Numerical simulations on 1D Schrödinger equation

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Abstract: Simple Euler, Modified Euler, 4th order Runge-Kutta and Split-Step methods are compared simulating a one-dimensional quantum particle colliding with a square potential barrier and transmission and reflection coefficients have been measured. Quantum tunneling effect appeares and our data fit well in quantum theory and experiments. Simple Euler method stands out for its low stability compared with the other three methods. Modified Euler shows a huge improvement in front of Simple Euler without any additional computing cost and gets closer to 4th order Runge-Kutta. RK4 performs as expected and prove its high stability. Finally, Split-Step method opens a hole new way to integrate Schrödinger equation and, also, preserve completely the norm of the wave-function.

I. INTRODUCTION AND NUMERICAL APPROACH

The aim of this project is to simulate the evolution of a one-dimensional quantum particle represented by a Gaussian wave-packet colliding with a potential barrier. The dynamics of that system is governed by the time-dependent Schrödinger equation:

$$i\hbar \frac{d}{dt}\left|\psi\right\rangle = \left[-\frac{\hbar}{2m}\nabla^2 + V\right]\left|\psi\right\rangle \quad (1)$$

which, in one-dimensional coordinates space, becomes

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x,t) \quad (2)$$

where ψ is the wave-function and x is the spatial coordinate.

The first step in numerical simulations is to discretize space and time. From now on, we will work on a discrete one-dimensional space with N points from $-L$ to L with $\Delta x = 2L/N$ so spatial coordinate will be defined as $x_n = -L + n\Delta x$. Also, we will have a fixed Δt so the wave-function ψ and the external potential V will follow that discretization.

In order to represent a localized quantum particle, ψ is initially defined by a Gaussian wave-packet with dispersion a, group velocity k_0 and centered at x_0. That is

$$\psi(x, t=0) = \sqrt[4]{\frac{a^2}{2\pi}} \exp\left\{ik_0 x - \frac{a(x-x_0)^2}{4}\right\} \quad (3)$$

which has an energy $E_{\text{wave}} = k_0^2/2m$ where m is the mass of the particle (see Figure 1).

And, in order to build a square potential wall with certain width centered at $x = 0$, we define

$$V(x_n) = \begin{cases} E_{\text{wall}}, & \text{if } |x_n| < \text{width}/2 \\ 0, & \text{otherwise} \end{cases} \quad (4)$$

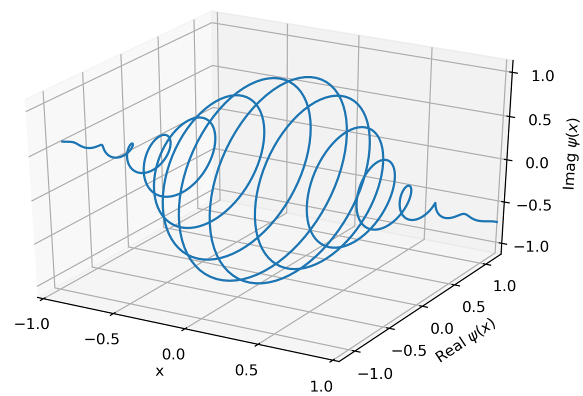

Figure 1: Representation of a Gaussian wave-packet

Now we just have to solve Schrödinger equation (2) and discretize the spatial second derivative.

II. INTEGRATION METHODS

A. Simple Euler

Euler methods are the simplest and most intuitive integration methods. The main idea is to convert differentials into small finite increments like

$$\frac{\partial \psi(x,t)}{\partial t} \approx \frac{\Delta \psi(x,t)}{\Delta t} = \frac{\psi(x, t+\Delta t) - \psi(x,t)}{\Delta t} \quad (5)$$

which is known as Newton's difference quotient with an error of $\mathcal{O}(\Delta t)$.

Also, we still have to express second derivative in space for a discretyzed system. Using a similar idea as before

$$\frac{\partial^2 \psi(x_n,t)}{\partial x^2} \approx \frac{\psi(x_{n+1},t) - 2\psi(x_n,t) + \psi(x_{n-1},t)}{\Delta x^2} \quad (6)$$

Now, putting equations (5) and (6) on (2) and defining

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our units so that $\hbar \equiv 1$ we get

$$\psi(x_n, t+\Delta t) = \psi(x_n, t) + \\ i\Delta t \left[\frac{\psi(x_{n+1}, t) - 2\psi(x_n, t) + \psi(x_{n-1}, t)}{2m\Delta x^2} - V(x_n)\psi(x_n, t)\right] \tag{7}$$

We end up with an iterative equation that, giving an initial configuration $\psi(x, t = 0)$, can give us the state at any time.

B. Modified Euler

Using the same idea as previous method, we make a huge improvement simply if we redefine equation (5) as

$$\frac{\partial\psi(x,t)}{\partial t} \approx \frac{\psi(x, t+\Delta t) - \psi(x, t-\Delta t)}{2\Delta t} \tag{8}$$

which is known as the symmetric difference quotient. In this case first-order errors cancel and the method becomes $\mathcal{O}(\Delta t^2)$.

Now, putting equations (8) and (6) on (2) we get

$$\psi(x_n, t+\Delta t) = \psi(x_n, t-\Delta t) + \\ i2\Delta t \left[\frac{\psi(x_{n+1}, t) - 2\psi(x_n, t) + \psi(x_{n-1}, t)}{2m\Delta x^2} - V(x_n)\psi(x_n, t)\right] \tag{9}$$

Which we will call the Modified Euler method. It is very similar to Simple Euler method and has the same computational cost but it is way more accurate.

C. Runge-Kutta

Runge-Kutta methods are a family of iterative methods and, perhaps, the most used ones on numerical integration due to their high accuracy and stability. We will see 4th order Runge-Kutta (RK4) which error goes like $\mathcal{O}(\Delta t^4)$.

We are not going to dive into the ideas behind these methods because they are not trivial and this is not the aim of this paper. Instead we take the final algorithm:

$$\psi(x, t+\Delta t) = \psi(x, t) + \frac{\Delta t}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right) \tag{10}$$

$$\begin{aligned} k_1 &= f(\psi \qquad\quad , t) \\ k_2 &= f(\psi + k_1\frac{\Delta t}{2}, t + \frac{\Delta t}{2}) \\ k_3 &= f(\psi + k_2\frac{\Delta t}{2}, t + \frac{\Delta t}{2}) \\ k_4 &= f(\psi + k_3\Delta t\ , t + \Delta t) \end{aligned}$$

with

$$f(\psi, t) = \frac{\partial\psi}{\partial t} \tag{11}$$

With that integrator and using our discretized spatial second derivative of equation (6) we are able to integrate and make our system evolve in time.

D. Split-Step Method

Finally we arrive to Split-Step method which uses a totally different approach. This method uses the Fourier transform of the wave-function defined as

$$\widetilde{\psi}(k, t) = \frac{1}{\sqrt{2\pi}}\sum_{n=0}^{N}\psi(x_n, t)e^{-ikx_n}\Delta x \tag{12}$$

where $\widetilde{\psi}$ denotes the wave-function on momentum space (Fourier-space) and k is the specific momentum.

Now, Schrödinger equation in Fourier-space becomes

$$i\hbar\frac{\partial\widetilde{\psi}}{\partial t} = \frac{\hbar^2k^2}{2m}\widetilde{\psi} + V(i\frac{\partial}{\partial k})\widetilde{\psi} \tag{13}$$

We can see some similitude between the two forms of Schrödinger equations. Both have a simple linear term multiplying ψ (or $\widetilde{\psi}$) and a more complicated one which involves derivative on x (or k). If we cut both equations on the linear term

$$\begin{aligned} i\hbar\frac{\partial\psi}{\partial t} &= V(x)\psi \\ i\hbar\frac{\partial\widetilde{\psi}}{\partial t} &= \frac{\hbar^2k^2}{2m}\widetilde{\psi} \end{aligned} \tag{14}$$

for a small time step Δt, these have a solution of the form

$$\begin{aligned} \psi(x, t+\Delta t) &= \psi(x, t)e^{-iV(x)\Delta t/\hbar} \\ \widetilde{\psi}(k, t+\Delta t) &= \widetilde{\psi}(k, t)e^{-i\hbar k^2\Delta t/2m} \end{aligned} \tag{15}$$

which $e^{-iV(x)\Delta t/\hbar}$ can be understand as the real-space operator and $e^{-i\hbar k^2\Delta t/2m}$ as the Fourier-space operator.

The idea of Split-Step method, in order to progress the system by a time-step Δt and starting on real-space, is:

1. Apply half time-step with real operator
2. Change to Fourier-space
3. Apply a whole time-step with Fourier operator
4. Change again to real-space
5. Apply again half time-step with real operator

This method can be very fast using discreet Fast Fourier Transform and precalculating evolution operators.

III. NUMERICAL SIMULATIONS

Getting back to the aim of this paper, we make the quantum particle to collide with a square potential wall of a certain width and height. We end up measuring the reflection and transmission coefficients of the barrier (R and T).

At $t = 0$ the wave-function is set with equation (3) centered on one side of the wall which is located at $x = x_{N/2} = 0$. Taking into account the fully normalization of the wave-funtion ($\Delta x \sum_{n=0}^{N} |\psi(x_n, t)|^2 = 1 \ \forall t \geq 0$) we let the wave-packet collide with the wall using one of the exposed integration methods and wait until the two resulting parts of the collision are detached from enough from the wall (at measure time t_m), then we measure the coefficients as

$$R = \Delta x \sum_{n=0}^{N/2} |\psi(x_n, t_m)|^2$$

$$T = \Delta x \sum_{n=N/2}^{N} |\psi(x_n, t_m)|^2$$

The parameters used in our simulations are:

- $L = 8$
- $a = 5$
- $m = 1$
- $N = 1000$
- $k_0 = 20$
- $x_0 = -2$

Using animated plots we determine the correct time to measure R and T at $t_m = 0.2$ (a video .mp4 is provided in order to prove it).

We first simulate the system with a width set to $20\Delta x \approx 0.32$ and a variable height from $E_{\text{wall}} = 0$ to $E_{\text{wall}} = 1.5E_{\text{wave}}$ in 50 steps. Then we set $E_{\text{wall}} = 0.9E_{\text{wave}}$ and the width goes from 0 to $20\Delta x$ in 20 steps.

Simulation program is written in Python language and using personal Fortran subroutines to run numerical calculus in all methods except for Split-Step method which uses only the Numpy library.

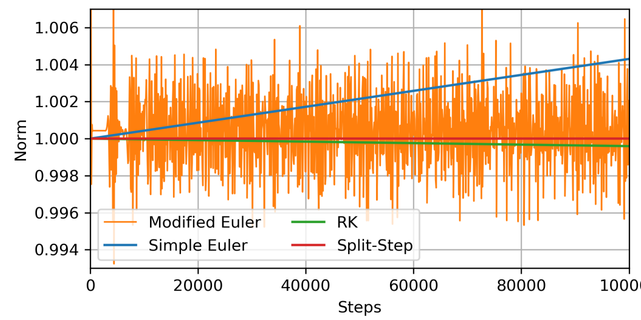

Figure 2: Norm of the wave-function evolving through time-steps of critical Δt for each integration method

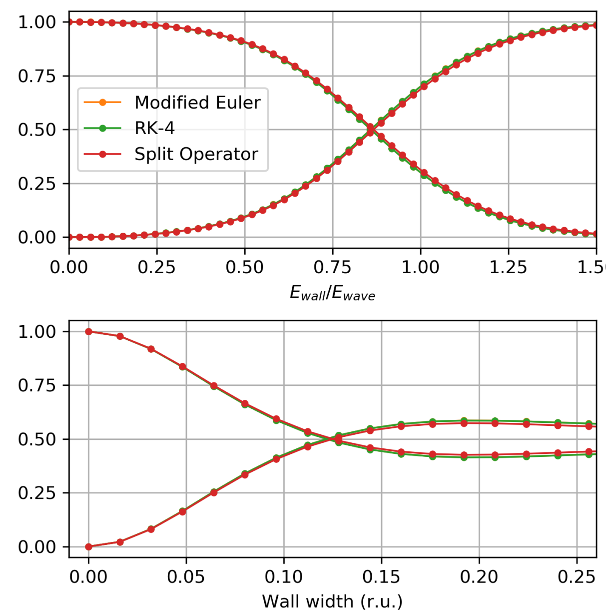

Figure 3: Transmission and Reflection (T and R) of different potential barriers using $\Delta t = 10^{-4}$ and the 3 integration methods. **Top:** varying barrier's height. **Bottom:** varying barrier's width.

IV. RESULTS

Comparing all 4 methods, Simple Euler method stands out for being highly unstable. We realize that Euler methods as well as Runge-Kutta have a maximum stable Δt. Beyond that threshold the method becomes unstable and it doesn't preserves the norm of the wave-function. Simple Euler and Runge-Kutta 4 show a slowly deviation in time of the norm (growing or decreasing) while Modifier Euler shows oscillation of the norm as we increase the time-step (see Figure 2 and Table I). Below threshold, all three methods have a very similar response and simulate the same physics.

But Slit-Step method is different. Due to its formulation it is 100% stable for any Δt and always preserves the norm. Also, its results show a slightly difference from previous methods. Nevertheless, as N is increased, that difference becomes smaller.

The results for all wall widths and heights appear on Figure (3). We can see quantum tunneling effect and how all methods converges at the same result overlapping each other, except for Simple Euler which needs a much smaller time-step to work and doesn't appears on the Figure.

	Simple Euler	Modified Euler	RK4	Split-Step
max Δt	$1.0 \cdot 10^{-6}$	$1.0 \cdot 10^{-4}$	$3.5 \cdot 10^{-4}$	None
Instability type	Slowly diverging	Oscillations	Slowly diverging	unreal results

Table I: Critical time-steps