Duplication, Collapse, and Escape of Magnetic Skyrmions Revealed Using a Systematic Saddle Point Search Method

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Various transitions that a magnetic Skyrmion can undergo are found in calculations using a method for climbing up the energy surface and converging onto first order saddle points. In addition to collapse and escape through a boundary, the method identifies a transition where the Skyrmion divides and forms two Skyrmions. The activation energy for this duplication process can be similar to that of collapse and escape. A tilting of the external magnetic field for a certain time interval is found to induce the duplication process in a dynamical simulation. Such a process could turn out to be an important avenue for the creation of Skyrmions in future magnetic devices.

Localized, noncollinear magnetic states are receiving a great deal of attention, where Skyrmions have come under special focus. Along with interesting transport properties, Skyrmions exhibit particlelike behavior and carry a topological charge enhancing their stability with respect to a uniform ferromagnetic background. In addition to the interest in their intriguing properties, they have been suggested as a basis for technological applications, e.g., data storage or even data processing devices [1,2]. A racetrack design of a memory device has been outlined where a spin polarized current drives a chain of Skyrmions past a reading device [3,4]. The effect of temperature and external magnetic field on the stability of the Skyrmions needs to be studied, as well as ways to generate and manipulate them. The effect of defects is also an important consideration [5,6]. Two mechanisms for the annihilation of Skyrmions have been characterized by theoretical calculations of atomic scale systems: collapse of a Skyrmion to form a ferromagnetic state [7–11] and escape of a Skyrmion through the boundary of the magnetic domain [9–12]. The effect of a nonmagnetic impurity has also been calculated [11]. By using harmonic transition state theory for magnetic systems [13,14], the lifetime of Skyrmions has been estimated [11,12]. Parameter values obtained from density functional theory [15] are found to give results that are consistent with experimental observations [16,17]. The challenge is to design materials where magnetic Skyrmions are small enough, while being sufficiently stable at ambient temperature, and to develop methods for manipulating them.

Theoretical calculations can help accelerate this development by identifying the various possible transformations that a Skyrmion can undergo at a finite temperature on a laboratory timescale. This can be achieved by the use of rate theory where the major challenge is to find the relevant transition mechanisms. If the final state of a transition is specified, in addition to the initial state, the geodesic nudged elastic band (GNEB) method [7,18] can be used to find the minimum energy path of the transition and, thereby, the activation energy, which is the highest rise in energy along the path. However, the final states of possible transitions are not always known. Another category of methods for identifying possible transition mechanisms where the final states are not specified, only the initial state, has turned out to be highly valuable in a different context, namely in studies of atomic rearrangements, such as chemical reactions and diffusion events [19,20]. Unexpected transition mechanisms have in many cases turned out to be preferred over mechanisms that seem *a priori* most likely [21].

Here, we describe a method that can be applied to identify transition mechanisms in magnetic systems without specifying final states. It represents an adaptation of a method that has been used extensively in studies of atomic rearrangements. A complication arises from the fact that magnetic systems are characterized by the orientation of the magnetic moments while the length of the magnetic moments is either fixed or obtained from self-consistency calculations [22]. The configuration space is therefore curved. The method is first described briefly, with more

detailed information in Supplemental Material [23], and then an application to a magnetic Skyrmion is presented, where, in addition to collapse and escape, the method gives a mechanism and activation energy that has not been reported before: duplication of a Skyrmion. Finally, a dynamical simulation is described where a time-dependent external field is used to induce such an event.

Within harmonic transition state theory [13,14,19], the mechanism and rate of a thermally induced transition is characterized by the first order saddle point [24] representing the bottleneck for the transition. Given an initial state corresponding to a local energy minimum, the various possible transitions the system may undergo can be identified by climbing up the energy surface and converging on the various first order saddle points on the energy ridge surrounding the minimum. A version of this approach, referred to as minimum mode following [25,26], is illustrated for a single-spin test system in Fig. 1. The method is based on the evaluation of eigenvalues and corresponding eigenvectors of the Hessian H. First, the region near the minimum, the convex region where all eigenvalues of the Hessian are positive, is escaped by following, for example, the gradient of the energy. Alternatively, a random vector or one of the eigenvectors of
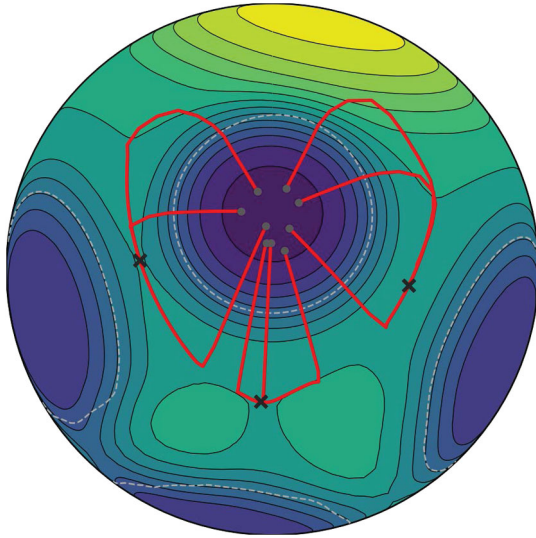

FIG. 1. An illustration of a method for climbing up the energy surface from an initial state minimum to a first order saddle point. The system contains only a single spin (see [23]) and because only the orientation of the magnetic vector can change, the energy surface can be mapped onto a sphere. The local energy minima (blue) are separated by an energy ridge, where points of low energy correspond to first order saddle points (black ×). The red curves illustrate saddle point search paths starting from various points. In this illustration, the system is made to follow the gradient of the energy until the lowest eigenvalue of the Hessian becomes negative (at the white dashed line). Beyond that point, the system is displaced along the effective force given by Eq. (1). This brings the system to a first order saddle point on the energy surface.

H can be followed to escape the convex region. Once an eigenvalue turns negative, an effective force

$$F^{\text{eff}} = F - 2(\hat{\lambda} \cdot F)\hat{\lambda}, \qquad (1)$$

is followed, where $F = -\nabla \mathcal{H}$ is the negative gradient of the energy and $\hat{\lambda}$ is the normalized eigenvector corresponding to the negative eigenvalue. Note that these vectors are $3N$-dimensional for a system with N spins. As the system is displaced in the direction of the effective force, it moves to higher energy along $\hat{\lambda}$, but to lower energy along the orthogonal degrees of freedom. Eventually, this brings the system to a first order saddle point on the energy surface. The final state of the transition can be obtained by a slight displacement further along $\hat{\lambda}$, followed by energy minimization.

This approach has not, to the best of our knowledge, been applied previously to a magnetic system. Here, the configuration space $\mathcal{M}_{\text{phys}}$ is given by the direct product of N spheres. In order to apply the mode following method, knowledge of second order derivatives is required, but, as is well known from the theory of Riemannian manifolds, they need to be treated with special care. The Hessian can be calculated by application of covariant derivatives, but their evaluation in spherical coordinates is usually cumbersome and suffers from singularities at the poles.

A more convenient approach is offered by viewing the configuration space as being embedded in a surrounding euclidean space $\mathcal{E} \supset \mathcal{M}_{\text{phys}}$. In this larger space, second order derivatives are easily performed. The Hessian in the physical subspace can then be reconstructed by a projection operator approach [27]. For any scalar function f on the manifold $\mathcal{M}_{\text{phys}}$, this true Hessian is defined as

$$\text{Hess } f(x)[z] = P_x \partial^2 \bar{f}(x) z + W_x(z, P_x^{\perp} \partial \bar{f}), \qquad (2)$$

where z is a vector tangent to the manifold, P_x and $P_x^{\perp}$ are the projectors onto the tangent space and onto the normal space, respectively, to the surface of the manifold at a point x on the sphere, $\bar{f}$ is the smooth extension of f to the Euclidean space, and W_x is the Weingarten map at x. The Weingarten map, sometimes also referred to as the shape operator, describes the curvature of 2D surfaces in terms of an embedding space.

For a Hamiltonian $\mathcal{H}$ of a spin system, the matrix representation of the Hessian is obtained by its action on the basis vectors (see [23]), i.e.,

$$H_{ij} = T_i^T \bar{H}_{ij} T_j - T_i^T I(\mathbf{n}^j \cdot \nabla^j \bar{\mathcal{H}}) T_j, \qquad (3)$$

where the indices i and j denote spins, $\bar{H} = \partial^2 \mathcal{H}(x)$, I is the 3×3 unit matrix, and T_i is the 3×2 matrix that transforms into the tangent space of spin i. As the Hessian matrix given by Eq. (3) is represented in $2N$, the evaluation

of an eigenmode in the $3N$ representation requires a transformation, i.e., $\lambda|^{3N} = T\lambda|^{2N}$ (see [23]).

The formulation of the constrained Hessian given by Eq. (3) and the saddle point search method described above have been implemented in the SPIRIT [28] software and used here to analyze transitions from a magnetic Skyrmion state. The energy of the system is described by an extended Heisenberg model

$$\mathcal{H} = -\mu_S \sum_{i=1}^{N} \mathbf{H} \cdot \mathbf{n}_i - J \sum_{\langle ij \rangle} \mathbf{n}_i \cdot \mathbf{n}_j - D \sum_{\langle ij \rangle} \hat{\mathbf{d}}_{ij} \cdot (\mathbf{n}_i \times \mathbf{n}_j),$$

(4)

where $\mathbf{H}$ is a uniform external magnetic field, $\mathbf{n}_i$ is the magnetic moment of spin i, J is the exchange coupling between nearest neighbor spins, the parameter D and unit vector $\hat{\mathbf{d}}_{ij}$ give the Dzyaloshinskii-Moriya vector in the plane of the lattice parallel to the vector connecting the two nearest neighbors i and j. The sums include only distinct nearest neighbor pairs. The system consists of 40×40 spins on a square lattice with free boundary conditions, and the parameter values and field strength are chosen to be the same as in a recent theoretical study [29] (values are given in [23]). The Bloch Skyrmion, shown in Fig. 2, is metastable with respect to the ferromagnetic phase.

Figure 2 shows an illustration of the eigenvectors corresponding to the three lowest eigenvalues. They correspond to translation, breathing, and elliptical distortion [30]. In order to escape from the convex region, we have chosen here to follow each one of these three modes until the corresponding eigenvalue becomes negative. After that, the system is displaced in the direction of the effective force given by Eq. (1), where $\hat{\lambda}$ is the eigenvector of the initially selected mode rather than the one with lowest eigenvalue.

By following the translational mode, the mode that has lowest eigenvalue initially, the Skyrmion moves towards the edge of the system and eventually, as it is pushed along the effective force, converges on a saddle point corresponding to an escape through the edge. Relaxation of the system after a slight displacement along the unstable mode at the saddle point brings the system to the ferromagnetic state. Similarly, by following the breathing mode, the second lowest eigenvalue mode, the Skyrmion shrinks and eventually converges to a saddle point corresponding to collapse. Again, the final state of the transition is the ferromagnetic state. However, by following the elliptical mode, the Skyrmion becomes stretched and converges on a saddle point corresponding to a division of the Skyrmion and formation of two Skyrmions. While the initial state contains one Skyrmion, the final state contains two.

The energy along the minimum energy paths for the three transitions is shown in Fig. 2. These were calculated using the geodesic nudged elastic band method [7], using an initial path formed by linear interpolation between the
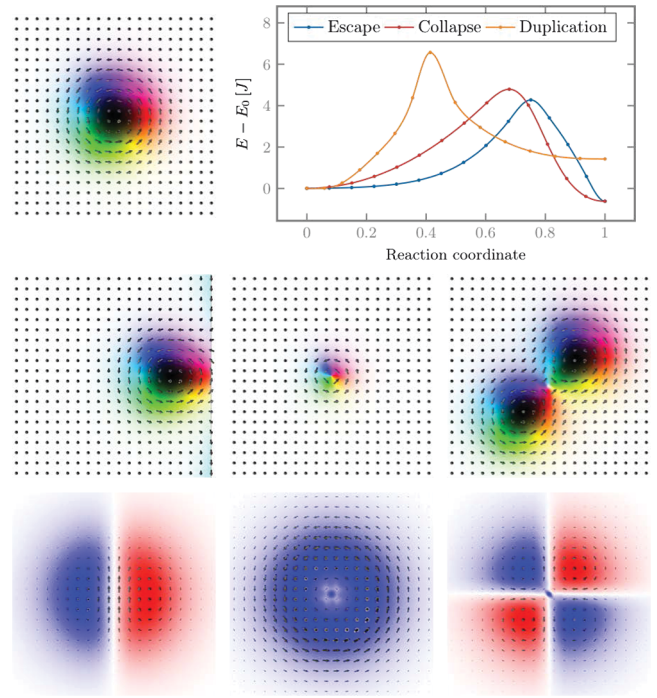

FIG. 2. (Top, left) Minimum energy configuration of the Skyrmion. (Top, right) Minimum energy paths for the three types of transitions found: duplication, collapse, and escape. The reaction coordinate is the scaled total displacement along the path. The energy is given in units of the exchange coupling constant J. (Middle row) Saddle point configurations found for escape through a boundary (left), radial collapse (middle), and duplication (right). (Bottom) The translational, breathing, and elliptical eigenmodes of the Skyrmion in the minimum energy configuration, each leading to the saddle point displayed directly above.

initial state and the saddle point, as well as between the saddle point and the final state. The activation energy for the collapse and escape is quite similar, but the activation energy for the duplication is higher in this case. The relative height of the energy barriers for the three processes depends on the parameter values. A calculation using a 10% smaller field and 60% larger value of D/J gives a lower activation energy for duplication than the other two transitions [23].

The shape of the three curves is quite different. The total displacement along the paths from the initial state to the saddle point is shortest for the duplication, while the displacement of the Skyrmion to the boundary and to the saddle point for escape involves the largest displacement. The energy profile for the collapse is similar to what has been presented before, a gradual shrinkage of the Skyrmion to the saddle point followed by an abrupt drop of the energy to that of the ferromagnetic state [7,8].

The duplication of the Skyrmion leads to an increase in the energy of the system because the Skyrmion is only metastable with respect to the ferromagnetic state for this set of parameters, while the other two transitions lead to a decrease in the energy. The energy along the minimum

energy path past the saddle point for duplication contains important information about Skyrmion interaction. It shows how the repulsive interaction between Skyrmions varies with the distance between them. Going from right to left along the minimum energy path in Fig. 2 shows how two Skyrmions can merge to form one Skyrmion.

The duplication transition identified here has not been described previously, but may turn out to be an important mechanism for generating Skyrmions. The first order saddle point on the energy surface corresponding to this mechanism can be found for a wide range of parameter values, as will be described in detail in a later publication. For example, we have found the duplication saddle point for a Pd/Fe bilayer on an Ir(111) substrate, a system that has been studied extensively, using parameter values that give close agreement with experimental results [12,15]. There, the energy barrier for duplication turns out to be slightly lower than that of collapse, 78 vs 80 meV.

The question now arises whether it is possible to induce the duplication event dynamically. We address this by performing a dynamical simulation where a short magnetic pulse is applied in addition to the stationary magnetic field. The pulse is represented by a uniform magnetic field which has both in-plane and out-of-plane components. For the duration of the pulse, 200 ps, the total magnetic field is tilted (see [23]). This is known to be an efficient way of exciting nonlinear Skyrmion dynamics [31]. The saddle point searches show that an excitation of the elliptical mode can induce duplication. Figure 3 shows snapshots from the simulation. During the pulse, an elongated structure is formed. After the pulse has been turned off, it splits up and eventually two Skyrmions remain in the system. In addition to the elliptic elongation, the duplication also requires the deformed structure to be bent in order for it to divide up. The bending corresponds to another eigenmode of the elongated Skyrmion. More efficient and/or reliable ways of achieving the duplication process could be devised, for example, by pinning the Skyrmion, introducing defects, or by other more elaborate external stimuli. The simulation described here is merely meant to show that it is possible to induce Skyrmion duplication in a rather simple way.

We have presented here a method that can be used to search for transition mechanisms and determine the activation energy for transitions in magnetic systems. It represents an adaptation of mode following methods that have been used for several years in studies of atomic rearrangements. The fact that magnetic transitions involve rotations of the magnetic vectors leads to constraints that need to be incorporated into the Hessian matrix in order to determine the low lying eigenvalues and corresponding eigenvectors. Saddle point searches where only the initial state of the transition is specified, such as the ones carried out here, are more challenging than a minimum energy path calculation where both the initial and final states are specified, but they have the advantage of being able to reveal unexpected transitions and unknown final states. In the application calculations presented here, we have chosen to drive the system out of the convex region by following a particular mode. We note that eigenvalues may cross and modes change direction as the system is pushed along a specific mode, so care should be taken to remain on the same mode throughout the saddle point search (see [23]).

Applications of the saddle point search method presented here to three-dimensional systems can be expected to yield an even larger variety of mechanisms than for two-dimensional systems since more possibilities open up with the additional dimension. For example, cylindrical Skyrmions can contract and form bobbers [29] and possibly other previously unknown magnetic structures.

A saddle point search method that only requires the initial state as input (unlike the GNEB method, where the final state also needs to be specified) can be used to sample an energy surface in a systematic way and search for possible states of the system, each state corresponding to a local energy minimum. The search takes the system from one local minimum to another via first order saddle points. This can be used as the basis of a simulation of the long timescale evolution of a system that undergoes thermally activated transitions, possibly enhanced by an external field. For each state visited, multiple saddle point searches are carried out to identify the most relevant low energy saddle points. The transition rate corresponding to each saddle point can be estimated using harmonic transition state theory and a random number used to choose which transition will occur next based on the normalized rates. This is referred to as the adaptive kinetic Monte Carlo
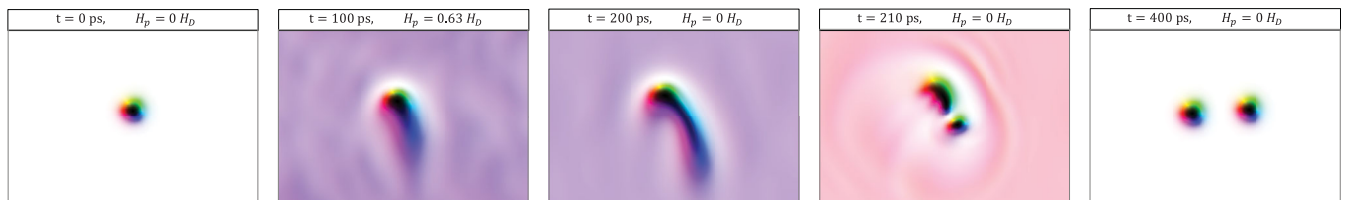

FIG. 3. Snapshots from a dynamical simulation where the duplication of a Skyrmion is induced by applying a magnetic pulse over 200 ps, giving a total field that is tilted with respect to the normal of the plane (see [23] for parameter values). The labels on top of the frames give the time and magnetic field of the pulse (which adds to a constant field in the direction of normal to the plane). The pulse is applied at time $t = 0$ and lasts until $t = 200$ ps. At the end of the pulse, an elongated defect is formed that later splits up (at $t = 209$ ps) to form two Skyrmions.

algorithm [32]. The simulated time can be estimated from the sum of rates. This approach has been used as the basis for simulations of long timescale evolution of complex atomic systems, where atomic rearrangement events can involve nonintuitive displacements of multiple atoms [33,34]. The adaptation presented here of the saddle point search method to spins opens the possibility of carrying out such long timescale simulations of magnetic systems.

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