Thermal Collapse of a Skyrmion

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Thermal collapse of an isolated skyrmion on a two-dimensional spin lattice has been investigated. The method is based upon solution of the system of stochastic Landau-Lifshitz-Gilbert equations for up 10⁶ spins. Recently developed pulse-noise algorithm has been used for the stochastic component of the equations. The collapse rate follows the Arrhenius law. Analytical formulas derived within a continuous spin-field model support numerically- obtained values of the energy barrier and the pre-exponential factor, and their dependence on the magnetic field. Our findings agree with experiments, as well as with recent numerical results obtained by other methods.

I. INTRODUCTION

Skyrmions are whirls of spins stabilized by topology. The topological protection of skyrmions has motivated recent research on their nucleation and manipulation in thin magnetic films. It arises from the mapping of a three-component fixed-length spin field on a two-dimensional (2D) coordinate space. Topological properties of skyrmions were first derived for the 2D Heisenberg exchange model. In practice they are violated by the discreteness of the atomic lattice that breaks the continuity of the spin field and the scale invariance of the exchange model. Other interactions such as Zeeman, dipole-dipole interaction (DDI), interaction of skyrmions with defects and thermal phonons, etc., further break the symmetry and stability of skyrmions, leading to their uncontrolled collapse or expansion. For that reason they are typically observed in non-centrosymmetric materials. The lack of inversion symmetry results in the Dzyaloshinskii-Moriya interaction (DMI). It competes with other material-dependent interactions, providing stability of skyrmions within a certain area of the phase diagram. Stable isolated skyrmions have been experimentally observed even at room temperatures.

Skyrmions provide a promising avenue for new forms of memory storage because information can be encoded in them as bits. Recent advances in nucleation methods have accelerated interest in skyrmions by demonstrating the feasibility of skyrmion writing devices. One promising method involves application of a spin-polarized current using a scanning tunneling microscope. Such a method can both nucleate and erase skyrmions, as was demonstrated on a PtFe/Ir(111) system. Additionally, recent experimental and theoretical work has explored the possibility of skyrmion creation by temperature by local heating and with the help of the magnetic force microscope (MFM) tip or a magnetic dipole. The ability of a stable skyrmion to form depends on both the material parameters and the external conditions, such as the magnetic field and temperature. It has been experimentally demonstrated that the size of a skyrmion can be tuned by the external field, with its radius shrinking on increasing the field until the skyrmion disappears.

In practice the stability of skyrmions against thermal or quantum collapse provides a limit on potential applications. Quantum decay of a skyrmion has been recently studied by a method based upon finding an instanton solution of the imaginary-time equations of motion. The statistical mechanics problem of the thermal collapse of a skyrmion is more involved. It has been explored for various systems, both for a skyrmion in a racetrack and an isolated skyrmion in a thin film. Although most of the investigators have studied purely 2D systems, some have considered multilayered systems as well. The latter are relevant to recent experimental advances in creating room temperature skyrmions, while numerical models of purely 2D systems apply to skyrmions found in B20 materials. All previous work relies on either Monte Carlo simulations or micromagnetic methods that search for the minimum energy path between two equilibrium states.

In this paper we present results of skyrmion stability computations on a 2D lattice using the stochastic Landau-Lifshitz-Gilbert (LLG) equation, where the stochastic component is accounted for with a pulse-noise algorithm. The latter, while being a powerful mathematical tool, also closely mimics interactions of spins with thermal phonons. Such a strategy has been previously implemented in examining phase transitions in various magnetic systems and thermal stability of single-domain magnetic particles. Here we extend the pulse-noise method to an isolated skyrmion on a 2D lattice. This allows us to compute the collapse rate of the skyrmion as the function of temperature. In evaluating the stochastic LLG in the presence of the pulse noise, we do not assume any particular collapse path. Instead, we solve numerically the system of stochastic differential equations that governs the motion of each spin in the lattice. The results fit the Arrhenius dependence is typical for overbarrier transitions driven by temperature. It has been observed experimentally in the decay of the array of skyrmions in a film.

The paper is organized as follows. In Section II the analytical model is discussed. In Section III details of the numerical method are presented. In Section IV results of the numerical computation and comparison to the analytical model are given. Lastly, a discussion of the results is given in Section V.

II. MODEL

We consider a two-dimensional square lattice of spins, \( s_i = S_i/|S_i| \) where \( S_i \) is a three-dimensional vector and \( i \) refers to
the lattice site. The Hamiltonian of the system is given by
\[
\mathcal{H} = -J \sum_{ij} s_i \cdot s_j - A \sum_i (s_i \times s_{i+\hat{x}}) \cdot \hat{x} + (s_i \times s_{i+\hat{y}}) \cdot \hat{y} - \mathbf{H} \cdot \sum_i s_i, \tag{1}
\]

The first term represents the Heisenberg exchange energy with the exchange constant \( J \) and sum being taken over the nearest neighbors. The second term represents the Dzyaloshinskii-Moriya interaction (DMI). For certainty we have chosen a Bloch type DMI. The last term is the Zeeman interaction energy due to the external field, \( \mathbf{H} \). The skyrmion that we consider will be stabilized by a field applied into the plane so that the Zeeman term becomes \( H \sum s_i z \).

The continuous analog of this energy is
\[
\mathcal{H} = \frac{1}{2} JS^2 \int dxdy \left[ \left( \frac{\partial s}{\partial x} \right)^2 + \left( \frac{\partial s}{\partial y} \right)^2 \right] - \frac{1}{24} JS^2 \int dxdy \left[ \left( \frac{\partial^2 s}{\partial x^2} \right)^2 + \left( \frac{\partial^2 s}{\partial y^2} \right)^2 \right] + AS^2 \int dxdy \left[ (s \times \frac{\partial s}{\partial x}) \cdot \hat{x} + (s \times \frac{\partial s}{\partial y}) \cdot \hat{y} \right] - HS \int dxdy s_z, \tag{2}
\]

where all lengths are measured in the units of the lattice spacing \( a \). The second term in this expression arises from taking into account the next derivatives in the expansion of the discrete form of the exchange energy that dominates spin interactions at small distances.

The continuous unit-length field \( s \) is characterized by the topological charge:
\[
Q = \frac{1}{4\pi} \int dxdy \cdot s \times \left( \frac{\partial s}{\partial x} \times \frac{\partial s}{\partial y} \right), \tag{3}
\]

that takes discrete values \( Q = 0, \pm 1, \pm 2, \ldots \).

The first, dominant, term in Eq. (2) gives rise to the Belavin-Polyakov (BP) skyrmion \(^3\) with the spin components
\[
s_x = 2\lambda r \left( \cos \phi \cos \gamma - \sin \phi \sin \gamma \right) \frac{1}{r^2 + \lambda^2},
\]
\[
s_y = 2\lambda r \left( \sin \phi \cos \gamma + \cos \phi \sin \gamma \right) \frac{1}{r^2 + \lambda^2},
\]
\[
s_z = \frac{\lambda^2 - r^2}{\lambda^2 + r^2},
\]

written as functions of polar coordinates, \( r = \sqrt{x^2 + y^2} \) and \( \phi \), in the \( xy \) plane. Here \( \lambda \) is the skyrmion size and \( \gamma \) is the chirality angle. It is the energy minimum of the first term in Eq. (2) within the homotopy class \( Q = 1 \). That energy minimum is independent of \( \lambda \) and \( \gamma \) and equals \( E = 4\pi JS^2 \).

Interactions weaker than the ferromagnetic exchange that are present in Eqs. (1) and (2) deform the BP skyrmion and make its energy depend on \( \lambda \) and \( \gamma \). However, for the smallest skyrmions the extremal solution of the corresponding equations of motion are still close to the BP shape. \(^2\) This allows one to estimate the energy of a small skyrmion by substituting Eq. (4) into Eq. (2). The result reads
\[
E = 4\pi JS^2 - \frac{2\pi JS^2}{3\lambda^2} - 4\pi AS^2 \lambda \sin \gamma + 4\pi |H|S^2 \lambda^2 \gamma (\lambda). \tag{5}
\]

The second term in Eq. (5) comes from the discreteness of the lattice. It favors the shrinkage of the skyrmion. \(^3\) The third and the fourth terms come from the integration of the DMI and Zeeman interactions. The factor \( I(\lambda) \) depends logarithmically on \( \delta_H/\lambda \) and \( L/\lambda \), with a shorter of the two lengths, \( \delta_H = \sqrt{JS/H} \) or the size of the system \( L \), dominating the dependence. Stabilizing magnetic field is applied opposite to the magnetic moment of the skyrmion, making the sign of the Zeeman term positive.

The energy in Eq. (5) is minimized by the Bloch-type skyrmion with \( \gamma = \pi/4 \). It is plotted in Fig. 1 for different fields, as function of the skyrmion size \( \lambda \). On increasing the field the energy minimum shifts towards smaller \( \lambda \). At \( H > H_{\text{crit}} \) the minimum no longer exists, making skyrmions of size \( \lambda < \lambda_{\text{crit}} \) absolutely unstable against the collapse.

With the logarithmic accuracy \( |H_{\text{crit}}|/(JS) \sim (A/J)^{1/3} \) and \( \lambda_{\text{crit}}/a \sim (J/A)^{1/3} \). Close to the critical field the energy barrier in Eq. (5) scales as \( U/(JS^2) \sim (A/J)^{2/3} (1 - |H|/H_{\text{crit}})^{3/2} \). The frequency of the oscillation of the skyrmion size near the bottom of the potential well scales as \( \omega_a/(JS) \sim (A/J)^{4/3} (1 - |H|/H_{\text{crit}})^{1/4} \). If one assumes that thermal fluctuations make the skyrmion to climb the energy barrier by shrinking without changing its shape, the expected thermal collapse rate should be \( \Gamma = \Gamma_0 \exp(-U/T) \), with the pre-exponential factor given by the attempt frequency, \( \Gamma_0 = \omega_a/(2\pi) \), at low damping. This assumption is confirmed by our numerical experiment (see below) illustrated in Fig. 2.
FIG. 2. Stages of skyrmion thermal collapse. From left to right: The skyrmion shrinks while preserving its shape. Color code: green/yellow = negative/positive $s_i$.

III. NUMERICAL METHODS

We approach the problem of skyrmion thermal collapse by evaluating the stochastic LLG equation on a 2D spin lattice. The time evolution of each spin in the lattice satisfies

$$\mathbf{s} = \gamma [\mathbf{s} \times (\mathbf{H}_{\text{eff},i} + \xi_i)] - \gamma \alpha [\mathbf{s} \times (\mathbf{s} \times \mathbf{H}_{\text{eff},i})],$$

(6)

where $\gamma = g \mu_B / \hbar$ is the gyromagnetic ratio (with $\mu_B$ being the Bohr magneton and $g$ being the gyromagnetic factor), $\alpha$ is a dimensionless damping parameter, $\mathbf{H}_{\text{eff},i} = -\partial \mathcal{H} / \partial \mathbf{s}_i$ is the effective field acting in the $i$-th spin, and $\xi_i$ is the stochastic field due to thermal fluctuations.

To begin, we compute a stable skyrmion spin configuration at zero temperature and some specified magnetic field by integrating the LLG equation. The skyrmion evolution converges to a minimum. By then applying Eq. (6) with a thermal noise of $\xi_i$, one can induce the collapse of the skyrmion and record the amount of time it takes. One way to quantify this collapse is through monitoring the topological charge given by Eq. (3). Collapse events are marked by sharp drops in the topological charge.

Typical numerical approaches to stochastic differential equations use white noise, which amounts to generating a random noise generator and the order of the numerical solver leads to relatively slow integration. While there have been advances in using midpoint and self-correcting midpoint methods, the approaches have still proven to not be advantageous. The problems with stochastic numerical solvers have been addressed in recent implementations of a pulse-noise method, where evaluation of the stochastic LLG where carried out using any numerical scheme, permitting higher order ones like fourth- and fifth-order Runge-Kutta methods.

The motivation behind the pulse-noise method relies on the separability of the noise-free and noise-induced time evolution of the spins, where $\Delta t$ is the length of the free zero-temperature evolution and $\delta t$ is the length of the noise evolution. By isolating the noise-evolution, we reduce the amount of time spent on generating random numbers and increase the efficiency of the noise-free numerical solver. The pulse-noise method has been used in analyzing the thermal magnetization switching of single-domain particles and phase transitions in classical spin systems, see Refs. 26,27 for details.

In our work, we use a fourth-order Runge-Kutta discretization scheme for the noise-free evaluation. Then each spin is rotated by a random angle whose magnitude and direction come from the stochastic field, $\xi_i$, given by

$$\xi_i = \sqrt{2aT / \gamma \mu_0} G_i,$$

(7)

Here $G_i$ is a normalized three dimensional vector with components generated from a random Gaussian distribution, $T$ is the temperature, and $\mu_0 = g \mu_B S$ is the magnetic moment associated with $s$. Each pulse-noise implementation corresponds to a rotation of the spins by the angle

$$\phi_i = \sqrt{\Lambda N \Delta t} G_i,$$

(8)

where $\Lambda N = 2 \gamma \hbar T / \mu_0$. The random noise must be Gaussian in order for the equation to reduce to the Fokker-Plank equation,

$$\langle \xi_{ij}(t), \xi_{kj}(t') \rangle = 2aT / \gamma \mu_0 \delta_{ij} \delta(t-t').$$

(9)

With these relations, we are able to compute the thermal collapse times of a single skyrmion. Previous work in calculating skyrmion lifetimes has been done using variations of the Nudged Elastic Band Method (NEBM) in which the minimum energy path between two equilibrium states was found. In this way, it was possible to find the energy barrier against various types of collapse and subsequently calculate the skyrmion mean lifetime for particular collapse mechanisms. The rate of collapse found by the NEBM requires guessing the path between the two equilibrium states and then varying that guess to find the minimum energy path between the states. Our method differs from these in that it relies on the equations of motion of the spins themselves, with an additional stochastic component. It does not assume any particular collapse path.

Our numerical computations were done on a $100 \times 100$ lattice with periodic boundary conditions. All energies have been measured in units of $JS^2 = 1$, while times have been measured in units of $\hbar / JS$. The DMI constant $A$ was set to 0.02 $J$. A maximum time of $10^6$ was set in all thermal collapse computations, and a noise-free evolution of $\delta t = 0.2$ was used. The thermal collapse computation was run 300 times for each temperature in parallel on a 40-node computing cluster. For the damping parameter in the LLG equation we chose $\alpha = 0.01$. In order to calculate the collapse rate, $\Gamma$, we calculated the probability of the skyrmion collapse within a time $t_i$ and determined the collapse rate and the energy barrier by fitting them to the Arrhenius law $\Gamma = \Gamma_0 \exp (-U / T)$.
IV. THERMAL COLLAPSE

We compute the thermal collapse rate of an isolated skyrmion by numerically solving the system of stochastic LLG equations at various temperatures. Our initial state is a BP skyrmion given by Eq. (4). By solving the equations of motion for the spins we first determine the equilibrium spin configuration at zero temperature. We then examine this skyrmion’s stability against thermal collapse by turning on temperature in the stochastic LLG equation. After some time the skyrmion collapses and the system transitions into the uniformly magnetized ferromagnetic state. By repeating this procedure several hundred times, we collect data on the collapse rate at a particular temperature. By then repeating the process at various temperatures we find an exponential dependence of $\Gamma$ on $1/T$ in agreement with the Arrhenius law, as shown in Fig. 3.

The energy barriers obtained from the Arrhenius law at various magnetic fields are presented in Fig. 4. It is interesting to compare the values determined numerically to the ones found by analytically computing the difference between the maximum and minimum of the energy curve in Eq. (5). Notice that the analytical model assumes continuity of the spin-field. Consequently, the results obtained analytically for the continuous spin field and numerically with the discrete model are expected to be close to each other only when spins rotate by a small angle from one lattice cite to the neighboring one. This is certainly not the case for small skyrmions, see Fig. 2.

Nevertheless, a qualitative agreement should be expected. While one cannot directly compare values at the same external field in both models, comparison of the barriers at the same displacement from the critical field offers some interesting agreement. The critical field in the discrete numerical model is $H_{\text{crit},N} = 0.00259 JS$, while the one in the analytical model (determined by the inflection point in the energy vs $\lambda$ in Fig. 1) is $H_{\text{crit},A} = 0.00134 JS$. Away from the critical field, we show that the barriers obtained by the two methods are approximately the same when computed as functions of $1 - |H|/H_{\text{crit}}$, see Fig. 5.

In order to predict the lifetime of a skyrmion, one must also examine the pre-exponential factor in the Arrhenius law, as this establishes the time scale for the collapse. Its typical values in problems of thermal collapse range from $10^9$ to $10^{11}$ Hz. We present our results in Fig. 6. The order of magnitude of the prefactor found in our computations is in agreement with the previous numerical work that uses spin dynamics computations, as presented in Fig. 6. Values of $\Gamma_0$ are on the order of $10^{11}$ Hz, when using $J = 10^3$ K. It has been shown experimentally that the pre-exponential factor varies with small changes in the external magnetic field, which we also observe in our data. Close to the critical field we see a drop in the attempt frequency to the values on the order of $10^9$ Hz. This is expected, since the energy minimum in which the skyrmion lives flattens out as the external field approaches the critical field, see Fig. 1.

Further quantitative analysis of the pre-exponential factor poses a challenge because of its possible dependence on temperature besides dependences on the external field and other parameters in the problem. A temperature-dependent analysis of the prefactor has been given in Ref. 28, in which the authors used the presence of Goldstone modes to derive the influence of the temperature. In our approach to the problem we must...
also take into account the influence that the damping parameter, $\alpha$, in the LLG equation has on the pre-exponential factor. It has already been shown analytically in a simpler problem of thermally activated escape rates of single spins\textsuperscript{[26,40]} that the $\alpha$-dependence of the pre-exponential factor has a few regimes. Similar problem for the skyrmion decay remains a challenging task.

Having derived in Section\textsuperscript{[11]} the analytical relationship between the energy barrier and small displacements from the critical field, we can compare it with our numerical results. To do this, we find the critical field in the discrete model and then compute the energy barriers at field values close to this critical one. We run the LLG equation at zero temperature on a BP skyrmion until the system’s energy converges to a minimum, then we increase the external field in small increments. We observe that the skyrmion shrinks, as has been demonstrated in experiments\textsuperscript{[23,35]}. Increasing the field further, we find the value of the field at which the skyrmion disappears. This is the critical field at which the energy minimum shown in Fig. 1 disappears. It is now possible to create a small energy barrier by slightly varying the external field and compute the collapse rate for a skyrmion by applying the stochastic LLG equation to the spin lattice. We again fit the collapse times to the Arrhenius law and determine the energy barriers at various magnetic fields. Our numerical results close to the critical field agree with the analytical ones, as shown in Fig. 7. Here we fit the computed energy barriers to the function $\ln U = c + n \ln \varepsilon$. The value of $n = 1.45$ is close to the analytical result $n = 3/2$.

\section{Discussion}

We have numerically modeled the thermal collapse of a skyrmion stabilized by the ferromagnetic exchange, DMI, and external magnetic field in a two-dimensional lattice. Using the stochastic Landau-Lifshitz-Gilbert equation and approximating thermal fluctuations through a pulse-noise algorithm, we have computed the time evolution of each spin in the lattice. In this way, we modeled the evolution of the skyrmion in time.

The values used in the computations were $S = 1$ for the spin, $A/J = 0.02$ for the ratio of DMI to exchange, and $\alpha = 0.01$ for the damping parameter. The value of the exchange constant $J = 10^3 K$ was chosen for estimates of the attempt frequency.

These are typical parameters of magnetic materials used in the experiments with skyrmions.

With the parameters chosen the energy barriers for the skyrmion collapse ranged from a few meV to a few tens of meV depending on the field. Such a strong dependence of the energy barrier on the magnetic field in the same ball park has been observed experimentally in a skyrmion lattice\textsuperscript{[13]}. There has been much discussion of entropy and the effect that it has on the pre-exponential factor in the Arrhenius law for thermal decay of skyrmions\textsuperscript{[26,28,38]}. The complicated phase space of a skyrmion in a two-dimensional lattice leads to many possible collapse paths, which means that the entropy plays a role in the collapse. This problem, however, is no different from other nucleation problems in statistical mechanics and the method we used is well suited for solving it.

The previous work has suggested that the skyrmion collapse rate may be affected by changes in the pre-exponential factor alongside with the changes in the energy barrier\textsuperscript{[26,38]}. We found evidence of this effect on our simulations. This motivates further research on how the pre-exponential factor impacts the skyrmion lifetime at elevated temperatures.

Since we considered a system with periodic boundary conditions, the only way for the skyrmion to vanish (besides quantum decay\textsuperscript{[24]}), was its spontaneous over-barrier shrinking due to thermal fluctuations to the size below which it collapses. This is a generic problem of skyrmion thermal collapse that must be of interest for experiments with skyrmions at elevated temperatures, as well as for applications of skyrmions in logic devices.

It has been shown previously\textsuperscript{[26]} that in systems with boundaries there is a range of external fields for which skyrmion escape through the boundary has a lower energy barrier than that for the internal collapse. This possibility has sparked interest in methods of suppressing such escape by, e.g., altering the DMI at the boundary\textsuperscript{[24]}. It has been shown that skyrmion stability can also be increased by the exchange frustration\textsuperscript{[45]}. Our method can be easily generalized for the study of these effects as well as for the studies of bilayers\textsuperscript{[14]} and slabs.
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