NANOSYSTEMS:
PHYSICS, CHEMISTRY, MATHEMATICS

Potkina M.N., et al. *Nanosystems: Phys. Chem. Math.*, 2023, **14** (2), 216–222.
http://nanojournal.ifmo.ru
DOI 10.17586/2220-8054-2023-14-2-216-222

Original article

Nucleation and collapse of magnetic topological solitons in external magnetic field

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ABSTRACT The dependence of the lifetimes and rates of spontaneous nucleation of topological magnetic solitons on the external magnetic field is calculated within the framework of the harmonic transition state theory for magnetic degrees of freedom. For two-dimensional magnetic skyrmions, the influence of the magnetic field on the collapse rate was found to be greater than on the nucleation rate. This is explained by the weaker dependence of the energy of the transition state on the external field compared to the energy of the metastable skyrmion. The balance of the nucleation and collapse of skyrmion rates makes it possible to determine the average equilibrium concentration of skyrmions in a thin film as a function of the external field and temperature. It is shown that skyrmion and antiskyrmion states can exist simultaneously in quasi-two-dimensional thin films in tilted external magnetic field. The minimum energy paths for the collapse of these topological solitons and magnetic configurations in the vicinity of saddle point have been found and compared.

KEYWORDS transition state theory, topological magnetic solitons, nucleation, collapse, lifetime.

ACKNOWLEDGEMENTS The study was supported by the Russian Science Foundation grant No. 22-72-00059, https://rscf.ru/en/project/22-72-00059/.

FOR CITATION Potkina M.N., Lobanov I.S., Uzdin V.M. Nucleation and collapse of magnetic topological solitons in external magnetic field. *Nanosystems: Phys. Chem. Math.*, 2023, **14** (2), 216–222.

1. Introduction

Magnetic skyrmions, antiskyrmions and other structures with a topological charge are currently considered as promising elements for creating a new generation of magnetic racetrack memory [1]. This technology assumes that information is encoded in localized magnetic structures that can move at speeds of up to several kilometers per second along magnetic tracks. Devices for writing and reading information do not move, which increases the performance and energy efficiency of magnetic memory. The small size of the information carriers makes it possible to achieve high density of information storage [2–4].

The fundamental issues of using topological solitons as bits of magnetic memory are their stability with respect to thermal fluctuations and the ability to write, read, delete and move information contained in a sequence of magnetic structures.

The problem of stability becomes especially relevant as the size of magnetic elements, which determine the density of information storage, decreases. From a theoretical point of view, the quantitative estimate of the stability and calculation of the lifetime of magnetic states are complex problems associated with the fundamental problem of “rare events”. The rate of magnetic transitions associated with the nucleation and collapse of localized topological magnetic structures as a whole is 10–12 orders of magnitude lower than the frequency of oscillations of individual magnetic moments in the system. Therefore, stochastic modeling can be carried out in a very limited range of high temperatures, and standard stochastic methods do not allow one to determine quantitative characteristics of stability, such as the lifetimes of long-lived topological magnetic states. However, due to the difference in the time scales of the collective and individual motion of magnetic moments, statistical approaches such as the transition state theory (TST) [5] or the Kramers-Langer method can be used to analyze the rates of magnetic transitions [6].

These approaches are based on the analysis of the multidimensional energy surface of the system, the search for minimal energy paths (MEP) between states corresponding to certain magnetic configurations, the calculation of energy barriers between such states and the rates of overcoming these barriers [7]. Methods of statistical physics have shown their effectiveness for describing the thermal stability of a wide class of magnetic systems from clusters of several atoms [8] to micromagnetic structures [9]. The TST was used to estimate the activation barriers for the decay of skyrmions in thin chiral films under conditions of restricted sample geometry, in an external magnetic field, and in the presence of impurities [10–12]. This theory has also been used to evaluate the lifetime of three-dimensional hopfions [13], as well as quasi-two-dimensional skyrmions in antiferromagnets [14] and synthetic antiferromagnets [15].

The task and technology of recording information by creating specific topological magnetic configurations is even more difficult, since it is necessary to take into account both thermal fluctuations and certain external impacts that should cause the transition [16]. The process of nucleation of topological structures can be induced by an additional magnetic field [17], polarized spin current [18] or electric field impulses [19]. Furthermore, for any practical application of topological solitons, it is necessary to take into account thermal fluctuations, the presence of impurities and structural defects [20]. Therefore, TST for magnetic degrees of freedom, which was used to quantify the lifetime of magnetic states at an arbitrary temperature, is an adequate method for describing such effects.

The problem of nucleation of topological structures under the influence of thermal fluctuations has much in common with the TST-estimation of the stability of such structures. In this case, the topologically trivial ground state of the system should be chosen as the initial state, and the metastable state with a magnetic skyrmion should be considered as the final state. After finding the MEP, the activation barrier is determined by the energy difference between the transition and ground states of the system. If a skyrmion is metastable, the activation barrier for nucleation is higher than for its collapse. The pre-exponential factor in the Arrhenius law for the nucleation of skyrmions can be computed in harmonic approximation to TST if the energy surface near the initial ferromagnetic (FM) state and near the saddle point (SP) on the energy surface corresponding to the transition state is approximated by a quadratic expansions.

Of particular interest are the effects associated with a change in the topological charge during the nucleation of localized topological solitons. As in the case of collapse, topological protection on a discrete lattice should manifest itself through the magnitude of the energy barrier separating a spatially homogeneous state and a state with a nonzero topological charge. A decrease in the lattice constant with respect to the size of a topological soliton, while maintaining its shape, corresponds to the transition to a continuous distribution of magnetization and should shed light on the nature of topological effects in such systems. For magnetic skyrmions, such a transition gives the energy of the transition state corresponding to the minimum energy ($8\pi A$) of the topological soliton in the σ-model with the exchange stiffness A [21], regardless of other magnetic parameters – anisotropy, magnetization, and Dzyaloshinskii-Moriya interaction (DMI) [22]. Therefore, the barrier for the nucleation of a skyrmion must be the same in the continuous limit, regardless of all interactions, except for the symmetric exchange.

For skyrmions with sizes on the order of several lattice constants, the nucleation barriers depend on the entire set of magnetic parameters. The size of a skyrmion and, consequently, the processes of nucleation can be controlled by applying an external magnetic field [23, 24]. In thin films in an inclined magnetic field, solitons of different types with different topological charges can be nucleated. In particular, skyrmions and anti-skyrmions were simultaneously observed in quasi-two-dimensional films of Heusler alloys, and transitions between these states were stimulated by changing the magnetic field in the film plane [25, 26].

In the present work, we study the dependence of the nucleation rate of topological magnetic solitons on an external magnetic field, taking into account thermal fluctuations. The next section describes the model and method for calculating the intensity of the nucleation process at a given temperature and external magnetic field. Next, we present the results of calculations of the rate of spontaneous generation of magnetic skyrmions and their equilibrium concentration in magnetic fields perpendicular to the film, and study the stability of coexisting skyrmions and anti-skyrmions in an inclined field.

2. Methodology of calculations and simulated system

We consider quasi-two-dimensional topological solitons in the system described by the generalized Heisenberg model with the energy

$$E = -J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j - \sum_{\langle i,j\rangle}\mathbf{D}_{ij}\cdot(\mathbf{S}_i\times\mathbf{S}_j) - \mu\sum_i \mathbf{B}\cdot\mathbf{S}_i - K\sum_i(\mathrm{S}_i^z)^2, \quad (1)$$

where $\mathbf{S}_i$ is a three-dimensional vector of unit length in the direction of the magnetic moment at site i of a two-dimensional lattice. The first term describes the Heisenberg exchange with the parameter J for the magnetic moments of the nearest neighbors, the second term takes into account the DMI with the Dzyaloshinskii-Moriya vector $\mathbf{D}_{ij}$ lying in the plane of the sample perpendicular to the vector connecting the nodes of atoms i and j. The third and fourth terms correspond to the interaction with the magnetic field and the contribution of magnetic anisotropy with an easy axis along the z-axis perpendicular to the film plane. The magnetic moments μ, external field $\mathbf{B}$ and anisotropy parameters K are assumed to be the same for all lattice sites. The summation $\langle i,j\rangle$ in (1) runs over all pairs of nearest neighbor sites.

We will use two sets of parameters: the first of them corresponds to the experimentally observed skyrmions in the Pd/Fe bilayer on the Ir(111) [27] substrate: $\mu B = 0.093J$, $K = 0.07J$, D=$|\mathbf{D}_{ij}|$ = $0.32J$, J = 7 meV. Skyrmions are placed on a two-dimensional triangular lattice and have a size of the order of several nanometers. The second set describes stable at room temperature antiskyrmions 150 nm in diameter in Mn-Pt-Pd-Sn Heusler alloys [28, 29]. The numerical values of the parameters are $\mu B = 2.2\times10^{-4}J$, K=0, D=0.016 J, J = 1.83 eV.

Note that the value of the exchange parameter J is proportional to the film thickness, which was several tens of nm. Calculations with these parameters were carried out for magnetic moments at the nodes of a two-dimensional square lattice. To reduce computational costs, we used the scaling method, which allowed us to reduce the size of the system while maintaining the shape and energy of topological solitons [29]. The system under consideration was taken $N = 20$ times less dense and the model parameters were changed accordingly ($D' = ND, \mu' = \mu N^2$) [22].

The multidimensional energy surface of the system is a functional of variables that uniquely determine the magnetic configuration. As such variables for model (1), one can use the angles that specify the directions of the magnetic moments.

Then, the "geodesic nudged elastic band method" [30] can be used to find a MEP between locally stable states. Instead we will use here the Cartesian coordinates for the vectors of magnetic moments, and the condition of the constancy of the magnitude of the magnetic moments at each site will be taken into account by introducing Lagrange multipliers. This approach allows to avoid singularities and simplifies computations of Hessians of energy [7,31]. For the rate of nucleation processes k_{nuc} in the harmonic approximation of TST, one can obtain an expression corresponding to the Arrhenius law

$$k_{nuc} = k_0 \exp\left(-\frac{E_{SP}}{k_B T}\right). \tag{2}$$

The activation energy of the skyrmion nucleation process is equal to the energy of the SP on the MEP E_{SP} relative to the FM state.

The pre-exponential factor, as in the case of collapse, can be written as the product of the dynamic and entropy parts:

$$k_0 = \frac{1}{2\pi} k_{dyn} k_{ent}. \tag{3}$$

The dynamic prefactor k_{dyn} depends only on the shape of the energy surface near the transition state. In the framework of TST, this contribution arises from the calculation of the rate of crossing the transition state from FM to the skyrmion state. Within the harmonic approximation, the dynamic prefactor for nucleation and collapse of skyrmion is the same. This factor can be calculated as follows [13]:

$$k_{dyn} = \sqrt{\frac{\boldsymbol{b} \cdot \mathcal{H}^{SP} \boldsymbol{b}}{|\zeta_s^1|}}, \quad b_i = \frac{\gamma}{\mu} \zeta_s^1 S_i^{SP} \times e_i. \tag{4}$$

Here S_i^{SP} is the spin configuration at the SP, $\mathcal{H}^{SP}$ is the Hessian of energy in this point, and $\boldsymbol{e}$ is the unit eigenvector corresponding to the only negative eigenvalue ζ_s^1 of the operator $\mathcal{H}^{SP}$. The constant γ is the gyromagnetic ratio. The entropy prefactor is the square root of the ratio of the modulus of determinants of Hessians $\mathcal{H}^{FM}$ and $\mathcal{H}^{SP}$ at homogeneous FM state and the SP respectively.

$$k_{ent} = \sqrt{\frac{\det \mathcal{H}^{FM}}{|\det \mathcal{H}^{SP}|}}. \tag{5}$$

If the harmonic expansion of energy near the saddle point contains zero modes corresponding to degrees of freedom for which the energy does not change significantly, then the entropy prefactor contains an additional factor k_{ZM} depending on temperature:

$$k_{ZM} = \frac{V_{SP}}{(2\pi k_B T)^{\frac{P_{SP}}{2}}}, \tag{6}$$

where V_{SP} give the volume corresponding to zero modes while P_{SP} the number of such modes. The dimensionality of $\mathcal{H}^{SP}$ in this case decreases by P_{sk}. It is worth noting that for the reverse process corresponding to the collapse of a topological soliton into a FM state, zero modes can also exist in the initial state. In this case, a factor similar to (6) will appear in the denominator of the expression for the entropy factor (5).

Knowing the rate of collapse k_{col} and nucleation k_{nuc} of skyrmion states makes it possible to estimate the equilibrium concentration of skyrmions n at arbitrary temperatures. In the equilibrium, the number of generated and decayed skyrmions per unit time should be the same. A skyrmion can be nucleated at any site of the lattice, and can be destroyed only where it was. The concentration is governed by the balance equation:

$$n k_{col} = n_s k_{nuc}. \tag{7}$$

where n_s is the density of sites in the lattice. Substituting the values of the rates and taking into account that the dynamic prefactor for decay and nucleation are the same, we obtain

$$n = n_s \frac{V_{SK}}{(2\pi k_B T)^{\frac{P_{SK}}{2}}} \exp\left(-\frac{E_{SK}}{k_B T}\right) \cdot \sqrt{\frac{\det \mathcal{H}^{FM}}{\det \mathcal{H}^{SK}}}, \tag{8}$$

where E_{SK} is the energy of the skyrmion state relative to the FM state. By P_{SK} and V_{SK} we have denoted, respectively, the number of zero modes and their volume for the equilibrium skyrmion state. The equilibrium concentration does not depend on the shape of the surface near the SP and the height of the energy barrier between the states. Only the time of equilibrium establishment depends on these quantities.

3. Results

Let us first consider the possibility of controlling the process of skyrmion nucleation due to thermal fluctuations in the PdFe bilayer on the Ir(111) surface. Tunneling microscopy methods have shown that in this system the equilibrium size of skyrmions and their lifetime depend on the strength of the external magnetic field. At a temperature of 4.2 K, the skyrmion structure remains stable up to fields of 5–6 T [27] . This means that skyrmions do not appear or disappear during the observation time if the current from the tip of the tunneling microscope used to observe the skyrmions is small enough [17]. As the temperature rises, the nucleation and collapse of skyrmions occur more and more often, and then the system passes into a fluctuation-disordered state, in which, along with skyrmions, there are also high-energy non-collinear localized and delocalized magnetic states [32].

Fig. 1 shows the temperature dependence of the average lifetime of skyrmion states, the average waiting time for the nucleation of a skyrmion at a selected lattice site, and the equilibrium concentration of skyrmions after the establishment of thermodynamic equilibrium. Circles and squares correspond to external magnetic fields $B = 3.75$ T and $B = 4.6$ T, respectively.

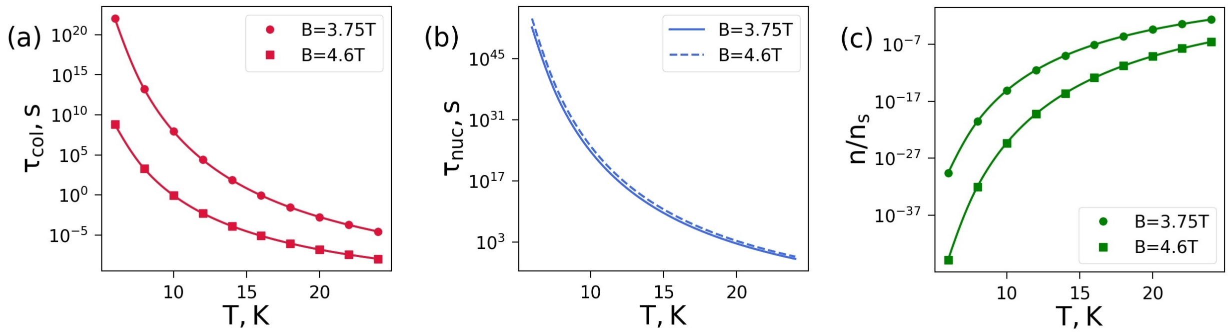

FIG. 1. Temperature dependence of the average waiting time for the collapse of a skyrmion τ_{col} (a), its nucleation τ_{nuc} (b) and the equilibrium number of skyrmions per lattice site (c) for two values of the external magnetic field $B = 3.75$ T (circles) and $B = 4.6$ T (squares)

At low temperatures up to 10 K, the spontaneous nucleation of skyrmions due to thermal fluctuations is practically impossible. The lifetime of already existing skyrmions ranges from a few seconds at a field of 3.75 T to several years at 4.6 T, as seen in Fig. 1a. In this case, the equilibrium concentration of skyrmions is negligible. As the temperature rises, the probability of collapse and nucleation also increases, but for nucleation it occurs faster in accordance with Fig. 1b. As a result, the equilibrium concentration of skyrmions increases, and in the region of 1000×1000 lattice sites, one can expect the appearance of several skyrmions in moderate magnetic fields and temperature 15–20 K, as follows from Fig. 1c.

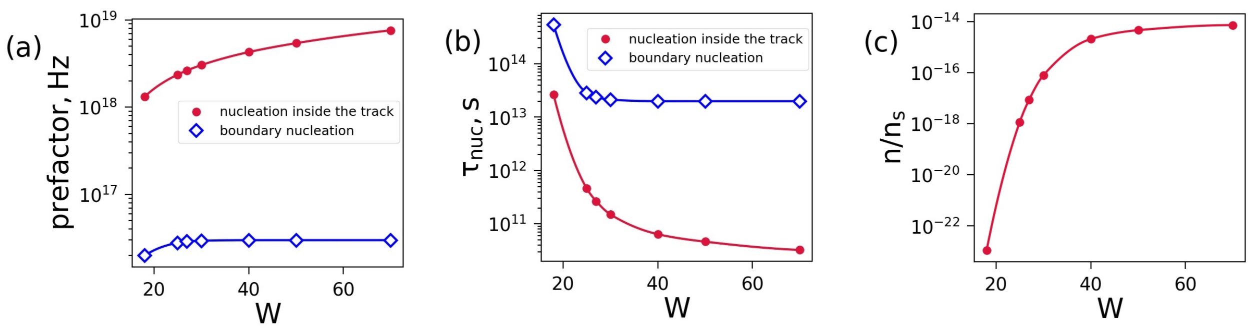

FIG. 2. The pre-exponential factor k_{nuc} for the rate of skyrmion nucleation on the magnetic track (a) and the average waiting time τ_{nuc} for nucleation at a particular lattice site (b) depending on the track width W. Filled red circles and empty blue rhombuses correspond to nucleation in the middle and at the border of the track, respectively. Equilibrium skyrmion concentration inside the track n/n_s as function of track width (c). T=15 K, B =4.6 T

The increase in concentration with temperature is associated with both energy and entropy effects. Note that the skyrmion and the transition state for collapse (nucleation) are metastable. As the temperature increases, the exponential factor in the Arrhenius law for the lifetime decreases, and the entropy factor $1/k_{ent}$ plays an increasingly important role. The entropy of the skyrmion state is greater than that of the transition state, and in the transition state it is greater than that of the ground state. This leads to the relation $k_{nuc} \gg k_{col}$. Therefore, with an increase in temperature, the rate of nucleation processes rapidly increases and can be comparable with the rate of skyrmion collapses and even exceed it. In which state it is more likely to detect a system at a fixed temperature depends on the magnitude of the external magnetic field. This has been done to write and delete single magnetic skyrmions using current injection from the tip of tunnel microscope [17].

In the practical development of technologies based on the use of topological solitons, it is necessary to take into account structural defects and the influence of boundaries on the stability, collapse, and nucleation of localized topological states [10, 12]. The nucleation of skyrmions under the action of the current from the tip of tunneling microscope occurs usually near local defects [17]. Such defects and the proximity of the sample boundary reduce the energy of the transition

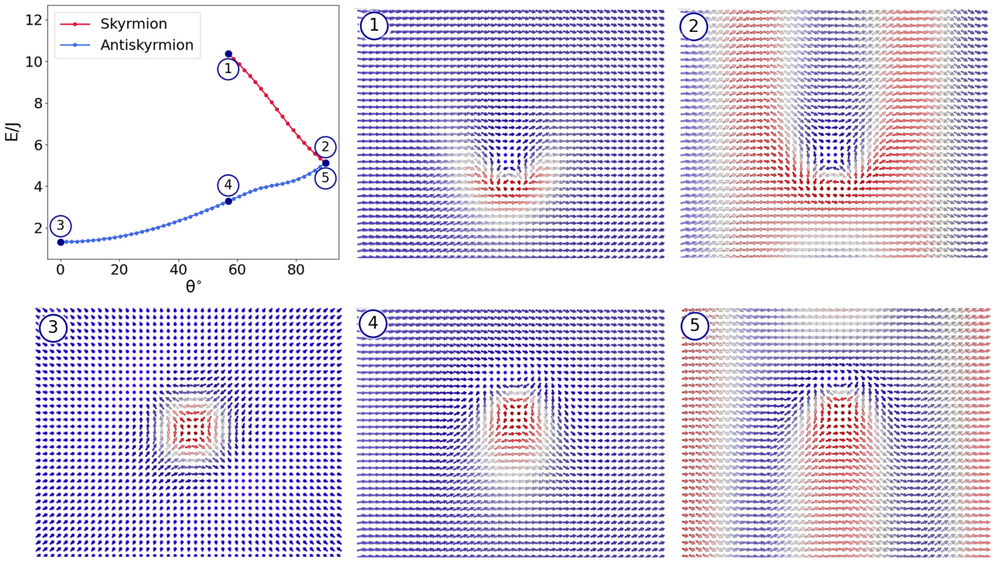

FIG. 3. Energy of antiskyrmion and skyrmion states as a function of the angle θ of inclination of the magnetic field. Configurations (1), (2), (3), (4) and (5) correspond to the marked points on the graph and show the evolution of the skyrmion and antiskyrmion states with an increase in angle θ

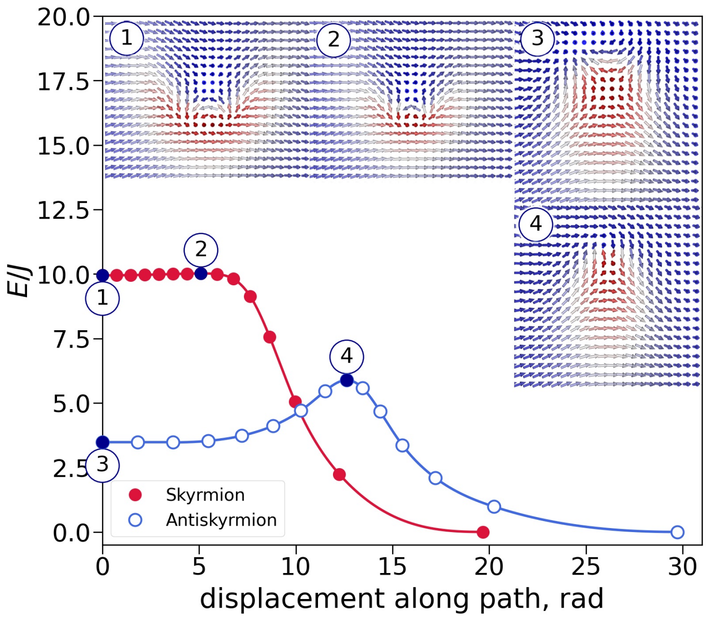

FIG. 4. MEPs for the collapse of a skyrmion (solid red circles) and an antiskyrmion (empty blue circles) in an inclined magnetic field (angle of inclination 60°). The insets show the magnetic configurations corresponding to equilibrium skyrmion (1), transition state during the decay of a skyrmion (2), equilibrium antiskyrmion (3), and the transition state during the decay of the antiskyrmion

state and, consequently, the activation barrier for collapse and nucleation of skyrmions. In addition, another way for the creation (annihilation) of skyrmions at the border has appeared [7, 22]. Therefore, nucleation processes, taking into account the finite size of the system, such as magnetic track of finite width, are of particular interest.

Fig. 2a shows the dependence of the pre-exponential factor for skyrmion nucleation inside the magnetic track and at its boundary on the track width W. It can be seen that the prefactor for nucleation at the boundary is significantly lower than for such a process inside the sample, and the characteristic waiting time for nucleation at the boundary is much longer, as can be seen in Fig. 2b. Besides, there are fewer atoms at the border of the track than inside it. Therefore, when calculating the average concentration, nucleation at the boundary can be neglected. Fig. 2c shows the equilibrium concentration of skyrmions localized in the magnetic track. It is negligibly small for narrow layers, but with increasing width it reaches a value corresponding to the concentration in an unlimited sample.

Let us now turn to the behavior of topological solitons in an inclined magnetic field. Here, we study the antiskyrmion state in magnetic field tilted with respect to the normal of the sample surface of Heusler alloy [28]. Plot in Fig. 3 (top left) shows the energy of antiskyrmion state as a function of slope angle θ (blue curve). When θ reaches a value of about 57°, the coexistence of the skyrmion state with the antiskyrmion state is observed (red curve). Fig. 3 (1)-(5) show the evolution of skyrmion and antiskyrmion state with an increase in the angle of inclination of the magnetic field. Coexisting particles with opposite topological charges were discovered in experimental works [25, 26]. There, counterpart state was obtained from antiskyrmion by tilting the magnetic field, which is in agreement with our simulation.

Fig. 4 shows the MEPs for the collapse of an antiskyrmion and a skyrmion into a homogenious FM ground state. These topological solitons simultaneously exist in a tilted magnetic field with inclination angle $\theta = 60^\circ$ but the energy of a skyrmion is greater than that of an antiskyrmion, and the barrier for the collapse of the skyrmion is much lower. However, increasing θ to 90° which correspond to an in-plane magnetic field leads to the identic MEPs and barriers. In the inserts of Fig. 4 the magnetic configurations in the initial states and at saddle points are shown. It is worth to note that the size of a noncollinear structure in the saddle point in an inclined magnetic field does not decrease significantly, in contrast to the case of a field perpendicular to the surface. This may be important for the value of entropy prefactor in Arrhenius law for lifetime and therefore affect the stability of the states [33].

4. Conclusion

The possibility of controlling the processes of spontaneous nucleation and collapse of topological magnetic solitons can be implemented by choosing the temperature regime and the external magnetic field. This allows writing and deleting information encoded in a sequence of topological magnetic structures. In an inclined magnetic field, localized magnetic configurations with different topological charges can simultaneously exist. Their stability and the activation energy of the nucleation and collapse can be operated by changing the angle of inclination of the magnetic field.

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Submitted 15 March 2023; revised 14 April 2023; accepted 15 April 2023

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Conflict of interest: the authors declare no conflict of interest.