Numerical simulation of the 2+1 dimensional Schrödinger equation

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NB! Abstract here!

I. INTRODUCTION

PDEs ect.

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

The Crank-Nicholson scheme

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

$$u_{ij}^{n+1} - r\left[u_{i+1,j}^{n+1} - 2u_{ij}^{n+1} + u_{i-1,j}^{n+1}\right] \tag{7}$$

$$- r\left[u_{i,j+1}^{n+1} - 2u_{ij}^{n+1} + u_{i,j-1}^{n+1}\right] + \frac{i\Delta t}{2}v_{ij}u_{ij}^{n+1} \tag{8}$$

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

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

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

$$A\vec{u}^{\,n+1} = B\vec{u}^{\,n}. \tag{11}$$

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