

Tridiagonal matrix solution for the time-dependent Schrödinger equation

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I. INTRODUCTION

A quantum mechanical system is described by a wave function ψ . The evolution of ψ through space and over time, in the non-relativistic regime, is described by 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

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

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

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

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:

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

the norm is $\langle \psi | \psi \rangle_{t+\Delta t} = \langle \psi | \psi \rangle_t + \langle \psi | \hat{H}^2 | \psi \rangle_t \Delta t^2 / \hbar^2$. To circumvent this 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]

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

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

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

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 $\psi(x, t)$.

III. 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:

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

Accordingly, Eq. (4) is discretised as

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

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

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

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

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

reduces the problem to a sparse matrix equation:

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

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).

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