Final Project of Numerical Linear Algebra course

Crank-Nicolson technique for solving the Schrodinger equation

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Problem statement

The time-dependent Schrödinger equation (TDSE) is the fundamental equation of non-relativistic quantum mechanics. The equation has found widespread application in many fields of physical science, for example in atomic, molecular, optical, nuclear and solid-state physics, among others.

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

Importance/Relevance

For TDSE, it is challenging to acquire their analytic solutions. A forward difference Euler method has been used to compute the TDSE numerical solutions. Nevertheless, the Euler scheme is instability in some cases. That is why the Crank-Nicolson technique, which is unconditional stable was proposed to overcome this disadvantage

The method itself

The Crank-Nicolson method, when applied to the Schrödinger equation, performs the following approximation at each time step

$$(2 + i\Delta t\mathbf{H}/\hbar)\vec{u}^{j+1} = (2 - i\Delta t\mathbf{H}/\hbar)\vec{u}^{j}.$$

which results in the (Nx + 1 × Nx + 1)-matrix system

$$\begin{pmatrix} A_1 & 1 & 0 & 0 & \dots \\ 1 & A_2 & 1 & 0 & \dots \\ 0 & 1 & A_2 & 1 & \dots \\ .. & .. & .. & .. & \dots \\ 0 & 0 & .. & 1 & A_{L-1} \end{pmatrix} \begin{pmatrix} \Psi_1^{n+1} \\ \Psi_2^{n+1} \\ \Psi_3^{n+1} \\ \dots \\ \Psi_{L-1}^{n+1} \end{pmatrix} = \begin{pmatrix} B_1 \\ B_2 \\ B_3 \\ \dots \\ B_{L-1} \end{pmatrix}$$

Initial state Ψ_i^0

Boundary conditions Ψ_0^n, Ψ_L^n

Thomas algorithm

Simplified Gaussian elimination, complexity *O(n)*

Forward step:

$$U_1 = \frac{1}{A_1} \text{ and } R_1 = B_1 U_1$$

$$U_i = \frac{1}{A_i - U_{i-1}} \text{ and } R_i = (B_i - R_{i-1}) U_i$$

Backward step:

$$\Psi_i^{n+1} = \begin{cases} R_{L-1} & i = L-1 \\ R_i - U_i \Psi_{i+1}^{n+1} & i < L-1 \end{cases}$$

$$\begin{bmatrix} 1 & U_1 & 0 & \dots & 0 \\ 0 & 1 & U_2 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix} \begin{bmatrix} \Psi_1^{n+1} \\ \Psi_2^{n+1} \\ \Psi_3^{n+1} \\ \dots \\ \Psi_{L-1}^{n+1} \end{bmatrix} = \begin{bmatrix} R_1 \\ R_2 \\ R_3 \\ \dots \\ R_{L-1} \end{bmatrix}$$

Our implementation

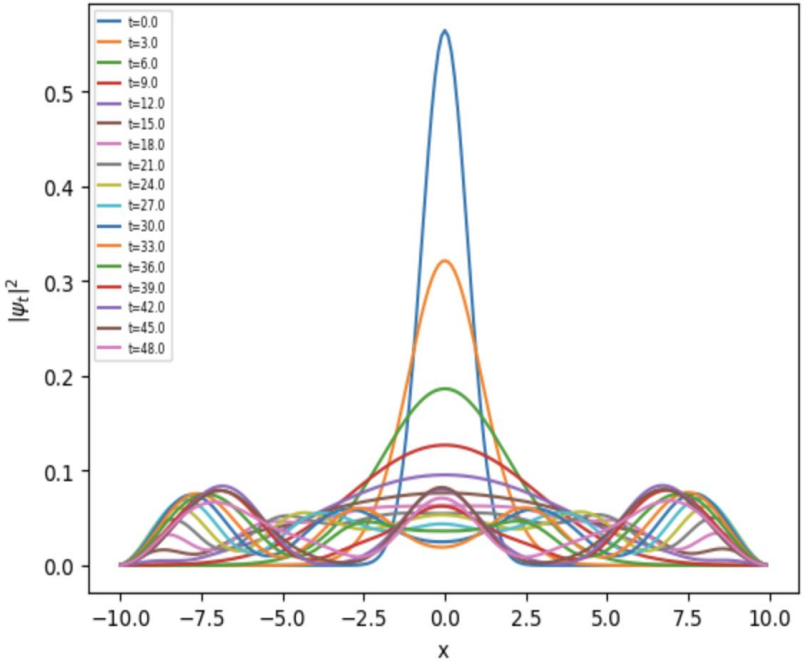
Initial condition - Gaussian wave packet:

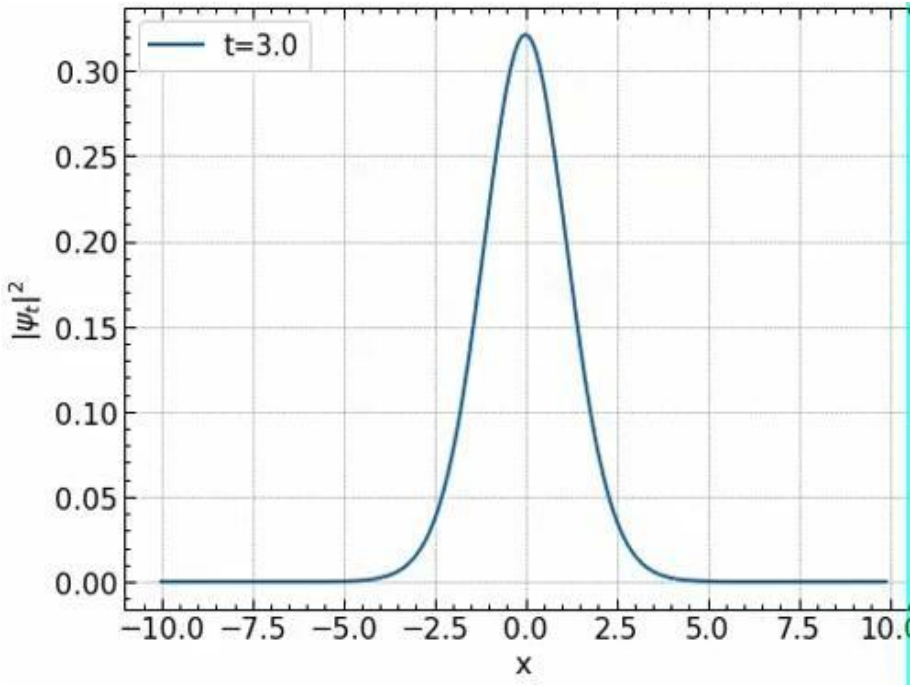
$$\Psi(t=0) = \frac{1}{\pi^{1/4}\sqrt{\sigma}} \exp\left(\frac{-(x-\mu)^2}{2\sigma^2}\right) \exp\left(ip_0 x/\hbar\right)$$

$x \in [-10,10]$
$t \in [0,50]$
$m = 1$
$\triangle x = 0.1$
$\triangle t = 0.5$
$p_0 = 0$
Boundary conditions: $\Psi(0, t) = \Psi(L, t) = 0$

Our implementation

Potential V(x) = 0





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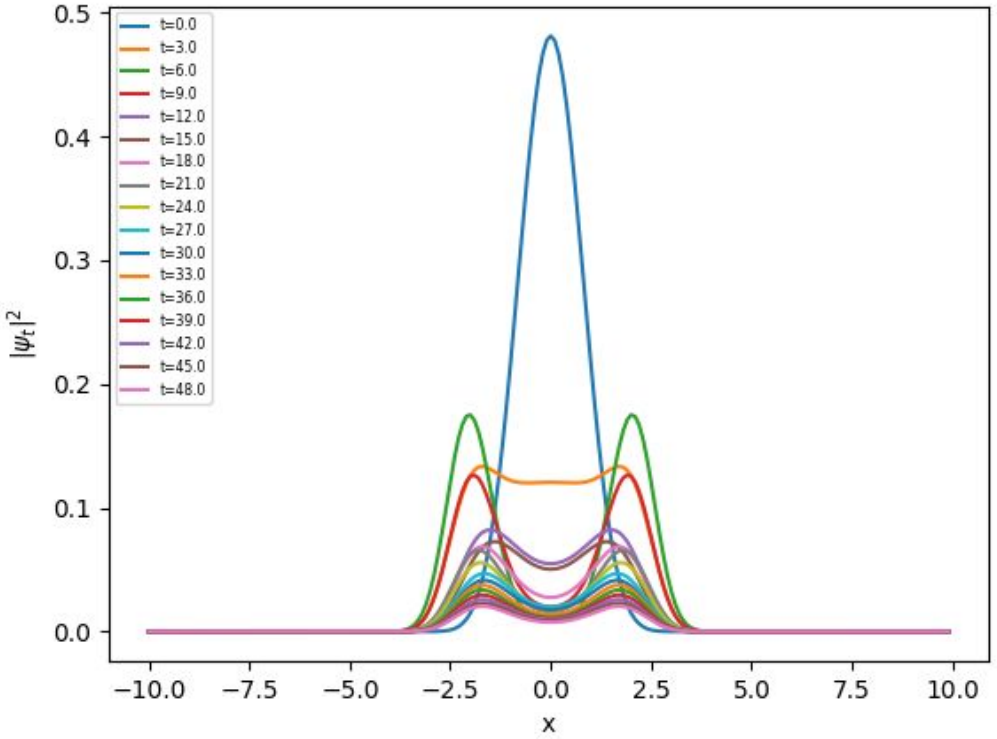
Double-well potential



Potential:

$$V(x) = \frac{a}{x_0^4}(x^2 - x_0^2)^2$$

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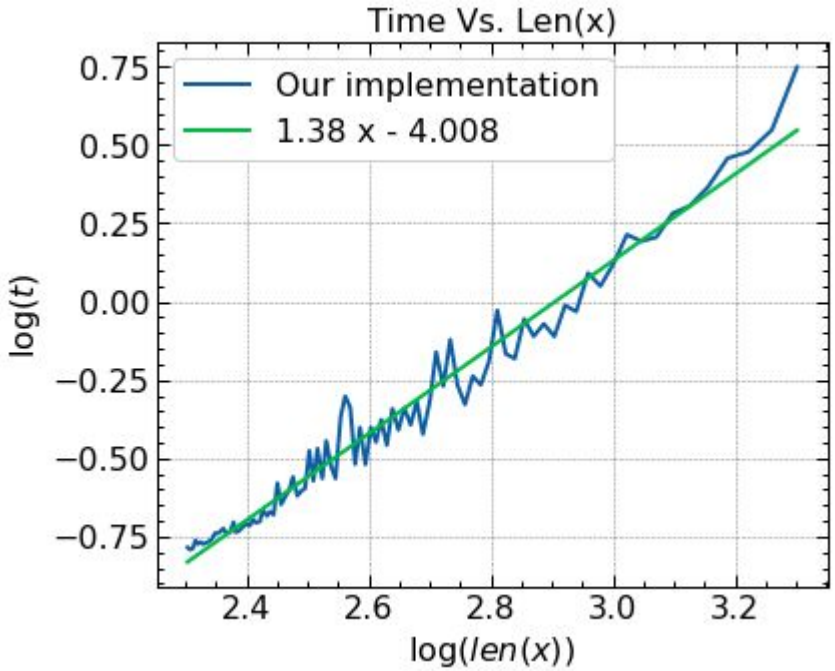
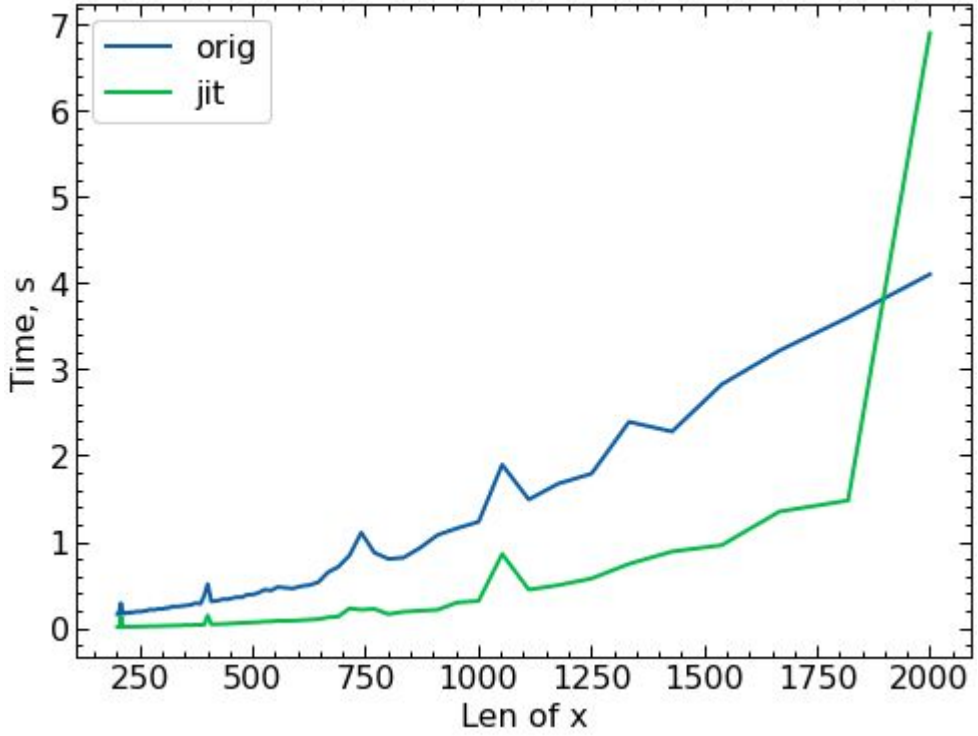
Complexity

Potential V(x) = 0

O(n)



Speed up


orig
jit
Time, s
Len of x
0
1
2
3
4
5
6
7
250
500
750
1000
1250
1500
1750
2000

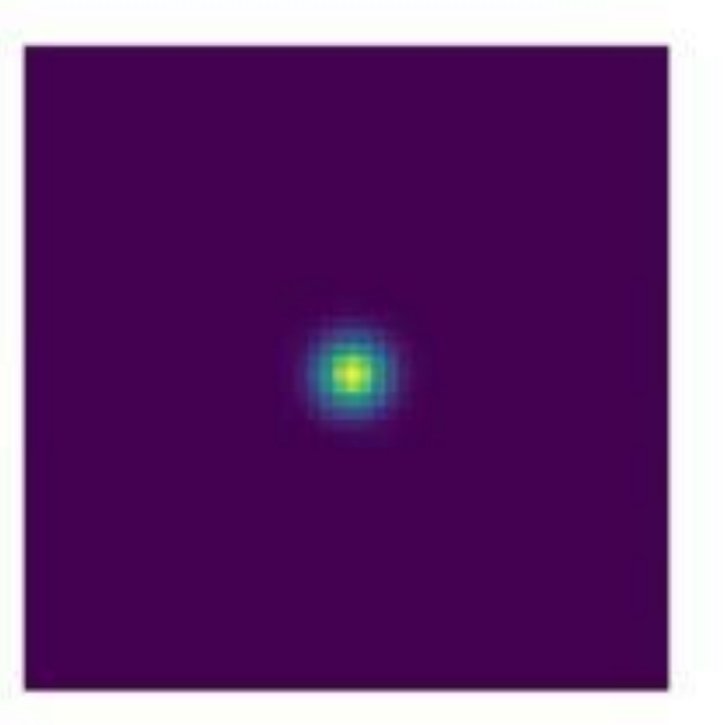
2D case

$$\mathbf{A}\cdot\mathbf{x}=\begin{pmatrix} a_{00} & -r_x & 0 & 0 & \cdots & 0 & -r_y & 0 & 0 & \cdots & 0 \\ -r_x & a_{10} & -r_x & 0 & \cdots & & 0 & -r_y & 0 & \cdots & 0 \\ 0 & -r_x & a_{20} & -r_x & & & & & -r_y & & \\ 0 & 0 & -r_x & \ddots & \ddots & & & & & \ddots & \\ \vdots & \vdots & & \ddots & & & & & & & \\ 0 & & & & & & & & & & \\ -r_y & 0 & & & & & & & & & \\ 0 & -r_y & & & & & & & & & \\ 0 & 0 & -r_y & & & & & & & \ddots & \\ \vdots & \vdots & & \ddots & & & & & \ddots & \ddots & -r_x \\ 0 & 0 & & & & & & & & -r_x & a_{(N-1),(N-1)} \end{pmatrix} \begin{pmatrix} \psi_{0,0}^{n+1} \\ \psi_{1,0}^{n+1} \\ \psi_{2,0}^{n+1} \\ \\ \vdots \\ \\ \psi_{i,j}^{n+1} \\ \\ \vdots \\ \\ \psi_{(N-1),(N-1)}^{n+1} \end{pmatrix}.$$

For 2D problem we have considered a 2-dimensional spatial grid (the xy plane) of N points in the x direction and N points in the y direction.

Our implementation

Time evolution of free potential particle in two-dimensional case:



Literature

1. David G. Robertson. “Solving the Time-Dependent Schrodinger Equation.”

2. Medium: “Quantum Mechanics with Python. Solving the 1D Time Independent Schrödinger Equation Numerically”

3. B. Ducomet AND A. Zlotnik “On stability of the Crank-Nicholson scheme with approximate transparent boundary condition for the Schrodinger equation”.

4. Amin Khan. “Numerical Solution of Schrödinger Equation by Crank–Nicolson Method”

thx.

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