Chebyshev time propagation method for the time-dependent Shrödinger equation

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1 Introduction

The Chebyshev time propagation method is used to solve the time development of quantum systems. This method works with any functional form of Hamiltonian operator, provided an estimate of the eigenvalue range can be made. It is not recommended for time-dependent Hamiltonians, but is very efficient for time-independent ones. Although the method does not inherently conserve norm or energy [1], it is nonetheless very accurate.

With this method a 1D-wavefunction is simulated in a time-independent potential. The simulation consists of an initially gaussian wavepacket colliding with a potential wall. The simulation code is provided as an attachment.

2 The time-dependent Shrödinger equation

One of the postulates in quantum mechanics is that wavefunctions evolve according to the time-dependent Schrödinger equation (1D)

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

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x,t) \tag{2}$$

For the case of time-independent potential, this equation has the solution (simple integration)

$$\Psi(x,t) = e^{-\frac{i}{\hbar}\hat{H}(x)t}\Psi(x,t) \tag{3}$$

$$= \hat{U}(t)\Psi(x,t) \tag{4}$$

where $\hat{U}(t)$ is called the time evolution operator. The main challenge in numerically calculating the time-development with this formula is thus the exponentiation of the Hamiltonian operator, which is a possibly large matrix.

3 Representation of the problem in a subspace of the position basis

For computational purposes it is convenient to represent the state vector in a subspace of the position basis as a finite column vector

$$|\Psi\rangle \approx \begin{bmatrix} \Psi(x_1) \\ \Psi(x_2) \\ \vdots \\ \Psi(x_n) \end{bmatrix} \tag{5}$$

where the coordinates x_i refer to the ith position in the discretized space, the space being divided to n sites.

The Hamiltonian operator has to be also presented in this basis. The main focus in this work is on the time propagation so we use the relatively simple centered second order finite-difference approximation for the second derivative

$$\frac{\partial^2}{\partial x^2}\Psi(x,t) = \frac{\Psi(x+\Delta x,t) - 2\Psi(x,t) + \Psi(x-\Delta x,t)}{\Delta x^2} + \mathcal{O}(\Delta x^2) \tag{6}$$

To simplify calculations we assume that the wavefunction vanishes beyond the grid which corresponds to an infinite potential beyond the boundaries. In this way the Hamiltonian can be represented as a tridiagonal matrix which is computationally less intensive. This assumption may create unwanted boundary effects that have to be taken into account.

With these approximations the Hamiltonian becomes

$$\mathbf{H} = \hat{\mathbf{K}} + \mathbf{V} \tag{7}$$

$$= -\frac{\hbar^2}{2m\Delta x^2} \begin{bmatrix} -2 + \frac{2m\Delta x^2 V(x_1)}{\hbar^2} & 1 & 0 & \cdots & 0 \\ 1 & -2 + \frac{2m\Delta x^2 V(x_1)}{\hbar^2} & 1 & \ddots & 0 \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & 1 & -2 + \frac{2m\Delta x^2 V(x_\mathrm{n})}{\hbar^2} \end{bmatrix} \tag{8}$$

assuming an equal site distance: $\forall\ \mathrm{i} : x_\mathrm{i} - x_{\mathrm{i}-1} = \Delta x$.

4 Chebyshev time propagation method

In the Chebyshev method the matrix exponent in the time evolution operator is approximated with a set of complex Chebyshev polynomials of the first kind $\Phi_n(\omega)$ defined by the recurrence relation [1]

$$\Phi_0(\omega) = 1 \tag{9}$$

$$\Phi_0(\omega) = -i\omega \tag{10}$$

$$\Phi_{n+1}(\omega) = -2i\omega\Phi_n(\omega) + \Phi_{n-1}(\omega) \tag{11}$$

It is known that the complex Chebyshev polynomial approximation is optimal if the function is approximated in the interval $[-i, i]$, since the maximum error in the approximation is minimal compared to almost all possible polynomial approximations.

Due to the range of definition of the Chebyshev polynomials the Hamiltonian operator has to be renormalized by dividing by $\Delta E_{\text{grid}} = E_{\max} - E_{\min}$, where $E_{\max}$ and $E_{\min}$ are the minimum and maximum eigenvalues of the Hamiltonian. In real space grid calculations these can be estimated as [2]

$$E_{\min} = V_{\min} \tag{12}$$

$$E_{\max} = V_{\max} + T_{\max} \tag{13}$$

$$T_{\max} = \frac{\hbar^2}{2m}\left(\frac{\pi}{\Delta x}\right)^2 \tag{14}$$

Also, for maximum efficiency, the range of eigenvalues is positioned between $[-1, 1]$ by shifting the Hamiltonian. After these operations we get the normalized Hamiltonian $\hat{\mathbf{H}}_{\text{norm}}$

$$\hat{\mathbf{H}}_{\text{norm}} = \frac{2\hat{\mathbf{H}} - \mathbb{1}\left(\frac{E_{\min}+E_{\max}}{2}\right)}{\Delta E_{\text{grid}}} \tag{15}$$

Now we can expand the time evolution operator $\hat{\mathbf{U}}(t)$ as [1]

$$\hat{\mathbf{U}}(t) = e^{-\frac{i}{\hbar}\hat{\mathbf{H}}t} \tag{16}$$

$$\approx e^{-\frac{i}{\hbar}\frac{E_{\min}+E_{\max}}{2}t} \sum_{n=0}^{N} a_n\left(\frac{\Delta E_{\text{grid}}t}{2\hbar}\right)\Phi_n\left(-i\hat{\mathbf{H}}_{\text{norm}}\right) \tag{17}$$

where the polynomial coefficients can be calculated from the following inner product [1]

$$a_n(\alpha) = \int_{-i}^{i} \frac{e^{i\alpha x}\Phi_n(x)}{(1-x^2)^{\frac{1}{2}}}\,\mathrm{d}x = \begin{cases} 2J_n(\alpha)\,, n \neq 0 & (18) \\ J_0(\alpha)\,, n = 0 & (19) \end{cases}$$

where J_n refers to the Bessel function of the first kind.

Examining the expansion coefficients as a function of n, one finds that when n becomes larger than α, the Bessel functions $J_n(\alpha)$ decay exponentially [1]. This means that in a practical implementation, the maximum number of terms N can be chosen such that the accuracy is dominated by the accuracy of the computer.

For time-independent Hamiltonians and a constant time step Δt, one can notice that the time evolution operator has to be calculated only once. This makes the method very efficient as the propagation consists only of a matrix-vector multiplication.

5 Simulation example

An example simulation was performed on a grid of 300 sites, with a time step of 0.0003. The Chebyshev polynomial expansion was terminated when the factor $a_n(\alpha)$ became less than 10^{-10}. Atomic units are used in the calculation, i.e. $m = \hbar = 1$.

The initial wavefunction $\Psi(x, 0)$ in this example is a gaussian wavepacket with an initial average momentum p_0

$$\Psi(x,0) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2} + ip_0 x} \tag{20}$$

The following series of images shows the time-development of this wave packet when it encounters a potential wall:

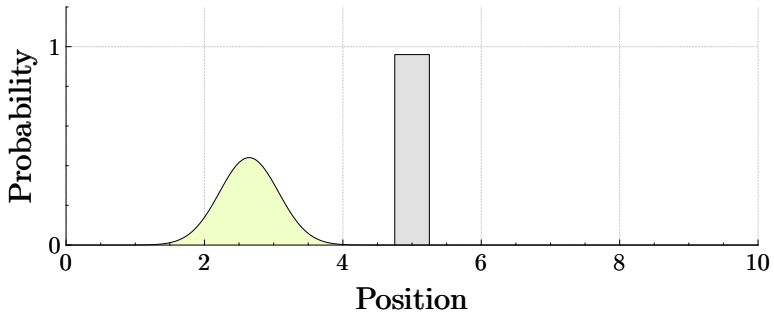

Figure 1: Initially gaussian wavepacket traveling to the right

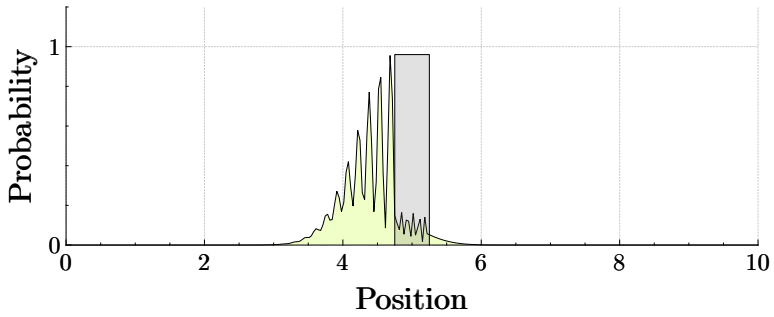

Figure 2: Transmission and reflection at the wall

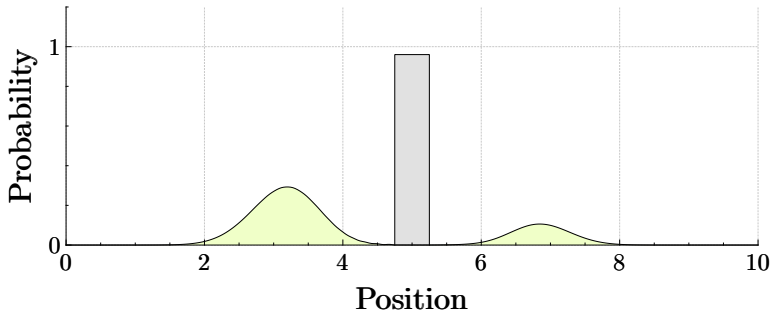

Figure 3: Transmitted and reflected parts

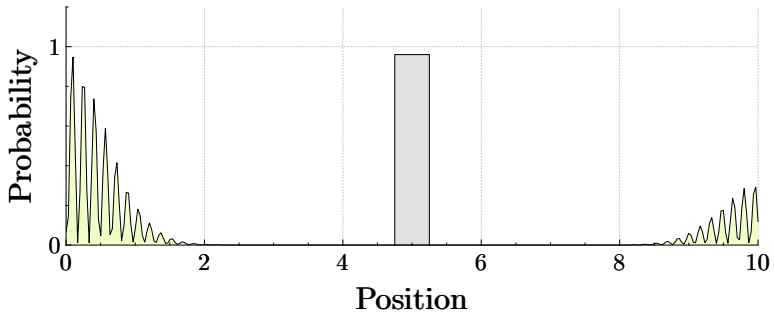

Figure 4: The grid boundary acts as an infinite potential wall, thus the reflection

References

[1] C Leforestier et al. "A comparison of different propagation schemes for the time dependent Schrödinger equation". In: *Journal of Computational Physics* 94.1 (1991), pp. 59 –80. ISSN: 0021-9991.

[2] Kalman Varga and Joseph Andrew Driscoll. *Computational nanoscience : applications for molecules, clusters, and solids*. Cambridge New York: Cambridge University Press, 2011. ISBN: 978-1-107-00170-1.