Poster for Stern-Gerlach Simulation

Researchers: Andrew Durkiewicz, Nate Simon, Greg Vetaw

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.

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 Schrödiner to be solved for the electron in the region of space containing the magnetic field is stated as,

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

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

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 Schrödiner equation can be approximated by using the central difference approximation and the forward difference approximation respectively,

$$\frac{\partial \Psi(x,z,t)}{\partial t} \approx \frac{\Psi(x,z,t+\Delta t)-\Psi(x,z,t)}{\Delta t} + O(\Delta t),$$

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

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

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

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, it the specific units were chosen to be ignored as they would only scale the relationships that our data demonstrated (note figure 1). 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.

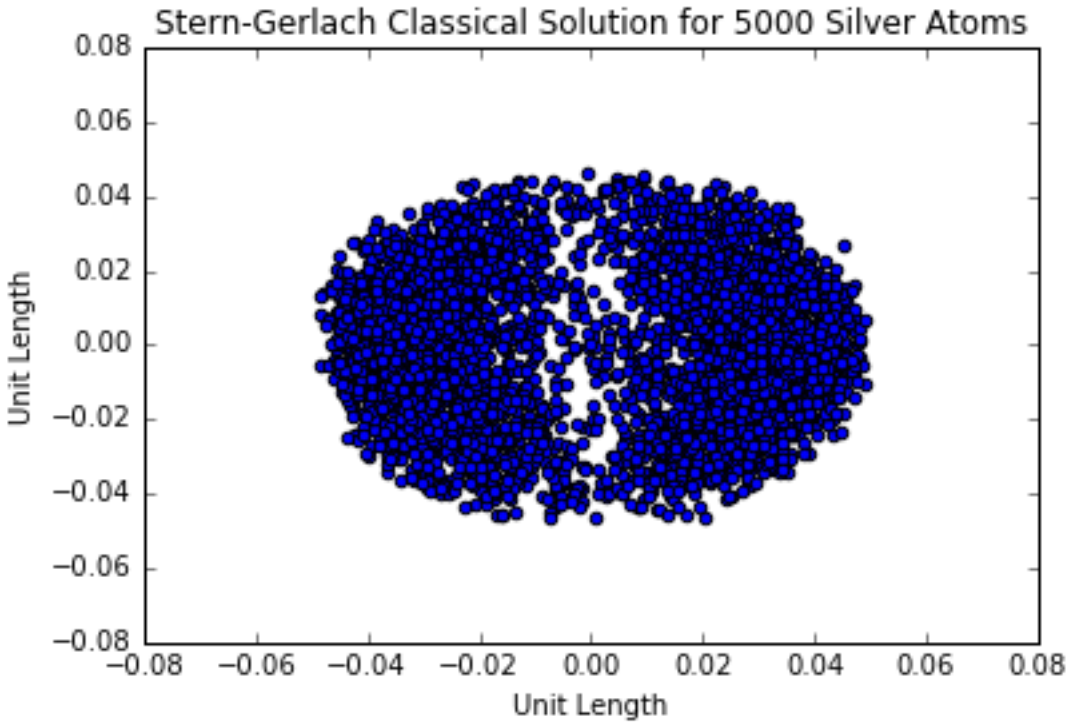

Figure 1 Semi-classical simulation for 5000 Ag atoms.

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 Guassian 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

Bulnes. Diaz, J. and Oliveira. I.S. 2001. Construction of exact solutions for the Stern-Gerlach effect. http://www.scielo.br/scielo.php?script=sci_arttext&pid=S0103-97332001000300023

Griffiths, David. 2005. *Introduction to Quantum Mechanics (2nd ed)*. Upper Saddle River, NJ. Person Prentice Hall.

Stenson, Jared Rees. 2012. *Representations for Understanding the Stern-Gerlach Effect. Journal of Blahology* 1:1-2.

Yosprakob, Atis and Suwanna, Sujin. 2016. *Time Evolution of Gaussian Wave Packets under Dirac Equation with Fluctuating Mass and Potential.* Bangkok, Thailand. arXiv:1601.03827v1.

Zettili, Nouredine. 2009. *Quantum Mechanics: Concepts and Applications (2n ed.)*. Jacksonville, USA. Wiley.