Tridiagonal matrix solution for the time-dependent Schrödinger equation

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Reference: Ankit Kumar *et al.*, *Quantum* **5**, 506 (2021) [quant-ph]

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.

I. CAYLEY'S FORM OF EVOLUTION OPERATOR

The idea of Cayley's approximation 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

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agreement at time $t + \Delta t/2$ [1–5]::

$$\exp\left(+i\frac{\hat{H}\Delta t}{\hbar}\right)\psi(x,t+\Delta t) = \exp\left(-i\frac{\hat{H}\Delta t}{\hbar}\right)\psi(x,t). \tag{4}$$

This way, the bidirectional stability in time is inbuilt into the theoretical framework. We can now truncate the operators on the left and the right up to the first order to arrive at an Implicit-Explicit relation:

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

The corresponding evolution operator now looks like:

$$\hat{U}(t+\Delta t, t) \approx \left(\hat{\mathbb{1}} + i\frac{\hat{H}\Delta t}{2\hbar}\right)^{-1}\left(\hat{\mathbb{1}} - i\frac{\hat{H}\Delta t}{2\hbar}\right). \tag{6}$$

It can be easily proved that this form of $\hat{U}$ is unitary, which means that the norm is preserved over time, i.e., $\langle\psi|\psi\rangle_{t+\Delta t} = \langle\psi|\psi\rangle_t$. We now discuss the numerical method for an efficient and accurate solution of Eq. (5).

II. 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:

$$f''(x) \approx \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{\Delta x^2} + \mathcal{O}(\Delta x^2). \tag{7}$$

Accordingly, Eq. (6) is discretised as

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

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

$$\psi_j^n - \frac{i\Delta t}{2\hbar}\left[-\frac{\hbar^2}{2m}\left(\frac{\psi_{j+1}^{n} - 2\psi_j^{n} + \psi_{j-1}^{n}}{\Delta x^2}\right) + V_j\psi_j^{n}\right] = \zeta_j^n, \tag{9}$$

$$a_j = 1 + \frac{i\Delta t}{2\hbar}\left(\frac{\hbar^2}{m\Delta x^2} + V_j\right), \quad \text{and} \tag{10}$$

$$b = -\frac{i\hbar\Delta t}{4m\Delta x^2}, \tag{11}$$

reduces the problem to a sparse matrix equation:

$$\begin{pmatrix} a_1 & b & & & & & \\ \ddots & \ddots & \ddots & & & & \\ & b & a_{j-1} & b & & & \\ & & b & a_j & b & & \\ & & & b & a_{j+1} & b & \\ & & & & \ddots & \ddots & \ddots \\ & & & & & b & a_{J-1} \end{pmatrix} \cdot \begin{pmatrix} \psi_1^{n+1} \\ \vdots \\ \psi_{j-1}^{n+1} \\ \psi_j^{n+1} \\ \psi_{j+1}^{n+1} \\ \vdots \\ \psi_{J-1}^{n+1} \end{pmatrix} = \begin{pmatrix} \zeta_1^n \\ \vdots \\ \zeta_{j-1}^n \\ \zeta_j^n \\ \zeta_{j+1}^n \\ \vdots \\ \zeta_{J-1}^n \end{pmatrix}, \tag{12}$$

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). We have avoided the Thomas algorithm by performing a LU factorisation of the tridiagonal matrix, and the equation is thereafter solved by forward and backward substitution of the ζ vector on the right.

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