THEORETICAL STUDY OF CURRENT-INDUCED
DYNAMICS OF AN ANTIFERROMAGNETIC
SKYRMIONIUM

A Thesis Presented to the Department of Theoretical and Applied Physics
African University of Science and Technology, Abuja
In partial fulfilment of the requirements for the award

MASTER OF SCIENCE DEGREE

By

ABAYOMI SAMUEL OBADERO

Supervised by

Dr. Collins Ashu Akosa
Co-Supervisor

Dr. Yuta Yamane

African University of Science and Technology

www.aust.edu.ng

P.M.B 681, Garki, Abuja F.C.T, Nigeria.

June, 2019
THEORETICAL STUDY OF CURRENT-INDUCED DYNAMICS OF AN ANTIFERROMAGNETIC SKYRMIONIUM

By

ABAYOMI SAMUEL OBADERO

A THESIS APPROVED BY THE DEPARTMENT OF THEORETICAL AND APPLIED PHYSICS

RECOMMENDED:

Supervisor: Dr. Collins Ashu Akosa

Head, Department of Theoretical Physics

APPROVED:

Chief Academic Officer (Prof. C. E. Chidume)

Date
Theoretical study of current-induced dynamics of antiferromagnetic skyrmionium

Abayomi Samuel Obadero

In this thesis, we present a theoretical study on the current-induced nucleation and propagation of antiferromagnetic skyrmionium. A skyrmionium, also known as 2π-skyrmion, is a vortex-like magnetic structure characterized by zero topological charge. We show by means of micro-magnetic simulation that an antiferromagnetic skyrmionium can be nucleated via a local injection of spin current with toroidal distribution. Our systematic study of the current-induced dynamics shows that a spatially uniform spin current induces propagation of antiferromagnetic skyrmionium with measurable distortion at high current densities. We derive expression for the velocity of the antiferromagnetic skyrmionium based on the collective-coordinate model and obtain good agreement with our numerical results.
DEDICATION

This thesis is dedicated to God Almighty the giver of life; the source of all wisdom and inspiration.

To my parents Mr. and Mrs. Obadero for their love and encouragement and to my uncle, Dr. Leke Olulana for his moral and financial support.
ACKNOWLEDGEMENTS

First of all, I would like to express my sincere gratitude to the Almighty God for His love, kindness, mercy and favours He has chosen to bestow upon me. My appreciation goes to my thesis supervisor, Dr. Collins Ashu Akosa for his trust in my ability as a student and support towards my trip to RIKEN as an intern. His guidance, encouragement and insightful comment helped me throughout the course of this work. I also express deep appreciation to my co-supervisor; Dr. Yuta Yamane for his patience, enthusiasm, motivation, and dedication to improving my knowledge in micro-magnetic simulations. He demonstrated immense effort in sharing his knowledge and expertise in the area of micromagnetism with me. Special thanks also goes to Prof. Gen Tatara, Head of the Spin Physics Theory Research Team at RIKEN, for his kindness and hospitality. He granted me full access to the facilities at his disposal for my research while at RIKEN.

I will also like to acknowledge my Head of Department of Physics, Prof. Kenfack Anatole and my all Lecturers for their advise and guidance. My sincere appreciation goes to my friends Iyaro Oluwanishola Jephthah (through whom I got to know about AUST), Oyeniran Gbenga, Ademola Michael e.t.c. To my colleagues who made my time in AUST fun-filled, worthwhile and educative, I want to say a very big thank you for the love we share and the struggles we have been through; see you all at the top.

Also to my aunt Mrs. Bunmi Olaboshinde whose financial support, prayers, and well wishes cannot be over emphasized, I want to say a very big thank you. I will also like to show my gratitude to Pastor Femi Alonge for his mentorship, God bless your home and Ministry. Finally, I will like to appreciate my family for their love and support, especially my mother for her care, teachings, prayers and encouragement. To my fiancé, Adetola, thank you for your assistance, prayers and words of wisdom. To every one who has directly or indirectly contributed to my achievements, I really want to say a very big thank you.
# TABLE OF CONTENTS

Abstract i  
Dedication ii  
Acknowledgements iii  
List of Figures viii  

1 Introduction  
  1.1 Spintronics 3  
  1.2 Non-collinear magnetic textures 4  
  1.3 Antiferromagnetic textures 6  
  1.4 Motivation 6  
  1.5 Objectives and contributions 7  

2 Theoretical Background  8  
  2.1 Magnetism in Brief 8  
  2.2 Magnetic Moment of an electron 8  
    2.2.1 Ferromagnetic Materials (FM) 12  
    2.2.2 Ferrimagnetic Materials 12  
    2.2.3 Antiferromagnetic Materials (AFM) 12  
    2.2.4 Paramagnetic Materials 13  
    2.2.5 Diamagnetic Materials 13  
  2.3 Magnetization 14  
  2.4 Micromagnetics 14  
    2.4.1 Exchange interaction 15  
    2.4.2 Anisotropy energy 16  
    2.4.3 Zeeman Energy 16  
    2.4.4 Magnetostatic Energy 17  
    2.4.5 Spin Orbit Coupling (SOC) 18  
    2.4.6 Dzyaloshinskii - Moriya Interaction 19  
    2.4.7 Effective Field 21  
  2.5 Magnetization Dynamics 21
## Research Contribution

3.1 Theoretical model ................................................. 33

3.2 Nucleation of Skyrmionium ...................................... 35

3.3 Propagation of Skyrmionium .................................... 37

3.3.1 Small Ferromagnetic-Canting Approximation ............... 38

3.3.2 Collective-Coordinate Model .................................. 39

3.4 Results and Conclusion ......................................... 42

3.4.1 Skyrmionium core displacement and velocity as a function of time . 42

3.4.2 Skyrmionium velocity as a function of charge current $j_c$ ............. 44

3.5 Conclusion .......................................................... 46

## Future Outlook

4. Future Outlook ...................................................... 47

## APPENDICES

A Emergent Magnetic and Electric field .................................. 49

B Topological Charge .................................................. 54

C Numerical Method and Fortran code ................................ 55

C.1 Runge-Kutta Method ............................................. 55

C.2 Forward, backward and central difference derivative method ....... 56

C.3 Algorithm of our Fortran code .................................... 57

C.4 Fortran code ....................................................... 58

## References

vi
LIST OF FIGURES

1.1 The basic cell of Spin-Transfer Torque MRAM (STT-MRAM) which consist of one MTJ and one accessing transistor. Image from [1] .......................... 4
1.2 Schematic diagram of a race track memory in a ferromagnetic nanowires, Image from[2] .......................................................... 5
1.3 Diagram of Domain wall, Skyrmion and Skyrmionium respectively ...... 6
1.4 An illustration of a spin structure for an antiferromagnetic Skyrmion, Image from[3] ......................................................... 7

2.1 A schematic diagram of current loop and an electron orbiting the nucleus in an Hydrogen atom. Image extracted from [4] ......................... 9
2.2 A schematic diagram of a ferromagnetic ordering ............................... 12
2.3 A schematic diagram of an antiferromagnetic ordering ......................... 13
2.4 Schematic description of different forms of DMI. (a) Rashba SOC arising from the interaction of heavy metal atom (grey) and magnetic moments of the ferromagnetic atoms result in Interfacial DMI. (b) Bulk DMI interaction due to Drsselhaus SOC. Figure extracted from [5] .................. 20
2.5 schematic representation of time-domain study of Magnetization ........... 23
2.6 Illustration of spin transfer torque mechanism. (a) Transport through a spin valve made up of thick ferromagnetic layer FM 1 , nonmagnetic spacer NM and a thin ferromagnetic layer FM 2 . (b) Interface of NM/FM 2 : the absorption of the transverse spin component in FM 2 causes a spin transfer torque on the magnetization of the free layer ..................... 24
2.7 An illustration of SOT due to SHE. Charge current ($j_c$) flows into the nonmagnetic material(NM) to cause spin accumulation of spin-up and spin-down electrons at the edges, as a result, spin current flows in such a way that it is mutually orthogonal to spin polarization and charge current as shown. This spin current diffuse into the Ferromagnetic Material(FM) to exert spin orbit torque (SOT) on the local magnetization of the FM ....................... 26
2.8 Illustration of a 2D magnetic Skyrmion with mapping from the Skyrmion configuration to the unit sphere; The arrows denote the spin direction and the out-of-plane spin component is represented by the color: red is out of the plane, green is in-plane, and blue is into the plane. The 2D magnetic Skyrmion is mapped into a unit 3D spherical surface with spins pointing in all directions. Figure extracted from [6] ................................. 27

2.9 A Schematic diagram of a single electron moving through a Skyrmion in the adiabatic approximation, in which the electron spin aligns perfectly with the local magnetic moment. Figure extracted from [7] ................................. 28

2.10 shows different Skyrmion structures with varying vorticity q and helicity c. The arrows and colours represent in-plane spin directions. ................................. 30

2.11 A schematic diagram of Skyrmion Hall effect with spin textures represented by arrows. Figure extracted from [8] ................................. 31

2.12 A schematic diagram of a ferromagnetic Skyrmionium. Figure extracted from [9] 32

3.1 (a) Schematic of our system; bilayer of antiferromagnet (AFM) and nonmagnetic metal (NM). For the nucleation process, a 9 ps pulse of spin current $j_s$ (green arrows) is locally injected within the toroidal region indicated by the black circles, i.e., between the inner and outer circles, followed by a 2.5 ns of relaxation. (b)-(e) Snapshots of the $n_3$ profile around the toroidal region ($0 \leq x_1 \leq 150$ nm and $0 \leq x_2 \leq 160$ nm) at selected times. In (b), the spatial profile of $p$ is schematically shown by white arrows ................................. 36

3.2 (a) Schematic motion process of our system; bilayer of antiferromagnet (AFM) and nonmagnetic metal (NM). For the motion process, a 6ns pulse of spin current $j_s$ (green arrows) is applied allover the sample. The white arrow represents the spin polarization $p$ with its direction in the $-x_2$ axis while the yellow arrow shows the direction of motion of the Skyrmionium. (b) shows snapshots of the $n_3$ profile at $t = 0$, $t = 1.5$, $t = 3.0$, $t = 4.5$ and $t = 6$ ns for $j_c = 0.2 \times 10^{12}$ and $j_c = 1.0 \times 10^{12}$ A/m$^2$ respectively ................................. 41

3.3 fig.3.3(a&b) shows the $x_1$ and $x_2$ components of the Skyrmionium core displacement, $R(m)$ and velocity $v_{x_1}$ and $v_{x_2}$ as a function of time, $t(s)$ for charge current $j_c = 0.2 \times 10^{12}$Am$^{-2}$ while fig.3.3(c&d) shows the $x_1$ and $x_2$ components of the Skyrmionium core displacement, $R(m)$ and velocity $v_{x_1}$ and $v_{x_2}$ as a function of time, $t(s)$ for charge current $j_c = 1.0 \times 10^{12}$Am$^{-2}$ respectively ................................. 43

3.4 Skyrmionium velocities $v_1$ and $v_2$, in the $x_1$ and $x_2$ directions, respectively, as functions of electric current density $j_c$. The analytical (numerical) results are represented by the solid lines (circles). For the Skyrmionium propagation, the spin current injection is spatially uniform ................................. 44
3.5 shows the Skyrmionium center of mass $M_1, M_2$ in the $x_1$ and $x_2$ directions respectively, and its effective mass $M$ as functions of time ($ns$) for charge currents $j_c = 0.2 \times 10^{12}$, $j_c = 0.4 \times 10^{12}$, $j_c = 0.8 \times 10^{12}$, and $j_c = 1.0 \times 10^{12}$.
Chapter 1

Introduction

Data storage which has to do with the collective ways and technologies involved in the capturing and retaining of digital information on optical, electromagnetic or silicon-based storage media is an important aspect of human lives, as we rely on it to preserve information that ranges from personal to critical business or general information. Magnetic memory or magnetic data storage is an important component in computer operation. It depends on the ability of magnets to magnetize other materials and the ability of those materials to retain their magnetization until they are forced to change the direction of their magnetization under the influence of an external magnetic field. Data are stored in storage devices as set of 0’s and 1’s or binary codes; this is achieved by using an electromagnetic (or the write head) to magnetize the magnetic materials in a specific direction (e.g up direction with bit registered as 1) as it moves over the magnetic material. The direction of magnetization of the magnetic material can be flipped by changing the direction of the current flowing in the electromagnet coil. Once written, the read head reads the encoded information or bits. The process of reading and writing information described above uses the principle of Faraday’s law of electromagnetic induction and Oersted field respectively. Apart from these mechanisms, other mechanism that prove to be more efficient than the Faraday’s electromagnetic induction is the anisotropic Magnetoresistance (AMR) effect[10] where relative angle between local magnetization and electric current affects the electrical resistance of the magnetic sample. Specifically in the year 1988 with the discovery of giant Magnetoresistance (GMR) [11, 12] and tunneling Magnetoresistance (TMR) [13] effects, it was revealed that electrical resistance of a multilayer device is a function of the relative
direction of the magnetization between the layers. This discovery gave birth to another area of research and interest known as *Spintronics*.

### 1.1 Spintronics

In our day to day experiences with electronic devices, charge of electrons are used to achieve functionalities in conjunction with semi conducting materials for logical operation and magnetic materials for storage. Spintronics (which means SPIN TRANSfer electrONICS, also known as magneto electronics) on the other hand takes advantage of the spin degree of freedom and resulting magnetic moment of an electron (in addition to its fundamental electronic charge in solid-state devices) to achieve improved functionalities for processing and storage of information.

Spintronic devices are based on Magnetic Tunnel Junctions (MTJs)[14, 15] which are seen (because of their high-speed, non-volatility and strong complementary metal-oxide-semiconductor, CMOS compatibility) to be next generation memory and logic chips. The way these devices operate in data storage for Magnetic random access memory (MRAM) is to make use of Magnetoresistance effect to write binary data on the magnetization of small multi-layered device that consist of magnetically fixed and free layers. The design of MRAM has witnessed great improvement compared to conventional memories because of it’s non-volatility, low power consumption, and increased read and write times. However, the drawbacks in this technology is in the fact that it uses Oersted field generated from transverse current in the wires to write binary data. This Oersted field because of its long-range effect, affect neighboring cells in what is referred to as cross-talking (non-locality) which results in read-write errors. The other drawback is in the fact that current density and heating increases with reduction in the cell’s size (this effect is known as *scaling*).

With it’s theoretical prediction[16, 17] and experimental verification[18, 19, 20, 18], spin transfer torque magnetic random access memories (STT-MRAM) was a major breakthrough in overcoming the cross-talking setback. In STT-MRAM, the magnetic configuration of the MRAM is altered by current transversing it through the transfer of angular momentum to local magnetization that store information as bit. In it’s set up, spin-polarized current flows
through a particular memory cell such that it does not influence neighboring cells as it were in field-driven MRAMs. However, the need of an external polarizer sets the floor a new way of generating spin torque without the need of external polarizers. A lot of research efforts was targeted at harnessing spin-orbit coupling, which exploits the inter-play between spin and orbital angular momentum to create spin currents from which spin-orbit torque can be exerted on ferromagnetic or antiferromagnetic materials [21, 22].

Figure 1.1: The basic cell of Spin-Transfer Torque MRAM (STT-MRAM) which consist of one MTJ and one accessing transistor. Image from [1].

1.2 Non-collinear magnetic textures

Non-collinear magnetic textures refers to magnetization or magnetic spins that are not on the same parallel line; such textures include domain wall, vortices, Skyrmion and the much talked about in the field of Spintronics; Skyrmionium (or $2\pi$ Skyrmion). With the development in computing power and advancement in lithographically patterning techniques, it is indeed possible to critically study the domain walls, Skyrmion, vortices or Skyrmionium by performing micromagnetic simulations on their static and dynamics. As a matter of fact, Stuart Parkin proposed a novel memory device known as the Racetrack memory[23]. The racetrack memory uses spin-polarized electric current to move magnetic textures along a nanoscopic permalloy wire. As spin polarized current flows through the wire, the domains are ’pushed’ through the wire over magnetic read or write heads that are positioned near the wire which changes the domains to record patterns of bits. This technology allows for higher bit densities in information storage at low cost, high speed of solid state memory and non volatility of stored information[24]. The discovery of this technology has opened an avenue for research and scientific investigation of magnetic domain walls, Skyrmion and
Figure 1.2: Schematic diagram of a race track memory in a ferromagnetic nanowires, Image from[2].

the most recent magnetic texture, the $2\pi$ Skyrmion.

Domain wall is a boundary between two neighbouring domains such that in between these two domains, the magnetization varies continuously. The wall is formed as a result of the competition between several magnetostatic energies like the exchange energy, dipolar energy and the magneto-crystalline anisotropy.

Skyrmion is a two-dimensional topological stable field states. As a topological object, it is important in solid state physics, especially in the technology of Spintronics. Skyrmion is formed as a result of energy interactions just as domain wall but with the addition of the Dzyaloshinskii-Moriya interaction. Magnetic Skyrmions have been observed experimentally[25, 26]. Single Skyrmions are very rich candidate for digital bit encoding with application in magnetic devices such as magnetic memory [27, 28, 29, 30, 31] and Skyrmion logic gates[32].

Skyrmionium on the other hand is pair of Skyrmion of opposite topological number. It can be created in a magnetic nanodisk and remain stable with Dzyaloshinskii-Moriya interaction (DMI). It has been observed experimentally [33], and it was discovered that Skyrmionium is stabilized at high DMI constant compared to a Skyrmion[32].
1.3 Antiferromagnetic textures

In past years, ferromagnetic textures formed from ferromagnetic materials had been gaining much attention than other magnetic materials such as ferrimagnetic, antiferromagnetic materials. This is because of the difficulty and complexity the other magnetic materials appears to have (example in the case of antiferromagnetic materials with two sublattices). But recent discoveries have shown that antiferromagnetic materials can be more robust and available than their ferromagnetic counterpart. Part of these robustness is found in the fact that they:

- can be easily integrated with ferromagnetic components
- have no stray fields
- are characterized by ultrafast response (in order of THz range compared to ferromagnetic materials of GHz range frequency switch).

Apart from all the advantages mentioned above, ferromagnetic texture (Skyrmion to be precise) suffers Skyrmion Hall Effect (SHE); an effect where the Skyrmion is seen to deviate from its translational path due to the Magnus force that stems from the topological charge of the Skyrmion[34, 31]. But with antiferromagnetic Skyrmion, it is expected that SHE is overcome as the transverse motion of the two sub-lattices cancel each other.

1.4 Motivation

The potential breakthrough that can be achieved in storing and transferring information through the use of electric current to control magnetic texture position is continuing to
attract a lot of attention due to its application in memory and logic devices. Therefore, a well detailed understanding of what is going on in the world of spin transport from the perspective of Physics will boost the performance of recent Spintronic devices and help in designing better devices for future applications. Although, the Skyrmionium had been studied extensively in ferromagnetic system in the past few years, its statics and dynamics in the antiferromagnetic (AFM) system is still elusive as the antiferromagnetic Spintronics and topological spins are two hot topics in the field of Spintronics.

1.5 Objectives and contributions

The objective of this thesis is to investigate and understand the statics and dynamics of antiferromagnetic Skyrmionium from Physics perspective. As we will further discuss in this thesis, the velocity of a current driven Skyrmionium depends on the current density used and at high current densities, the Skyrmionium experiences distortion which is traceable to the coupled motion of two nested Skyrmions of different topological numbers.

After reviewing some theoretical background in Chapter 2, we move ahead to present a novel way of nucleating a Skyrmionium from a uniform antiferromagnetic state. We then move ahead to propagate the nucleated antiferromagnetic Skyrmionium by spin transfer torque (STT) and present some analytical calculations of the Skyrmionium velocity using the small ferromagnetic canting and the collective coordinate model (Chapter 3). Both nucleation and propagation process was carried in micromagnetic simulations with codes written in Fortran. In what follows (Section 3.4), we discuss some results obtained from our numerical simulations and then give some concluding remark.
Chapter 2

Theoretical Background

2.1 Magnetism in Brief

What is Magnetism?

Magnetism can be defined as the attractive or repulsive effect caused by electromagnetic force (which is one of the four forces of nature) as a result of a moving or rotating electric charge. The region around the moving charge is affected by this motion and consist of both electric and magnetic field which creates an electromagnetic field and an electromagnetic force as a result. The most familiar example of magnetism is the bar magnet which can be attracted or repelled (to/from each other) in a magnetic field; (Law of polarity). Another example is the earth (Which is always referred to as a giant magnet). The definition and description above are all classical way of explaining Magnetism. The quantum mechanical approach gives a better understanding and thus predicts that all matter is magnetic in nature to some degree depending their atomic configuration.

2.2 Magnetic Moment of an electron

An electron is an elementary charged particle that has angular momentum coming from it’s orbital motion around the nucleus of the atom and it’s spin. From the Amperian loop model, it was discovered that electric current produces a magnetic field since two current carrying wires attract or repel each other just as magnets would do depending on the direction of current. It is then natural to think that all magnets are made up of sufficiently small amperian loop with magnetic dipole moment. This analogy holds good for an electron as
well. The orbiting electron therefore possesses a magnetic moment that is derived as follows:

\[
\text{Current} (I) = \frac{\text{charge}(-e)}{\text{period}(T)} \quad (2.1)
\]

The negative comes from the fact that an electron has a negative charge. Eq. (2.1) can then be re-written as

\[
I = -\frac{e v}{2\pi r} \quad (2.2)
\]

Where \( T = \frac{2\pi}{\omega} \). The magnetic moment is given by the relation \( \mu = I \times A \) and Substituting Eq. (2.1) into this relation, noting that the area swept by the charged particle is given by \( A = \pi r^2 \) we obtain the following relation:

\[
\mu = g \frac{e}{2m_e} L \quad (2.3)
\]

Eq. (2.3) suggests that associated to the orbital momentum \( L \) of an electron is the magnetic moment \( \mu \) and also that the orbital angular momentum and the magnetic moment of an electron are in opposite direction due to the charge of the electron, where \( g \) is the Lande g-factor in which for an electron, it’s taken to be 2.

![Figure 2.1: A schematic diagram of current loop and an electron orbiting the nucleus in an Hydrogen atom. Image extracted from [4]](image)

In Quantum mechanics, the orbital angular momentum of an electron is given by the formula:

\[
L = \sqrt{\ell(\ell + 1)} \hbar \quad (2.4)
\]

Where \( \ell \) in Eq. (2.4) is the azimuthal quantum number which describes the sub-shell in an atom and gives the magnitude of the orbital angular momentum and takes the value \( \ell = 0, 1, 2, \ldots n - 1 \) and \( n \) is the orbital quantum number.
In the S-orbital (with $\ell = 0$), we should therefore expect no magnetic moment from the electron in this orbital. But from the Stern-Gerlach experiment[35], it was observed that an electron in the S-orbital has magnetic moment. This magnetic moment is due to the Spin of the electron. From Eq. (2.4), we can therefore replace the orbital angular momentum of the electron ($L$) by the Spin ($S$) so that Eq. (2.4) now becomes:

$$S = \sqrt{S(S + 1)}\hbar$$  \hspace{1cm} (2.5)$$

and the corresponding magnetic moment due to spin from Eq. (2.3)(if we measure $\mu$ in the $z$-direction) is given by:

$$\mu_z = -\frac{e}{m_e}S_z = -\frac{e}{m_e}m_p\hbar$$  \hspace{1cm} (2.6)$$

Where $m_p = \pm \frac{1}{2}$. The magnetic moment due to spin and that due to orbital motion in the first Bohr orbit ($n = 1$) are exactly equal. Because of it’s fundamental nature, this amount of magnetic moment is given a special symbol and a special name known as $\mu_B$ and Bohr magneton respectively($\mu_B = \frac{eh}{2m_e}$). Therefore, Eq. (2.6) is re-written as :

$$\mu_z = \pm \mu_B = 9.24 \times 10^{-27} Am^{-2}$$  \hspace{1cm} (2.7)$$

Atom contains many electrons, each spinning about (as one of the fundamental particles of nature) and these electrons have angular momentum (due to their orbital motion around the nucleus in a quantized state and its Spin) and these momenta (spin and orbital angular momentum) both combine vectorially to give the atom as a whole a definite angular momentum[36]. The magnetic moment of the atom is the vector sum of all it’s electronic moments and two(2) possibilities arise:

- The magnetic moment of the electrons may orient such that they cancel each other. As a result, the atom may have no magnetic moment. This condition leads to diamagnetism.

- The cancellation of the electrons magnetic moment is not total but partial and the
atom is left with some magnetic moment. Materials that composed of this kinds are the para-, ferro-, antiferro- or ferrimagnetic. The macroscopic magnetic effect is felt when a sufficient amount of these unpaired electrons combinations are aligned with their spins in the same direction.

Therefore, the total magnetic moment ($\mu$) due to spin ($S$) and angular momentum ($L$) is given by:

$$J = \sqrt{J(J+1)}\hbar$$

(2.8)

Where $J = L + S$. It is worth mentioning that although the values of $J$, $L$ and $S$ can be known for an isolated atom, it is generally impossible to calculate the magnetic moment $\mu$ for the atoms of a solid unless we make the following valid assumption for many substances: There is no orbital contribution to the moment, which means that $J = S$ i.e the orbital moment is quenched. This quenching condition comes from the crystalline or crystal field produced by the surrounding atoms to the atom been considered in the solid. This field has the symmetry of the crystal involved. For example, if the electron orbits in a particular isolated atom is circular, when the atom now forms part of a cubic crystal, the orbits might become elongated along the three orthogonal axes due to the electric fields created by the neighbours on the axes. In such a case, the orbits are now "coupled" or bound strongly to the crystal lattice. On the other hand, the spins are loosely bound to the orbits. Now when a magnetic field is applied along some arbitrary directions, the strong orbit-lattice coupling often does not allow the orbits and their associated orbital magnetic moments to align towards the field’s direction whereas, the spins are free to align due to the relatively weak spin-orbit coupling compared to the orbit-lattice coupling counterpart. This simply means that only the spin contribute to the magnetization process and the resultant magnetic moment of a solid material; the orbital moments acts as though they were not there. Quenching may be complete or partial[36]. Due to atomic configuration, magnetic materials can be classified into the following:
2.2.1 Ferromagnetic Materials (FM)

In a ferromagnetic material, we have a lattice such that the spin/magnetic moment which are localized on the lattice points all point in the same direction. A ferromagnetic material has unpaired electronic electrons and can form permanent magnet when exposed to a stronger external magnetic field i.e the spin of the electrons tends to stay aligned even when the external field is removed. Examples of such materials are iron, cobalt, nickel, e.t.c

![Figure 2.2: A schematic diagram of a ferromagnetic ordering](image)

2.2.2 Ferrimagnetic Materials

Ferrimagnetic materials just like ferromagnetic materials retain their magnetization when removed from the presence of an external magnetic field, but the difference is that neighbouring pair of electron spins points in opposite directions. Due to the lattice arrangement of a ferrimagnetic material, the magnetic moment pointing in one direction is stronger than the ones pointing in another direction. Ferrimagnetism occur in magnetite and other ferrites and just like ferromagnets, they(ferrimagnets) are attracted to magnets.

2.2.3 Antiferromagnetic Materials (AFM)

In contrast to a ferromagnetic ordering, the intrinsic spins of valence electrons in an AFM point in opposite direction. In an antiferromagnetic ordering, points on each alternate lattice point in the same direction whereas adjacent spins are pointing in opposite direction. This lattice could be decomposed into two sub-lattices say lattice A and B which are fer-
romagnetically ordered within itself but the two lattices have antiferromagnetic coupling among themselves. Therefore, this antiferromagnetic state can be written as the superposition of ferromagnetically ordered states in which the two lattices are antiferromagnetically coupled with each other. In AFM, the magnetic moment/spin of site A and site B are equal in magnitude but opposite in direction so that the whole domain is going to be unmagnetized i.e overall magnetization is zero. Examples of materials that exhibit this kind of structure are: nickel oxide (NiO), hematite (such as FeMn, Cr) e.t.c.

Figure 2.3: A schematic diagram of an antiferromagnetic ordering

2.2.4 Paramagnetic Materials

In a paramagnetic material, we have electrons that are unpaired and free to align their magnetic moments. In the presence of an external magnetic field, the magnetic moments are magnetized and therefore align in the direction of the external field at least for the moment the field is present because when the external field is removed, the magnetic moments return back to their original direction and the memory (of spin alignment direction in the presence of external field is lost). Example of such materials are: Lithium(Li), Magnesium(Mg), Molybdenum(Mo), e.t.c

2.2.5 Diamagnetic Materials

Diamagnetism is simply the tendency to be repelled by a magnetic field. This effect is observed only in materials that have no unpaired electrons. In the presence of an external
magnetic field, diamagnetic materials are weakly magnetized in the direction opposite to the external field. Diamagnetism results from the orbital motion of electrons creating tiny current loops that produces weak magnetic fields. All materials are repelled by permanent magnet; but the resulting force from this effect is too weak to be observed but there are some noticeable exceptions. Examples of Paramagnetic materials are graphite, e.t.c. It should be noted that all the different magnetic materials or ordering highlighted/explained above are strongly dependent on temperature as a ferromagnetically ordered material beyond the critical temperature can become a paramagnet in which the magnetic moment points in arbitrary directions such that the overall magnetization is zero.

2.3 Magnetization

Magnetization is defined as the volume density of the permanent or induced magnetic moment in a magnetic material. It can be referred to as the degree to which a magnetic material response to an external magnetic field. It can also be seen as the average magnetic moments over several atoms so that magnetization changes in space in a continuous fashion. Mathematically, magnetization can be written as:

\[ \mathbf{m} = \frac{1}{V} \sum_i \mu_i \]  

(2.9)

Where \( V \) is the volume in space. The magnitude of magnetization is usually referred to as the saturation magnetization i.e \( M_s = |\mathbf{M}| \)

2.4 Micromagnetics

Micromagnetics is a phenomenological description of magnetic behaviours at sub-micrometer length scales designed to model the non-uniformity of magnetization in a very efficient way. It doesn’t describe the behaviour of the magnetization associated with each atom but rather adopts a continuous description much like in elastic theory. In micromagnetics, the magnetization is represented by a continuous function of position with each magnetization represented by the unit vector \( \mathbf{m} = \mathbf{M}/M_s \) where \( M_s \) is the saturation magnetization.
The aim of micromagnetics is to find a spatial distribution function for the magnetization unit vector direction $m(r, t)$ which minimizes the total energy of the system [37]. In this thesis, we carry out micromagnetism simulation using the torque formulation described by Landau-Lifshitz equation and modified by Gilbert[38]; via the addition a viscous damping term in a way that the precession of the magnetic dipole is described by the dynamics of a "magnetic top". Furthermore, the numerical integration of the LLG equation for each elementary cell in subsequent fractions of the time of precession(for each picosecond as an example) is done with the elementary cell considered to be homogeneous. The direct integration of the LLG equation is carried out until the change in the magnetization ($\frac{dm}{dt}$) is smaller than a preset tolerance value for each elementary cell with the damping parameter chosen arbitrarily. In what follows, we look at some of the interactions that competes for energy minimization of the overall system using the torque formulation.

### 2.4.1 Exchange interaction

The major mechanism through which spins (or magnetic moments) interact with each other is called the exchange interaction. This means that the magnetic moments are coupled with one another to form magnetically ordered states. This coupling is quantum mechanical in nature which arises from the overlap of electrons together with the Pauli exclusion principle. The exchange interaction is an electrostatic effect in conjunction with symmetrization. In a ferromagnetic or antiferromagnetic material, the exchange interaction occurs between magnetic ions and "forces" the magnetic moment of each neighbour to either align parallel or anti-parallel to each other or one another as the case may be.

**Exchange Energy**

The essential characteristics of ferromagnet is the parallel arrangement/alignment of local magnetic moments. Any deviation from this ideal alignment causes more energy for the system and this is not preferable. The exchange energy is given by the expression:

$$E_{\text{exch}} = A \int (\nabla m)^2 dV$$  \hspace{1cm} (2.10)
Where $A$ is the exchange constant or exchange stiffness constant. The exchange energy does not depend on direction i.e it is Isotropic in nature.

### 2.4.2 Anisotropy energy

This is the directional dependence of a material’s magnetic properties. With respect to the crystallographic axis of a material, the energy of a ferromagnet depend on the direction of the magnetization. The magnetic moment (spin) of magnetically anisotropic material tend to align with the easy axes, which is an energetically favourable direction of spontaneous magnetization. Two opposite directions along an easy axis are usually equivalent, and the actual direction of magnetization can be along either of them. This directional dependence basically arises from the spin-orbit interactions which is described by the anisotropy energy.

#### Uniaxial Anisotropy

When more than one kind of crystal material has a single axis of high symmetry, such a material is said to have a uniaxial anisotropy, which is the direction of the lowest energy known as the "easy axis". When the magnetization $m$ with a polar angle $\theta$ is away from this "easy axis", the general form of the energy density can be expressed as $u_{\text{ani}} = K \sin^2 \theta$ where $K$ is the magnitude of the anisotropy energy density or the energy density constant. Writing the energy density in Cartesian coordinate, we therefore have that:

$$E_{\text{ani}} = K \sin^2 \theta = K - \frac{1}{2} m \cdot H_{\text{ani}}$$

(2.11)

Where $H_{\text{ani}} = 2Km_z = H_k(n \cdot m)n$. This formula is valid in the case of random uniaxial anisotropy, also. $H_k$ is called local anisotropy field strength, $n$ is the easy direction unit vector, and $M$ is the magnetization $m = M/M_s$.

### 2.4.3 Zeeman Energy

The Zeeman energy is the potential energy of a magnetized material in an external magnetic field. This interaction energy between the magnetization and external magnetic field is given
2.4.4 Magnetostatic Energy

Otherwise known as the stray field (outside the magnet) is the demagnetizing field. This is the magnetic field generated by the magnetization. This stray field has the tendency to act on the magnetization so as to reduce the total magnetic moment. It gives rise to shape anisotropy in a ferromagnet with single magnetic domain and to magnetic domains in larger ferromagnet. The demagnetizing field is a long-range interaction and as a result, it difficult to estimate numerically as it consumes most of the time during a micromagnetic simulation.

It is worth mentioning that in an antiferromagnet, the stray field cancels out and therefore no demagnetizing field effect in an antiferromagnet. This is because in an antiferromagnet, the magnetization in each sub-lattice points in opposite direction which causes the stray field effect of local magnetization in sub-lattice A for example to be canceled by the stray field effect of local magnetization in sub-lattice B and the over-all sum of this effect over the material sample for an antiferromagnet gives zero (theoretically).

The demagnetizing field is responsible for the formation of domains in a ferromagnet, i.e. the relaxation towards the demagnetized state as two interactions alone (anisotropy and exchange) do not lead to the formation of domain pattern as the exchange favours the parallel alignment of the magnetizations in any direction, the anisotropy determines the energetically lowered crystallographic direction. As a result of these two interactions alone, we have a single domain structure. This single domain structure however causes energy to the system; in order to reduce this energy, the magnetic structure breaks into multiple domain configuration to reduce the stray field effect. If we assume that a ferromagnetic body with magnetization \( m \) occupies a region \( V \), the demagnetizing field at the position

\[
E_{\text{ext}} = -J_s \int H_{\text{ext}} \cdot m dV
\]
vector $\mathbf{r}$, $H_{\text{demag}}$ can be written from magnetostatics as:

$$H(r)_{\text{demag}} = -\int_{V} \frac{(r - r') \nabla \cdot m(r')}{|r - r'|^3} \, d\tau' + \oint_{\partial V} \frac{(r - r') m(r') \cdot n(r')}{|r - r'|^3} \, ds'$$  \hspace{1cm} (2.13)

Where $d\tau'$, $ds'$ are the volume and area element respectively. Eq. (2.13) is over the space variable $r$, $\partial V$ is the boundary of the volume $V$ and $n(r')$ is the outward normal at $r'$. It is obvious from Eq. (2.13) that $H_{\text{demag}}$ depend on the whole distribution of $m$.

Before we discuss the next interaction which is the Dzyaloshinskii - Moriya Interaction (DMI), we will like to lay the foundation for the cause of this interaction which is the Spin Orbit Coupling.

### 2.4.5 Spin Orbit Coupling (SOC)

The interaction between the spin of an electron and its orbital motion around the nucleus is referred to as Spin Orbit Coupling (SOC). In Section (2.2), we discussed the concept of angular momentum of the electron due to the orbital motion of the electron around the nucleus (in the rest frame of the proton). If we assume an electron frame, then in this frame, the proton orbits the electron. Associated to the electric current as a result of the orbital motion is the magnetic field at the position of the electron which is given by:

$$B = \frac{\mu_0 e}{4\pi m r^3} L$$ \hspace{1cm} (2.14)

Since the electron has a magnetic moment, there will be an interaction of the magnetic field with the magnetic moment and the energy resulting from this interaction is given by:

$$\mathcal{E}_{\text{soc}} = -\mu \cdot B = -\frac{\mu_0 e^2}{4\pi m^2 r^3} L \cdot S = \frac{1}{2} \frac{e^2}{4\pi m^2 r^3 \epsilon_0 c^2} L \cdot S$$ \hspace{1cm} (2.15)

Eq. (2.15) is the energy for the spin-orbit coupling. The factor $1/2$ comes from the non-inertial frame of the electron with velocity $\mathbf{v}$ and effective magnetic field $\mathbf{B}_{\text{eff}} = -\mathbf{v} \times \mathbf{E}/2c^2$ known as the Thomas precession. The SOC is a smaller effect that drives on top of the
Bohr energy and the exchange interaction.

In most inorganic solids, there are two main contributions to the SOC which are the Dresselhaus and Rashba contribution. Dresselhaus SOC occurs in the material crystal with bulk inversion symmetry breaking which means that there is a net electric field for certain crystal direction [39, 40]. On the other hand, the Rashba SOC occurs in materials with interfacial inversion symmetry breaking; i.e. systems with net electric field due to structural inversion asymmetry[41, 42].

2.4.6 Dzyaloshinskii - Moriya Interaction

In 1960, Dzyaloshinskii proposed a theoretical model to explain weak ferromagnetism observed in some antiferromagnets by introducing an asymmetric exchange term in the Hamiltonian based on symmetry arguments [43]. This interaction which was later termed called Dzyaloshinskii - Moriya Interaction (DMI), is present in systems with both large SOC and breaking inversion symmetry. DMI in materials can be classified based on the nature of inversion symmetry breaking as Interfacial or Bulk DMI as shown in Figure 2.4

Interfacial DMI

When an ultra-thin magnetic film is placed on top of heavy-metal substrate with strong SOC along the material’s interface at atomic scale, there is an inversion symmetry breaking along this interface such as Fe/Ir[44]. This type of SOC is called Rashba SOC and the associated DMI energy for a discrete system reads [45]

$$H_{DMI}^I = -d_{DMI}^I \sum_{i,j} \left( u_{ij} \times z \right) \cdot \left( m_i \times m_j \right)$$

where $m_i$ and $m_j$ represent classical unit vector in the direction of the local magnetic moments at site $i$ and $j$, respectively, $d_{DMI}^I$ is the strength of the interface-induced DMI, $u_{ij}$ is the unit vector between sites $i$ and $j$, and $z$ is the normal to the interface (inversion asymmetric direction). In micromagnetic models, the magnetization is assumed to change
continuously, in which case, the corresponding energy density is given as \[46\]

\[
\mathcal{E}_{iDMI} = D_{DMI}^I [m_z (\nabla \cdot \mathbf{m}) - (\mathbf{m} \cdot \nabla)m_z] \tag{2.17}
\]

\[
= D_{DMI}^I [m_z (\partial_x m_x + \partial_y m_y) - m_x \partial_x m_z - m_y \partial_y m_z],
\]

where \(D_{DMI}^I\) is the continuous effective interfacial DM constant in unit of \(Jm^{-2}\).

**Bulk DMI**

Unlike interfacial DMI, bulk DMI involves materials with bulk inversion symmetry breaking and strong SOC such as in B20 compounds like MnSi [25]. This type of SOC is called Dresselhaus SOC in the material bulk, with associated DMI energy for a discrete system given by

\[
\mathcal{H}_{DMI}^B = -d_{DMI}^B \sum_{i,j} u_{ij} \cdot (\mathbf{m}_i \times \mathbf{m}_j), \tag{2.18}
\]

where \(d_{DMI}^B\) is the strength of the bulk DMI. Similarly the energy density for continuous model is given as

\[
\mathcal{E}_{DMI}^B = -D_{DMI}^B \left[ m \cdot (\nabla \times \mathbf{m}) \right] \tag{2.19}
\]

\[
= D_{DMI}^B \left( m_z (\partial_y m_x - \partial_x m_y) - m_x \partial_y m_z + m_y \partial_x m_z \right),
\]

where \(D_{DMI}^B\) is the continuous effective bulk DM constant in unit of \(Jm^{-2}\).

---

Figure 2.4: Schematic description of different forms of DMI. (a) Rashba SOC arising from the interaction of heavy metal atom (grey) and magnetic moments of the ferromagnetic atoms result in Interfacial DMI. (b) Bulk DMI interaction due to Drsselhaus SOC. Figure extracted from [5]
2.4.7 Effective Field

The effective field $H_{\text{eff}}$ represent the sum of all internal (such as the exchange, magneto-static, anisotropy and DM) and external magnetic fields, calculated as

$$H_{\text{eff}} = -\frac{1}{\mu_0 M_s} \frac{\partial \mathcal{E}}{\partial \mathbf{m}},$$  \hspace{1cm} (2.20)

where $\mathcal{E}$ is the energy density which includes contributions from the exchange, DM, magnetic anisotropy, Zeeman, and magneto-static energies. In this thesis, we do not take into consideration the magnetostatic energy as we assumed that in an antiferromagnets, the stray fields emanating from the tow sublattices cancels out due to the opposite alignment of spins in the sublattices.

2.5 Magnetization Dynamics

The Landau Lifshitz equation popularly known as the LL equation is an ordinary differential equation that describes the precessional motion of magnetization\cite{38, 47} When an external field is applied to magnetization, the magnetization precesses around the external field. This precessional motion can be simply described by Newton’s law of motion: the rate of change of angular momentum $\mathbf{L}$ associated with the magnetization is equal to the torque $\tau$ causing the motion.

$$\frac{d\mathbf{L}}{dt} = \tau$$  \hspace{1cm} (2.21)

The torque experienced by the magnetization is due to the presence of the external field and this $\tau$ can be expressed as

$$\tau = \mathbf{m} \times H_{\text{eff}}$$  \hspace{1cm} (2.22)

From the concept of orbital angular momentum and spin(Magnetization) in Quantum mechanics, the relationship between orbital angular momentum ($\mathbf{L}$) and spin is give as Eq. \hspace{1cm} (2.3): where $g$ is the Lande g-factor (for an electron, the value is 2).

$$\mathbf{m} = -\gamma \mathbf{L}$$  \hspace{1cm} (2.23)
Where $\gamma = g\mu_B/\hbar$ and $\mu_B = e\hbar/2m_e$, Eq. (2.22) can therefore be re-written as follows:

$$\frac{dL}{dt} = -\frac{1}{\gamma} \frac{dm}{dt} \quad (2.24)$$

Also from Eq. (2.3), we can re-write Eq. (2.22) as

$$\frac{dm}{dt} = -\gamma m \times H_{\text{eff}} \quad (2.25)$$

The steady state is achieved when the magnetization $m$ aligns along the direction of the effective field. This is because in real system, the precession of the magnetization does not continue indefinitely but stops due to damping or dissipative forces. Landau and Lifshitz predicted the damping term as a torque that orient towards the external field which forces the magnetization to align along the external field, $H_{\text{eff}}$, so that the overall equation of motion is the sum of the precessional term and the damping term which can be written in an explicit form as follows:

$$\frac{dm}{dt} = -\gamma m \times H_{\text{eff}} + \gamma \lambda \left( m \times (m \times H_{\text{eff}}) \right) \quad (2.26)$$

Eq. (2.26) above is valid in the case where we have small damping parameter, $\lambda$. In the year 1955, Gilbert proposed an equation that models the case of a strong damping ($\alpha$) in thin film[38] which is given by the equation below:

$$\frac{dm}{dt} = -\gamma m \times H_{\text{eff}} + \gamma \alpha \left( m \times \frac{dm}{dt} \right) \quad (2.27)$$

To eliminate $dm/dt$ on the RHS, we multiply Eq. (2.27) by $\alpha m$ to obtain

$$\alpha m \times \frac{dm}{dt} = -\gamma \alpha m \times (m \times H_{\text{eff}}) + \alpha^2 m \times \left( m \times \frac{dm}{dt} \right). \quad (2.28)$$

Substituting Eq. (2.28) into Eq. (2.26), and making use of vectorial triple product algebra, we see that we can re-cast Eq. (2.26) into

$$\frac{\partial m}{\partial t} = -\frac{\gamma}{1 + \alpha^2} m \times H_{\text{eff}} - \frac{\gamma \alpha}{1 + \alpha^2} m \times (m \times H_{\text{eff}}) \quad (2.29)$$
Eq. (2.29) is the popular LLG equation which predicts the dynamics of magnetization vector \( \mathbf{m}(\mathbf{r}, t) \) as time progresses.

Just like electric currents carried by moving charges, spin current also occur due to moving spins. The spin current carries angular momentum which can be transferred to the magnetization, a phenomenon known as spin-transfer torques\cite{48}. This phenomenon was first theorized by Sloncwezki and Berger\cite{17, 16}. A flow of spin angular momentum or simply spin current arises when there is an imbalance between the spin-up and spin-down electrons, the interaction between electron spin and a thin ferromagnetic layer results in the re-orientation of electron spin on transmission or reflection from the ferromagnetic layer. From the law of conservation of momentum, a change in electron spin angular momentum direction results in a torque on the ferromagnet. When the direction of the electron spin is in plane with the torque experienced by the magnetization of the ferromagnet, we have an in-plane (or adiabatic) spin transfer torque. When the torque experienced by the magnetization of the ferromagnet is perpendicular to the direction of the electron spin, then we have a non-adiabatic (or field-like torque). The adiabatic and non-adiabatic STT terms are given by the expressions\cite{49}:

\[
\tau_{\text{non-adiabatic}} = -\beta u \left( \mathbf{m} \times \frac{\partial \mathbf{m}}{\partial x} \right)
\]  
(2.30a)
\[ \tau_{\text{adiabatic}} = -um \times \left( m \times \frac{\partial m}{\partial x} \right), \]  

(2.30b)

where \( \beta \) is the non-adiabatic parameter, \( u = \frac{\gamma h}{\mu_0 e P} \) has the dimension of velocity, \( \hbar \) is the reduced Planck’s constant, \( e \) is the electronic charge, \( j_e \) is the charge current density, and \( P \) is the current polarization coefficient. The incorporation of these torque terms into Eq. (2.26) yields the equation of motion that governs the dynamics of the magnetization given by

\[
\frac{dm}{dt} = -\gamma m \times H + \alpha \left( m \times \frac{dm}{dt} \right) - \beta u \left( m \times \frac{\partial m}{\partial x} \right) - um \times \left( m \times \frac{\partial m}{\partial x} \right) \tag{2.31}
\]

Figure 2.6: Illustration of spin transfer torque mechanism. (a) Transport through a spin valve made up of thick ferromagnetic layer \( \text{FM}_1 \), nonmagnetic spacer \( \text{NM} \) and a thin ferromagnetic layer \( \text{FM}_2 \). (b) Interface of \( \text{NM}/\text{FM}_2 \): the absorption of the transverse spin component in \( \text{FM}_2 \) causes a spin transfer torque on the magnetization of the free layer.

Fig. 2.6 above shows a schematic diagram of the representation of spin-transfer torque. A spin polarized current enters a ferromagnetic material. The interaction between the spin-polarized current and the magnetization results in a change in the spin direction of the outgoing electron compared to the incident electron. The difference in spin polarization give rise to torques on the ferromagnet (both adiabatic and non-adiabatic). The bold vertical arrow represents the magnetization of the ferromagnetic layer.
2.5.2 Spin Hall effect and Spin-orbit torques

Spin Hall effect (SHE) is a transport phenomenon that involves the appearance of spin accumulation on the lateral surface of a current-carrying heavy-metal (e.g., Platinum) layer with strong spin-orbit coupling. This occurrence is analogous to the classical Hall effect where a current-carrying conductor when placed in a magnetic field, the positive and negative charges drift and accumulate on the lateral surface of the current-carrying conductor (due to Lorentz force acting on the charges in the conductor) but the difference is that in SHE, there is no need for magnetic field to drift the charges.

If a Ferromagnetic (FM) layer is placed on the heavy metal, the spin current will propagate into the FM layer and exert spin-orbit torques (SOT) on the FM layer. The direction of charge current ($j_c$), spin current ($j_s$) and the spin polarization ($p$) are mutually orthogonal to one another. The SOT is written as [50, 51]:

\[
\tau_{IP} = -m \times (m \times p) \quad (2.32a)
\]

\[
\tau_{OOP} = -\xi (m \times p) \quad (2.32b)
\]

Eq. (2.32a) is the in-plane SOT while Eq. (2.32b) is the out-of-plane SOT. $p$ measures the strength of the SOT, $\xi$ is the amplitude of out-of-plane torque relative to the in-plane torque and

\[
p = \frac{\gamma h}{2\mu_0 c M_s} \frac{\theta_{SHE}}{t_F} j_e, \quad (2.33)
\]

where $\gamma$ is the gyromagnetic ratio, $\theta_{SHE}$ is the Spin Hall angle (efficiency of charge to spin current conversion, $j_s = \theta_{SHE} j_e$). The LLG equation (Eq. 2.26) re-written with the SOTs is given as

\[
\frac{dm}{dt} = \gamma m \times H_{eff} + \alpha (m \times \frac{dm}{dt}) - \left[m \times (m \times p) - \xi (m \times p)\right] \quad (2.34)
\]

It is worthy to note here that for metallic systems $\xi \ll 1$ and in the rest of this thesis, we consider only the term $\tau_{IP}$.
Figure 2.7: An illustration of SOT due to SHE. Charge current ($j_c$) flows into the non-magnetic material (NM) to cause spin accumulation of spin-up and spin-down electrons at the edges, as a result, spin current flows in such a way that it is mutually orthogonal to spin polarization and charge current as shown. This spin current diffuse into the Ferromagnetic Material (FM) to exert spin orbit torque (SOT) on the local magnetization of the FM.

### 2.6 Magnetic Skyrmion

In the field of Micromagnetics, the behaviour of magnetic materials at sub-micrometer length scale is studied. This length scale considered is large enough for the atomic structure of the material to be ignored but small enough to resolve magnetic structures such as Domain wall, Vortices, Skyrmion, Skyrmionium, e.t.c. In this length scale, the gradual change of magnetization with time is continuously described by the LLG equation through micromagnetic simulation in what is referred to as the continuous approximation.

In what follows, we take a brief look at different Magnetic Skyrmion (at static equilibrium) and the different interactions that are necessary for it’s formation, although this thesis, we focus on the antiferromagnetic Skyrmionium ($2\pi$ Skyrmion).

Skyrmions are topologically stable field configuration (by topologically stable, we mean they are invariant under continuous deformation). It is a non-collinear configuration of magnetizations with a whirling magnetic structure[52]. Skyrmion is described by an integer invariant which is always referred to as the topological charge which comes to play in the mapping from a physical two-dimensional space to the target space $S_2$. This topological charge tells how many times magnetizations are wrapped around a unit circle in the map-
Skyrmion was originally proposed by the British nuclear physicist Tony Skyrme in the year 1960, it was proposed as a quasi-particle-like topological excitation in the description of interaction of pions[53]. In the year 1994, Bogdanov et al. theoretically suggested that the topologically protected Skyrmions can exist as a stable or metastable state with DMI in magnetic materials[54]. Bogdanov and Rößler theoretically predicted Skyrmion in magnetic thin films in the year 2001[55] while in 2009, Mühlbauer et al. was first to observe the magnetic Skyrmion lattice in B20-type bulk chiral magnet MnSi with broken inversion symmetry[25]. After these times, Skyrmions have been observed experimentally, created, and manipulated in many materials including magnetic materials[26, 44, 56, 57], multiferroic materials[58], ferroelectric materials[59], and semiconductor materials.[60]

Figure 2.8: Illustration of a 2D magnetic Skyrmion with mapping from the Skyrmion configuration to the unit sphere; The arrows denote the spin direction and the out-of-plane spin component is represented by the color: red is out of the plane, green is in-plane, and blue is into the plane. The 2D magnetic Skyrmion is mapped into a unit 3D spherical surface with spins pointing in all directions. Figure extracted from[6]

2.6.1 Skyrmion Dynamics and Topological Effect

Motion of an electron through a Skyrmion in an Adiabatic approximation

The next interesting phenomenon to look at is the effect a Skyrmion has on a spin-polarized electron when it propagates through the Skyrmion. In Physics, adiabatic approximation states that provided the perturbation acting on a physical system is slow enough, the physical system remains in its instantaneous eigenstate. Applying this approximation to our electron-Skyrmion system, we can assume that in the adiabatic approximation, the exchange coupling, $J$ is more larger than the kinetic energy of the electron such that the electron spin aligns to the texture spin at time-scale shorter than its motion. This is achieved
if the charge density is low and the Skyrmion size is larger than the Fermi wavelength of
the electron such that in this approximation, although the Hamiltonian of the electron is
changing continuously, the wavefunction that describes the conduction electron only gains
a phase factor known as the **Berry phase**. This phase factor causes an incredible physical
effect which stems from the effective electromagnetic fields traceable to the Skyrmion. This
means that the Skyrmion acts on the electron as a flux of magnetic field which is quantized.
In this thesis, We shall derive the effective fields (electric and magnetic) from the Skyrmion,
and then describe some of its properties.

![Schematic diagram of a single electron moving through a Skyrmion in the
adiabatic approximation, in which the electron spin aligns perfectly with the local magnetic
moment. Figure extracted from[7]](image)

The motion of an electron through a Skyrmion can be described by the Schrödinger
equation:

\[
\frac{i\hbar}{\partial t}\Psi = -\left[\frac{\hbar^2 \nabla^2}{2m} - J\sigma \cdot m(r,t)\right]\Psi
\]

(2.35)

Where \(\Psi\) and \(m\) are the wavefunction and mass of the electron respectively, \(\sigma\) is the Pauli
matrices vector, \(J\) is the exchange coupling constant and \(m\) is the vector that describes
Skyrmion spin texture. Eq. (2.35) is non-diagonal due to the exchange term added to the
Kinetic energy term. We therefore perform a unitary transformation \(U = n^\alpha \sigma_\alpha\) which
diagonalize Eq. (2.35) i.e. \(\Psi \rightarrow U\Phi\) and \(\Psi^\dagger \rightarrow \Phi^\dagger\Phi U^\dagger\). This procedure yields fictitious vector
and scalar potentials

\[
A_\mu = i\hbar U\partial_\mu U
\]

(2.36)

\[
A_0 = -i\hbar U\partial_0 U
\]
and the transformed Schrödinger equation in the rotating given as

$$i\hbar \partial_t \Phi = \frac{(P - \mathbf{A})^2}{2m} \Phi + J\sigma_z \Phi + A_0 \Phi \quad (2.37)$$

In the Lab frame, these potentials are given as (see Appendix A for details)

$$A_\mu = -\frac{\hbar}{2} \left( m \times \partial_\mu m \right) \cdot m + \frac{\hbar}{2} \left( 1 - \cos \theta \right) \partial_\mu \phi$$

$$A_0 = \frac{\hbar}{2} \left( m \times \partial_t m \right) \cdot m - \frac{\hbar}{2} \left( 1 - \cos \theta \right) \partial_t \phi \quad (2.38)$$

Where the additional term in Eq. (2.38) $\frac{\hbar}{2} \left( 1 - \cos \theta \right) \partial_\mu \phi$ is known as the Adiabatic Gauge field. To make use of the Maxwell Relation ($\mathbf{B}^{em} = \nabla \times \mathbf{A}, \mathbf{E}^{em} = -\partial_t \mathbf{A} - \partial_i A_0$) in order to derive the emergent electric and magnetic field from the Scalar and vector potential respectively, we make use of the Semi-Classical assumption *that the magnetization aligns in the direction of the Pauli matrices* so that according to the derivations in Appendix (A), we can obtain an expression for the emergent Magnetic and electric field as:

$$\mathbf{B}^{em} = \frac{\hbar}{2} m \cdot \left( \partial_z m \times \partial_y m \right)$$

$$\mathbf{E}^{em} = -\frac{\hbar}{2} m \cdot \left( \partial_t m \times \partial_x m \right) \quad (2.39)$$

**Topological Charge**

Topological charge, also known as Topological number is any quantity in physical theory that takes only one of a set of discrete values as a result of Topological consideration. It is the total flux of the emergent magnetic field. This immediately means that from Eq. (2.39), we can obtain the Topological number of a 2D Skyrmion by integrating Eq. (2.39) as below:

$$Q = \frac{1}{4\pi} \int \int m \cdot \left( \partial_x m \times \partial_y m \right) d^2r \quad (2.40)$$

From Appendix A, we can show that for a Skyrmion, the topological number is $Q = \pm 1$. A Skyrmion can also be characterized by helicity and chirality which depends on energy and the mechanism of stabilization of the Skyrmion[61]. The diagram below shows Skyrmions
with vorticity (or chirality) $q = \pm 1$ and helicity $c = 0, c = \pm 1$ and $c = 2$.

![Skyrmion structures with varying vorticity $q$ and helicity $c$.](image)

Figure 2.10: shows different Skyrmion structures with varying vorticity $q$ and helicity $c$. The arrows and colours represent in-plane spin directions.

**Skyrmion Hall Effect (SHE)**

In Physics, Hall effect arises when charged particles like electrons or holes passing through a conductor get deflected (due to the Lorentz force) in opposite direction in the presence of a magnetic field. This causes accumulated charges (of opposite signs) on opposite sides of the conductor thereby creating what is known as the Hall Voltage.

Now, in the case of a magnetic Skyrmion, it has been shown that similar effect occurs where the topological charge rather than the electrical charge causes Skyrmions to travel in a curved path which is away from the direction of the application of current as a result of Magnus force, thus the name **Skyrmion Hall effect**. We can immediately see that in order to explain well the phenomenon of Skyrmion Hall effect, one has to attribute this effect to the emergent magnetic field that is produced by the Skyrmion itself in order to compare it with the hall effect that we know. SHE gives a new dimension for the manipulation of Skyrmion trajectories. As said earlier, it pushes Skyrmion toward the edge of the patterned device where it can be either be destroyed or bounce back. Theoretical analysis and results predicts that the Skyrmion hall effect may be decreased by canceling the topological Magnus force in two coupled Skyrmions which has opposite topological charge thereby, resulting in
a zero net topological charge (since the direction of the of the Skyrmion’s deflection is a function of the sign topological number, then spin states that have a zero topological charge must not deviate). This can be made possible for example in Skyrmions made from an antiferromagnetic materials[32] or in an antiferromagnetically exchange-coupled trilayers with Skyrmions on two sides[34]. This brings us to the next promising magnetic texture for spintronics applications, the **Skyrmionium or 2π Skyrmion**

![Skyrmion Hall effect diagram](image)

Figure 2.11: A schematic diagram of Skyrmion Hall effect with spin textures represented by arrows. Figure extracted from[8]

### 2.6.2 Skyrmionium or 2π Skyrmion

Just as we have discussed in Sec. 2.6.1 above, the promising way of overcoming the SHE is by having a Skyrmion with zero topological charge, a Skyrmionium is a good candidate for this. What then is a Skyrmionium? It is a Skyrmion-like structure with topological number of $Q = 0$[62]. It can be viewed as two nested Skyrmions with opposite topological number $Q$ forming a donught-like out-of-plane spin distribution[32]. As a result of zero topological charge, it is free from Magnus force when driven into motion. A Skyrmionium can be created in a magnetic nanodisk and remain stable with the Dzyaloshinkii-Moriya interaction (DMI)[62, 63, 45]. The first experimental observation of a Skyrmionium was achieved on a ferromagnetic thin film by laser radiation with high energy as compared with the Skyrmion generation in which each Skyrmionium created has been found stable over few years[33]. According to Zang2016, the energy of a Skyrmionium is lower than that
of a Skyrmion for high DMI constant of about $4 \times 10^{-3}\text{Jm}^{-2}$\cite{32}. It was also predicted theoretically that Skyrmionium can be driven by magnetic field gradient as well as in-plane spin-polarized current\cite{64} which reveals its application in future electronics and spintronics applications.

While both Skyrmion and Skyrmionium have been experimentally observed and investigated in ferromagnets, their antiferromagnetic counterparts have only been theoretically predicted recently\cite{65, 34, 66}. Antiferromagnetic materials have been widely projected as a viable replacement of ferromagnets deployed in some of the existing technologies due to their advantageous features\cite{67, 68, 69}. They are robust against external magnetic fields, produce no or negligibly small demagnetizing field, and display ultrafast dynamics. Antiferromagnetic Skyrmion or Skyrmionium will therefore play pivotal roles in the next generation of spintronics applications. Compared to the antiferromagnetic Skyrmion, however, relatively little study has been devoted to the antiferromagnetic Skyrmionium thus far. In this thesis, we propose a novel way of nucleating an antiferromagnetic Skyrmionium, and also investigate a current-driven propagation of Skyrmionium. Micromagnetic simulation reveals that a local spin current injection with toroidal distribution can generate a Skyrmionium. We then derive the Skyrmionium velocity driven by uniform spin current injection, based on a collective-coordinate model. The numerically-observed Skyrmionium motion agrees well with the analytical result, confirming the absence of Magnus force.

Figure 2.12: A schematic diagram of a ferromagnetic Skyrmionium. Figure extracted from\cite{9}
Chapter 3

Research Contribution

In this section, we present a systematic theoretical study on the current-induced nucleation and propagation of antiferromagnetic skyrmionium. We also derive expression for the velocity of the antiferromagnetic skyrmionium based on the collective-coordinate model and compare with our numerical results.

3.1 Theoretical model

We consider a two-dimensional bipartite square lattice with antiferromagnetic-coupled magnetic moments sitting at each equivalent magnetic lattice sublattice $a$ and $b$, with saturation magnetization $M_s$. The spatial variation of the magnetic moments within each sublattice is assumed to be sufficiently slow compared to the atomic length scale, such that the antiferromagnet (AFM) can be appropriately modeled by performing coarse graining for each sublattice [70]. Before we proceed, let us define some notations we adopted to make our analysis trackable. The magnetic moment of atoms in the $i$-unit cell for $\zeta$-sublattice is represented by the classical unit vector $m_i^\zeta$, from which the total magnetization and Néel order parameter of the $i$-unit cell is computed as $m^i = (m^i_a + m^i_b)/2$ and $n^i = (m^i_a - m^i_b)/2$, respectively. In this representation $m^i$ and $n^i$ are always perpendicularly to each other i.e. $n \cdot m^i = 0$. This classical treatment is appropriate when the atomic magnetic moment is sufficiently large and the spatial variation of each magnetization is slow compared to the atomic length scale. In the continuous limit, we model the AFM by the following magnetic energy density $\mathcal{E}$ [65]
\[ E = \frac{J_0}{2} \sum_{i,\zeta} \mathbf{m}_i^\zeta \cdot \mathbf{m}_\zeta + A_1 \sum_{i,\zeta,\mu} \left( \frac{\partial \mathbf{m}_i^\zeta}{\partial x_\mu} \right)^2 - \frac{A_2}{2} \sum_{i,\zeta,\mu} \frac{\partial \mathbf{m}_i^\zeta}{\partial x_\mu} \cdot \frac{\partial \mathbf{m}_i^\zeta}{\partial x_\mu} \] (3.1)

\[-K \sum_{i,\zeta} \left( \mathbf{m}_i^\zeta \cdot \mathbf{e}_3 \right)^2 - D \sum_i \mathbf{n}_i \cdot (\mathbf{e}_3 \times \nabla) \times \mathbf{n}_i\]

where \( J_0 (> 0) \) is the homogeneous exchange coupling energy, \( A_1 \) and \( A_2 \) are the isotropic exchange stiffnesses, \( K (> 0) \) is the uniaxial anisotropy constant along the \( x_3 \) axis, \( D (> 0) \) characterizes the Dzyaloshinskii-Moriya interaction (DMI), and \( \mathbf{e}_\mu \) is the unit vector along the \( x_\mu \) axis. From Eq. (3.1), it is obvious that the dipolar (or magnetostatic) energy has been neglected in our model; this is because long term interaction in a perfect AFM is theoretically considered zero as the magnetizations of the two sublattices in an AFM align in an opposite direction such that the effect of dipolar field is canceled. The dynamics of \( \mathbf{m}_i^\zeta \) are described by the coupled Landau-Lifshitz-Gilbert equation;

\[ \frac{\partial \mathbf{m}_i^\zeta}{\partial t} = -\mathbf{m}_i^\zeta \times \gamma \mathbf{H}_i^\zeta + \alpha \mathbf{m}_i^\zeta \times \frac{\partial \mathbf{m}_i^\zeta}{\partial t} - \mathbf{m}_i^\zeta \times (\mathbf{m}_i^\zeta \times \mathbf{p}_i) \] (3.2)

where \( \gamma \) and \( \alpha \) are the gyromagnetic ratio and the Gilbert damping constant, respectively, (which are assumed for simplicity to be sublattice-independent) and \( \mathbf{H}_i^\zeta = -(\mu_0 M_S)^{-1} \delta E/\delta \mathbf{m}_i^\zeta \) is the effective magnetic field for the \( \zeta \)-sublattice in the \( i \)-unit unit. The last term in Eq. (3.18) is the Sloncwezski-Berger spin-transfer torque[16] due to spin current injection into the AFM, with \( \mathbf{p}_i \) is proportional the magnitude and polarization of the applied spin current [see in Sec. 2.5.1 for details]. Here, we have assumed that the injected spin is transferred in equal proportion to each sublattice.

In this thesis, we consider the spin current injection realized through spin Hall effect (as in Sec. 2.5.1) in a nonmagnetic metal (NM)/AFM bilayer as shown in Fig. (3.1). The spin current \( \mathbf{j}_s \) induced in NM due to spin Hall effect diffuses into the adjacent AFM and exerts the spin-transfer torque on the magnetizations[71] (the spin-transfer torque of this mechanism is also called spin orbit torque or spin Hall torque). The directions of the electric current density \( \mathbf{j}_c \) in NM, the spin current flow \( \mathbf{j}_s \), and the polarization of the spin current
\( \mathbf{p} \) satisfy the relationship \( \mathbf{j}_c \propto \mathbf{j}_s \times \mathbf{p} \). The spatial distribution of \( \mathbf{p}(x, t) \) is thus determined by that of \( \mathbf{j}_c(x, t) \), as \( \mathbf{j}_s \) is along the \( x_3 \) axis (the film-normal direction). In the following sections, we will consider a spatially-nonuniform as well as uniform \( \mathbf{p} \). The magnitude of \( \mathbf{p} \) carried by the injected spin current is given by Eq. (2.33) where \( \theta_{\text{SHE}} \) is the spin Hall angle of NM, and \( d \) which in this case represented as \( t_{\text{AFM}} \) is the thickness of the AFM thin film (along the \( x_3 \) axis).

### 3.2 Nucleation of Skyrmionium

To apply a Skyrmionium in the racetrack memory, it is necessary to be able to control the nucleation and propagation processes of this quasi-particle inside nanotrails. To generate the Skyrmionium, we need to switch the magnetization of the Skyrmionium shell in the opposite direction relative to the Skyrmionium core. The configuration of our system for the nucleation is similar to that of Ref. [72], except that they studied ferromagnetic Skyrmionium. In the micromagnetic simulation (with code written in Fortran), we consider an AFM rectangular thin film of dimensions 6000\( \times \)160\( \times \)1 \( \text{nm}^3 \) [Fig. (3.1a)], and divide it into \( 1 \times 1 \times 1 \) \( \text{nm}^3 \) unit cells (We consider a long rectangular thin film of the above dimension because we are interested in the steady state motion of the Skyrmionium since it takes sometime for the Skyrmionium to recover from its transient motion and move in steady state). Both sublattice magnetizations \( \mathbf{m}_A \) and \( \mathbf{m}_B \) are defined at each unit cell in the spirit of coarse graining. As the model parameters, we employ \( J_0 = 10^8 \text{ J/m}^3 \), \( A_1 = 2.5 \times 10^{-12} \text{ J/m} \), \( A_2 = 10^{-11} \text{ J/m} \), \( D = 4.2 \times 10^{-3} \text{ J/m}^2 \), \( K_z = 4 \times 10^5 \text{ J/m}^3 \), \( \alpha = 0.2 \), \( M_S = 5.8 \times 10^5 \text{ A/m} \), \( \gamma = 2.211 \times 10^5 \text{ s}^{-1} \text{(A/m)}^{-1} \), \( \theta_{\text{SHE}} = 0.15 \) and \( t = 5.0 \times 10^{-14} \text{s} \) (We use the time of such magnitude in order to capture the magnetization dynamics at that level). Starting from the initial state with \( \mathbf{n} \) homogeneous pointing in the \( +x_3 \) direction, spin current \( \mathbf{j}_s \) is locally injected within the toroidal region [indicated by two black circles in Fig. (3.1a and b)] for 9 ps to switch the magnetization of the Skyrmionium shell in the opposite direction relative to the Skyrmionium core(For the Skyrmionium nucleation, in order to account for some parameters like the Skyrmionium radii, the anisotropy, exchange coupling, we found the current density \( j_c = 1.18 \times 10^{13} \text{ A/m}^2 \) to be the right value in the nucleation process as
any other current density might not be able to begin the nucleation process), followed by a 2.5 ns of relaxation without applying any external torque; the center of the toroid is located at \( x_0^1 = 75 \) nm and \( x_0^2 = 80 \) nm, while the inner and outer radii of the toroid are 12 and 60 nm, respectively. This way of nucleating a Skyrmionium can be realized experimentally by placing one electrode at the circumference of the inner radius and the other electrode at the circumference of the outer radius, then allow the charge current from the both electrodes flow in a radial manner in the toroidal region where the magnetization will be switched relative to the core\[72\]. The spatial profile of \( p \) within the toroid is given by

\[
 p = |p|(\sin \varphi e_1 + \cos \varphi e_2), \tag{3.3}
\]

as indicated by white arrows in Fig. (3.1b), with \( \varphi = \tan^{-1}\left(\frac{x_2 - x_0^2}{x_1 - x_0^1}\right) \), while \( p = 0 \) outside the toroid. Such a spin current injection corresponds to applying an electric

![Figure 3.1: (a) Schematic of our system; bilayer of antiferromagnet (AFM) and nonmagnetic metal (NM). For the nucleation process, a 9 ps pulse of spin current \( j_s \) (green arrows) is locally injected within the toroidal region indicated by the black circles, i.e., between the inner and outer circles, followed by a 2.5 ns of relaxation. (b)-(e) Snapshots of the \( n_3 \) profile around the toroidal region (0 \( \leq x_1 \leq 150 \) nm and 0 \( \leq x_2 \leq 160 \) nm) at selected times. In (b), the spatial profile of \( p \) is schematically shown by white arrows.](image)
current pulse in Corbino geometry, i.e., a radially symmetric \( j_c = j_c(\cos \varphi e_1 + \sin \varphi e_2) \) within the toroid region in NM. Recently, it had been demonstrated that such an ultrashort electric pulse can be optically excited by utilizing a photosensitive switch[72].

In Fig. 3.1 (b)-(e), the snapshots of the \( n_3 \) profile around the center of the toroid at selected times are displayed. At \( t = 3 \) ps [Fig. (3.1c)], it is seen that the “seed” of a Skyrmionium has been generated, where the in-plane components of \( n \) has been developed in the toroidal region. The spin current injection is then completely turned off at 9 ps [Fig. (3.1d)], when \( n \) inside the toroidal region has flipped to the \( -x_3 \) direction. After 2.5 ns of relaxation without current, the system reaches the state with a Skyrmionium stabilized [Fig. (3.1e)].

### 3.3 Propagation of Skyrmionium

Now that we have successfully nucleated a Skyrmionium, we consider the propagation of the created Skyrmionium induced by spatially uniform spin current injection. We address the Skyrmionium propagation by an analytical as well as numerical approach. Our analytical result reveals the dependence of the Skyrmionium velocity on the material and injected spin current. We proceed in the analytical calculation of the equation of motion for the nucleated Skyrmionium as follows:

Then, the LLG equation which is derived according to Eq. (2.29) in Sec. (2.5) with the addition of the in-plane STT term is given by:

\[
\frac{\partial m_\zeta}{\partial t} = -m_\zeta \times \frac{\gamma}{1+\alpha^2} \left( H_\zeta - \frac{\alpha}{\gamma} p \right) - m_\zeta \times \frac{\gamma}{1+\alpha^2} \left( m_\zeta \times \left( H_\zeta + \frac{\alpha}{\gamma} p \right) \right) \quad (3.4)
\]

In terms of \( m \) and \( n \), Eq. (3.4) can be rewritten as:

\[
\frac{\partial n}{\partial t} = -n \times \left( \gamma H_m - \frac{\alpha}{\gamma} \frac{\partial m}{\partial t} - m \times \left( \gamma H_n - \frac{\alpha}{\gamma} \frac{\partial n}{\partial t} \right) - n \times (m \times p) - m \times (n \times p) \right)
\]

\[
\frac{\partial m}{\partial t} = -m \times \left( \gamma H_n - \frac{\alpha}{\gamma} \frac{\partial n}{\partial t} - m \times \left( \gamma H_m - \frac{\alpha}{\gamma} \frac{\partial m}{\partial t} \right) - n \times (n \times p) - m \times (m \times p) \right) \quad (3.5)
\]

Where \( H_m = H_A + H_B/2 \) and \( H_n = H_A - H_B/2 \) i.e the effective field in sublattice A and
B. By explicitly expressing \(H_m\) and \(H_n\), we have:

\[
\frac{\partial n}{\partial t} = -n \times \left[ \left( \nu_n \nabla^2 - \alpha \frac{\partial}{\partial t} \right) m + \gamma \left( H^{\text{ext}} - 2H_E m + H^{\text{ani}}_m \right) \right] - m \times \left[ \left( \nu_n \nabla^2 - \alpha \frac{\partial}{\partial t} \right) n \right.
\]
\[
\left. + \gamma \left( H^{\text{dmi}}_{rd} + H^{\text{ani}}_n \right) \right] - n \times (m \times p) - m \times (n \times p)
\]

(3.6)

\[
\frac{\partial m}{\partial t} = -n \times \left[ \left( \nu_n \nabla^2 - \alpha \frac{\partial}{\partial t} \right) n + \gamma \left( H^{\text{dmi}}_{rd} + H^{\text{ani}}_n \right) \right] - m \times \left[ \left( \nu_m \nabla^2 - \alpha \frac{\partial}{\partial t} \right) m + \gamma \left( H^{\text{ext}} + H^{\text{ani}}_m \right) \right] - n \times (n \times p) - m \times (m \times p)
\]

(3.7)

Where \(H_E = J_0 / \mu_0 M_s\), \(\nu_n = 2\gamma (2A_1 + A_2) / \mu_0 M_s\), \(\nu_m = \gamma (2A_1 - A_2) / \mu_0 M_s\), \(H^{\text{ani}}_n = \frac{2K}{\mu_0 M_s} n_z e_z\), and \(H^{\text{ani}}_m = \frac{2K}{\mu_0 M_s} m_z e_z\).

3.3.1 Small Ferromagnetic-Canting Approximation

Due to the fact that AFM exchange coupling between the sublattice magnetization is most often dominant over the other energy scales, we can safely assume \(|m(r, t)| \ll 1|\)
and \(|n(r, t)| \simeq 1|\); the dynamics of the AFM is described by the directional motion of \(n(r, t)\), which is well approximated by a unit vector, and the small transverse magnetization \(m(r, t)\).

This means that we ignore all the \(m(r, t)\)-dependent terms but the \(H_E\) term in Eq. (3.6), then:

\[
\frac{\partial n}{\partial t} \simeq -n \times \gamma \left( H^{\text{ext}} - 2H_E m \right)
\]

(3.8)

Multiplying the above equation by \(n \times \) and performing some vector algebra, one obtains:

\[
m = -\frac{1}{2H_E} n \times \left( \frac{1}{\gamma} \frac{\partial n}{\partial t} + n \times H^{\text{ext}} \right)
\]

(3.9)

Eq. (3.9) thus predicts that once the dynamics of \(n\) is known, the FM canting \(m\) is determined. Up to the first order of \(m\), Eq. (3.7) on the other hand reduces to:

\[
\frac{\partial m}{\partial t} = -n \times \left[ \frac{1}{\gamma} \left( \nu_n \nabla^2 - \alpha \frac{\partial}{\partial t} - p \times \right) n + H^{\text{dmi}}_{rd} + H^{\text{ani}}_n \right] - m \times \gamma H^{\text{ext}}
\]

(3.10)
Finding the derivative of Eq. (3.9) and substituting the result into Eq. (3.10), we obtain:

\[
0 = n \times \left( n \cdot \gamma H^{ext} \right) \left[ \gamma H^{ext} - 2n \times \frac{\partial n}{\partial t} \right] - n \times \gamma \left( \frac{\partial H^{ext}}{\partial t} - 2H_E p \right) + 2\gamma H_E \left[ \gamma (H_d^{rd} + H_n^{rd}) - \alpha \frac{\partial n}{\partial t} \right]
\]

(3.11)

Where \( \Box = \nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \) with \( c^2 = 2\nu_n \gamma H_E \)

### 3.3.2 Collective-Coordinate Model

If we assume that the dynamics of \( n(r, t) \) is described by the time evolution of a set of collective coordinates say \( X_1 \) and \( X_2 \) so that \( n(r, t) = n(r - vt) \) where \( v \equiv (\frac{dX_1}{dt}, \frac{dX_2}{dt}) \), then:

\[
\frac{\partial n}{\partial t} = \sum_{X_\mu = X_1, X_2} \frac{\partial n}{\partial X_\mu} \frac{dX_\mu}{dt}
\]

\[
\frac{\partial^2 n}{\partial t^2} = \sum_{X_\mu = X_1, X_2} \frac{\partial n}{\partial X_\mu} \frac{d^2 X_\mu}{dt^2} + \sum_{\mu, j} \frac{\partial n}{\partial X_\mu} \frac{dX_\mu}{dt} \frac{dX_k}{dt}
\]

(3.12)

In linear response analysis, the second term in Eq. (3.12) may be neglected. Eq. (3.11) has the form of \( n \times A = 0 \) meaning that the vector \( A \) is parallel to \( n \) i.e \( A = c n \). We then proceed by substituting to this Eq. (3.11) then multiplying the result by \( \frac{\partial n}{\partial X_i} \) and finally integrating the subsequent equation over the sample volume, we obtain the equation of motion for the collective coordinate as:

\[
\sum_{\mu} \left[ M_{i\mu} \frac{d^2 X_\mu}{dt^2} + (2\alpha \gamma H_E M_{i\mu} + G_{i\mu}) \frac{dX_\mu}{dt} \right] = F_0^i + F_{i}^{stt}
\]

(3.13)

where

\[
M_{i\mu} = \int d^2 r \left( \frac{\partial n}{\partial X_\mu} \frac{\partial n}{\partial X_i} \right)
\]

\[
G_{i\mu} = 2 \int d^2 r (n \cdot \gamma H^{ext}) n \cdot \left( \frac{\partial n}{\partial X_\mu} \times \frac{\partial n}{\partial X_i} \right)
\]

\[
F_0^i = \int d^2 r \frac{\partial n}{dX_i} \cdot \left[ c^2 \nabla^2 n - n \times \gamma \frac{\partial H^{ext}}{\partial t} - (n \cdot \gamma) \gamma H^{ext} + 2\gamma^2 H_E (H_d^{rd} + H_n^{rd}) \right]
\]

\[
F_{i}^{stt} = 2\gamma H_E \int d^2 r \frac{\partial n}{dX_i} \cdot (n \times p)
\]

(3.14)
Since we did not move our Skyrmionium with an external magnetic field, $H_{\text{ext}} = 0$ then, $G_{\mu} = 0$. Also, when $i \neq \mu$, $M_{i\mu} = 0$ and finally, in our rigid Skyrmionium motion assumption, $F_{\mu}^0 = 0$. Therefore, the equation of motion of the Skyrmionium is given by:

$$M_{\mu} \frac{d^2 X_{\mu}}{dt^2} + 2\alpha \gamma H_E M_{\mu} \frac{dX_{\mu}}{dt} = F_{\mu}^{\text{stt}}$$  \hspace{1cm} (3.15)$$

Where

$$M_{\mu} = \int d^2r \left( \frac{\partial n}{\partial X_{\mu}} \right)^2$$

$$F_{\mu}^{\text{stt}} = 2\gamma H_E \int d^2r \frac{\partial n}{\partial X_{\mu}} \cdot (n \times p) = 2\gamma H_E \sum_i p_i I_{\mu i}$$  \hspace{1cm} (3.16)$$

To compute Eqs. (3.16), we rely on the numerical profile of $n$ (since the analytical expression for a Skyrmionium solution is unavailable). With the equilibrium Skyrmionium structure obtained in Section (3.2), we find $M_1 \simeq M_2 \simeq 73.4$ and $I_{12} \simeq -I_{21} \simeq -4.6 \times 10^{-7}$ m; For a Néel type Skyrmionium, the other components of $I_{\mu j}$ (i.e. $I_{11}, I_{13}, I_{22}$ and $I_{23}$) are vanishingly small in general[72]. A spin current with the polarization $p$ along the $+x_1$ ($-x_2$) axis, therefore, drives a Skyrmionium propagation in the $+x_2$ ($+x_1$) direction. [corresponding to $j_c$ flowing in the $+x_2$ ($+x_1$) direction.]

Let us now examine the Skyrmionium dynamics in the presence of spin current polarized in the $-x_2$ direction, i.e., $p \parallel -e_2$. In this case, $F_2 = 0$ and thus $dX_2/dt = 0$, while a general solution $dX_1/dt$ for Eq. (3.6) is given by

$$\frac{dX_1(t)}{dt} = v_1 \left( 1 - e^{-2\alpha \gamma H Et} \right) ,$$  \hspace{1cm} (3.17)$$

where the initial velocity being zero ($dX_1/dt|_{t=0} = 0$) has been assumed, and $v_1$ is the terminal velocity defined by

$$v_1 \equiv \left. \frac{dX_1}{dt} \right|_{t \to \infty} = \frac{|I_{12}|}{\alpha M_1} |p| .$$  \hspace{1cm} (3.18)$$

On the other hand, using our numerical tool, we wrote a code in Fortran to simulate the Skyrmionium motion (see Appendix C.4). In the code, we made use of the fourth order
Runge Kutta method to solve the time dependent Landau Lifshitz Gilbert (LLG) equation (using the form of LLG equation in Eq. 3.4). The figure below shows the schematic diagram of the motion process and $n_3$ profile position of the Skyrmionium at $t = 0 ns$, $t = 1.5 ns$, $t = 3 ns$, $t = 4.5 ns$ and $t = 6 ns$ for charge current density $j_c = 0.2 \times 10^{12} A/m^2$ and $j_c = 1.0 \times 10^{12} A/m^2$ respectively. We can see an increase in the Skyrmionium velocity $v$ with current density $j_c$, and the distortion of the Skyrmionium for higher current densities ($j_c = 1.0 \times 10^{12} A/m^2$ is displayed).

Figure 3.2: (a) Schematic motion process of our system; bilayer of antiferromagnet (AFM) and nonmagnetic metal (NM). For the motion process, a 6ns pulse of spin current $j_s$ (green arrows) is applied allover the sample. The white arrow represents the spin polarization $p$ with its direction in the $-x_2$ axis while the yellow arrow shows the direction of motion of the Skyrmionium. (b) shows snapshots of the $n_3$ profile at $t = 0$, $t = 1.5$, $t = 3.0$, $t = 4.5$ and $t = 6 ns$ for $j_c = 0.2 \times 10^{12}$ and $j_c = 1.0 \times 10^{12}$ $A/m^2$ respectively.

In the next section, we shall move on to discuss some of the results obtained from the micromagnetic simulation and the analytical calculations done in this chapter. We shall also check the validity of the collective coordinate model by comparing its prediction with micromagnetic simulations.
3.4 Results and Conclusion

3.4.1 Skyrmionium core displacement and velocity as a function of time.

In this chapter, we want to see how the core of the Skyrmionium evolves in time as the Skyrmionium moves under the application of spin current $j_s$ uniformly over the sample. One of the plausible ways of estimating Skyrmionium core displacement ($X_1, X_2$) is to calculate the moment of the third component of the Néel order parameter $n_3(-1 \leq n_3 \leq 1)$ which is given by the expression:

$$X_\mu = \frac{\int x_\mu (1 - n_3) d^2x}{\int (1 - n_3) d^2x}$$  \hspace{1cm} (3.19)

where $\int (1 - n_3) d^2x$ is the total magnetization of the Skyrmionium. Eq. (3.19) represents the average $x_1$ and $x_2$ displacement of Skyrmionium core as it moves under the application of spin current. To understand how Eq. (3.19) works, let us consider the motion of the Skyrmionium on $x_1$ direction with magnetizations positioned on the real line and the core been at a particular point on the real line. If the core is positioned at the origin for example, the numerator of Eq. (3.19) gives zero (since $x = 0$ and also because of the symmetric property of the $2\pi$ Skyrmion and the real line such that when we sum over the product of position and total magnetization, one obtains zero) and also when the magnetization is pointing up, the whole of Eq. (3.19) gives zero. We can then immediately see that the only time we obtain a non-zero result from Eq. (3.19) is when the core is positioned on the real line such that it’s not symmetric with it and when the magnetization points in an arbitrary direction or down. Using the understanding from this equation, we numerically estimate the average displacement and a linear graph was obtained for the $x_1$ (horizontal displacement) of the Skyrmionium core with time while the $x_2$ (vertical displacement) is zero as time elapses i.e. the Skyrmionium does not move practically in the $x_2$-direction. The Skyrmionium velocity was also numerically estimated from the data obtained for the Skyrmionium core displacement. The diagram below shows the Skyrmionium core displacement and velocity as a function of time for current density $j_c = 0.2 \times 10^{12} Am^{-2}$ and $j_c = 1.0 \times 10^{12} Am^{-2}$. From the graph above, it can be seen that for both current densities, a linear graph is obtained for the $x_1$ - component of Skyrmionium core displacement. While charge current
Figure 3.3: fig.3.3(a&b) shows the $x_1$ and $x_2$ components of the Skyrmionium core displacement, $R(m)$ and velocity $v_{x1}$ and $v_{x2}$ as a function of time, $t(s)$ for charge current $j_c = 0.2 \times 10^{12} Am^{-2}$ while fig.3.3(c&d) shows the $x_1$ and $x_2$ components of the Skyrmionium core displacement, $R(m)$ and velocity $v_{x1}$ and $v_{x2}$ as a function of time, $t(s)$ for charge current $j_c = 1.0 \times 10^{12} Am^{-2}$ respectively.

of $j_c = 0.2 \times 10^{12} Am^{-2}$ moves the Skyrmionium over about 500 lattice sites, charge current of $j_c = 1.0 \times 10^{12} Am^{-2}$ moves the Skyrmionium over 3000 lattice sites. Although it’s subtle to talk of steady state motion for the Skyrmionium driven with $j_c = 1.0 \times 10^{12} Am^{-2}$ at 10ns, for charge current of $j_c = 0.2 \times 10^{12} Am^{-2}$, the Skyrmionium is already in it’s steady state motion at about 0.3ns (with velocity of about $93 ms^{-1}$). This means that the higher the current density, the longer time it takes for the Skyrmionium to adjust its structure in order to attain steady state motion according to Newton’s law of motion. This long time
required for the Skyrmionium stability can be attributed to the fact that the Skyrmionium structure is such that it is made up of two skyrmions of opposite topological number nested together so that under the whole structure has to move collectively under the application of an external driving force. With such kind of structure and high force (or current density), it is therefore natural to expect stable motion of the system after some time as the system tries to find a stable state after the application of an external force.

In the next section, we try to look at the velocity of the Skyrmionium as a function of charge current $j_c$.

### 3.4.2 Skyrmionium velocity as a function of charge current $j_c$

To study the dependence of the Skyrmionium velocity as a function of the current density $j_c$, we numerically estimated the Skyrmionium velocities from the displacement of $(X_1, X_2)$ during the application of spin-transfer torque as shown in the figure below: In Fig. (3.4),

![Figure 3.4: Skyrmionium velocities $v_1$ and $v_2$, in the $x_1$ and $x_2$ directions, respectively, as functions of electric current density $j_c$. The analytical (numerical) results are represented by the solid lines (circles). For the Skyrmionium propagation, the spin current injection is spatially uniform.](image)

the numerically estimated Skyrmionium velocities were plotted by circles as functions of $j_c$. To an extent, our micromagnetic simulation agrees with the collective coordinate model especially for lower charge current $j_c$; the Skyrmionium velocity exhibits a linear dependence
on the current density (for lower current density), and the relation between directions of $\mathbf{p}$ and the Skyrmionium propagation is consistent. The quantitative discrepancy between the two approaches in $v_1$, may be attributed to the distortion of the Skyrmionium shape as it can be seen from fig. (3.2) that at larger current density, the relative shift of the inner and outer skyrmions as well as the overall deformation becomes more appreciable, reducing the accuracy of the rigid-motion approximation in our collective coordinate model. To ascertain this claim, we take a look at the Skyrmionium mass (in the $x_1$ and $x_2$) direction as a function of charge current from our micromagnetic simulation and we observe that the Skyrmionium mass increases in the course of its motion and the overall shifting of its center of mass in the $x_1$ and $x_2$ direction were captured as shown in the diagram below: From Fig. (3.5)

![Diagram showing Skyrmionium mass as a function of charge current](image)

Figure 3.5: shows the Skyrmionium center of mass $M_1$, $M_2$ in the $x_1$ and $x_2$ directions respectively, and its effective mass $M$ as functions of time ($\text{ns}$) for charge currents $j_c = 0.2 \times 10^{12}$, $j_c = 0.4 \times 10^{12}$, $j_c = 0.8 \times 10^{12}$, and $j_c = 1.0 \times 10^{12}$,

shown above, it is clearly seen that for lower charge current ($j_c = 0.2 \times 10^{12}$ and less), the $x_1$ and $x_2$ component of the Skyrmionium mass almost remains the same as the initial mass, $M = 73.4$ and there was no distortion whatsoever as both mass components share the same center but for higher charge current density (precisely starting from $j_c = 0.4 \times 10^{12}$), the mass in $x_1$ and $x_2$ direction increases especially the $x_2$ component of the Skyrmionium mass (which suggests that the Skyrmionium experiences more distortion in this direction than in the direction of motion, $x_1$ as it can also be confirmed in Fig. 3.2) and there is
an overall shifting of the Skyrmionium center of mass as it moves along which therefore means that our rigid motion assumption of the Skyrmionium fails to predict it’s motion for high charge current density. As a result of this increase in the Skyrmionium mass, we immediately see that Eq. (3.18) does not capture the increase in Skyrmionium mass as it moves under the application of charge current. This means that the Skyrmionium terminal velocity calculated in Eq. (3.18) of Sec. (3.3) is not independent of the Skyrmionium center of mass as we have assumed in our rigid motion assumption of the Skyrmionium.

3.5 Conclusion

In conclusion, we have theoretically studied current-driven nucleation and propagation of antiferromagnetic Skyrmionium. Micromagnetic simulations have been performed to demonstrate that a local spin current injection with a toroidal distribution can nucleate a Skyrmionium, and a spatially-uniform spin current can drive the Skyrmionium into motion (with a code written in Fortran by the author to demonstrate these processes). An analytical expression for the Skyrmionium velocity derived based on a collective-coordinate model is consistent with the numerical result. Our findings offer a way of nucleating an antiferromagnetic Skyrmionium, as well as an estimation of the current-driven Skyrmionium velocity for a given material. In visualizing the motion process of our simulation, we were able to see distortion in the structure of the Skyrmionium (which becomes evident for large current density). We attributed the acceleration of the Skyrmionium to this distortion. Finally, we observe a little deviation of our simulation from analytical calculation especially for high charge current.
Chapter 4

Future Outlook

In this section, we will like to look at areas where this work could be improved as regarding the distortion experienced by the Skyrmionium under the application of charge current and also the deviation observed between our numerical simulation and analytical prediction of the Skyrmionium terminal velocity especially for high current density as we discussed in Sec. (3.4) and also obvious in Fig. (3.2) from Sec. (3.3).

Talking about the deviation observed between the analytic and numerical results, we saw from Eq. (3.18) that an increase in the Skyrmionium center of mass as it moves along (especially for higher charge current density) was not accounted for. It therefore means that a more general analytics (where the change in Skyrmionium center of mass depends on the charge current) is therefore required to correctly predicts the terminal Skyrmionium velocity in the course of its motion. In doing this, the analytical and numerical prediction of the Skyrmionium terminal velocity should agree in accordance with Eq. (3.18).

Talking about Skyrmionium distortion, one of the possible ways of reducing the distortion experienced by the Skyrmionium during its motion under the application of charge current (especially for high charge current) is by increasing the inner radius relative to the outer radius. This can be viewed from the perspective that for a smaller inner Skyrmion radius, the outer Skyrmion suffers more distortion as compared to the inner radius. Therefore, if the inner radius can be made larger relative to the outer Skyrmionium radius, this can reduce the distortion experienced by the Skyrmionium and with this, the rigid assumption may therefore be valid. In doing this, we then have to carefully find the charge current \( j_c \) that will be sufficient to begin the nucleation process as discussed in Sec. (3.2).
Still talking about the distortion, another possible cause of this may arise from the material parameter which is the *Damping parameter, α*. The damping parameter can be viewed as a dissipative term that inhibits the terminal velocity of the Skyrmionium. When the damping parameter is too large, the Skyrmionium might lose energy very fast such that the structure of the system has to compensate for this energy loss. One way to study the effect of this damping is to perform numerical simulations for different damping parameters and compare the distortion experienced by the Skyrmionium for different damping parameters.
APPENDICES

A  Emergent Magnetic and Electric field

\[ \sigma_\mu \sigma_\beta = \delta_\mu_\beta + i \epsilon_{\mu_\beta j} \sigma_j \]  \hspace{1cm} (1)

\[ (a \times b)^j = \epsilon_{\mu_\beta j} a_\mu b_\beta \]  \hspace{1cm} (2)

\[ \epsilon_{ijk} \epsilon_{ilm} = \left[ \delta_{jl} \delta_{km} - \delta_{jm} \delta_{kl} \right] \]  \hspace{1cm} (3)

\[ \Psi \rightarrow U \Phi \]  \hspace{1cm} (4)

\[ \Psi^\dagger \rightarrow \Phi^\dagger U^\dagger \]  \hspace{1cm} (5)

since \( U \) is Hermitian. so, we define \( U = n^\alpha \sigma_\alpha \)

\[ U^\dagger \sigma_\mu U = n^\alpha n^\beta \sigma_\alpha \delta_{\mu_\beta} = n^\alpha n^\beta \sigma_\alpha [\sigma_\mu \sigma_\beta] \]  \hspace{1cm} (6)

\[ U^\dagger \sigma_\mu U = n^\alpha n^\beta \sigma_\alpha \left[ \delta_{\mu_\beta} + i \epsilon_{\mu_\beta j} \delta_{\alpha j} \right] \]  \hspace{1cm} (7)

similifying this using Eq. (1) we have,

\[ U^\dagger \sigma U = n^\alpha n^\beta \sigma_\alpha \delta_{\mu_\beta} + i n^\alpha n^\beta \epsilon_{\mu_\beta j} \left[ \delta_{\alpha j} + i \epsilon_{\alpha jm} \right] \]  \hspace{1cm} (8)

\[ U^\dagger \sigma_\mu U = n^\alpha n^\mu \sigma_\alpha + i n^\alpha n^\beta \epsilon_{\mu_\beta j} \delta_{\alpha j} - n^\alpha n^\beta \epsilon_{\mu_\beta j} \delta_{\alpha j} \epsilon_{\alpha jm} \sigma_m \]  \hspace{1cm} (9)

\[ U^\dagger \sigma_\mu U = n^\alpha n^\mu \sigma_\alpha + i n^\alpha n^\beta \epsilon_{\mu_\beta j} \delta_{\alpha j} + n^\alpha n^\beta \epsilon_{\mu_\beta j} \delta_{\alpha j} \epsilon_{\alpha jm} \sigma_m \]  \hspace{1cm} (10)
Using the relation Eq. (3) shown above, we can re-write Eq. (10) as follows:

\[ U^\dagger \sigma U = n^\alpha n^\mu \sigma_\alpha + in^\alpha n^\beta \epsilon_{\mu \beta \alpha} + n^\alpha n^\beta \delta_{\mu \alpha} \delta_{\beta m} \sigma_m - n^\alpha n^\beta \delta_{\mu m} \delta_{\beta \alpha} \sigma_m \quad (11) \]

But

\[ in^\alpha n^\beta \epsilon_{\mu \beta \alpha} = 0 \]

Therefore, Eq. (11) reduces to:

\[ U^\dagger \sigma U = n^\alpha n^\mu \sigma_\alpha + n^\mu n^\beta \sigma_\beta - n^\alpha n^\alpha \sigma_\mu \quad (12) \]

But \( n^\alpha n^\alpha = 1 \) and \( \sigma_\mu \) can be re-written as: \( \sigma_\mu = \delta_{\mu \alpha} \sigma_\alpha \) so that Eq. (12) reduces to:

\[ U^\dagger \sigma U = \left( 2n^\alpha n^\mu - \delta_{\mu \alpha} \right) \sigma_\alpha \quad (13) \]

\[ \Phi^\dagger U \partial_\mu \left(U \Phi \right) = \Phi^\dagger U \partial_\mu U \Phi + \Phi^\dagger \partial_\mu \Phi = \Phi^\dagger \left(U \partial_\mu U + \partial_\mu \right) \Phi \quad (14) \]

\[
m = \begin{pmatrix} \cos \phi \sin \theta \\ \sin \phi \sin \theta \\ \cos \theta \end{pmatrix}, \quad n = \begin{pmatrix} \cos \phi \sin \theta/2 \\ \sin \phi \sin \theta/2 \\ \cos \theta/2 \end{pmatrix} \quad (15)\]

\[ \partial_\mu \Psi^\dagger \cdot \partial_\mu \Psi = \left( \Phi^\dagger \partial_\mu U + \Phi^\dagger \partial_\mu \Phi \right) \cdot \left(U \partial_\mu U + U \partial_\mu \Phi \right) = \Phi^\dagger \partial_\mu U \cdot \left(U \partial_\mu \Phi + \Phi^\dagger \partial_\mu U \cdot U \partial_\mu \Phi \right) = \Phi^\dagger \left( \partial_\mu + U \partial_\mu \Phi \right) \cdot \left( \partial_\mu + U \partial_\mu \Phi \right) \quad (16) \]
\[
\Phi^\dagger U \sigma_x m_x U \Phi = \left( 2n^x n^x - 1 \right) \sigma_x + 2n^x n^y \sigma_y + 2n^x n^z \sigma_z \right] m_x
\]
\[
\Phi^\dagger U \sigma_y m_y U \Phi = \left( 2n^y n^y - 1 \right) \sigma_y + 2n^x n^y \sigma_y + 2n^x n^z \sigma_z \right] m_y
\]
\[
\Phi^\dagger U \sigma_z m_z U \Phi = \left( 2n^z n^z - 1 \right) \sigma_z \right] m_z
\]

(17)

Applying Eq. (15), and adding the components of Eq. (17) we can show that \( \Phi^\dagger U \sigma \cdot m U \Phi(r, t) = \sigma_z \) If we define
\[
A = i\hbar U \partial_\mu U
\]
and
\[
A_0 = -i\hbar \partial_t U
\]
Recall that \( U = n^\alpha \sigma_\alpha \). Therefore, we can re-write Eq. (18) as follows:
\[
A_\mu = i\hbar n^\alpha \sigma_\alpha \left( \partial_\mu n^\beta \sigma_\beta \right)
\]
(20)

but \( \partial_\mu \sigma_\beta = 0 \). Then, Eq. (20) reduces to:
\[
A_\mu = i\hbar n^\alpha \sigma_\alpha \left( \partial_\mu n^\beta \right) \sigma_\beta
\]
(21)

from Eq. (1), Eq. (22) becomes
\[
A_\mu = i\hbar n^\alpha \left( \delta_{\alpha, \beta} + i\epsilon_{\alpha \beta \gamma} \sigma_\gamma \right) \partial_\mu n^\beta
\]
(23)

Nothing the meaning of the kroneckera symbol and observing that \( \epsilon_{\alpha \beta \gamma} \sigma_\gamma = 0 \) in the permutation notation, we see that Eq. (23) reduces to:
\[
A_\mu = i\hbar \left( n^\alpha \partial_\mu n^\alpha + i\epsilon_{\alpha \beta \gamma} n^\alpha \sigma_\gamma \partial_\mu n^\beta \right)
\]
(24)
But \( n^\alpha \partial_\mu n^\alpha = 0 \). Therefore, Eq. (24) reduces to:

\[
A_\mu = i\hbar \left( i\epsilon_{\alpha\beta\gamma} n^\alpha \partial_\mu n^\beta \right) \sigma_\gamma
\]

Eq. (25) can be written as:

\[
A_\mu = -\hbar \left( \mathbf{n} \times \partial_\mu \mathbf{n} \right) \cdot \sigma
\]

The vector potential in the rotating frame thereby given by:

\[
A_\mu = -\hbar \left( \mathbf{n} \times \partial_\mu \mathbf{n} \right)
\]

To obtain the vector potential in the lab frame, we multiply Eq. (27) by the Hermitian conjugate of the rotation matrix \( R_{\mu\alpha} \) given in Eq. (13). Then we have:

\[
R A = -\hbar \left( 2n^\alpha n^\mu - \delta_{\mu\alpha} \right) \left( \mathbf{n} \times \partial_\mu \mathbf{n} \right)
\]

\[
R A = -\hbar \begin{pmatrix}
2 \cos^2 \phi \sin^2 \frac{\theta}{2} - 1 & \sin 2\phi \sin^2 \frac{\theta}{2} & \cos \phi \sin \theta \\
\sin 2\phi \sin^2 \frac{\theta}{2} & 2 \sin^2 \phi \sin^2 \frac{\theta}{2} - 1 & \sin \phi \sin \theta \\
\cos \phi \sin \theta & \sin \phi \sin \theta & 2 \cos^2 \frac{\theta}{2} - 1
\end{pmatrix}
\times
\begin{pmatrix}
-\frac{1}{2} (\sin \phi \partial_\mu \theta + \cos \phi \sin \theta \partial_\mu \phi) \\
-\frac{1}{2} (\sin \phi \sin \theta \partial_\mu \phi - \cos \phi \partial_\mu \theta) \\
\frac{1}{2} (1 - \cos \theta) \partial_\mu \phi
\end{pmatrix}
\]

\[
(29)
\]

\[
R A = -\frac{\hbar}{2}
\begin{pmatrix}
\cos \phi \sin \theta \partial_\mu \phi + \sin \phi \partial_\mu \phi \\
\sin \phi \sin \theta \partial_\mu \phi - \cos \phi \partial_\mu \phi \\
(\cos \theta - 1) \partial_\mu \phi
\end{pmatrix}
\]

Eq. (30) is in the form of \( \mathbf{m} \times \partial_\mu \mathbf{m} \) with an additional term \((1 - \cos \theta) \partial_\mu \phi \mathbf{m}\) which is the Adiabatic Gauge field.

\[
\mathbf{m} \times \partial_\mu \mathbf{m} = \begin{pmatrix}
-\sin \phi \partial_\mu \theta - \cos \phi \cos \theta \sin \theta \partial_\mu \phi \\
\cos \phi \partial_\mu \theta - \sin \phi \sin \theta \cos \theta \partial_\mu \phi \\
\sin^2 \theta \partial_\mu \phi
\end{pmatrix}
\]

\[
(1 - \cos \theta) \partial_\mu \phi \mathbf{m} = \begin{pmatrix}
(\cos \phi \sin \theta - \cos \theta \cos \phi \sin \theta) \partial_\mu \phi \\
(\sin \phi \sin \theta - \cos \theta \sin \phi \sin \theta) \partial_\mu \phi \\
(\cos \theta - \cos^2 \theta) \partial_\mu \phi
\end{pmatrix}
\]

Adding \((1 - \cos \theta) \partial_\mu \phi \mathbf{m}\) from \( \mathbf{m} \times \partial_\mu \mathbf{m} \), we can then explicitly obtain the vector potential
matrix in the "lab frame" i.e.

\[
A = R A = -\frac{\hbar}{2} \left( \mathbf{m} \times \partial_{\mu} \mathbf{m} \right) \cdot \mathbf{\sigma} + \frac{\hbar}{2} \left( 1 - \cos \theta \right) \partial_{\mu} \phi \mathbf{m} \cdot \mathbf{\sigma} = \begin{pmatrix} \cos \phi \sin \theta \partial_{\mu} \phi + \sin \phi \partial_{\mu} \theta \\ \sin \phi \sin \theta \partial_{\mu} \phi - \cos \phi \partial_{\mu} \theta \\ (\cos \theta - 1) \partial_{\mu} \phi \end{pmatrix}
\] (32)

The scalar potential \(A_0\) can be obtained by following similar procedure for calculating the vector potential so that:

\[
A_0 = \frac{\hbar}{2} \left( \mathbf{m} \times \partial_{\mu} \mathbf{m} \right) \cdot \mathbf{\sigma} - \frac{\hbar}{2} \left( 1 - \cos \theta \right) \partial_{\mu} \phi \mathbf{m} \cdot \mathbf{\sigma}
\] (33)

Now, we will make use of the Maxwell’s relation in calculating the emergent magnetic and electric field, using the assumption that the magnetization align in the direction of the Pauli matrices (Semi-Classical assumption) so that the vector potential becomes:

\[
\mathbf{A} = -\frac{\hbar}{2} \left( \mathbf{m} \times \partial_{\mu} \mathbf{m} \right) \cdot \mathbf{m} + \frac{\hbar}{2} \left( 1 - \cos \theta \right) \partial_{\mu} \phi \mathbf{m} \cdot \mathbf{\sigma}, \quad \mathbf{A}_0 = \frac{\hbar}{2} \left( \mathbf{m} \times \partial_{\mu} \mathbf{m} \right) \cdot \mathbf{m} - \frac{\hbar}{2} \left( 1 - \cos \theta \right) \partial_{\mu} \phi
\] (34)

\[
\mathbf{B}^{em} = \nabla \times \mathbf{A}, \quad \mathbf{E}^{em} = -\partial_t \mathbf{A} - \partial_i \mathbf{A}_0
\] (35)

Using the Levi-civita symbol,

\[
B_{z}^{em} = \epsilon_{xyz} \partial_x A_y \\
A_y = -\frac{\hbar}{2} \epsilon_{pqy} m_p (\partial_q \mathbf{m}) m_y + \frac{\hbar}{2} (1 - \cos \theta) \partial_y \phi \\
B_{z}^{em} = -\frac{\hbar}{2} \left[ \epsilon_{xyz} \epsilon_{pqy} \partial_x \left( m_p (\partial_q \mathbf{m}) m_y \right) - \left( \epsilon_{xyz} \sin \theta \partial_x \theta \partial_y \phi \right) \right] \\
B_{z}^{em} = -\frac{\hbar}{2} \left[ \delta_{xp} \delta_{zq} - \delta_{xq} \delta_{zp} \partial_t \left( m_p (\partial_q \mathbf{m}) m_y \right) - \left( \epsilon_{xyz} \sin \theta \partial_x \theta \partial_y \phi \right) \right] \\
B_{z}^{em} = -\frac{\hbar}{2} \left[ \partial_p \left( m_p (\partial_z \mathbf{m}) m_y \right) - \partial_q \left( m_z (\partial_q \mathbf{m}) m_y \right) - \left( \epsilon_{xyz} \sin \theta \partial_x \theta \partial_y \phi \right) \right] \\
B_{z}^{em} = -\frac{\hbar}{2} \epsilon_{xyz} \sin \theta \partial_x \theta \partial_y \phi \\
= \frac{1}{2} \epsilon_{xyz} \frac{\hbar}{2} \sin \theta \left( \partial_x \theta \partial_y \phi - \partial_y \theta \partial_x \phi \right)
\] (36)
We can show that $\sin \theta$ times the term in brackets in Eq. (36) is equal to the mixed product $\mathbf{m} \cdot \left( \partial_x \mathbf{m} \times \partial_y \mathbf{m} \right)$. Therefore, the emergent magnetic field is given by the equation:

$$
\mathbf{B}_{\text{em}} = \frac{\hbar}{2} \mathbf{m} \cdot \left( \partial_x \mathbf{m} \times \partial_y \mathbf{m} \right) \quad (37)
$$

We can equally show that the emergent magnetic field is given by the expression:

$$
\mathbf{E}_{\text{em}} = -\frac{\hbar}{2} \mathbf{m} \cdot \left( \partial_t \mathbf{m} \times \partial_x \mathbf{m} \right) \quad (38)
$$

### B Topological Charge

The Topological charge of a Skyrmion derived from Eq. (37) is:

$$
Q = \frac{1}{4\pi} \int \int \mathbf{m} \cdot \left( \partial_x \mathbf{m} \times \partial_y \mathbf{m} \right) d^2r \quad (39)
$$

Using Eq. (39), the Topological charge can be written in spherical coordinate as:

$$
Q = \frac{1}{4\pi} \int \int \sin \theta \left( \partial_x \theta \partial_y \phi - \partial_y \theta \partial_x \phi \right) d\theta d\phi \quad (40)
$$

The term $\left( \partial_x \theta \partial_y \phi - \partial_y \theta \partial_x \phi \right)$ is the inverse Jacobian:

$$
J^{-1} = \left[ \det \begin{pmatrix} \partial_x \theta & \partial_x \phi \\ \partial_y \theta & \partial_y \phi \end{pmatrix} \right]^{-1}
$$

of our transformation $x = \sin \theta \cos \phi$ and $y = \sin \theta \sin \phi$

$$
Q = \frac{1}{4\pi} \int \int J \sin \theta J^{-1} d\theta d\phi \quad (41)
$$

Using the radial symmetry of the Skyrmion i.e in the cylindrical coordinate where $r = (x, y) = (\rho \cos \varphi, \rho \sin \varphi)$, and the pin direction is $\mathbf{m}(r) = \left( \sin \theta(\rho) \cos \phi(\varphi), \sin \theta(\rho) \sin \phi(\varphi), \cos \theta(\rho) \right)$ we can write:

$$
\theta = \theta(\rho)
$$
\[ \phi = \phi(\varphi) = m\varphi + \gamma \]

Where \( m \) is the vorticity \( (m = \pm 1) \) and \( \gamma \) is the Helicity. Therefore, Eq. (41) is written as:

\[ Q = \frac{m}{4\pi} \int_0^\infty \sin\theta(\rho)d\theta(\rho) \int_0^{2\pi} d\phi(\varphi) \]

\[ Q = \frac{m}{4\pi} \cos\theta(\rho)|_{0}^{\infty} \phi(\varphi)|_{0}^{2\pi} \] (42)

\[ Q = \frac{m}{4\pi} \cos\theta(\rho)|_{0}^{\infty} \phi(\varphi)|_{0}^{2\pi} \] (43)

In the case of a Skyrmion where spins points in the positive z-direction (up) then \( \theta(\rho = \infty) = 0 \) and at the center of the Skyrmion, the spin points down and as such, \( \theta(\rho = 0) = \pi \), so that

\[ \cos\theta(\rho)|_{0}^{\infty} = 2 \]

and

\[ \phi(\varphi)|_{0}^{2\pi} = 2\pi \]

Then,

\[ Q = \pm 1 \] (44)

**C Numerical Method and Fortran code**

**C.1 Runge-Kutta Method**

The method adopted in this thesis to solve the LLG equation (a first order differential equation in time) is the fourth order Runge-Kutta method. It is the most robust and consistent methods used in the numerical integration of differential equations. The problem to be solved is of the type \( \dot{u} = g(u, t) \), \( u(0) = u_0 \), this method find the approximate value at a particular order \( N \) of the function at time \( t + dt \), by knowing the function and it’s derivative at a given time \( t \), as a weighted average of \( N \) points interpolated in the time interval \( dt \) with different estimations of the gradient \( x \). In the case of the fourth order
Runge-Kutta (or RK4), the algorithm reads:

\begin{align}
  k_1 &= g(t, y(t)) \\
  k_2 &= g\left(t + \frac{dt}{2}, u(t) + \frac{dt}{2} \cdot k_1\right) \\
  k_3 &= g\left(t + \frac{dt}{2}, u(t) + \frac{dt}{2} \cdot k_2\right) \\
  k_4 &= g\left(t + dt, u(t) + dt \cdot k_3\right) \\
  u(t + dt) &= u(t) + \frac{dt}{6} (k_1 + 2k_2 + 2k_3 + k_4)
\end{align}

The local truncation error of the RK4 is of \(O(dt^5)\) while the total accumulated error of the method is of the order \(O(dt^4)\). In the simulation for this thesis, such equations for each of the sublattices of our system with each sublattice having three components of magnetization and \(g\) is a vector given by the LLG equation.

### C.2 Forward, backward and central difference derivative method

In order to correctly estimate the energy terms that has to do with first and second order derivatives (especially at the boundary of our system), we rely on the forward, backward and central derivative for our numerical simulations. To do this, we use the following derivations of first and second order derivatives from Taylor’s theorem \([73]\):

**Forward difference**

\begin{align}
  f'(x_i) &= \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2) \\
  f''(x_i) &= \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2} + O(h^2)
\end{align}

**Backward difference**

\begin{align}
  f'(x_i) &= \frac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h} + O(h^2) \\
  f''(x_i) &= \frac{-f(x_{i-3}) + 4f(x_{i-2}) - 5f(x_{i-1}) + 2f(x_i)}{h^2} + O(h^2)
\end{align}
Central difference

\begin{align}
  f'(x_i) &= \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2) \\
  f''(x_i) &= \frac{f(x_{i+1}) - 2f(x_i) - f(x_{i-1})}{h^2} + O(h^2)
\end{align} \tag{48}

We made use of the central derivative for points in the bulk, forward and backward for points at the edges. The error associated with the central, forward and backward derivative is $O(h^2)$ i.e $(4.0 \times 10^{-18}$, since $h$ which is our mesh size is $2.0 \times 10^{-9})$. This means that the accuracy of our numerical simulation is quite good.

C.3 Algorithm of our Fortran code

![Schematics of the Fortran code algorithm](image)

Figure 1: Schematics of the Fortran code algorithm
C.4 Fortran code

```fortran
! Nucleation stage
MagNuca = mag_iNi(Nx,Ny,1,0)
MagNuca = mag_iNi(Nx,Ny,-1,0)
ST = STT(initial = 0)

open(1, file='mag_iNiA.txt', status='new')
open(2, file='mag_iNiB.txt', status='new')

do k=0,Nx*Ny-1
   ix = modulo(k,Nx)
   iy = k/Nx
   write(1,*) MagNuca(k,0), MagNuca(k,1), MagNuca(k,2)
   write(2,*) MagNuca(k,0), MagNuca(k,1), MagNuca(k,2)
end do
close(1)
close(2)

do t=0,20
   call Mag_relax(MagNuca, MagNuca, al, ga, dx, Nx, Ny, k, x, y, k, x, z, al, a2, mu_0, Ms, do, 01, ST, dt, t, 0, 68)
   do k = 0, Nx*Ny-1
      write(1,*) MagNuca(k,0), MagNuca(k,1), MagNuca(k,2)
      write(2,*) MagNuca(k,0), MagNuca(k,1), MagNuca(k,2)
   end do
end do
close(3)
close(4)

! Relaxation stage

open(5, file='magrelA.9ps.txt', status='old')
open(6, file='magrelB.9ps.txt', status='old')

do k=0,Nx*Ny-1
   ix = modulo(k,Nx)
   iy = k/Nx
   write(5,*) Magrelaxa(k,0), Magrelaxa(k,1), Magrelaxa(k,2)
   write(6,*) Magrelaxb(k,0), Magrelaxb(k,1), Magrelaxb(k,2)
end do
close(5)
close(6)

open(7, file='magrelaxA.txt', status='new')
open(8, file='magrelaxB.txt', status='new')
ST = STT(initial = 1)

call Mag_relax(Magrelaxa, Magrelaxb, al, ga, dx, Nx, Ny, k, x, y, k, x, z, al, a2, mu_0, Ms, do, 01, ST, dt, t, 0, 500080)

do k = 0, Nx*Ny-1
   ix = modulo(k,Nx)
   iy = k/Nx
   write(7,*) Magrelaxa(k,0), Magrelaxa(k,1), Magrelaxa(k,2)
   write(8,*) Magrelaxb(k,0), Magrelaxb(k,1), Magrelaxb(k,2)
end do
!
!
!
! Motion stage

open(9, file='magrelaxA.txt', status='old')
open(10, file='magrelaxB.txt', status='old')

do k = 0, Nx*Ny-1
   ix = modulo(k, Nx)
   write(9,*) Magmotiona(k,0), Magmotiona(k,1), Magmotiona(k,2)
   write(10,*) Magmotionb(k,0), Magmotionb(k,1), Magmotionb(k,2)
end do

ST = STT(initial = 2)

do t = 0, tmax-1
   call Mag_relax(Magmotiona, Magmotionb, al, ga, dx, Nx, Ny, k, x, y, k, x, z, al, a2, mu_0, Ms, do, 01, ST, dt, t, 0, 5)
   do k = 0, Nx*Ny-1
      write(11,*) Magmotiona(k,0), Magmotiona(k,1), Magmotiona(k,2)
      write(12,*) Magmotionb(k,0), Magmotionb(k,1), Magmotionb(k,2)
   end do
   end do
   close(11)
   close(12)
```

58
REFERENCES


63


