Operator Splitting Method for Schrödinger Equation

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Summary

This article introduces the application of the operator splitting method in solving the Schrödinger equation, focusing on the decomposition of the Hamiltonian operator and its time discretization implementation. Through the decomposition of the operator, it demonstrates a divide-and-conquer numerical strategy.

1 Introduction for Operator Splitting

1.1 Rewriting the Schrödinger Equation

For the Schrödinger equation

$$\mathrm{i}\frac{\partial \psi(\boldsymbol{x},t)}{\partial t} = \hat{H}\psi(\boldsymbol{x},t),$$

where $\hat{H}$ is the Hamiltonian operator, defined as

$$\hat{H} = -\frac{1}{2}\frac{\partial^2}{\partial \boldsymbol{x}^2} + V(\boldsymbol{x}) = \hat{T} + \hat{V}.$$

The equation can be rewritten as

$$\frac{\partial \psi(\boldsymbol{x},t)}{\partial t} = -\mathrm{i}\hat{H}\psi(\boldsymbol{x},t) \quad \Leftrightarrow \quad \psi_t = -\mathrm{i}\hat{H}\psi,$$

treating $\boldsymbol{x}$ as a parameter, the solution in time satisfies

$$\psi(t,\cdot) = e^{-\mathrm{i}\hat{H}(\cdot)t}.$$

Considering time discretization, we obtain

$$\psi(t+\Delta t,\cdot) = e^{-\mathrm{i}\hat{H}(\cdot)(t+\Delta t)} = e^{-\mathrm{i}\hat{H}(\cdot)\Delta t}\psi(t,\cdot).$$

1.2 Operator Splitting Method

The operator splitting method, as the name suggests, achieves a divide-and-conquer numerical solution by decomposing the Hamiltonian operator into a sum of sub-operators. A simple approach is to split the operator $\hat{H}$ into the kinetic energy term $\hat{T}$ and the potential energy term $\hat{V}$, i.e.,

$$\hat{H} = \hat{T} + \hat{V}.$$

Expanding the exponential operator,[1]

$$e^{-\mathrm{i}\Delta t\hat{H}} = e^{-\mathrm{i}\Delta t(\hat{T}+\hat{V})} = \sum_{n=0}^{\infty}\frac{(-\mathrm{i}\Delta t)^n(\hat{T}+\hat{V})^n}{n!}.$$

We find that due to

$$\hat{T}\hat{V} \neq \hat{V}\hat{T},$$

[2] the operator

$$e^{\hat{H}} = e^{\hat{T}+\hat{V}} \neq e^{\hat{T}}\cdot e^{\hat{V}}.$$

The proof is presented in Appendix A, which interested readers can explore. So, how do we compute $e^{\hat{H}}$? This requires the Baker-Campbell-Hausdorff (BCH) formula.

[1] The exponential operator is defined as

$$e^{\hat{A}} = \sum_{n=0}^{\infty}\frac{\hat{A}^n}{n!}.$$

[2] In fact, we say that operators satisfying

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0$$

are commutative, which is equivalent to

$$\hat{A}\hat{B} = \hat{B}\hat{A}.$$

Theorem 1.1. [Baker-Campbell-Hausdorff Formula] Let $\hat{A}$ and $\hat{B}$ be two non-commutative operators in a Lie algebra (i.e., $[\hat{A}, \hat{B}] \neq 0$), where $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ denotes the commutator. Then their exponential product can be expressed as:

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{C}},$$

where the operator $\hat{C}$ is given by:

$$\hat{C} = \hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}] + \frac{1}{12}\left([\hat{A}, [\hat{A}, \hat{B}]] + [\hat{B}, [\hat{B}, \hat{A}]]\right) + \frac{1}{24}[\hat{B}, [\hat{A}, [\hat{A}, \hat{B}]]] + \cdots,$$

This series includes higher-order nested commutators. If $[\hat{A}, \hat{B}] = 0$, then $\hat{C} = \hat{A} + \hat{B}$, and thus $e^{\hat{A}} e^{\hat{B}} = e^{\hat{A}+\hat{B}}$.

1.2.1 Analysis of Lie-Trotter Splitting Using BCH

One form of Lie-Trotter splitting (first-order) is:

$$e^{-\mathrm{i}\Delta t(\hat{T}+\hat{V})} \approx e^{-\mathrm{i}\Delta t\hat{T}} e^{-\mathrm{i}\Delta t\hat{V}} = e^{\hat{X}} e^{\hat{Y}},$$

According to the BCH formula, the second-order expansion of the product $e^{-\mathrm{i}\Delta t\hat{T}} e^{-\mathrm{i}\Delta t\hat{V}}$ is:

$$\hat{Z}_{LT} = \hat{X} + \hat{Y} + \frac{1}{2}[\hat{X}, \hat{Y}] + O((\Delta t)^3),$$

Computing the commutator:

$$[\hat{X}, \hat{Y}] = [-\mathrm{i}\Delta t\hat{T}, -\mathrm{i}\Delta t\hat{V}] = (-\mathrm{i}\Delta t)^2[\hat{T}, \hat{V}] = -(\Delta t)^2[\hat{T}, \hat{V}],$$

Thus,

$$\begin{aligned}\hat{Z}_{LT} &= -\mathrm{i}\Delta t\hat{T} - \mathrm{i}\Delta t\hat{V} + \frac{1}{2}(-(\Delta t)^2[\hat{T}, \hat{V}]) + O((\Delta t)^3) \\ &= -\mathrm{i}\Delta t(\hat{T} + \hat{V}) - \frac{(\Delta t)^2}{2}[\hat{T}, \hat{V}] + O((\Delta t)^3).\end{aligned}$$

Therefore, the Lie-Trotter approximation is:

$$e^{-\mathrm{i}\Delta t\hat{T}} e^{-\mathrm{i}\Delta t\hat{V}} = \exp\left(-\mathrm{i}\Delta t(\hat{T} + \hat{V}) - \frac{(\Delta t)^2}{2}[\hat{T}, \hat{V}] + O((\Delta t)^3)\right),$$

Compared to the target operator $e^{-\mathrm{i}\Delta t(\hat{T}+\hat{V})}$, the exponent includes an additional error term, primarily $-\frac{(\Delta t)^2}{2}[\hat{T}, \hat{V}]$. This error term is $O((\Delta t)^2)$, making the Lie-Trotter splitting a globally first-order accurate method.

1.2.2 Analysis of Strang (Symmetric) Splitting Using BCH

One form of Strang splitting (second-order) is:

$$e^{-\mathrm{i}\Delta t(\hat{T}+\hat{V})} \approx e^{-\mathrm{i}\frac{\Delta t}{2}\hat{V}} e^{-\mathrm{i}\Delta t\hat{T}} e^{-\mathrm{i}\frac{\Delta t}{2}\hat{V}}.$$

Through a more detailed BCH expansion, for Strang splitting, we have:

$$e^{-\mathrm{i}\frac{\Delta t}{2}\hat{V}} e^{-\mathrm{i}\Delta t\hat{T}} e^{-\mathrm{i}\frac{\Delta t}{2}\hat{V}} = \exp\left(-\mathrm{i}\Delta t(\hat{T} + \hat{V}) + C_3(-\mathrm{i}\Delta t)^3 + O((\Delta t)^5)\right),$$

where C_3 is a specific combination related to nested commutators of $\hat{T}$ and $\hat{V}$. Notably, the $O((\Delta t)^2)$ term (proportional to $[\hat{V}, \hat{T}]$) is eliminated. Thus, the local error of Strang splitting is $O((\Delta t)^3)$, making it a globally second-order accurate method.

2 Solving the Schrödinger Equation Using Lie-Trotter Splitting

Our goal is to compute the wave function $\psi(\boldsymbol{x}, t_n)$ at subsequent times $t_n = n\Delta t$, starting from the initial wave function $\psi(\boldsymbol{x}, 0)$ at $t_0 = 0$.

2.1 Application of Operators

Having split the operator $\hat{H}$ into simpler sub-operators, how do we apply these operators in our algorithm? Here, we discuss the two exponential operators separately.

Applying the Potential Evolution Operator $e^{-\mathrm{i}\Delta t\hat{V}}$: The potential exponential operator acts on the wave function (or a general function):

$$\Psi(\boldsymbol{x}, \cdot) = e^{-\mathrm{i}\Delta t\hat{V}(\boldsymbol{x})}\psi(\boldsymbol{x}, \cdot),$$

This step can be performed directly.

Applying the Kinetic Evolution Operator $e^{-\mathrm{i}\Delta t\hat{T}}$: Next, we apply the exponential kinetic operator to the wave function:

$$\Psi(\boldsymbol{x}, \cdot) = e^{-\mathrm{i}\Delta t\hat{T}}\psi(\boldsymbol{x}, \cdot),$$

The kinetic operator $\hat{T} = -\frac{1}{2}\nabla^2$ is a differential operator. We can compute it in Fourier space, where the kinetic operator corresponds to a simple multiplication operator:

$$\mathcal{F}\{e^{\hat{T}}u(\boldsymbol{x})\}(\boldsymbol{k}) = e^{\frac{-\mathrm{i}\Delta t|\boldsymbol{k}|^2}{2}}\tilde{u}(\boldsymbol{k}).$$

The detailed derivation is provided in Appendix B. Thus, the general procedure for applying the exponential kinetic operator is:

1. **Fourier Transform**: Transform the intermediate wave function $\psi(\boldsymbol{x})$ in position space to its momentum representation $\tilde{\psi}(\boldsymbol{k})$ using the Fast Fourier Transform.

2. **Fourier Space Evolution**: In Fourier space, multiply each component of $\tilde{\psi}(\boldsymbol{k})$ by the corresponding phase factor:
$$\tilde{\psi}(\boldsymbol{k}, \cdot) = e^{-\mathrm{i}\Delta t\frac{|\boldsymbol{k}|^2}{2}}\tilde{\psi}(\boldsymbol{k}, \cdot);$$

3. **Inverse Fourier Transform**: Transform the evolved result back to physical space using the Inverse Fast Fourier Transform.

2.2 Overall Algorithm

We can divide the time evolution into three steps:

- Initialization: Specify the initial wave function $\psi(\boldsymbol{x}, t = 0)$ at all spatial grid points.
- Time Iteration: For each time step, from t_n to $t_{n+1} = t_n + \Delta t$, update the wave function.
- Repeat: Update t_n to t_{n+1}, $\psi(\boldsymbol{x}, t_n)$ to $\psi(\boldsymbol{x}, t_{n+1})$, and repeat the above steps until the desired final evolution time is reached.

Through this iterative approach, we can use the Lie-Trotter splitting method to simulate the time evolution of the wave function. Its pseudocode is shown in Algorithm 1.

Algorithm 1 Time Evolution Using Lie-Trotter Splitting

Require: Initial wave function $\psi_0(\boldsymbol{x})$ (on spatial grid points)
Require: Potential function $V(\boldsymbol{x})$ (on spatial grid points)
Require: Time step Δt
Require: Total evolution time T
Ensure: Wave function $\psi_n(\mathbf{x})$ at final time T, where $n = [T/\Delta t]$

▷ 1. Initialization

$\psi_{temp}(\boldsymbol{x}) \leftarrow \psi_0(\boldsymbol{x})$
$t \leftarrow 0$

▷ 2. Time Iteration Loop

while $t < T$ **do** ▷ Step A: Apply potential evolution operator $e^{-\mathrm{i}\Delta t\hat{V}}$ (in position space)
  for all spatial grid points $\boldsymbol{x}_j$ **do**
    $\psi_{temp}(\boldsymbol{x}_j) \leftarrow e^{-\mathrm{i}\Delta t V(\boldsymbol{x}_j)} \cdot \psi_{temp}(\boldsymbol{x}_j)$
  end for

▷ Step B: Apply kinetic evolution operator $e^{-\mathrm{i}\Delta t\hat{T}}$ (in Fourier space)

  $\tilde{\psi}_{temp}(\mathbf{k}) \leftarrow \mathrm{FFT}(\psi_{temp}(\mathbf{x}))$ ▷ 1. Transform to frequency space
  for all momentum space grid points $\boldsymbol{k}_j$ **do**
    $\tilde{\psi}_{temp}(\boldsymbol{k}_j) \leftarrow e^{-\mathrm{i}\Delta t|\boldsymbol{k}_j|^2/2} \cdot \tilde{\psi}_{temp}(\boldsymbol{k}_j)$ ▷ 2. Multiply by phase factor
  end for
  $\psi_{temp}(\boldsymbol{x}) \leftarrow \mathrm{IFFT}(\tilde{\psi}_{temp}(\boldsymbol{k}))$ ▷ 3. Inverse transform to position space

▷ 3. Update time

  $t \leftarrow t + \Delta t$
end while

$\psi_n(\boldsymbol{x}) \leftarrow \psi_{temp}(\boldsymbol{x})$
return $\psi_n(\boldsymbol{x})$

2.3 Strang Splitting Numerical Scheme

In practice, the Strang splitting method is more commonly used. On one hand, it guarantees third-order convergence; on the other hand, its numerical implementation is equally straightforward. The time iteration numerical solution is given by:

$$\psi(\boldsymbol{x}, t+\Delta t) = e^{-\mathrm{i}\frac{\Delta t}{2}\hat{V}} e^{-\mathrm{i}\Delta t\hat{T}} e^{-\mathrm{i}\frac{\Delta t}{2}\hat{V}} \psi(\boldsymbol{x}, t).$$

Its practical implementation is essentially the same as the previous method.

2.4 Numerical Examples

We now test several numerical examples, including the evolution of a free particle and a harmonic oscillator.

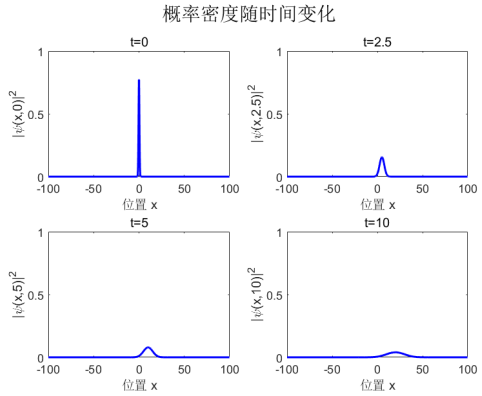
Example 2.1. For a free particle, where

$$V(x) = 0,$$

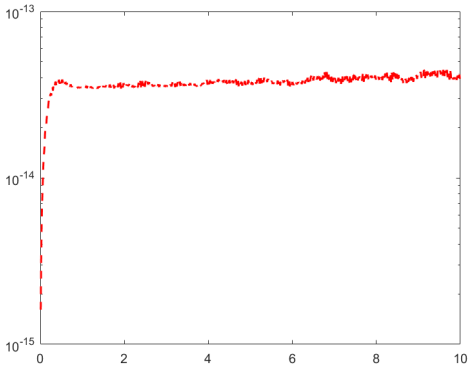
this represents particle evolution without the influence of a potential field in physics. The analytical solution is:

$$\psi = \left(\frac{2}{\pi}\right)^{1/4} \cdot (1+2\mathrm{i}t)^{-1/2} \cdot \exp\left(-\frac{(x-2t)^2}{1+2\mathrm{i}t} + 2\mathrm{i}x - 2\mathrm{i}t\right).$$

Using Lie-Trotter splitting for approximation, we set the spatial domain to $[-L, L]$, with $L = 300$, Fourier degrees of freedom $N = 800$, time step $\Delta t = 0.01$, and $t \in [0, 10]$. The probability density of the wave function is shown on the left of Figure 1, and the error variation over time is on the right. Next, we compare the two splitting methods under different time steps, as shown in Figure 2. It is evident that their error curves align, as the operators are commutative in the absence of a potential field.



(a) Probability density of free particle wave function



(b) Error variation over time

Figure 1: No potential field

Example 2.2. Consider a harmonic oscillator, where

$$V(x) = \frac{1}{2}x^2,$$

representing particle evolution under the influence of an oscillator field in physics. The analytical solution is:

$$\pi^{-1/4} \cdot \exp\left(-\frac{x^2}{2}\right) \cdot \exp\left(-\frac{\mathrm{i}t}{2}\right).$$

We set the spatial domain to $[-L, L]$, with $L = 7.5$, Fourier degrees of freedom $N = 200$, time step $\Delta t = 0.01$, and $t \in [0, 10]$. Using Lie-Trotter splitting for approximation, the probability density of the

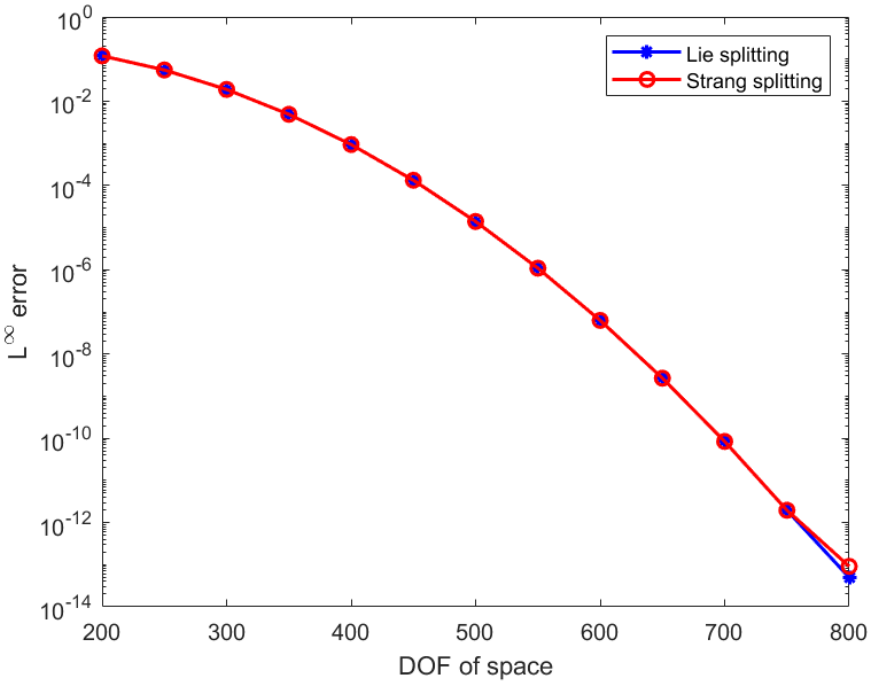
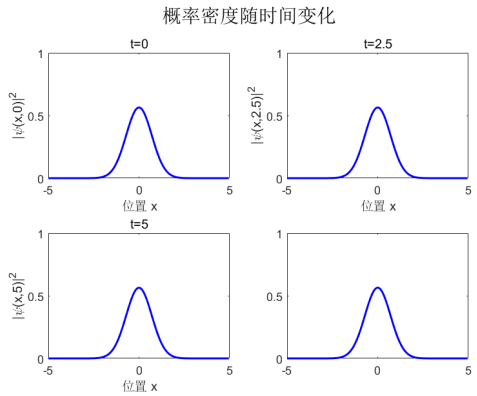
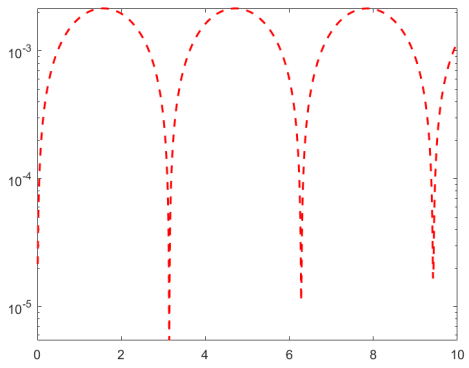


Figure 2: Error comparison of two splitting methods

wave function is shown on the left of Figure 3, and the error variation over time is on the right. Compared to the free particle, the harmonic oscillator's error increases significantly over time. Comparing the errors of the two splitting methods (Figure 4), it is clear that Strang splitting significantly outperforms Lie-Trotter splitting.



(a) Probability density of harmonic oscillator wave function



(b) Error variation over time

Figure 3: Harmonic oscillator potential field

3 Solving the Cubic Nonlinear Schrödinger Equation

The primary challenge of the Schrödinger equation lies in its nonlinear component. The nonlinear model equation is:

$$\mathrm{i}\frac{\partial \psi(\boldsymbol{x},t)}{\partial t} = \hat{H}\psi(\boldsymbol{x},t) = \left(\frac{\partial^2}{\partial \boldsymbol{x}^2} + 2V(\boldsymbol{x})\right)\psi(t,\boldsymbol{x}),$$

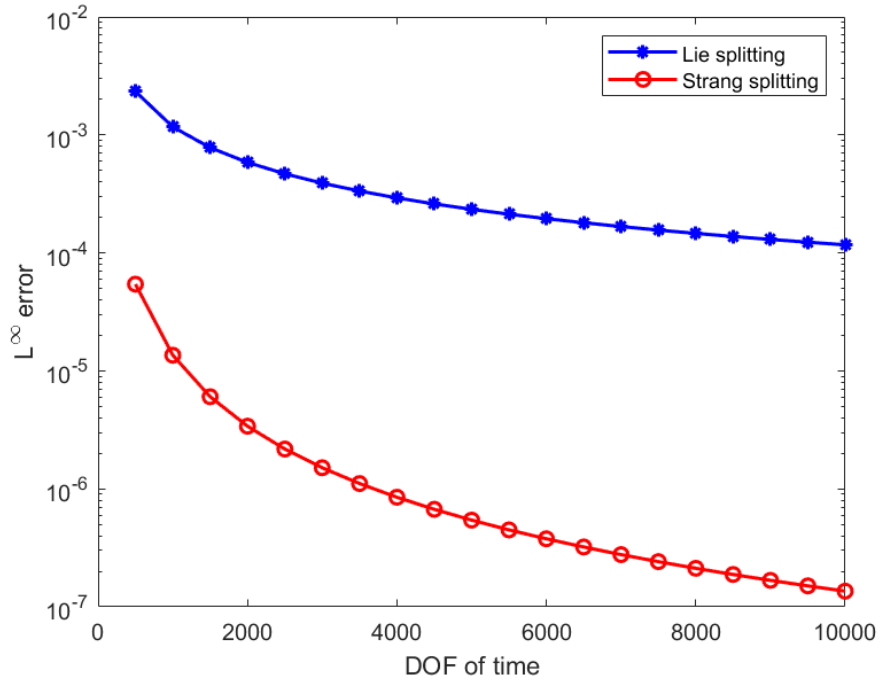


Figure 4: Error comparison of two splitting methods

where

$$V = |\psi(t,\boldsymbol{x})|^2, \quad \hat{V} = |\psi(t,\boldsymbol{x})|^2(\cdot).$$

We solve the equation in the following steps:

- Solve the linear subproblem:

$$\mathrm{i}\frac{\partial \psi(\boldsymbol{x},t)}{\partial t} = \frac{\partial^2}{\partial \boldsymbol{x}^2}\psi(\boldsymbol{x},t) = \Delta\psi(\boldsymbol{x},t), \quad t \in [t_n, t_n + \Delta t/2],$$

  with solution denoted as:

$$\psi_{1/2}^{-} = \psi(\boldsymbol{x}, t_n + \Delta t/2).$$

- Solve the nonlinear subproblem:

$$\begin{cases} \mathrm{i}\frac{\partial \psi_m(\boldsymbol{x},t)}{\partial t} = \hat{V}[\psi_{1/2}^{-}]\psi_m(\boldsymbol{x},t), & t \in [t_n, t_n + \Delta t], \\ \psi_m(\boldsymbol{x}, t_n) = \psi_{1/2}^{-}, \end{cases}$$

  with solution denoted as:

$$\psi_{1/2}^{+} = \psi_m(\boldsymbol{x}, t_n + \Delta t).$$

- Solve the linear subproblem:

$$\begin{cases} \mathrm{i}\frac{\partial \psi_f(\boldsymbol{x},t)}{\partial t} = \Delta\psi_f(\boldsymbol{x},t), & t \in [t_n + \Delta t/2, t_n + \Delta t], \\ \psi_f(\boldsymbol{x}, t_n + \Delta t/2) = \psi_{1/2}^{+}, \end{cases}$$

  with solution:

$$\psi_1(\boldsymbol{x},t) = \psi(\boldsymbol{x}, t + \Delta t).$$

Consider an example, with numerical results provided by [Chang et al.(1999)Chang, Jia, and Sun].

Example 3.1. The analytical solution is a solitary wave function:

$$\psi = \operatorname{sech}(x + 2 - 4t) \exp(-\mathrm{i}(2x + 4 - 3t)).$$

With $L = 70$, $t \in [0, 1]$, using the Strang splitting method, we obtain the following error, as shown in Figure 5.

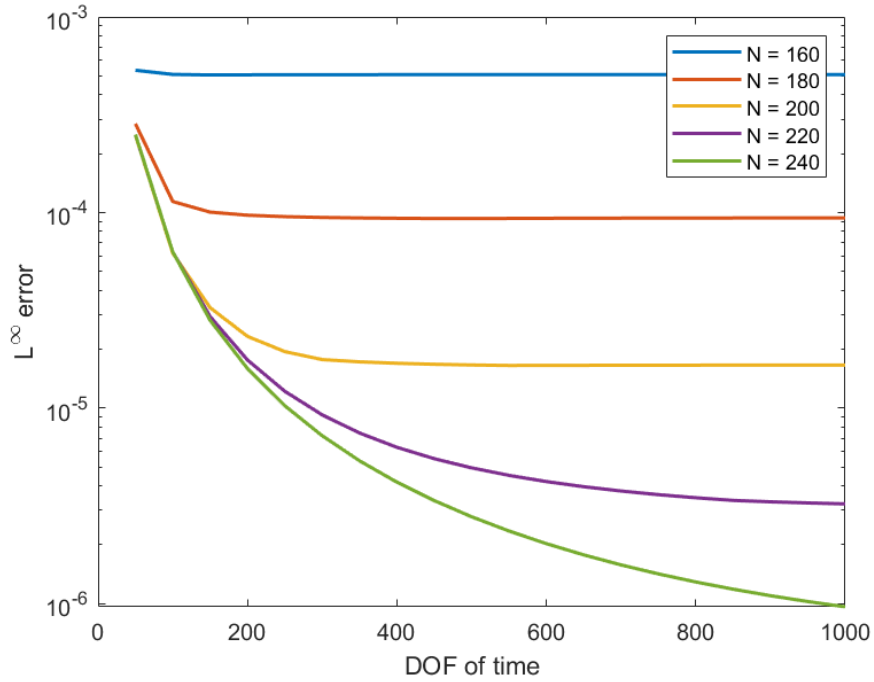


Figure 5: Error comparison under different time grids

A Non-Additivity of Exponential Non-Commutative Operators

First, expanding $e^{\hat{T}+\hat{V}}$, we obtain:

$$\begin{aligned} e^{\hat{T}+\hat{V}} &= 1 + (\hat{T} + \hat{V}) + \frac{1}{2!}(\hat{T} + \hat{V})^2 + O((\hat{T} + \hat{V})^3) \\ &= 1 + \hat{T} + \hat{V} + \frac{1}{2}(\hat{T}^2 + \hat{T}\hat{V} + \hat{V}\hat{T} + \hat{V}^2) + O((\hat{T} + \hat{V})^3). \end{aligned} \tag{1}$$

Next, expanding $e^{\hat{T}} e^{\hat{V}}$:

$$\begin{aligned} e^{\hat{T}} e^{\hat{V}} &= (1 + \hat{T} + \frac{1}{2}\hat{T}^2 + \cdots)(1 + \hat{V} + \frac{1}{2}\hat{V}^2 + \cdots) \\ &= (1 + \hat{V} + \frac{1}{2}\hat{V}^2) + (\hat{T} + \hat{T}\hat{V} + \frac{1}{2}\hat{T}\hat{V}^2) + \left(\frac{1}{2}\hat{T}^2 + \frac{1}{2}\hat{T}^2\hat{V}\right) + \cdots, \end{aligned}$$

Collecting terms up to second order:

$$e^{\hat{T}} e^{\hat{V}} = 1 + \hat{T} + \hat{V} + \left(\frac{1}{2}\hat{T}^2 + \hat{T}\hat{V} + \frac{1}{2}\hat{V}^2\right) + \cdots. \tag{2}$$

Comparing the expansions (1) and (2), for $e^{\hat{T}+\hat{V}} = e^{\hat{T}} e^{\hat{V}}$ to hold, all corresponding terms must be equal, leading to the following coefficient matching:

- Zeroth order: $1 = 1$,
- First order: $\hat{T} + \hat{V} = \hat{T} + \hat{V}$,
- Second order:
  (1): $\frac{1}{2}(\hat{T}^2 + \hat{T}\hat{V} + \hat{V}\hat{T} + \hat{V}^2)$,
  (2): $\frac{1}{2}\hat{T}^2 + \hat{T}\hat{V} + \frac{1}{2}\hat{V}^2$.

Equating the second-order terms:

$$\frac{1}{2}\hat{T}^2 + \frac{1}{2}\hat{T}\hat{V} + \frac{1}{2}\hat{V}\hat{T} + \frac{1}{2}\hat{V}^2 = \frac{1}{2}\hat{T}^2 + \hat{T}\hat{V} + \frac{1}{2}\hat{V}^2.$$

Canceling identical terms $\frac{1}{2}\hat{T}^2$ and $\frac{1}{2}\hat{V}^2$:

$$\frac{1}{2}\hat{T}\hat{V} + \frac{1}{2}\hat{V}\hat{T} = \hat{T}\hat{V}.$$

Moving $\frac{1}{2}\hat{T}\hat{V}$ to the right:

$$\frac{1}{2}\hat{V}\hat{T} = \frac{1}{2}\hat{T}\hat{V}.$$

This implies:

$$\hat{V}\hat{T} = \hat{T}\hat{V},$$

which is the condition for $\hat{T}$ and $\hat{V}$ to commute, i.e., $[\hat{T}, \hat{V}] = \hat{T}\hat{V} - \hat{V}\hat{T} = 0$. Thus, only when $\hat{T}$ and $\hat{V}$ commute do the series expansions of $e^{\hat{T}+\hat{V}}$ and $e^{\hat{T}}e^{\hat{V}}$ match up to second order.

B Fourier Transform Form of the Kinetic Operator

Our goal is to derive the Fourier transform of the function $e^{\hat{T}}u(\boldsymbol{x})$, i.e., $\mathcal{F}\{e^{\hat{T}}u(\boldsymbol{x})\}(\boldsymbol{k})$. The kinetic operator $\hat{T}$ in Fourier space is given by:

$$\mathcal{F}\{\hat{T}u(\boldsymbol{x})\}(\boldsymbol{k}) = \frac{|\boldsymbol{k}|^2}{2}\tilde{u}(\boldsymbol{k}),$$

where $\tilde{u}(\boldsymbol{k}) = \mathcal{F}\{u(\boldsymbol{x})\}(\boldsymbol{k})$. For an operator function $f(\hat{T})$ in Fourier space, if an operator $\hat{O}$ satisfies:

$$\mathcal{F}\{\hat{O}u\}(\boldsymbol{k}) = o(\boldsymbol{k})\tilde{u}(\boldsymbol{k}),$$

then for any function $f(\hat{O})$, its action in Fourier space is multiplication by $f(o(\boldsymbol{k}))$:

$$\mathcal{F}\{f(\hat{O})u\}(\boldsymbol{k}) = f(o(\boldsymbol{k}))\tilde{u}(\boldsymbol{k}).$$

Applying this to $f(\hat{T}) = e^{\hat{T}}$, the Fourier transform of $e^{\hat{T}}u(\boldsymbol{x})$ is:

$$\mathcal{F}\{e^{\hat{T}}u(\boldsymbol{x})\}(\boldsymbol{k}) = e^{\frac{|\boldsymbol{k}|^2}{2}}\tilde{u}(\boldsymbol{k}).$$

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[Lubich(2008)] Christian Lubich. On splitting methods for schrödinger-poisson and cubic nonlinear schrödinger equations. *Mathematics of computation*, 77(264):2141–2153, 2008.