Tridiagonal matrix solution for the time-dependent Schrödinger equation

Ankit Kumar
Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, India

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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

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

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 $\langle\psi|\psi\rangle_{t+\Delta t} = \langle\psi|\psi\rangle_t + \langle\psi|\hat{H}^2|\psi\rangle_t\,\Delta t^2/\hbar^2$. 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]

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

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 $\psi(x,t)$.

Ankit Kumar: akvyas1995@gmail.com

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:

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

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).

[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).