

EXPLORING LONGTIDUNAL SPIN WAVE-PACKAGE SEPARATION IN A
MAGENTIC MATERIAL

By

KUSH AGGARWAL

A Thesis Submitted to The W.A. Franke Honors College

In Partial Fulfillment of the Bachelors degree
With Honors in

Physics and Mathematics

THE UNIVERSITY OF ARIZONA

M A Y 2 0 2 3

Approved by:

Dr. Shufeng Zhang
Department of Physics

Exploring Longitudinal Spin Wave Package Separation

15 April 2023

ABSTRACT

The Stern-Gerlach experiment was the first experimental evidence of the fact that the electrons have discrete spin states in contrary to continuous spectrum earlier hypothesized. Motivating their work, we explored the spin wave package separation for longitudinal waves as they pass through a medium with non-zero magnetization. Our analysis is based on the assumption that the wave packets have a Gaussian waveform up to a leading order. We give a analytical solution that proves that the wave package separates into up spin and down spin wave packets in the magnetic material. We backed up our results by numerical simulations. Our results show that indeed the initial wave package separates into two Gaussian wave packages. One with a positive amplitude which corresponds to spin up and one with negative amplitude which corresponds to spin down. For the experimental detection of the separated wave packages it is important that the peak to peak separation between them increase with time. Indeed, we showed that the ratio of the distance between the peaks and full width at half maximum is a increasing function of time. However, the observed separation is much smaller than the currently available probe wavelength in the industry, hence it would might be possible in the future that this result could be used for practical applications.

1 ANALYSIS

In this section, we briefly present the derivation of how the resulting wave packets travel in the magnetized medium. Let us start by describing the general problem. The ensemble of particles is propagating in the x-direction. Now consider two Magnetic layers:

$$M(x) = \begin{cases} \vec{M}_1, & x < 0 \\ \vec{M}_2, & x > 0 \end{cases}$$

where \vec{M}_1 is oriented along z direction (i.e., parallel to the direction of motion of the particles) and \vec{M}_2 is oriented at an angle θ with the x axis (in x - z plane).

Using the general definition of Hamiltonian in a magnetized material, we can write the Hamiltonian as :

$$\hat{H} = \frac{p^2}{2m} - J\vec{\sigma} \cdot \vec{M} \quad (1)$$

where p , m , J , and $\vec{\sigma}$ are the momentum, the mass of particle, the total angular momentum, and the Pauli vector. For simplification, we can resolve the momentum vector, and therefore the magnitude p^2 into the p_x and the p_\perp components. Furthermore, we know that the magnitude of momentum and the Plancks constant are related as $p = \hbar^2 k$, where

k is the wave number of the particle's wave function. Thus, equation 1 can be re-written as:

$$\hat{H} = \frac{\hbar^2}{2m}(k_x^2 + k_\perp^2) - J\vec{\sigma} \cdot \vec{M} \quad (2)$$

As the magnetization for $x > 0$ is oriented at angle θ with respect to the direction of motion (x-axis), we can resolve the magnetization into two components - $\sigma_z \cos \theta + \sigma_y \sin \theta$. Therefore, we can write two separate equations:

for $x < 0$:

$$\hat{H} = \frac{\hbar^2}{2m}(k_x^2 + k_\perp^2) - J\sigma_z \quad (3)$$

and for $x > 0$:

$$\hat{H} = \frac{\hbar^2}{2m}(k_x^2 + k_\perp^2) - J(\sigma_z \cos \theta + \sigma_y \sin \theta) \quad (4)$$

Let us now solve for the wavefunctions of the particles. Starting with the region $x < 0$, let the initial wavefunction be:

$$\begin{aligned} \psi(x) = & A e^{\iota(k_x x)} e^{\iota(k_y y + k_z z)} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + B e^{-\iota(k_x x)} e^{\iota(k_y y + k_z z)} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ & + C e^{-\iota(k'_x x)} e^{\iota(k_y y + k_z z)} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned}$$

(5)

where, $kx^2 + ky^2 + kz^2 = (\frac{2m}{\hbar^2})(E_f + J)$ and $kx'^2 + ky'^2 + kz'^2 = (\frac{2m}{\hbar^2})(E_f + J)$.

Let us now write the general wavefunction for $x > 0$:

$$\psi(x) = D e^{\iota(k_x x)} e^{\iota(k_y y + k_z z)} |\uparrow\rangle_\theta + E e^{-\iota(k'_x x)} e^{\iota(k_y y + k_z z)} |\downarrow\rangle_\theta \quad (6)$$

where $|\uparrow\rangle_\theta$ and $|\downarrow\rangle_\theta$ represent the eigenvectors for spin-up and spin-down wavepackets. A detailed derivation of these eigenvectors is given in Appendix A. We can directly substitute equations A7 and A8 in equation 6. The wave function has to be continuous at $x = 0$. Therefore, we now equate equations 5 and 6 at $x = 0$. This gives us:

$$D \begin{pmatrix} \cos \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{pmatrix} + E \begin{pmatrix} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} \end{pmatrix} = A \begin{pmatrix} 1 \\ 0 \end{pmatrix} + B \begin{pmatrix} 1 \\ 0 \end{pmatrix} + C \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (7)$$

On simplification, we get:

$$\begin{pmatrix} D \cos \frac{\theta}{2} + E \sin \frac{\theta}{2} \\ D \sin \frac{\theta}{2} - E \cos \frac{\theta}{2} \end{pmatrix} = \begin{pmatrix} A + B \\ C \end{pmatrix} \quad (8)$$

Therefore, we now get set of two equations:

$$D \cos \frac{\theta}{2} + E \sin \frac{\theta}{2} = A + B \quad (9)$$

$$D \sin \frac{\theta}{2} - E \cos \frac{\theta}{2} = C \quad (10)$$

Now we make the derivatives on both sides of equations 5 and 6 equal (as the derivatives have to be continuous as well) and we get:

$$A k_x \begin{pmatrix} 1 \\ 0 \end{pmatrix} - B k_x \begin{pmatrix} 1 \\ 0 \end{pmatrix} - C k'_x \begin{pmatrix} 0 \\ 1 \end{pmatrix} = D k_x \begin{pmatrix} \cos \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{pmatrix} + E k'_x \begin{pmatrix} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} \end{pmatrix} \quad (11)$$

On comparing the rows on both sides of equation 11 we get:

$$D \cos \frac{\theta}{2} + E \sin \frac{\theta}{2} = A + B \quad (12)$$

$$D \sin \frac{\theta}{2} - E \cos \frac{\theta}{2} = C \quad (13)$$

On simplification, we get:

$$C = E \cos \frac{\theta}{2} - D \frac{k_x}{k'_x} \sin \frac{\theta}{2} \quad (14)$$

$$A - B = D \cos \frac{\theta}{2} + E \frac{k_x}{k'_x} \sin \frac{\theta}{2} \quad (15)$$

On combining equations (13) and (14), we get:

$$D \sin \frac{\theta}{2} - E \cos \frac{\theta}{2} = E \cos \frac{\theta}{2} - D \frac{k_x}{k'_x} \sin \frac{\theta}{2} \quad (16)$$

On solving equation (16), we get:

$$E = \frac{D}{2} \tan \frac{\theta}{2} \left(1 + \frac{k_x}{k'_x} \right) \quad (17)$$

Putting (17) into (15) we can write:

$$A - B = D \cos \frac{\theta}{2} + \frac{D}{2} \tan \frac{\theta}{2} \left(1 + \frac{k_x}{k'_x} \right) \left(\frac{k'_x}{k_x} \right) \sin \left(\frac{\theta}{2} \right) \quad (18)$$

Putting equation 17 into equation 12 we get:

$$A + B = D \cos \frac{\theta}{2} + \frac{D}{2} \tan \frac{\theta}{2} \left(1 + \frac{k_x}{k'_x} \right) \sin \left(\frac{\theta}{2} \right) \quad (19)$$

Adding equations 18 and 19 we get:

$$\frac{D}{A} = \frac{2}{2 \cos \frac{\theta}{2} + \frac{1}{2} \tan \frac{\theta}{2} \sin \frac{\theta}{2} \left(\frac{(k'_x + k_x)^2}{k'_x k_x} \right)} \quad (20)$$

Putting equation 20 in equation 17 we get :

$$\frac{E}{A} = \frac{1}{2 \cos \frac{\theta}{2} + \frac{1}{2} \tan \frac{\theta}{2} \sin \frac{\theta}{2} \left(\frac{(k'_x + k_x)^2}{k'_x k_x} \right)} \tan \frac{\theta}{2} \left(1 + \frac{k_x}{k'_x} \right) \quad (21)$$

We define $A = 1$ as our normalization.

Now, we have all the information for describing our full-time-dependent incident and transmitted wavefunctions.

For our analysis, we are not working on the reflected wave, so, we do not need C and D . Hence, our full-time dependent incident wave function for $x < 0$ is:

$$\psi_i(x, t) = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \int_{0.95k_0}^{1.05k_0} e^{\iota k_x (x - x_0)} e^{-\iota k_x^2 \frac{\hbar t}{2m}} dk_x \quad (22)$$

and for $x > 0$, we get:

$$\begin{aligned} \psi_{tr}(x, t) = & \frac{1}{\sqrt{2\pi}} \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix} \int_{0.95k_0}^{1.05k_0} D e^{\iota(k_x)(x-x_0)} e^{-\iota k_x^2 \frac{\hbar t}{2m}} \\ & + \frac{1}{\sqrt{2\pi}} \begin{pmatrix} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} \end{pmatrix} \int_{0.95k_0}^{1.05k_0} E e^{\iota k'_x(x-x_0)} e^{-\iota k_x'^2 \frac{\hbar t}{2m}} \end{aligned} \quad (23)$$

where $k'_x = \sqrt{k_x^2 - \frac{1}{2}}$. The coefficients D and E can be extracted from equations 20 and 21 with A = 1. Therefore, we can define the transmitted spin-up and spin-down wave functions as:

$$\psi_{t,up}(x, t) = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix} \int_{0.95k_0}^{1.05k_0} D e^{\iota(k_x)(x-x_0)} e^{-\iota k_x^2 \frac{\hbar t}{2m}} dk_x \quad (24)$$

$$\psi_{t,down}(x, t) = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} \end{pmatrix} \int_{0.95k_0}^{1.05k_0} E e^{\iota(k_x)'(x-x_0)} e^{-\iota k_x'^2 \frac{\hbar t}{2m}} dk_x \quad (25)$$

By performing the numerical integration routines on equations 24 and 25 we get $\psi_{t,up}$ and $\psi_{t,d}$ as a function of x for a particular time t . Now we introduce a separate de-phasing factor in $\psi_{t,up}$ and $\psi_{t,down}$. So we get :

$$\psi_{t,up}(x, r_1) = \psi_{t,up}(x) e^{\left(\frac{xr_1}{L}\right)} \quad (26)$$

and

$$\psi_{t,down}(x, r_2) = \psi_{t,down}(x) e^{\left(\frac{xr_2}{L}\right)} \quad (27)$$

where L is defined as the length of the magnetic layer. Now we want to calculate the spin density of the transmitted wave in the x,y, and z directions. For that, we start by defining the Pauli matrices: $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -\iota \\ \iota & 0 \end{pmatrix}$, and $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. We also define $\chi = \psi_{t,up}(r_1) + \psi_{t,down}(r_2)$ Using these definitions, we define the corresponding spin densities for a fixed position x as:

$$S_x = \int_{-1}^1 (\chi)^\dagger \sigma_x(\chi) \quad dr \quad (28)$$

$$S_y = \int_{-1}^1 (\chi)^\dagger \sigma_y(\chi) \quad dr \quad (29)$$

$$S_z = \int_{-1}^1 (\chi)^\dagger \sigma_z(\chi) \quad dr \quad (30)$$

where $r = r_1 + r_2$.

We will now describe how to calculate these spin densities, we shall describe the procedure for S_x , and the same follows for S_y and S_z . The equations 26 and 27 when evaluated at a particular x , give a constant vector and each of the σ_x , σ_y , and σ_z are constant quantities. Therefore, in equation 28, only variables are r_1 and r_2 in the de-phasing factors $e^{\left(\frac{xr_1}{L}\right)}$ and $e^{\left(\frac{xr_2}{L}\right)}$ respectively. On combining this we get, $e^{\left(\frac{x(r_1+r_2)}{L}\right)}$ and the choice of $r = (r_1+r_2)$ follows from there. More exhaustively, the equation for S_x will look like this:

$$S_x = \int_{-1}^1 c_1 \sigma_x c_2 e^r \quad dr$$

where c_1 and c_2 are constants. S_y and S_z can be calculated in the same way for some x .

For our analysis we are considering $\theta = \frac{\pi}{2}$ in equation 4. This means that magnetization for $x > 0$ is along the x-axis and there is no magnetization along the y or z directions. Therefore, the spin density in the x direction would scatter into spin-up and spin-down components and we would expect dephasing in y and z direction, i.e., spin density in y and z would eventually decay to zero.

2 RESULTS

In this work, we analyzed the spin wave package separation when an ensemble of particles enters a new medium with non-zero magnetization oriented at an angle of 90° with the direction of travel. We numerically integrated the wavefunctions for transmitted spin-up and spin-down wave packages and then calculated the spin densities in the x direction using our simulations. We varied the value of $k^2 - k'^2$ and calculated the spin densities as a function of x . The results are plotted in Figure 1.

We now briefly discuss and compare the analytical solutions with the numerical estimates. The wave packets of the spin densities (both spin-up and spin-down) follow a Gaussian function. Along the x direction, the spin-up wavepacket is a Gaussian wavepacket with positive amplitude while the spin-down wavepacket is a Gaussian wavepacket with negative amplitude, i.e., it is inverted. Assuming that the peak of these two Gaussian wavepackets is getting separated by a constant velocity v . Therefore, the distance between the peaks of these wavepackets increases as vt , where t is the time. On the other hand, the Full-Width-Half-Maxima (FWHM) of a Gaussian wavepacket varies as $\sqrt{\alpha^2 + \beta^2 t^2}$, where α and β are some constants depending on the value of K_0 . Thus we expect to measure the ratio of the distance between the peaks of spin density wavepackets and the half sum of the FWHM width of two peaks (denoted by σ) as:

$$\sigma \propto \frac{vt}{\alpha^2 + \beta^2 t^2} \quad (31)$$

Ratio of separation between peaks ($X_U - X_D$) and $0.5*(FWHM_U + FWHM_D)$ Vs. Time

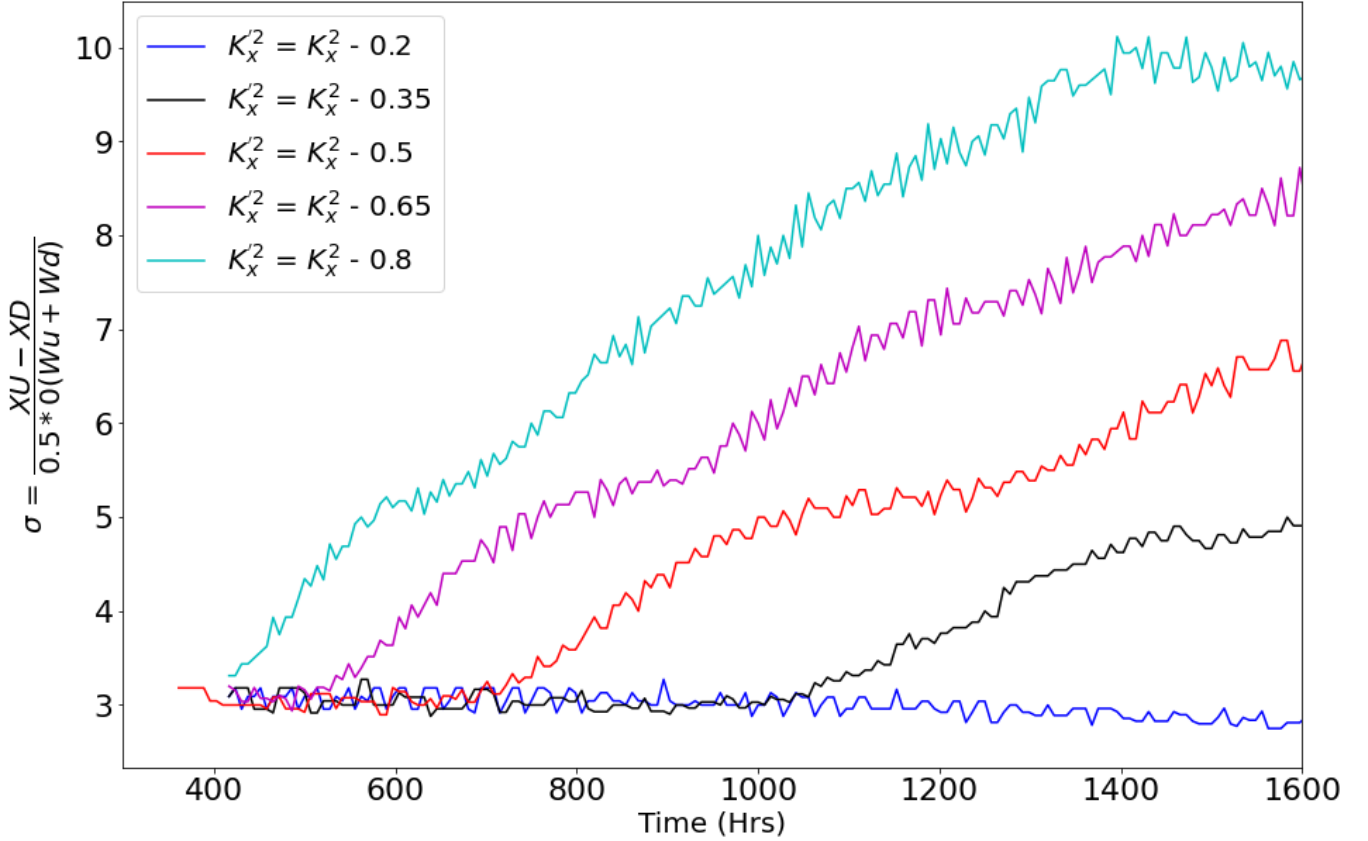


Figure 1. This figure shows the ratio of the distance between the peaks (up and down spin) and the half sum of their FWHM widths for varying peak velocities.

On differentiating this function, one can see that this function has no extremum. It rises slowly with time for a while and then stays almost constant, i.e., asymptotic along x axis. The initial increase in σ is evident from Figure 1. Due to high computational time, we did not plot the results for later times, but our simulations indicate that the σ does get asymptotic to the x axis at later times.

APPENDIX A: DERIVATION OF SPIN-UP AND SPIN-DOWN EIGENVECTORS

In this section, we will derive the spin-up ($|\uparrow\rangle_\theta$) and spin-down ($|\downarrow\rangle_\theta$) eigenvectors. Starting with the characteristic equation, we can write:

$$(\sigma_x \sin \theta + \sigma_z \cos \theta)\psi = \lambda\psi \quad (\text{A1})$$

Using the matrix form of the Pauli matrices σ_x and σ_z , we can write equation A1 as:

$$\left[\begin{pmatrix} 0 & \sin(\theta) \\ \sin(\theta) & 0 \end{pmatrix} + \begin{pmatrix} \cos(\theta) & 0 \\ 0 & \cos(\theta) \end{pmatrix} \right] \psi = \lambda\psi \quad (\text{A2})$$

On simplification, we can write equation A2 as:

$$\begin{pmatrix} \cos(\theta) & \sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \psi = \lambda\psi \quad (\text{A3})$$

We can now begin solving the characteristic equation for equation A3:

$$\begin{vmatrix} \cos(\theta) - \lambda & \sin(\theta) \\ \sin(\theta) & \cos(\theta) - \lambda \end{vmatrix} \psi = 0 \quad (\text{A4})$$

On solving this determinant gives, we get the characteristic equation $\lambda^2 = 1$. This means that λ can have only two eigenvalues: ± 1 . We shall now find the corresponding Eigenvectors: Let the eigenvector corresponding to $\lambda = 1$ be $|\uparrow\rangle$ and the eigenvector corresponding to $\lambda = -1$ be $|\downarrow\rangle$.

For $\lambda = 1$:

$$\begin{pmatrix} \cos(\theta) - 1 & \sin(\theta) \\ \sin(\theta) & \cos(\theta) - 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad (\text{A5})$$

From equation A5, we get $a \sin(\theta) = b \cos(\theta) + b$ and $a = b \cot \theta + b \csc \theta$. Therefore, the eigenvector for this eigenvalue is:

$$|\uparrow\rangle = a \begin{pmatrix} \cot \theta + \csc \theta \\ 1 \end{pmatrix} \Rightarrow |\uparrow\rangle = b \begin{pmatrix} \cot \frac{\theta}{2} \\ 1 \end{pmatrix} \quad (\text{A6})$$

On normalizing this eigenvector we find that $b^2 \cot^2(\frac{\theta}{2}) + b^2 = 1$. Therefore, we get $b = \sin(\frac{\theta}{2})$. Consequently, we can write the normalized eigenvector as:

$$|\uparrow\rangle = \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix} \quad (\text{A7})$$

Similarly, we can derive the eigenvector for $\lambda = -1$ as:

$$|\downarrow\rangle = \begin{pmatrix} \sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{pmatrix} \quad (\text{A8})$$