Solution of Time-dependent Schrodinger Equation with different absorbing Boundary Conditions

(Crank-Nicolson Method)

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Derivation

For Spatial domain, take x $= x_j + j\Delta x$, where j $\epsilon[0, J]$ and t $=$ n Δt, with n$\epsilon[0, N]$

$$\psi\left(x_j, t_n\right) \equiv \psi_j^n$$

After applying this discretization to the time-evolution, we obtain

$$\psi_j^{n+1} = e^{-i\hat{H}\Delta t}\psi_j^n = \hat{U}(\Delta t)\psi_j^n$$

Now, we approximate our U to a new Unitary function

$$\hat{U}(\Delta t) = e^{-i\hat{H}\Delta t} \simeq \frac{\left(1 - \frac{i\hat{H}\Delta t}{2}\right)}{\left(1 + \frac{i\hat{H}\Delta t}{2}\right)}$$

Derivation (Continued)

Applying Finite difference approximation-

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

Finally, we introduce the vector $\psi^n = \left(\psi_0^n, \cdots, \psi_j^n, \cdots, \psi_J^n\right)$, a matrix equation:

$$\mathcal{U}_1\boldsymbol{\psi}^{n+1} = \mathcal{U}_2\boldsymbol{\psi}^n$$

Here $\mathcal{U}_1$ and $\mathcal{U}_2$ represent two tridiagonal $(J+1)\times(J+1)$ matrices

Derivation

$$\mathcal{U}_1 = \begin{pmatrix} \xi_0 & -\alpha & & & \\ -\alpha & \xi_1 & -\alpha & & \\ & \ddots & \ddots & \ddots & \\ & & -\alpha & \xi_{J-1} & -\alpha \\ & & & -\alpha & \xi_J \end{pmatrix}, \quad \mathcal{U}_2 = \begin{pmatrix} \gamma_0 & \alpha & & & \\ \alpha & \gamma_1 & \alpha & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha & \gamma_{J-1} & \alpha \\ & & & \alpha & \gamma_J \end{pmatrix}$$

with

$$\alpha = \frac{i\Delta t}{2\Delta x^2}, \xi_j = 1 + \frac{i\Delta t}{2}\left(\frac{2}{\Delta x^2} + V_j\right), \gamma_j = 1 - \frac{i\Delta t}{2}\left(\frac{2}{\Delta x^2} + V_j\right).$$

Now, We are ready to implement this to the code.

Problem Statement

- We have used the travelling wave solutions for One-D Schrodinger wave equation.
- While numerically solving it, we need to fix the range to a finite 1D box.
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Video Example

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Problem

Reflections at the boundaries

- Undesirable Reflection occurs at the boundaries.
- Reason of the Reflection - Our Simulation box/range is very small.

How do you think we can overcome from this problem?

Solutions discovered so far-

Some of the solutions proposed are-

- Increase the box size such that the analysis region is very small compared to the range of the simulation box - **increases computation time**
- Introducing negative imaginary potential near the boundary.
- Applying Absorbing Boundary Condition on the system - **Our Solution**

ABC

We have solved our Absorbing Boundary condition via three different methods-

- Linear approximation method
- Rational Function approximation
- New Absorbing Boundary Conditions

Absorbing Boundary conditions are applied by satisfying the dispersion relation at the Boundaries. Dispersion relation is given by -

$$\psi(x,t) = \exp i(kx - \omega t)$$

$$\hbar^2 k^2 = 2m(\hbar\omega - V)$$

Manipulating and approximating the dispersion relation differently gives us three different methods with different accuracies.

To transform the dispersion relation back into the x-t space, one needs an approximation for the square root, which can be easily transformed into a differential equation at the boundaries.
Here, We approximate the parabolic solution of the plane wave Schrodinger equation to a straight line.

Disadvantages -

- Parameters α_1 and α_2 introduced in the derivation are completely unphysical, hence selected randomly. This leads to inaccuracy in our ABC.

Simulation

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Here, We approximate the dispersion relation by rational function approximation-

$$\sqrt{z - z_0} \approx \sqrt{z_0}\,(1 + 3z/z_0)\,/\,(3 + z/z_0) \tag{1}$$

Advantages -

- It gives the physical meaning to the parameters α_1 and α_2 relating then with g_1 and g_2 which are directly related with energy.

Simulation

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Here, We calculate the group velocity (from the dispersion relation) and manipulate them.

- We want wave passing from right boundary, hence we assume group velocity to be positive. $v_g = \hbar k/m$
- We approximate that $v_g = q$,where q is positive and real.
- In general, Waves can possess more than one component of group velocities. Hence, we have solved the equation for $\mathbf{p} = 2$, 3 and 4.

Solving for p = 2, (p - number of different group velocities of a travelling Wave)

$$\zeta_1 \psi^{n+1}_{(0,J)} + \zeta_2 \psi^{n+1}_{(1,J-1)} = \zeta_3 \psi^{n}_{(0,J)} + \zeta_4 \psi^{n}_{(1,J-1)}$$

where

$$\zeta_1 = \left(-\frac{i}{2\Delta x} - \frac{ic_1}{2\Delta t} + \frac{\left(c_1 V_{(0,J)} - c_2\right)}{4} \right),$$

$$\zeta_2 = \left(\frac{i}{2\Delta x} - \frac{ic_1}{2\Delta t} + \frac{\left(c_1 V_{(0,J)} - c_2\right)}{4} \right),$$

$$\zeta_3 = \left(\frac{i}{2\Delta x} - \frac{ic_1}{2\Delta t} - \frac{\left(c_1 V_{(0,J)} - c_2\right)}{4} \right),$$

$$\zeta_4 = \left(-\frac{i}{2\Delta x} - \frac{ic_1}{2\Delta t} - \frac{\left(c_1 V_{(0,J)} - c_2\right)}{4} \right).$$

$$\mathcal{U}_1 = \begin{pmatrix} \zeta_1 & \zeta_2 & & & \\ -\alpha & \xi_1 & -\alpha & & \\ & \ddots & \ddots & \ddots & \\ & & -\alpha & \xi_{J-1} & -\alpha \\ & & & \zeta_2 & \zeta_1 \end{pmatrix}, \quad \mathcal{U}_2 = \begin{pmatrix} \zeta_3 & \zeta_4 & & & \\ \alpha & \gamma_1 & \alpha & & \\ & \ddots & \ddots & \ddots & \\ & & \alpha & \gamma_{J-1} & \alpha \\ & & & \zeta_4 & \zeta_3 \end{pmatrix}$$

Modifying the initial matrix to this new matrix and implementing it on the code gives us the result as shown below.

NOTE - Refer to the project report for a detailed derivation of p =3, 4.

Simulation

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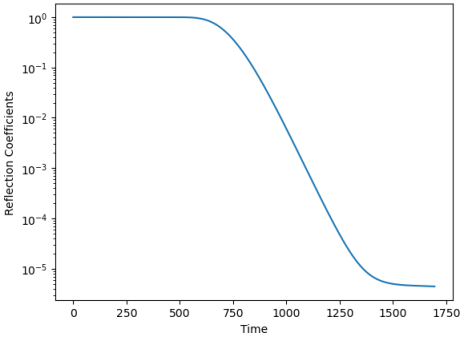
The reflection ratio/reflection coefficient is a parameter that describes how much of a wave is reflected by an impedance discontinuity in the transmission medium. It is equal to the ratio of the amplitude of the reflected wave to the incident wave.

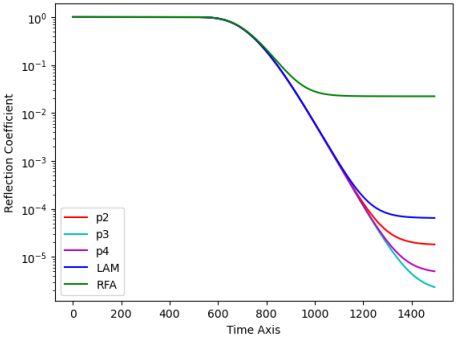
$$R = \frac{\sum_{j=0}^{J} \left|\psi_j^n\right|^2 \Delta x}{\sum_{j=0}^{J} \left|\psi_j^0\right|^2 \Delta x}$$

- If R = 1, The wave packet is completely reflected.
- If R = 0, The wave packet is completely absorbed.

- We observe that the reflection ratio vs time curve dies from 1 to 0 as the wave progress towards the boundaries.
- It's a one-step decay curve.



Comparing Reflection Coefficient Vs time Curve for all methods-



- As we can observe, Rational Function approximation is the poor method of all the methods.
- New Absorbing Boundary condition for p = 3 is the best method that gives the answer with high accuracy.

Theoretical Predictions

- The solution of the Schrodinger equation is composed of three different components of group velocities as the reflection coefficient is minimum for p =3.
- Initial value of R = 1 can be explained by the restriction of Numerical methods and their initial conditions.
- The reason for decreasing amplitude of the wave packet with time can be predicted by R = 1 at the initial point of time, indicating the reflected wave superimpose on our initial Gaussian wave packet and reduces its amplitude.

Introducing the Potential Barrier

The main aim of applying ABC was to get an accurate simulation of the scattering of waves. So now, we introduce the rectangular potential barrier in between the path of the traveling wave packet.

Simulation

Developments in the field-

- Crank-Nicolson Method can be used to solve the non-linear time-dependent Schrodinger equation.
- More accurate and Novel methods can be devised by using some other approximations on ABC to get higher accuracies.

References

1. Christoph Wachter in "Numerical Solution of the Time-Dependent 1D-Schrodinger Equation using Absorbing Boundary Conditions"
2. J.-P. Kuska in "Absorbing boundary conditions for the Schrodinger equation on finite intervals"
3. Tsugumichi Shibata in "Absorbing boundary conditions for the finite-difference time-domain calculation of the one-dimensional Schrodinger equation"

Thank You