# Simulating the 1-D Time-Dependent Schrödinger Equation

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## Introduction

Ever since Schrödinger first formulated his revolutionary theory describing the behavior of particles in terms of a newly invented wavefunction, $\psi$, the implications for modern physics have been nearly endless. The time-dependent Schrödinger equation (TDSE) compactly describes the evolution of a particle's $\psi$ in the presence of a potential energy function. While very powerful, Schrödinger's equation is only directly solvable in special cases. For this reason, accurate and efficient numerical methods are an active area of research. We will describe two methods that we plan to pursue: the Euler method described by MacDonald, and the Chebyshev-FFT method [2]. We will then test our algorithms against systems whose analytical solutions are well-known in order to check our accuracy. We hope to implement both methods to the level where analytical solutions can be closely approximated.

## Background and Theory

The time-dependent Schrödinger equation (1) (TDSE) describes the evolution of a wavefunction in a potential $V$:

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = H\left|\Psi(t)\right\rangle. \tag{1}$$

The Dirac notation of $|\Psi(t)\rangle$ is the most generalized, and reflects that the wavefunction is in some state (not necessarily given in position basis) at time $t$. The Hamiltonian operator $H$ is classically analogous to the total energy of the wavefunction. It is given in the 1-D position basis (which we will be using for the remainder of this paper) by

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t), \tag{2}$$

and "operating" it on some wavefunction in the same basis $\psi(x,t)$ will result in observing the wavefunction's total energy $E$, given by the time independent Schrödinger equation, an eigenvalue equation for $H$ of the form

$$H\psi = E\psi.$$

(The difference of notation between $\Psi$ and $\psi$ will be described in a moment).

In quantum mechanics, most of the analytically solvable situations are where the potential $V$ does not change with time, so that (1) can be solved by assuming $\Psi$ is composed of the product of two, separable equations dependent on only position or time, respectively. Switching to a $V$ that *does* change with time greatly complicates things, so for this project, we will only be dealing with the time-independent potential case. If the potential is time independent, the wavefunction solution $\Psi(x,t)$ can be written as the multiplication of two separable functions

$$\Psi(x,t) = \psi(x,t)\phi(t). \tag{3}$$

By applying the method of separation of variables and plugging (3) into (1) and discretizing the time with step size $\Delta t$, we achieve the solutions

$$\phi(t) = e^{-iHt/\hbar} \qquad \Rightarrow \qquad \Psi(x, t_0 + \Delta t) = e^{-iH\Delta t/\hbar}\psi(x,t_0), \tag{4}$$

or

$$\psi(t_0 + \Delta t) = e^{-iH\Delta t/\hbar}\psi(t_0), \tag{5}$$

which describes the time evolution of some state $\psi(x,t)$ from some initial time $t$ to $t + \Delta t$; this exponential is known as the time-evolution operator.

# Possible Methods

When exploring methods within our capabilities for solving the TDSE, we decided that implementing two different methods and comparing/contrasting the accuracy of their results was the best way to go about our investigation. From the possible methods we mulled over, the first that we have chosen is an average over explicit and implicit Euler approaches combined with Fourier analysis and complex arithmetic (as suggested by MacDonald). The second method uses Chebyshev polynomials to compute the time-evolution operator combined with fast Fourier transforms to propagate the wavefuntion (as suggested by Tal-Ezer and Kosloff).

## MacDonald Method

For this method, we begin with a simple forward Euler approximation of the TDSE:

$$\psi^{n+1} = \psi^n - \frac{i\Delta t}{\hbar} H\psi^n \tag{6}$$

with the "slope" term times $\Delta t$ coming from a rearranging of terms in the TDSE. To approximate the $\partial^2/\partial x^2$ term that appears in the Hamiltonian operator, we use the central difference scheme to second order in x-spacing:

$$\frac{\partial \psi_k^n}{\partial x^2} = \frac{\psi_{k+1}^n - 2\psi_k^n + \psi_{k-1}^n}{\Delta x^2} + \mathcal{O}(\Delta x)^2$$

where n is the particular time at which we are evaluating the position of our particle, k is the x-location of the particle, and $\Delta x$ is our chosen spacing between x-locations. Placing this into equation (6), with $V(x,t) = 0$ for a free particle, we get:

$$\psi_k^{n+1} = \psi_k^n + iQ(\psi_{k+1}^n - 2\psi_k^n + \psi_{k-1}^n), \qquad Q = \frac{\hbar\Delta t}{2m\Delta x^2}$$

Normally, we could solve an Euler step such as this with a transformation of the variable, x, to Fourier space and back again, but this treatment would yield solutions that grow without limit in Fourier space due to an amplifying factor, $\alpha$, with possible magnitude greater than 1 (we will explain how this factor comes about in more detail in our final paper). Thus, we need to set up a new, but very similar, method of Euler approximating the next iteration that limits the growth of the wavefunction and maintains the condition that the integral over all space $(-\infty, \infty)$ of the mod-squared wavefunction (the probability density) is equal to 1 (i.e. unitarity must be preserved; the wavefunction must stay normalized). To do this, we implement a method that averages explicit and implicit Euler methods. Using the same process as described for the explicit Euler method on the implicit Euler method, we get:

$$\psi_k^{n+1} = \psi_k^n + i\frac{Q}{2}(\psi_{k+1}^{n+1} - 2\psi_k^{n+1} + \psi_{k-1}^{n+1}) + i\frac{Q}{2}(\psi_{k+1}^n - 2\psi_k^n + \psi_{k-1}^n)$$

which produces an amplifying factor, $\alpha$, when transformed to Fourier space that has magnitude equal to 1 over all possible values of the new variable (this results from the new $\alpha$ being $\alpha_{explicit}/\alpha_{implicit}$, which are complex conjugates with quotient amplitude always equal to 1). Taking this approach, including a potential function, $V(x_k, t_n) = V_k^n$, and rearranging terms, we get:

$$\psi_k^{n+1} - i\frac{Q}{2}(\psi_{k+1}^{n+1} - 2\psi_k^{n+1} + \psi_{k-1}^{n+1}) + i\frac{\Delta t}{2\hbar}V_k\psi_k^{n+1} = \psi_k^n + i\frac{Q}{2}(\psi_{k+1}^n - 2\psi_k^n + \psi_{k-1}^n) - i\frac{\Delta t}{2\hbar}V_k\psi_k^n$$

Although this looks more like a jumbled mess of Greek and English letters than a solvable equation, it actually takes on the very simple form of a tridiagonal matrix with complex coefficients. Taking the unknowns

to be our $\psi^{n+1}$ terms, applying this equation to each x-position, $k$, and solving for them independently with their counterpart terms in each equation, we get a sparse matrix of complex coefficients that we can use to solve for each value of $\psi$ at position $k$ and time $n+1$. This process can be repeated for as many time steps as we would like. We will describe in more detail exactly how we go about solving for these wavefunction values using Fourier Analysis and complex arithmetic in our final paper and presentation.

## The Chebyshev-FFT Method

### The Time-Dependence of the Wavefunction

The following method is from van Dijk et al. [2]. First, we discretize $x$ and $t$ with the standard approach $x_j = x_0 + j\Delta x$ and $t_n = t_0 + n\Delta t$, with $j \in \{0, 1, \cdots J\}$ and $n \in \{0, 1, 2\cdots\}$. Next, note that equation (5) describes the basic prescription for the "stepping" of the wavefunction through time. There are multiple ways to compute the time-evolution operator; for example, Tal-Ezer and Kosloff describe in [2] writing the operator as an expansion of Chebyshev polynomials $T_n(x)$, which are orthogonal and defined over the interval [-1, 1].

$$\langle T_n(x)|T_m(x)\rangle = \int_{-1}^{1} \frac{T_n(x)T_m(x)}{\sqrt{1-x^2}}\,\mathrm{d}x = C_n\delta_{nm} \qquad C_n = \begin{cases} \pi & n = 0 \\ \pi/2 & n = 1, 2, 3\cdots \end{cases}.$$

Because the time evolution operator $e^{-iH\Delta t/\hbar}$ has a complex argument, we need to use the generalized complex Chebyshev polynomials, $\phi_n(y) = i^n T_m(-iy)$, in the expansion of the operator. The orthogonality statement of these polynomials (with weight function $-i/\sqrt{1-|y|^2}$) is given by

$$\langle \phi_n(y)|\phi_m(y)\rangle = -i\int_{-i}^{i} \frac{\phi_n(y)\phi_m^*(y)}{\sqrt{1-|y|^2}}\,\mathrm{d}y = (-1)^n C_n\delta_{nm},$$

where $\phi_m^*(y)$ is the complex conjugate of $\phi_m(y)$. These polynomials can be found by the recursion relationship

$$\phi_n(y) = 2y\phi_{n-1}(y) + \phi_{n-2}(y) \qquad \begin{cases} \phi_0(y) = 1 \\ \phi_1(y) = y \end{cases}. \tag{7}$$

Tal-Ezer and Kosloff [2] use an interesting approach of scaling the Hamiltonian (2) such that it's energy eigenvalues all lie within $[-1, 1]$ (so that the Chebyshev polynomials can be correctly applied). If the eigenvalues, $E$, of $H$ satisfy

$$E \in [E_{\min}, E_{\max}] \qquad \begin{cases} E_{\min} \equiv V_{\min} \\ E_{\max} \equiv \hbar^2\pi^2/2m(\Delta x)^2 + V_{\max} \end{cases}$$

where $V_{\min}$ and $V_{\max}$ are the minimum and maximum values that the potential $V$ reaches in the domain of interest, then the scaled Hamiltonian can be found with

$$H_{\text{scaled}} = \frac{H}{\Delta E} - \left(1 + \frac{E_{\min}}{\Delta E}\right),$$

where $\Delta E \equiv (E_{\max} - E_{\min})/2$. We then define $y \in [-i, i]$ as

$$y \equiv -iH_{\text{scaled}} = \frac{z}{\Delta E\Delta t/\hbar} + i\left(1 + \frac{E_{\min}}{\Delta E}\right), \qquad z \equiv -iH\Delta t/\hbar.$$

From this, as $z$ can be expressed in terms of $y$, and because the Chebyshev polynomials (including their complex variants) are complete and orthogonal, they can be expanded:

$$e^z = \sum_{n=0}^{\infty} a_n\phi_n(y),$$

where the coefficients $a_n$ can be found with

$$a_n \equiv -ie^{-i(\Delta E + E_{\min})\Delta t/\hbar} \int_{-i}^{i} \frac{e^{\Delta E \Delta t y/\hbar}\phi_n^*(y)}{\sqrt{1-|y|^2}}\,\mathrm{d}y$$

$$a_n \equiv e^{-i(\Delta E + E_{\min})\Delta t/\hbar} D_n J_n(\Delta E \Delta t/\hbar), \qquad D_n = \begin{cases} 1 & n = 0 \\ 2 & n \geq 1 \end{cases},$$

where $J_n$ is the Bessel function of the first kind of order $n$ (which can be implemented into Python with `scipy.special.jv()`). Equation (6) says that the time evolution of the wavefunction from some time $t$ to $t + \Delta t$ is described by

$$\psi(t+\Delta t) = e^{-iH\Delta t/\hbar}\psi(t) \equiv e^z \psi(t) \equiv \sum_{n=0}^{\infty} a_n \phi_n(y)\psi(t).$$

From here, define $\Phi_n \equiv \phi_n(y)\psi(t)$ such that

$$\psi(t+\Delta t) = \sum_{n=0}^{\infty} a_n(\Delta t)\Phi_n(x), \tag{8}$$

and apply the recurrence relationship (7) to obtain

$$\begin{aligned} \Phi_0 &= \psi(t) \\ \Phi_1 &= y\psi(t) = y\Phi_0 = -\frac{i}{\Delta E}H\Phi_0 + i\left(1 + \frac{E_{\min}}{\Delta E}\right)\Phi_0 \\ \Phi_n &= -\frac{2i}{\Delta E}H\Phi_{n-1} + 2i\left(1 + \frac{E_{\min}}{\Delta E}\right)\Phi_{n-1} + \Phi_{n-2}. \end{aligned} \tag{9}$$

Equation (8) can be used to compute the wavefunction at some time $t$ from some initial wavefunction at an earlier time, presumably with the infinite series truncated at some point. The coefficients $a_n$ can be obtained in advance of the process, although because (8) needs to be completed for each new step in the iterations, it will be computationally intensive to do so.

**Applying Position-Dependence of the Wavefunction**

Consider that for our numerical purposes, the grid of position steps (domain of $x$) will be equally spaced with mesh size $h$. From (2), for some function $\chi(x)$, the hamiltonian acting on $\chi(x)$ will give

$$H\chi(x) = -\frac{\hbar^2}{2m}\chi''(x) + V(x)\chi(x), \tag{10}$$

where $\chi''(x)$ denotes $\partial^2\chi/\partial x^2$. Now, we can apply our discretization of $x$ by $x = x_0, x_1, \cdots, x_j, \cdots, x_J$ with

$$(H\chi)_j = -\frac{\hbar^2}{2m}\chi_j'' + V_j\chi_j \qquad (V_j \equiv V(x_j)).$$

From here, there are multiple methods to the obtain the $\chi''$ of equation (10). The most elegant (and fastest, according to [2]), is the so-called fast-Fourier-transform (FFT) method.

Recall that the Fourier transform and the inverse Fourier transform of some $\chi(x)$ are defined as

$$X(\xi) = \int_{-\infty}^{\infty} \chi(x)e^{2\pi i\xi x}\,\mathrm{d}x \quad \text{and} \quad \chi(x) = \int_{-\infty}^{\infty} X(\xi)e^{-2\pi i\xi x}\,\mathrm{d}\xi.$$

Due to a useful differentiation property of Fourier transforms, differentiating $\chi(x)$ twice gives

$$\chi''(x) = -4\pi^2 \int_{-\infty}^{\infty} \xi^2 X(\xi) e^{-2\pi i \xi x} \, \mathrm{d}\xi.$$

Thus, $\chi''(x)$ can therefore be found be taking the (fast) Fourier transform of $\chi(x)$, multiplying that by $-4\pi^2\xi^2$, and then taking the inverse Fourier transform of the result. So, the $H\chi(x)$ of (10) can be found in a fairly straight-forward manner in this way. This can then be used to compute the $H\Phi_{n-1}$ term of (9) for the expansion of the time-evolution operator, thus giving us a way to numerically solve for the wavefunction at that point.

This method is fairly computationally intensive, it seems, and we will thus need to find ways to reduce our computing time when implementing and running this method.

# Testing

The TDSE has a broad range of applications in situations where classical physics fails. While our methods are restricted to the somewhat limiting case of systems with constant potential energy functions, we have collected several common examples of these cases with known analytical solutions. To test our method's effectiveness, we will compare numerical solutions for each of the following cases to the analytical solutions.

## Free Particle

The simplest application of the TDSE is in determining the wavefunction of a free particle with 0 potential energy. Plugging 0 into $V(x)$ into the general Schrodinger's Equation gives a first order ODE, which can be solved without separating into time-dependent and spatially-dependent equations. The solution for the wavefunction is simply that of a plane wave:

$$\psi(x,t) = Ae^{i(kx-\omega t)}.$$

While a numerical solution can be achieved using much more simple methods than our TDSE solver, testing our method against this edge case first will provide a good test before more complicated systems are analyzed.

## Infinite Well

Consider the case of a particle confined in an infinite square well of length $a$ and centered at $x = \frac{a}{2}$. The potential energy, $V(x)$, can be expressed by the following piece-wise function:

$$V(x) = \begin{cases} 0 & 0 \leq x \leq a \\ \infty & x < 0,\, x > a. \end{cases}$$

The analytical solution for the evolution of the wavefunction over time is [1]

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \text{ For } n \equiv 1, 2, 3....$$

We can use this analytical solution to check the accuracy of our solvers against how the particle should behave in a situation with a nonzero potential function.

## Radial Component of the Ground State Hydrogen Atom

Consider a hydrogen-like atom consisting of a nucleus with a single electron. It has been shown that the classical understanding of the electron as a point particle leads to many inconsistencies with observation. The TDSE yields a much more accurate representation of the atom, and correctly predicts not only the atom's wavefunction but also its possible energy levels. In fact, the hydrogen atom is the only realistic

application of the TDSE whose analytical solution is known, as all other cases require assumptions that are unlikely to occur in reality.

According to Coulomb's Law, the potential between two particles of charge $\pm e$ (in this case the electron and nucleus) is

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}.$$

We will state without derivation that the wavefunction for the Hydrogen atom's electron is given by

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r)Y_l^m(\theta, \phi)$$

where $n$, $m$, $l$ are the electron's quantum numbers, and $Y_l^m$ are spherical harmonics. To get rid of angular dependence, we will narrow our investigation to the ground state, which has a wavefunction of

$$\psi_{100} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0},$$

where $a_0$ is the Bohr radius. Using what we have left after these approxiamtions, we can solve for the behavior of the radial component of the ground state Hydrogen atom through our TDSE solver.

# Motivation

Although our plans for implementing a numerical approach to solving the TDSE are limited to basic quantum mechanical situations, they can be extended to real-world applications through application of more rigorous methods and potential functions fairly easily. For example, if we had wished to represent the behavior of qubits in a quantum computer, all we would need to do is modify our potential well function such that we can easily change the conditions within the well to allow the system to exist at many different harmonics as they would in a quantum computing situation.

Additionally, as mentioned above, we can use this tool to simulate the actual behavior of a Hydrogen atom numerically. This peak into the quantum world is a fascinating way to understand the basics of how the fundamental components of matter work. With more rigorous methods and an applicable potential function correctly derived, we could also implement our TDSE solver such that we could approximate the behavior of other atoms that lack analytical solutions. The drawback to doing this is that the potential functions and computing power needed to model these situations are far beyond the scope of our current knowledge and technological resources, which is why we only stick to a basic Hydrogen atom simulation.

# References


[1] V. Jelic and F. Marsiglio. The double well potential in quantum mechanics: a simple, numerically exact formulation. *University of Alberta*, Sep 2012.

[2] W. van Dijk, J. Brown, and K. Spyksma. Efficiency and accuracy of numerical solutions to the time-dependent schrödinger equation. *Phys. Rev. E*, 84:056703, Nov 2011.