A Review of Conventional and Machine Learning-Based Solutions to the Schrödinger Equation

Mark Ruel D. Chua

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This paper is dedicated to exploring conventional numerical methods and machine learning-based approach in solving 1-dimensional harmonic oscillator govern by the time-dependent Schrödinger equation.

1 The Simple Harmonic Oscillator

The simple harmonic oscillator is one of the fundamental problems illustrating the basic concepts and methods of quantum mechanics [1].

Recall. The Time-Dependent Schrödinger Equation (TDSE)

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t) = H\Psi(\mathbf{x},t) \tag{1}$$

For the simple harmonic oscillator, the Hamiltonian is given by

$$H = \frac{\mathbf{p}^2}{2m} + \frac{m\omega^2\mathbf{x}^2}{2} \tag{2}$$

Using Eq. 1 with the Hamiltonian given by Eq. 2, we can find a partial differential equation satisfied by the energy eigenfunctions $u_n(\mathbf{x})$. For simplicity, let's consider the 1-dimensional time-independent Schrödinger wave equation given by

$$-\frac{\hbar^2}{2m}\frac{d}{dx^2}u_n(x) + \frac{1}{2}m\omega^2x^2u_n(x) = E_nu_n(x) \tag{3}$$

where the energy eigenvalues* follows the quantization relation

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad , \qquad n = 0, 1, 2, 3, ... \tag{4}$$

*Can be determined using ladder operators $\hat{a}$ and $\hat{a}^\dagger$.

The wave functions satisying Eqs. 3 and 4 are given by

$$u_n(x) = c_n H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right)\exp\left\{\frac{-m\omega x^2}{2\hbar}\right\} \tag{5}$$

where H_n are Hermite polynomials[†] given by

$$H_0(x') = 1 \tag{6}$$
$$H_1(x') = 2x' \tag{7}$$
$$H_2(x') = 4x'^2 - 2 \tag{8}$$
$$H_3(x') = 8x'^3 - 12x' \tag{9}$$
$$\dots \tag{10}$$

and c_n is a normalization constant[‡] given by

$$c_n = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4}(2^n n!)^{-1} \tag{11}$$

The analytical solution to the 1-dimensional simple harmonic oscillator follows to be the superposition of the Eq. 5 eigenstates. For instance, we can consider a 50-50 superposition of n-state and m-state

$$\Psi(x,t) = u_{n,m}(x,t) = \frac{1}{\sqrt{2}}e^{-iE_n t}u_n(x) + \frac{1}{\sqrt{2}}e^{-iE_m t}u_m(x) \tag{12}$$

2 Statement of the Problem

The analytical solution for the 1-dimensional simple harmonic oscillator is given in Sec. 1. Now, we want to explore numerical solutions to this problem. In particular, we want to find a solution for the TDSE[§] given by

$$i\Psi_t = 0.5\left(-\Psi_{xx} + \omega^2 x^2 \Psi\right) \tag{13}$$

within the domain spatial domain $x \in [-\pi, \pi]$ and temporal domain $t \in [0, 2\pi]$.

We suppose that the wave function vanishes on the boundaries, that is, it follows the Dirichlet boundary conditions

$$\Psi(x_0, t) = 0 \quad , \qquad \text{for} \quad x \in \{-\pi, \pi\} \tag{14}$$

Then, using Eq. 12, we assume that the initial condition is given by

$$\Psi(x, 0) = u_{n,m}(x, 0) \tag{15}$$

[†]In Eq. 5, the Hermite polynomials are functions of $x' = x\sqrt{m\omega/\hbar}$

[‡]Determined using the orthogonality relationship $\int_{-\infty}^{+\infty} H_n(x')H_m(x')e^{-x'^2}dx' = \sqrt{\pi}2^n n!\delta_{nm}$

[§]In this case, we used Hartree atomic units, that is, $\hbar = m_e = 1$. Moreover, we also used this shorthand notation for derivatives: $\frac{\partial f}{\partial x} = f_x$, $\frac{\partial^2 f}{\partial x^2} = f_{xx}$, etc.

3 Conventional Numerical Methods

We now implement various conventional methods to solve the problem presented in Sec. 2. The calculations in this section mainly follows Ref. [2].

3.1 Diagonalization of the Hamiltonian

We now consider a general numerical method used to solve time-evolution equations[¶] based on a (pseudo) Hermitian structure given by

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t) = \hat{H}(t)\Psi(\mathbf{x},t) \tag{16}$$

We may find a solution to Eq. 16 using Dyson's time-ordering operator[‖] $\hat{T}$, that is

$$\Psi(\mathbf{x},t+\Delta t) = \hat{T}\exp\left(-\frac{i}{\hbar}\int_t^{t+\Delta t}\hat{H}(t')dt'\right)\Psi(\mathbf{x},t) \tag{17}$$

Expanding this using Dyson series, we find

$$\Psi(\mathbf{x},t+\Delta t) = \left(\hat{I} - \frac{i}{\hbar}\int_{t_0}^{\Delta t}dt_1\hat{H}(t_1) + \frac{i^2}{\hbar^2}\int_{t_0}^{\Delta t}dt_1\int_{t_0}^{t_1}dt_2\hat{H}(t_1)\hat{H}(t_2) + \ldots\right)\Psi(\mathbf{x},t) \tag{18}$$

To implement this in a numerical scheme, we need to approximate the solution. If we neglect the time-ordering operator and approximate Eq. 18, our calculations will have an error on the order of $\mathcal{O}(\Delta t^3)$ and Eq. 17 can be approximated as

$$\Psi(\mathbf{x},t+\Delta t) = \exp\left(-\frac{i}{\hbar}\int_t^{t+\Delta t}\hat{H}(t')dt'\right)\Psi(\mathbf{x},t) + \mathcal{O}(\Delta t^3) \tag{19}$$

Conventional numerical approaches typically requires us to discretize the equation and domain of the problem. It follows that the operator

$$\hat{\mathcal{H}}(t,\Delta t) = \frac{1}{\hbar}\int_t^{t+\Delta t}\hat{\mathcal{H}}(t')dt' \tag{20}$$

of the time-evolution operator in Eq. 19 needs to be discretized. The time evolution of the wave function will now involve calculating matrix exponentials of $\boldsymbol{\mathcal{H}}(t,\Delta t)$[**]. We assume that the discretization preserves the (pseudo) Hermiticity of $\boldsymbol{\mathcal{H}}(t,\Delta t)$.

In general, the exponential of an arbitrary $n\times n$ matrix $\mathbf{X}$ is given by the power series

$$\exp(\mathbf{X}) = \sum_{k=0}^{\infty}\frac{1}{k!}\mathbf{X}^k \tag{21}$$

[¶] This is also equivalent to the integral equation $\Psi(\mathbf{x},t) = \hat{I} - \frac{i}{\hbar}\int_{t_0}^{t}dt_1\hat{H}(t_1)\Psi(\mathbf{x},t_1)$

[‖] This operator reorder operators in a product such that the operators with later times appear to the left of operators with earlier times

[**] $\boldsymbol{\mathcal{H}}$ is the matrix representation of Eq. 20

where $\mathbf{X}^0$ is defined to be the identity matrix $\mathbf{I}$ with the same dimension as $\mathbf{X}$, or equivalently, we an write Eq. 21 as

$$\exp(\mathbf{X}) = \lim_{k\to\infty}\left(\mathbf{I} + \frac{\mathbf{X}}{k}\right)^k \tag{22}$$

for integer-valued k. Another standard procedure to compute the exponential of some matrix is to calculate its eigendecomposition[††]. To do this, let's consider a square matrix $\mathbf{Q}$ whose columns are the normalized eigenvectors of $\boldsymbol{\mathcal{H}}(t, \Delta t)$ in any order. Then, this square matrix $\mathbf{Q}$ must satisfy

$$\boldsymbol{\mathcal{H}}(t, \Delta t)\mathbf{Q} = \mathbf{Q}\boldsymbol{\Lambda} \tag{23}$$

where $\boldsymbol{\Lambda}$ represents the diagonal matrix of the real eigenvalues of $\boldsymbol{\mathcal{H}}(t, \Delta t)$. Preserving the (pseudo) Hermiticity of $\boldsymbol{\mathcal{H}}(t, \Delta t)$ ensures that the inverse of $\mathbf{Q}$ exists. It follows that

$$\boldsymbol{\Lambda} = \mathbf{Q}^{-1}\boldsymbol{\mathcal{H}}(t, \Delta t)\mathbf{Q} \tag{24}$$

Furthermore, we can write the matrix exponential of $\boldsymbol{\mathcal{H}}(t, \Delta t)$ in Eq. 19 as

$$\exp\left(-\frac{i}{\hbar}\int_t^{t+\Delta t}\hat{H}(t')dt'\right) = \exp\left(-i\boldsymbol{\mathcal{H}(t, \Delta t)}\right) \tag{25}$$

Using Eq. 21, we find

$$\exp\left(-i\boldsymbol{\mathcal{H}(t, \Delta t)}\right) = \sum_k \frac{1}{k!}\left(-i\boldsymbol{\mathcal{H}(t, \Delta t)}\right)^k \tag{26}$$

$$= \sum_k \frac{(-i)^k}{k!}\left(\mathbf{Q}\mathbf{Q}^{-1}\boldsymbol{\mathcal{H}(t, \Delta t)}\mathbf{Q}\mathbf{Q}^{-1}\right)^k \tag{27}$$

$$= \sum_k \frac{(-i)^k}{k!}\mathbf{Q}\left(\mathbf{Q}^{-1}\boldsymbol{\mathcal{H}(t, \Delta t)}\mathbf{Q}\right)^k\mathbf{Q}^{-1} \tag{28}$$

Using Eq. 24, we further simplify the equation as

$$\exp\left(-i\boldsymbol{\mathcal{H}(t, \Delta t)}\right) = \mathbf{Q}\sum_k \frac{(-i)^k}{k!}\left(\boldsymbol{\Lambda}\right)^k\mathbf{Q}^{-1} = \mathbf{Q}\exp(-i\boldsymbol{\Lambda})\mathbf{Q}^{-1} \tag{29}$$

Now, the matrix exponential of $\boldsymbol{\mathcal{H}}(t, \Delta t)$ is easier to compute using Eq. 29, as $\boldsymbol{\Lambda}$ is a diagonal matrix. Meaning, we only need to find the exponential of the energy eigenvalues $\exp(-iE_k)$ which are the diagonal elements of $\boldsymbol{\Lambda}$. Moreover, if $\boldsymbol{\mathcal{H}}(t, \Delta t)$ is Hermitian, then $\mathbf{Q}^{-1} = \mathbf{Q}^\dagger$.

The diagonalization of the Hamiltonian can be interpreted as its discretization, while the differential equation involving them are discretized using various schemes such as

[††]Eigendecomposition is the factorization of a matrix into a canonical form, whereby the matrix is represented in terms of its eigenvalues and eigenvectors. Only diagonalizable matrices can be factorized in this way.

finite differences method, where a function is evaluated on a regular rectangular grid with spatial spacing Δx and temporal spacing Δt. In general, the first- and second-order differential operators can be approximated using

$$\frac{df(x)}{dx} = -\frac{f(x-\Delta x)}{2\Delta x} + \frac{f(x+\Delta x)}{2\Delta x} + \mathcal{O}(\Delta x^3) \tag{30}$$

$$\frac{df(x)}{dx} = \frac{f(x-2\Delta x)}{12\Delta x} - \frac{3f(x-\Delta x)}{2\Delta x} + \frac{3f(x+\Delta x)}{2\Delta x} - \frac{f(x+2\Delta x)}{12\Delta x} + \mathcal{O}(\Delta x^5) \tag{31}$$

$$\frac{d^2f(x)}{dx^2} = \frac{f(x-\Delta x)}{\Delta x^2} - 2\frac{f(x)}{\Delta x^2} + \frac{f(x+\Delta x)}{\Delta x^2} + \mathcal{O}(\Delta x^3) \tag{32}$$

$$\frac{d^2f(x)}{dx^2} = -\frac{f(x-2\Delta x)}{12\Delta x^2} + \frac{4f(x-\Delta x)}{3\Delta x^2} - \frac{5f(x)}{2\Delta x^2} + \frac{4f(x+\Delta x)}{3\Delta x^2} - \frac{f(x+2\Delta x)}{12\Delta x^2} + \mathcal{O}(\Delta x^5) \tag{33}$$

3.1.1 Discretization of the given problem

The TDSE in Eq. 1 follows the (pseudo) Hermitian structure of Eq. 16. Thus, we can implement the approach discussed in Sec. 3.1 to the problem presented in Sec. 2. We begin with the discretization of the Hamiltonian presented in Eq. 2. Explicitly writing the momentum operator $\mathbf{p}$ in Hartree atomic units, we have

$$\hat{H} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{\omega^2 x^2}{2} \tag{34}$$

Using second-order finite differences, Eq. 34 can be approximated as

$$\hat{H}f(x) = -\frac{1}{2}\left(\frac{f(x-\Delta x)}{\Delta x^2} - 2\frac{f(x)}{\Delta x^2} + \frac{f(x+\Delta x)}{\Delta x^2}\right) + \frac{\omega^2 x^2}{2}f(x) \tag{35}$$

It follows that, if we represent the discretized function $f(x)$ as

$$f(x) := \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ \dots \\ f_N \end{bmatrix} \tag{36}$$

Then, we can write the matrix representation of the discretized Hamiltonian as

$$\hat{H} := -\frac{1}{2\Delta x^2}\begin{bmatrix} -2 & 1 & 0 & 0 & \dots \\ 1 & -2 & 1 & 0 & \dots \\ 0 & 1 & -2 & 1 & \dots \\ 0 & 0 & 1 & -2 & 1 \\ \vdots & \vdots & \vdots & 1 & -2 \end{bmatrix} + \frac{\omega^2 x^2}{2}\begin{bmatrix} 1 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ 0 & 0 & 0 & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots & 1 \end{bmatrix} \tag{37}$$

which is consistent with the second-order finite difference expression in Eq. 35.

3.2 Crank-Nicolson Method

3.3 Fourier Split Operator Method

4 Machine Learning-Based Approach

We now implement a machine learning-based approach to solve the problem. The calculations in this section mainly follows Ref. [3].

4.1 The Physics-Informed Neural Network

References

[1] J. J. Sakurai and J. Napolitano, *Modern Quantum Mechanics*, Cambridge University Press, 2020, ISBN 978-0-8053-8291-4, 978-1-108-52742-2, 978-1-108-58728-0 doi:10.1017/9781108587280

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