JOINT INSTITUTE FOR NUCLEAR RESEARCH
Bogoliubov Laboratory of Theoretical Physics (BLTP)

FINAL REPORT ON THE INTEREST PROGRAMME

Micromagnetic simulation for magnetization dynamics in ferromagnetic thin film

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Participation period:
March 01 – April 20,Wave 12

Dubna, 2025

CONTENTS

Abstract

During the practice the domain structure of ferromagnet thin films has been studied according to Ising model. The numerical realization of this model has been created. It has shown adequate behavior for different temperatures.

Landau-Lifshitz-Gilbert (LLG) model has been under consideration in application to thin film dynamics. Magnetization film dynamic has been investigated for several cases of magnetic particles interaction conditions. The analysis of the difficult evolution has been carried out.

Introduction

Information technology plays a significant role in the modern world across all areas of human activity. Thin-film technologies have become the foundation of modern electronics, photonics, and spintronics.

The main feature of all modern information processing devices is the nonlinear nature of the dynamic equations for these systems. Nonlinear equations require special approaches for their numerical solution, as well as for the selection of the mesh and time step.

In this practice, attention was focused on modeling magnetic phenomena in ferromagnetic thin films. These films are understood as those for which the variation of magnetic characteristics with thickness can be neglected. Under this assumption, the problem becomes two-dimensional. The magnetic properties of the film are determined by the presence of a magnetic moment of atoms the film consists of. The presence of a magnetic moment of a charged particle is related to the presence of angular momentum of the particle or, in the simplest case, spin. The effects arising in magnetic systems and the dynamics of such systems are studied by spintronics. Therefore, modeling magnetic phenomena in thin films is a relevant task.

1. Ising model

1.1. Microscopic Theory

The simplest model of a two-dimensional spin system is the Ising model. Within this model, a value S_i – the projection of the spin at the i-th node in a certain direction – is assigned to the nodes of a square lattice. In this model, the value of the projection takes on the values ± 1. If we assume that the main contribution to the energy of the system comes from the pair exchange interaction of neighboring spins, then the energy of the system in this model, in the absence of an external magnetic field, can be expressed as follows:

$$E = -J \sum S_i S_j, \tag{1}$$

where the summation is performed over all neighboring nodes. Most often, four nearest neighbors are considered – two vertically and two horizontally. J is the exchange interaction energy of a pair of neighboring spins. Periodic boundary conditions are usually used. For the one-dimensional Ising model, an analytical solution for the canonical ensemble was obtained by Ising himself [1]. For the two-dimensional case it was obtained slightly later by Onsager [2].

This model has advantageous due to its relative simplicity and its ability to predict the presence of fundamental properties of ferromagnets within the structure of the system. Such properties include the presence of a domain structure, the existence of temperature regions with ferromagnetic and paramagnetic properties, and the transition from a paramagnetic state to a ferromagnetic state through a second-order phase transition for a two-dimensional system.

The Ising model is microscopic model; all parameters can be derived from the properties of both the spin particles themselves and the wave functions localized near the lattice nodes. However, for modeling relatively large inhomogeneous or nonequilibrium systems, this class of models is poorly suited due to the enormous number of particles. The Ising model, as a statistical model, can predict the thermodynamic properties of an equilibrium magnetic system, but it cannot describe nonequilibrium dynamics, which is of great importance for applied research.

1.2 Numerical Implementation

To demonstrate the emergence of a domain structure in a thin film at low temperatures, a numerical program implementation was developed using the Monte Carlo simulation method in the Wolfram Mathematica software package. A 100x100 node lattice with periodic boundary conditions was considered. Spin exchange interaction was considered only between neighboring nodes vertically and horizontally. Simulations were performed for 21 values of the parameter $\tau = \beta/J$ ranging from 0.32, до 3.2, representing the dimensionless thermodynamic beta normalized by the exchange energy. For each temperature value, the same randomly generated spin distribution on the lattice was used. At each step of the cycle in the algorithm a node was randomly selected and the spin value at that node was erased. A new spin value was chosen with the following probability:

$$p_{\pm}(\beta) = \frac{e^{-\beta E_{\pm}}}{e^{-\beta E_{+}} + e^{-\beta E_{-}}}, \tag{8}$$

where $E_{\pm}$- are the system energies corresponding to the spin value of the selected node. To allow the system's energy to reach a saturation, a typical value for the necessary number of steps for this system is on the order of 10^6. Figure 1 shows the spin configurations at different temperatures and the dependence of the system energy on the step number for two different temperatures. It can be seen that with decreasing temperature (increasing parameter τ), a domain structure forms. However, this model is statistically small for observing the jump in heat capacity at the second-order phase transition.

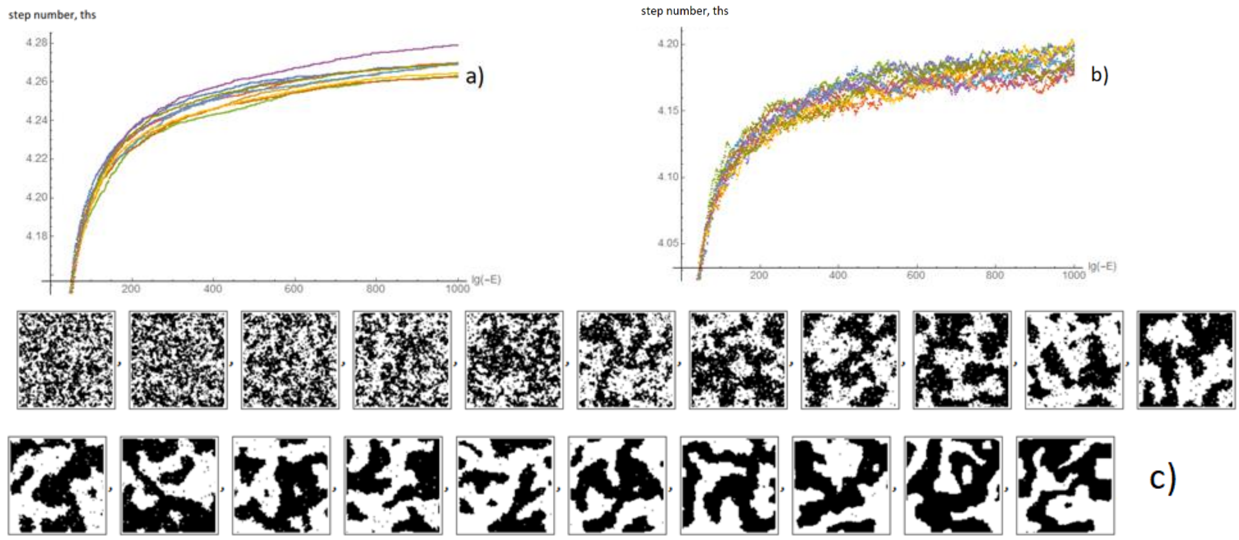

Figure 1. Dependence of the system energy, calculated according to (1), on the step number for a) $\tau = 3.2$ (low temperatures), b)$\tau = 0.32$ (high temperatures). Each figure shows the results of 10 algorithm realizations. c) Spin distribution at different values of the parameter $0.32 < \tau < 3.2$.

2. Continuous model of a magnetic system

2.1 Description within a continuous medium

As mentioned earlier, the presence of spin in a charged particle allows us to introduce the particle's magnetic moment to describe its interaction with a magnetic field. If we assume that electrons make the main contribution to the magnetic properties, then the magnitude of their magnetic moment is related to their spin as follows:

$$\mu = -\gamma_S \hbar \boldsymbol{S} \qquad (2)$$

Let's now suppose that we are interested in the state of each individual magnetic particle within a system. This is valid because the size of the probe of our magnetic property detector is much larger than both the magnetic particle itself and the distance between them. In such a case, we are interested in some average value of the magnetization in the region of our probe, created by individual elementary magnets.

Consider a region Ω containing a magnetic body. Let's isolate a small volume dV within it, located at a point defined by the radius vector $\boldsymbol{r}$. This volume, on the one hand, contains a thermodynamically large number of magnetic particles characterized by magnetic moments μ_i. On the other hand, it is small enough that the average value of the magnetic moment in the vicinity of the isolated volume changes smoothly. We call this average value of the magnetic moment the magnetization vector and define it as follows:

$$\boldsymbol{M}(\boldsymbol{r}) = \frac{\sum_i \mu_i}{dV} \qquad (3)$$

Thus, we arrive at a description of the magnetic system by specifying a vector field throughout the volume of the magnetic sample. At each point this vector field will interact with the external magnetic field as an isolated individual magnetic moment. The phenomenological Landau-Lifshitz-Gilbert (LLG) model is used to describe the dynamics of this vector field.

2.2 Landau-Lifshitz-Gilbert model

This model is phenomenological and attempts to describe phenomena in a dissipative system with strong interactions between individual subsystems. For an isolated magnetic moment in an external magnetic field $\boldsymbol{H}$, the dynamic equation is given by:

$$\frac{\partial \boldsymbol{M}}{\partial t} = -\gamma \boldsymbol{M} \times \boldsymbol{H}. \qquad (4).$$

The model of a particle's magnetic moment is related to the model of a magnetic dipole, which not only describes the effect of an external field on the particle but also defines the magnetic field created by the particle itself. Therefore, if an initially isolated dipole is placed in an environment of other magnetic dipoles, the external field for this dipole in the right-hand side of equation (4) should be understood as both the magnetic field external to the system and the field created by all other sources, which depend on the magnitude of magnetization in other points of the system. If we want to limit ourselves to a local model, we postulate the hypothesis of a self-consistent effective magnetic field $\boldsymbol{H}_{eff}(\boldsymbol{r})$, which itself depends on the magnetization at that same point with radius vector $\boldsymbol{r}$:

$$\frac{\partial \boldsymbol{M}}{\partial t} = -\gamma \boldsymbol{M} \times \boldsymbol{H}_{eff}. \qquad (5).$$

The form of $\boldsymbol{H}_{eff}(\boldsymbol{r})$ can be determined from a microscopic model of the interaction between the particles of the medium [3,4]. The effective field model is a Hamiltonian model, the basis for constructing the functional of which is the thermodynamic functional of the system's free energy. Dissipation in the system is accounted for by specifying a suitable Rayleigh dissipation function, which leads to the appearance of an additional term in the system's dynamic equation.

The final form of the dynamic equation can be written as follows:

$$\frac{\partial \boldsymbol{m}}{\partial t} = -\gamma\, \boldsymbol{m} \times \boldsymbol{H}_{eff} + \frac{\alpha}{M_s} \boldsymbol{m} \times \frac{\partial \boldsymbol{m}}{\partial t}, \qquad (6)$$

where α>0 – is the Gilbert damping parameter, which is a characteristic of the material. The microscopic model assumes the conservation of the magnitude of the magnetic moment of each particle, and the LLG model possesses this same property. M_S – is the saturation magnetization, representing the state when all magnetic moments in the considered small volume *dV* are aligned in the same direction. Equation (6) is written in a dimensionless form (normalized by M_S) for the magnetization vector $\boldsymbol{m} = \boldsymbol{M}/M_S$.

2.3 Types of interactions

The effective field $\boldsymbol{H}_{eff}$ in (6) is a function of magnetization according to the self-consistent field theory. For the main known magnetic materials to date, the macroscopic consequences of the interaction between the particles of the substance can be described by specifying the effective magnetic field in the form:

$$\boldsymbol{H}_{eff} = A\nabla^2\boldsymbol{m} + K(\boldsymbol{e}_K \cdot \boldsymbol{m})\boldsymbol{e}_K + \boldsymbol{H} + \boldsymbol{H}_{DMI} + \boldsymbol{H}_T. \qquad (7)$$

The first term is related to the tendency of magnetic moments to align parallel to each other. It is directly obtained from the generalization of the Ising model to the Heisenberg spin model, where the energy is determined by the dot product of the spin vectors. Expanding this energy for small angles allows us to determine a simplified form of the interaction energy. In equation (7), A denotes the exchange stiffness coefficient, proportional to the exchange energy J in the Ising model (see section 1.1.).

The second term in equation (7) is related to the presence of anisotropy in the magnetic crystal. The simplest case of anisotropy is the presence of one preferred direction in the crystal, the direction of which is given by the vector $\boldsymbol{e}_K$. The coefficient K can be either positive, in which case it is referred to as an easy-axis towards which the magnetic moments of the system tend to align, or negative, in which case it is referred to as a hard-axis, and the magnetic moments tend to align perpendicular to the specified direction. The third term in equation (7) describes the magnetic field external to the magnetic material, which would be present at that point if only this magnetic material were removed from the system. The fourth term in equation (7) describes the Dzyaloshinskii-Moriya interaction, which is relevant when studying specific materials. The fifth term in equation (7) reflects the interaction of the magnetic material with a current flowing through it from an external source.

This effective field model is implemented in the Micromagnetics module of the commercially available software package COMSOL Multiphysics [5].

2.4 Micriomagnetics simulation

2.4.1 External field

To test the capabilities of the Micromagnetics module in COMSOL Multiphysics, calculations were performed within the framework of the LLG model for the dynamics of a section of thin film with dimensions of 100×100 nm in an external magnetic field perpendicular to the magnetic material. The magnetic field was defined as a 4-lobe spiral, smoothed in such a way that there was no uncertainty at the center and vanishing at the boundary of the magnetic material. Figure 2 shows the distribution of the external magnetic field. The field was chosen to be sufficiently weak (on the order of 10^3 A/m) to have a perturbative effect on the system in order to test the solver and mesh settings. The initial unit magnetization vector was set uniform across the film with initial state components $m_x = m_z = 1/\sqrt{2}$. Periodic boundary conditions were used.

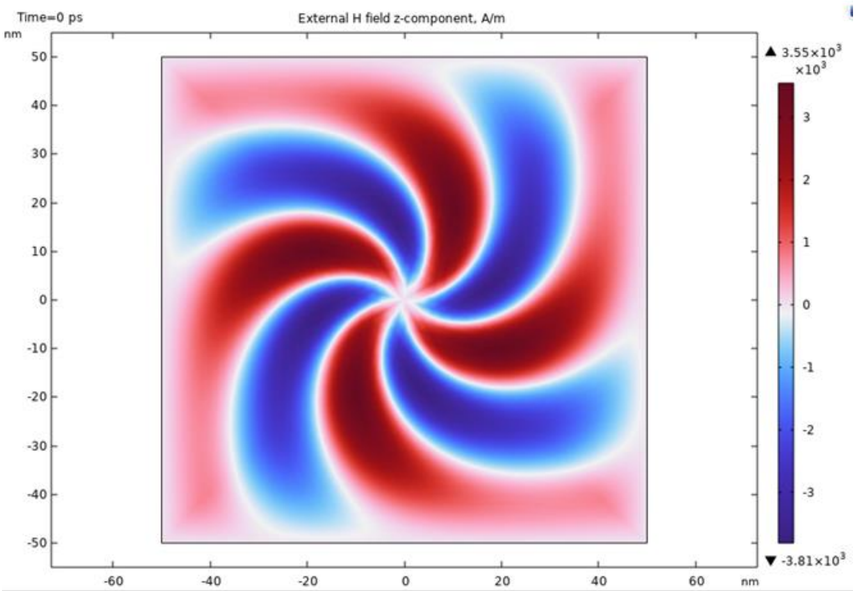

Figure 2. Distribution of the z-component of the external magnetic field in the film.

An unstructured mesh with a total of 6282 elements was used to calculate the dynamics of this state, which corresponds to a mesh element size on the order of 2 nm. Computations on a coarser mesh converged for this problem, but these parameters were chosen as the most suitable after a mesh convergence study. The temporal dynamics were considered for a time interval of 1 ns with a field distribution recording step of 10 ps. The time step in the solver did not exceed 0.1 ps. The typical calculation time with these parameters was 30 minutes.

Figure 3 shows some intermediate magnetization distributions in the sample; the characteristic time between two distinguishable states is on the order of 5 ps, which means that the field passes through approximately 200 states during the simulation time, each of which possesses a symmetry of the fourth-order axis.

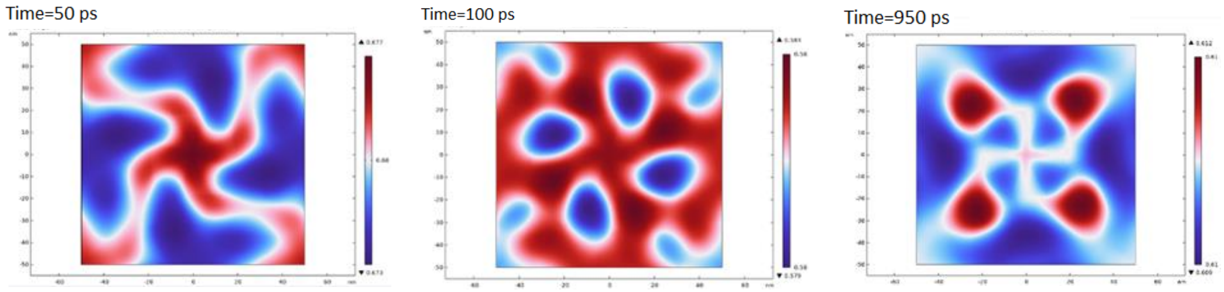

Figure 3. Intermediate distributions of the z-component of the unit magnetization vector during intrinsic dynamics.

To analyze the dynamics of the system, the distributions of the components of the normalized magnetization vector were read to file at all mesh nodes, after which a Fourier transform was performed over time. Figures 4a and 4b show the time dependence and Fourier spectra for two points: the center (0,0) and the “antinode” - the point with coordinates (25,10), where maxima for the z-component of the magnetization vector typically occurred. From the graphs, it can be seen that the spectrum is not continuous, but contains many harmonics, which indicates a complex, but not chaotic, evolution regime. In Figure 5b, precession with the Larmor frequency is clearly visible for the given parameters.

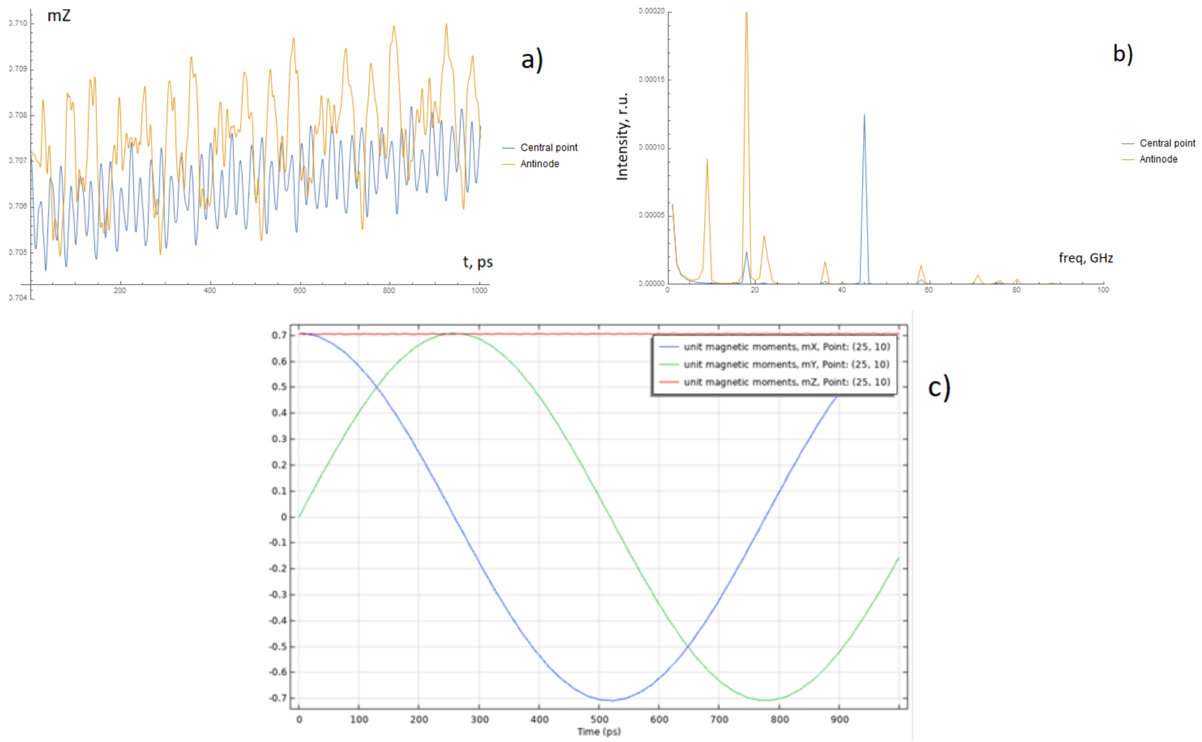

Figure 4. a) Time dependence of the z-component of magnetization at reference points. b) Fourier spectrum of the signal. c) Three components of magnetization on a single scale.

Figure 5a presents a map of the frequency distributions in the sample, constructed as follows: for each point, two frequencies with the highest intensities were selected from the Fourier spectrum (assuming that two main harmonics are sufficient for a rough but adequate reproduction of the system’s evolution over time), and maps of these frequencies were constructed and then superimposed on each other. The colored regions represent:

- yellow: regions in which the higher frequency has a higher intensity,
- blue: regions in which the higher frequency has a lower intensity.

Figure 5b takes into account frequencies with the third-highest harmonic intensity, and Figure 5c shows the Fourier spectra obtained for the blue and red points marked in Figure 5b, respectively. It can be seen that the system is a structure of a set of disjoint regions with sufficiently long-lived high-amplitude oscillations, separated by regions with faster oscillations. Also of interest is that the intensity distributions for the two frequencies (Fig. 5a) possess not only axial symmetry of the 4th order but also mirror symmetry with respect to the vertical and horizontal planes, while taking into account the third frequency preserves axial symmetry but violates mirror symmetry.

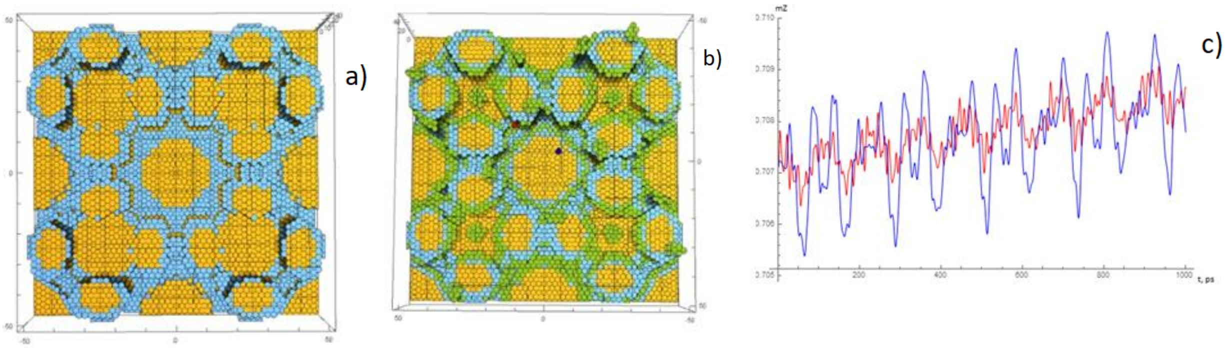

Figure 5. Maps of a) two- and b) three-frequency distribution of contributions from intense harmonics. c) Dependence of the z-component of the unit magnetization vector on time at the corresponding points in figure b).

2.4.2 Intrinsic dynamics of a complex initial state

Calculations were also performed for the same film within the LLG model for dynamics in the absence of an external magnetic field. Now, the initial state itself was chosen as a 4-lobe spiral. The distributions of the x and z components of the unit magnetization vector in the initial state are shown in Figures 6a and 6b, respectively.

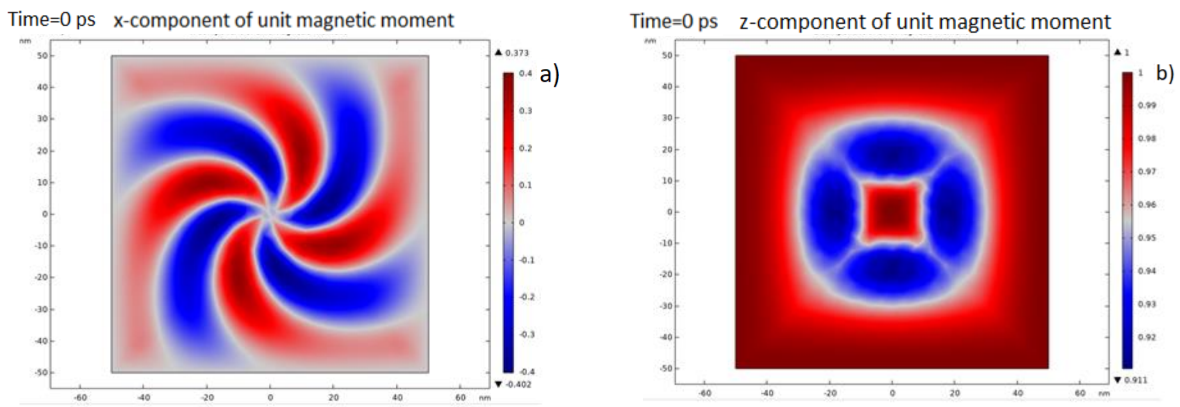

Figure 6. Initial states of the a) x- and b) z-components of the unit magnetization vector in the calculation domain.

The calculations were performed on a mesh with the same parameters. The temporal dynamics were considered for a time interval of 1 ns with a field distribution recording step of 1 ps. The time step in the solver did not exceed 5 fs.

This boundary value of the step ensured stable convergence of the solver throughout the calculation time. When increasing the maximum step size, the solution diverged or converged much slower, as the solver, in an attempt to find a suitable, even larger, time step, could make around 20 selection attempts. The typical calculation time with these parameters was 3.5 hours. The values of the interaction parameters are given in Table 1.

Table 1. Interaction parameters in the LLG model.

α	γ, m/($s \cdot A$)	$A, A \cdot m$	$M_s, A/m$	$K, A/m$	e_K
5×10^{-4}	2.21×10^{5}	3.28×10^{-11}	1.94×10^{5}	-3.88×10^{4}	(0,0,1)

Figure 7 shows some intermediate magnetization distributions in the sample.

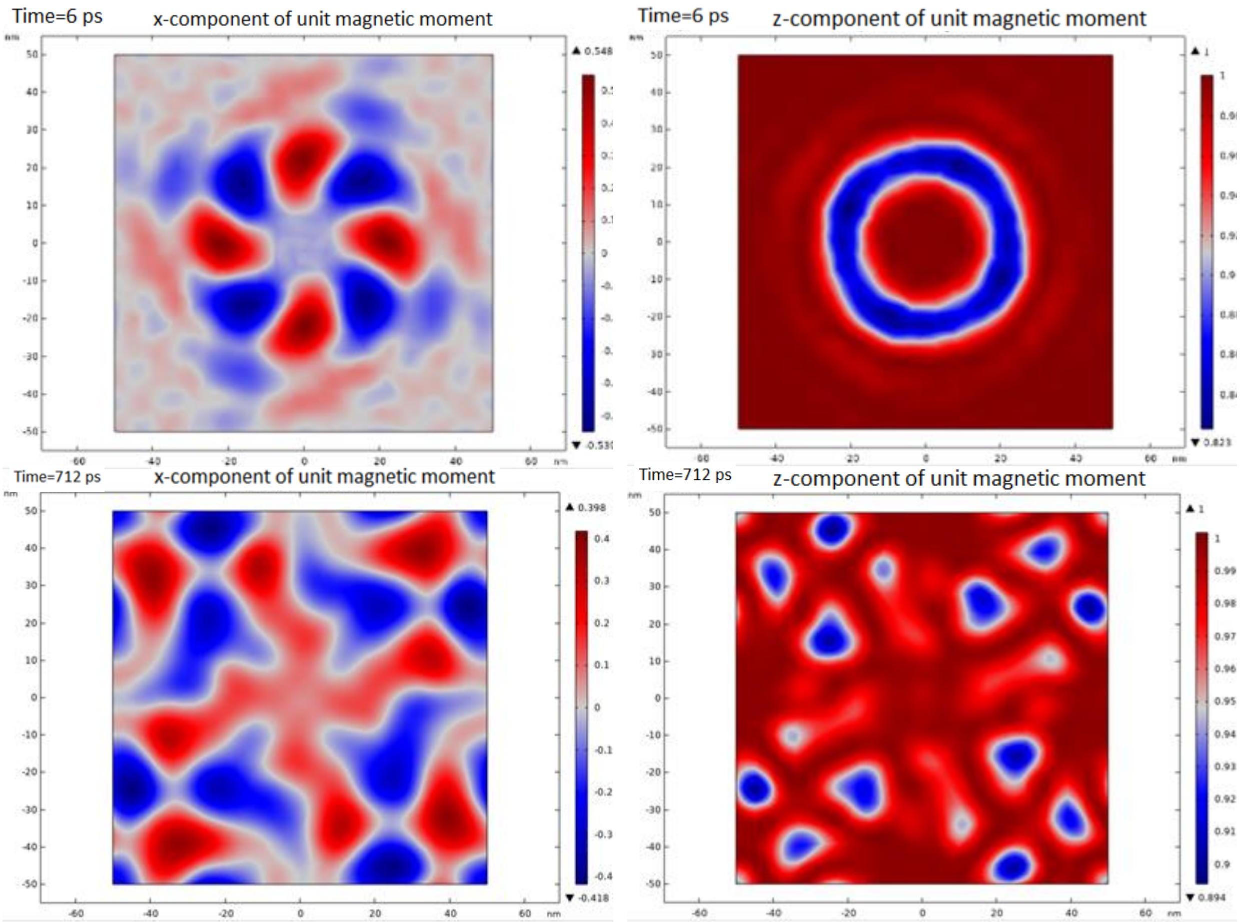

Figure 7. Intermediate values of the x- and z-components of the unit magnetization vector in the calculation domain.

2.4.3 Dzyaloshinskii-Moriya interaction

Separately, the dynamics of the initial state from the previous section were investigated when the Dzyaloshinskii-Moriya interaction was included in the model. The field distributions with an interaction parameter of D=0.01 A are presented in Figure 8. With the same mesh and solver parameters for a time interval of 15 ps, the computation time increases by a factor of 4-5.

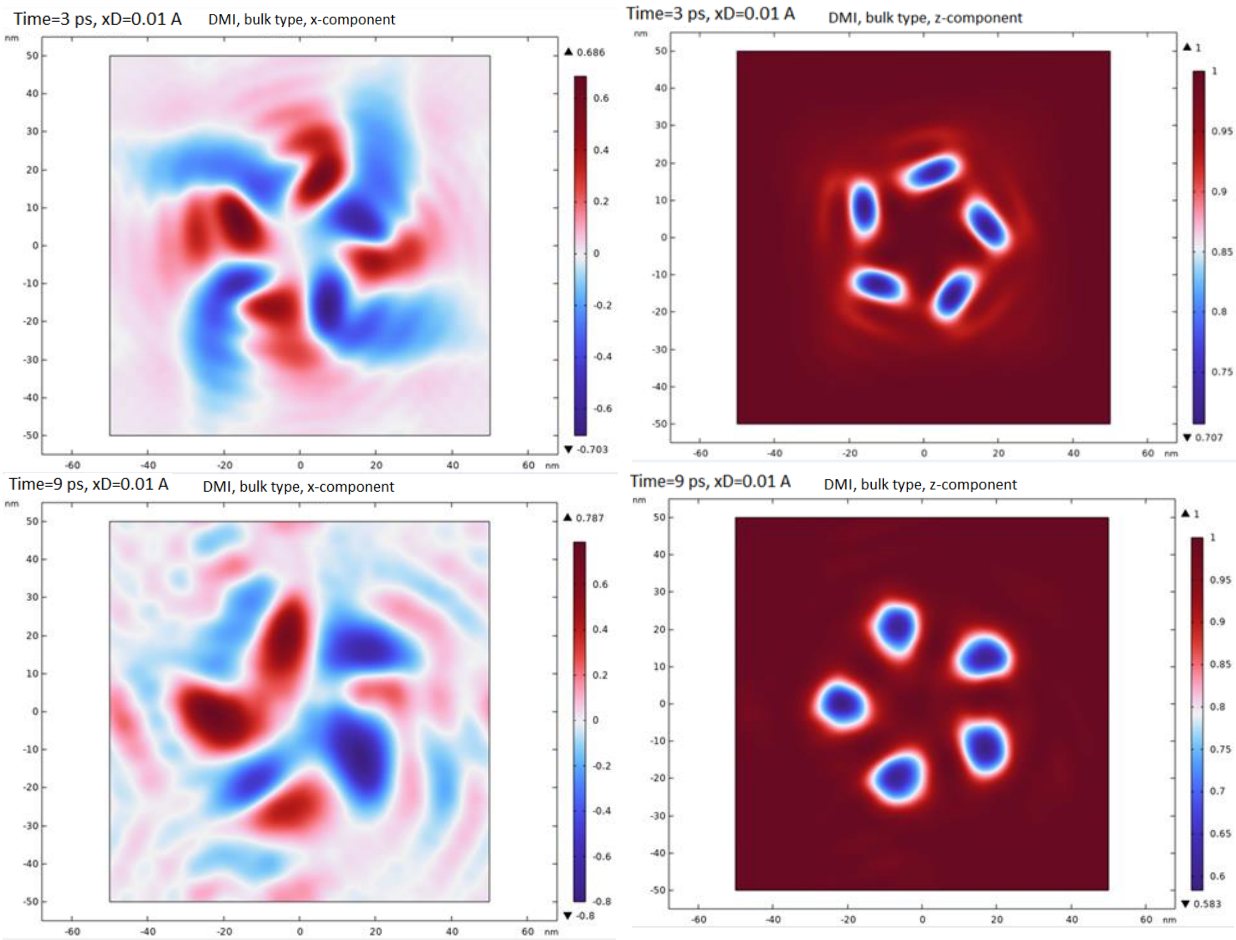

Figure 8. Intermediate values of the x- and z-components of the unit magnetization vector in the calculation domain when considering the DM interaction.

It can be immediately noted that the axial symmetry for the tangential component of magnetization is violated during its own dynamics. A small introduction of noise, for example, in the form of restructuring the mesh while maintaining its parameters, leads to the appearance of magnetization distributions that are close to each other in shape but rotated relative to each other by 90, 180, or 270 degrees.

Conclusion

During the practice, the main focus was on modeling magnetic phenomena in thin films under various conditions. The modeling was carried out in two stages.

In the first stage, a program was created for the numerical implementation of the microscopic Ising model. This program predicts the presence of a domain structure in the temperature range below a certain critical temperature. It was only possible to calculate the structure of a statistically small system within a reasonable time. It did not allow observing signs of a phase transition in the thermodynamic quantities. However, qualitatively, this program correctly predicts the structure of the system.

In the second stage, the dynamics of the magnetic system were simulated within the framework of the Landau-Lifshitz-Gilbert model for various system parameters. Particular attention was paid to analyzing the convergence of the numerical model. The correct selection of mesh and solver parameters depends not only on the geometric features of the computational domain but also on the considered interactions and states.

Acknowledgments

I would like to express my sincere gratitude to Dr. Majed Nashaat for the excellent organization of his lectures and practice including careful planning, attention to details and methodological guidance. Taking part in INTEREST program was a great possibility to work with him for solving interesting and difficult problems.

I would like to express my heartfelt appreciation to organizers of JINR INTERST program. This program is a great chance to work on the frontier of the modern physics and deepen our knowledge in advanced topics.

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