Simulating Particle Creation and Annihilation in Quantum Physics

Matthew Harper
Mentor:Roderich Tumulka

Rutgers University

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Goals of the Project

- Our main goal was to create a toy model for particle creation and annihilation using Maple
- We wrote code from scratch to numerically solve the Schrödinger equation, this allowed us to more easily implement additional terms

Some Basics

- In quantum mechanics the probability of particles in a given location is described by a wave-function $\psi(\boldsymbol{x}, t)$
- ψ is complex valued function in some configuration space. For example, if we have N particles then $\psi : \mathbb{R}^{3N} \times \mathbb{R} \to \mathbb{C}$
- ψ evolves with time by the Schrödinger equation

Schrödinger Equation Example

$$i\partial_t \psi = H\psi$$
$$i\partial_t \psi = \left(-\nabla^2 + q\frac{\boldsymbol{x}-\boldsymbol{r}}{|\boldsymbol{x}-\boldsymbol{r}|^2}\right)\psi$$

Introducing Numerics

- In order for us to "solve" this PDE we need initial conditions.
- For our purposes we will have $\psi(\boldsymbol{x}, 0) = f(\boldsymbol{x})$ and we will be considering the interval $[0, 1)$ with a periodic boundary
- Our method also replaces space with a lattice and the Laplace operator now becomes a difference operator.

Difference Operator

$$\frac{d}{dx}\psi = \frac{\psi(x+\epsilon) - \psi(x)}{\epsilon} \qquad \frac{d}{dx}\psi = \frac{\psi(x) - \psi(x-\epsilon)}{\epsilon}$$

$$\frac{d^2}{dx^2}\psi = \frac{\psi(x+\epsilon) - 2\psi(x) + \psi(x-\epsilon)}{\epsilon^2}$$

Fourier Transforms

- The difference operator; however, caused ψ to blow up during our trials
- We were able to use the form of the difference operator to generate a tri-diagonal matrix

$$\frac{d^2}{dx^2}\psi = \frac{\psi(x+\epsilon) - 2\psi(x) + \psi(x-\epsilon)}{\epsilon^2}$$

- By applying the Discrete Fourier Transform and Inverse Transform Matrices to the periodic matrix we get a diagonal matrix with entries: $\frac{1}{\epsilon}(4 - 2\cos(\epsilon\pi * [i-1]))$

Taking a Time Step

- We have effectively found the eigenvalues for the derivative operator
- By Fourier transforming ψ, multiplying it by our diagonal matrix, then transforming back we have the "periodic" second derivative of ψ
- The Schrödinger equation tells us that $\psi(t + \Delta t) = e^{-iH\Delta t}\psi(t)$ so we can now generate time evolutions since we can take second derivatives

First Results

- Let us choose our initial wave-function $\psi(x, 0) = e^{-100(x-.5)^2}$
- Notice that it spreads evenly in both directions and that the function is periodic with time

Gaussian

Some More from the Simple Case

- Here we see the interference between two incoming waves, and 'waves' now seems to be an appropriate name
- $\psi(x,0) = e^{-100(x-.25)^2+50ix} + 1.2e^{-100(x-.75)^2-50ix}$ is the initial wave-function, also note that the time scale is smaller

Interference

Introducing A Potential

- In this quantum mechanical context, think of a potential as an obstacle for ψ to pass over (or through)
- This is the first additional term we add to H
- We only need to multiply by $e^{-i(V(\boldsymbol{x}))\Delta t}$ to incorporate it into the time step for ψ, V is not an operator on ψ so we do not need to perform any other steps

Schrödinger Equation with Potential

$$i\partial_t\psi = \left(-\nabla^2 + V\right)\psi$$

Results for a Potential

- Using $e^{-100(x-.5)^2}$ from before and a potential of $1000\cos(2\pi x)$, observe that the well keeps the peak of the function contained in the center

Potential Well

Creation and Annihilation

- Suppose we have an electron at a fixed position $\boldsymbol{r}$ and it can absorb and emit photons, which have wave-function ψ
- The configuration space of ψ is $\mathcal{F} = \bigcup_{N=0}^{\infty} \mathbb{R}^{3N}$
- The modified Hamiltonian now has this form

C/A Equation

$$H_{C/A}\psi = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \delta(\boldsymbol{x} - \boldsymbol{r})\psi^{(i-1)}(\boldsymbol{x}) + \sqrt{N} \int d^3\boldsymbol{x}\delta(\boldsymbol{x} - \boldsymbol{r})\psi^{(i+1)}(\boldsymbol{x})$$

Creation and Annihilation in 0 and 1 Dimensions

- If we restrict the maximum number of photons to 1 the wave-function will have sectors for $N = 0$ and $N = 1$ particles
- This animation shows the "creation" of a photon at the center and how its wave-function interferes with another
- The wave function is .05 in the 0 sector and $e^{-100((x-.25)^2+(y-.25)^2+I(50x+50y)}$ in the 1 sector

0 Sector

1 Sector