Numerical Time-Dependent Schrödinger Equation

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Abstract

The Time-Dependent Schrödinger Equation (TDSE) describes the quantum state of a particle in the non relativistic regime. The lack of analytical solutions for most cases of interest motivates its study with numerical methods. We present a numerical scheme for the TDSE using the Finite Element Method and Crank-Nicolson.

Introduction

The TDSE is, in natural units ($\hbar = 1$):

$$i\partial_t |\psi\rangle = \hat{H} |\psi\rangle \tag{1}$$

and takes the following form in position basis:

$$i\partial_t \psi = \left[-\frac{1}{2m}\nabla^2 + V(\mathbf{r})\right]\psi \tag{2}$$

The probability density for the particle's position is given by:

$$|\psi(\mathbf{r}, t)|^2 \tag{3}$$

Numerical method

Due to its geometric flexibility, finite element method with quadratic elements was preferred. The chosen timestepping method is Crank-Nicolson because it is unitary, meaning the norm of the solution is preserved and thus is probability. Applying these two methods requires computing the potential-weighted mass matrix, C, given by:

$$C_{ij} = \int \phi_i \phi_j V(\mathbf{r})\, d\mathbf{x} \tag{4}$$

In terms of the global finite element matrices A (stiffness), B (mass), and potential-weighted mass C, the timestepping operator (equivalent to the quantum mechanical propagator in the position basis) is:

$$U = \left[B + \frac{i\Delta t}{2}\left(\frac{A}{2m} + C\right)\right]^{-1}\left[B - \frac{i\Delta t}{2}\left(\frac{A}{2m} - C\right)\right] \tag{5}$$

which satisfies:

$$\psi^{n+1} = U\psi^n \tag{6}$$

Test case

The test problem is the 2D infinite square well, defined by:

$$V = 0, \quad \Omega = [0,1]^2, \quad \psi = 0 \text{ on } \partial\Omega \tag{7}$$

This has an analytical solution, given an initial wavefunction, which is shown below. The initial wavefunction used was a superposition of two eigenstates, $n_x = 1$, $n_y = 1$ and $n_x = 2$, $n_y = 2$.

$$E_n = \frac{\pi^2}{2ml_x l_y}(n_x^2 + n_y^2) \tag{8}$$

$$\psi(x, y, t) = \sum_{n_x, n_y} \frac{1}{4}\frac{\sqrt{2}}{l_x}\frac{\sqrt{2}}{l_y}\sin(n_x \pi x)\sin(n_y \pi y)e^{-iE_n} \tag{9}$$

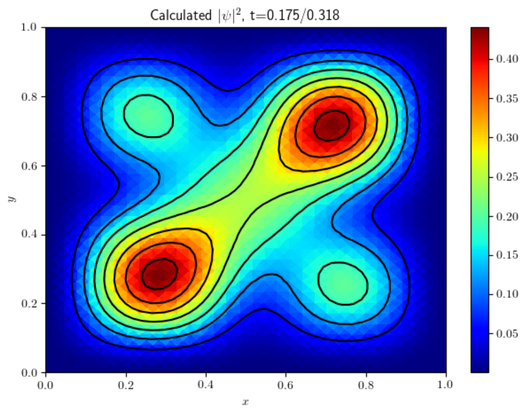

Figure: Graph of the calculated probability distribution.

The error measurements taken were of the relative infinity norm at $t_f = \frac{1}{\pi}$. The estimated algebraic convergence rate is 2 in Δt and 3 in Δx. This is expected because Crank-Nicolson is second order in time and quadratic basis functions are used.

Grid Δx	Error	Timestep Δt	Error
2.5×10^{-1}	5.73×10^{-2}	3.18×10^{-2}	2.54×10^{-1}
6.25×10^{-2}	9.00×10^{-4}	3.18×10^{-3}	6.02×10^{-3}
3.125×10^{-2}	1.28×10^{-4}	3.18×10^{-4}	1.32×10^{-4}

Table: Summary of convergence properties.

Double slit experiment

The domain is similar to $\Omega = [-1,1]^2$ with a division at $x = 0$ and two slits at around $y = 0$ connecting the two halves. $V = 0$ with homogeneous Dirichlet boundary conditions and a plane wave initial condition e^{ikx}

DoubleSlit0.png

Figure: Initial conditions for double slit.

The wave travels to the right and hits the slits. A part is reflected, and the transmitted one experiences interference:

DoubleSlit115.png

Classically, the expected result is to detect particles in regions with the same shape as the slits, but this does not happen. This shows the inability to explain properties of quantum-scale objects by considering them as exclusively particles or waves, and leads to the concept of wave-particle duality.

Conclusion

A numerical realization of the double slit experiment was presented, showing that the Time-Dependent Schrödinger equation predicts wave-like behavior for objects in the quantum scale.
It was also shown that Crank-Nicolson is a reasonable timestepping scheme for this problem based on the error statistics and the conservation of probability.

Future Work

In order to address many systems of physical importance, the current work could be modified to make a general solver for the TDSE. This process involves the following:

- Generalize boundary conditions.
- Improve spatial resolution.
- Use time-dependent potentials.
- Implement in 3D.

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