An accurate pentadiagonal matrix solution for the time-dependent Schrödinger equation

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Abstract

One of the unitary forms of the quantum mechanical time evolution operator is given by Cayley's approximation. The standard practice is to approximate the second derivatives in the Hamiltonian with the three-point formula, which leads to a tridiagonal system of linear equations. In this work, we implement the highly accurate five-point stencil to derive a pentadiagonal system. Given the same grid size and the time step, the resultant numerical solutions achieve a much higher degree of accuracy than the standard ones.

I. INTRODUCTION

A non-relativistic quantum mechanical system is described by a wave function ψ, which evolves in time in accordance with the Schrödinger equation. For the one-dimensional case of a particle of mass m interacting with a potential V, the time-dependent Schrödinger equation (TDSE) is

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right)\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t). \tag{1}$$

In case the potential is static, $V(x,t) = V(x)$, the problem reduces to an implementation of the unitary operator U:

$$\psi(x,t+\Delta t) = \hat{U}(t+\Delta t,t)\ \psi(x,t) = \exp\left(-i\frac{\hat{H}\Delta t}{\hbar}\right)\psi(x,t), \tag{2}$$

where $\hat{H} = -(\hbar^2/2m)\partial^2/\partial x^2 + V(x)$ is the Hamiltonian. Any truncation in the series expansion of $\hat{U}$ leads to a loss of unitarity, and consequently, there is a change in the norm of the wave function over time. For example, if we truncate $\hat{U}$ up to the first order:

$$\hat{U}(t+\Delta t,t) \approx \hat{\mathbb{1}} - i\frac{\hat{H}\Delta t}{\hbar}, \tag{3}$$

the norm is $\langle\psi|\psi\rangle_{t+\Delta t} = \langle\psi|\psi\rangle_t + \langle\psi|\hat{H}^2|\psi\rangle_t \Delta t^2/\hbar^2$. Moreover, $\psi(x,t) \neq \hat{U}^{-1}(t+\Delta t,t)\psi(x,t+\Delta t)$, i.e., the solutions are not bidirectionally stable in time. To circumvent these problems we implement the Cayley's form of evolution operator.

II. CAYLEY'S FORM OF EVOLUTION OPERATOR

A Cayley's approximation for the unitary operator $\hat{U}$ reads [1–5]

$$\hat{U}(t+\Delta t,t) \approx \left(\hat{\mathbb{1}} + i\frac{\hat{H}\Delta t}{2\hbar}\right)^{-1}\left(\hat{\mathbb{1}} - i\frac{\hat{H}\Delta t}{2\hbar}\right), \tag{4}$$

This means that $\psi(x,t)$ and $\psi(x,t+\Delta t)$ are related by an Implicit-Explicit expression:

$$\left(\hat{\mathbb{1}} + i\frac{\hat{H}\Delta t}{2\hbar}\right)\psi(x,t+\Delta t) = \left(\hat{\mathbb{1}} - i\frac{\hat{H}\Delta t}{2\hbar}\right)\psi(x,t). \tag{5}$$

As clear from the above equation, the idea is to evolve $\psi(x,t)$ by half of the time step forward in time, and $\psi(x,t+\Delta t)$ by half of the time step backward in time, such that there is an agreement at time $t+\Delta t/2$. This way, the bidirectional stability in time is inbuilt into the theoretical framework. Moreover, the functional form of $\hat{U}$ in Eq. (4) is unitary, which implies that the norm is preserved over time: $\langle\psi|\psi\rangle_{t+\Delta t} = \langle\psi|\psi\rangle_t$. We now discuss the numerical methods for an efficient and accurate calculation of $\psi(x,t)$.

A. The tridiagonal discretisation

The standard practice for solving Eq. (5) is to approximate the second derivative in Hamiltonian with the three-point central difference formula:

$$f''(x) \approx \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{\Delta x^2} + \mathcal{O}(\Delta x^2). \tag{6}$$

Accordingly, Eq. (4) is discretised as

$$\begin{aligned}\psi_j^{n+1} + \frac{i\Delta t}{2\hbar}\left[-\frac{\hbar^2}{2m}\left(\frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{\Delta x^2}\right) + V_j\psi_j^{n+1}\right] \\ = \psi_j^n - \frac{i\Delta t}{2\hbar}\left[-\frac{\hbar^2}{2m}\left(\frac{\psi_{j+1}^{n} - 2\psi_j^{n} + \psi_{j-1}^{n}}{\Delta x^2}\right) + V_j\psi_j^{n}\right],\end{aligned} \tag{7}$$

where $f_j^n \equiv f(x_j,t_n)$, $\Delta x = x_{j+1} - x_j$ is the grid size, and $\Delta t = t_{n+1} - t_n$ is the time step. Denoting

$$\psi_j^n - \frac{i\Delta t}{2\hbar}\left[-\frac{\hbar^2}{2m}\left(\frac{\psi_{j+1}^{n} - 2\psi_j^{n} + \psi_{j-1}^{n}}{\Delta x^2}\right) + V_j\psi_j^{n}\right] = \zeta_j^n, \tag{8}$$

$$a_j = 1 + \frac{i\Delta t}{2\hbar}\left(\frac{\hbar^2}{m\Delta x^2} + V_j\right), \quad \text{and} \tag{9}$$

$$b = -\frac{i\hbar\Delta t}{4m\Delta x^2}, \tag{10}$$

reduces the problem to a sparse matrix equation:

$$\begin{pmatrix} a_1 & b & & & & & \\ \ddots & \ddots & \ddots & & & & \\ & b & a_{j-1} & b & & & \\ & & b & a_j & b & & \\ & & & b & a_{j+1} & b & \\ & & & & \ddots & \ddots & \ddots \\ & & & & & b & a_{J-1} \end{pmatrix} \cdot \begin{pmatrix} \psi_1^{n+1} \\ \vdots \\ \psi_{j-1}^{n+1} \\ \psi_j^{n+1} \\ \psi_{j+1}^{n+1} \\ \vdots \\ \psi_{J-1}^{n+1} \end{pmatrix} = \begin{pmatrix} \zeta_1^n \\ \vdots \\ \zeta_{j-1}^n \\ \zeta_j^n \\ \zeta_{j+1}^n \\ \vdots \\ \zeta_{J-1}^n \end{pmatrix}, \tag{11}$$

where J is the dimension of the position grid. We now have a tridiagonal system of linear equations for $J-1$ unknown wave function values at time t_{n+1}. Usually, this is solved for ψ^{n+1} by utilizing the Thomas algorithm (which is nothing but Gaussian elimination in a tridiagonal case).

B. The pentadiagonal discretisation

A numerical method is as good as the underlying finite difference approximations. The three-point formula for the second derivative has an error of $\mathcal{O}(\Delta x^2)$. In an improvement, we implement the five-point stencil, which is accurate within $\mathcal{O}(\Delta x^4)$:

$$f''(x) \approx \frac{-f(x+2\Delta x) + 16f(x+\Delta x) - 30f(x) + 16f(x-\Delta x) - f(x-2\Delta x)}{12\Delta x^2} + \mathcal{O}(\Delta x^4). \tag{12}$$

Eq. (5) is now discretised as

$$\begin{aligned} \psi_j^{n+1} + \frac{i\Delta t}{2\hbar}\left[-\frac{\hbar^2}{2m}\left(\frac{-\psi_{j+2}^{n+1} + 16\psi_{j+1}^{n+1} - 30\psi_j^{n+1} + 16\psi_{j-1}^{n+1} - \psi_{j-2}^{n+1}}{12\Delta x^2}\right) + V_j\psi_j^{n+1}\right] \\ = \psi_j^n - \frac{i\Delta t}{2\hbar}\left[-\frac{\hbar^2}{2m}\left(\frac{-\psi_{j+2}^{n} + 16\psi_{j+1}^{n} - 30\psi_j^{n} + 16\psi_{j-1}^{n} - \psi_{j-2}^{n}}{12\Delta x^2}\right) + V_j\psi_j^{n}\right]. \end{aligned} \tag{13}$$

Following the similar approach as in the previous section, we now denote

$$\psi_j^n - \frac{i\Delta t}{2\hbar}\left[-\frac{\hbar^2}{2m}\left(\frac{-\psi_{j+2}^{n} + 16\psi_{j+1}^{n} - 30\psi_j^{n} + 16\psi_{j-1}^{n} - \psi_{j-2}^{n}}{12\Delta x^2}\right) + V_j\psi_j^{n}\right] = \zeta_j^n, \tag{14}$$

$$a_j = 1 + \frac{i\Delta t}{2\hbar}\left(\frac{5\hbar^2}{4m\Delta x^2} + V_j\right), \tag{15}$$

$$b = -\frac{i\hbar\Delta t}{3m\Delta x^2}, \quad \text{and} \tag{16}$$

$$c = \frac{i\hbar\Delta t}{48m\Delta x^2}. \tag{17}$$

which reduces the problem to

$$\begin{pmatrix}
a_1 & b & c & & & & & & & \\
\ddots & \ddots & \ddots & \ddots & & & & & & \\
 & \ddots & \ddots & \ddots & \ddots & \ddots & & & & \\
 & & c & b & a_{j-1} & b & c & & & \\
 & & & c & b & a_j & b & c & & \\
 & & & & c & b & a_{j+1} & b & c & \\
 & & & & & \ddots & \ddots & \ddots & \ddots & \ddots \\
 & & & & & & \ddots & \ddots & \ddots & \ddots \\
 & & & & & & & c & b & a_{J-2}
\end{pmatrix} \cdot \begin{pmatrix} \psi_1^{n+1} \\ \vdots \\ \psi_{j-2}^{n+1} \\ \psi_{j-1}^{n+1} \\ \psi_j^{n+1} \\ \psi_{j+1}^{n+1} \\ \psi_{j+2}^{n+1} \\ \vdots \\ \psi_{J-2}^{n+1} \end{pmatrix} = \begin{pmatrix} \zeta_1^n \\ \vdots \\ \zeta_{j-2}^n \\ \zeta_{j-1}^n \\ \zeta_j^n \\ \zeta_{j+1}^n \\ \zeta_{j+2}^n \\ \vdots \\ \zeta_{J-2}^n \end{pmatrix}. \tag{18}$$

This represents a pentadiagonal system of linear equations for $J-2$ unknown wave function values at time t_{n+1}. The Thomas algorithm can no longer be used, and we solve for ψ^{n+1} by performing a LU-factorisation of the matrix on the left, followed by forward and backward substitutions of the vector on the right [4, 5].

III. PERFORMANCE

For a comparison between the standard tridiagonal solutions and the pentadiagonal solutions of this work, we simulate the evolution of a Gaussian wave packet in the harmonic oscillator potential $V(x) = m\omega^2 x^2/2$. Given an arbitrary initial position spread σ, the Heisenberg uncertainty product is given by (calculated by solving the Ehrenfest's differential equations)

$$\mathbf{\Delta}x\mathbf{\Delta}p = \frac{\hbar}{2}\sqrt{\cos^4(\omega t) + \sin^4(\omega t) + \frac{1}{4}\left(\frac{\omega_0^2}{\omega^2} + \frac{\omega^2}{\omega_0^2}\right)\sin^2(2\omega t)}, \tag{19}$$

where $\omega_0 = \hbar/2m\sigma^2$, and $\mathbf{\Delta}$ denotes the standard deviation. Assuming $\hbar = 1$, $m = 1$, and $\omega = 0.1$, in Fig. 1 we plot the errors in the uncertainty product calculated with both methods. It can be easily seen that, irrespective of the choice of the grid size and the time step, our pentadiagonal solutions are far more accurate than the standard ones. This

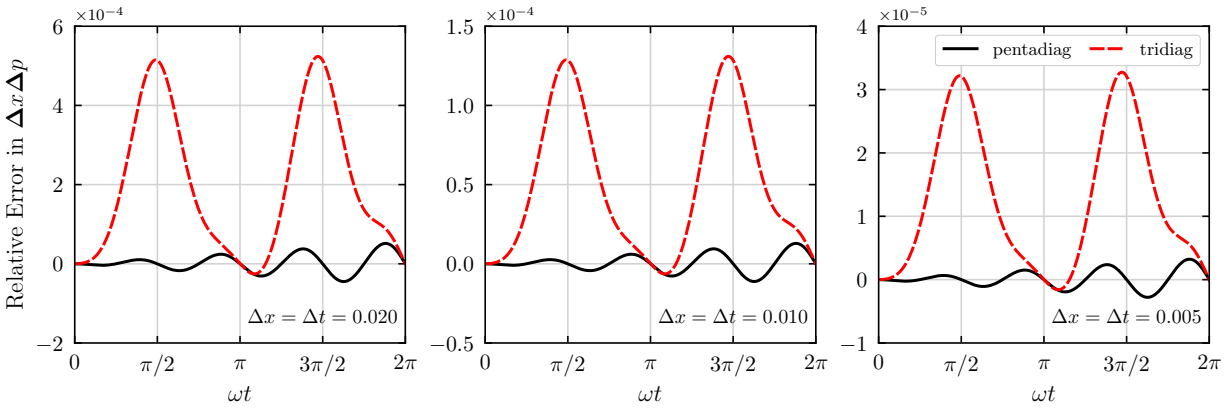

FIG. 1. Comparison of errors in the tridiagonal and the pentadiagonal solutions of TDSE for the harmonic oscillator potential ($\hbar = 1$, $m = 1$, and $\omega = 0.1$). The initial wave packet is centered at $x = -10$ with a width of 2 units. The error in uncertainty product $\boldsymbol{\Delta} x \boldsymbol{\Delta} p$ is evaluated w.r.t. to the analytical result of Eq. (19). Δx denotes the grid size, and Δt is the time step. Note different vetical scales in each panel.

makes it an excellent method for implementation in situations where the potential is weak and highly accurate simulations are required, e.g., in case of a wave packet evolving in the gravitational potential.

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[1] W. Press *et al.*, *Numerical Recipes: The Art of Scientific Computing*, 3rd ed. (Cambridge University Press, USA, 2007).

[2] F. J. Vesely, *Computational Physics*, 2nd ed. (Springer, USA, 2001).

[3] J. Thomas, *Numerical Partial Differential Equations: Finite Difference Methods*, 1st ed. (Springer-Verlag, USA, 1995).

[4] P. Puschnig, Computerorientierte Physik (2016).

[5] A. Kumar, T. Krisnanda, P. Arumugam, and T. Paterek, Quantum **5**, 506 (2021).