar\omega \quad (4)$$

Consider the following 1+1 dimension matter wave

$$\Psi(x, t) = e^{i(kx - \omega t)} \quad (5)$$

By differentiating with respect to position ( $x$ ) twice we find

$$\frac{\partial \Psi}{\partial x} = ik e^{i(kx - \omega t)} = ik \Psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} = (ik)^2 e^{i(kx - \omega t)} = (ik)^2 \Psi$$

By (3) and  $i^2 = -1$  we can express the second position derivative as

$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{p^2}{\hbar^2} \Psi \quad (6)$$

therefore

$$\hbar^2 \frac{\partial^2 \Psi}{\partial x^2} = p^2 \Psi \quad (7)$$

furthermore by (2)

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = \frac{p^2}{2m} \Psi = T \Psi \quad (8)$$

The wavefunction is assumed to be composed of a time and space factor

$$\Psi(\hat{r}, t) = \psi(\hat{r})\phi(t)$$

now by factoring and dividing  $\phi$  and recalling the hamiltonian (1) we can write the Time Independent Schrödinger Equation [TISE]

$$E\psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \quad (9)$$

This is often written with  $\psi$  factored such that

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

Now consider differentiating our matter wave with respect to time

$$\frac{\partial \Psi}{\partial t} = -i\omega e^{i(kx - \omega t)} = -i\omega \Psi \quad (10)$$

(4) suggests  $E\Psi = \hbar\omega\Psi$  which motives the manipulation

$$-\frac{i}{\hbar} E\Psi = -i\omega\Psi = \frac{\partial \Psi}{\partial t}$$

so

$$E\Psi = -i\hbar \frac{\partial \Psi}{\partial t}$$

Considering (9) we may write the Time Dependent Schrödinger Equation [TDSE]

$$i\hbar \frac{\partial}{\partial t} \Psi = \left[ -\frac{\hbar^2}{2m} \left( \frac{\partial}{\partial x} \right)^2 + V \right] \Psi \quad (11)$$

TDSE expressed in multiple dimensions utilizes the gradient operator to replace the spacial derivative with respect to  $x$



$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}, t) \right] \Psi(\vec{r}, t)$$

Admittedly, deriving the Schrödinger Equation teaches little to understand quantum mechanics, yet the focus of this report is to introduce an alternative method to DO quantum mechanics. This derivation provides some insight to topics which will be developed further. Before delving into the numerical approach described below, I shall introduce the concepts fundamental to understanding what a valid wavefunction is. TDSE Wavefunctions are  $\Psi \equiv \Psi(\hat{r}, t)$  while the time independent  $\psi \equiv \psi(\vec{r})$ .

Valid Wavefunctions are complex value functions which describe a probability distribution which is piecewise-smooth. A real value distribution is obtained by integrating a wavefunction against its conjugate. Equation (13)

For any complex number  $z \in \mathbb{C}$ , the product of  $z$  and its conjugate ( $z^*$ ) is always real.

$$z = a + bi \ni a, b \in \mathbb{R}$$

$$|z|^2 = z^* z = (a - bi)(a + bi) = a^2 + b^2$$

Similarly  $|\Psi|^2 = \Psi^* \Psi \in \mathbb{R}$

Quantum mechanics is the study of quantized elements; the simplest problems consider a single particle. All well-behaved wavefunctions exhibit the following properties.

$$\lim_{x \rightarrow \pm\infty} \Psi(x) = 0 \tag{12}$$

This states the wavefunction must approach zero at the end of the domain. By convention the inner product of the wavefunction over all space is one; an intuitive statement for wavefunctions which describe a single quantum of particle.

$$\int_{\forall \mathbb{R}^3} \Psi^* \Psi d\vec{r} = 1 \tag{13}$$

When represented in one dimension.

$$\int_{-\infty}^{\infty} \Psi^* \Psi dx = 1 \tag{14}$$

Below I shall discuss the concept of even and odd parity which will be useful in later sections.

we say  $f$  has even parity if  $f(x) = f(-x)$

we say  $f$  has odd parity if  $f(x) = -f(-x)$

Alternatively we may describe an even function as having a reflection symmetry over the y-axis while odd parity functions have a  $180^\circ$  rotational symmetry with respect to the origin. This is relevant for its consequences on a valid wavefunction with an even potential. Assume  $\psi$  is a valid wavefunction [Eigenfunction],  $E$  is its associated eigenvalue and  $V$  has even parity. From 1-D TISE

$$E\psi(x) = \left[ -\frac{\hbar^2}{2m} \left( \frac{\partial}{\partial x} \right)^2 + V(x) \right] \psi(x) \quad (15)$$

Applying the reflection  $x \rightarrow -x$

$$E\psi(-x) = \left[ -\frac{\hbar^2}{2m} \left( \frac{\partial}{\partial x} \right)^2 + V(-x) \right] \psi(-x) \Rightarrow$$

$$E\psi(-x) = \left[ -\frac{\hbar^2}{2m} \left( \frac{\partial}{\partial x} \right)^2 + V(x) \right] \psi(-x)$$

Notice  $\psi(-x)$  now satisfies the original equation as  $\psi$  is a factor of both sides. Any function  $u(x) = a\psi(\pm x)$  will satisfy equation (15) for any  $a \in \mathbb{C}$ , yet we must restrict  $a = \pm 1$  for the wavefunction to remain normalized [equation (13)]. Therefore for an even potential we expect a wavefunctions with odd or even symmetries to exist.

### 1.3 Numerical Method

Analytic solutions to quantum mechanics rely on solving differential equations which usually motivates an educated guess or ansatz. Methods developed here utilize implicit finite difference schemes on TISE to find energy eigenvalues and Crank-Nicolson time dependent solutions by straightforward calculation. To begin constructing centered-difference schemes consider the finite difference definition of a derivative evaluated at  $x$  and  $x - \Delta x$  to construct a finite difference representation of the second derivative.

$$\left. \frac{df}{dx} \right|_x = \lim_{\Delta x \rightarrow 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

and

$$\left. \frac{df}{dx} \right|_{x-\Delta x} = \lim_{\Delta x \rightarrow 0} \frac{f(x) - f(x-\Delta x)}{\Delta x}$$

So the second derivative of some function  $f$  on  $x$  maybe expressed

$$\begin{aligned}\frac{d^2 f}{dx^2} &= \lim_{\Delta x \rightarrow 0} \frac{\frac{df}{dx}\big|_x - \frac{df}{dx}\big|_{x-\Delta x}}{\Delta x} \\ \frac{d^2 f}{dx^2} &= \lim_{\Delta x \rightarrow 0} \frac{\lim_{\Delta x \rightarrow 0} \frac{f(x+\Delta x) - f(x)}{\Delta x} - \lim_{\Delta x \rightarrow 0} \frac{f(x) - f(x-\Delta x)}{\Delta x}}{\Delta x} \\ &= \lim_{\Delta x \rightarrow 0} \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{\Delta x^2}\end{aligned}$$

When discretizing the spacial grid  $\Delta x \neq 0$  (thus a finite difference). Therefore the approximate second derivative is written

$$\frac{d^2 f}{dx^2} \approx \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2} \quad (16)$$

The second derivative approximation (16) is essential to the energy eigenvalue sieve and Crank-Nicolson method. To evaluate both time and space derivatives numerically we exchange a continues resolution for step sizes  $\Delta x$  &  $\Delta t$  and introduce  $j$  &  $n$  to identify the discrete grid so a general function  $U(x, t)$  may be expressed

$$U(x, t) \approx U(j\Delta x, n\Delta t)$$

To develop the Crank-Nicolson method, here I shall assume a function  $U(x, t)$  and rewrite (16) to approximate  $U''$

$$U'' = \frac{d^2 U}{dx^2} = F_j^n = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2} \quad (17)$$

The Crank-Nicolson method approximates the time derivative as an average of the second derivatives of space one evaluated at  $t = n\Delta t$  and another evaluated at  $t = (n + 1)\Delta t$ . For a partial differential equation of the form

$$\frac{\partial U}{\partial t} = \frac{\partial^2}{\partial x^2} U$$

the Crank-Nicolson centered-difference approximation is a combination of implicit ( $\nu = 1$ ) and explicit ( $\nu = 0$ ) Euler schemes. Haberman [2012]

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \left[ (\nu) F_j^{n+1} + (1 - \nu) F_j^n \right] \quad (18)$$

The Crank-Nicolson scheme averages implicit and explicit Euler (CN:  $\nu = \frac{1}{2}$ )

By a simple 1 dimensional diffusion example with time and space discretization  $U(j\Delta x, n\Delta t)$  approximates the following differential equation

$$\frac{\partial U}{\partial t} = a \frac{\partial^2 U}{\partial x^2}$$

Applying both time discretization on the left hand side and spacial discretization to the right gives the resulting CN-type equation

$$\begin{aligned} \frac{U(x, t + \Delta t) - U(x, t)}{\Delta t} = \\ = \frac{a}{2\Delta x^2} [ [U(x + \Delta x, t + \Delta t) - 2U(x, t + \Delta t) + U(x - \Delta x, t + \Delta t)] + [U(x + \Delta x, t) - 2U(x, t) + U(x - \Delta x, t)] ] \end{aligned} \quad (19)$$

The following equations are represented using notation introduced earlier [see (17 )] using the substitution  $r = \frac{a\Delta t}{2\Delta x^2}$  and some algebra (19) may be arranged as

$$-ru_{i+1}^{n+1} + (1 + 2r)u_i^{n+1} - ru_{i-1}^{n+1} = -ru_{i+1}^n + (1 - 2r)u_i^n - ru_{i-1}^n \quad (20)$$

from the Crank-Nicolson method we have arrived at a system of equations

$$\begin{bmatrix} (1+2r) & -r & 0 & 0 & 0 & \dots \\ -r & (1+2r) & -r & 0 & 0 & \dots \\ 0 & -r & (1+2r) & -r & 0 & \dots \\ \dots & & & & & \\ & \dots & & & & \\ 0 & \dots & 0 & 0 & -r & (1+2r) \end{bmatrix} \begin{bmatrix} u_1^{n+1} \\ u_2^{n+1} \\ \vdots \\ u_{i-1}^{n+1} \\ u_i^{n+1} \\ u_{i+1}^{n+1} \\ \vdots \\ u_j^{n+1} \end{bmatrix} = \begin{bmatrix} (1-2r) & -r & 0 & 0 & 0 & \dots \\ -r & (1-2r) & -r & 0 & 0 & \dots \\ 0 & -r & (1-2r) & -r & 0 & \dots \\ \dots & & & & & \\ & \dots & & & & \\ 0 & \dots & 0 & 0 & -r & (1-2r) \end{bmatrix} \begin{bmatrix} u_1^n \\ u_2^n \\ \vdots \\ u_{i-1}^n \\ u_i^n \\ u_{i+1}^n \\ \vdots \\ u_j^n \end{bmatrix}$$

Compressed into matrices and arrays

$$[L]\vec{U}^{n+1} = [R]\vec{U}^n \quad (21)$$

while it is tempting to solve for  $\vec{U}^{n+1}$  by matrix inversion such that

$$\vec{U}^{n+1} = [L]^{-1}[R]\vec{U}^n$$

Matrix inversion techniques on matrices of size  $n \times n$  scales in difficulty on order  $\mathcal{O}(n^3)$ ; we may take advantage of the tridiagonal nature of these systems which can be solved much faster  $\mathcal{O}(n)$  using reduced row-echelon methods. Next we construct the analogous Crank-Nicolson system for TDSE.

$$i\hbar \frac{\partial}{\partial t} \Psi = \left( \frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right) \Psi \quad (22)$$

Applying Crank-Nicolson method to the TDSE and using the substitution  $\rho = \frac{i\hbar \Delta t}{4m \Delta x^2}$

$$-\rho \psi_{i+1}^{n+1} + (1 + 2\rho) \psi_i^{n+1} - \rho \psi_{i-1}^{n+1} = -\rho \psi_{i+1}^n + (1 - 2\rho + \frac{\Delta t V_i^n}{i\hbar}) \psi_i^n - \rho \psi_{i-1}^n \quad (23)$$

As with CN on diffusion-like models CN on TDSE is also representable by a tridiagonal system of equations. CN on TDSE is symbolically identical with an additional term on the center diagonal of the right hand side matrix containing the potential information.

Higher dimensional numerical schemes will either lack the quick tridiagonal system or an alternative schemes may retain the 1-dimensional derivative approximation (16) applied three times for each spacial dimension to preserve the tridiagonal matrices.. Approximating the second derivative for higher dimensions considers nearest values in both y and z dimensions. Similar to equation 16

$$\left[ \left( \frac{\partial}{\partial x} \right)^2 + \left( \frac{\partial}{\partial y} \right)^2 + \left( \frac{\partial}{\partial z} \right)^2 \right] f = \nabla^2 f \approx$$

$$\frac{f(x+\Delta x, y, z) - 2f(x, y, z) + f(x-\Delta x, y, z)}{\Delta x^2} + \frac{f(x, y+\Delta y, z) - 2f(x, y, z) + f(x, y-\Delta y, z)}{\Delta y^2} + \frac{f(x, y, z+\Delta z) - 2f(x, y, z) + f(x, y, z-\Delta z)}{\Delta z^2}$$

When represented as a matrix, each interior row will contain seven nonzero elements - six  $(x, y, \&z)$  neighbors + one potential & center) for both the  $L$  &  $R$  matrices.

## 2 Applications

### 2.1 Time Independent Energy Eigenvalue Sieve

Treating the Time Independent Schrödinger Equation as an eigenvalue-eigenfunction differential equation motivates utilizing a finite difference method to sieve for valid energies.

The application of the finite difference approximation for the second derivative (16) on TISE (9)

$$E\psi = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \right] \psi \Rightarrow$$

$$E\psi_j = -\frac{\hbar^2}{2m} \left[ \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{\Delta x^2} \right] + V_j\psi_j \quad (24)$$

Note the potential is discretized on an identical interval  $\ni \psi(x) \approx \psi(j\Delta x)$  and  $V(x) \approx V(j\Delta x)$  To sieve we use the finite difference TISE to solve for  $\psi_{j+1}$ . By rearranging (24) [Harris [2008]]

$$\psi_{j+1} = \left[ \frac{2m\Delta x^2}{\hbar^2} [E - V_j] + 2 \right] \psi_j - \psi_{j-1} \quad (25)$$

In the form of equation 25, the finite difference method provides a straight forward computation to test possible possible eigenvalues of energy  $E$ . When sieving for solutions to introductory quantum mechanics problems, orientating the basis and potential wisely simplifies the work load. For finite-difference solutions we want to exploit symmetries whenever possible. Many introductory problems are even prompting an approach to sieve in two cases one for even and another for odd wavefunctions. See discussion in Sec 1.2.

- For Even Wavefunctions  $\Psi(x=0) = \psi_0 = 1$
- For Odd Wavefunctions  $\Psi(x=0) = \psi_0 = 0$
- Compute  $\psi_1$  by (24)
- Compute  $\psi_{j+1}$  by (24) to the end of the domain
- Build negative end of domain by symmetry
- Enforce (13) to normalize wavefunction
- Reject Wavefunctions and energy  $E$  which do not satisfy boundary conditions (12)

Enforcing boundary conditions is different for every potential and locating an energy eigenvalue which yields a wavefunction with exactly 0 at the boundary is very unlikely. The following sections use 'natural units'  $\ni \hbar = m = 1$  and identify the particularly tolerance used to consider an eigenvalue.

### 2.1.1 Particle in a Box

$$V(x) = \begin{cases} 0 & : x \in [-2, 2] \\ \infty & : x \notin [-2, 2] \end{cases}$$

With  $V = 0$ , inside the well TISE takes the simple form

$$E\psi = \left[ -\frac{1}{2} \frac{\partial^2}{\partial x^2} \right] \psi \quad (26)$$

The general solution has the form

$$\psi(x) = A \sin(kx) \quad (27)$$

$A$  is some normalization constant and  $k$  the allowed wave numbers  $k \ni k = \frac{n\pi}{L}$ . By the general solution and TISE suggests the energy levels. Griffiths [2005]

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2} \quad (28)$$

When using natural units and the above potential ( $L = 4$ )

$$E_n = \frac{n^2 \pi^2}{32} \quad (29)$$

Particle in a Box sieved solutions were considered valid if the boundary value was below the tolerance  $\psi(x = L/2) \leq 10^{-4}$ . Often many energies will satisfy this boundary condition. When sieving, I often tested energies in steps of  $\Delta E = 10^{-3} - 10^{-4}$ . If multiple energies satisfy the boundary tolerance, then the wavefunction with the lowest boundary value is selected as the eigenfunction. All subsequent sections use a spacial step  $\Delta x = 0.01$

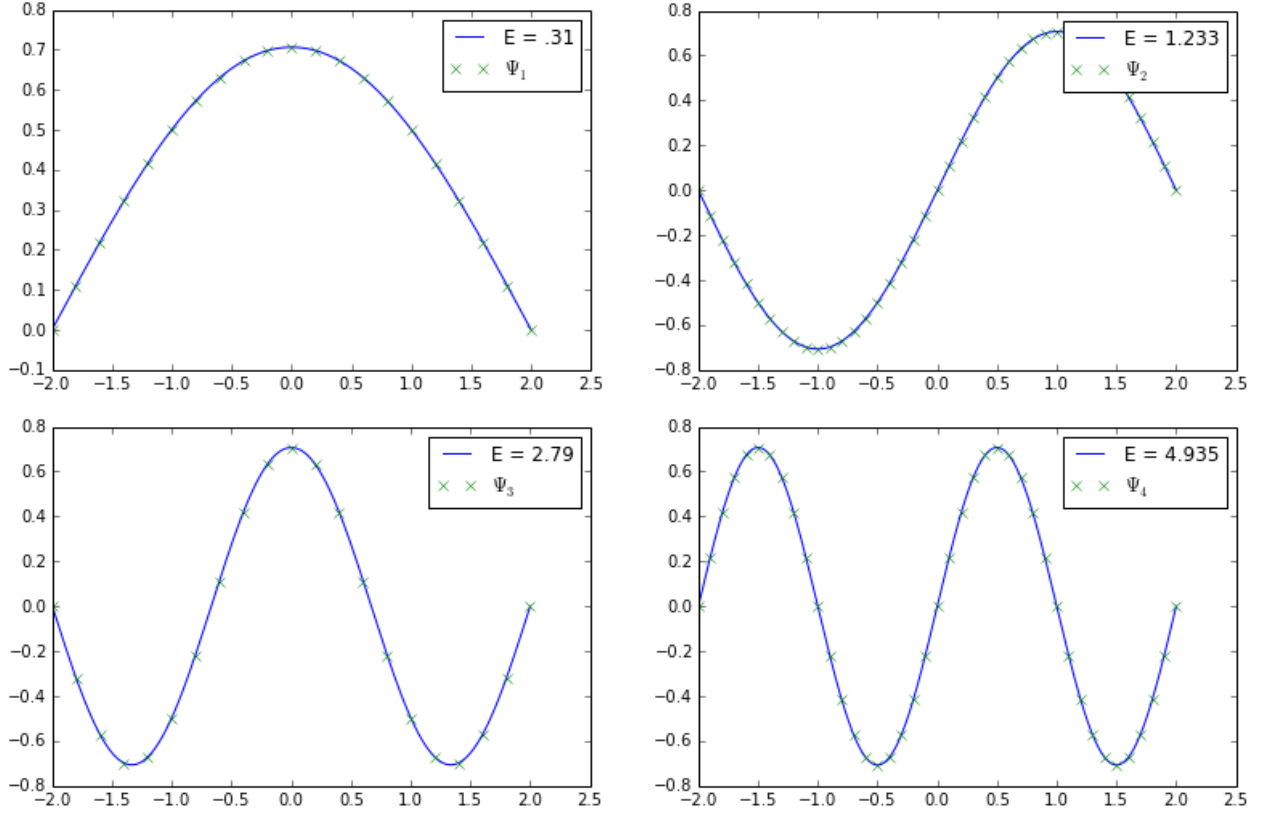


Figure 1: First 4 sieved Quantum Box Wavefunctions (solid) and corresponding analytic functions  $\Psi_n$

Quantum Number	1	2	3	4	5	6	7	8	9	10	11	12	13	15	17
Analytic $E$	$\pi^2/32$	$\pi^2/8$	$9\pi^2/32$	$\pi^2/2$	$25\pi^2/32$	$9\pi^2/8$	$49\pi^2/32$	$2\pi^2$	$81\pi^2/32$	$25\pi^2/8$	$121\pi^2/32$	$9\pi^2/2$	$169\pi^2/32$	$225\pi^2/32$	$289\pi^2/32$
Approximation	0.308	1.234	2.776	4.935	7.711	11.103	15.113	19.739	24.982	30.843	37.319	44.413	52.124	69.396	89.135
Numerical Method	.31	1.233	2.79	4.935	7.75	11.101	15.183	19.733	25.1	30.827	37.48	44.381	52.34	69.67	89.44



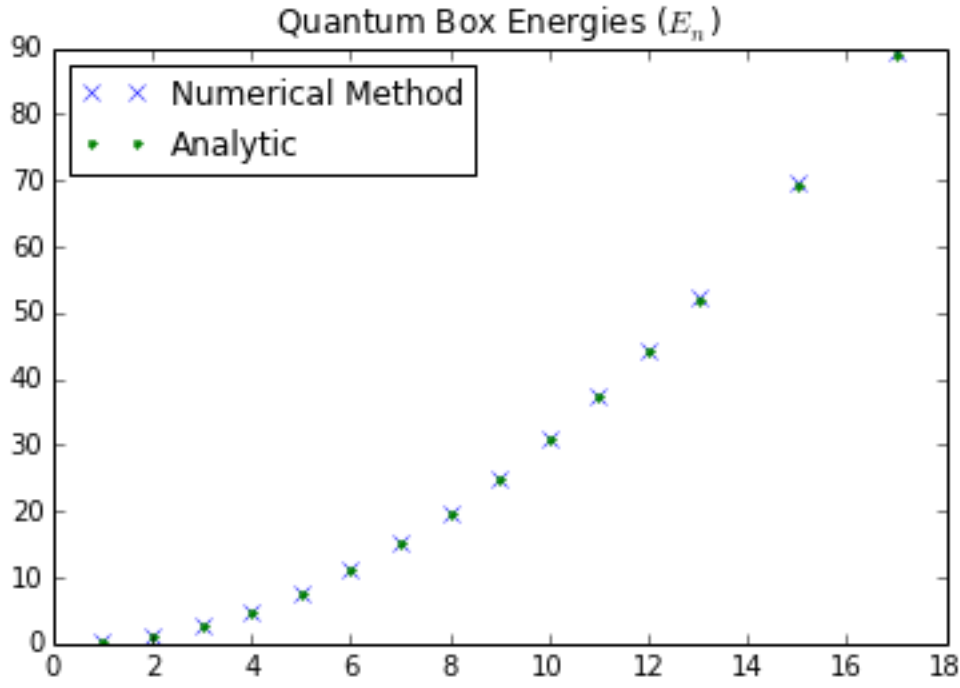


Figure 2:  
Corresponding  
energies for  
analytic and  
numerical  
Wavefunctions  
for the Particle  
in a Quantum  
Box  $E_n \propto n^2$ .  
Largest error  
 $\approx 65$  parts in  
10,000 for  $E_1$

### 2.1.2 Quantum Harmonic Oscillator

For potentials of the form  $V(x) \propto x^2$  analytic solutions yield evenly spaced energies. This potential is analogous to the harmonic oscillator of classical mechanics also studied as Hooke's Law. The strength of the classical potential - the stiffness of a spring is related to the spring constant  $k$  which relates to the frequency of oscillations  $\omega \ni \omega = \sqrt{\frac{k}{m}}$ . Hamiltonians ( $\hat{H}$ ) of this type produce wavefunctions which approach zero at infinity  $\lim_{x \rightarrow \infty} \psi(x) = 0$ . It is impossible to compute the centered-difference sieve infinite times so the checking criteria is relaxed.

$\hat{H}$  for QHO is written in general:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}\omega^2 m \hat{x}^2$$

Yields an energy spectra:

$$E_n = \hbar\omega(n + 1/2)$$

And first several wavefunctions. Griffiths [2005]

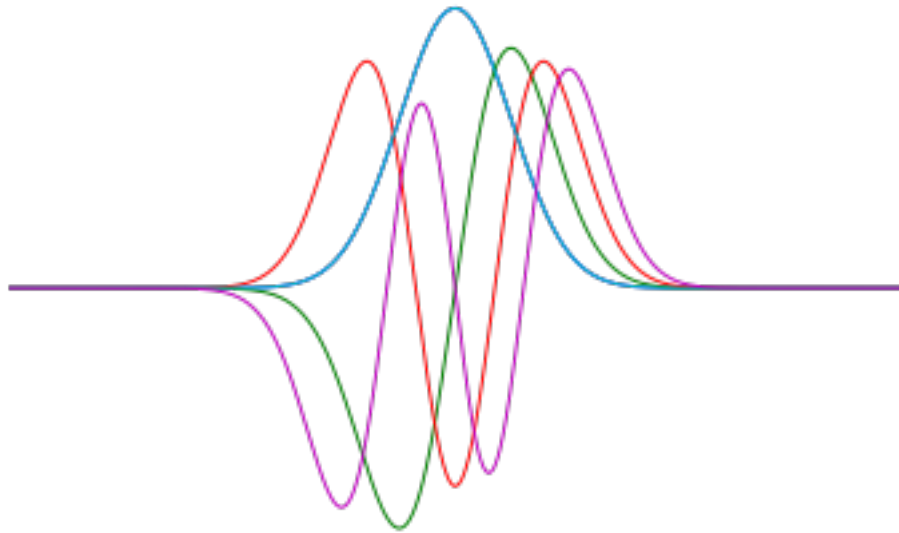


Figure 3:  $n = 0, 1, 2, 3$  Analytic QHO Wavefunctions

QHO ground state energy corresponds to  $n = 0$

If  $V(x) = \frac{x^2}{2}$

then  $E_n = \hbar\omega(n + 1/2) = \hbar(1)(n + 1/2)$

In natural units we expect

$$E_n = n + \frac{1}{2}$$

The first few valid wavefunctions may be sieved with criteria  $\psi(x = 4.5) \leq 10^{-1}$

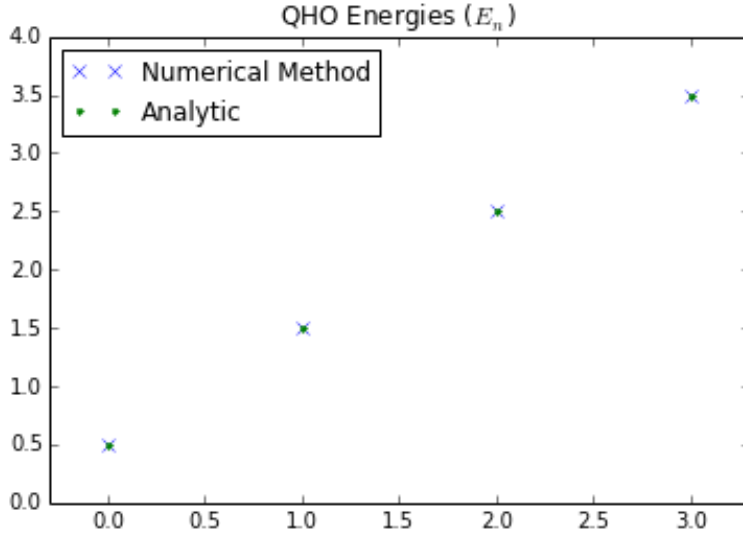


Figure 5: Corresponding energies for analytic and numerical solutions for Quantum Harmonic Oscillator  $E_0, E_1, E_2, E_3, E_n = n + \frac{1}{2}$  Largest error  $\approx 57$  parts in 10,000 for  $E_0$

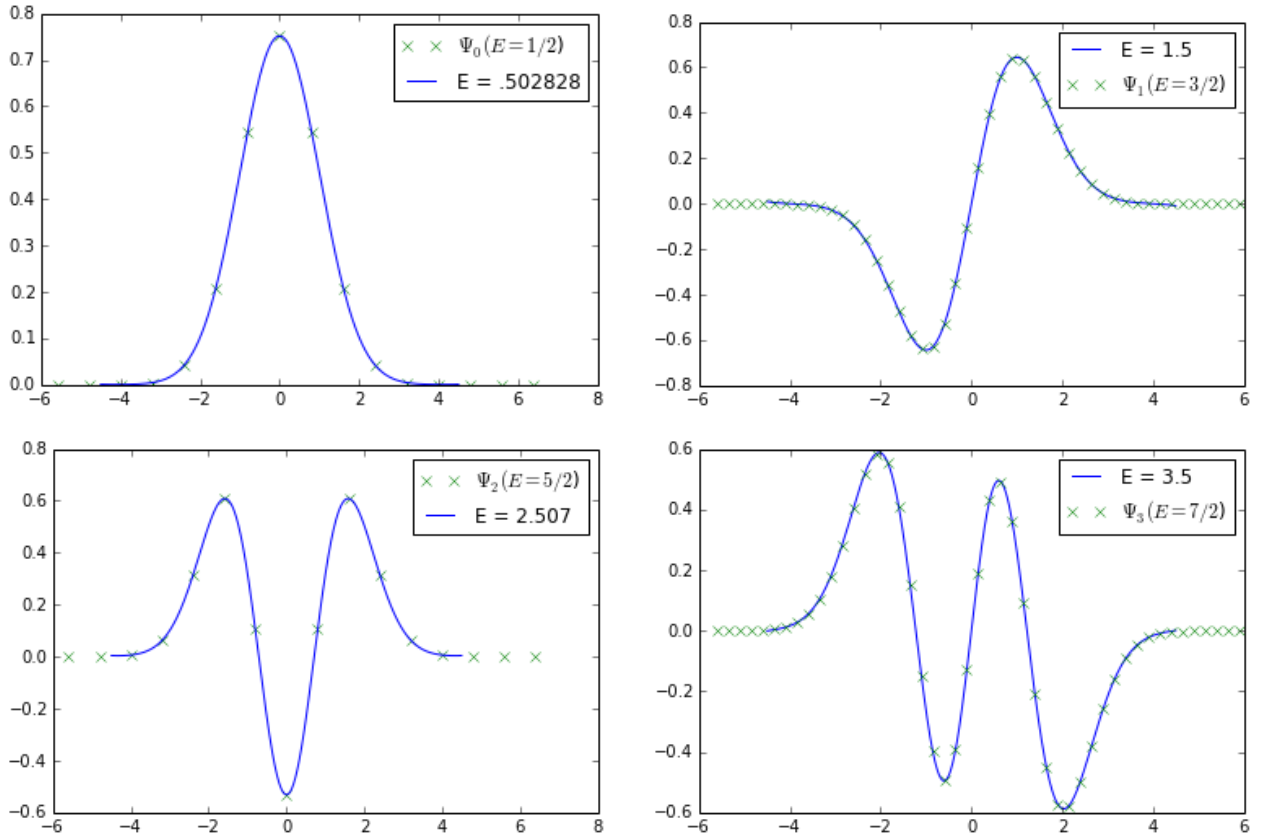


Figure 4: First 4 sieved SHO Wavefunctions (solid) and corresponding analytic functions  $\Psi_n$

### 2.1.3 Nonanalytic solutions

If we perturb the infinite potential box by a constant, degenerate perturbation theory tells us the eigenvalue of the perturbed ground state will shift

$$E_0^1 = E_0 + a \quad (30)$$

Griffiths [2005]

Setting  $V_{bump} = a = 1$  so

$$V(x) = \begin{cases} 1 & : x \in [-2, 2] \\ \infty & : x \notin [-2, 2] \end{cases}$$

In section 2.1.1 centered difference sieve found a ground energy  $E_{Ground} = 0.31$  the centered difference sieve for the perturbed potential with  $V_{bump} = 1$  yields an eigenvalue  $E_0^1 = 1.31$

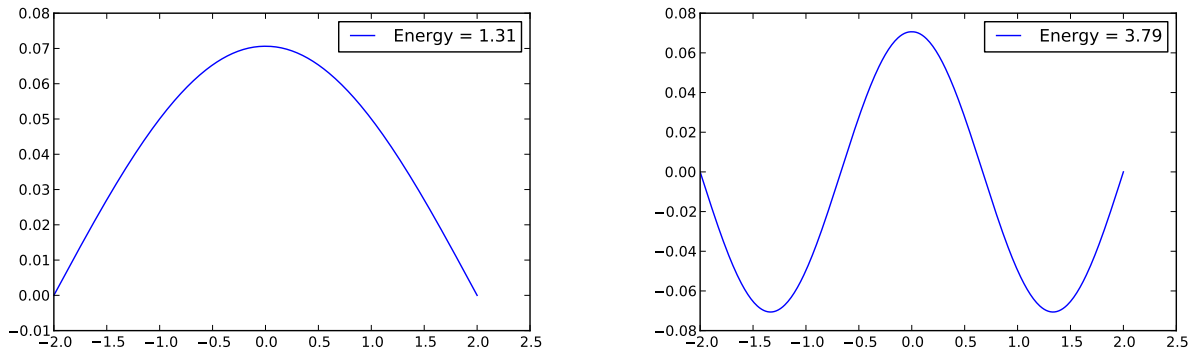


Figure 6: Raised Quantum Box Wavefunctions

Once again the centered difference sieve excels in lieu of convoluted analytic methods. Consider the following potential with finite bumps.

$$V(x) = \begin{cases} -5 & : x \in [-2, 2] \\ 0 & : x \in [-4.5, -2] \cup [2, 4.5] \\ \infty & : x \notin [-4.5, 4.5] \end{cases}$$

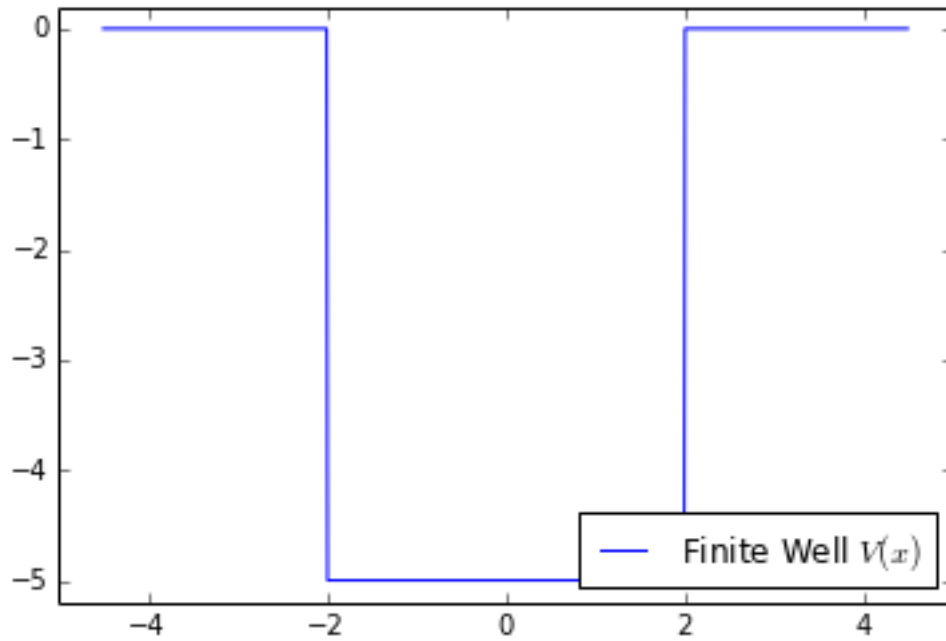


Figure 7: Finite Well Potential

Solving problems with piecewise-constant potentials analytically, even with an ansatz to Airy functions, requires lengthy boundary matching. The center difference sieve quickly builds wavefunctions and selects valid energy eigenvalues.

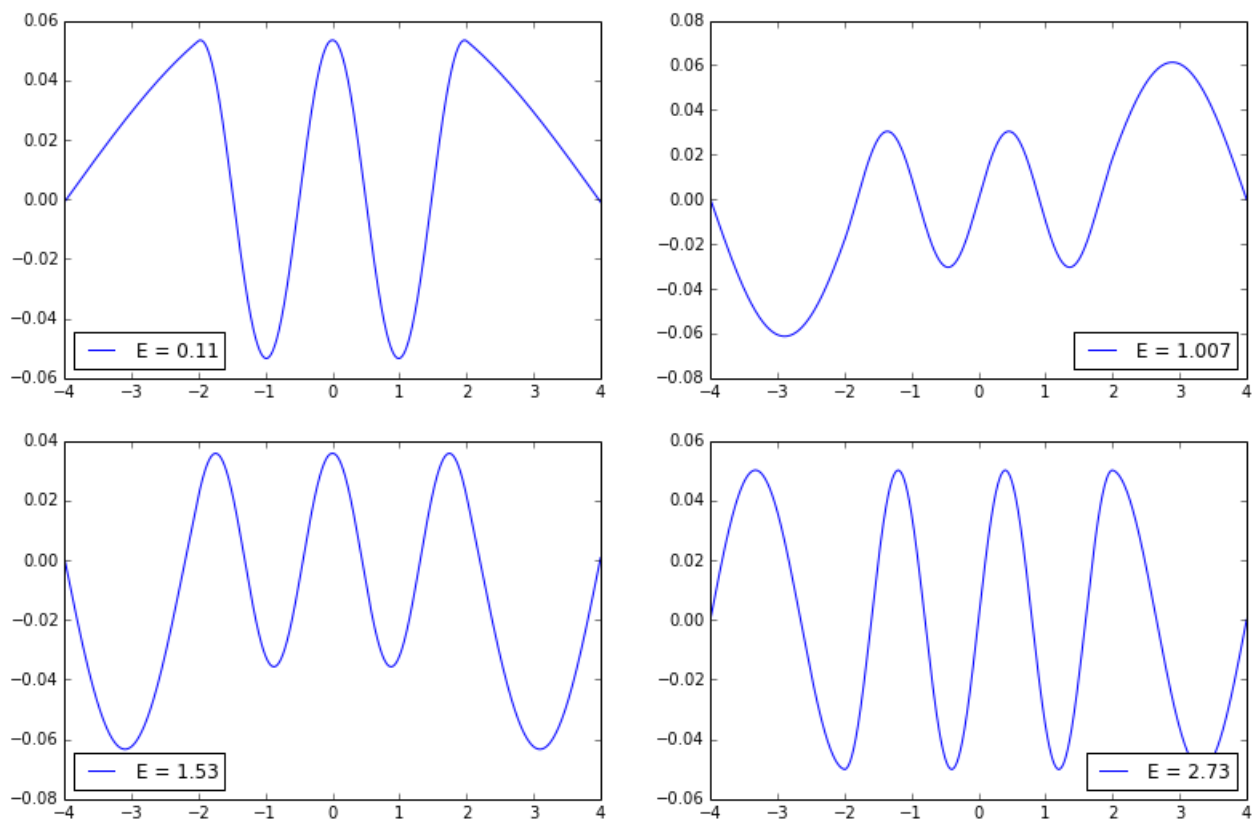


Figure 8: Finite Well Wavefunction Solutions

Next consider

$$V(x) = \begin{cases} -5 & : x \in [-8, -4.5] \cup [-2, 2] \cup [4.5, 8] \\ 0 & : x \in [-4.5, -2] \cup [2, 4.5] \\ \infty & : x \notin [-8, 8] \end{cases}$$

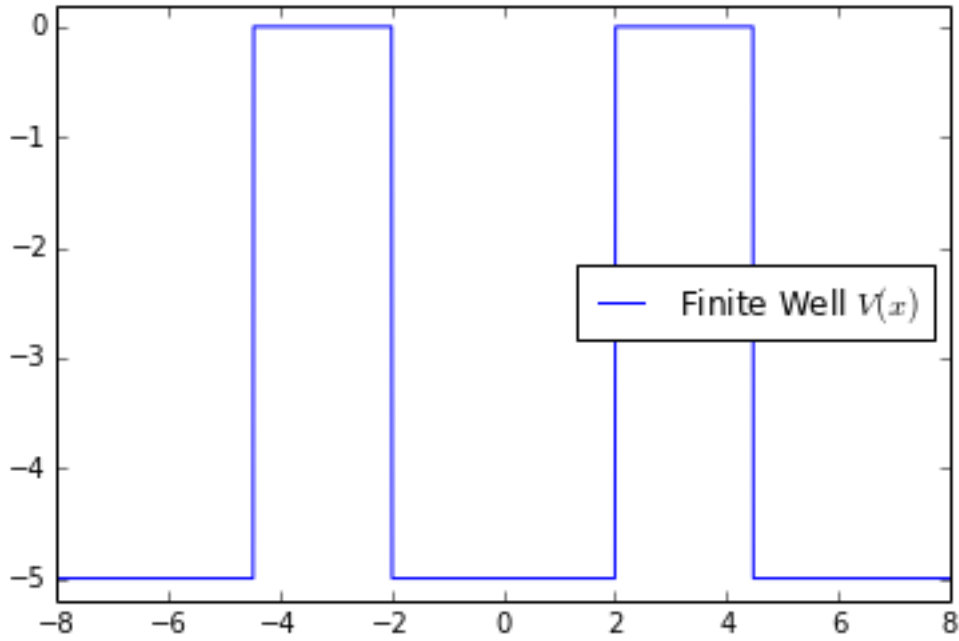


Figure 9: Finite Hills

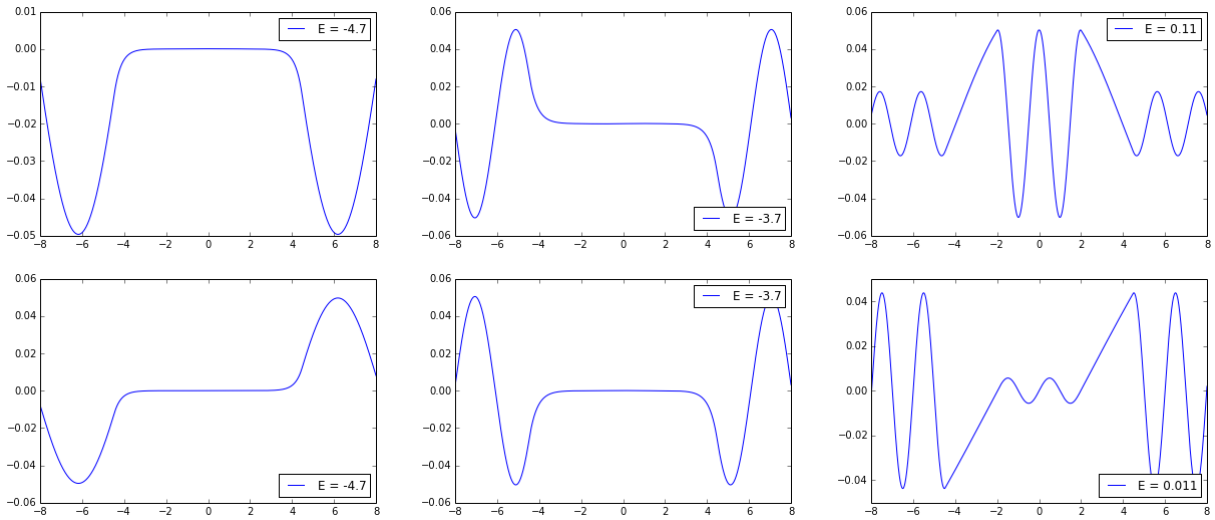


Figure 10: Solutions to potential with two finite hills

Now we consider a similar potential shifted up five units

$$V(x) = \begin{cases} 0 & : x \in [-8, -4.5] \cup [-2, 2] \cup [4.5, 8] \\ 5 & : x \in [-4.5, -2] \cup [2, 4.5] \\ \infty & : x \notin [-8, 8] \end{cases}$$

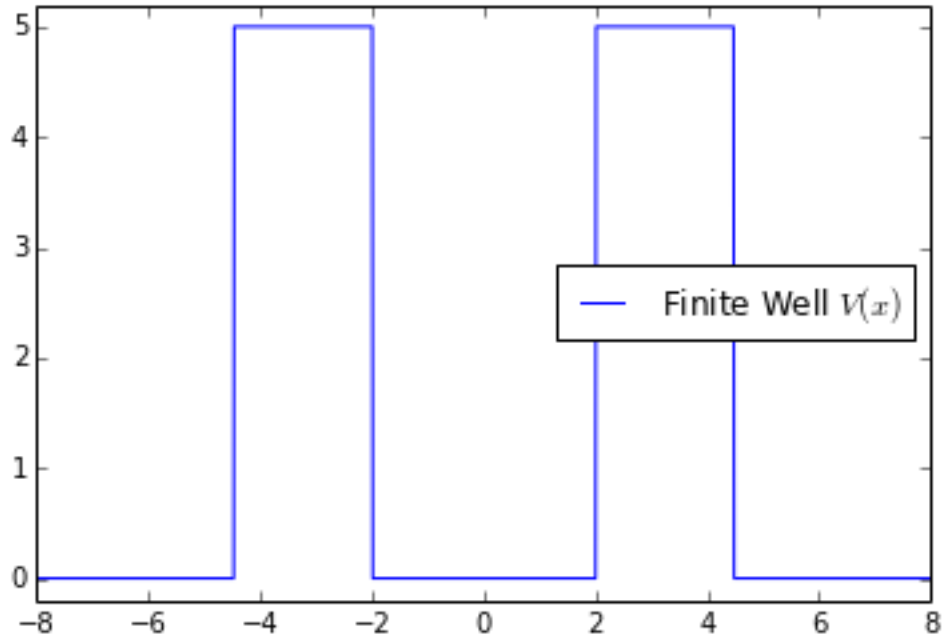


Figure 11: Raised Finite Hills

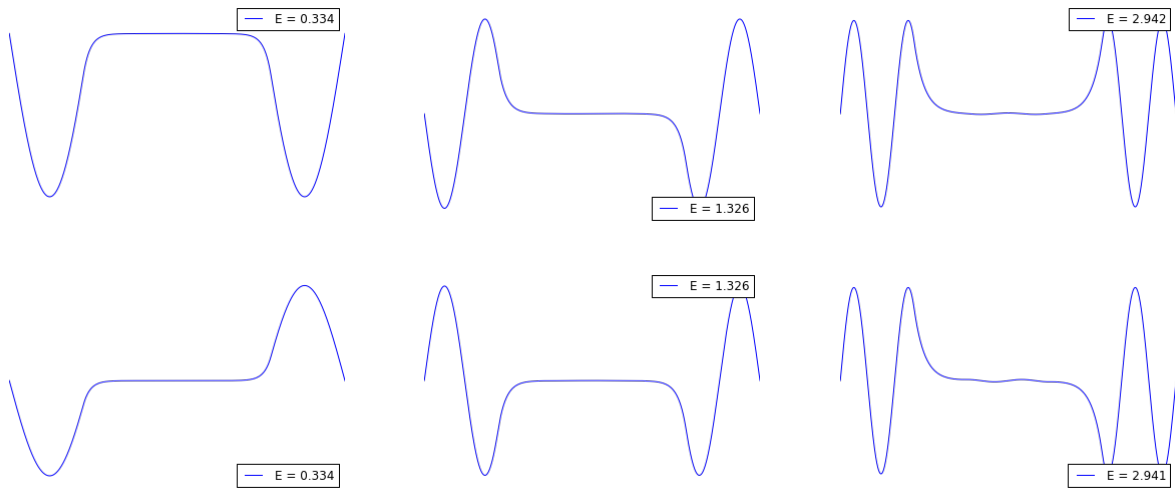


Figure 12: Solutions to raised potential with finite well

From the two previous potentials we can observe a unique degeneracy as eigen energy values have an even and odd form.



## 2.2 Crank-Nicolson on Schrödinger's Equation

The following results apply equation (23) to wavefunctions found using the centered difference sieve utilized in the previous section.

### 2.2.1 Stationary States

Crank-Nicolson schemes are unconditionally stable while the explicit Euler methods [Equation (18)  $\nu = 0$ ] is only stable with a relation criteria for the time-step ( $\Delta t$ ) and spacial discretization ( $\Delta x$ ).

Because of unconditional stability, the Crank-Nicolson scheme may be analyzed for any time-step large or small.

For a particle in a quantum box the time dependent solution has the form

$$\Psi_n(x, t) = \begin{cases} A \sin(k_n x) e^{-i\omega_n t} & : x \in [-L/2, L/2] \\ 0 & : \text{Otherwise} \end{cases}$$

Since  $e^{i\theta}$  oscillates quantum box solutions will retain their  $|\Psi|^2$  shape while the wavefunction  $\Psi$  will lose real magnitude into the complex domain. The following figures demonstrate this oscillation and the stability with a variety of time-steps ( $\Delta t$ ) and iterations of CN-scheme on the first excited state of a particle in a box.

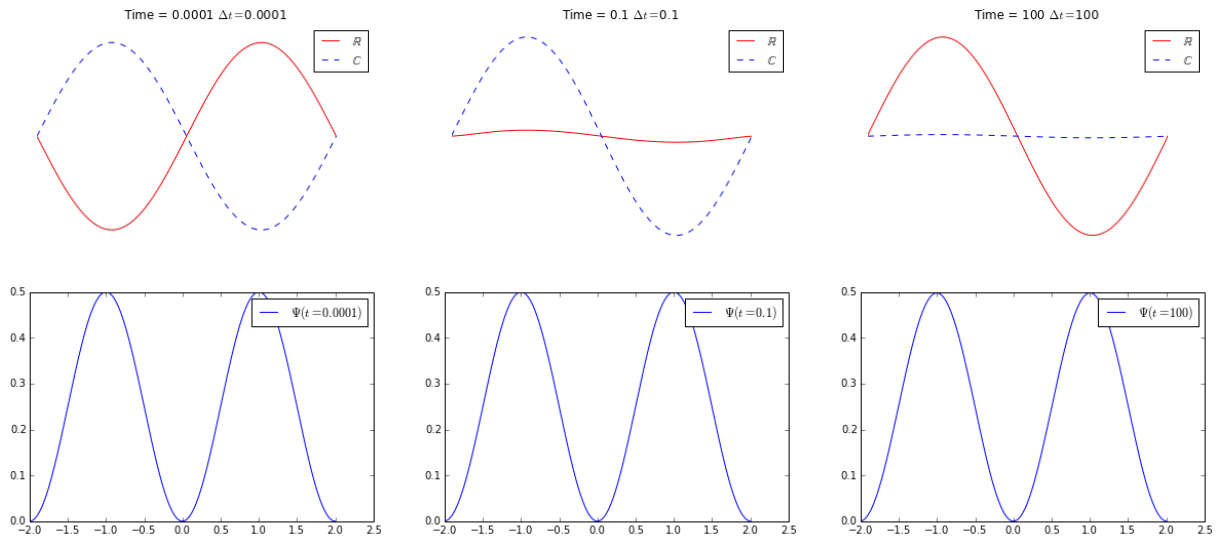


Figure 13: Single Iteration of various time-steps  $\Delta t$

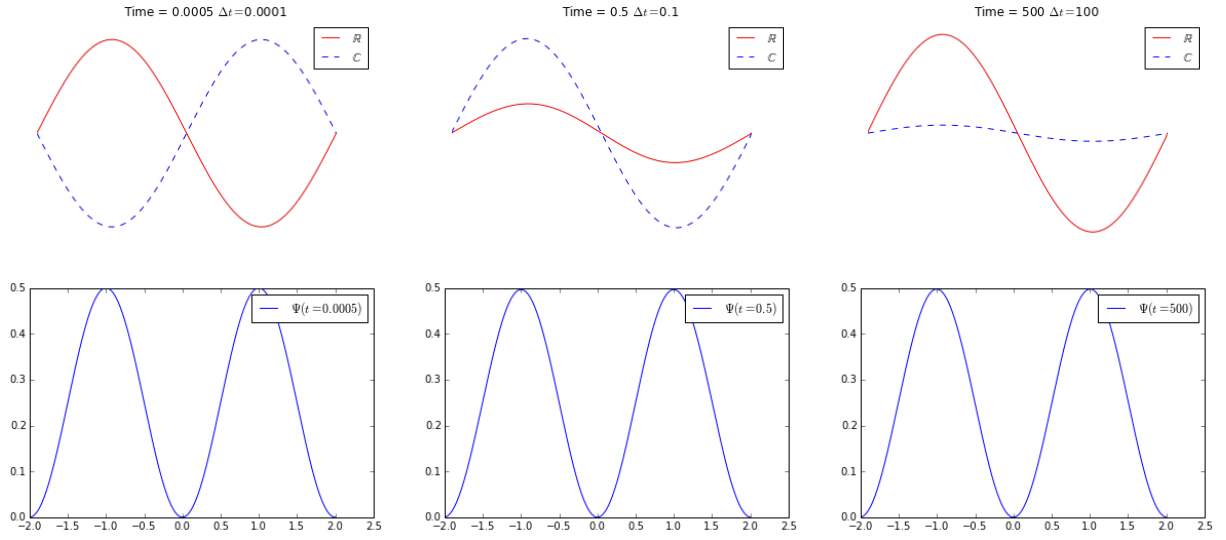


Figure 14: The Fifth Iteration of various time-steps  $\Delta t$

After a large number of iterations the first excited state relaxes to the ground state. Additional steps of this transition are shown in the appendix.

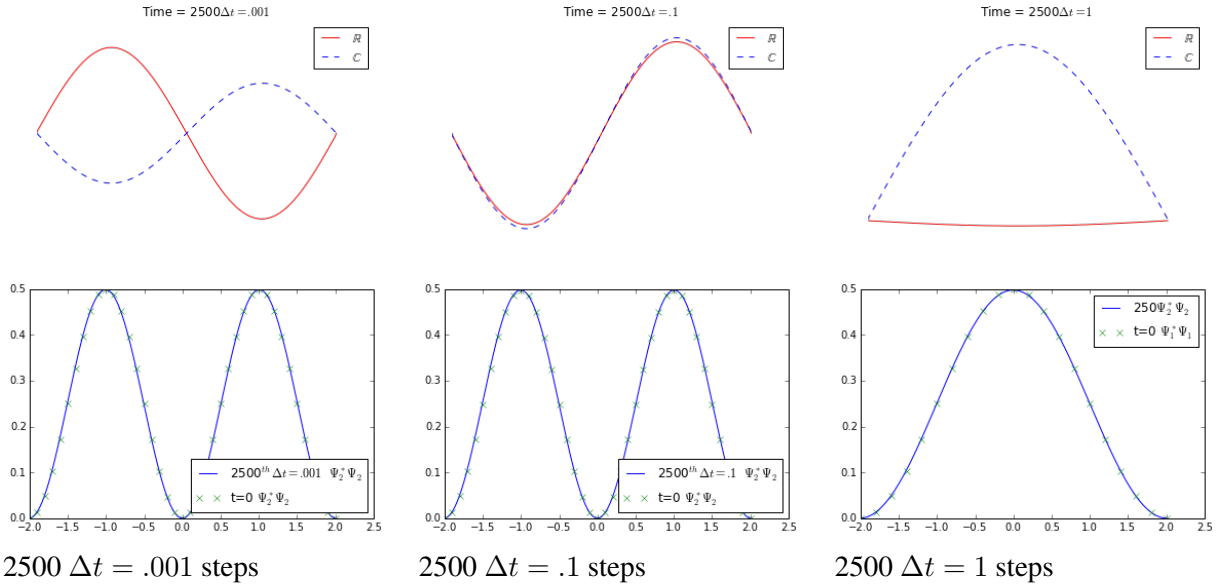


Figure 15: Stability of Quantum Box Time Dependent Wavefunction at the 2500<sup>th</sup> CN iteration

Although analytic time dependent solutions to the simple harmonic oscillator remain stationary, wavefunctions found utilizing a centered difference sieve exist on a truncated domain. While it is

possible to construct a Crank-Nicolson schemes utilizing tridiagonal matrices on a truncated domain, such schemes are beyond this discussion. To correctly time evolve on a truncated domain the tridiagonal matrices must handle the non-zero domain boundary. Below we observe the consequence of the truncated domain. For the Crank-Nicolson scheme in this report, the tridiagonal matrices  $L$  &  $R$  assume there exists a zero-valued wavefunction outside of the domain.

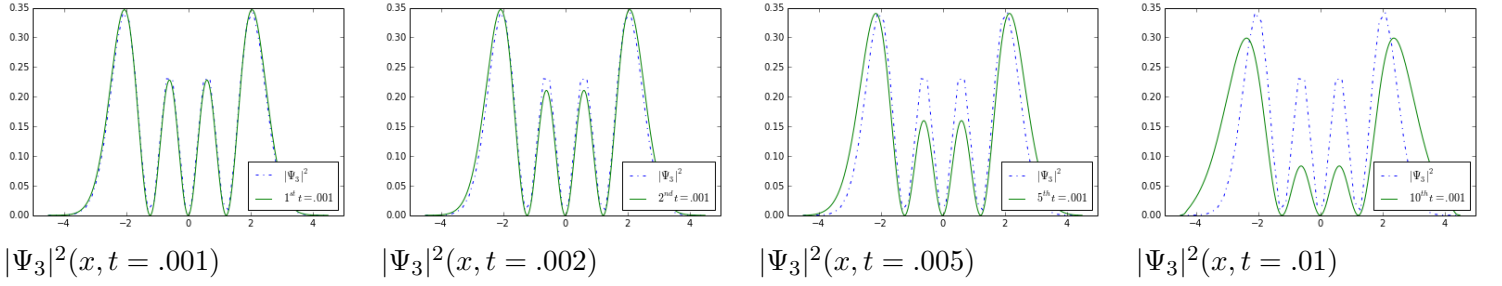


Figure 16:  $\Delta t = .001$  Time Evolutions for the third excited state QHO square wavefunction  $|\Psi_3|^2$

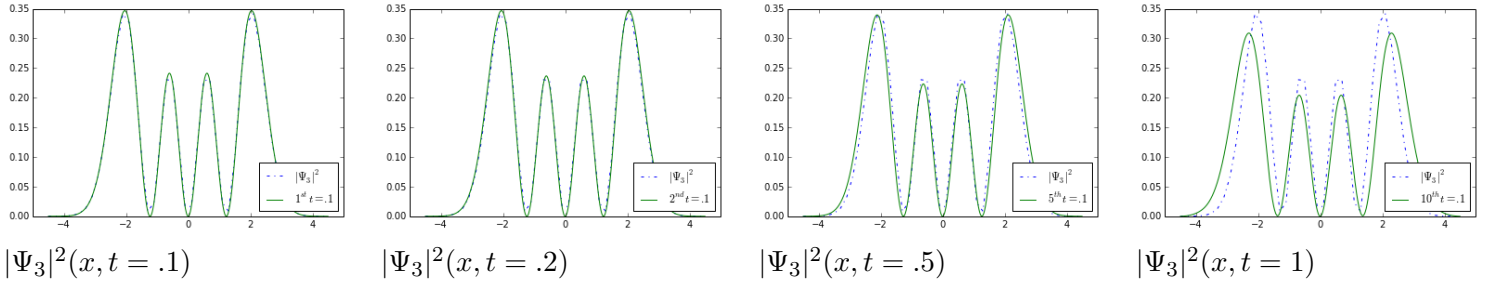


Figure 17:  $\Delta t = 0.1$  Time Evolutions for the third excited state QHO square wavefunction  $|\Psi_3|^2$

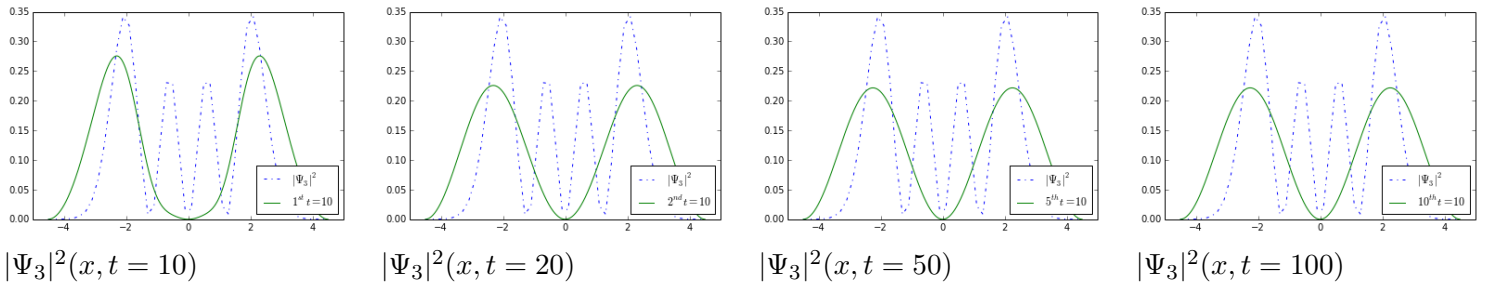


Figure 18:  $\Delta t = 10$  Time Evolutions for the third excited state QHO square wavefunction  $|\Psi_3|^2$

### 2.2.2 Tunneling

In this section, I demonstrate using the Crank-Nicholson scheme to explore the quantum phenomenon of tunneling. There exists no classical analogous to quantum tunneling - classically particles are bound by the surrounding topology if they do not have sufficient kinetic energy to escape. Consider a ball in 1 dimension between two hills whose peaks correspond to 5 joules of potential if the ball were to reach either summit - similar to figure: (11). If this ball is placed between these hills with 2 joule of kinetic energy, the ball will always exists between them and never outside. The small particles in the quantum regime may exist on on either side of a finite hill even if the particle has less energy than the well.

Below a trapped quantum box wavefunction is moved from the infinite boundary to the wider domain of figure: (11)

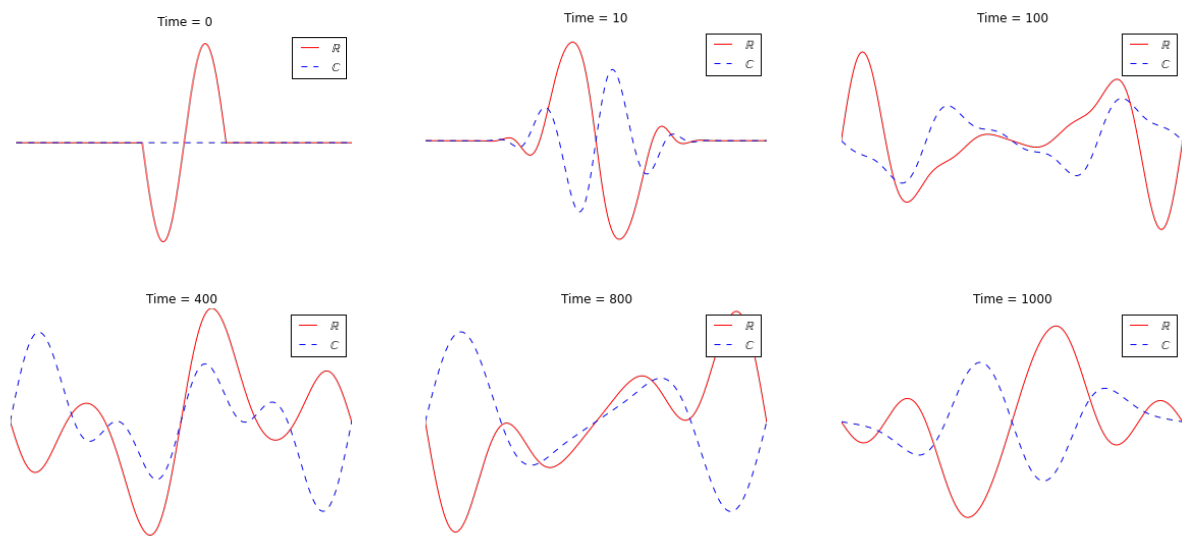


Figure 19: Evolution of Quantum Box  $\Psi_2$  in a potential with finite hills

### **3 Concluding Remarks**

Centered-difference methods provides a quick and accurate approximation to solving differential equations. Sieved energy eigenvalues correlated to analytic energies with less than 1% error. Since so many situations one may describe using Schrödinger's Equation have no analytic solutions, the swift iterative method of centered difference sieves and the Crank-Nicolson Scheme provide a method to investigate the vast quantum world.

## 4 Appendix

### 4.1 More on Time Independent Wavefunctions $\psi$

Additional Quantum Box Solutions

Figure 20: Quantum Box Wavefunctions

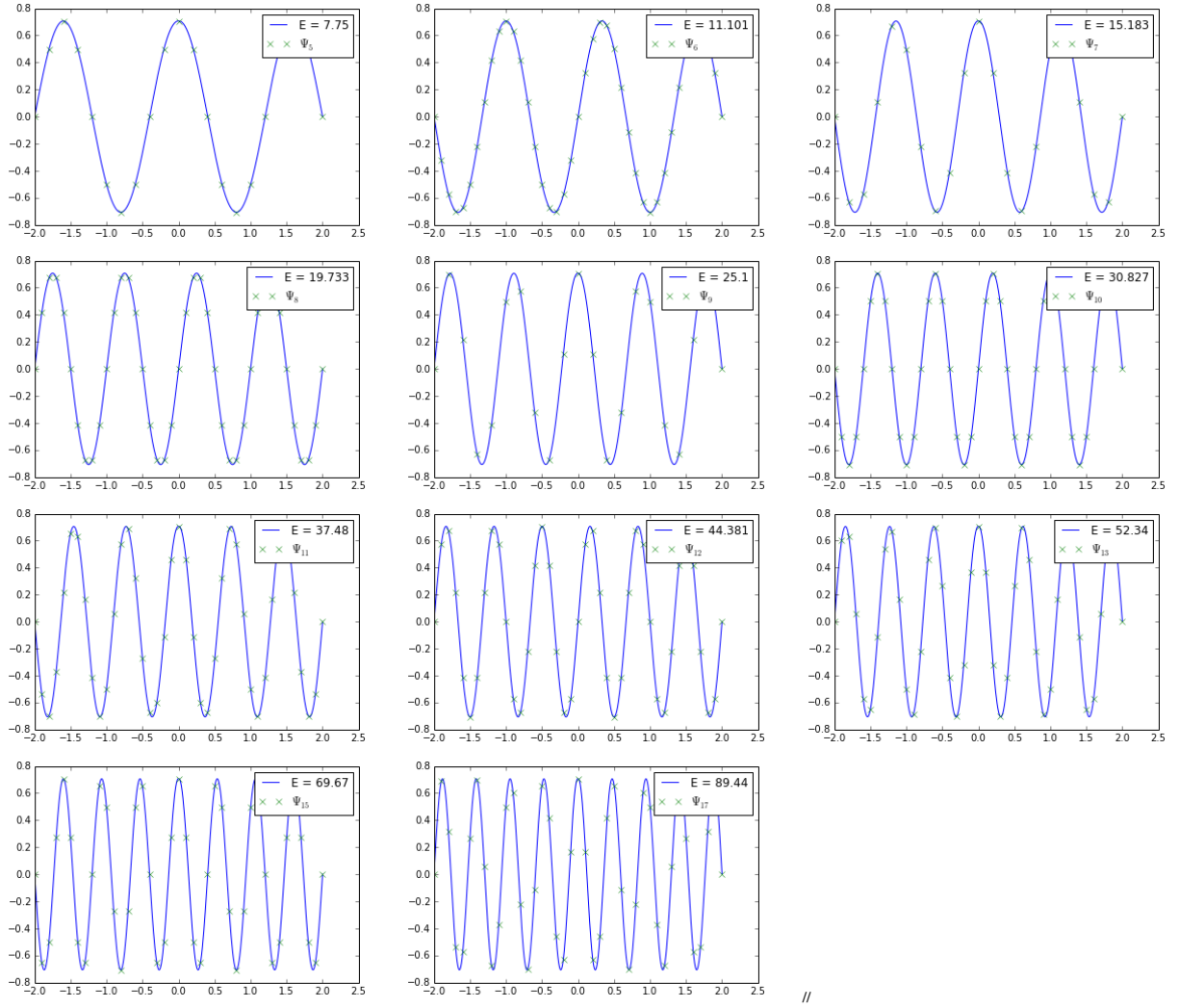


Figure 21: Additional sieved Quantum Box Wavefunctions (solid) and corresponding analytic functions  $\Psi_n$

## 4.2 More on Time Dependent Wavefunctions $\Psi$

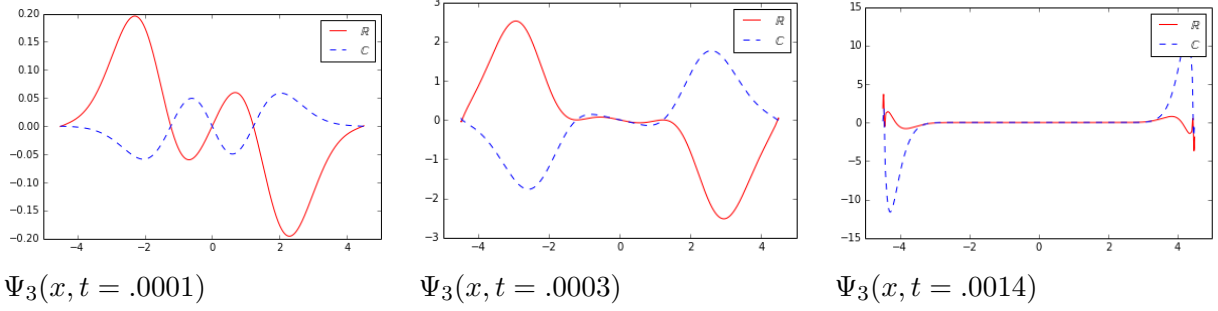


Figure 22:  $\Delta t = 0.0001$  Time Evolutions for the third excited state QHO Wavefunction  $\Psi_3$

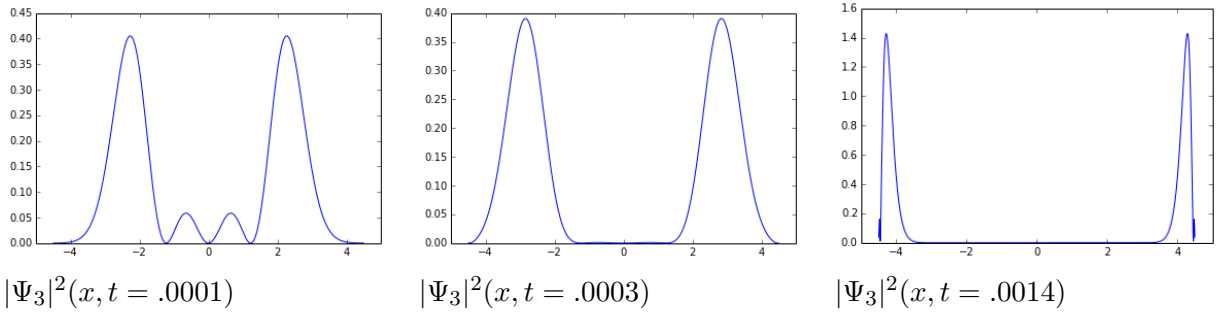


Figure 23:  $\Delta t = 0.0001$  Time Evolutions for the third excited state QHO square wavefunction  $|\Psi_3|^2$

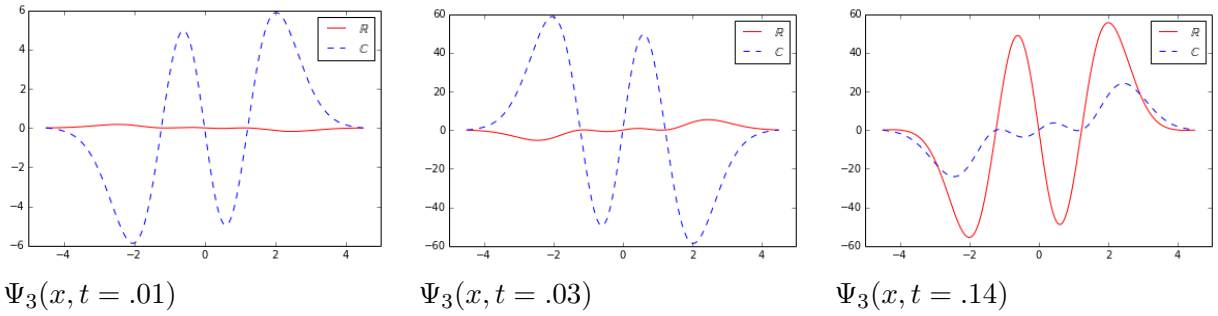


Figure 24:  $\Delta t = 0.01$  Time Evolutions for the third excited state QHO Wavefunction  $\Psi_3$

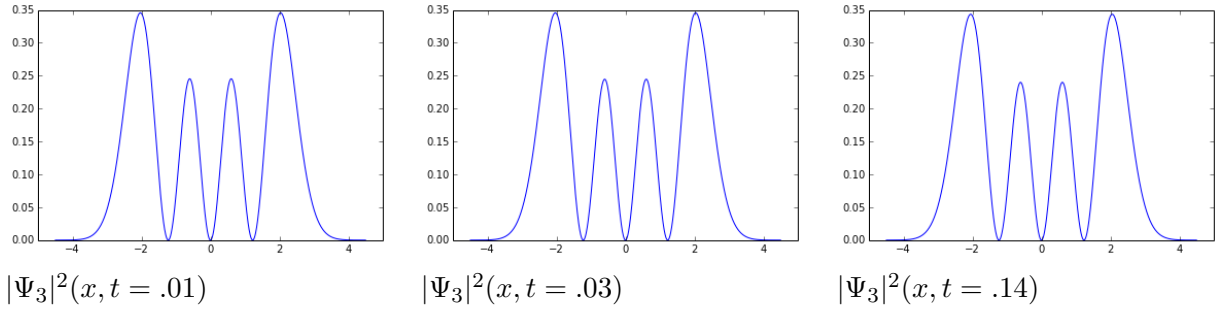


Figure 25:  $\Delta t = 0.01$  Time Evolutions for the third excited state QHO square wavefunction  $|\Psi_3|^2$

#### 4.2.1 Relax Transition

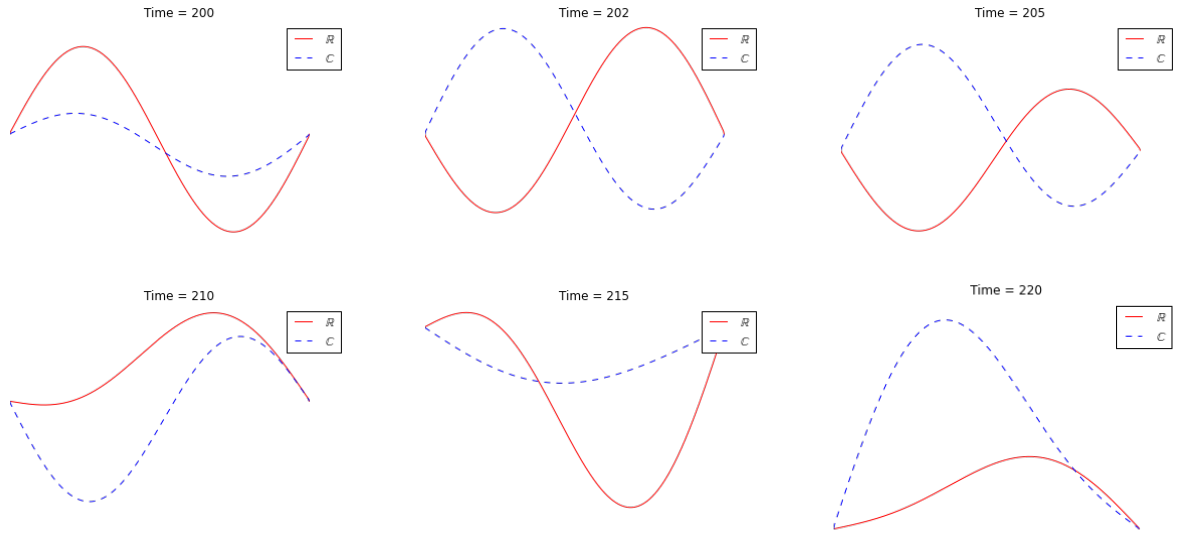


Figure 26:  $\Delta t = 1$  Relaxing Time Evolutions for the first excited state Quantum Box wavefunction  $\Psi_2$



### 4.2.2 Tunneling

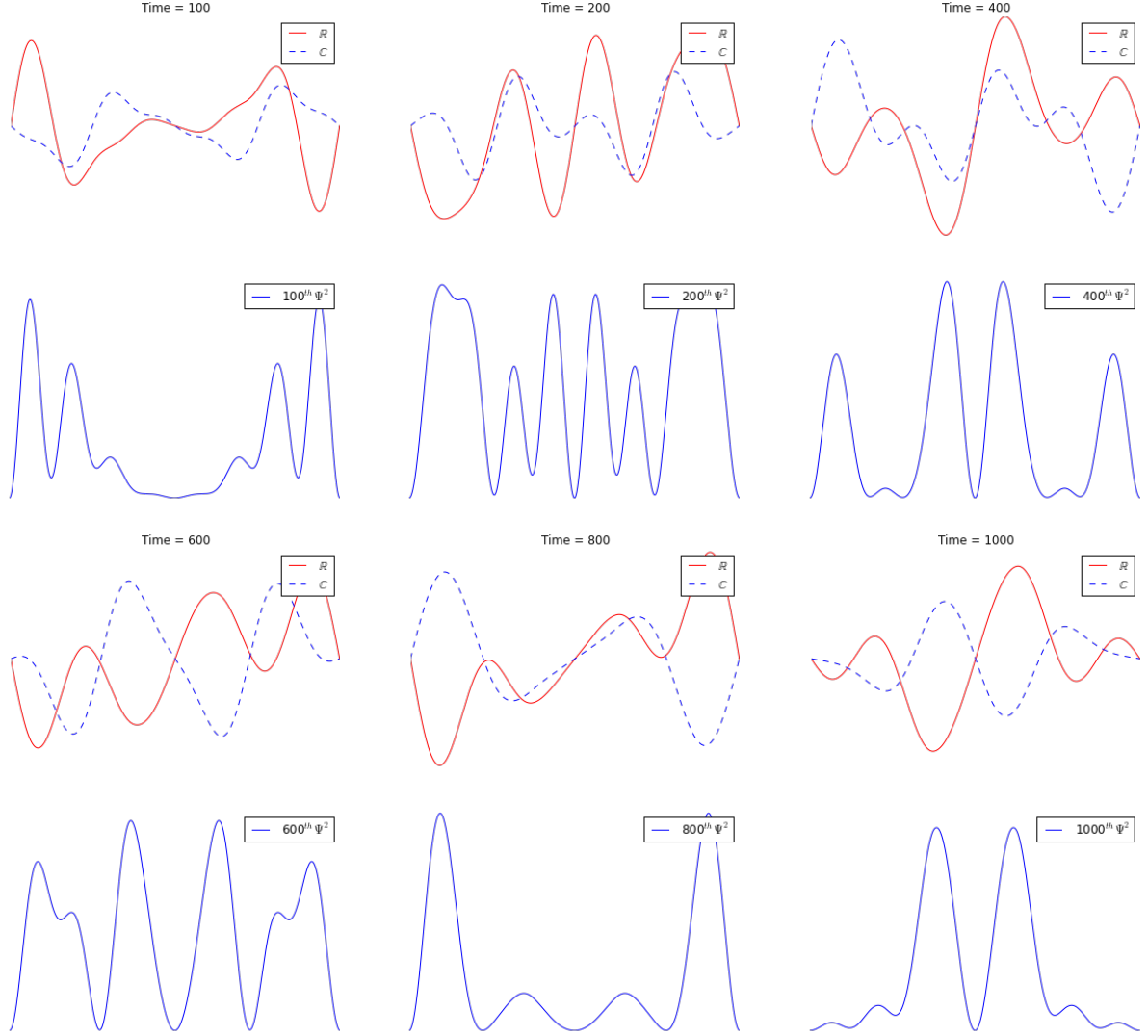


Figure 27:  $\Delta t = 0.01$  Time Evolutions for the third excited state QHO square wavefunction  $|\Psi_3|^2$

## 5 Glossary

Symbol	Expansion
$x, y, z$	Spatial Coordinates
CN	Crank-Nicholson
TISE	Time Independent Schrödinger Equation
$\psi$	Time Independent Wavefunction
TDSE	Time Dependent Schrödinger Equation
$\Psi$	Time Dependent Wavefunction
$\in$	In the Set
$\ni$	Such That
$\forall$	For All
$\mathbb{Z}$	Integer Set
$\mathbb{R}$	Real Set
$\mathbb{C}$	Complex Set
$\cup$	Set Union
$\mathcal{O}$	Order
$\nabla$	Gradient Operator
$F$	Finite Difference Function
$\Delta t$	time-step Interval
$\Delta x$	Spatial Step Interval

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