REVERSIBLE SIMULATION AND VISUALIZATION OF QUANTUM EVOLUTION

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Introduction

Current techniques in quantum simulations are often used to provide insight into a variety of particle interaction phenomenon. These techniques are varied and in recent times have become highly specialized. However, the focus of this project is a more general technique: the finite difference method. Unlike other techniques in quantum simulation, a certain form of finite difference scheme has been shown to be bit-level reversible ([6] pp.337-348). It is this scheme which is analyzed and simulated.

Simulations are becoming more common as learning aids as well. Visualization of elementary phenomenon as well as complex interactions can be useful to the student overwhelmed with the myriad of equations shown in many quantum mechanics courses. Having a method to "see" particle behavior can be an invaluable tool, either when attempting to grasp a concept or interpret complex numerical data. Several methods of visualization are explored for one-dimensional and two-dimensional systems.

For the reversible finite difference scheme, a formal analysis of its consistency, convergence, and stability are presented. In addition, an extension of this scheme into multidimensional systems is provided. A Java simulation of this finite difference scheme is used to verify many results experimentally and investigate other issues. Different visualization methods are explored in Java as well.

Chapter 2

Particle Evolution

To begin investigations into different finite difference schemes, several basic ideas from quantum mechanics are necessary. A knowledge of quatum mechanics is not required to understand the basics of the discrete simulation, but familiarity with the results will help in interpreting certain physical aspects of the simulation.

To move into the realm of quantum mechanics, one must replace the classical concept of a particle as a point with the analogous concept of a particle as a wave function $\psi(\overrightarrow{r}, t)$. The wave function represents all the information one can obtain about the particle. Whereas the classical state of a particle can be completely determined by specifying the position and velocity at a given time, the quantum state requres a specification of the function $\psi(\overrightarrow{r}, t)$. This wave function propagates over time (much as a classical particle simply moves from one point to another). It is this evolution that is modelled mathematically by the Schrödinger equation.

2.1 The Schrödinger Equation

When any particle is subject to a potential $V(\overrightarrow{r}, t)$ the corresponding motion of that particle is given approximately by

$$i\hbar\frac{\partial}{\partial t}\psi(\overrightarrow{r}, t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\overrightarrow{r}, t) + V(\overrightarrow{r}, t)\psi(\overrightarrow{r}, t)$$

where m is the mass of the particle, $\hbar$ is Plank's constant divided by 2π, and $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$. This is the widely used Schrödinger equation. It is a linear differential equation that is second order in space and first order in time. It gives a description of the motion of $\psi(\overrightarrow{r}, t)$. It should be noted that the wave function $\psi(\overrightarrow{r}, t)$ is usually complex, this can be seen from the constant i written on the left-hand side of the Schrodinger equation. In order for equality to be maintained, it is necessary that the wave function $\psi(\overrightarrow{r}, t)$ have an imaginary component (or trivially, $\psi(\overrightarrow{r}, t) = 0$).

When considering a particle in one dimension, the Schrödinger equation takes the slightly simpler form

$$i\hbar\frac{d}{dt}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x,t) + V(x,t)\psi(x,t).$$

It is this form which is the basis for the majority of the analysis and simulations. Although exact solutions are known for several systems, in general the solution to this equation can be quite difficult. Knowing simple formulas for approximating the derivative of a function gives several ways to rewrite this equation in a discrete form. However, before considering discrete schemes it is useful to determine what happens in the continuous case.

For the reader without a prior physical undertanding of the problem, the basic goal lies in simulating a discrete version of this differential equation. Given some initial condition $\psi(\vec{r},0)$, we wish to be able to determine the state of the system $\psi(\vec{r},t)$ at any time t > 0. The relationship between $\psi(\vec{r},t)$ and $\psi(\vec{r},0)$ can be determined by using the Schrödinger equation.

One of the basic assumptions of nonrelativistic quantum mechanics is that the variables describing space are independent of those describing time. Because of this, we can consider solutions of the form $\psi(x,t) = \varphi(x)\chi(t)$ and use the separation of variables technique ([8] p.213). If the potential $V(x,t)$ has no time dependence, the Schrödinger equation can be rewritten in its time-independent form

$$E\varphi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi(x) + V(x)\varphi(x) \tag{2.1}$$

where $\psi(x,t) = \varphi(x)e^{-i\omega t}$ gives the time-dependent wavefunction and $E = \hbar\omega$. For a more detailed introduction to the Schrödinger equation, the reader is advised to consult [8].

2.2 Evolution of a Free Particle

The most natural question when one first encounters the Schrödinger equation is what predictions does it make for a particle with no forces acting on it. This simplifies the equation greatly, and allows a general insight to be gained into the evolution of any particle. To begin, we simply rewrite the Schrodinger equation in one dimension with the potential $V(\vec{r},t) = 0$. With this constraint, the equation simplifies into

$$i\hbar\frac{d}{dt}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x,t).$$

It is important to notice that this equation is solved by "plane waves," wave functions of the form $\psi(x,t) = e^{i(kx-\omega t)}$ whenever $\omega = \frac{\hbar k^2}{2m}$. This result is obtainable through the separation of variables given above and easily verifiable through direct substitution (see [8] pp. 210-211).

Since the Schrödinger equation is linear, then any linear combination of these plane waves is also a solution. Superpositions of plane waves give a mathematical model of the evoluion of a free particle. Considering ω as a function of k, any superposition of these plane waves may be written as

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(k) e^{i(kx - \omega(k)t)} dk \tag{2.2}$$

for some function $g(k)$ (see [1] pp. 22-23). Any wave function that can be written as a superposition of plane waves is said to be a "wave packet". The complicated movement of a free particle is then reduced to specifying a single equation of one variable: $g(k)$. Determining $g(k)$ completely determines the movement of the wavefunction at any time t in this case. Fortunately, there is a simple method of determining $g(k)$ for any set of good initial conditions $\psi(x,0)$.

If we take $t = 0$, then immediately

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(k) e^{ikx} dk$$

and it can be seen that $\psi(x,0) \Leftrightarrow g(k)$ form a Fourier transform pair.

It is important to realize the power of this set of equations. For any set of good initial conditions $\psi(x,0)$, the state of the system at any time $t > 0$ can now be determined in two simple steps:

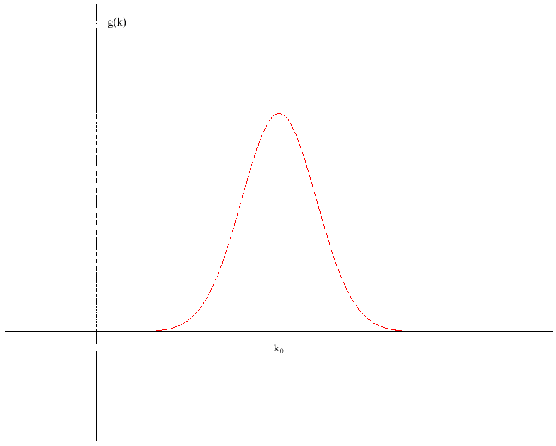
1. Find $g(k)$, the Fourier transform of $\psi(x,0)$.
2. Use 2.2 to determine the value of the wave function at an arbitrary time t.

Even in the event that these steps cannot be performed analytically, these equations can be integrated numerically. This numerical integration is usually far less computationally expensive than the discrete style of simulation which is the focus of this paper. However, these equations hold only when $V(\vec{r},t) = 0$. In the case of a stationary potential $V(\vec{r})$ or a time-varying potential $V(\vec{r},t)$, these simple method will not work. For many stationary potentials $V(\vec{r})$, a similar trick may be used, however. The time-varying potential $V(\vec{r},t)$ is the case where direct simulation of the quantum system is usually considered the best approach. Therefore, for a simulation to be truly useful, it should be able to work with a time-varying potential $V(\vec{r},t)$.

2.3 Evolution of a Free Gaussian Wave Packet

The one-dimensional Gaussian wave packet is defined to be the superposition of plane waves e^{ikx} with the function $g(k)$ taken to be a Gaussian distribution [2]. It is useful to have an intuitive idea of the shape of this wave packet, and explicit formulas for its evolution. Recall that specifying $g(k)$ for a free particle completely determines the entire solution. In this case it is possible to write explicit formulas for both the initial state $\psi(x,0)$ and the state at any time

Figure 2.1: Gaussian Distribution



t: $\psi(x,t)$. First, let $g(k) = \frac{\sqrt{a}}{(2\pi)^{\frac{1}{4}}} e^{-\frac{a^2}{4}(k-k_0)^2}$ (see Figure 2.1), the direct formula for a gaussian distribution.

From this formula for $g(k)$, the inital state of the wave packet is easily determined. Recall that $\psi(x,0) \Leftrightarrow g(k)$ form a Fourier transform pair. This gives:

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(k) e^{ikx} dk.$$

Substituting the gaussian expression for $g(k)$,

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \left(\frac{\sqrt{a}}{(2\pi)^{\frac{1}{4}}} e^{-\frac{a^2}{4}(k-k_0)^2} \right) e^{ikx} dk.$$

This expression can be integrated directly, and the wave function $\psi(x,0)$ is given explicitly by ([2])

$$\psi(x,0) = \left(\frac{2}{\pi a^2} \right)^{\frac{1}{4}} e^{ikx} e^{-\frac{2x}{a^2}^2}. \tag{2.3}$$

As expected, the Fourier transform of a gaussian distribution is gaussian. Finally, the wave function at $t \geq 0$ is determined by substituting our specified function $g(k)$ into equation 2.2:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(k) e^{i(kx - \omega(k)t)} dk.$$

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \left(\frac{\sqrt{a}}{(2\pi)^{\frac{1}{4}}} e^{-\frac{a^2}{4}(k-k_0)^2} \right) e^{i(kx - \omega t)} dk.$$

This integral can also be evaluated analytically, the result being the general formula for the evolution of a gaussian wave function when $V(x,t) = 0$:

$$\psi(x,t) = \left(\frac{2a^2}{\pi}\right)^2 \frac{e^{i\phi}}{\left(a^4 + \frac{4\hbar^2 t^2}{m^2}\right)^{\frac{1}{4}}} \exp\left\{-\frac{\left(x - \frac{\hbar k_0}{m}t\right)^2}{a^2 + \frac{2i\hbar t}{m}}\right\} e^{ik_0 x} \qquad (2.4)$$

where $\phi = -\theta - \frac{\hbar k_0^2}{2m}t$, and $\tan 2\theta = \frac{2\hbar t}{ma^2}$ ([2] p. 64). Though this function appears complicated, there is no need to work with it any further aside from simulation. Also it should be noted that when $t = 0$ then $\phi = 0$ and the equation simplifies into equation 2.3.

Each of these formulas and results are useful for even a discrete simulation. To initialize any simulation, it is necessary to provide initial conditions. Usually these inital conditions are taken to be gaussian wave packet. Also, it is useful to compare the simulated free particle evolution to the analytic solution given above. Comparing a simulated result to the exact solution gives an empirical method to determine the accuracy in certain cases. Since in many instances the Schrödinger equation is difficult to solve, the solution to the free particle case is useful because it is realtively easy to obtain analytically and easy to implement.

2.4 One-Dimensional Harmonic Oscillator

A final case to consider in simulation and theory is that of the simple harmonic oscillator. In classical mechanics, this corresponds to a mass-spring system. The mass on the spring feels a "restoring" force proportional to the distance x that it has traveled away from its resting point. Since the force is proportional to x, the particle is trapped in a parabolic potential energy "well." The classical particle remains trapped and oscillates around its resting point indefinitely.

In quantum mechanics, the simple harmonic oscillator gives a similar result. The motion of the particle is given when one sets $V(x)$ to a quadratic in Schrödinger's equation. However, to provide useful results, we need to first consider what happens in the stationary case. From the time-independent Schrödinger equation

$$E\varphi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi(x) + V(x)\varphi(x)$$

the potential $V(x)$ is set to a quadratic $V(x) = \frac{1}{2}m\omega^2 x^2$.The solution to this equation is somewhat involved[1] and we simply present the result without proof. Solutions to this equation have the form ([3] p. 533)

$$\varphi_n(x) = \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} e^{-\beta^2 x^2/2} H_n(\beta x)$$

[1] For a detailed discussion of the solution to the harmonic oscillator and its solution, see [3], chap. 5.

where H_n are the Hermite polynomials, and $\beta = \sqrt{\frac{m\omega}{\hbar}}$. This result will be used later, when simulating systems of this type.

Chapter 3

Finite Difference Schemes

The finite difference method provides a simple and powerful idea for simulating or numerically solving differential equations. However, when used naively, the results obtained are often unsatisfactory. Fortunately, there are established theories which allow the effectiveness of particular schemes to be determined analytically.

In a finite difference scheme, the derivatives in a differential equation are replaced by finite differences on a grid. This grid is a set of evenly spaced points: a discretization of any variables involved in the differential equation. In the case case of Schrödinger's equation, the continuous variables x and t need to be replaced by discrete versions x_i and t_n. Based on this grid, formulas approximating derivatives can be determined, and used to simulate a differential equation.

A simple example of this is the formula

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{\triangle x}$$

where $\triangle x$ is the spacing between grid points, i.e. $x_{i+1} - x_1 = \triangle x$. The key idea in making this substitution is that if the grid spacing $\triangle x$ approaches 0, then the finite difference formula must approach the actual derivative. In this case,

$$f'(x_i) = \lim_{\triangle x \to 0} \frac{f(x_{i+1}) - f(x_i)}{\triangle x}$$

is simply the definition of the derivative, and the finite difference formula must be valid. When a difference formula does approach the derivative it seeks to approximate, that formula is said to be consistent.

3.1 Centered Difference Formulas

The only type of finite difference used in the reversible Schrödinger system is the centered difference. Because of this, the centered differences should be mentioned before presenting the discrete version of Schrödinger's equation.

The centered difference formula for the first derivative in one dimension is given as

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{2h}. \tag{3.1}$$

In this formula, $x_{i+1} - x_i = h$. The validity of this formula, if not immediately apparent, can be seen by writing out the Taylor expansions for $f(x+h)$ and $f(x-h)$:

$$f(x+h) = f(x) + f'(x)h + f''(x)h^2 + O(h^3)$$
$$f(x-h) = f(x) - f'(x)h + f''(x)h^2 - O(h^3).$$

The $O(h^3)$ term is written using the useful "Big Oh" notation[1]. Taking the difference of these Taylor expansions gives

$$f(x+h) - f(x-h) = 2f'(x)h + 2O(h^3)$$

which can be rewritten in the form of equation 3.1.

$$2f'(x)h = f(x+h) - f(x-h) - 2O(h^3)$$
$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{O(h^3)}{h}$$
$$f'(x) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2),$$

where we have used $x_{i+1} = x_i + h$, and the definition of the "Big-Oh" notation. This equation is called a centered difference formula since to approximate the derivative at each point x_i we evaluate f at two points centered around x_i, namely points x_{i+1} and x_{i-1}.

The centered difference formula for the second derivative in one dimension is given as

$$f''(x_i) \approx \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{2h^2}. \tag{3.2}$$

The validity of this formula is also verified by considering the Taylor expansions for the various terms:

$$f(x+h) = f(x) + f'(x)h + f''(x)h^2 + f^{(3)}(x)h^3 + O(h^4)$$
$$f(x-h) = f(x) - f'(x)h + f''(x)h^2 - f^{(3)}(x)h^3 + O(h^4).$$

Instead of their difference, now consider their sum:

$$f(x+h) + f(x-h) = 2f(x) + 2f''(x)h^2 + 2O(h^4).$$

Rearranging terms gives the form of equation 3.13:

$$2f''(x)h^2 = f(x+h) + f(x-h) - 2f(x) - 2O(h^4).$$

[1] For a mathematical definition of "Big Oh" and "Little Oh" notation in the context of finite difference schemes, see [7] p.21.

$$f''(x) = \frac{f(x+h) + f(x-h) - 2f(x)}{2h^2} - \frac{O(h^4)}{h^2}.$$

$$f''(x) = \frac{f(x_{i+1}) - 2f(x) + f(x_{i-1})}{2h^2} + O(h^2)$$

after absorbing the constant -1 into the $O(h^2)$ term.

With an understanding of centered differences, one can derive the particular reversible finite difference scheme analyzed here.

3.2 Finite Difference Scheme for the Schrödinger Equation

When the Schrodinger equation is discretized by replacing derivatives with centered difference formulas, it has been shown previously ([4] pp. 381-384) that it is possible to implement it in a completely reversible fashion. It is this discrete version that we consider now for simulation and analysis. In particular we investigate the convergence, consistency, and stability, and are able to show analytically that this scheme will converge under certain conditions.

The "derivation" of the finite difference scheme in question has been presented elsewhere ([4] pp. 377-381) and repeating the algebraic steps in the derivation is unnecessary. However, it is important to note the substitutions and ideas used in creating this formula. The main idea used in coming up with the finite difference scheme is to substitute centered differences for both the time derivative and spatial derivative. With this substitution, an "update rule" can be determined; specifically, an expression for the state at time t_{n+1} can be written in terms of the state at previous times. This expression can be used to compute the state at successive steps in time, and the goal of simulating quantum evolution is realized. Because the centered difference formulas are used, this scheme is called a "central-time, central-space" scheme[2].

Since the Schrodinger equation is first order in time, the centered difference formula 3.1 must be substituted for this derivative. Similarly, the centered difference formula 3.13 must be substitued for the spatial derivative. Making these substitutions gives:

$$i\hbar\frac{d}{dt}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x,t) + V(x,t)\psi(x,t)$$

$$i\hbar\frac{\psi(x_m,t_{n+1}) - \psi(x_m,t_{n-1})}{2k} \approx$$

$$-\frac{\hbar^2}{2m}\frac{\psi(x_{m+1},t_n) - 2\psi(x_m,t_n) + \psi(x_{m-1},t_n)}{2h^2} + V(x_m,t_n)\psi(x_m,t_n). \quad (3.3)$$

[2]This naming convention is introduced in [7], where schemes with similar derivations are also referred to as "Leapfrog" schemes.

In this formula, the grid spacings are $k = t_{n+1} - t_n$ and $h = x_{m+1} - x_m$. Instead of writing $\psi(x_m, t_n)$, we adopt the useful notation $\psi(x_m, t_n) \equiv \psi_m^n$, where the discrete time index is written in the superscript and the discrete spatial index is written as a subscript. With this new notation, the cumbersome equation 3.3 is rewritten as

$$i\hbar \frac{\psi_m^{n+1} - \psi_m^{n-1}}{2k} \approx -\frac{\hbar^2}{2m} \frac{\psi_{m+1}^n - 2\psi_m^n + \psi_{m-1}^n}{2h^2} + V_m^n \psi_m^n$$

After some algebra ([4] pp. 377-381) and replacing the approximate equality symbol with equality, the following useful formula is obtained.

$$\psi_m^{n+1} = \psi_m^{n-1} + i \left[\alpha \frac{k}{h^2} \left(\psi_{m+1}^n - 2\psi_m^n + \psi_{m-1}^n \right) + \beta k V_m^n \psi_m^n \right] \tag{3.4}$$

where the physical constants have been grouped together as $\alpha = \frac{\hbar}{2m}$, $\beta = \frac{-2}{\hbar}$ for simplification. In this equation, the value of the wave function at time t_{n+1} is written explicitly in terms of the wave function at times t_n, t_{n-1}.

By separating the wavefunction into real and imaginary components, an update rule can be derived explicitly in terms of these components. This update rule can be implemented in a reversible fashion ([6] pp. 337-348). When the components of the wavefunction are written as $\psi = X + iY$, the discrete update rule becomes

$$X_m^{n+1} = X_m^{n-1} - \left[\alpha \frac{k}{h^2} \left(Y_{m+1}^n - 2Y_m^n + Y_{m-1}^n \right) + \beta k V_m^n Y_m^n \right]$$

$$Y_m^{n+1} = Y_m^{n-1} + \left[\alpha \frac{k}{h^2} \left(X_{m+1}^n - 2X_m^n + X_{m-1}^n \right) + \beta k V_m^n X_m^n \right].$$

This can be implemented in a series of C-like statements,

$$X_m - = \left[\alpha \frac{k}{h^2} \left(Y_{m+1} - 2Y_m + Y_{m-1} \right) + \beta k V_m^n Y_m \right] \tag{3.5}$$

$$Y_m + = \left[\alpha \frac{k}{h^2} \left(X_{m+1} - 2X_m + X_{m-1} \right) + \beta k V_m^{n+1} X_m \right]. \tag{3.6}$$

This exact update rule that is implemented in the simulation. It is important to note that there is a subtle difference between this two-step update and the original (equation 3.4). At a given time t, the two-step update affects only either the real or the imaginary component. However the original rule, written with complex numbers, specifies that both should be updated at each time t. The result is that the original rule (equation 3.4) contains two separate, noninteracting systems. Each of these systems is like the two-step update rule given above, but they are completely isolated from each other. Since the original rule can be viewed this way, any result on convergence, stability, and consistency of the original scheme extends to the two-step scheme.

3.3 Consistency

In order to begin investigation into the behavior of this finite difference scheme, we must first consider its consistency. Conceptually speaking, a finite difference scheme is consistent if it approaches the differential equation as the grid spacing is reduced. Although it would appear that this is implied by using the centered difference formulas (which were shown to be consistent by Taylor expansions), it is important to verify this directly for the complete scheme.

Within the context of a finite difference scheme, consistency has a precise mathematical definition ([7] p. 20). Given a partial differential equation $Pu = f$ and a finite difference scheme, $P_{k,h}v = f$, the finite difference scheme is consistent with the partial differential equation if for any smooth function $\psi(t,x)$

$$\lim_{k,h\to 0} [P\psi - P_{k,h}\psi] = 0$$

(where P is a differential operator and $P_{k,h}$ is a difference operator). From this definition, we can show that the scheme represented in 3.4 is consistent.

To facilitate analysis of the scheme 3.4, the case of the free particle is considered. The potential $V(x,t)$ is completely arbitrary and cannot be accounted for completely in steps of the analysis. However, if the free particle is not both consistent and stable, cases where the potential $V(x,t)$ is nontrivial will be inherently unstable. When the potential $V(x,t) = 0$, the finite difference scheme in 3.4 simplifies to

$$\psi_m^{n+1} = \psi_m^{n-1} + i\alpha\frac{k}{h^2}\left(\psi_{m+1}^n - 2\psi_m^n + \psi_{m-1}^n\right). \tag{3.7}$$

Collecting all terms of this equation and the Schrödinger equation onto one side gives a formula for the operator P and the difference operator $P_{k,h}$:

$$i\hbar\frac{d}{dt}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x,t)$$

$$i\hbar\frac{d}{dt}\psi(x,t) + \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x,t) = 0.$$

$$i\hbar\frac{\psi_m^{n+1} - \psi_m^{n-1}}{2k} \approx -\frac{\hbar^2}{2m}\frac{\psi_{m+1}^n - 2\psi_m^n + \psi_{m-1}^n}{2h^2}$$

$$i\hbar\frac{\psi_m^{n+1} - \psi_m^{n-1}}{2k} + \frac{\hbar^2}{2m}\frac{\psi_{m+1}^n - 2\psi_m^n + \psi_{m-1}^n}{2h^2} \approx 0,$$

where we have used the form of the update rule before simplification. It can be seen now that the operators P and $P_{k,h}$ are given by

$$P\psi(x,t) = \left(i\hbar\frac{d}{dt} + \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi(x,t) = 0$$

$$P_{k,h}\psi_m^n = i\hbar\frac{\psi_m^{n+1}-\psi_m^{n-1}}{2k} + \frac{\hbar^2}{2m}\frac{\psi_{m+1}^n - 2\psi_m^n + \psi_{m-1}^n}{2h^2} \approx 0.$$

Now we may proceed from the definition of convergence, namely to determine the value of

$$\lim_{k,h\to 0}\left[P\psi - P_{k,h}\psi\right]. \tag{3.8}$$

It may appear that since $P = 0$ and $P_{k,h} \approx 0$, that this limit should identically be zero, however this is not the case. The argument $P\psi - P_{k,h}\psi$ is nonzero when (k,h) are significantly different from zero. Substituting for P and $P_{k,h}$,

$$\lim_{k,h\to 0}\left[P\psi - P_{k,h}\psi\right]$$

$$\lim_{k,h\to 0}\left[\left(i\hbar\frac{d}{dt} + \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi - \left(i\hbar\frac{\psi_m^{n+1}-\psi_m^{n-1}}{2k} + \frac{\hbar^2}{2m}\frac{\psi_{m+1}^n - 2\psi_m^n + \psi_{m-1}^n}{2h^2}\right)\right].$$

A Taylor expansion can be written for ψ_{m-1}^n and ψ_{m+1},

$$\psi_{m+1} = \psi_m + \psi_m' h + \psi_m'' h^2 + \psi_m^{(3)} h^3 + O(h^4)$$

$$\psi_{m-1} = \psi_m - \psi_m' h + \psi_m'' h^2 - \psi_m^{(3)} h^3 + O(h^4).$$

Taking the sum of these gives

$$\psi_{m+1} + \psi_{m-1} = 2\psi_m + 2\psi_m'' h^2 + O(h^4).$$

Direct substitution for this sum now gives

$$\lim_{k,h\to 0}\left[\left(i\hbar\frac{d}{dt} + \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\right.$$

$$\left. - \left(i\hbar\frac{\psi_m^{n+1}-\psi_m^{n-1}}{2k} + \frac{\hbar^2}{2m}\frac{\left[2\psi_m + 2\psi_m'' h^2 + O(h^4)\right] - 2\psi_m^n}{2h^2}\right)\right].$$

Simplifying,

$$\lim_{k,h\to 0}\left[\left(i\hbar\frac{d}{dt} + \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi - \left(i\hbar\frac{\psi_m^{n+1}-\psi_m^{n-1}}{2k} + \frac{\hbar^2}{2m}\frac{2\psi_m'' h^2 + 2O(h^4)}{2h^2}\right)\right] = 0,$$

$$\lim_{k,h\to 0}\left[\left(i\hbar\frac{d}{dt}\right)\psi - \left(i\hbar\frac{\psi_m^{n+1}-\psi_m^{n-1}}{2k} + \frac{\hbar^2}{2m}O(h^2)\right)\right] = 0.$$

A similar Taylor expansion can be written for ψ^{n+1} and ψ^{n-1},

$$\psi^{n+1} = \psi^n + \frac{d\psi^n}{dt}k + \frac{d^2\psi^n}{dt^2}k^2 + O(k^3)$$

$$\psi^{n-1} = \psi^n - \frac{d\psi^n}{dt}k + \frac{d^2\psi^n}{dt^2}k^2 - O(k^3).$$

Taking the difference of these gives

$$\psi^{n+1} - \psi^{n-1} = 2\frac{d\psi^n}{dt}k + 2O(k^3).$$

Substituion of this difference gives

$$\lim_{k,h\to 0}\left[\left(i\hbar\frac{d}{dt}\right)\psi - \left(i\hbar\frac{2\frac{d\psi^n}{dt}k + 2O(k^3)}{2k} + \frac{\hbar^2}{2m}O(h^2)\right)\right] = 0.$$

Simplifying,

$$\lim_{k,h\to 0} -\left[i\hbar O(k^2) + \frac{\hbar^2}{2m}O(h^2)\right] = 0,$$

$$\lim_{k,h\to 0}\left[O(k^2) + O(h^2)\right] = 0. \tag{3.9}$$

Clearly, as $k, h \to 0$, both $O(k^2)$ and $O(h^2)$ approach zero (by definition). Thus the scheme 3.7 is consistent with Schrödinger's equation.

3.4 Convergence and Stability

Since the scheme 3.7 has been shown to be consistent, we now seek to establish bounds on its stability. In doing experiments with different parameters of the simulation, certain values of (h, k) caused a noticable and quick explosion of values, while others yielded totally satisfactory results. We now will place this intuition on a firm, analytical ground.

Convergence of a finite difference scheme is equivalent to requiring that given a solution to the differential equation, then the approximation (given by the difference equation) must converge to this solution as the grid spacing is made arbitrarily small. Stability is the requirement that the solution remain bounded. Although both of these terms have a precise mathematical definition, considering each of them independently is not required because of the Lax-Richmyer Equivalence Theorem ([7] p. 222). This theorem states simply that convergence is a necessary and sufficient condition for stability. Because of this, we may limit our investigation to finding when the scheme 3.7 is stable. The following calculations do not take into account the finite precision of computer number systems. It is assumed, for simplicity, that each operation has an infinite precision.

The stability of scheme 3.7 has a precise mathematical definition, but in practice it is not neccessary to work directly with this definition. By using Fourier analysis on the state ψ at any time t_n a simpler method can be determined that is equivalent to stability. To motivate this, one must simply realize that any upper bound on the growth of the norm of the vector $\|\psi^n\|$ (when such a norm is properly defined[3]) translates into an equivalent bound on the the

[3]In general, this will be the L^2 norm $\|\psi\|_h \equiv \sqrt{\left(h\sum_{m=-\infty}^{\infty}|\psi_m|^2\right)}$ ([7] p. 24) for which Parseval's relation can be verified by direct substitution.

norm of the Fourier transform $\left\|\widehat{\psi}^n\right\|$ because of Parseval's relation. A complete introduction to the Fourier analysis of finite difference schemes can be found in [7], we simply state the key results necessary to determine the stability of this scheme.

To begin, the Fourier transform in one dimension for a grid of discrete points ψ is defined as

$$\widehat{\psi}(\xi) \equiv \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} e^{-imh\xi}\psi_m h$$

where h is the grid spacing, and $\xi \in \left[-\frac{\pi}{h}, \frac{\pi}{h}\right]$ ([7] p. 33). Similarly, the inverse formula is given by

$$\psi_m \equiv \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} e^{imh\xi}\widehat{\psi}(\xi)d\xi. \tag{3.10}$$

These two formulas form the basis of the analysis. As mentioned before, one would like to establish a bound on the growth $\|\psi^n\|$, a measure of the the system. If this growth is unbounded for some reason, then almost any initial condition will eventually become a state with arbitrarily large values. Since the true solution of the differential equation is bounded, then if the same initial conditions simulate into arbitrarily large values, the system must be unstable and nonconvergent.

For a particular finite difference scheme, we can get a measure of its growth of the state ψ^n at each step by rewriting the update rule in terms of the Fourier transform $\widehat{\psi}(\xi)$ by using formula 3.10. Each term ψ_m in the update rule can be replaced by the integral in 3.10. For the update rule 3.7 we have the following

$$\psi_m^{n+1} = \psi_m^{n-1} + i\alpha\frac{k}{h^2}\left(\psi_{m+1}^n - 2\psi_m^n + \psi_{m-1}^n\right)$$

$\frac{1}{\sqrt{2\pi}}\int_{-\pi/h}^{\pi/h} e^{imh\xi}\widehat{\psi}^{n+1}(\xi)d\xi =$

$$\frac{1}{\sqrt{2\pi}}\int_{-\pi/h}^{\pi/h} e^{imh\xi}\widehat{\psi}^{n-1}(\xi)d\xi + i\alpha\frac{k}{h^2}\left(\frac{1}{\sqrt{2\pi}}\int_{-\pi/h}^{\pi/h} e^{i(m+1)h\xi}\widehat{\psi}(\xi)d\xi\right.$$
$$\left. -2\frac{1}{\sqrt{2\pi}}\int_{-\pi/h}^{\pi/h} e^{imh\xi}\widehat{\psi}(\xi)d\xi + \frac{1}{\sqrt{2\pi}}\int_{-\pi/h}^{\pi/h} e^{i(m-1)h\xi}\widehat{\psi}(\xi)d\xi\right)$$

The terms can be collected, giving

$\frac{1}{\sqrt{2\pi}}\int_{-\pi/h}^{\pi/h}\left[e^{imh\xi}\widehat{\psi}^{n+1}(\xi) - e^{imh\xi}\widehat{\psi}^{n-1}(\xi)\right.$

$$\left. - i\alpha\frac{k}{h^2}\left(e^{i(m+1)h\xi}\widehat{\psi}(\xi) - 2e^{imh\xi}\widehat{\psi}(\xi) + e^{i(m-1)h\xi}\widehat{\psi}(\xi)\right)\right] d\xi = 0$$

Finally, since the Fourier transform is unique, then the integrand itself must be identically zero, and

$$e^{imh\xi}\widehat{\psi}^{n+1}(\xi)-e^{imh\xi}\widehat{\psi}^{n-1}(\xi)-i\alpha\frac{k}{h^2}\left(e^{i(m+1)h\xi}\widehat{\psi}(\xi)-2e^{imh\xi}\widehat{\psi}(\xi)+e^{i(m-1)h\xi}\widehat{\psi}(\xi)\right)=0$$

$$e^{imh\xi}\left[\widehat{\psi}^{n+1}(\xi)-\widehat{\psi}^{n-1}(\xi)-i\alpha\frac{k}{h^2}\left(e^{ih\xi}\widehat{\psi}(\xi)-2\widehat{\psi}(\xi)+e^{-ih\xi}\widehat{\psi}(\xi)\right)\right]=0$$

$$e^{imh\xi}\left[\widehat{\psi}^{n+1}(\xi)-\widehat{\psi}^{n-1}(\xi)-\alpha\frac{k}{h^2}\left(\widehat{\psi}(\xi)2i\cos(h\xi)-2i\widehat{\psi}(\xi)\right)\right]=0$$

$$\widehat{\psi}^{n+1}(\xi)-\widehat{\psi}^{n-1}(\xi)-\alpha\frac{k}{h^2}\left(2i\cos(h\xi)-2i\right)\widehat{\psi}(\xi)=0.$$

This recurrence relation on $\widehat{\psi}^n$ gives the method for determining the growth of the system. Specifically, consider the substitution $\widehat{\psi}^n = g^n$ where the superscript on g represents a power and the superscript on $\widehat{\psi}^n$represents the index. The function $g(h\xi)$ is called the amplifaction factor ([7] p.41). It is a function of $h\xi$ which is equivalent to a frequency. For each frequency, $g(h\xi)$ gives the amount that frequency is amplified during a particular update. As the reader may suspect, it is usually required that $|g(h\xi)| \leq 1$ since when $|g(h\xi)|$ exceeds 1 (g is independent of the time step n) then for some particular frequency $h\xi$ we will see an exponential growth.

For clarity, if the finite difference scheme were a single step scheme then,

$$\widehat{\psi}^n(\xi) = g(h\xi)\widehat{\psi}^0(\xi).$$

That is, one can determine the state at any step n (in the frequency domain) by repeated multiplication by the amplification factor $g(h\xi)$. However, this simple formula *cannot* be used in general for the two-step scheme 3.7. Instead a more complicated form is used. Fortunately we do not need this result directly, however it is useful to obtain a picture of what the amplification factor's purpose is.

For the scheme of 3.7, we can proceed with the substitution $\widehat{\psi}^n = g^n$ obtaining

$$\widehat{\psi}^{n+1}(\xi)-\widehat{\psi}^{n-1}(\xi)-\alpha\frac{k}{h^2}\left(2i\cos(h\xi)-2i\right)\widehat{\psi}(\xi)=0$$

$$g^{n+1}-g^{n-1}-\alpha\frac{k}{h^2}\left(2i\cos(h\xi)-2i\right)g^n=0.$$

Since both k, h are fixed constant, we will replace them with $\lambda = k/h^2$ and simplify.

$$g^{n+1}-g^{n-1}-\alpha\lambda\left(2i\cos(h\xi)-2i\right)g^n=0.$$

$$(g^{n-1})(g^2-1-\alpha\lambda\left(2i\cos(h\xi)-2i\right)g)=0.$$

$$g^2 - \alpha\lambda\left(2i\cos(h\xi) - 2i\right)g - 1 = 0.$$

Similarly, we will replace $h\xi$ with $\theta = h\xi$ and consider g a function of θ.

$$g^2 - \alpha\lambda\left(2i\cos\theta - 2i\right)g - 1 = 0.$$

This form is called the amplification polynomial $\Phi(g,\theta)$.

$$\Phi(g,\theta) = g^2 - \alpha\lambda\left(2i\cos(h\xi) - 2i\right)g - 1.$$

Now, it may be possible to relate the constraint on $g(\theta)$ to a constraint on $\alpha\lambda$ directly. However, this is unnecessary as there is a useful theorem ([7] p. 91) which takes into account several subtleties in doing so. It is this theorem which leads to the desired result.

Strikwerda states the theorem as follows: If $\Phi(g,\theta)$ is explicitly independent of h, k, then the necessary and sufficient condition for the finite difference scheme to be stable is that all roots, $g_v(\theta)$, satisfy

- $|g_v(\theta)| \leq 1$
- if$|g_v(\theta)| = 1$, then $g_v(\theta)$ must be a simple root.

For our particular finite difference scheme, the result can be easily determined. Since $\Phi(g,\theta)$ is quadratic, the roots $g_v(\theta)$ can be determined easily. Directly from the quadratic equation,

$$\Phi(g,\theta) = g^2 - \alpha\lambda\left(2i\cos\theta - 2i\right)g - 1 = 0$$

$$g_\pm = \frac{\alpha\lambda\left(2i\cos\theta - 2i\right) \pm \sqrt{-\alpha^2\lambda^2\left(2\cos\theta - 2\right)^2 + 4}}{2}$$

$$g_\pm = i\alpha\lambda\left(\cos\theta - 1\right) \pm \sqrt{-\alpha^2\lambda^2\left(\cos\theta - 1\right)^2 + 1} \tag{3.11}$$

Instead of determining the cases where $|g_v(\theta)| \leq 1$, we can use the equivalent condition $|g_v(\theta)|^2 \leq 1$. It is immediately apparent that when the expression under the radical is nonnegative, then we obtain

$$|g_+|^2 = |g_-|^2 = |g_+ g_-|$$

$$|g_+ g_-| = \left|\alpha^2\lambda^2\left(\cos\theta - 1\right)^2 - \alpha^2\lambda^2\left(\cos\theta - 1\right)^2 + 1\right| = 1.$$

Thus when the expression under the radical is nonnegative, $|g_\pm(\theta)| = 1$. In order for this expression to be nonnegative, we have

$$-\alpha^2\lambda^2\left(\cos\theta - 1\right)^2 + 1 \geq 0$$

$$\alpha^2\lambda^2\left(\cos\theta-1\right)^2\leq 1.$$

Since we desire this to hold for every value of θ, it suffices to consider the maximum value of $\left(\cos\theta-1\right)^2$ in order to impose the most constrain on this system.

$$\alpha^2\lambda^2\left(\cos\theta-1\right)^2\leq 4\alpha^2\lambda^2\leq 1.$$

Equivalently,

$$\alpha^2\lambda^2\leq\frac{1}{4}$$

or,

$$|\alpha\lambda|\leq\frac{1}{2}.$$

However, this condition is *not* sufficient per se, there is the additional requirement that $g_+\neq g_-$when $|g_\pm(\theta)|=1$, according to this theorem. To avoid this case, we must not allow the radical in equation 3.11 to be identically zero or else

$$g_\pm=i\alpha\lambda\left(\cos(h\xi)-1\right)\pm\sqrt{-\alpha\lambda\left(\cos(h\xi)-1\right)^2+1}=i\alpha\lambda\left(\cos(h\xi)-1\right)$$

and $g_+=g_-$. With this restriction, we may begin an analogous calculation

$$-\alpha^2\lambda^2\left(\cos\theta-1\right)^2+1>0,$$

and end with an analogous result

$$|\alpha\lambda|<\frac{1}{2}.$$

Finally we must consider the case when the expression under the radical in equation 3.11 is negative. In this case, factor out i from the radical and obtain a positive result:

$$g_\pm=i\alpha\lambda\left(\cos\theta-1\right)\pm\sqrt{-\alpha^2\lambda^2\left(\cos\theta-1\right)^2+1}$$

$$g_\pm=i\alpha\lambda\left(\cos\theta-1\right)\pm i\sqrt{\alpha^2\lambda^2\left(\cos\theta-1\right)^2-1}$$

$$g_\pm=i\left[\alpha\lambda\left(\cos\theta-1\right)\pm\sqrt{\alpha^2\lambda^2\left(\cos\theta-1\right)^2-1}\right].$$

Now,

$$|g_-|=\left|\alpha\lambda\left(\cos\theta-1\right)-\sqrt{\alpha^2\lambda^2\left(\cos\theta-1\right)^2-1}\right|.$$

The bound $|g_-|\leq 1$ must hold for any θ in order to be stable. In particular, it must hold when $\theta=\pi$,

$$|g_-|=\left|\alpha\lambda\left(\cos\pi-1\right)-\sqrt{\alpha^2\lambda^2\left(\cos\pi-1\right)^2-1}\right|.$$

$$|g_-| = \left|-2\alpha\lambda - \sqrt{4\alpha^2\lambda^2 - 1}\right|$$
$$|g_-| = \left|2\alpha\lambda + \sqrt{4\alpha^2\lambda^2 - 1}\right|. \tag{3.12}$$

Clearly, for any value of $|\alpha\lambda| > \frac{1}{2}$ (since for other values of $|\alpha\lambda|$, it has been shown that $|g_-| = 1$ and that equation 3.12 does not arise) the radical in equation 3.12 is positive while the term $2\alpha\lambda$ exceeds 1. It must be true then that $|g_-| > 1$ for at least some points θ for any value of $|\alpha\lambda| > \frac{1}{2}$.

Consequently, in order for the scheme 3.7 to be stable and convergent, we must require that $|\alpha\lambda| < \frac{1}{2}$.

This result is quite important for setting up the parameters of the simulation. Recall that the constant α is a combination of physical constants, and cannot be altered. However, $\lambda = k/h^2$ and these parameters are set at run-time. In practice, because the equation is consistent then for any value of h one can pick an arbitrarily small, positive k so that the system will converge. However, this trial and error method is unsatisfactory for several reasons. First and foremost, there is no guarantee of convergence without an understanding of the system. Also, if a smaller k does not improve the accuracy of the simulation greatly, then there is no real need to reduce it further than the point of convergence (this will be investigated later).

Another important point to notice is that $|g_\pm(\theta)| = 1$ identically whenever the simulation is stable. Recall that for the time independent Schrödinger equation (equation 2.1) to convert a time-independent solution is related to a time-dependent one by $\psi(x,t) = \varphi(x)e^{-i\omega t}$. That is, the time-independent solutions are simply rotated by a phase factor and the norm of these solutions is not changed. In fact it can be shown[4] that for any wave function ψ, the norm defined as

$$\int_\infty \overline{\psi}\psi dV$$

is conserved (over time) by Schrödinger's equation[5]. Since this norm is conserved in reality, we should expect an analagously defined discrete norm to be conserved as well. This indeed appears to be the case since $|g_\pm(\theta)| = 1$ and Parseval's relation tells us that $\|\psi\|$ and $\left\|\widehat{\psi}\right\|$ are equivalent when defined discretely as above.

Finally, it is important to note what happens when $|\alpha\lambda|$ exceeds $\frac{1}{2}$ by a small amount. In this case, we notice that only near the point $\theta = \pi$ will the root g_- have a magnitude greater than 1. This anomaly manifests itself by causing an exponential increase in frequencies that have $h\xi \approx \pi$. Other frequencies will remain "norm conserved" as $|g_\pm(\theta)| = 1$ since the radical in equation 3.11 will still be positive in most cases.

[4]This follows a priori from showing $\frac{\partial}{\partial t}\int_\infty \overline{\psi}\psi dV = 0$ by interchanging the derivative and integral, then substituting for $\frac{\partial\psi}{\partial t}, \frac{\partial\overline{\psi}}{\partial t}$ by the Schrödinger equation.

[5]In this definition, $\overline{\psi}$ is the complex conjugate of ψ.

3.5 Two-Dimensional Finite Difference Scheme

While mathematically simpler, a one-dimensional finite difference simulation leaves much to be desired in the way of visualization. Since visualization is a goal of this project, it becomes necessary to consider a reversible extension of the simulation into multiple dimensions. Consider the original update rule of equation 3.4:

$$\psi_m^{n+1} = \psi_m^{n-1} + i\left[\alpha\frac{k}{h^2}\left(\psi_{m+1}^n - 2\psi_m^n + \psi_{m-1}^n\right) + \beta k V_m^n \psi_m^n\right].$$

This equation has bit-level reversibility when implemented properly because it can be separated into real and imaginary update steps. The only difference between the one-dimensional Schrödinger equation

$$i\hbar\frac{d}{dt}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x,t) + V(x,t)\psi(x,t)$$

and its multidimensional counterpart

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

is that one uses the Laplacian ∇^2 while the other uses a second derivative. The second derivative has a direct correspondence with certain terms of the finite difference scheme:

$$\psi_m^{n+1} = \psi_m^{n-1} + i\left[\alpha\frac{k}{h^2}\overbrace{\left(\psi_{m+1}^n - 2\psi_m^n + \psi_{m-1}^n\right)}^{\frac{d^2}{dx^2}} + \beta k V_m^n \psi_m^n\right].$$

Thus, any change to the terms included here would not affect the ability to separate the equation into real and imaginary update steps. Because of this, to develop a two-dimensional update rule, we simply need a difference operator to replace the Laplacian[6]. This can be devoloped by considering Talyor's formula[7] for the centered difference approximation to the second derivative (equation 3.13). Recall

$$f''(x_i) \approx \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{2h^2}. \tag{3.13}$$

In this case, we need a Taylor approximation for $\nabla^2\psi = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2}$. We may consider each term independently and make the restriction that the grid spacing in the x,y direction is the same, i.e. $x_{i+1} - x_i = y_{j+1} - y_j = h$. In the

[6]The reasoning applies equally well to three-dimensional implementation.

[7]There is no need to consider Taylor's formula in multiple dimensions, since each derivative we approximate is only taken in one dimension. Using a multidimensional Talyor formula ([5] p. 331) simplifies into the same result.

interest of making the notation simpler, we will write $\psi^n_{u,v} = \psi(\langle x, y\rangle, t)$ when $t = kn$, $x = hu$, and $y = hv$. Since

$$f''(x) = \frac{f(x_{i+1}) - 2f(x) + f(x_{i-1})}{2h^2} + O(h^2)$$

we may write

$$\frac{\partial}{\partial x^2}\psi(\langle x, y\rangle, t) = \frac{\psi^n_{u+1,v} - 2\psi^n_{u,v} + \psi^n_{u-1,v}}{2h^2} + O(h^2).$$

Similarly, in the y direction,

$$\frac{\partial}{\partial y^2}\psi(\langle x, y\rangle, t) = \frac{\psi^n_{u,v+1} - 2\psi^n_{u,v} + \psi^n_{u,v-1}}{2h^2} + O(h^2).$$

Finally, by summing these, we have the desired difference operator

$$\nabla^2\psi = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = \frac{\psi^n_{u+1,v} + \psi^n_{u-1,v} + \psi^n_{u,v+1} + \psi^n_{u,v-1} - 4\psi^n_{u,v}}{2h^2} + O(h^2).$$

Making similar substitutions as the one-dimensional update rule, we may derive the following:

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

$$i\hbar\frac{\psi^{n+1}_{u,v} - \psi^{n-1}_{u,v}}{2k} \approx -\frac{\hbar^2}{2m}\frac{\psi^n_{u+1,v} + \psi^n_{u-1,v} + \psi^n_{u,v+1} + \psi^n_{u,v-1} - 4\psi^n_{u,v}}{2h^2} + V^n_m\psi^n_m$$

$$\frac{\psi^{n+1}_{u,v} - \psi^{n-1}_{u,v}}{k} = -i\left[\alpha\frac{\psi^n_{u+1,v} + \psi^n_{u-1,v} + \psi^n_{u,v+1} + \psi^n_{u,v-1} - 4\psi^n_{u,v}}{h^2} + \beta V^n_m\psi^n_m\right]$$

$$\psi^{n+1}_{u,v} - \psi^{n-1}_{u,v} = i\left[\alpha\lambda\left(\psi^n_{u+1,v} + \psi^n_{u-1,v} + \psi^n_{u,v+1} + \psi^n_{u,v-1} - 4\psi^n_{u,v}\right) + \beta V^n_m\psi^n_m\right]$$

$$\psi^{n+1}_{u,v} = \psi^{n-1}_{u,v} + i\left[\alpha\lambda\left(\psi^n_{u+1,v} + \psi^n_{u-1,v} + \psi^n_{u,v+1} + \psi^n_{u,v-1} - 4\psi^n_{u,v}\right) + \beta V^n_m\psi^n_m\right]. \tag{3.14}$$

It is this update rule that is used in two-dimensional simulations. When separated into real and imaginary components as $\psi = X + iY$ this update rule becomes

$$X_{u,v} - = i\left[\alpha\lambda\left(Y_{u+1,v} + Y_{u-1,v} + Y_{u,v+1} + Y_{u,v-1} - 4Y_{u,v}\right) + \beta V_m Y_m\right]$$

$$Y_{u,v} + = i\left[\alpha\lambda\left(X_{u+1,v} + X_{u-1,v} + X_{u,v+1} + X_{u,v-1} - 4X_{u,v}\right) + \beta V_m X_m\right]$$

Just as in the one-dimensional case, the separation of the wavefunction into two update steps will allow it to be implemented reversibly.

Chapter 4

Simulations

Using Java, the update rules for the one-dimensional and two-dimensional systems were implemented. A framework was created which allowed the results of the simulations to be displayed. Each simulation required a small amount of code to be modified, however. In each of the following sections, a particular aspect of the simulation code is highlighted and the results are analyzed.

Within the implementation, the discrete wave functions are stored as `int`'s while the math necessary to initialize and update the wave functions is computed using `double`'s. In order for the scheme 3.5 to be completely reversible, the update to the wave function must be done using an integer addition or subtraction. To maintain precision, the largest value in the initial state is scaled up near the maximum value for an integer. Since the Schrödinger equation is linear, this scaling has no effect on the update rule.

4.1 Initialization Routines

Before the results of particular simulations are discussed, it is important to note the way that the initial conditions are created and the simulation is setup. In general, with a n-step scheme such as the scheme 3.7 one must initialize n steps of the simulation. Accordingly, if scheme 3.7 is used, ψ^0 and ψ^1 must be provided. In this implementation (using the two-step update 3.5) we must provide the real component at one time and the imaginary component at the following time.

In these simulations, we consider particles roughly equivalent to electrons. For the mass m in the Schrödinger equation, we use the electron mass $m_e = 9.1094e-31\text{kg}$, and we restrict our spatial dimensions to the order of magnitude associated with the electron. The initial wave function $\psi(x,0)$ is taken to be the Gaussian wave packet (equation 2.3)

$$\psi(x,0) = \left(\frac{2}{\pi a^2}\right)^{\frac{1}{4}} e^{ikx} e^{-\frac{2x}{a^2}^2}.$$

Figure 4.1: Initial wave function

In most cases, to compute the first step ψ^1 a single-step scheme is used. Once enough initial conditions exist, then the multi-step scheme is used. However, in the interest of simplicity, the order 0 approximation $\psi^1 = \psi^0$ is used. In this case, since the initial state X^0 is purely real, while the following state Y^1 is purely imaginary, this approximation gives the formula $\psi(x,0) = X^0 + iY^1$. From this we can determine the first two states, necessary to simulate using the update rule 3.5.

In cases where we compare simulation with an analytic solution, the analytic solution is usually used to initialize both X^0 and Y^1.

4.2 Free Particle Evolution

In this simulation, the evolution of a free particle is simulated while running side-by-side with the analytic solution. To begin the simulation, only the simulated result will be shown. A comparison with the analytic solution will then follow.

The initial conditions as mentioned above are shown in the simulation in Figure 4.1. The real portion of the wavefunction is drawn in blue, while the complex portion is in yellow. Unfortunately, this paper was probably printed and archived using a black and white system. The complex part of the wave function is the higher peaking one. This makes sense, as $\psi(x,0)$ has a phase factor of e^{ikx}. When $x = 0$, then $\cos kx = 1$ and this represents the peak of the wave function. Also notice that the real portion of the wavefunction is even and the imaginary component is odd.

This wave function evolves in the simulation and spreads out over time (see Figures4.2, 4.3). The Gaussian wave packet spreads over time in a free particle system.

Finally, it is important to note what happens when this is plotted directly against the analytic solution for the Gaussian wavefunction. The Java program is capable of generating the analytic values at a given time t. These two plots are superimposed upon one another. The result for $t = 0$ is just that the values are perfectly aligned, since the discretized version of the wave function was initialized using the analytic version[1]. However letting the simulation run

[1] and, of course, our image resolution is not good enough to discern the rounding error as

Figure 4.2: Wave function after some simulation.

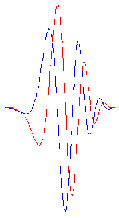


Figure 4.3: Wave function spreading after more simulation.

a short time gives the layout in Figure where a very small difference can be discerned. This difference might not be noticable at first, so the analytic solution has been labelled in this figure.

If the simulation runs long enough, we reach the end of the grid of points in the +x direction. This causes endpoint values to be clamped, so in effect there is an additional restriction placed on the simulation. The result of this, shown in Figure , clearly marks a discrepancy between the two methods. Since the endpoints are clamped to 0 in the code, this has the effect of introducing an infinite potential[2] at the edges of the grid.

4.3 Simple Harmonic Oscillator

In these simulations, similar initial conditions are used. However, the potential is replaced by a quadratic. This causes an oscillatory behaviour in the simulation, as the wave packet shifts from left to right.

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most of the bits in each integer value are not wasted.

[2]This was suggested by Dr. Michail Frank during an informal discussion of his simulations. Consult [4], Appendix E for more insight into this simulation.

Figure 4.4: The simulated and analytic solutions.

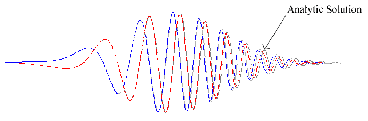


Figure 4.5: Reaching the edge of the simulation.

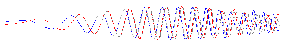
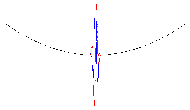


Figure 4.6: Quadratic potential simulation in initial state



4.4 Orders of Magnitude

Within the free particle framework, we have shown that stability is guaranteed for $|\alpha\lambda| < \frac{1}{2}$. It is interesting to place several systems with different λ (each stable) in a free particle framework. While we cannot ever achieve the true free particle because of endpoint conditions we may wrap the grid around so that it forms an loop by letting the leftmost point on the grid become adjacent to the rightmost point. While this violates our physical understanding of this system, it will form a framework in which edge effects do not introduce "artificial" error and the accuracy of the scheme can be observed.

In doing this, we superimpose three separate, noninteracting simulations, with $\lambda_1 = 10\lambda_2 = 100\lambda_3$. The goal of this simulation is to get an intuitive feel for the accuracy of the system.

After 20,000 of the largest time step (2,000,000 of the smallest time step) we arrive at the point of simulation in Figure 4.9. In this figure, a small discrepancy has appeared between the simulation of smallest timestep and the simulation of largest timestep. It is apparent that at least two simulations are occurring simultaneously (as it usually is not when one overlaps the other).

After more simulation (n>3,500,000), simulation 2 ($\lambda_1 = 10\lambda_2$) begins to become noticable. After this many time steps, the simulation with the largest time step is noticably different than the other simulations. This can be seen in Figure 4.10.

By observing the behaviour after a relatively large time t, we hope to recognize the significance of having a small time step in this system. Even once the system is guaranteed to be stable, reducing the time step does cause error to be reduced further.

Figure 4.7: Quadratic potential simulation moving right

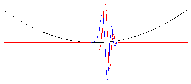


Figure 4.8: Quadratic potential simulation returning left

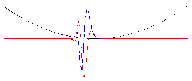
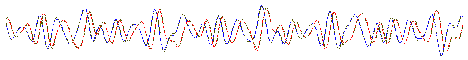


Figure 4.9: Simulation when n=2,000,000



4.5 Visualization in Two Dimensions

To conclude this work, two-dimensional potentials were created and simulated. The result is an "overhead" view of the particle. From this perspective, the particle initially appears as it would to us intuitively: as a round ball. However, as it spreads out (as Gaussian wave packets do) we are reminded of the quantum aspects of the simulation.

The method of displaying the data was to color each point on the grid based on the amplitude $|\psi|$ of the wavefunction. Larger amplitudes were given lighter colored points. The background was taken to be black. Since this scheme will not print well, pictures were modified after simulation and before being inserted into the reporrt. The result is an "inverse" image of the screen, which still conveys all necessary information about the simulation.

A sample simulation consists of a particle given an inital velocity moving towards a step potential barrier. This step potential has a break in it, allowing the particle to partially pass through. However part of the wave function is reflected. The initial setup can be seen in Figure 4.11 and after interaction with the barrier, we arrive at the setup of Figure 4.12. Finally, once most of the particle has passed the barrier, we arrive at the setup in Figure 4.13.

Figure 4.10: Simulation when n>3,500,000

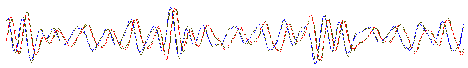


Figure 4.11: Two-dimensional initial setup.

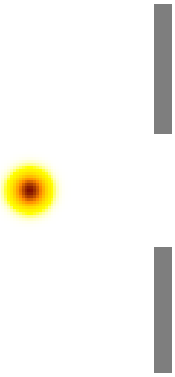


Figure 4.12: Two-dimensional interaction

Figure 4.13: Two-dimensional system after interaction

Chapter 5

Conclusions, Future Work

With this project, many goals were achieved. For the free particle system, an analysis showed that the finite difference scheme was both consistent and stable for certain λ. In addition the effectiveness of this tool to simulate arbitrary systems was investigated through experiment. The visualization of quantum evolution in one dimension and two dimensions was a useful addition.

There are many steps to take after this. For the finite difference scheme, the question of a global propagator needs to be investigated. If the potential $V(x,t)$ was time independent, then the discrete operations used in updating the wave function should correspond to multiplication of the entire system by some matrix M. If M were written explicitly, it would not change with respect to time (since the potential is time independent). Consequently, it appears that to calculate the state at some step n, one can simply find M^n. This could reduce the simulation time logarithmically. This avenue would be interesting to explore, as well as to consider stability and accuracy of this type of scheme.

For the two-dimensional visualization aspect, the idea of placing a different color at each point in the simulation based on the phase should be implemented. This would provide an alternate method of visualizing the data. Finally a three-dimensional surface plot could be done of the wave function. Visualization of a three-dimensional wave function opens other interesting avenues as well.

The role of reversibilty in the finite difference scheme needs to be addressed. Each of these are possible steps that can be taken.

Bibliography

[1] Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloë. *Quantum Mechanics*, chapter I. John Wiley & Sons, 1977.

[2] Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloë. *Quantum Mechanics*, chapter G1. John Wiley & Sons, 1977.

[3] Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloë. *Quantum Mechanics*. John Wiley & Sons, 1977.

[4] Michael P. Frank. *Reversibility for Efficient Computing*. PhD thesis, M.I.T., 1999.

[5] Watson Fulks. *Advanced Calculus*. John Wiley & Sons, 1978.

[6] Anthony J.G. Hey, editor. *Feynman and Computation: Exploring the Limits of Computation*. Perseus Books, 1999.

[7] John C. Strikwerda. *Finite Difference Schemes*. Chapman & Hall, 1989.

[8] Stephen T. Thornton and Andrew Rex. *Modern Physics for Scientists and Engineers*. Saunders, 1993.