Fine energy structure of a magnetic skyrmion localized on a nonmagnetic impurity in an external magnetic field

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Abstract. The Localization of a magnetic skyrmion on a nonmagnetic defect in a two-dimensional triangular lattice is investigated within the framework of the generalized Heisenberg model, which includes exchange, anisotropy, Dzyaloshinskii–Moriya interaction, and interaction with an external magnetic field. It is shown that there is a threshold magnetic field, below which there are two locally stable positions of the defect inside the skyrmion. The energy difference between the states with a different localization of defects results in a fine energy structure of skyrmions, depending on the strength of the magnetic field.

Keywords: saddle point, minimum energy path, skyrmion, logic device, racetrack memory.

Introduction

A magnetic skyrmion (Sk) is a localized non-collinear state that has been observed, in particular, in thin films of 3d metals on the surface of heavy metals (Hagemeister et al. 2015). The small size and high mobility under the action of ultra-low current density make this system attractive for use in spintronic applications. Sks, like particles, can move freely in a magnetic film while maintaining their size and shape. For their practical use, it is important to be able to localize Sks in a certain area and move them along a definite trajectory. This can be achieved by a local change in the strength of the magnetic interactions or values of those magnetic moments in the media where the Sk is located. Elongated domains (Castell-Queralt et al. 2019) or sample boundaries (Zhang et al. 2015) provide "rails" for the movement of the skyrmion, while local point defects can lead to the formation of a center of attraction or repulsion, or to anchoring the Sk in a certain place (Stosic et al. 2017).

Local point defects can affect the current-induced motion of Sks. Calculations have shown that the introduction of local anisotropy in some sites of the two-dimensional lattice does not change the Sk velocity/current ratio (Iwasaki et al. 2013), but nonmagnetic local impurities change the trajectory of Sks and can pin them, so that a small current will not move the skyrmion along the sample at all (Müller, Rosch 2015).

Nonmagnetic defects also change the activation energy for skyrmion annihilation and nucleation from a ferromagnetic state. Consequently, it may turn out that most of the Sks that will be produced by recording devices will be localized (Romming et al. 2013).

A non-magnetic defect modifies the energy surface of the system and reduces the energy of the transition state. The inclusion of an external magnetic field also leads to a change in the shape of the energy surface, which also reduces the stability of the Sk if the field is directed antiparallel to the magnetization in the skyrmion core (Uzdin et al. 2018). In this paper, we include both factors and study the field dependence of the energy surface of a Sk localized at a nonmagnetic defect.

Model and methods

A thin magnetic film was modelled in a Heisenberg type model with a triangular lattice. Energy E of a magnetic state is given by

$$E = -J\sum_{<i,j>}\vec{S}_i \cdot \vec{S}_j - \sum_{<i,j>}\vec{D}_{ij}\cdot\left[\vec{S}_i \times \vec{S}_j\right] - K\sum_i S_{i,z}^2 - \mu\vec{B}\sum_i \vec{S}_i \ . \tag{1}$$

Here J is the exchange parameter, which is assumed to be non-zero only for the nearest-neighbor sites, $\vec{D}_{ij}$ is the Dzyaloshinskii-Moriya (DM) vector laying in a plane orthogonal to the line connecting atomic sites i and j. The vector of anisotropy is perpendicular to the lattice plane along the z-axis. $K > 0$ is the constant of easy axis anisotropy. Magnetic field $\vec{B} = B\vec{z}$ is directed along the magnetization in homogeneous ferromagnetic state. $\vec{S}_i$ are three-dimensional vectors of unit length along the magnetic moment on site i; μ is the magnitude of the magnetic moments.

A single site is assumed to be a nonmagnetic impurity. The summation $<i, j>$ in (1) is taken over all pairs of the nearest neighbor sites in the triangular lattice excluding the impurity. The values of the parameters taken from (Hagemeister et al. 2015) correspond to the experimentally observed skyrmions in the Pd/Fe/Ir(111) system, $\mu B = 0.093\,J$, $K = 0.07\,J$, $D = \left|\vec{D}_{ij}\right| = 0.32\,J$, $J = 7$ (meV).

The system supports the Neel (hedgehog) Sk slightly disturbed by the presence of impurity. We considered a strip of a triangular lattice containing 80×61 atoms with periodic boundary conditions, which is large enough to host an isolated skyrmion, namely, the energy perturbation due to self-interaction across the boundary is about 0.0002%. The dipolar interaction or the demagnetizing field is not taken into account, since the Sks under study have a diameter less than 4.6 nm (the lattice constant for Fe / Ir (111) is 0.27 nm). The impurity is a local disturbance, which should not be affected by the demagnetizing field.

The metastable states of Sks were calculated numerically using the conjugate gradient method in Cartesian coordinates (Lobanov, Uzdin 2020). The transformations of a magnetic Sk localized on an impurity were studied by calculating the minimum energy paths MEPs between the Sk state and the other (meta) stable states on the energy surface of the system. The MEPs were calculated using the geodesic nudge elastic band method (Bessarab et al. 2015).

Localization of an Sk on an impurity in the external magnetic field

The appending of a non-magnetic impurity to the ferromagnetic phase creates an energy vertex around this magnetic defect that repels Sks nearby. However, if the distance from the impurity to the Sk center is approximately equal to the Sk radius, then the Sk is pinned to the impurity, see Fig. 1a, c. The energy landscape has a local minimum for a specific location of the impurity, and the Sk must overcome the activation barrier for the dissociation from the impurity. The equilibrium positions of the defect correspond to the plane orientation of the magnetization $S_z = 0$ and form a "ring". This behavior has been observed experimentally using the scanning tunneling microscopy technique (Hanneken et al. 2016).

We found out that for the external magnetic field weaker than a critical value B_c there exists another possibility for pinning, when the impurity is located exactly in the center of the Sk, see Fig. 1b. For such weak fields, the magnetization in the central part of the Sk is almost uniform and opposite to the magnetization in the ferromagnetic phase, however, the local maximum of energy density is formed in the Sk center. According to our numerical simulation $\mu B = 0.067\,J$, for the parameters under consideration. For larger $B > B_c$, the impurity in the center is not a stable position and the Sk domain wall is attracted by a nonmagnetic hole.
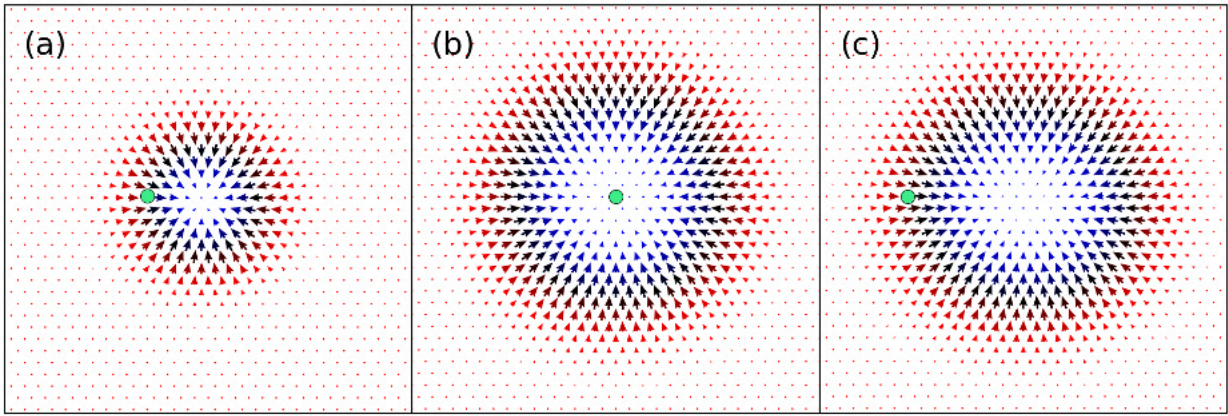
Fig. 1. An isolated Sk with the impurity in the boundary (panels a, c) and in the center (b) for $\mu B = 0.093\,J$ (panel a) and $\mu B = 0.046\,J$ (b, c). The Sk with the impurity in the center is metastable only for B below the critical field $\mu B_c = 0.067\,J$, whereas the impurity at the boundary is metastable down to $\mu B = 0.13\,J$, and the skyrmion without impurities is stable down to $\mu B = 0.21\,J$

The energy barriers for the transition from a state with an impurity in the Sk center to a state with an impurity at the boundary were found by calculating the MEP shown in Fig. 2a. An increase in the external field raises both the energy of the initial and transition states, but the former grows faster than the latter. This is why the energy barrier between the initial and final states tends to zero as $B \rightarrow B_c$, which leads to the instability of the central position of the nonmagnetic defect for high fields, see Fig. 2b.
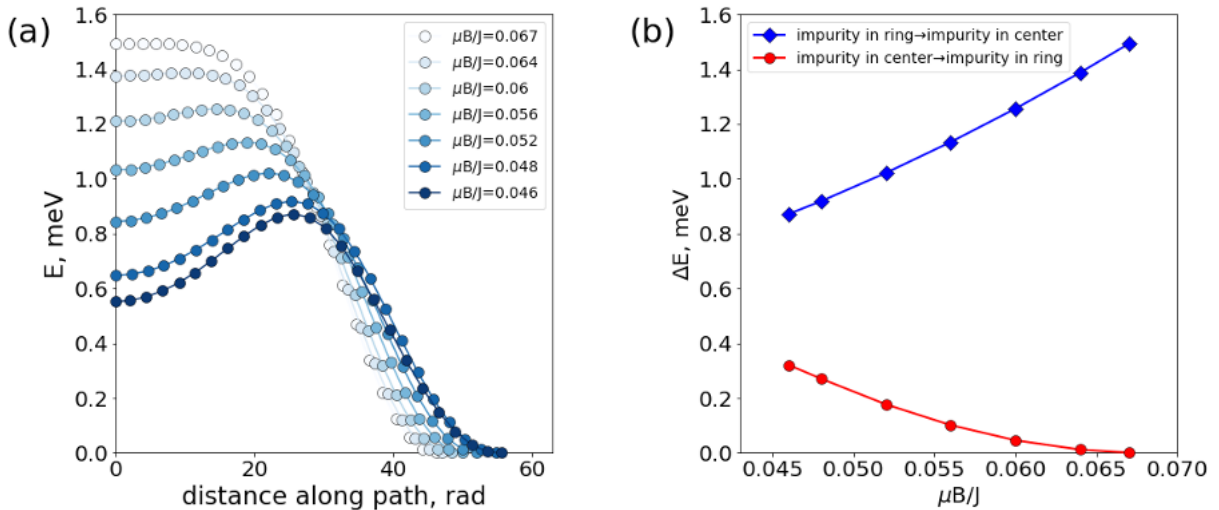

Fig. 2. (a) The minimum energy paths between the states with an impurity in the Sk center and at the Sk boundary for a magnetic field range of $0.046\,J \leq \mu B \leq 0.067\,J$. The zero energy corresponds to the skyrmion with the impurity at the boundary. (b) The energy barriers for transitions from the state with an impurity in the Sk center to the state with an impurity at the Sk boundary and backward as a function of the magnetic field

To a first approximation, a nonmagnetic impurity can be regarded as the absence of a single spin in an Sk. Then the stable positions of the impurity should correspond to the maximum energy density in the skyrmion. All contributions to the energy of the metastable Sk state are shown in Fig. 3 for two values of the magnetic field below and above the critical one. It can be seen that an Sk is stabilized by the DM interaction, since only this contribution is negative. The impurity at the Sk boundary is, indeed, in the local maximum of the energy density.

When the magnetic field decreases below the critical value B_c, the density of the DM interaction energy increases in the Sk center. Then the second local maximum of total energy density appears near the defect (Fig. 3, lower row) and the removal of the magnetic site from the Sk center gives a maximal local energy reduction.
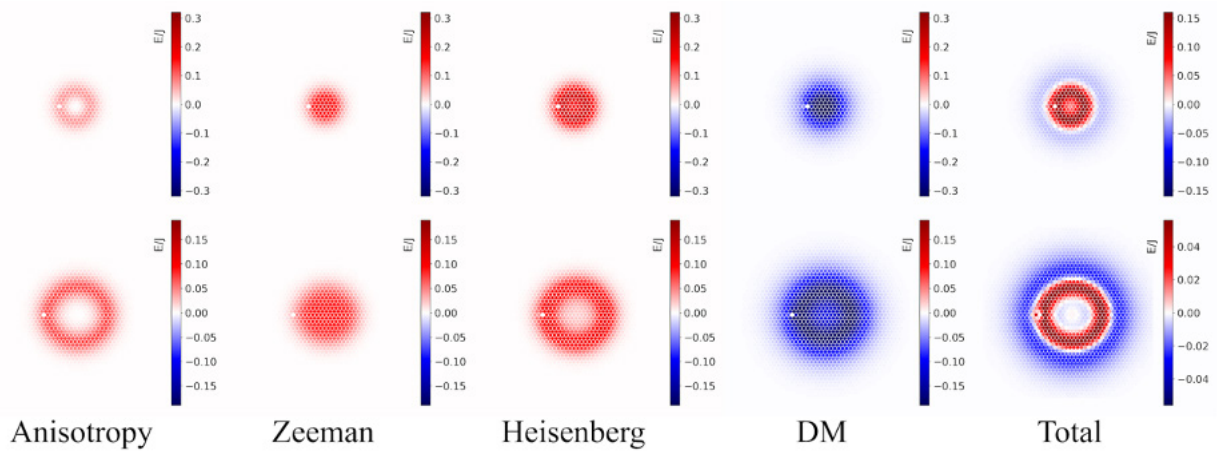

Fig. 3. Contributions of energy per spin in a magnetic field $\mu B = 0.093 \, J$ (top row)
and $\mu B = 0.046 \, J$ (bottom row), the columns correspond to the different contributions of energy.
The position of the impurity is shown with a white dot

Conclusions

Calculation of the energy Sk localized at a nonmagnetic defect showed the presence of two local energy minima below the threshold magnetic field B_c. They correspond to the location of the defect at the border and in the very center of the Sk. The energies of these Sk configurations depend on the magnitude of the magnetic field. Therefore, one can expect resonant energy absorption caused by the interaction with current or spin waves in such systems.

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