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.*:

$$\begin{aligned} R^{n+1}_{i,j,k} = R^{n-1}_{i,j,k} + 2[(4\alpha + \frac{1}{2}\Delta t V_{i,j,k}) I^n_{i,j,k} - \alpha(I^n_{i+1,j,k} + I^n_{i-1,j,k} \\ + I^n_{i,j+1,k} + I^n_{i,j-1,k} + I^n_{i,j,k+1} + I^n_{i,j,k-1})] \end{aligned} \tag{1}$$

$$\begin{aligned} I^{n+1}_{i,j,k} = I^{n-1}_{i,j,k} + 2[(4\alpha + \frac{1}{2}\Delta t V_{i,j,k}) R^n_{i,j,k} - \alpha(R^n_{i+1,j,k} + R^n_{i-1,j,k} \\ + R^n_{i,j+1,k} + R^n_{i,j-1,k} + R^n_{i,j,k+1} + R^n_{i,j,k-1})] \end{aligned} \tag{2}$$

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

1. Simulate the time-dependent behavior of a Gaussian wave packet in 2D using initial conditions of $\Psi(0,t) = \Psi(L,t) = 0$ and $V(x,t) = \infty$ for $x < 0$ and $x > L$.
2. Test algorithm by simulating the behavior of a quantum wavepacket in enclosed 2D spaces.
3. Move to 3D particle simulation enclosed in a box and in a harmonic oscillator.
4. Visualize and animate these 3D behaviors in an intuitive and robust manner.
5. BONUS: Implement 3D quantum tunneling effects for potential barriers.