

PHY494 - Spring 2017 - Final Project Proposal

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Problem

The mechanics of quantum physics are strange. One of the (many) difficulties of understanding the quantum world is the reliance of simplified one-dimensional situations to introduce students to a particle's odd wave-like behavior. But we, as far as I know, live in a three-dimensional world and I want to know what a 3D particle looks like. How does it interact over time with rigid or dynamic potential barriers? What does quantum tunneling look like in 3D? Can these be modeled accurately by a computer?

Approach

The main obstacle to answering these questions will be solving Schrödinger's equation in three dimensions. It will be necessary to include a time-dependence to model the dynamic situations we will create by answering the questions above. Specifically, we will be attempting to use the real/imaginary position integration scheme by Maestri *et al.*:

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

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

To visualize the particle's behavior, we will model the *probability* of detecting the particle at any position. The value of the probability at a data point will be calculated from the above integration scheme. Visualizing a probability density in 3D can be difficult, so we'll be using the yt package which can be installed into the Anaconda distribution of Python.

Objectives

- Test algorithm by simulating the behavior of a quantum wavepacket in enclosed 2D spaces.
- Move to 3D particle simulation enclosed in a box and in a harmonic oscillator.
- Visualize and animate these 3D behaviors in an intuitive and robust manner.
- BONUS: Implement 3D quantum tunneling effects for potential barriers.