Visualizing Quantum Wave Packets

Nate Chrisman, Brian Pickens, Andrew Shurman

Background

An electron which is placed in a region with a known potential has behavior that can be determined by solving the time-dependent Schrödinger Equation in 2D, which is presented as

$$i\frac{\partial \psi(x,y,t)}{\partial t} = -\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right) + V(x,y)\psi$$

Given that the electron's initial momentum and position via calculation of a Gaussian, the behavior of the electron can be modeled over time and a calculation of probability density can be made.

Methods

Using the real and imaginary position integration scheme by Maestri *et al.*, the function is separated into real and imaginary parts. A leapfrog integration is performed.

$$R_{i,j}^{n+1} = R_{i,j}^{n-1} + 2\left[(4\alpha + \frac{1}{2}\Delta t V_{i,j})I_{i,j}^{n} - \alpha(I_{i+1,j}^{n} + I_{i-1,j}^{n} + I_{i,j+1}^{n} + I_{i,j-1}^{n})\right]$$

$$I_{i,j}^{n+1} = I_{i,j}^{n-1} + 2\left[(4\alpha + \frac{1}{2}\Delta t V_{i,j})R_{i,j}^{n} - \alpha(R_{i+1,j}^{n} + R_{i-1,j}^{n} + R_{i,j+1}^{n} + R_{i,j-1}^{n})\right]$$

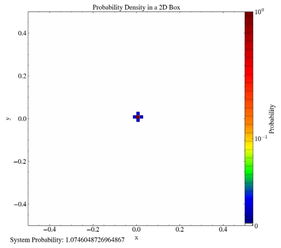
The probability density, ρ, is given for the real and imaginary parts at integer and half-integer time step "t" values, respectively.

$$\rho(t) = \begin{cases} R^2(t) + I\left(t + \frac{\Delta t}{2}\right) I\left(t - \frac{\Delta t}{2}\right), & \text{for integer t} \\ R^2(t) + I\left(t + \frac{\Delta t}{2}\right) I\left(t - \frac{\Delta t}{2}\right), & \text{for half-integer t} \end{cases}$$

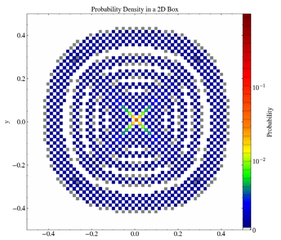
For visualization, Python modules **yt** and **imageio** were used to capture the probability density at each time step. Each frame was then compiled into a .gif file for visualization over time.

Results

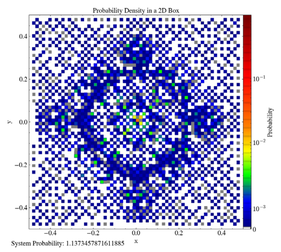
2D Harmonic



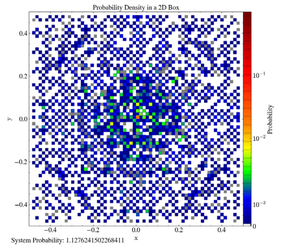
Time Step: 0
Seconds Elapsed: 0.000



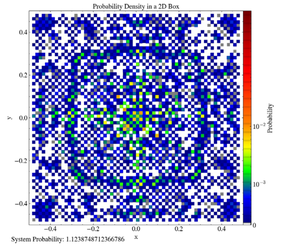
Time Step: 65
Seconds Elapsed: 2.708



Time Step: 221
Seconds Elapsed: 9.208

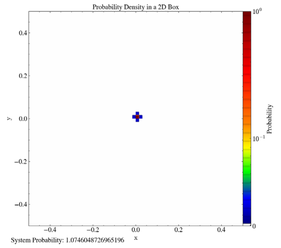


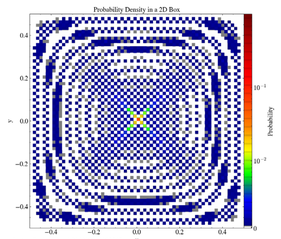
Time Step: 500
Seconds Elapsed: 20.833

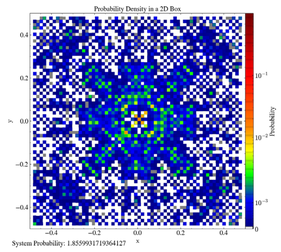


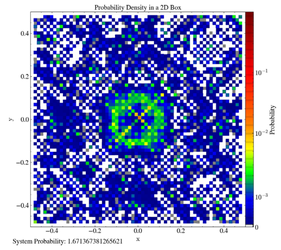
Time Step: 1664
Seconds Elapsed: 69.333

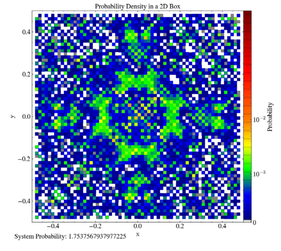
2D Infinite Box





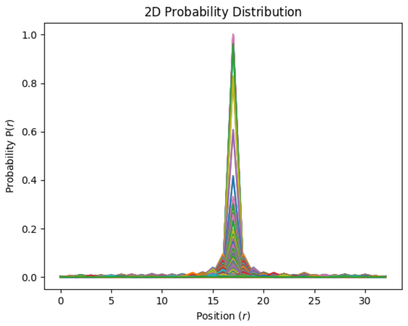






Results

The algorithm does not conserve probability over time accurately:



For a 2D simulation of lattice size 32, the probability per frame is seen to stay somewhat near 1.00, but errors do accumulate over time.

Summary

While initial visualization of 2D wave packet behavior was accomplished, too much error accumulated to see quantum revival. The 3D algorithms diverged in all cases.

A more robust testing suite would allow development of a much more robust conditions for the algorithm.

References & Acknowledgments

- Algorithms pulled from *Computational Physics: Problem Solving With Computers 3rd Edition* (Landau, Páez, Bordeianu)
- Frames rendered using code from **The yt Project**.
  Website: yt-project.org
  GitHub: https://github.com/yt-project/yt
- Frames animated using code from the **imageio** package.
  Website: https://imageio.github.io/
  GitHub: https://github.com/imageio/imageio