Imperial College London

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Department of Earth Science and Engineering

MSc in Applied Computational Science and Engineering

Independent Research Project
Project Plan

Isolated skyrmion state stability exploration using mean-field models

by

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1 Introduction

The growing demand for data storage requires that storage technologies and materials continue to be researched and developed. Magnetic storage is the most economical data storage method [1], among which thin-film magnetic materials are widely used in hard disk drives, and their thickness is usually less than 1 micron. Today, hard disk drive technology encodes binary data (0 or 1) in perpendicular recording media using magnetic particles pointed upwards or downwards [2], which in practice requires balancing three conflicting: signal-to-noise ratio, thermal stability and imprinting information [3, 4]. Therefore, other magnetic storage methods need to be investigated in the further progress.

Relevant research showed that topologically stable magnetic skyrmions can be used as new materials to develop data storage and information processing devices. Skyrmions were first introduced to describe local particle-like configurations in field theory [5, 6], and have recently been highly correlated with spin structures in condensed matter systems. The structure can be regarded as the distribution of spin directions around a unit sphere and this texture is the result of Dzyaloshinskii-Moriya Interaction(DMI) [7]. They can be easily manipulated using very small spin-polarized currents, are in the nanometer-scale shapes and can be stabilized easily. Skyrmions therefore have the potential to enable new types of high-density, energy-efficient storage and logic devices [3, 8, 9].

The main challenge in the development of skyrmion-based devices is their thermal and magnetic stability [10]. In order realize efficient data storage using skyrmions, we need to explore the range of temperatures and magnetic fields in which skyrmions exist. In addition, the size of the disk is also discussed in the study, the thin-film materials have been used in magnetic storage, the thickness and diameter of this material also have an effect on skyrmion stability [3]. Therefore, it is particularly important to explore the effects of temperature, magnetic field and disk diameter on the existence of skyrmions.

There are two distinct spin textures in the helical magnet: helical and skyrmion [11] which can be transformed. The research [8] used a novel magnetic material, $Fe_{1-x}Co_xSi$ [12], and explored their field and temperature dependence in details by applying an external magnetic field normal to the thin film and changing the environmental temperature. It demonstrated the region where the skyrmion appeared in the experimental and simulated phase diagrams. Taking the temperature of 25 K as an example, skyrmions start to appear when a weak magnetic field of 20 mT was applied, then completely replaced helical at 50 mT, and the material demagnetized when the field strength increases to 80 mT [8]. Notably, the results showed there are no skyrmions exist in the zero magnetic field, which makes the application of disk storage more difficult.

To explore the zero-field stability of skyrmions textures, this study [3] focuses on the dependence of skyrmions on disk size and magnetic field strength. It simulated nanostructured thin-film helical magnetic FeGe disks of different thicknesses and diameters, and obtains a d-B plane phase diagram by applying a magnetic field perpendicular to the thin film to observe the spin texture. It proved that skyrmionics can exist in zero-field with disk diameter $d > 140\,\text{nm}$, and importantly, in the absence of an external magnetic field and without magnetocrystalline anisotropy, skyrmionic textures are the lowest energy state in the helicalmagnetic thin-film nanostructures [3]. This study did not take temperature into account (T=0 K), the effect of temperature can continue to be discussed.

2 Problem Description and Objectives

2.1 Problem Description

As demonstrated above, temperature, magnetic field and disk diameters have effects on the existence of skyrmions, and in order for topologically stable magnetic skyrmions to be better used in data storage and information processing devices, we need to further explore their properties and characteristics. This project is proposed based on the above researches and focuses on the temperature and magnetic field dependence of skyrmions in the magnetic disk of a certain size and we only consider the isolated skyrmion states(only one skyrmion exists). According to the related paper [3], we choose the continuous three-dimensional disk model with d=150 nm as the research object, because this case exists skyrmion in zero-field when the temperature is 0 K.

Skyrmions exist when the system is under lowest energy magnetisation state, mean-field approximation is used in this project to identify the states, which can ignore the collective effects of thermal fluctuations and obtain qualitative characteristics of the phase diagrams more efficiently. Different from the Monte-Carlo simulation with high computational cost, the mean-field model uses the concept of effective field to uniformly change the state of the particles in the magnetic field, which greatly improves the computational efficiency and reduces the computational cost. In addition, mean-field can use temperature as one of the parameters to study the properties of thermodynamic phases. However, the accuracy of the results will be reduced in this method, and the critical temperature and critical exponent cannot be predicted [13]. Our project focuses on the qualitative analysis of temperature and magnetic fields, so this shortcoming will not cause much impact.

In this project we use thin-film helical magnetic FeGe disks, a popular material in skyrmion-related research with a critical temperature of $T_\mathrm{C} = 278.7$ K [14], the crystal lattice constant $a = 4.7$ Å [15], the saturation magnetisation $M_\mathrm{S} = 384$ kAm^{-1} and the DMI material parameter D is $|D| = 1.58$ mJm^{-2} [3].

2.2 Objectives

The project is divided into two parts: programming and simulation. We need to complete mean-field algorithm in code to identify the lowest energy states and do simulation to explore physic problem of skyrmions. The key technical objectives of the research on this topic are listed as follows,

2.2.1 Code development

For coding part, first target is to randomly initialize a three-dimensional continuous model and and use the finite difference method(FDM) to discretize the model into an aggregate of cuboids. FDM is intuitive and easy to implement and solve numerically. It concentrates on solving the problem of the regular model of the cuboid [16], which is very suitable for the thin film material that our project focuses on. Neumann boundary condition has been applied to the 3D system.

We can calculate the efficient field for the domain using

$$\mathbf{H}_\mathrm{eff} = \mathbf{H}_\mathrm{eff}^\mathrm{ex} + \mathbf{H}_\mathrm{eff}^\mathrm{dmi} + \mathbf{H}_\mathrm{eff}^\mathrm{z} + \mathbf{H}_\mathrm{eff}^\mathrm{a} + \mathbf{H}_\mathrm{eff}^\mathrm{d}, \tag{1}$$

The first term is the effective field of exchange energy $\mathbf{H}_{\text{eff}}^{\text{ex}} = \frac{2A}{\mu_0 M_S}\nabla^2\mathbf{m}$ with material parameter A, and $\mathbf{m} = \frac{\mathbf{M}}{M_S}$. The second term is for the Dzyaloshinskii-Moriya Interaction(DMI) $\mathbf{H}_{\text{eff}}^{\text{dmi}} = -\frac{2D}{\mu_0 M_S}\nabla\times\mathbf{m}$, where D is the material parameter. The third term is the Zeeman energy field $\mathbf{H}_{\text{eff}}^{\text{z}} = \mathbf{H}$, which is equal to the external field. The $\mathbf{H}_{\text{eff}}^{\text{a}}$ is the anisotropy energy term $\frac{2K}{\mu_0 M_s}\mathbf{m}\cdot\hat{\mathbf{u}}$, where K is the anisotropy constant, $\hat{\mathbf{u}}$ is the unit vector along the preferential anisotropy axis. The last term represents the demagnetisation energy field [3, 16].

The core idea of mean-field algorithm is to update all cuboids of the domain at once, using

$$\mathbf{m}' = \mathscr{L}(\beta\,|\mathbf{H}_{\text{eff}}|)\cdot\frac{\mathbf{H}_{\text{eff}}}{|\mathbf{H}_{\text{eff}}|}, \tag{2}$$

Here $\mathscr{L}(x) = \coth x - x^{-1}$ is the Langevin function, and $\beta = (k_B T)^{-1}$ adds the temperature into mean-field model with k_B is the Boltzmann constant [13].

then do

$$\mathbf{m}' = \mathbf{m}' + \lambda(\mathbf{m}' - \mathbf{m}), \tag{3}$$

where λ in the range of 0.4-0.6 leads to a good convergence rates [11].

As model is updated and new magnetic field is calculated, the system energy is continuously decreased. Iterative these steps until the domain has been revisited enough times, and any differences between the previous mean field $\mathbf{m}$ remains within the specified tolerance 10^{-5}. Then we can find the lowest energy states of the three-dimensional model to do the simulation.

The flow chart of the code is shown in the Figure. 1 below.

2.2.2 Simulated T-B phase diagram

In order to discuss the existence of skyrmions, the number of skyrmion in three-dimensional model $S^{3\text{D}}$ can be computed using skyrmion number formula:

$$S^{3\text{D}} = \frac{1}{8\pi}\int \mathbf{m}\cdot\left(\frac{\partial\mathbf{m}}{\partial x}\times\frac{\partial\mathbf{m}}{\partial y}\right)\mathrm{d}^3 r, \tag{4}$$

we also define the scalar value $S_{\text{a}}^{3\text{D}}$ for three-dimensional models are:

$$S_{\text{a}}^{3\text{D}} = \frac{1}{8\pi}\int \left|\mathbf{m}\cdot\left(\frac{\partial\mathbf{m}}{\partial x}\times\frac{\partial\mathbf{m}}{\partial y}\right)\right|\mathrm{d}^3 r, \tag{5}$$

In order to explore the T-B plane, we will randomly initialize a three-dimensional disk with diameter d=150 nm and parameters of FeGe, apply different values of temperature and magnetic field in mean-field algorithm, that is, using different (T,B) points and identifying their lowest energy states. The skyrmion number formula will be used to find the isolated skyrmion situations. Also, we can implement a visualization model to observe the states of skyrmions more clearly, and the states of all particles can be displayed on the three-dimensional disk model, which also increases the readability of the results.

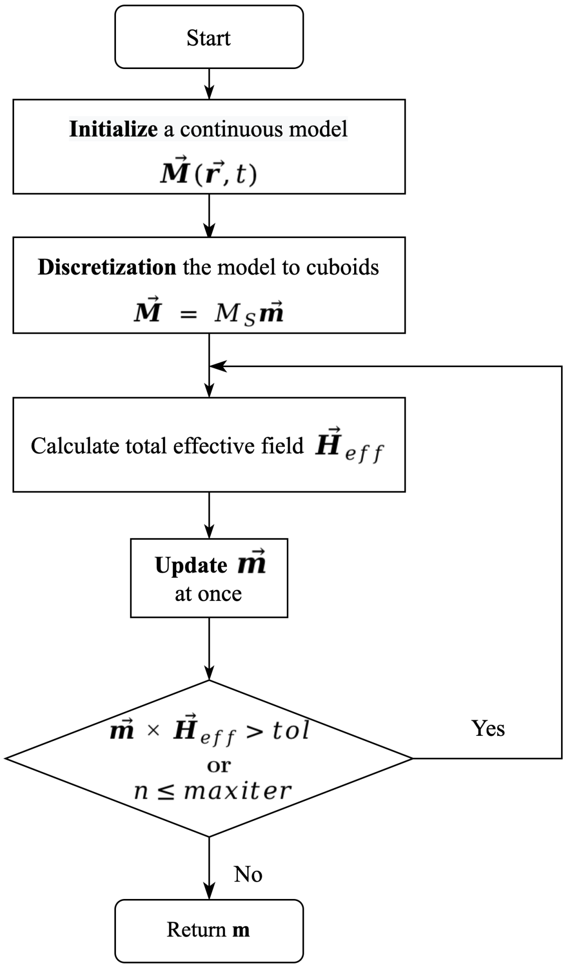

Figure 1: Flow chart of the code.

3 Progress to Date and Future Plan

3.1 Progress to Date

From the beginning of the project, I completed several tasks by collaborating with team members.

1) Learning physic background about magnetism, energy terms: Zeeman, Exchange, Anisotropy and DMI, simple Monte-Carlo and mean-field algorithm.

2) Initializing a model both in atomistic and continuous model.

3) Implementing calculation of energies and effective fields for the four terms, and applying some test cases for them.

4) Implementing an atomistic mean-field and simple Monte-Carlo algorithm to compare the differences.

5) Doing literature review for the relevant researches.

3.2 Future Plan

The Gantt chart Figure. 2 shows the detailed plans for the entire project.

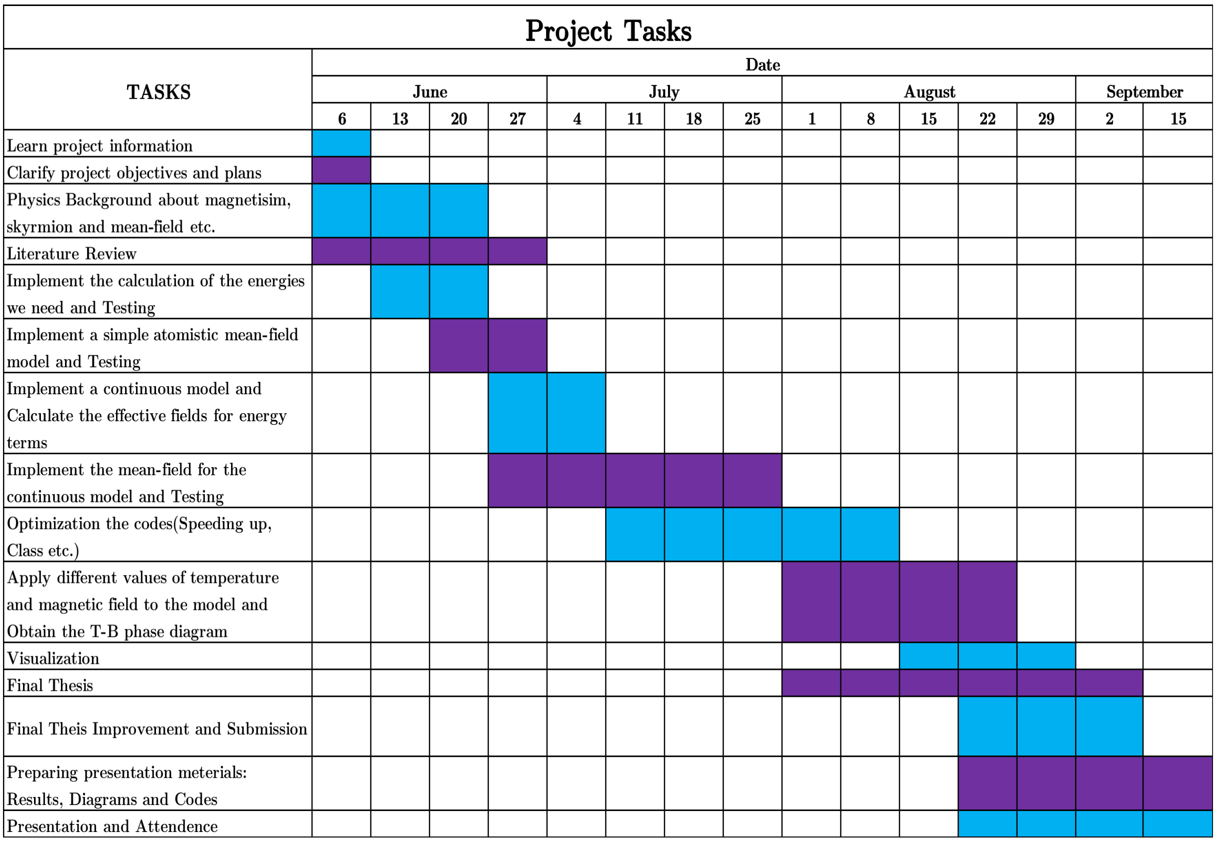

Figure 2: Gantt Chart for the project plan.

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