

Figure 1 Wave Distribution with the B-field in one direction for the quantum mechanics simulation of the wave-packet simulation. Dark regions demonstrate the split in propagation.

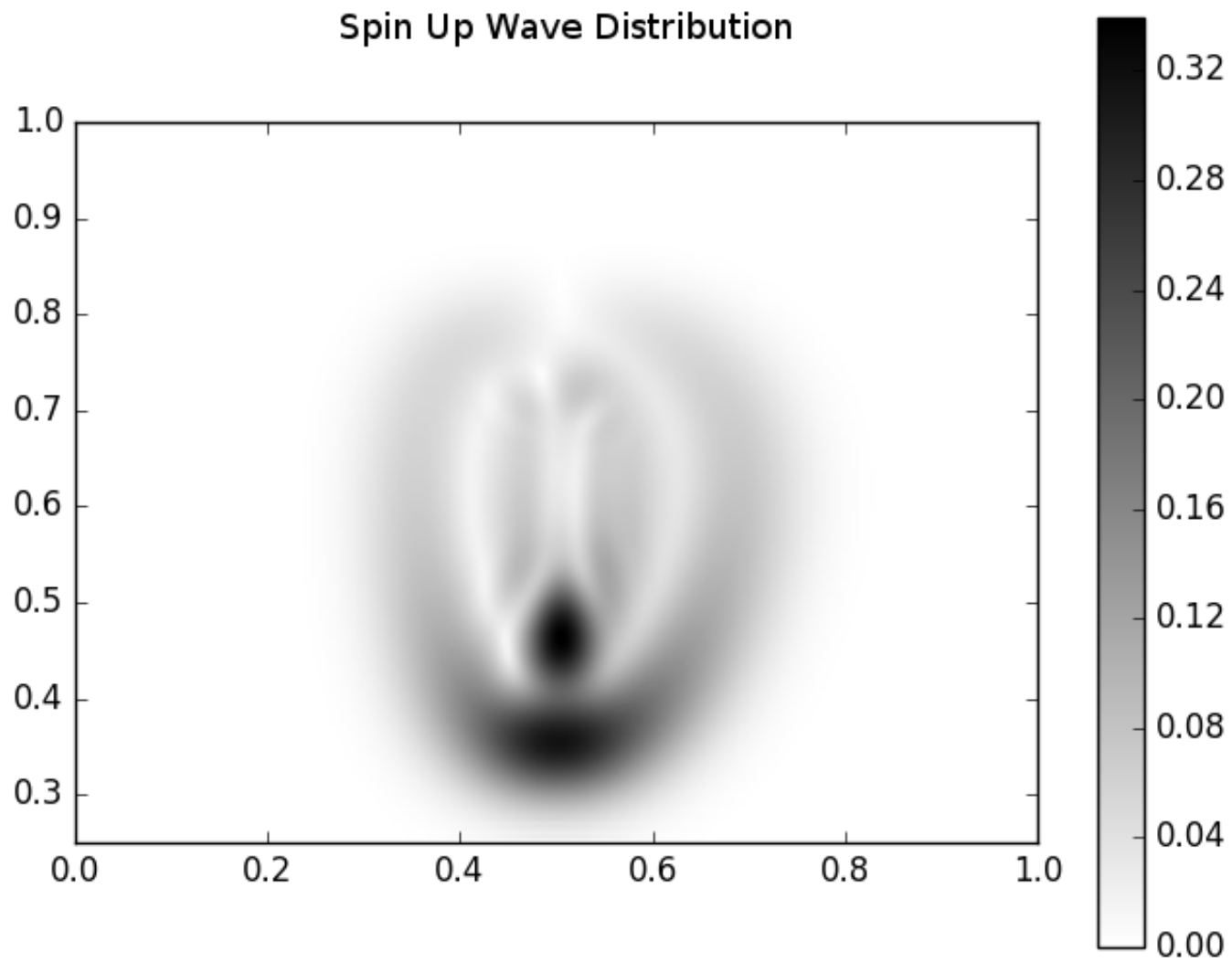


Figure 2 Spin-up wave distribution in the quantum simulation of wave packet propagation.

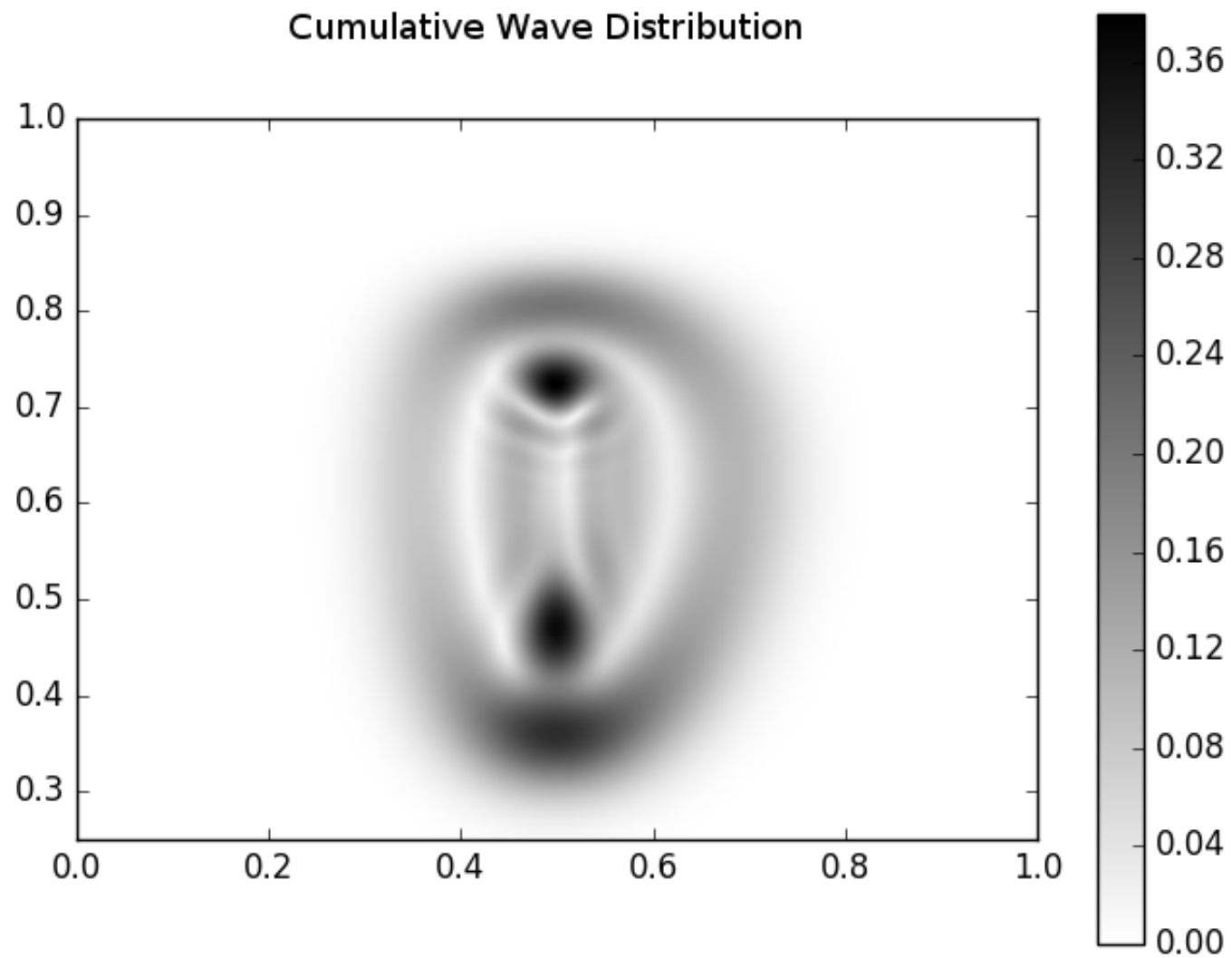


Figure 3 Complete solution with cumulative magnitudes of both spin up and down distributions.

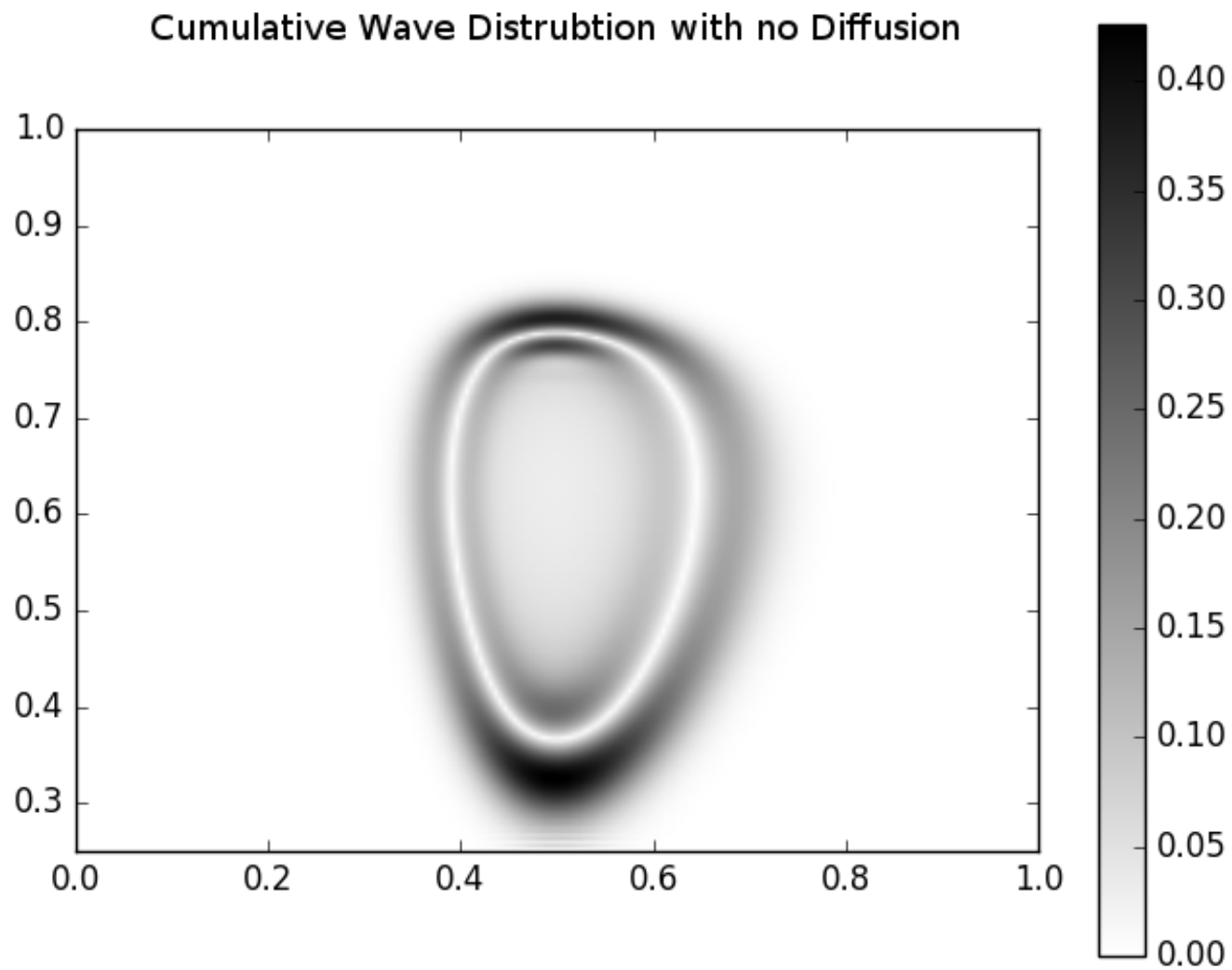


Figure 4 Removing the coefficient of diffusion (Hamiltonian momentum term) better illustrates system evolution as a result of only the magnetic field interaction.

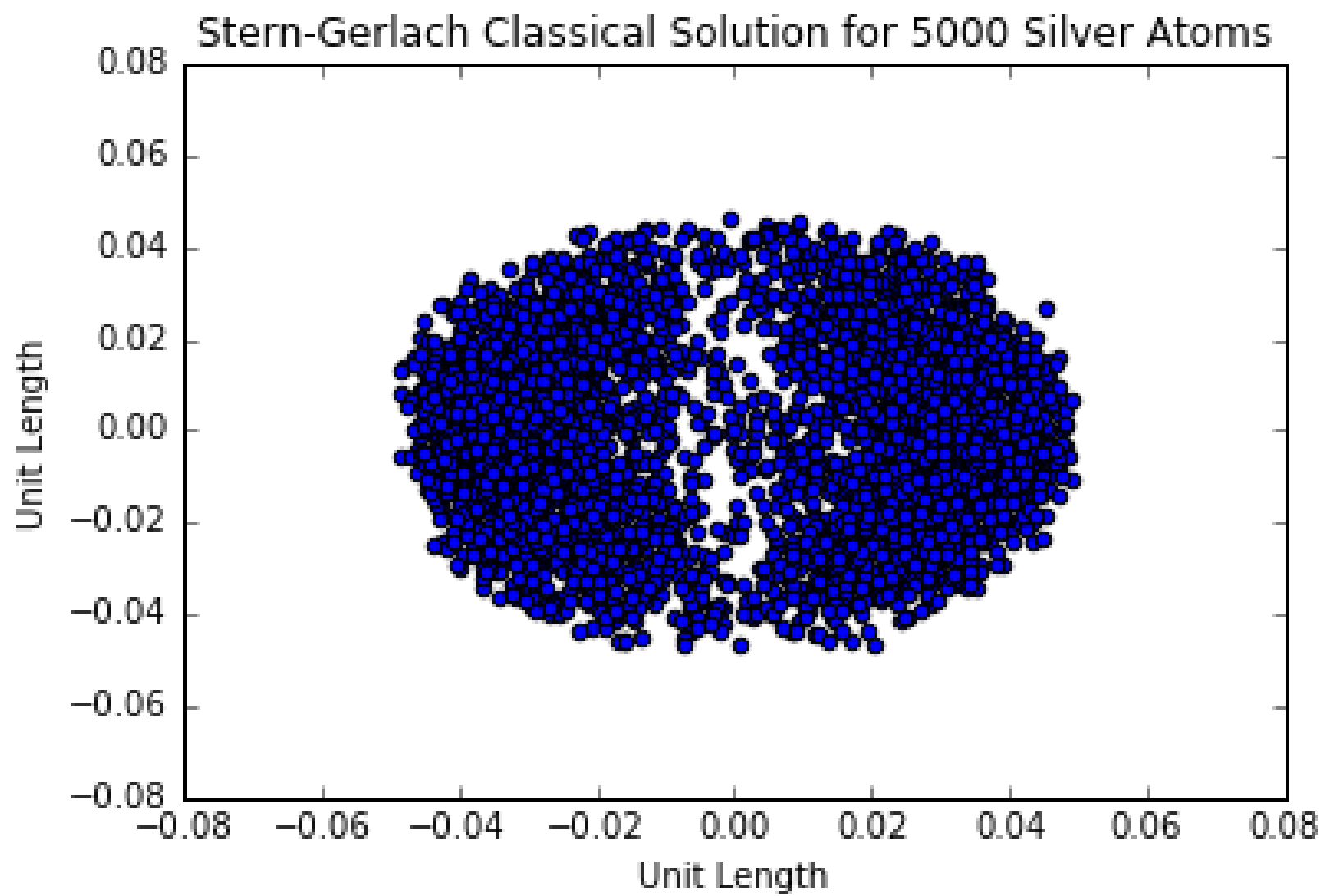


Figure 5 Semi-classical simulation for 5000 Ag Atoms.

Stern-Gerlach Simulation

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Code is available at <https://github.com/ASU-CompMethodsPhysics-PHY494/final-stern-gerlach-simulation.git> under the CC0 license

Abstract

In 1922 Otto Stern and Walther Gerlach confirmed that microscopic particles have a quantized intrinsic degree of freedom called spin angular momentum when they sent a beam of silver atoms through an inhomogeneous magnetic field. Since silver atoms have an extra electron in the 5s orbital, the result showed that the spin of the electron is $\pm\hbar/2$. Thus, for this project we sought out to simulate the Stern-Gerlach experiment by using the finite difference method with a Gaussian wave packet implemented in Python. We also wished to reconstruct the results of the experiment in the classical limit where the states of the electron were assumed to be a continuous band symmetric about the axis where the beam splits. The major hurdle that was encountered was trying to get the states to split and discretize in a manner that made sense for both the classical limit and the quantum limit. The results that were obtained in the semi-classical limit showed that when electrons exit the magnetic field they can populate any state that is symmetric about their initial axis of motion between $\pm\hbar$. The quantum result showed an interference distribution that was heavily peaked about the initial axis of motion which differed from the classical result. For future work we are anticipating simulating the experiment by using the Crank-Nicolson method.

Results

For the semi-classical simulation, 5000 silver atoms were given an initialized velocity with random variance in their Cartesian velocity reference frame. Each atom was given a unique randomized S_x and S_y spin value between the values of -1 and +1, such that the S_z could be calculated from the values of S_x and S_y . This was done to maintain that the spin vector maintained a value of 1 for each atom ($S_x^2 + S_y^2 + S_z^2 = 1$). The atoms were under a constant force, and thus we calculated their positions as time evolved using Newtonian mechanics. The point of this simulation was to explore how the results would play out for the Stern-Gerlach experiment, had a classically allowed spin-angular momentum been possible. For this simulation specifically, we were interested in the relationships between the magnetic field and the force that it caused on the atoms themselves, choosing to neglect specific units of length. For that case, if the specific units were chosen to be ignored as they would only scale the relationships that our data demonstrated (note figure 5). The quantum result showed an interference distribution that was heavily peaked about the initial axis of motion which differed from the classical result. We were able to model the results in the form of a video, which demonstrated the split we hoped to model (note Figures 2 and 3). What we also found was that removing the coefficient of the diffusion term gave a better illustration of the system interaction as it illustrated the magnetic field interaction uniquely (see figure 4). This contrast the complete solution with the diffusion term (see figure 3).

Introduction

The Stern-Gerlach experiment demonstrates that when a beam of silver atoms, which have 46 coupled electrons forming a spherically symmetric configuration and one single electron in the 5s orbital, passes through an inhomogeneous magnetic field the beam splits into two discrete states being spin up or spin down. This effect is purely quantum mechanical and it is due to an inherent property possessed by particles called Spin angular momentum. Spin is an intrinsic degree of freedom that is separate from moving particles' spatial degrees of freedom. In this project we wished to reconstruct the results of the Stern-Gerlach experiment in the classical limit where the states of the electron were assumed to be a continuous distribution band symmetric about the initial axis of motion, $z = 0$. After this was accomplished we sought out to simulate the correct distribution of states of the electron, spin up or spin down, by using the finite difference method with a Gaussian wave packet implemented in Python.

Conclusion

The results that were obtained in the classical limit showed that when electrons exit the magnetic field as they can populate any state that is symmetric about their initial axis of motion between $\pm \hbar$ (this was an arbitrary choice states for the randomized states). The quantum result showed an interference distribution that was heavily peaked about the initial axis of motion when the diffusion coefficient (1/mass) was considered which differed from the classical result because it was not a continuous band.

When the diffusion coefficient was set to unity the result showed two Gaussian distributions splitting about the initial axis of motion which imitated the same initial behavior as the result with diffusion, but noticeable difference was that there was not any interference behavior. What showed was two distributions heavily peaked at what could be considered as two “quantum” states.

When removing the $\gamma\alpha x\sigma_y$ term in the magnetic field the result showed two simple Gaussian distributions splitting about the initial axis and populating into two symmetric states. For future work we are anticipating simulating the experiment by using the Crank-Nicolson method.

Literature cited

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Theory

The magnetic dipole moment, μ , due to electrons is given by,

$$\vec{\mu} = \gamma \vec{S}$$

where \vec{S} is the spin operator that holds the Pauli spin matrices and γ is the gyromagnetic ratio.

The inhomogeneous magnetic field is given by,

$$\vec{B}(x, y, z) = -\alpha x \hat{x} + (B_0 + \alpha z) \hat{z}.$$

The time-dependent two-dimensional Schrödinger to be solved for the electron in the region of space containing the magnetic field is stated as,

$$\hbar \frac{\partial \Psi(x, z, t)}{\partial t} = \left[\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} \right) - (\gamma \alpha z \sigma_z + B_0) \frac{\partial}{\partial z} - \gamma \alpha x \sigma_y \frac{\partial}{\partial x} \right] \Psi(x, z, t)$$

So that the energies and eigenstates are,

$$E_{\pm} = \mp \gamma \frac{\hbar}{2} \sqrt{(\alpha x)^2 + (B_0 + \alpha z)^2}$$

$$\Psi(x, z, t) = \psi e^{\frac{-iE_{\uparrow}t}{\hbar}} \chi_{\uparrow} + \psi e^{\frac{-iE_{\downarrow}t}{\hbar}} \chi_{\downarrow}$$

$$\psi = \int \frac{d^2p}{(2\pi)^2} \left(\frac{2\pi}{\beta} \right) e^{-\frac{1}{2\beta^2}(\vec{p}-\vec{k})^2} e^{\frac{i}{\hbar}(xp_x + zp_z)}$$

Method

For the semi-classical simulation, Newtonian mechanics were used to project the individual atoms forward in time to calculate their final positions. This was done under the assumption that the magnetic force is constant in direction and time. The velocities were broken down into their directional components, where y points directly into the magnet. Since the magnetic field had no y component, we used the initial y-velocity to calculate the time of travel. This served as the basis for all the mechanical calculations.

To solve the two-dimensional Schrödinger equation numerically the finite difference method was utilized where space and time were discretized onto a lattice and the wave function was solved at each site on the lattice. When using the finite difference method, the second-ordered spatial derivatives, the first-ordered spatial derivatives, and the time derivative in Schrödinger equation can be approximated by using the central difference approximation and the forward difference approximation respectively,

$$\begin{aligned}\frac{\partial \Psi(x, z, t)}{\partial t} &\approx \frac{\Psi(x, z, t + \Delta t) - \Psi(x, z, t)}{\Delta t} + O(\Delta t), \\ \frac{\partial \Psi(x, z, t)}{\partial x} &\approx \frac{\Psi(x + \Delta x, z, t) - \Psi(x - \Delta x, z, t)}{2\Delta x} + O(\Delta x^2), \\ \frac{\partial^2 \Psi(x, z, t)}{\partial x^2} &\approx \frac{\Psi(x + \Delta x, z, t) + \Psi(x - \Delta x, z, t) - 2\Psi(x, z, t)}{\Delta x^2} + O(\Delta x^2).\end{aligned}$$

Here the errors are second ordered and the z – spatial derivatives are of the same form as the x-spatial derivatives.

For the quantum simulation the finite difference method was used to project the wave function forward in time and central in space:

```
for k in range(Nt):

    # Solve this Hamiltonian: http://mathurl.com/zwzt59e.png

    Psi_next[1:-1, 1:-1] = Psi1[1:-1, 1:-1] + 1j/(2*m) * (dt * ( \
    (Psi1[2: , 1:-1] - 2*Psi1[1:-1, 1:-1] + Psi1[ :-2, 1:-1])/dz**2 + \
    (Psi1[1:-1, 2: ] - 2*Psi1[1:-1, 1:-1] + Psi1[1:-1, :-2])/dx**2)) + \
    z_sq*(B0 + alpha*z_sq)*dt/(2*dz) * (Psi1[ :-2, 1:-1] - Psi1[2:, 1:-1]) + \
    1j * x_sq*alpha * dt/(2*dx) * (Psi2[1:-1, :-2] - Psi2[1:-1, 2:]) * FULL_EQ \
    Psi2[1:-1, 1:-1] = Psi2[1:-1, 1:-1] + 1j/(2*m) * (dt * ( \
    (Psi2[2: , 1:-1] - 2*Psi2[1:-1, 1:-1] + Psi2[ :-2, 1:-1])/dz**2 + \
    (Psi2[1:-1, 2: ] - 2*Psi2[1:-1, 1:-1] + Psi2[1:-1, :-2])/dx**2)) + \
    -z_sq*(B0 + alpha*z_sq)*dt/(2*dz) * (Psi2[ :-2, 1:-1] - Psi2[2:, 1:-1]) + \
    -1j * x_sq*alpha * dt/(2*dx) * (Psi1[1:-1, :-2] - Psi1[1:-1, 2:]) * FULL_EQ \
    Psi1[:, :] = Psi_next \
```

