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2D Scattering of Quantum Wave Packets

Introduction

In the Schrödinger model of quantum mechanics, we can model particles as being defined by complex wave functions ψ. Using the Schrödinger equation,

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,t)+V(x,y)\psi(x,y,t)=i\hbar\frac{\partial\psi(x,y,t)}{\partial t}=H\psi \qquad \text{Eq. 1}$$

we can see how a particle's wave function ψ(*x,y,t*) evolves in time with a given potential *V*(*x,y*). An interesting aspect to look at is how the wave packet can interact with the potential in reflecting, transmitting, or interfering. When dealing with scattering of particles in quantum mechanics, we need to take into account the Heisenberg uncertainty principle: $\Delta x\Delta p \geq \hbar/2$. This effectively means that we cannot know both a particle's momentum and position absolutely. To model this inherently probabilistic phenomenon, one can represent a particle by a distribution of positions and momentums, each weighted by a probability. For simplicity, we often find that a Gaussian is a logical model for a localized lump of energy or particle. The probability density of finding the particle is found by the magnitude squared of the wave function, i.e. $\psi^*\psi$ since ψ is complex.

Analytically, we can calculate the probability that a particle will be reflected or transmitted through a barrier or well, but even with this case, we are limited in our choices of potential. They are usually only finite step functions and other simple shapes. To properly visualize how a particle scatters, we would like to calculate the probability of the particle being at any point in our system and watch it evolve in time, not simply the probability of reflection or transmission. I have chosen to model 2D scattering instead of

3D scattering to better visualize how the wave packet evolves in time. 2D scattering also offers much more interesting phenomena than 1D scattering, such as slits and finite width barriers.

Numerical Methods

To calculate the particle's wave function, I looked for some background work done in this field and found a paper on numerically modeling 1D scattering[1]. I used a method similar to the paper's to discritize my wave function in space and time. As seen in equation 1, the Schrödinger equation has two spatial derivatives in *x* and *y* and one in *t*. To model the space derivatives, I used a second order centered finite difference method with equal spatial step sizes in *x* and *y*. I chose *m* to scale away the constant on the spatial derivatives to get the spatial derivatives to look like

$$\frac{1}{\varepsilon^2}\left[\psi_{j+1,k} - 2\psi_{j,k} + \psi_{j-1,k}\right] + \frac{1}{\varepsilon^2}\left[\psi_{j,k+1} - 2\psi_{j,k} + \psi_{j,k-1}\right] \qquad \text{Eq. 2}$$

where *j* is the *x* mesh coordinate and *k* is the *y* mesh coordinate such that $j\varepsilon = k\varepsilon = L$ (the length of one side of the grid). We essentially have discretized space into a square mesh of equal spacings. To deal with the time derivative, we realize that we do not want to use a finite difference method after we use some insight into quantum mechanics. The time evolution operator is closely tied with the Hamiltonian or energy operator, Ĥ. We can evolve from one time step to another by

$$\psi_{j,k}^{n} = e^{i\delta H}\psi_{j,k}^{n+1} \qquad \text{Eq. 3}$$

where *n* is our time coordinate and δ is our time step. An additional concern we have when estimating our time operator, however, is that its magnitude stays 1, i.e. that it is unitary. Goldberg et al. show that we can do this using the Cayley form

$$(1 - i\delta H/2)/(1 + i\delta H/2) \qquad \text{Eq. 4}$$

which approximates the time operator, but leaves it unitary. Additionally, we now have the time operator correct to δ^2 instead of only δ as the finite difference method would have given us. After some manipulation, we can derive an implicit form for the wave function at each step based on stenciling of the previous time step and the current time step as shown below.

$$\begin{aligned} &\psi_{j+1,k}^{n+1} + \psi_{j,k+1}^{n+1} + \left[i \cdot \frac{2\varepsilon^2}{\delta} - 4 - \varepsilon^2 V_{j,k} \right] \psi_{j,k}^{n+1} + \psi_{j-1,k}^{n+1} + \psi_{j,k-1}^{n+1} = \\ &-\psi_{j+1,k}^{n} - \psi_{j,k+1}^{n} + \left[i \cdot \frac{2\varepsilon^2}{\delta} + 4 + \varepsilon^2 V_{j,k} \right] \psi_{j,k}^{n} - \psi_{j-1,k}^{n} - \psi_{j,k-1}^{n} \end{aligned} \qquad \text{Eq. 5}$$

Now that we have derived the equation to solve, we need a method to implicitly solve it. The Crank-Nicolson method seen in class seems like a good candidate. We need to modify the version seen in class to work for 2D by creating a sparse N^2 by N^2 matrix where N is the number of spatial steps in either direction. Instead of stepping in time each row as in 1D, we need to step in time a 2D grid. We accomplish this by changing the N by N grid into an N^2 by 1 column vector. We can now step in time using the method seen before. However, I have chosen periodic boundary conditions, which means in addition to having tridiagonal blocks along the diagonal plus 2 diagonals, we need to add in 4 more partial diagonals. The matrix is still sparse and now has the form of figure 1 below.

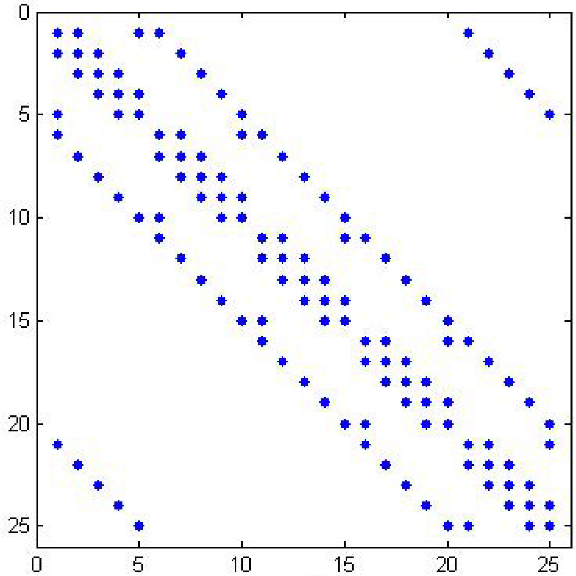

Figure 1: A look at the sparse matrix form for periodic boundary conditions. The furthest corner diagonals were added as well as the corners of the blocks along the diagonal. These extra conditions create periodic boundary conditions.

Results

As stated before, the spatial domain is a 2D square region with periodic boundaries. To simulate a 'particle in a box' as is done often in 1D, we can easily make the potential very large on the boundaries to prevent any transmission from one side to another. I started with a simple rectangular barrier of constant height and found that I could get the wave packet to tunnel through as well as reflect. The best way to visualize the wave packet is by viewing the movies I made or running the code. Matlab does not seem to let me save images anymore, so I must refer you to only movies. I also recreated other potentials, with which I am familiar such as a double slit or even no potential. I use a non rectangular shape by using a cylindrical potential barrier. I also tried a non uniform barrier using a cos^2 barrier. Furthermore, I tried to make a particle in a box to see if I could get standing waves. While I did get some interesting behavior, I did not find any modes. Included with my code, *QMscattering.m*, are some potentials I used to create these movies. Some movies include the potential barrier as well as the probability density.

Interesting behavior I found had to do with time steps. By changing the final time, the relative energies of the potential and wave packet changed. Usually increasing the final time increased the potential barrier. Changing the time step also affected the output. If I used too large of a final time or too large time steps, I found the system to react very strangely. I have included a movie of this behavior as well. I found the total probability by summing up the probability density over the grid and found it was constant over all of the runs I made. This is good news because it means that probability is conserved.

I think that by looking at the behavior of wave packets scattering in 2D, we can get a better sense of how particles really interact at the quantum level. Merely calculating the probability of reflection or transmission in 1D does not give the full picture of quantum mechanics. In the future, scattering movies of this nature could help introductory quantum physics students. Additionally, if modes could be found for particle in a box, then that could further help to visualize this behavior.

References

[1] Goldberg, Abraham et al. *Computer-Generated Motion Pictures of One-Dimensional Quantum-Mechanical Transmission and Reflection Phenomena*. American Journal of Physics 35, 177-186 (1967).