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Comment on "Path to collapse for an isolated Néel skyrmion"

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Rohart, Miltat and Thiaville [Phys. Rev. B **93**, 214412 (2016)] recently reported calculations indicating two mechanisms for the annihilation of a skyrmion in a Co monolayer on Pt(111). The path calculations were based on a method presented in the supplemental material of their article. It is pointed out here that their method does not in general converge on minimum energy paths, unlike the geodesic nudged elastic band method which is discussed for comparison. As a result, the maximum energy along the two paths presented does not provide an accurate estimate of the activation energy for the transition and the fact that two different paths were obtained should not be taken as an indication that the skyrmion annihilation can occur by two different mechanisms.

The task of finding minimum energy paths (MEPs) for transitions in magnetic systems arises in many contexts, the estimation of the thermal stability of skyrmions being one. An MEP is the path of highest statistical weight and gives clear information about the mechanism of the transition. The highest energy point along the MEP corresponds to the first order saddle point (SP) on a multidimensional energy surface of the system and gives an estimate of the activation energy for the transition within the harmonic transition state theory[1]. In a recent article[2], Rohart, Miltat and Thiaville (RMT) report two paths for the skyrmion annihilation in a Co monolayer on Pt(111), where the first path corresponds to a symmetrical shrinking of the skyrmion, while the second path involves a large rotation of the spins in the skyrmion center. This is taken to indicate two different mechanisms for skyrmion annihilation. In this comment, it is demonstrated that the method presented and used in Ref.[2] does not, in general, converge to an MEP. The method is contrasted with the geodesic nudged elastic band (GNEB) method[3] which does converge to an MEP and the key difference between these two methods are explained in detail.

A system of N magnetic moments can be described by a set of N unit vectors, $\boldsymbol{M} = \left(\vec{M}_1, \vec{M}_2, \ldots, \vec{M}_N\right)$, where each unit vector $\vec{M}_i$ defines orientation of the ith moment (here and below, symbols with an arrow above denote 3-dimensional vectors while bold symbols denote $3N$-dimensional vectors). The force acting on the system is defined as the antigradient of the total energy projected on the tangent space to the configuration manifold: $\boldsymbol{F} = \left(\vec{F}_1, \vec{F}_2, \ldots, \vec{F}_N\right)$, $\vec{F}_i = -\frac{\partial E(\boldsymbol{M})}{\partial \vec{M}_i} + \left(\frac{\partial E(\boldsymbol{M})}{\partial \vec{M}_i} \cdot \vec{M}_i\right)\vec{M}_i$, $i = 1, \ldots, N$. Projection on the tangent space is needed so as to satisfy constraints on the length of magnetic vectors.

Since SPs are stationary points on the energy surface, the following necessary condition must hold there:

$$\boldsymbol{F}|_{SP} = \boldsymbol{0}. \tag{1}$$

An energy maximum along the path obtained with the GNEB method satisfies this condition. Indeed, the GNEB method involves systematic adjustment of an initially generated path so as to zero the transverse component of the force at each point along the path:

$$\boldsymbol{F}|_\perp = \boldsymbol{F} - (\boldsymbol{F}\cdot\boldsymbol{\tau})\,\boldsymbol{\tau} \to \boldsymbol{0}, \tag{2}$$

which is equivalent to the following set of conditions:

$$\vec{F}_i|_\perp = \vec{F}_i - \vec{\tau}_i \sum_{j=1}^{N} \left(\vec{F}_j \cdot \vec{\tau}_j\right) \to \vec{0},\ i = 1, \ldots, N. \tag{3}$$

Observe, that the transverse force on the ith moment, $\vec{F}_i|_\perp$, is affected by the forces on all moments in the system through the dot product $(\boldsymbol{F}\cdot\boldsymbol{\tau}) = \sum_{j=1}^{N}\left(\vec{F}_j \cdot \vec{\tau}_j\right)$. Eq. (2) or (3), which defines the path obtained with the GNEB method, represents a necessary condition for an MEP. The unit tangent to the path, $\boldsymbol{\tau}$, is defined as follows:

$$\begin{aligned}\boldsymbol{\tau} = \dot{\boldsymbol{M}}/|\dot{\boldsymbol{M}}| &= \left(\frac{\dot{\vec{M}}_1}{|\dot{\boldsymbol{M}}|}, \frac{\dot{\vec{M}}_2}{|\dot{\boldsymbol{M}}|}, \ldots, \frac{\dot{\vec{M}}_N}{|\dot{\boldsymbol{M}}|}\right)\\ &= \left(\vec{\tau}_1, \vec{\tau}_2, \ldots, \vec{\tau}_N\right),\end{aligned} \tag{4}$$

where the dot denotes derivative with respect to some parameter of the path, e.g. displacement along the path, and $|\cdot|$ denotes the Euclidean norm:

$$|\dot{\boldsymbol{M}}| = \sqrt{\sum_{j=1}^{N}\left(\dot{\vec{M}}_j \cdot \dot{\vec{M}}_j\right)} \tag{5}$$

At an energy maximum along any transition path, the derivative of the total energy, E, with respect to the parameter of the path vanishes. This implies:

$$\begin{aligned}\dot{E}|_{max} = 0 &= \sum_{i=1}^{N}\left(\frac{\partial E}{\partial \vec{M}_i}\cdot\dot{\vec{M}}_i\right)\\ &= -|\dot{\boldsymbol{M}}|\sum_{i=1}^{N}\left(\vec{F}_i\cdot\vec{\tau}_i\right) = -|\dot{\boldsymbol{M}}|\,(\boldsymbol{F}\cdot\boldsymbol{\tau}),\end{aligned} \tag{6}$$

where use was made of the following identity:

$$\left(\vec{M}_i \cdot \dot{\vec{M}}_i\right) = |\dot{\boldsymbol{M}}|\left(\vec{M}_i \cdot \vec{\tau}_i\right) = 0,\ i = 1, \ldots, N. \tag{7}$$

Eqs. (2)-(3) and (6) ensure that Eq. (1) is fulfilled at an energy maximum along the path obtained with the GNEB method. Note that the GNEB method involves an approximation for the path tangent, i.e. using finite differences, and Eq. (7) must be enforced by projection of the approximate tangent on the tangent space to the configuration manifold.

RMT propose a different scheme for finding transition paths in magnetic systems. First of all, the tangent to the path is defined in their method as the set of unit vectors (see Eq. (1) in the supplemental material for Ref.[2]):

$$\boldsymbol{\tau}^{RMT} = \left(\vec{\tau}_1^{RMT}, \vec{\tau}_2^{RMT}, \dots, \vec{\tau}_N^{RMT}\right) = \left(\frac{\dot{\vec{M}}_1}{|\dot{\vec{M}}_1|}, \frac{\dot{\vec{M}}_2}{|\dot{\vec{M}}_2|}, \dots, \frac{\dot{\vec{M}}_N}{|\dot{\vec{M}}_N|}\right). \tag{8}$$

Observe that $\boldsymbol{\tau}^{RMT}$ and $\boldsymbol{\tau}$ (see Eq. (4)) point in the same direction only if $|\dot{\vec{M}}_1| = |\dot{\vec{M}}_2| = \ldots = |\dot{\vec{M}}_N|$, i.e. when all spins rotate with the same speed during the transition. Moreover, due to normalization of individual 3-dimensional vectors, some components of $\boldsymbol{\tau}^{RMT}$ become undefined if corresponding spins do not move during the transition, so a special treatment of such spins need to be invoked (see Eq. (3) in the supplemental material for Ref.[2] and a text therein). Below we assume that all components of $\boldsymbol{\tau}^{RMT}$ are well-defined.

In the RMT method, the path is relaxed along the direction $\boldsymbol{\eta} = (\vec{\eta}_1, \vec{\eta}_2, \dots, \vec{\eta}_N)$, which is defined for each spin as follows

$$\vec{\eta}_i = [\vec{M}_i \times \vec{\tau}_i^{RMT}], \tag{9}$$

so as to zero the constrained force (see Eq. (2) in the supplemental material for Ref.[2]):

$$\vec{F}_i^{RMT} = -\left(\frac{\partial E(\boldsymbol{M})}{\partial \vec{M}_i} \cdot \vec{\eta}_i\right)\vec{\eta}_i \to \vec{0},\ i = 1, \dots, N, \tag{10}$$

which is equivalent to:

$$\vec{F}_i - \left(\vec{F}_i \cdot \vec{\tau}_i^{RMT}\right)\vec{\tau}_i^{RMT} \to \vec{0},\ i = 1, \dots, N. \tag{11}$$

Eq. (11) which defines the path obtained with the RMT method is different from Eq. (2) or (3). It implies that a point along the RMT path is a stationary point on the energy surface, i.e. Eq. (1) is satisfied, only if N conditions are met simultaneously:

$$\left(\vec{F}_i \cdot \vec{\tau}_i\right) = 0,\ i = 1, \dots, N. \tag{12}$$

However, it is practically impossible that Eqs. (12) hold at any intermediate point along the RMT path. In particular, it is not guaranteed that Eqs. (12) are fulfilled at the energy maximum along the path, where only Eq. (6), a general case of Eqs. (12), holds. As a result, energy maxima along the path found within the RMT method can not be interpreted as SPs on the energy surface.

By defining a search direction according to Eq. (9), N additional constraints per a point along the path were essentially introduced in Ref.[2], see Eqs. (10)-(11), while only one additional constraint is needed, Eq. (2). These constraints prevent a path from converging on the MEP and relevant SPs are unlikely to be found in the RMT method.

It is important to realize that Eq. (1) is only a necessary condition for an SP, not sufficient. Therefore, even if some SP search method provides a candidate point where Eq. (1) is satisfied, further analysis is needed in order to verify that the point is indeed an SP. A reliable strategy for verification of an SP involves calculation of the Hessian matrix of the energy and making sure that one and only one eigenvalue is negative. In magnetic systems, calculation of the Hessian matrix is hampered by constraints on the length of magnetic moments. While this can be resolved by use of spherical coordinates, additional difficulties may arise when some of the spins point close to the poles, where azimuthal angle gets undefined. Instead, usual Cartesian components of the magnetic vectors can be used, while constraints are taken into account using Lagrange multipliers, see Ref.[4] for details.

In conclusion, while the two paths found in Ref.[2] can be realized in the system, they can not be interpreted as MEPs on the energy surface as it is not guaranteed that energy maxima along the paths satisfy a necessary condition for an SP. As a result, the maxima along the paths should not be used as estimates of the activation energy for a transition. The two separate paths obtained for skyrmion annihilation in Ref.[2] should not be taken as indications of two different mechanisms for skyrmion annihilation. Indeed, recent calculations carried out with the GNEB method for this system[5] have resulted in only one MEP which has a significantly lower maximum energy than the two paths reported in Ref.[2].

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