Numerical simulation of the 2+1 dimensional Schrödinger equation

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NB! Abstract here!

I. INTRODUCTION

Looking at the world around you there are an incredible variety of processes occurring. This can be the weather, how heat diffuses through your cooking utensils and burns you, or how light behaves and allows you to see it all. Most such physical processes are amazingly complex and depend on many variables. Partial differential equations (PDEs) allow us to model such processes. These PDEs can be incredibly difficult and often impossible to solve analytically. An example some readers might be familiar with are the famous Navier-Stokes equations, the solving of which would be rewarded with a million dollar prize. Thus, to simulate and at least approximate solutions to these equations we utilize the rapidly evolving tool of computational simulation by implementing a variety of finite difference schemes and letting a computer do the repetitive work. We will use the Crank-Nicholson scheme to solve a possibly even more famous PDE, the time-dependent Schrödinger equation. The equation is simplified to our specific case where we simulate arguably the most famous experiment in physics; the double slit experiment. It was originally performed by Thomas Young in 1802 resulting in the first demonstration of wave-particle duality.

Crank-Nicholson

conservation of probability to check stability

II. METHODS

To simulate the double-slit-in-a-box experiment we use the following theoretical framework. The time-dependent Schrödinger equation's general formulation is

$$i\hbar\frac{d}{dt}|\Psi\rangle = \hat{H}|\Psi\rangle. \tag{1}$$

Here $|\Psi\rangle$ is the quantum state and $\hat{H}$ is the Hamiltonian operator. For our purposes we consider a single, non-relativistic particle in two spatial dimensions. This allows $|\Psi\rangle$ to be expressed as $/Psi(x, y, t)$, a complex-valued function. In this case the Schrödinger equation can be expressed as

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

$$+V(x,y,t)\Psi(x,y,t). \tag{3}$$

In the first term on the RHS, $-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$ and $-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$ express kinetic energy equivalent to $\frac{p^2}{2m}$ in classical physics. Here m is the particle mass. Only the case of a time-independent potential $V = V(x, y)$ is considered. Working in this kind of position space the Born rule is

$$p(x,y;t) = |\Psi(x,y,t)|^2 = \Psi^*(x,y,t)\Psi(x,y,t). \tag{4}$$

Here $p(x, y; t)$ is the probability density of a particle being detected at a position (x, y) at a time t. Continuing we assume that all dimensions have been scaled away. This leaves us with a dimensionless Schrödinger equation

$$i\frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial y^2} - \frac{\partial^2 u}{\partial y^2} + v(x,y)u. \tag{5}$$

$v(x, y)$ is some potential and $u = u(x, y, t)$ our "wave function" which will hold a complex value ($u \in \mathbb{C}$). With this new notation the Born rule becomes

$$p(x,y,;t) = |u(x,y,t)|^2 = u^*(x,y,t)u(x,y,t). \tag{6}$$

Here we assume that the wave function u has been properly normalized.

Initial and boundary conditions

Dirichlet boundary conditions are implemented in the xy-plane as follows.

- $u(x = 0, y, t) = 0$
- $u(x = 1, y, t) = 0$
- $u(x, y = 0, t) = 0$
- $u(x, y = 1, t) = 0$

The initial wave function u^0_{ij} is given by the unnormalized quantum mechanical Gaussian wavepacket

$$u(x,y,t=0) = e^{-\frac{(x-x_c)^2}{2\sigma_x^2} - \frac{(y-y_c)^2}{2\sigma_y^2} + ip_x(x-x_c) + ip_y(y-y_c)}. \tag{7}$$

This is then normalized such that

$$\sum_{i,j} u^{0*}_{ij}u^0_{ij} = 1. \tag{8}$$

The Crank-Nicholson scheme

Using the Crank-Nicholson scheme, eq. 5 is discretized as

$$u_{ij}^{n+1} - r\left[u_{i+1,j}^{n+1} - 2u_{ij}^{n+1} + u_{i-1,j}^{n+1}\right] \tag{9}$$

$$- r\left[u_{i,j+1}^{n+1} - 2u_{ij}^{n+1} + u_{i,j-1}^{n+1}\right] + \frac{i\Delta t}{2} v_{ij} u_{ij}^{n+1} \tag{10}$$

$$= u_{ij}^{n} + r\left[u_{i+1,j}^{n} - 2u_{ij}^{n} + u_{i-1,j}^{n}\right] \tag{11}$$

$$+ r\left[u_{i,j+1}^{n} - 2u_{ij}^{n} + u_{i,j-1}^{n}\right] - \frac{i\Delta t}{2} v_{ij} u_{ij}^{n}. \tag{12}$$

Here $r \equiv \frac{i\Delta t}{2h^2}$. i indexes are not to be confused with the imangiary unit i. A more comprehensive analytical derivation can be found in appendix A. Considering the case with our specific boundary conditions, this can be expressed as the matrix equation

$$A\vec{u}^{\,n+1} = B\vec{u}^{\,n}. \tag{13}$$

III. RESULTS

IV. DISCUSSION

V. CONCLUSION

Appendix A: Analytical discretization of the 2+1 dimensional wave equation

The Schrödinger equation written as

$$i\frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} + v(x,y)u, \tag{A1}$$

can be discretized using the Crank - Nicholson scheme. This involves using the forward Euler approximation for time

$$\frac{\partial u}{\partial t} = \frac{u_{ij}^{n+1} - u_{ij}^{n}}{\Delta t}, \tag{A2}$$

and evaluating the second order spatial derivative in both the current and next time step to then use the average for both spatial dimension x and y. Using Taylor expansion results in

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{h^2}. \tag{A3}$$

Then evaluating in the current and next time step we have

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{2}\left[\frac{u_{i+1,j}^{n+1} - 2u_{ij}^{n+1} + u_{i-1,j}^{n+1}}{h^2} + \frac{u_{i+1,j}^{n} - 2u_{ij}^{n} + u_{i-1,j}^{n}}{h^2}\right] \tag{A4}$$

for the x dimension. Similarly, for the y dimension we have

$$\frac{\partial^2 u}{\partial y^2} = \frac{u_{i,j+1} - 2u_{ij} + u_{i,j-1}}{h^2} \tag{A5}$$

and evaluated in the current and next time step

$$\frac{\partial^2 u}{\partial y^2} = \frac{1}{2}\left[\frac{u_{i,j+1}^{n+1} - 2u_{ij}^{n+1} + u_{i,j-1}^{n+1}}{h^2} + \frac{u_{i,j+1}^{n} - 2u_{ij}^{n} + u_{i,j-1}^{n}}{h^2}\right]. \tag{A6}$$

Now to discretize eq. A1 we insert our results from eq. A2, A4 and A6. This gives

$$i\frac{u_{ij}^{n+1} - u_{ij}^{n}}{\Delta t} = -\frac{1}{2}\left[\frac{u_{i+1,j}^{n+1} - 2u_{ij}^{n+1} + u_{i-1,j}^{n+1}}{h^2} + \frac{u_{i+1,j}^{n} - 2u_{ij}^{n} + u_{i-1,j}^{n}}{h^2}\right] \tag{A7}$$

$$-\frac{1}{2}\left[\frac{u_{i,j+1}^{n+1} - 2u_{ij}^{n+1} + u_{i,j-1}^{n+1}}{h^2} + \frac{u_{i,j+1}^{n} - 2u_{ij}^{n} + u_{i,j-1}^{n}}{h^2}\right] + \frac{1}{2}\left[v_{ij}u_{ij}^{n+1} + v_{ij}u_{ij}^{n}\right], \tag{A8}$$

where the whole RHS is evaluated in the current and next time step including the last term. Then multiplying by $i\Delta t$ on both sides (remembering that $i^2 = -1$), we have

$$-u_{ij}^{n+1} + u_{ij}^{n} = -\frac{i\Delta t}{2}\left[\frac{u_{i+1,j}^{n+1} - 2u_{ij}^{n+1} + u_{i-1,j}^{n+1}}{h^2} + \frac{u_{i+1,j}^{n} - 2u_{ij}^{n} + u_{i-1,j}^{n}}{h^2}\right] \tag{A9}$$

$$-\frac{i\Delta t}{2}\left[\frac{u_{i,j+1}^{n+1} - 2u_{ij}^{n+1} + u_{i,j-1}^{n+1}}{h^2} + \frac{u_{i,j+1}^{n} - 2u_{ij}^{n} + u_{i,j-1}^{n}}{h^2}\right] + \frac{i\Delta t}{2}\left[v_{ij}u_{ij}^{n+1} + v_{ij}u_{ij}^{n}\right]. \tag{A10}$$

NB! Need to check if the above and below expressions are actually equal!

Collecting all the $n+1$ terms on the LHS we have the final expression

$$u_{ij}^{n+1} - r\left[u_{i+1,j}^{n+1} - 2u_{ij}^{n+1} + u_{i-1,j}^{n+1}\right] - r\left[u_{i,j+1}^{n+1} - 2u_{ij}^{n+1} + u_{i,j-1}^{n+1}\right] + \frac{i\Delta t}{2}v_{ij}u_{ij}^{n+1} \tag{A11}$$

$$= u_{ij}^{n} + r\left[u_{i+1,j}^{n} - 2u_{ij}^{n} + u_{i-1,j}^{n}\right] + r\left[u_{i,j+1}^{n} - 2u_{ij}^{n} + u_{i,j-1}^{n}\right] - \frac{i\Delta t}{2}v_{ij}u_{ij}^{n}, \tag{A12}$$

where $r \equiv \frac{i\Delta t}{2h^2}$.