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Switching of skyrmion states by uniaxial deformations and stability of skyrmions in elastic ferromagnetic film

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Abstract: Magnetic skyrmions represent a certain type of topologically protected quasiparticles, which are necessarily stable in relation to a wide range of external magnetic fields temperatures. Skyrmions retain their vortical magnetic structure in a physical space both in the ground state and at room temperatures thanks to the combination of competing exchange interaction, Dzyaloshinskii–Moriya interaction and external magnetic field, which may arise on the surface of magnetic layers. From the energy effectiveness point of view, the process of switching skyrmion states in magnetic multilayer structures is significantly more perspective for real world applications such as piezomagnetic switches, ultra-dense magnetic memory units, detectors of weak fields and other spintronic devices, compared to the classic domain reorientation process, despite the dependence of magnetic properties of such materials on film thickness. In this article a single-layer ferromagnetic film with triangular symmetry was simulated, in which the exchange interaction and the Dzyaloshinskii–Moriya interaction depend on the distance between neighboring spins, and lattice sites are represented as mobile point bodies with unit mass, connected to neighbor sites by elastic force. Film stretching was modeled by displacing the edge sites and calculating the equilibrium positions of the remaining sites, and the ground state was calculated using the steepest descent method. The processes of switching individual skyrmion states using a combination of external magnetic fields of various intensities and various uniaxial stretching as well as stability of the skyrmion lattice were studied.

Keywords: ground state, elastic deformations, magnetostriction, skyrmion lattice, ferromagnetism, Dzyaloshinskii–Moriya interaction, Hooke's law, phase transition

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1. Introduction

Magnetic skyrmions are of great interest in condensed matter physics for their ability to gain and retain ordered states at non-zero temperatures, which can be used for a variety of real-world applications, most notably for memory devices. Therefore, the study of their thermal behavior and possible phase transitions has been the main focus of research for last two decades.

Topology of magnetic quasiparticles is characterized by a topological charge [13] — a nonzero integer that describes the number of revolutions of the classical spin. Several classes of materials have emerged in which it is possible to stabilize magnetic skyrmion excitations, which has been observed experimentally [1,2]. In multilayer films Dzyaloshinsky–Moriya interaction necessary to stabilize the skyrmion texture can arise as a result of inversion, breaking the symmetry at the boundaries between layers. Competition of Dzyaloshinsky–Moriya interaction with exchange interaction and external field leads to the formation of skyrmions, which can exist in a wide temperature range, up to 500 K [3,4]. From the point of view of practical applications in real devices, it is necessary not only to stabilize the skyrmion phases at room temperature, which is possible in multilayer systems, for example in Ta/CoFeB/MgO [5], but also to manipulate skyrmions and control their states.

Although the classical lattice models such as Ising, Heisenberg, Potts models are consistent with thermodynamical and statistical predictions, the mechanism for thermal fluctuations of spins does not reflect the mechanical nature of the temperature — lattice sites are considered frozen in place and only spin states are changed according to Boltzmann distribution, thus more research into the role of mechanic deformations is needed. El Hog et al. numerically studied skyrmion stability/instability under uniaxial stresses using the Finsler geometry modeling technique and found out that the DMI anisotropy is caused by lattice deformations [6]. Jiangang et al. has attempted to build a comprehensive elasticity theory of ultrathin nanofilms [7]. In [8] the effect of epitaxial deformation on structural and magnetic properties of $YFeO_3$ on $SrTiO_3$ substrate was investigated. Thermal and structural magnetic evolution of Ni-Zr alloy clusters was numerically studied in [9]. In [10] the surface relief of randomly distributed magnetic particles on elastic matrix under the influence of external field has been studied. Finizio with colleagues has investigated the emergence of anisotropy in Nickel nanosquares induced by piezoelectric strain and measured the magnetostrictive constant of $\lambda_s = -26$ ppm [11].

Uniaxial anisotropy in $Co_{20}Fe_{60}B_{20}$ films under stress was found independent of film thickness by Gueye et al. [12].

In this paper we offer a model for elastic magnetic film with mobile lattice sites and distance-dependent exchange and Dzyaloshinskii–Moriya (DM) interactions and investigate the effect of uniaxial stress and weak magnetic fields on nucleation, destruction and switching skyrmion states, and study thermal stability of a skyrmion lattice. The paper is organized as follows: Chapter 1 — a brief overview of the topic and motivation for this article, Chapter 2 — a description of model and methods, Chapter 3 — study of uniaxial stress effect on skyrmions, Chapter 4 — simulation of thermal fluctuations of skyrmion lattice, Chapter 5 gives a summary of the article and conclusions.

2. Model description and methods

Consider a single-layer magnetic film with triangular symmetry and finite size, consisting of point bodies with unit mass as lattice sites. $\vec{r}_i$ and $\vec{S}_i$ denote the position and Heisenberg spin of i-th site. With this laid out we can write down the magnetic Hamiltonian of i-th site as follows:

$$\mathcal{H}_i=-H^z\cdot S_i^z-\Sigma_{j=1}^{6}\{J_0\exp(1-|\vec{d}_{ij}|)\vec{S}_i\cdot S_j+D_0\vec{d}_{ij}\cdot[\vec{S}_i\times S_j]\} \quad (1)$$

Here $\vec{d}_{ij}=\vec{r}_j-\vec{r}_i$ is the distance vector connecting sites i and nearest neighbor site j, J_0 — exchange parameter, D_0 — module of DM vector, H^z — external magnetic field perpendicular to the film's plane. The first term is responsible for Zeeman's energy, the second term describes the energy of exchange interaction which decreases exponentially with the distance, and the third term describes the energy of DM interaction which is proportional to the distance.

Additionally, we introduce a linear elastic force between sites i and j described by Hooke's law. The resultant force acting on the i-th site by its 6 neighbors can be written in the form:

$$\vec{F}(\vec{r}_i,\vec{r}_j)=\Sigma_{j=1}^{6}\vec{F}_j(\vec{r}_i)=\Sigma_{j=1}^{6}\sigma_0(|\vec{d}_{ij}|-1)\vec{n}_{ij} \quad (2)$$

Here σ_0 is module of elasticity, $\vec{n}_{ij}=\vec{d}_{ij}/|\vec{d}_{ij}|$ a unit vector directed from site i to site j. Note that the force $\vec{F}_j$ becomes attractive when $|\vec{d}_{ij}|>1$ and repulsive when $|\vec{d}_{ij}|<1$ and vanishes at equilibrium distance $|\vec{d}_{ij}|=1$ (Fig. 1).

For both Chapters 3 and 4 we will need to calculate the ground state by minimizing the Hamiltonian (Eq. (1)), which will be done by using steepest descent method, modified for our simulation using local field instead of gradient tensor: each spin is only influenced by its 6 neighbors and external field, so we can split all sites into three non-interacting groups and update each group of spins according to their local fields, created by spins from other two groups, in parallel.

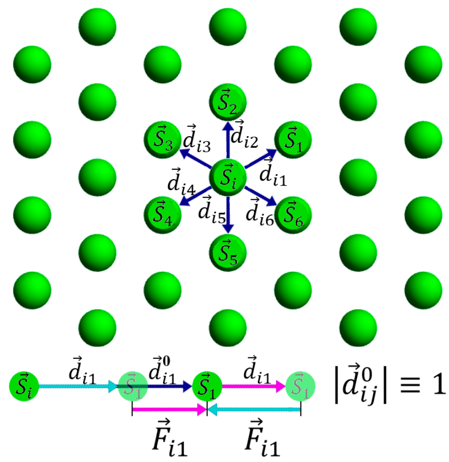


Fig. 1. (Color online) The model of elastic triangular lattice with free boundaries.

To calculate equilibrium positions of sites during film stretching, we will displace and fix sites on the left and right boundary (or top and bottom) according to the stretching factor and then relax the rest by displacing each non-fixed site in the direction of resulting elastic force in small steps and recalculating forces, until all forces have reach small values.

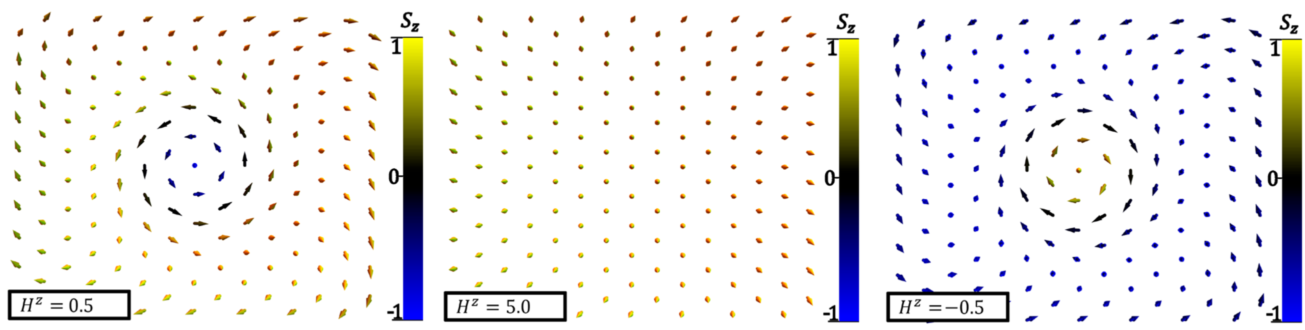
The precision of calculations was controlled by comparing the value of total energy decrease per step ΔE_{iter} relative to the mean energy E_{mean} (for ground states) and absolute values of elastic forces (for equilibrium positions) with the threshold value $\varepsilon=10^{-4}$.

Model parameters will be described in the corresponding chapters.

3. Switching skyrmion state with magnetic fields and uniaxial stretch

In this chapter we investigate how a combination of uniaxial deformation and weak magnetic field ($|H^z/J_0|<1$) causes nucleation, destruction and switching of skyrmions.

We will start by simulating a non-deformed single layer film with triangular symmetry (Fig. 2.) of size $L_{x0}\times L_{y0}$ where $L_{x0}=7\sqrt{3}a$, $L_{y0}=10a$ with lattice unit $a=1$, consisting of two



a b c

Fig. 2. (Color online) Skyrmion state switching with by application of strong and weak magnetic fields.

overlapping rectangular lattices: 8×10 sites (site columns #1, #3, etc. in Fig. 2 a) and 7×11 sites (site columns #2, #4, etc. in Fig. 2 a) and following parameters: J_0=1.0, D_0=0.75, σ_0=1.0.

During simulation we have discovered two ways to switch a skyrmion state (its topological charge and helicity).

First method involves the use of strong magnetic field.

We start with a skyrmion (Fig. 2 a) with topological charge Q_T=−1 in a weak magnetic field H^z=0.5 — this value was established in our previous research [13] as optimal in relation to other parameters J_0=1.0 and D_0=0.75 for which skyrmions have the most pronounced and stable configuration. To switch skyrmion state with magnetic field we first need to force it into ferromagnetic state but, as we have discovered, its central spin can only be flipped by a magnetic field H^z=5.0 (Fig. 2 b) or higher. After that we decrease the field intensity and flip its direction H^z=−0.5 — this creates a new skyrmion with opposite topological charge Q_T=1, as well as opposite chirality (Fig. 2 c). The same process with opposite fields can be used to switch the skyrmion state back.

For the second method we need to set L_x and L_y as lengths of the film in deformed state in *x*- and *y*-directions, as well as introduce stretching parameter $\alpha_x = L_x / L_{x0}$ and $\alpha_y = L_y / L_{y0}$ accordingly.

The second method: we start with a skyrmion with topological charge Q_T=−1 in a weak magnetic field H^z=0.5 (Fig. 3 a), uniformly stretch the film in the *y*-direction by a factor of α_y=1.2 (Fig. 3 b), restore the original size of the film α_y=1 and switch the direction of field to H^z=−0.5, uniformly stretch the film in the *x*-direction by a factor α_x=1.2 (Fig. 3 c), restore the original size $\alpha_x = \alpha_y$=1 and obtain a skyrmion with the opposite charge Q_T=1 and chirality (Fig. 3d).

We have considered many different combinations of stretching by various factors and various intensities of magnetic field applied and discovered that stretching by 15% or less the skyrmion state persists after restoring size, and that stretching by 50% or more the magnetic configuration change to a domain structure. The particular algorithm of switching skyrmion state described above is the optimal from the point of view of energy required and minimal number of steps.

4. Thermal fluctuations simulation and phase transition

Consider now the more general case with free oscillating sites in the presence of elastic forces between nearest neighbors (Eq. (2)). Simulation parameters were chosen as as J_0=1.0, D_0=0.75, H^z=0.5, σ_0=1.0, $L_{x0}=13\sqrt{3}a$, $L_{y0}=22a$, consisting of two overlapping rectangular lattices sized 14×22 sites (odd columns in Fig. 4) and 13×21 sites (even columns in Fig. 4).

With these parameters we start with a ground state containing 4 skyrmions (Fig. 4). As we warm up the system, we will slowly and randomly increase the amplitudes of displacements of film sites and recalculate the ground state

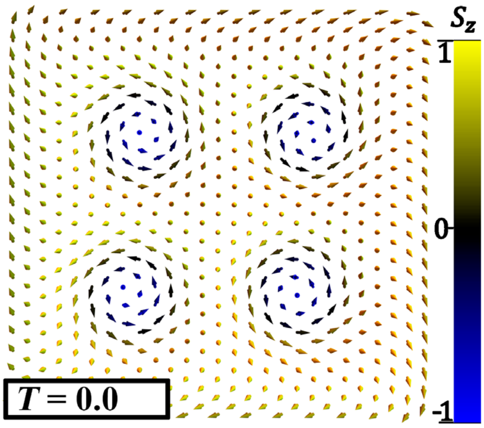


Fig. 4. (Color online) The ground state of the film with four skyrmions.

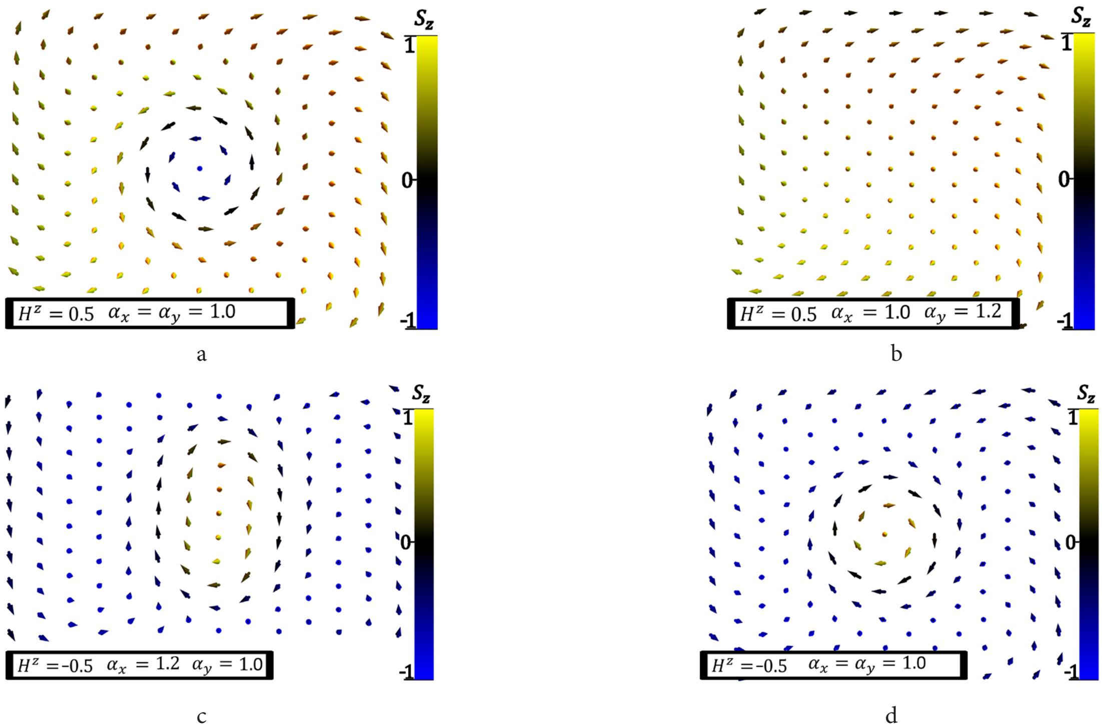


Fig. 3. (Color online) Skyrmion state switching by application of weak magnetic fields and uniaxial deformations.

at each step with exchange and DM parameters modified according to distances between sites. Using amplitude of displacements as a measure of temperature (as temperature is proportional to energy of oscillations which in turn is proportional to the square of amplitude) helps us avoid solving the huge system of equations of motions.

To calculate the order parameter $P_M(T)$ of the system we introduce two separate order parameters $P_s(T)$ and $P_r(T)$ for spins and positions, so that $P_M(T)=P_s(T)\cdot P_r(T)$:

$$P_s(T)=\left\langle \frac{1}{N}\sum_{i=1}^{N}\vec{S}_i^t(T)\cdot\vec{S}_i^0 \right\rangle_t, \quad (3)$$

$$P_r(T)=\left\langle \frac{1}{N}\sum_{i=1}^{N}\exp\left(-\left|\vec{r}_i^{\,t}(T)-\vec{r}_i^{\,0}\right|^2\right) \right\rangle_t. \quad (4)$$

Here $\vec{S}_i^0$, $\vec{r}_i^{\,0}$, $\vec{S}_i^t$ and $\vec{r}_i^{\,t}(T)$ denote i-th spin and position at the ground state and at temperature T accordingly, $\langle\ldots\rangle_t$ denotes averaging over 10 different states at the same temperature. . The parameters were chosen in this form such that at $T=0$ both are equal to 1.0, and at high temperatures and low order both tend to zero.

During the simulation we also calculated order parameter's susceptibility $\chi_m(T)$ as follows:

$$\chi_M(T)=\frac{\left\langle P_M(T)^2\right\rangle-\left\langle P_M(T)\right\rangle^2}{k_B T}. \quad (5)$$

To calculate topological charge of skyrmions described in Eq. (6) we first need to interpolate film's discrete spin field as a continuous magnetization field $\vec{M}(x,y)$:

$$Q_T=\frac{1}{4\pi}\iint \vec{M}\cdot\left[\frac{d\vec{M}}{dx}\times\frac{d\vec{M}}{dy}\right]dx\,dy. \quad (6)$$

To do so, we introduce an array of small neural networks, one network for every calculated state at every temperature step, so we will train $10\times 50=500$ individual networks. Each network consists of two hidden layers with 500 nodes each, input and output layers 3 node each: cartesian coordinates of sites $\vec{r}_i^{\,t}(T)$ as input signal and corresponding spin components $\vec{S}_i^t(T)$ as target output signal, total of 581 training data points for each neural network. After training each network is effectively becomes an interpolation function for the continuous spatial distribution of spin field, thus this function can be used as magnetization $\vec{M}(x,y)$ in Eq. (6). Networks were trained until the cost function went below 10^{-6}.

Order parameter, its susceptibility and topological charge at different temperatures are shown in Fig. 5. We have observed two distinct phase transitions corresponding to destruction of the first and second skyrmions.

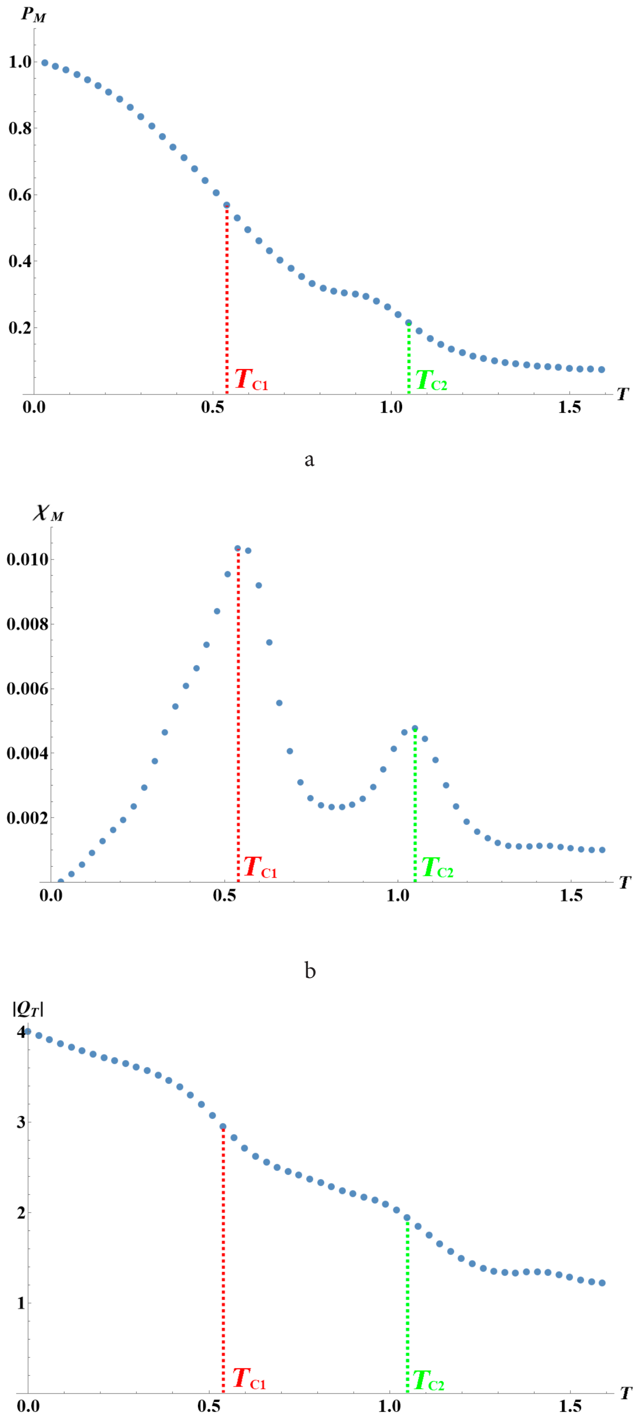


Fig. 5. (Color online) Order parameter, order parameter susceptibility and topological charge versus temperature. Red and green lines indicate two separate phase transitions when first and second skyrmions are destroyed.

5. Conclusion

We have investigated the effect of elastic uniaxial deformations and thermal fluctuations of crystal sites on the processes of skyrmion state switching and on the stability of skyrmions in the model with distance-dependent exchange and Dzyaloshinskii–Moriya interactions.

An energetically more favorable method of skyrmion states switching involving weak magnetic field and consecutive uniaxial deformations in orthogonal directions was developed, compared to the classic method using strong magnetic fields.

A simulation of thermal fluctuations of mobile crystal sites was carried out. We have discovered that the first two out of four initial skyrmions get destroyed at different critical points $T_{C1}\approx 0.54$ and $T_{C1}\approx 1.05$, which points at the topological stability of individual skyrmions and low correlation with other skyrmions.

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