SIMULATING SKYRMIONS IN SQUARE LATTICE CHIRAL MAGNETS

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BUCARAMANGA
2021

Contents

1. Introduction

Skyrmions originated as localized solutions to non-linear field theories (solitons) that, due to their non-trivial topology, had particle-like behaviour. These topologically stable solitons were introduced by T. H. R. Skyrme in the 1960s to model baryons in the atomic nucleus [1]. Since then, the term skyrmion has been used to identify localized and topologically non-trivial quasi-particles that have emerged in different fields of physics.

In magnetic materials, skyrmions were first predicted as possible metastable states of ferromagnets by Belavin and Polyakov in 1975 [2]. Later at the end of 1980's and for more than a decade, Bogdanov and collaborators established that chiral interactions (interactions that are not symmetric under spatial inversion), present in non-centrosymetric materials, can lead to thermodinamically stable skyrmions [3–8]. These chiral interactions are known as Dzyaloshinskii-Moriya interactions and tend to align spins perpendicular to each other [9, 10], in contrast to the normal exchange interaction which favors parallel spins.

Magnetic skyrmions were observed for the first time in the bulk of the chiral magnet MnSi, where they could detect skyrmion spin lattices in a small region of the phase diagram known as the A-phase [11]. Soon after, skyrmions lattices were observed in a thin film of $Fe_{0.5}Co_{0.5}Si$ crystal, where it was identified that skyrmions can be stabilized more easily in thin films and therefore skyrmion lattices can be found in a bigger region of the phase diagram [12]. After these initial observations, skyrmion lattices have been found in many different materials [13]. Since their experimental observation, magnetic skyrmions have become one of the most promising candidates to act as the information carrier in future racetrack memories, due to their great stability against fluctuations and efficient mobility when driven by external forces [14].

We propose studying the physical interactions behind the formation of magnetic skyrmions in chiral magnets and carry out simulations of square lattice chiral magnets, which approximate the real behavior thin films [12]. This proposal is organized as follows: the problem statement will put boundaries in the intended project and right after, in the objectives section, we will establish the concrete goals of the project. Subsequently, in the theoretical framework, we present the essential theoretical and computational tools with which magnetic materials are studied at a classical level. Finally we propose a methodology to meet the goals and the corresponded timeline of execution.

2. Problem statement

In view of the promising technological applications, establishing the conditions under which magnetic skyrmions are formed in chiral magnets has been the subject of great study. Both computer simulation and phenomenological models have guided the exploration of the phase space of many materials [13], which has resulted in the discovery of different types skyrmions CITE[Beyond Skyrmions].

The aim of this thesis is to obtain the magnetic phase diagram (B vs T) of square lattice chiral ferromagnetic and antiferromagnetic materials to identify regions of parameter space where skyrmion phases form. To do this, we will model magnetic materials using a classical spin model and use Monte Carlo simulations to construct the magnetic phase diagram. The results will be contrasted with those of existing computational and experimental works. This will allow to troubleshoot the code and optimize it to consider materials with more complex geometries in future projects.

3. Objectives

3.1 General objective

To identify regions of the parameter space of square lattice chiral ferromagnetic and antiferromagnetic materials where magnetic skyrmion phases are present.

3.2 Specific objectives

- To understand the magnetic interactions present in chiral magnets that allow formation of magnetic skyrmions.
- To simulate a square lattice chiral ferromagnetic material and construct its magnetic phase diagram.
- To simulate a square lattice antiferromagnetic chiral material and construct its magnetic phase diagram.

4. Theoretical Framework

This section starts with a description of the classical Heisenberg model with the essential interaction terms that are known to give rise to skyrmions. Then, a brief introduction to magnetic skyrmions and their topological properties. Finally, some of the reasoning behind the Monte Carlo method and a form of the Metropolis algorithm.

4.1 Classical Heisenberg Model

The classical Heisenberg model assumes each atom i in a magnetic material carries a net magnetic moment represented by a three-dimensional unit vector $\mathbf{S}_i = \boldsymbol{\mu}_i / \|\boldsymbol{\mu}_i\|$ where $\boldsymbol{\mu}_i$ is the atomic magnetic moment. The Hamiltonian of a magnetic material consists of multiple magnetic interaction terms which give rise to rich and complex physical phenomena. For this thesis, we will only consider three terms widely regarded as necessary for magnetic Skyrmions to form [15, 16]:

$$\mathcal{H} = \mathcal{H}_{\text{exc}} + \mathcal{H}_{\text{field}} + \mathcal{H}_{\text{DMI}}, \tag{4.1}$$

where $\mathcal{H}_{\text{exc}}$ is the Heisenberg exchange interaction, $\mathcal{H}_{\text{field}}$ is the interaction with an external magnetic field and $\mathcal{H}_{\text{DMI}}$ is the Dzyalonshinskii-Moryia interaction. In the following, we will give a short explanation of each term.

Exchange Interaction

The exchange interaction is a short range quantum effect introduced by Heisenberg to explain the long range ordering of atomic magnetic moments in ferromagnetic materials [17]. In the classical limit, the energy between neighboring magnetic moments is given by

$$\mathcal{H}_{\text{exc}} = -J \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{4.2}$$

where $\sum_{<i,j>}$ represents the sum over nearest neighbor magnetic moments. For $J > 0$ the ferromagnetic state (all magnetic moments parallel) is favored while for $J > 0$ the antiferromagnetic state (neighbor magnetic moments anti-parallel) is favored.

Interaction with an External Field

The energy describing the classical interaction of the moments with an external magentic field (sometimes called Zeeman energy) is given by

$$\mathcal{H}_{\text{field}} = -\mathbf{b} \cdot \sum_i \mathbf{S}_i, \tag{4.3}$$

where $\mathbf{b} = \|\boldsymbol{\mu}_i\|\mathbf{B}$ and $\mathbf{B}$ is the magnetic field.

Dzyalonshinskii-Moryia Interaction

The Dzyalonshinskii-Moryia interaction is an antisymmetrical interaction present in some non-centrosymmetric magnets and interfacially asymmetric multilayers that in the classical Heisenberg model can be written as [16]

$$\mathcal{H}_{\text{DMI}} = -\sum_{<i,j>} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j), \tag{4.4}$$

where $\mathbf{S}_i$ and $\mathbf{S}_j$ are two neighboring magnetic moments and $\mathbf{D}_{ij}$ is the DMI vector, which is dictated by the symmetry of the material or stack of materials. This interaction, in contrast to Heisenbergs' exchange interaction, favors perpendicular alignment of neighboring magnetic moments.

4.2 Magnetic Skyrmions

Magnetic skyrmions are localized magnetic moment configurations characterized by having a center where the magnetic moment is oriented opposite to its surroundings. The magnetic moments in

the inside of the skyrmion rotate progressively from the inside to the outside and the specific way in which they do defines different kinds of magnetic skyrmions (see Figure 4.1).

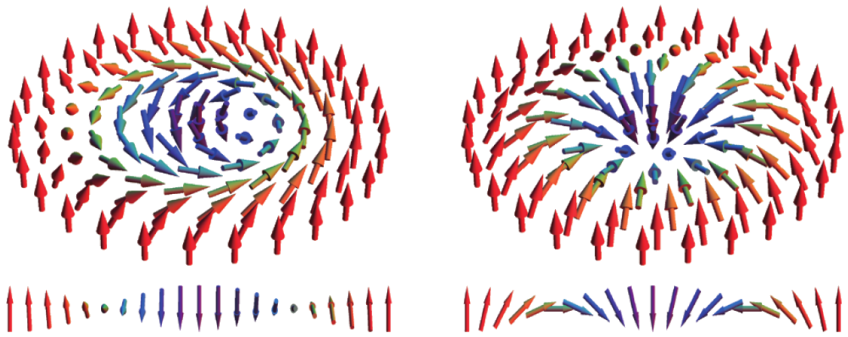

Figure 4.1: Left, Bloch-type skyrmion. The magnetics moments rotate perpendicular to the radial direction when moving from the center to the outside. **Right**, Néel-type skyrmion. The magnetic moments rotate in the radial direction when moving from the center to the outside. Figure taken from [18].

One of the main characteristics of magnetic skyrmions is their great stability, which is due to their non-trivial spatial topology that "protects" them from being deformed. This topological protection can be understood by working in a continuous picture, where we assume variations between neighboring spins are small, this allows us to write the magnetization as a continuous vector field $\mathbf{m}(\mathbf{r})$. In this picture, a skyrmion can be seen as the stereographic projection of a 3D hedgehog-like object projected to a plane (see Figure 4.2).

In topology, the stereographic representation of the magnetization $\mathbf{m}(\mathbf{r})$ defines a map from the 2-sphere to itself, identified by the number of times the magnetic moments rotate onto themselves when moving on the sphere along the azimuthal direction. This number is known as the winding number and according to topology, all $\mathbf{m}(\mathbf{r})$ with the same winding number are equivalent and constitute an homotopy class [15]. Homotopy classes are sets of mappings that can be continuously deformed into each other. It is in this sense that magnetic configurations with the same winding number are equivalent. Moreover, magnetic configurations with a different winding number cannot be continuously deformed into each other (they belong to different homotopy classes), which is the origin of the topological protection mentioned before.

For skyrmions in the continuous picture, the winding number (also called topological charge) of a magnetization configuration $\mathbf{m}(\mathbf{r})$ is given by [19]

$$Q = \frac{1}{4\pi} \int \mathbf{m}(\mathbf{r}) \cdot \left[\frac{\partial \mathbf{m}(\mathbf{r})}{\partial x} \times \frac{\partial \mathbf{m}(\mathbf{r})}{\partial y} \right] = \pm 1, \pm 2, \dots . \tag{4.5}$$

allowing only integer topological charges for the different types of skyrmions.

Even though the above explanation is enlightening, the expression (4.5) above has to be adapted to the discrete atomistic model we're considering in this proposal. This was done by Berg and Lüscher in [20], in the square lattice for example, the topological charge density q_l defined in a unit cell of the lattice is given by [21]

$$\tan\left(\frac{q_l}{2}\right) = \frac{\mathbf{m}_i \cdot (\mathbf{m}_j \times \mathbf{m}_k)}{1 + \mathbf{m}_i \cdot \mathbf{m}_j + \mathbf{m}_i \cdot \mathbf{m}_k + \mathbf{m}_j \cdot \mathbf{m}_k}, \tag{4.6}$$

where i, j, k denote sites in the unit cell forming the elementary triangle l and $\mathbf{m}_i$, $\mathbf{m}_j$, $\mathbf{m}_k$ are the magnetic moments in those sites (see Figure 4.3).

The total topological charge of the lattice is found by summing over all the elementary triangles in the lattice

$$Q = \frac{1}{4\pi} \sum_l q_l, \tag{4.7}$$

which is also an integer.

It is known that skyrmions tend to form lattices. Therefore, in a lattice of an specific type of skyrmion, the total topological charge (4.7) can also be used to determine the number of skyrmions of the system.

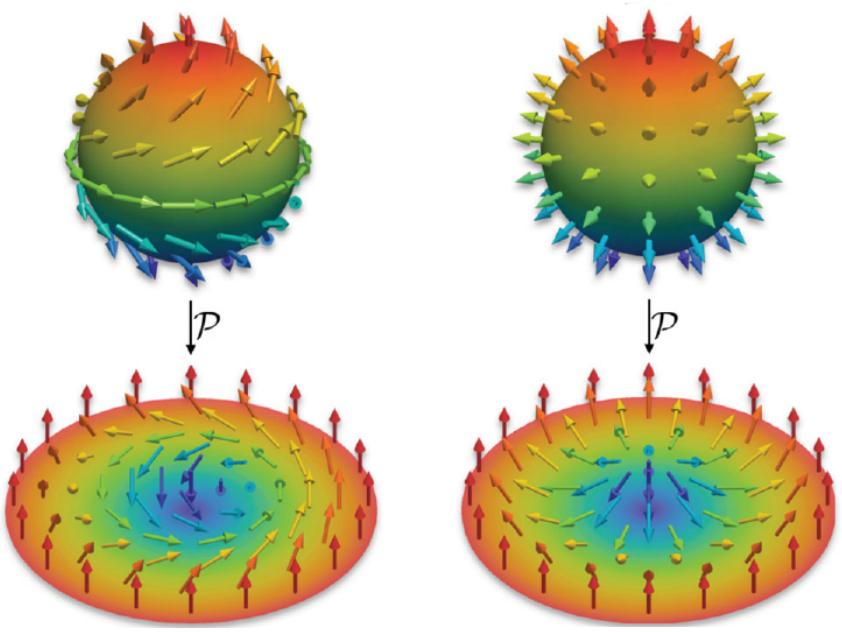

Figure 4.2: Left, Stereographic projection for Bloch-type skyrmion. **Right**, Stereographic projection for Néel-type skyrmion. Figure taken from [22].

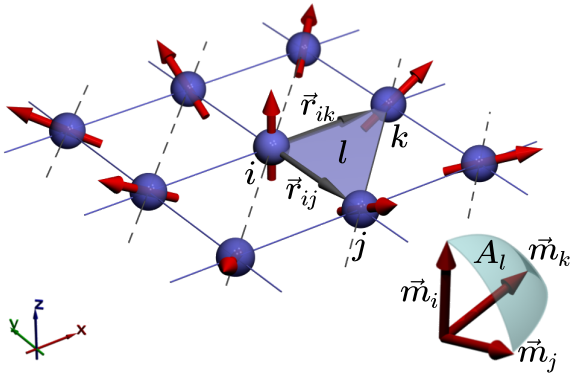

Figure 4.3: Elementary triangles defined in the square lattice and the vectors $\mathbf{m}_i$, $\mathbf{m}_j$ and $\mathbf{m}_k$ involved in the calculation of the topological charge density. Figure taken from [23].

4.3 Monte Carlo Method

To calculate equilibrium quantities like the magnetization or magnetic susceptibility, the standard analytical procedure consists in calculating the partition function of our model, given in the canonical ensemble by [24]

$$Z = \int_{\Omega_1} ... \int_{\Omega_N} \prod_{i=1}^{N} \frac{d\Omega_i}{4\pi} \exp\{-\beta\mathcal{H}\}, \tag{4.8}$$

where $d\Omega_i$ is the element of solid angle in the direction $\mathbf{S}_i$. With Z all thermodynamic quantities can be found by taking derivatives with respect to the parameters of the system. Nevertheless, the high dimensional integral appearing in Z can only be solved exactly in some special cases. Alternatively, approximations like the mean-field approximation, or computational methods like the Monte Carlo method have to be used.

In Monte Carlo simulations, the goal is to avoid calculating thermodynamic quantities via the partition function but rather to compute averages directly using a procedure known as importance sampling. The idea behind importance sampling is to choose a subset of states at random from a probability distribution $q(\mu)$, where μ is the state of the system, in such a way that we include the important areas in the phase space of the system.

Suppose we want to find the expectation value of a physical quantity Q, in the canonical ensemble this is given by

$$\langle Q \rangle = \int_{\Omega_1} ... \int_{\Omega_N} \prod_{i=1}^{N} \frac{d\Omega_i}{4\pi} Q(\mu)\, p(\mu), \tag{4.9}$$

where $p(\mu) = \frac{1}{Z} \exp\{-\beta\mathcal{H}(\mu)\}$. We can introduce importance sampling (if $q(\mu) \neq 0 \ \forall\mu$) in the following manner

$$\langle Q \rangle = \int_{\Omega_1} ... \int_{\Omega_N} \prod_{i=1}^{N} \frac{d\Omega_i}{4\pi} Q(\mu)\, p(\mu) \frac{q(\mu)}{q(\mu)} = \left\langle Q \frac{p(\mu)}{q(\mu)} \right\rangle_q . \tag{4.10}$$

This way, if we choose $q(\mu) = p(\mu)$ we have $\langle Q \rangle = \langle Q \rangle_q$ and a sample of states $\{\mu_1, ..., \mu_N\}$ drawn from $q(\mu)$ can be used to estimate $\langle Q \rangle$ by

$$\langle Q \rangle \simeq \frac{1}{N} \sum_{i=1}^{N} Q(\mu_i). \tag{4.11}$$

This approach allows us to compute expectation values using a small amount of states, namely, the most likely states according to the canonical distribution.

The remaining part of the method consists in finding a way to pick a sample of states whose distribution is the canonical distribution. There exists different algorithms that accomplish this, the most widely known being the Metropolis algorithm. To sample from the canonical distribution, the Metropolis algorithm starts by initializing the system in some state μ_n. Then repeating the following steps until convergence [25]:

1. Generate a new configuration ν from μ_n.
2. Calculate the energy difference between the two states ΔE.
3. Generate a random number $r \in [0, 1]$.
4. Choose the new state of the system according to

$$\mu_{n+1} = \begin{cases} \nu & \text{if } r \leq \min\left(\mathrm{e}^{-\beta \Delta \mathrm{E}}, 1\right) \\ \mu_n & \text{otherwise.} \end{cases}$$

This algorithm always accepts changes in the configuration that lower the total energy of the system. Additionally, when a new configuration has a higher energy it still has a probability of being accepted, with a probability given by the Botlzmann factor of the energy difference.

5. Methodology

To meet the proposed objectives, we suggest the following methodology.

1. **Phenomenological study of chiral magnets**
   Magnetic skyrmions were theoretically predicted as peculiar lowest energy configurations of phenomenological energy functionals for chiral magnets. In this step, we will review these seminal works and the works that followed, to understand how the different magnetic interactions present in chiral magnets allow the formation of magnetic skyrmions. Additionally, we will review some of the topological properties that make magnetic skyrmions interesting.

2. **Monte Carlo simulation design**
   After having an understanding of why magnetic skyrmions form in chiral magnets, we will proceed to code a Monte Carlo simulation for the classical Heisenberg model. In the theoretical framework we described the Metropolis algorithm, which is simplest Markov Chain Monte Carlo algorithm. In this step we will evaluate some key aspects of the simulation, like in which programming language to implement the algorithm and if the performance of the Metropolis algorithm is satisfactory or using more efficient algorithms like a cluster algorithm [26] may be needed.

3. **Exploration of the parameter space of square lattice chiral ferromagnets**
   With the Monte Carlo simulation ready, given a set of parameters $(T, b, J, \mathbf{D_{ij}})$ we can obtain the expected value of important observables (energy, magnetization, magnetic susceptibility, specific heat) and the skyrmion number. In this step we choose the parameter space we need to explore based on existing computational and experimental works. Then run the simulations and use the skyrmion number as the order parameter to construct the magnetic phase diagram.

4. **Exploration of the parameter space of square lattice chiral antiferromagnets**
   This step is analogous to the ferromagnetic case.

5. **Elaboration of manuscript**

6. Schedule

Table 6.1 presents the timeline for the execution of the methodology.

Step	Month											
	1	2	3	4	5	6	7	8	9	10	11	12
1. Phenomenological study												
Literature review												
Topology literature review												
2. Monte Carlo simulation design												
Metropolis implementation												
Test performance												
Code adaptation												
3. Chiral ferromagnets												
Literature review												
Creation of phase diagram												
4. Chiral antiferromagnets												
Literature review												
Creation of phase diagram												
5. Manuscript elaboration												

Table 6.1: Schedule

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