Competing Bulk and Interfacial DMI for designing non-trivial magnetic objects

Submitted by:

Dinesh Beniwal 1811061

Supervised by: Dr. Ajaya Kumar Nayak

Department of Physics

National Institute of Science Education and Research, Bhubaneswar

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Abstract

Symmetry breaking together with strong spin-orbit interaction give rise to many exciting phenomena in condensed matter physics. A recent example is the finding of chiral spin textures, named as magnetic skyrmions, in magnetic systems lacking inversion symmetry. In the last few years, the field of magnetic skyrmion has received enormous attention due to its potential use in the future technology, e.g. racetrack memory, skyrmion driven logic gates, etc. In this report, we discuss various aspects of magnetic skyrmions and the stabilization of novel magnetic objects that not explored yet.

In recent years scientist are trying to stabilize the skyrmions at room temperature for their possible use in spintronics. In general, two main type of skyrmions, Neel-skyrmions and Bloch-skyrmions, have been reported in systems with interfacial and bulk DMI, respectively. In this project report, we utilize micromagnetic simulation to design novel topological spin texture by combining both bulk and interfacial DMI in a single system. For this purpose we use Object Oriented MicroMagnetic Framework (OOMMF) pogram. Two different thin layer, one layer with Interfacial DMI and another layer with Bulk DMI are brought together and their interaction is studied. The two magnetic layers interact via Heisenberg exchange interaction. Interestingly, we are able to stabilize new kind of topological objects with topological number 1.

Chapter 1

Magnetic Interactions

Magnets are existed for a long time and people used them in campus and other instruments. Talking about a brief history, in 1820, Hans-Christian find out that a current caring wire deflects compass needle and this was scientific beginning of magnetism. After some years Michel Faraday discovered electromagnetic induction and in 1864 Maxwell gives us complete relation between electrostatics and magneto-statics by his unified theory of electricity, magnetism and light.

$$\Delta.\mathbf{E} = \frac{\rho}{\epsilon_o} \tag{1.1}$$

$$\Delta.\mathbf{B} = 0 \tag{1.2}$$

$$\Delta \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{1.3}$$

$$\Delta \times \mathbf{B} = \mu_o \mathbf{j} + \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} \tag{1.4}$$

1.1 Magnetostatics

We will start with classical physics of the magnetic fields, forces and energies associated with distributions of magnetic material. Magnetostatics refers to study the magnetism without time dependence.

1.1.1 The magnetic dipole moment

Magnetic moment **m** is the elementary quantity in solid state magnetism. On an atomic scale, intrinsic magnetic moments are associated with its orbital motion around the nucleus. In classical electromagnetism we can equate this with a current loop. If there is a current I around an elementary oriented loop of area **dS** then the magnetic moment **dm** is given by

$$\mathbf{dm} = I\mathbf{dS} \tag{1.5}$$

magnetic moment has the units of $A.m^2$. Simplifying using Ampere's law one can write

$$m = IA \tag{1.6}$$

Coming back to atomic magnetic moment we can define the local magnetization $\mathbf{M}(\mathbf{r}, \mathbf{t})$ as the time-averaged magnetic moment δm in a mesoscopic volume δV is

$$\delta m = \mathbf{M}\delta V \tag{1.7}$$

This magnetization also known as spontaneous magnetization $\mathbf{M_s}$ within a ferromagnetic domain. Magnetic moment and magnetization are axial vectors. They are unchanged under spatial inversion, $r \to -r$, but they do change sign under time reversal $t - t$.

1.1.2 Magnetic field (B)

Firstly magnetic field are observed by the magnets and proposed that the field via magnets are interacting are called magnetic fields. As magnets always have two poles and we have not yet found a magnetic mono pole implies that magnetic fields does not have any source and sink like electric field have. Hence as given by Maxwell's equation that the divergence of magnetic field is equal to zero.

$$\nabla.\mathbf{B} = 0 \tag{1.8}$$

Sources of the B-field are:

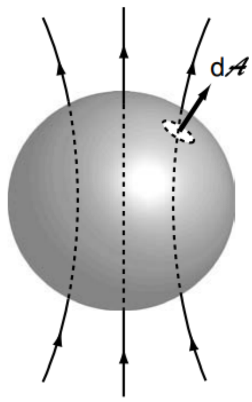

FIGURE 1.1: The B field is divergence-less, with no sources or sinks

- Electric current flowing in conductors.
- Moving charges
- Magnetic moments

Now as mentioned above electric fields are source of magnetic field, so the relation between the magnetic flux density **B** and the current density **j** is given by Maxwell's equation:

$$\nabla \times \mathbf{B} = \mu_o \mathbf{j} \tag{1.9}$$

The interactions happens between electric charges, currents and magnetic moments in space is by electric and magnetic fields. The fields provide the connection between charges, moments and currents, transferring information at the speed of light. All the sources of **B** are moving charges. So magnetic field interact with charges only when they move. So the fundamental force on a charged particle by electric and magnetic field is given by Lorentz law.

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \tag{1.10}$$

Uniform magnetic fields can also be generated, such as by a long solenoid, Helmholtz coils and a Halbach cylinder.

1.1.3 The H-field

H-field is known as the magnetic field strength or magnetizing force. When magnetic field(**B**) is passed through the material, it interact with the material (as atoms have moving electrons and other magnetic properties). So the resulted magnetic field in the material is given as:

$$\mathbf{H} = \mathbf{B}/\mu_o - \mathbf{M} \tag{1.11}$$

here symbols have same meaning as defined in the above sections. In the vacuum, there is no atoms so magnetization becomes zero and trivially:

$$\mathbf{H} = \mathbf{B}\mu_o \tag{1.12}$$

Now this new field(H) is no longer divergence-less, as a matter of face it's divergence is given as:

$$\nabla.\mathbf{H} = -\nabla.\mathbf{M} \tag{1.13}$$

In a greater analogy with electric field this field can be analogous with electric field and magnetic poles can be analogous with electric charges. For more detailed description refer to references [5].

1.1.4 The demagnetizing field

As described in above section that **H** can be treated as electric field of magnetism. So they have to start from a pole and end on another pole. Let's see the case of a bar magnet(Fig[2.2]). We see that the H lines, radiating out from the north pole and ending at the south pole and which is opposite of B field inside the magnet, thus tends to demagnetize the magnet. This is known as self demagnetization and field is call demagnetizing field.

The demagnetizing field $\mathbf{H_d}$ acts in the opposite direction to the magnetization **M** which creates it. The demagnetizing field $\mathbf{H_d}$ of a body is proportional to the magnetization

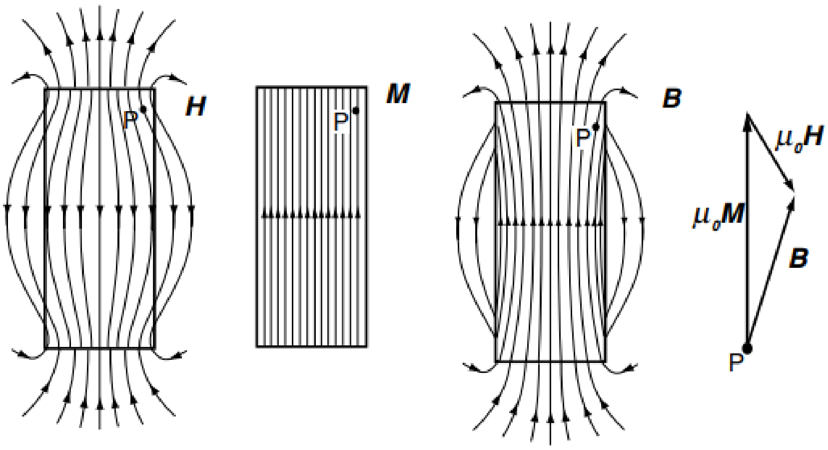

FIGURE 1.2: H, M, B for a magnet

which creates it:

$$\mathbf{H_d} = -N_d\mathbf{M} \tag{1.14}$$

here N_d is the demagnetizing factor. The value of N_d depends mainly on the shape of the body.

1.1.5 Permeability and susceptibility

In free space there is no magnetization, so the the magnetic field is linearly related to H field as:

$$\mathbf{B} = \mu_o\mathbf{H} \tag{1.15}$$

here $\mu_o = 4\pi \times 10^{-7}Hm^{-1}$ is the **permeability of free space**.

In the special case that the magnetization **M** is linearly related to magnetic field **H**, the solid is called linear material and the relation can be written as:

$$\mathbf{M} = \chi\mathbf{H} \tag{1.16}$$

here χ is a dimensionless quantity called the **magnetic susceptibility**. In this special case there is still a linear relation between **B** and **H**,:

$$\mathbf{B} = \mu_o(1+\chi)\mathbf{H} \tag{1.17}$$

$$\mathbf{B} = \mu_o\mu_r\mathbf{H} \tag{1.18}$$

here $\mu_r = 1 + \chi$ is the relative permeability of the material. Magnetic susceptibility is the degree to which a material can be magnetized in an external magnetic field. Based on the value of magnetic susceptibility(χ) that a material exhibits, we have different types of magnetic materials:

- χ is small and negative, it is known as diamagnetic.

- χ is small and positive, it is known as paramagnetic.
- χ is very large and positive, it is known as ferromagnetic.

1.2 Quantum picture of Magnetism

The magnetic moments in solids are associated with electrons. The microscopic theory of magnetism is based on the quantum mechanics of electronic angular momentum, which has two distinct sources – orbital motion and spin. They are coupled by the spin–orbit interaction. The description of magnetism in solids is fundamentally different depending on whether the electrons are localized on ion cores or delocalized in energy bands. Free electron leads to temperature independent Pauli para-magnetism and Landau diamagnetism and localized non-interacting electrons exhibit curie para-magnetism.

1.2.1 Orbital and spin moments

The electron is an elementary particle which has two distinct sources of angular momentum, one is associated with orbital motion around the nucleus, the other is spin.

Orbital moment

According to Bohr model the electron revolve around the nucleus, An circulating electron can be treated as current loop. So the magnetic moment associated with the current loop is $m = IA$, in the term of angular momentum $l = m_e\mathbf{r} \times \mathbf{v}$, the magnetic moment is related with angular momentum as:

$$\mathbf{m} = -\frac{e}{2m_e}\mathbf{l} \tag{1.19}$$

The orbital angular momentum is quantized quantity, so quantized magnetic moment is:

$$m_z = -\frac{e}{2m_e}m_l\hbar \tag{1.20}$$

here $\mu_B = e\hbar/2m_e$ is the Bohr magneton.

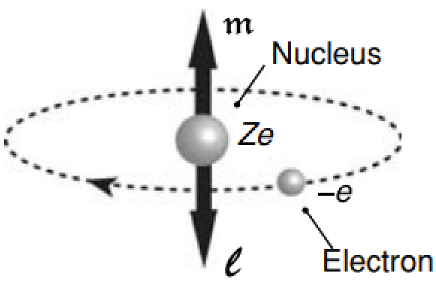

FIGURE 1.3: The electron moves in a circular orbit where its quantized angular momentum $\mathbf{l}$ and magnetic moment $\mathbf{m}$ are oppositely directed.

Spin moment

Electron have an intrinsic momentum of its own which is defined as spin moment of the electron. The name should not be confused as electron does not around its own axis(as it is point like particle and electron have to rotate faster than speed of light to generate observed momentum), the name is just as strange as quantum physics. It have quantum number s=1/2. The spin magnetic momentum have mathematical form:

$$\mathbf{m} = -\frac{e}{m_e}\mathbf{s} \tag{1.21}$$

The spin magnetic quantum number is $m_s = \pm 1/2$.

1.2.2 Spin-orbit coupling

Spin and angular momentum are vector quantities so, we can have vector superposition of them. After coupling by spin-orbit interaction we call it total angular momentum $\mathbf{j}$ defied as

$$\mathbf{m} = -\frac{e}{2m_e}\mathbf{j} \tag{1.22}$$

The interaction for a single electron is represented by the spin-orbit Hamiltonian:

$$H_{so} = \lambda \mathbf{l}.\mathbf{s} \tag{1.23}$$

here λ is the spin orbit coupling energy.

1.3 The free electron model

Now there are a lot of ways matter can interact with magnetic fields. Atom's surrounding effects its interaction with external and internal field. So while doing this project we limited ourselves to metals and other magnetic materials. As we know metals follow quit the free electron model, so we will be briefly discuss that in this and coming sections.

The electron are considered as free particle but they can not escape from atom so the electrons are described as non-interacting waves confined in a box of dimension L. The Hamiltonian have both kinetic and potential terms

$$H = \frac{p^2}{2m_e} + V(r) \tag{1.24}$$

As momentum vector $\mathbf{p}$ is can be written as $\mathbf{p} = \hbar\mathbf{k}$ the above equations solution i.e. energy can be projected on k-space where each point will represents a possible state for the electrons in a free-electron gas contained in the box. All electrons try to occupy the lowest available energy states, we get a sphere of radius k_f,the Fermi wave-vector. Similarly the energy of last electron is called Fermi energy and given as $\epsilon_f = (\hbar^2/2m_e)(3\pi^2 n)^{2/3}$. Each state have two-fold spin degeneracy. The density of states for either spin is given as:

$$D(\epsilon) = (1/4\pi^2)(2m_e/\hbar^2)^{2/3}\epsilon^{1/2} \tag{1.25}$$

by above equation we observed that density of states does not depend on L or shape of the box.

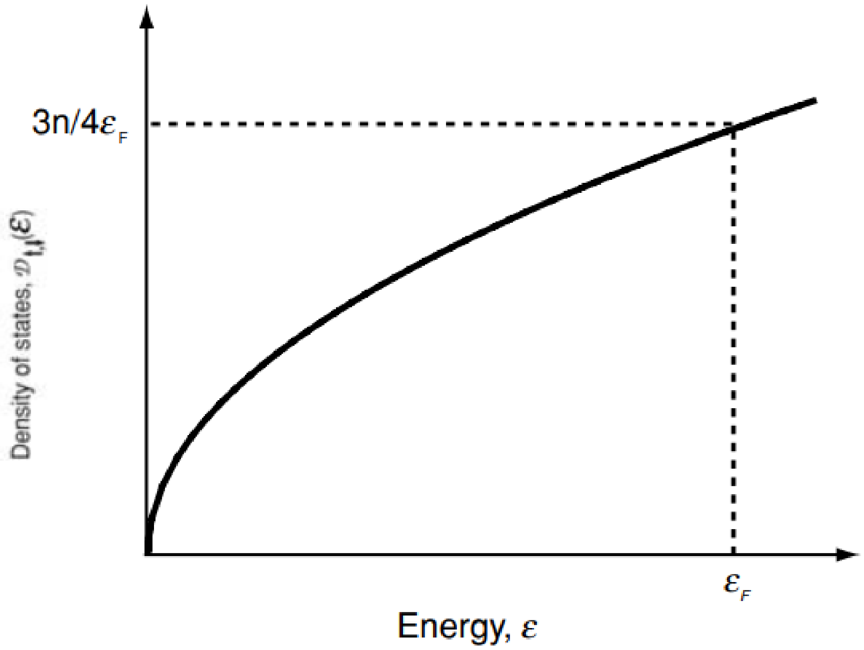

FIGURE 1.4: Density of up or down states in the free-electron model

1.4 Pauli paramagnetism

The effect of an external magnetic field on the metals is described by the Pauli. The interaction of metal and effects due to that interaction are described in this section. Magnetic field **B** can shift spin momentum into two sub-bands by $\pm\mu_b B$. This is because magnetic field try to align magnetic moments to external field. Applied external field gives rise to energy of electrons whose spin is parallel to field and lower the energy of the electrons whose spin anti-parallel to field[Fig[2.5]]. The magnetic susceptibility is given by:

$$\chi_p = 2\mu_o\mu_B^2\mathbf{D}(\epsilon_f) \tag{1.26}$$

1.5 Exchange Interactions

Till now we have seen the origin of magnetic moment from electrons, what are its properties, what are the different types magnetic fields, how magnetic moment interact with these fields. After that we move on to metals and behaviours of electrons in the

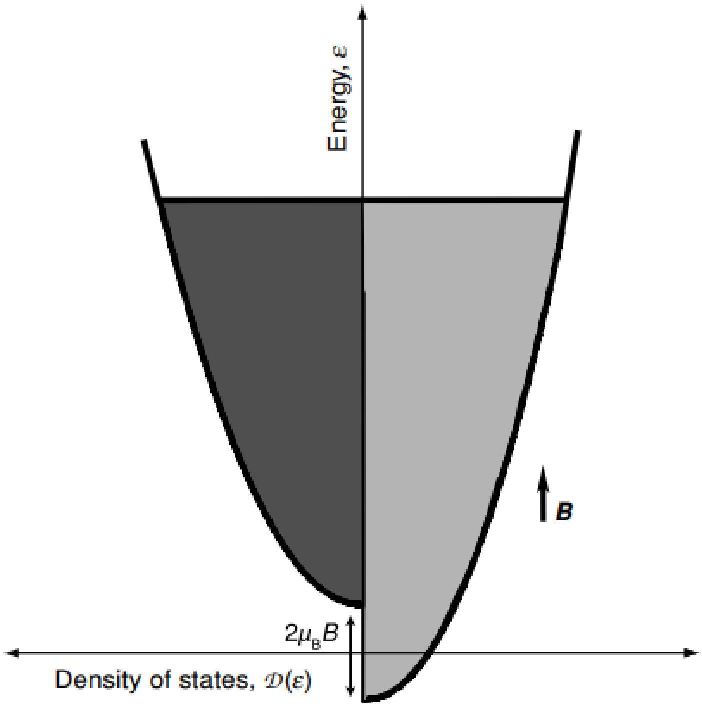

FIGURE 1.5: Spin splitting of the ↑ and ↓ densities of states in a magnetic field. A net moment results from the transfer of electrons at the Fermi level from the ↓ to the ↑ band

metals. In this section we will see how those atoms and electron interact with other atoms and electrons in the material. These interactions allows the magnetic moments in a solid to communicate with each other.

Exchange interactions are the core phenomenon of long range magnetic order. A ferromagnet is characterized by a a spontaneous magnetization associated with long range magnetic ordering. The energy of a magnetic system have different terms corresponding to different interactions of the magnetic moments with an external field, the crystal lattice and with the other magnetic moments. Equilibrium magnetization structures are found by minimizing the total energy of a system.

We consider an ensemble of N atoms on a lattice with lattice constant a. Each atom have a net magnetic moment $\mathbf{m_i} = \mathbf{M_i}/M_s$, here M_s is the saturation magnetization. The magnetic moment can be defined by atomic spin $\mathbf{S_i}$ as $\mathbf{M_i} = -g\mu_B\mathbf{S_i}$. The total energy of the assembly of spins in its atomic form is given by:

$$E = E_{ex} + E_{DM} + E_Z + E_{ani} \tag{1.27}$$

here E_{ex} is the isotropic exchange energy, E_{DM} is the DMI exchange energy, E_Z is the Zeeman energy, and E_{ani} the anisotropy energy.

1.5.1 Dipole-dipole interaction

In ferromagnetic materials, magnetic dipoles generate the demagnetization field $\mathbf{H_d}$ to minimize overall energy and surface charge/poles. The average energy density of the dipole-dipole interaction can be expressed as:

$$E_{DDI} = -\frac{\mu_o}{2}\mathbf{M}.\mathbf{H_D}\mathbf{DI} \tag{1.28}$$

[10]

1.5.2 Heisenberg exchange

The Heisenberg exchange interaction is due to overlap of electronic orbitals. The energy between two neighbouring sites can be expressed as:

$$E_i = -2J_{ij}\mathbf{m_i}.\mathbf{m_j} \tag{1.29}$$

here J_{ij} is the exchange integral between sites i and j. It decreases rapidly as a function of distance so this is a short range interaction. This exchange is known as ferromagnetic if it favours parallel spins, i.e.,if $J_{ij} > 0$, and antiferromagnetic if $J_{ij} < 0$, which favours anti-parallel spins. The total isotropic exchange energy of a system of N interacting spins is expressed as:

$$E_{ex} = -\sum J_{ij}\mathbf{m_i}.\mathbf{m_j} \tag{1.30}$$

In the continuum limit, Heisenberg exchange is expressed as:

$$E_{ex} = \int dV.A.((\Delta m_x)^2 + (\Delta m_y)^2 + (\Delta m_z)^2)) \tag{1.31}$$

here $A = J_{ex}n/a$ is the exchange constant(in units of J/m) with n number of atoms per unit cell. Fig[1.1] have more illustration of Heisenberg interaction.

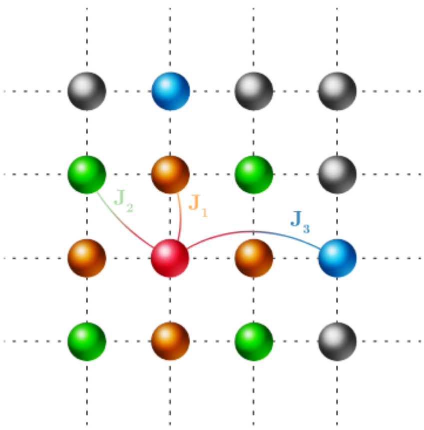

FIGURE 1.6: A simple cubic lattice, where J_1 is the isotropic exchange coupling between nearest neighbours, J_2 is between next-nearest neighbours, and J_3 is between next-next-nearest neighbours. Unless the exchange is frustrated, we restrict ourselves to nearest-neighbour interactions.[2]

1.5.3 Direct exchange

When neighbouring magnetic atoms interact via an exchange interaction, this is known as direct exchange. For this interaction the overlapping between two atoms must be sufficient because in some cases this interaction is not so common as there is insufficient direct overlap. Due to this reason direct exchange does not lead to the observed magnetic properties. This shows that the role of conduction electrons should not be neglected.

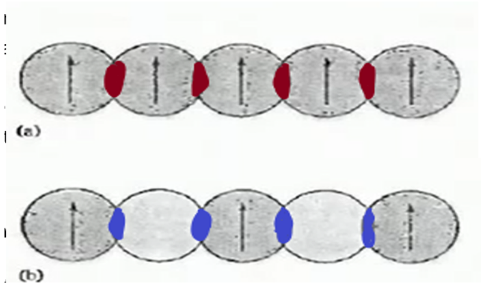

FIGURE 1.7: (a)Direct exchange as two magnetic atoms are overlapping directly and (b)Super exchange as there is still exchange even though two magnetic atoms are not overlapping.

1.5.4 Super exchange

This is also known as indirect exchange. A number of ionic solids, some oxides and fluorides shows magnetic properties. For example MnO and MnF_2 are both antiferromagnets. There is no direct overlap between the electron of Mn ions but they still show magnetic properties. This can explained by super exchange when two metal ions interact even when they have one non-metal atom in between them.

It can be defined as an indirect exchange between non-neighbouring magnetic ions. Fig[2.7] shows the positing and overlapping in direct and super exchange. Super exchange arises because there is a kinetic energy advantage for anti-ferromagnetism which is shown in Fig[2.8]. In some cases super exchange can be ferromagnetic.

1.5.5 RKKY interaction

In metals the exchange interaction between magnetic ions can be mediated by the conductive electrons.A localized magnetic moment spin-polarizes the conduction electrons and this polarization in turn couples to a neighbouring localized magnetic moment a distance r away[Fig.[2.9(a)]]. This interaction is also indirect interaction. RKKY interaction was discovered by the Ruderman, Kittel, Kasuya and Yosida.

The RKKY interaction which describes the interaction between two local impurity spins at the positions i and j in the form of an XYZ-type effective exchange Hamiltonian,

$$H_{RKKY} = J_x^{ij}(S_i^x S_j^x + S_i^y S_j^y) + J_z^{ij} S_i^z S_j^z \tag{1.32}$$

for 2D metals case

$$H_{RKKY} = J_n^{ij} \mathbf{S_i}.\mathbf{S_j} \tag{1.33}$$

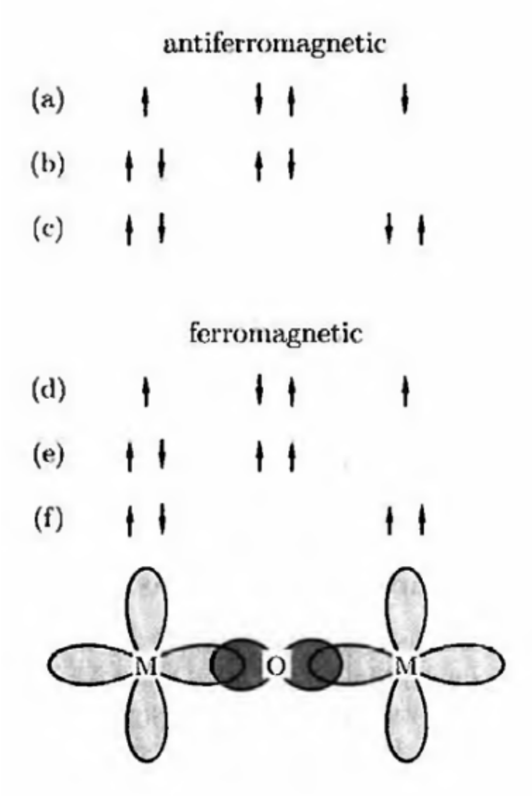

FIGURE 1.8: Super exchange in a magnetic oxide. If the moments on the transition metal atoms are coupled anti-ferromagnetically, the ground state is (a) and this can mix with excited configurations like (b) and (c). The magnetic electrons can thus be delocalized over the M-O-M thus lowering the kinetic energy. If the moments on the metal atoms are coupled ferromagnerically, the ground state(d), can not mix with excited states like (e) and (f) because these configurations are prevented by the Pauli exclusion principle [1]

here the J is r-dependent exchange and which is given as

$$J_{RKKY} \propto \frac{cos(2k_F r)}{r^3} \tag{1.34}$$

This interaction is a long rang interaction and has an oscillatory dependence on the distance between the magnetic moments. Hence depending on the separation it may be either ferromagnetic or anti-ferromagnetic[Fig[2.9(b)]].

1.5.6 Double exchange

While discussing super exchange we mentioned that some oxides can have ferromagnetic interaction. It occurs when magnetic ion have mixed valency i.e it can exist in more than one oxidation state. Fig[2.10] have an example of double exchange.

1.5.7 The Dzyaloshinksii-Moriya Interaction (DMI)

In the low symmetry crystals a interaction arises due to spin orbit coupling(SOC), which is known as Dzyaloshinksii-Moriya Interaction (DMI). The total DMI energy of a system

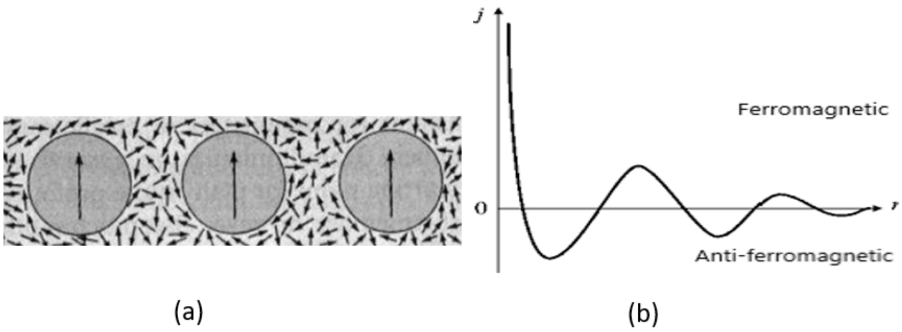

FIGURE 1.9: (a) the configuration of free electrons and atoms in the material. (b) how RKKY interaction change the properties of material based on the distance between two nearby interaction.

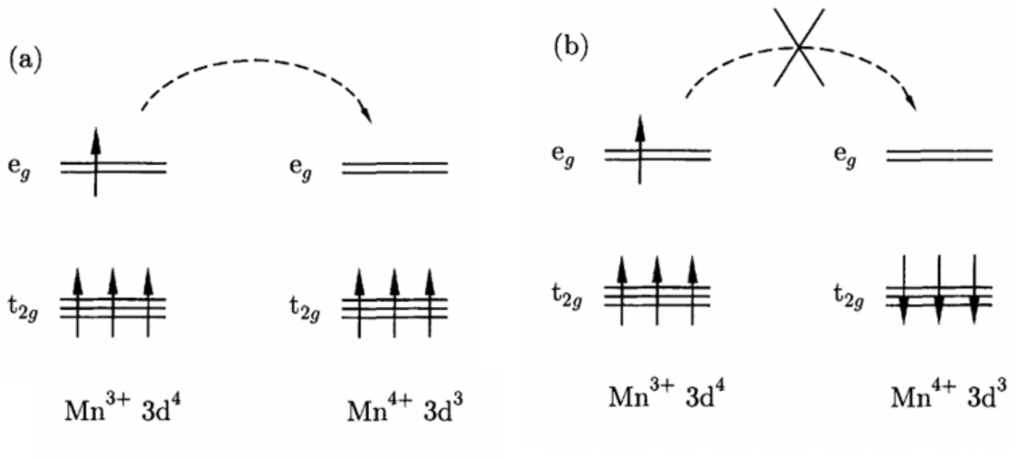

FIGURE 1.10: Double exchange mechanism gives ferromagnetic coupling between Mn^{3+} and Mn^{4+}. The single-centre exchange interaction favours hopping if (a) neighbouring ions are ferromagnetically aligned and no if (b) neighbouring ions are antiferromagnetically[1]

of N interacting spins is expressed as

$$E_{DMI} = -\sum \mathbf{D_{ij}}.(\mathbf{m_i} \times \mathbf{m_j}) \tag{1.35}$$

The DMI vector $\mathbf{D_{ij}}$ is dictated by the crystal symmetry. Under an inversion operation where the midpoint of two sites, $\mathbf{m_i}$ and $\mathbf{m_j}$ are exchanged, the energy consequently flips sign, which demonstrates the broken inversion symmetry. If two spins are lying in the plane normal to $\mathbf{D_{ij}}$ and perpendicular to each other gives minimum DMI energy.

As a consequence, the DMI tends to rotate spins with respect to other interactions and thus creating non-collinear magnetic configurations, such as skyrmions. In non-centrosymmetric magnets and/or interfacially asymmetric multilayers we have a broken(spatial) inversion symmetry. The broken inversion symmetry in these material systems leads to a noncollinear Dzyaloshinskii-Moriya interaction.

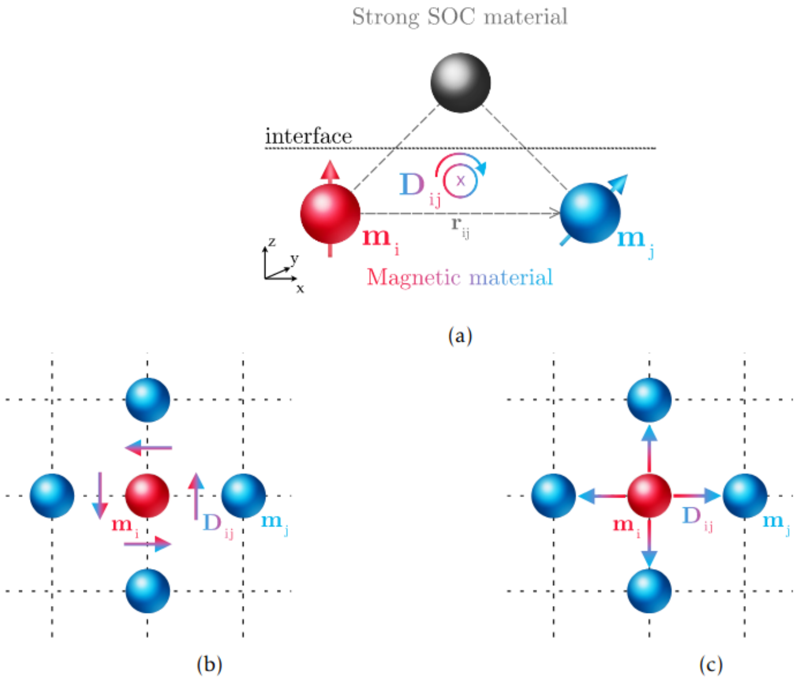

FIGURE 1.11: (a) DMI induced by the vertical breaking of the inversion symmetry along z at an interface between a magnetic material and a material exhibiting strong spin-orbit coupling. (a) and (b) show different symmetries of the DMI in the xy-plane on a simple square lattice. (b) In the case where the DMI is induced at an interface via breaking of the inversion symmetry along z, the **D**-vector is orthogonal to the displacement vector between neighbouring sites. (c) In bulk materials with horizontal breaking of the inversion symmetry induced by the crystal lattice, the **D**-vector is collinear to the displacement vector between neighbouring sites.[2]

Fig[2.11(b and c)] shows directions of D vector in different cases. In the continuum approximation DMI with symmetry breaking along z can be written as:

$$E_{DM} = \int dV.D.([m_z \frac{\partial m_x}{\partial x} - m_x \frac{\partial m_z}{\partial x}] + [m_z \frac{\partial m_y}{\partial y} - m_y \frac{\partial m_z}{\partial y}]) \tag{1.36}$$

here D is the DMI constant (in the unit of J/m^2).

1.6 Magnetic order and types of magnetic materials

From the previous section we have known the different types of magnetic interaction which operate between magnetic moments. Based on those interaction different types of magnetic materials have different type of arrangement of their magnetization and also react differently to the external field. In this section we will go through all those details.

1.6.1 Ferromagnetism

A ferromagnet has a spontaneous magnetization even in the absence of applied field. All the magnetic moments align in the one direction. This phenomena is called ferromagnetism and the material is described as ferromagnetic material. The Hamiltonian of ferromagnet in the external applied magnetic field is given by:

$$\mathbf{H} = -\sum_{ij} J_{ij}\mathbf{S_i}.\mathbf{S_j} + f\mu_B \sum_{j} \mathbf{S_j}.\mathbf{B} \tag{1.37}$$

and we know that in the case of ferromagnet the exchange constant J will be always positive and ensure the ferromagnetic alignment. The first term in the Hamiltonian is Heisenberg exchange energy. Magnetic susceptibility of ferromagnetic materials is given by:

$$\chi = \propto \frac{1}{T - T_c} \tag{1.38}$$

This is known as **Curie Weiss law**.

1.6.2 Antiferromagnetism

A antiferromagnet also have spontaneous magnetization. Here also all magnetic moments align in one direction but all the neighbour magnetic moments have opposite direction with respect to that moment. So the exchange interaction constant(J) is negative due to that the molecular field is oriented such that it is favourable for nearest neighbour magnetic moment to lie antiparallel to on another. This is called antiferromagnetism and the material is called antiferromagnetic material.

Fig[2.12] shows the configuration and arrangement of magnetic moments in the ferromagnetic, antiferromagnetic and ferrimagnetic materials.

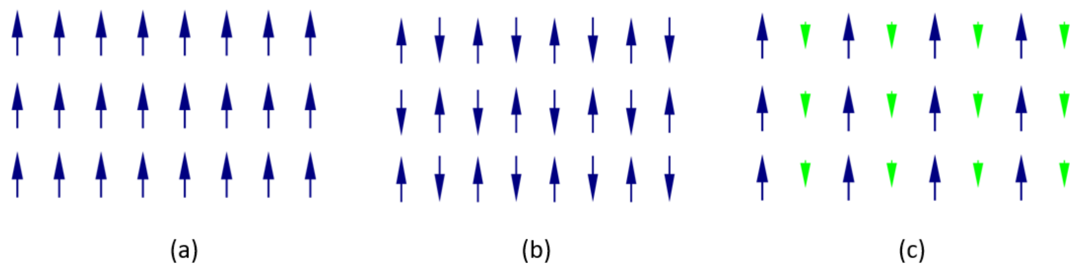

FIGURE 1.12: Arrangement of magnetic moments in the (a) Ferromagnetic, (b) Antiferromagnetic and (c) Ferrimagnetic materials.

1.6.3 Ferrimagnetism

In the antiferromagnetism two oppositely align magnetic moments have same magnitude. But in some materials the two magnetic moments align as antiferromagnetically but does not have same magnetization. Therefor they will not cancel out each other and we have a net magnetization. This phenomenon is known as ferrimagnetism and these materials are called ferrimagnetic materials. The magnetic susceptibilities of ferrimagnets do not follow the Curie Weiss law.

1.7 Micromagnetism

The basic premise of micro-magnetism is that a magnet is a mesoscopic continuous medium where atomic-scale structure can be ignored. A ferromagnet is characterized by a a spontaneous magnetization associated with long range magnetic ordering. The energy of a magnetic system have different terms corresponding to different interactions of the magnetic moments with an external field, the crystal lattice and with the other magnetic moments. Equilibrium magnetization structures are found by minimizing the total energy of a system. In ferromagnetic materials domains tend to form in the lowest energy state.

1.7.1 Micromagnetic energy

To get the most stable structure of material one should have minimum micromagnetic energy which have many components and can be written as:

$$E_{total} = E_{ex} + E_{ani} + E_{demag} + E_z + E_{stress} + E_{ms} \tag{1.39}$$

here first energy term is due to exchange interactions, second term E_{ani} is magnetocrystalline anisotropy energy, E_{demag} is demagnetizing field, E_z is due to applied external field and known as zeeman energy and the last terms are due to applied stress and magnetostriction.

Exchange energies are discussed in the exchange interaction section and demagnetizing field is also discussed In this section we will discuss the rest of the energies.

1.7.1.1 Anisotropy

There are some favourable axes in the magnetic material in which magnetization can be aligned along. The is known as magneto-crystalline anisotropy and energy associated with this is known as anisotropy energy. The spin interact with the orbital motion as SOC and the orbital motion interacts with the crystal as electrostatic fields and overlapping wave functions of neighbouring atoms, hence gives the following form:

$$E_{ani} = -K_u \sum_{i=1}^{N} (\mathbf{m_i}.\mathbf{e_{ani}})^2 \tag{1.40}$$

here $K_u > 0$ is the anisotropy constant and $\mathbf{e_{ani}}$ is easy axis. In the continuum form:

$$E_{ani} = -K_u \int dV (\mathbf{m}.\mathbf{e_{ani}})^2 \tag{1.41}$$

here K_u takes units of J/m^3. [2] Fig[2.13] shows the results from the interplay of uniaxial anisotropy and demagnetizing field.

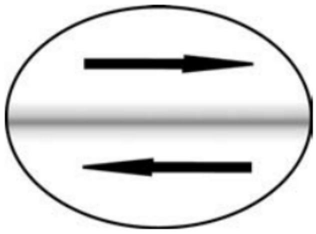

FIGURE 1.13: A ferromagnetic domain state resulting from the interplay of uniaxial anisotropy and demagnetizing field. The domain wall is the shaded region [5]

1.7.1.2 Zeeman Energy

Zeeman energy comes into picture when system interact with external magnetic field.

$$E_z = -M_s \sum_{i=1}^{N} \mathbf{m_i}.\mathbf{B} = 1 \tag{1.42}$$

Zeeman energy is minimum when all magnetic moments are song the external field. In the continuous form

$$E_z = -M_s \int dV \mathbf{m}.\mathbf{B} \tag{1.43}$$

1.7.1.3 Strain

An external stress σ_{ij} applied to a sample introduces a strain term in the energy:

$$E_{stress} = -\sigma_{i,j}\sigma_{ij}\epsilon_{ij} \tag{1.44}$$

where $\epsilon_{ij} = m_{ijkl}H_kH + l$ is the magneto-elastic strain tensor.

1.7.2 Domain theory

The micro-magnetic approach is capable, in principle, of predicting the equilibrium magnetic configurations of any system but the calculation are complex. Domain theory is an attempt to reduce this complexity. Domain in the ferromagnetic materials are defined as a large regions of uniform magnetization in macroscopic sample. These regions are separated by domain walls. An applied field changes the net magnetization of the sample either by causing the walls to move or in case of high amplitude magnetic field by rotating the magnetization of domains.

Bloch wall and Neel wall

A domain wall is classified as **Bloch wall** when rotation of magnetic moments are perpendicular to the plane. In the Bloch wall the divergence of the magnetization is zero. On the other hand **Neel wall**, where the magnetization rotates within the plane of the domain magnetization. Fig[2.14] shows the Bloch and Neel walls. Generally Neel wall have higher energy then Bloch wall. Neel wall is favoured in thin films.

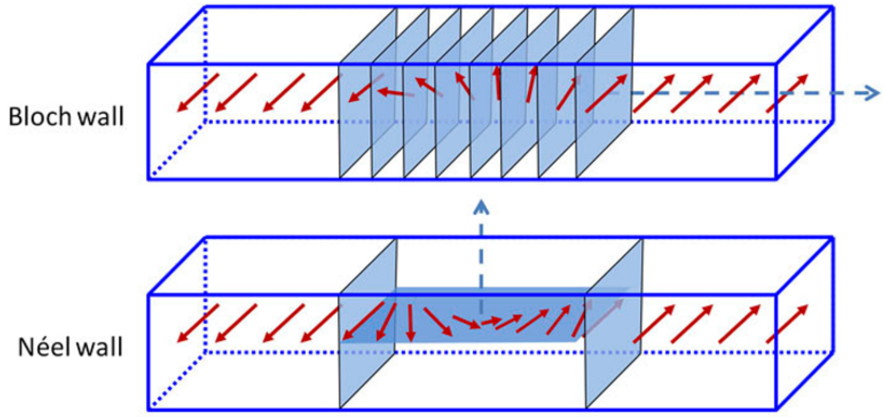

FIGURE 1.14: Bloch and Neel wall

1.7.3 Landau-Lifshitz-Gilbert equation

LLG equation in ferromagnetic material or Time evolution of magnetization in a ferromagnetic material is given as:

$$\frac{d\mathbf{M}}{dt} = -\gamma'\mathbf{M} \times \mathbf{H}_{eff} - \lambda\mathbf{M} \times (\mathbf{M} \times \mathbf{H}_{eff}) \tag{1.45}$$

here γ is the gyro-magnetic ratio, and α is the magnetic damping parameter and $\lambda = \alpha\gamma$. Here the first term causes the precession of $\mathbf{M}$ around $\mathbf{H}_{eff}$ and second term is the damping term.

$$\mathbf{H}_{eff} = \mathbf{H}/M_s + \mathbf{H}_{ani} + \mathbf{H}_{ex}$$

here the terms represents the same physical quantities as mentions in the above sections. LLG equation gives us the time evolution of magnetization due to all the factors interacting like anisotropy, DMI, exchange and external field. In our project we studied the skyrmions and the LLG equation is the best fit for see the effect of all the factors in the creation, annihilation and moving the skyrmions.

1.8 The Objected Oriented Micro-Magnetic Framework Simulation(OOMMF)

In this project all the simulations to study the skyrmions are performed using OOMMF simulations. The OOMMF is a public domain micromagnetics program developed at the National Institute of Standards and Technology. Our simulations are carried out by a set of the OOMMF extensible solver objects of the standard OOMMF distribution. We also include several OXS extension modules in order to model, for examples, the Bulk-DMI.

Basically in the OOMMF after giving all the parameters like Heisenberg exchange, DMI, anisotropy, Zeeman field, its evolver solves the LLG equation by Runge-kutta method. It can provide us real time evolution of magnetization, energy and many other parameters [3].

Chapter 2

Magnetic Skyrmion

> "**Magnetic skyrmions** are quasiparticles which have been predicted theoretically and observed experimentally in condensed matter systems. Skyrmions can be formed in magnetic materials in their 'bulk' such as in MnSi, or in magnetic thin films. They can be achiral, or chiral in nature, and may exist both as dynamic excitations or stable or meta-stable states [8]"

A magnetic skyrmion is the smallest possible perturbation to a uniform magnet: a point like region of reversed magnetization, surrounded by a whirling twist of spins. These quasiparticles do not exist in the absence of a magnetic state and their electrodynamics cannot be described by Maxwell's equations.

2.1 Discovery of Skyrmion

Skyrmions are named for British nuclear physicist Tony Skyrme, who first proposed their existence in 1961. It was discovered as effort to explain subatomic particles like protons and neutrons using convoluted twists in the quantum field that all particles possess. After all that theory was dropped but idea came into light when those topological structures observed in magnetic materials. In a magnetic skyrmion, the knotted magnetic field lines wrap around one another like key rings hooking into other key rings, crating a nanometer-scale shape [7].

2.2 Topological physics of magnetic skyrmion

If two spins are lying in the plane normal to $\mathbf{D_{ij}}$ and perpendicular to each other gives minimum DMI energy. Heisenberg exchange favors parallel/anti-parallel spin configurations. As a result of competition between DMI and Heisenberg exchange, the neighboring-spins thus extend a finite angle with respect to each other. This argument is known as Derrick's argument and gives us the emergence of magnetic skyrmion.

For magnetic multi layers with interfacial DMI, the electric current passing through the heavy metal layer injects a perpendicular spin current into the adjacent magnetic thin layer via the spin Hall effect. That causes skyrmion to move in the material. The complete magnetization evolution can be studied by a **Landau-Lifshitz-Gilbert(LLG)** equation:

$$\frac{\mathbf{dm}}{\mathbf{dt}} = -\gamma \mathbf{m} \times \mathbf{H}_{eff} + \alpha \mathbf{m} \times \frac{\mathbf{dm}}{\mathbf{dt}} + \frac{g\mu_B}{2eM_s}[(\mathbf{j_1}.\Delta)\mathbf{m} + \frac{\theta_{SH}}{t_f}\mathbf{m} \times (\mathbf{m} \times (\hat{z} \times \mathbf{j_e}))] \quad (2.1)$$

where γ is the gyro-magnetic ratio, and α is the magnetic damping parameter. $\mathbf{H_{eff}} = \frac{\partial F}{\partial(M_s \mathbf{m})}$, with F the magnetic free energy and M_s the saturation magnetization, is the effective field containing the external magnetic field and spin interaction. First term in bracket is the STT where $\mathbf{j_1}$ is electrical current density. The second term is spin Hall spin torque, where θ_{SH} is the spin Hall angle, $\hat{z}$ is the plane normal, t_f is the film thickness, and $\mathbf{j_e}$ is the density of electron current floating in the heavy metal, layer. [4]

The structures of skyrmions stabilized by DMI are not only limited to Bloch and Neel-type, it also stabilizes all types of skyrmion intermediate states, antiskyrmions etc. There are other mechanisms by which spin textures can be stabilized like frustrated exchange interactions, four-spin exchange interactions and long-range dipolar interactions. But for our project we will focused on the systems with DMI stabilized materials.

2.3 Types of Skyrmions

Generally in condensed matter physics, skyrmion are defined as being any spin structure in which the center magnetization is in opposite direction to its boundary and which can be mapped once to the sphere. So, by the definition skyrmion is characterized by two quantities, its radial profile and the twisting angle.

Another classification of spin structures can be based on their topology, defined by their skyrmion number which is given by as

$$n = \tfrac{1}{4\pi} \int \mathbf{M} \cdot \left(\frac{\partial \mathbf{M}}{\partial x} \times \frac{\partial \mathbf{M}}{\partial y} \right) dxdy \quad (2.2)$$

where n is the topological index, $\mathbf{M}$ is the unit vector in the direction of the local magnetization within the magnetic thin, ultra-thin or bulk film, and the integral is taken over a two dimensional space. Any structure for which n is an integer greater than equal to one, can be qualified as magnetic skyrmions. Fig[1.1] and Fig[1.2] shows different types of spin structures and their topological index.

2.4 Dynamics of Skyrmion

Creation, deleting and manipulating skyrmions can be explained by dynamics of skyrmions.

Creation and Annihilation of skyrmions

There are numerous methods has been discovered over the years to create and annihilate skyrmions. In this section we will walk through some of them. Here are some common methods to write or create a skyrmion.

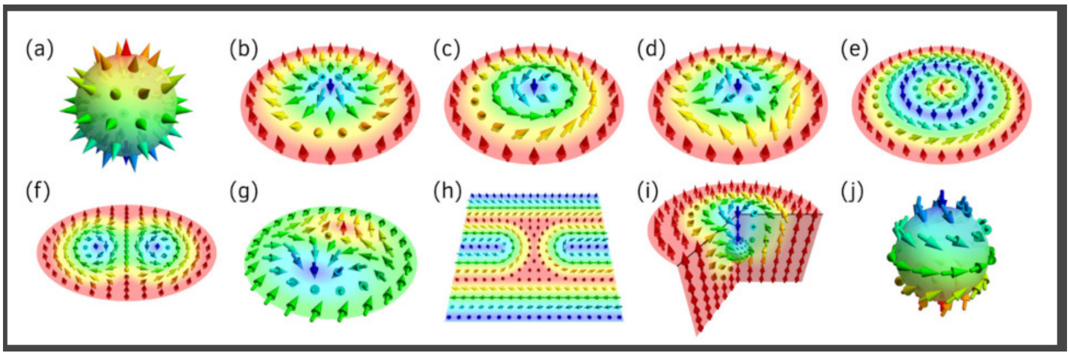

FIGURE 2.1: Zoo of (topological) spin textures with different winding numbers. (a) Hedgehog, (b) Néel-type skyrmion(n=1), (c) Bloch-type skyrmion(n=1), (d) antiskyrmionn=(-1),(e) skyrmionium(n=0), (f) biskyrmion(n=2), (g) example of an in-plane skyrmion(n=1), (h) skyrmion in helical background(n=1), (i) chiral bobber, (j) combed anti-hedgehogformed around the Bloch point in panel.[6]

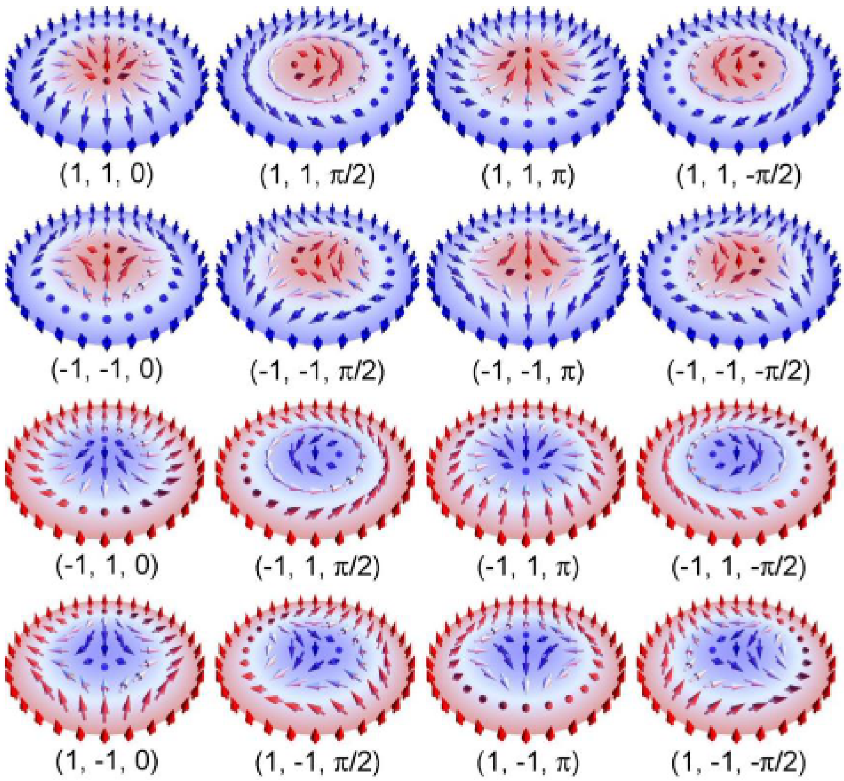

FIGURE 2.2: Illustrations of 2D magnetic skyrmions with different topological charge, vorticity number and helicity number, i.e. (Q, Q_v, Q_h).The arrow denotes the spin direction and the out-of-plane spin component(m_z)is represented by the color: red is out of the plane, white is in-plane, and blue is into the plane.[9]

- Generation by magnetic fields
- Generation by thermal excitations
- Generation by Spin torques

- Generation by electric fields

Moving Skyrmions

Currently the most widely discussed skyrmion-based application is a ”racetrack” type device. For such device shifting of skyrmions is a must condition. These are some methods proposed and experimentally proven methods of shifting skyrmion in the lattice.

- Magnetic field gradients
- Electric field
- Spin torques: Spin transfer and spin orbit torques.
- Magnons
- Temperature gradients

Their detailed description can be found in Ref. [6].

2.5 Application of Skyrmions

Skyrmions is a hot topic among the researcher due to its huge potential in future. Racetrack is the currently center of application of skyrmion. Racetrack memories are based on the idea of storing data by aligning quasi particle nature of magnetic spin states. It is also proposed to used them to build skyrmion based conventional logic devices.

Skyrmion can also be used in spin transfer nano-oscillators. These oscillators are attractive for applications as wide-band nano-scale electrical oscillators, sensitive magnetic field sensors and on-chip microwave signal sources.[6]

Chapter 3

Stabilization of Novel topological objects

Using the OOMMF simulation we first created single Neel and Bloch skyrmions. We studies how they evolve with time and how DMI, anisotropy effects them. After their individual study we created two layer thin film in which one have Interfacial DMI and another have Bloch DMI. This phenomenon never studied before and we encountered frustrated skyrmion like structures. Throughout the whole simulated figure red colour indicates the direction of +z axis(out of the plane).

3.1 Neel skyrmion

In the chapter one we have shown the structure of Neel skyrmion. It has skyrmion number +1. To simulate Neel skyrmion we structured a thin film of configuration $500nm \times 500nm \times 1nm(x-y-z)$. Providing Uniform Heisenberg exchange constant $A = 1.5 \times 10^{-11} J/m$, Anisotropy constant $K = 5 \times 10^5 J/m^3$ and DMI constant $D = 3.4mJ/m^2$.

Initial magnetization of each atom is taken as $M_s = 6 \times 10^5 A/m$. To see the evolution of the film we solved LLD equation by Rungekutta method in OOMMF and Results are shown in Fig[3.1]. Also simulated LTEM image is also shown in Fig[3.2], which is clean as expected and described in the previous chapters.

3.2 Bloch skyrmion

To simulate Bloch skyrmion we structured a thin film of configuration $500nm \times 500nm \times 1nm(x-y-z)$. Providing Uniform Heisenberg exchange constant $A = 1.5 \times 10^{-11} J/m$, Anisotropy constant $K = 5 \times 10^5 J/m^3$ and DMI constant $D = 3.4mJ/m^2$.

Initial magnetization of each atom is taken as $M_s = 6 \times 10^5 A/m$. To see the evolution of structure we solved LLD equation by Rungekutta method in OOMMF and Results are shown in Fig[3.1]. Also simulated LTEM image is also shown in Fig[3.3]

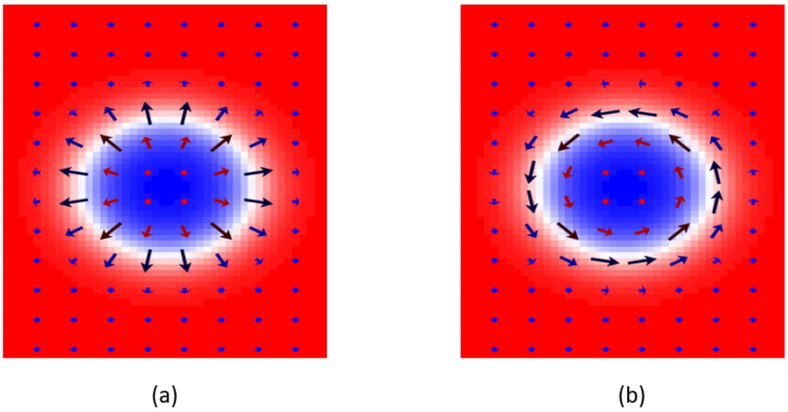

FIGURE 3.1: (a) Neel skyrmion (b) Bloch skyrmion

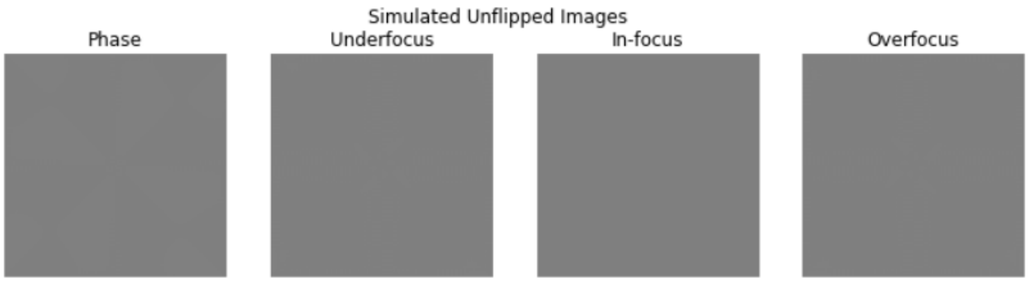

FIGURE 3.2: Simulated LTEM image of Neel Skyrmion

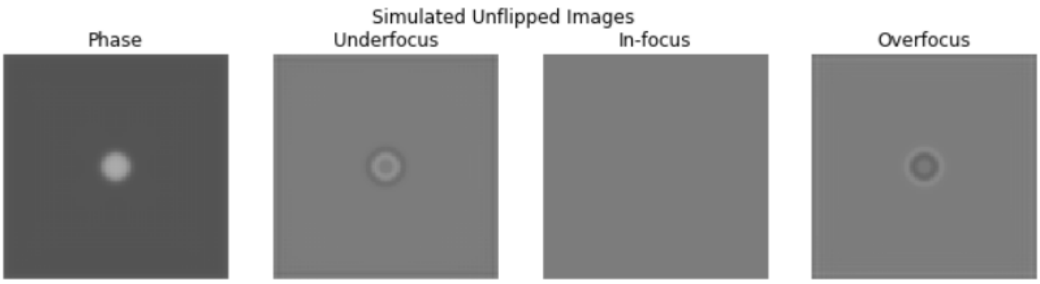

FIGURE 3.3: Simulated LTEM image of Bloch Skyrmion

3.3 Study of single skyrmion in multi-layer(two) thin film

Here we have carried out the results of our main simulation of the project. We introduced the Interfacial and Bloch DMI in two different separated layers and studied the behaviour of skyrmion when these layers only interact via Heisenberg interaction. For the simulation, first we created two identical layers of dimensions $200nm \times 200nm \times 1nm(x-y-z)$. Both layers are placed on top of each other and both have uniaxial Anisotropy constant $K = 4.5 \times 10^5 J/m^3$, Heisenberg constant $A = 1.5 \times 10^-11 J/m$ and initial magnetization of single atom is $M_s = 6 \times 10^5 A/m$. Fig[3.5] shows the described configuration for this experiment. First layer have Neel DMI ($D = 3.2mJ/m^2$) and second layer have Bulk DMI ($D = 3.2mJ/m^2$).

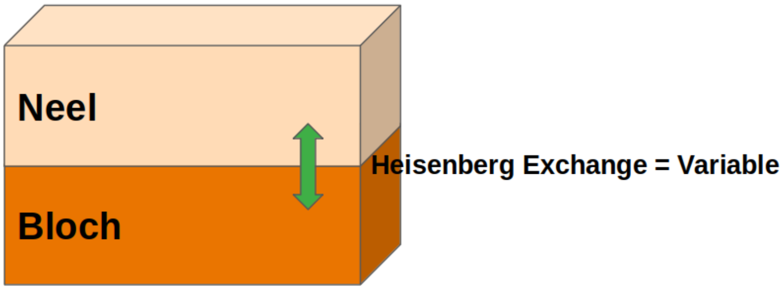

FIGURE 3.4: Configuration of Layers, top layer have Neel DMI ($D = 3.2mJ/m^2$) and bottom layer have Bulk DMI ($D = 3.2mJ/m^2$)

3.3.1 Absence of Heisenberg exchange interaction between the layers (i.e. $A = 0J/m$)

Initially Heisenberg exchange was limited to each layer and hence there was no interaction between these films. So, as expected both layers should have Neel and Bloch skyrmion respectively and it turns out to be the same. Fig[3.5] shows Neel skyrmion which is created in upper layer and Bloch skyrmion created in bottom layer.

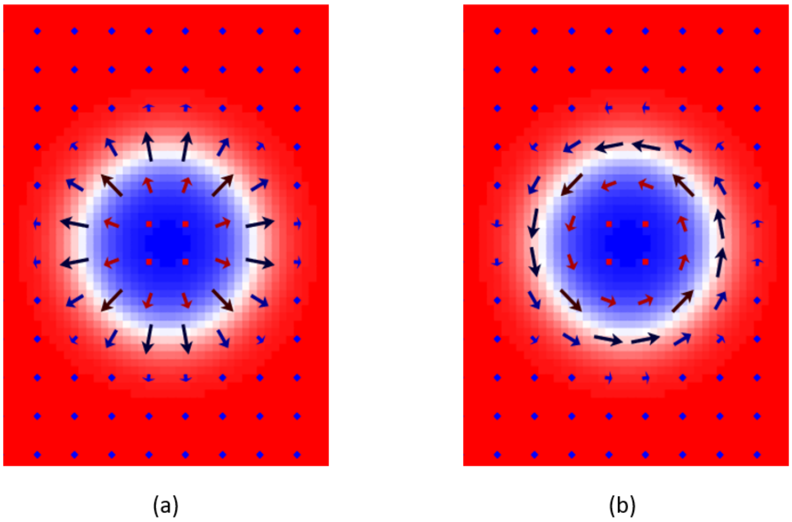

FIGURE 3.5: (a) Neel skyrmion formed in the top layer and (b) Bloch skyrmion formed in the bottom layer

3.3.2 Increment of Heisenberg exchange between the layers

In the second step we introduced Heisenberg exchange between two layers and keep increasing with a some increment and observed it's behaviour. This means we got two layers with two different types of DMI are interacting with each other. We started with Heisenberg exchange constant $A = 0.01 \times 10^{-11}/m$ and keep it increasing as $A = 0.05 \times 10^{-11}/m$, $A = 0.08 \times 10^{-11}/m$, $A = 0.14 \times 10^{-11}/m$ and $A = 0.1493 \times 10^{-11}/m$. Fig[3.7] shows the evolution of skyrmion with increment in Heisenberg exchange between layers.

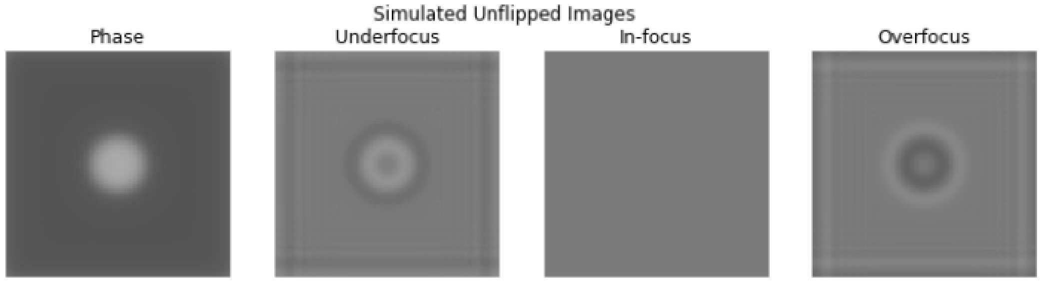

FIGURE 3.6: Simulated LTEM images of two layer configuration in the absence of Heisenberg exchange (i.e. $A = 0J/m$)

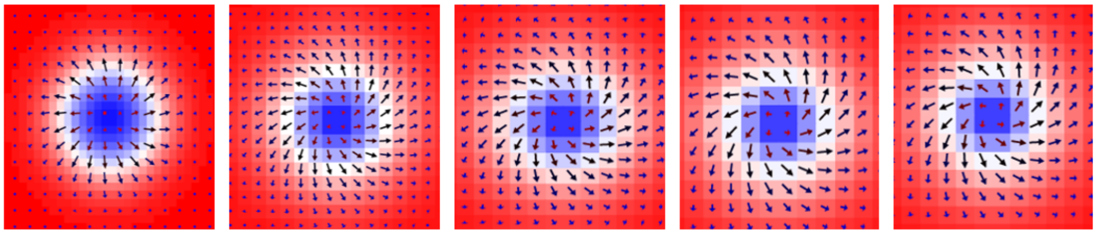

FIGURE 3.7: Evolution of skyrmion with the exchange. Heisenberg exchange constant (a) $A = 0.01 \times 10^{-11}/m$, (b) $A = 0.05 \times 10^{-11}/m$, (c) $A = 0.08 \times 10^{-11}/m$, (d) $A = 0.14 \times 10^{-11}/m$ and (e) $A = 0.1493 \times 10^{-11}/m$

We can observe that Neel and Bloch both skyrmions are stared to deform their structure. The resulted skyrmion looks like frustrated skyrmion. The size of skyrmion was also stated to decrease. We observed that for above configuration skyrmion vanishes for higher exchange.

3.3.3 Stabilized skyrmion for higher exchange interaction

After observing the behaviour we try to stabilize skyrmion for strong interaction, so we made some changes in the description in the film and created more stable skyrmion with the following configuration. First layer have Neel DMI ($D = 4.2mJ/m^2$) and second layer have Bulk DMI ($D = 4.2mJ/m^2$), Uniaxial Anisotropy constant $K = 4.5 \times 10^5 J/m^3$, Heisenberg constant $A = 1.8 \times 10^{-11} J/m$ (Individual layer) and Heisenberg constant $A = 20.5 \times 10^{-11} J/m$ (between two layers). Fig[3.8] shows the the spin twisted structure for above described structure. Fig[3.9] shows corresponding LTEM image.

3.4 Conclusion

We designed a two layer thin film and see the interaction between two different types of DMI. Such study with both Interfacial and Bulk DMI was never done before. The two magnetic layers interact via Heisenberg exchange interaction. Interestingly, we are able to stabilize new kind of topological objects with topological number 1[structure in fig[3.8] have skyrmion number +1]. Hence we can conclude that we have a topological object due to combined interaction between two layer.

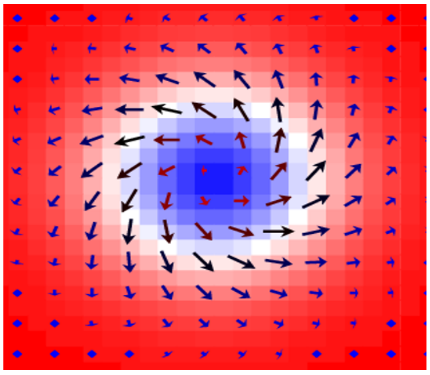

FIGURE 3.8: Spin texture for exchange constant $A = 20.5 \times 10^{-}11 J/m$

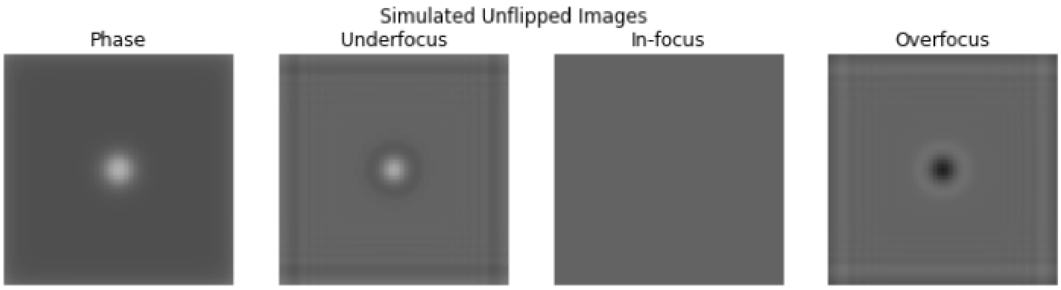

FIGURE 3.9: Simulated LTEM image of stabilized skyrmion ($A = 20.5 \times 10^{-}11 J/m$)

Skyrmion are very hot topic due to their potential use in new type of memory(racetrack memory). So to get a stabilized topological object which can also be stabilized on room temperature is pretty essential. Researchers are working on different types of structure, our proposed model also gives us a stable topological object. As we gave a simulated model, we do not have proof of stable structure on room temperature.

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