Three-dimensional chiral skyrmions with attractive interparticle interactions

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Abstract
We introduce a new class of isolated three-dimensional skyrmion that can occur within the cone phase of chiral magnetic materials. These novel solitonic states consist of an axisymmetric core separated from the host phase by an asymmetric shell. These skyrmions attract one another. We derive regular solutions for isolated skyrmions arising in the cone phase of cubic helimagnets and investigate their bound states.

Keywords: skyrmions, chiral magnets, Dzyaloshinskii–Moriya interaction

(Some figures may appear in colour only in the online journal)
where \( \mathbf{m} = (\sin \theta \cos \psi; \sin \theta \sin \psi; \cos \theta) \) is the unity vector along the magnetization \( \mathbf{M} \), \( A \) is the exchange stiffness constant, \( D \) is the Dzyaloshinskii–Moriya (DM) coupling energy, and \( H \) is the applied magnetic field.

Chiral modulations along the applied field with the period \( L_D = 4\pi A/|D| \) correspond to the global minimum of the functional (1) below the critical field \( \mu_D H_D = D^2/(2A M) \). The equilibrium parameters for the cone phase are expressed in analytical form [2] as:

\[
\theta_\ell = \arccos(H/H_D), \quad \psi_\ell = 2\pi \ell/L_D,
\]

where \( \ell \) is the spatial variable along the applied field.

At \( H = H_D \), the cone phase transforms into the saturated phase with \( \theta = 0 \). Within the saturated phase \((H > H_D)\), isolated chiral skyrmions are described by axisymmetric solutions of type

\[
\theta = \theta(\rho), \quad \psi = \varphi + \pi/2,
\]

that are homogeneous along the skyrmion axis \( z \) where \( r = (\rho \cos \varphi, \rho \sin \varphi, z) \) are cylindrical coordinates for the spatial variable [4]. The equilibrium solutions for \( \theta(\rho) \) are derived from the Euler equation for the energy functional [4]

\[
w_0(\theta) = A J_0(\theta) + D J_1(\theta) - \mu_D M H \cos \theta,
\]

\[
J_0(\theta) = \theta_0^2 + \frac{1}{\rho^2} \sin^2 \theta, \quad J_1(\theta) = \theta_0 + \frac{1}{\rho} \sin \theta \cos \theta,
\]

with the boundary conditions \( \theta(0) = \pi, \theta(\infty) = 0 \).

Below the saturation field \((H < H_D)\), the structure of two-dimensional skyrmions is imposed by the arrangement of the cone phase (2). These solutions should be periodic with period \( L_D \) along the \( z \)-axis and are confined by the following in-plane boundary conditions:

\[
\theta_{\rho=0} = \pi, \quad \theta_{\rho=\infty} = \theta_{\ell}, \quad \psi_{\rho=\infty}(z) = \psi_{\ell}(z).
\]

The solutions for \( \theta(\rho, \varphi, z), \psi(\rho, \varphi, z) \) are derived by the minimization of the energy functional (1):

\[
w = A J(\theta, \psi) + D J(\theta, \psi) - \mu_D M H \cos \theta,
\]

with the boundary conditions (5), where the exchange (\( J \)) and Dzyaloshinskii–Moriya (\( I \)) energy functionals are

\[
J(\theta, \psi) = \theta_0^2 + \theta_0^2 + \frac{1}{\rho^2} \theta_0^2 + \sin^2 \theta \left( \psi_0^2 + \psi_0^2 + \frac{1}{\rho^2} \psi_0^2 \right),
\]

\[
I(\theta, \psi) = \sin(\psi - \varphi)(\theta_0 + \frac{1}{\rho} \sin \theta \cos \theta \psi_0) + \sin^2 \theta \psi_0 + \cos(\psi - \varphi)(\theta_0 + \frac{1}{\rho} \sin \theta \cos \theta \psi_0).
\]

To investigate the solutions for asymmetric skyrmions, we use the discretized version of equation (1):

\[
w = J \sum_{\langle i, j \rangle} (S_i \cdot S_j) - \sum_i H \cdot S_i
\]

\[
- D \sum_i (S_i \times S_{i+\hat{x}} \cdot \hat{x} + S_i \times S_{i+\hat{y}} \cdot \hat{y} + S_i \times S_{i+\hat{z}} \cdot \hat{z})
\]

(8)

We consider classical spins of unit length on a three-dimensional cubic lattice. \( \langle i, j \rangle \) denotes pairs of nearest-neighbor spins. The Dzyaloshinskii–Moriya constant \( D \) defines the period of modulated structures \( p \) via the following relation: \( DJ = \tan(2\pi/p) \). Or vice versa, one chooses the period of the modulations for the computing procedures and defines the corresponding value of DM constant. In what follows, the Dzyaloshinskii–Moriya constant is set to 0.7265\( J \) which corresponds to one-dimensional modulations with a period of 10 lattice spacings in zero field [15]. We note that throughout this article we consider periodic boundary conditions in all three directions. The discrete model (8) is particularly useful when the continuum model becomes invalid for localized solutions with sizes of a few lattice constants [12, 16]. The model is also able to operate with smaller arrays of spins as compared with the continuum model. The size of our numerical grid is set to \( 100 \times 100 \times p \).

Numerical calculations for \( H = 0.57H_D \) (figures 1 and 2) show the main features of asymmetric skyrmions. The entire structure of a skyrmion within the cone phase can be thought of as a stack of layers (figure 1) rotating around the \( z \) axis with period \( L_D \). These specific solitonic states are characterized by three-dimensional chiral modulations: the cone modulations along their axis and a double-twist rotation in the perpendicular plane.

Figures 2(a)–(c) present the equilibrium structures within a layer with a fixed value of \( z \). The function \( m_z(\rho, \varphi) \) consists of a strongly localized axisymmetric core separated from the outer region with a fixed value of the magnetization \( m(\theta, \psi) \) (2) by a broad strongly asymmetric transitional region we call the shell.

The contour lines of equal \( m_z \) in figure 2(a) and magnetization profiles along the skyrmion diameter, \( m_z(\xi) \) in figure 2(c), display the details of the shell. Note especially, that the magnetization profile along \( \varphi = \psi_0 + \pi/2 \) reaches the value \( \theta = 0 \). In figure 2(a), this point is enclosed by crescent-shaped contours. The unit spheres in figure 2(d) demonstrate the difference between the solution for axisymmetric skyrmions in the saturated phase (3) and those within the cone phase (5).
The former are described by $O O_1$ lines connecting the skyrmion center with $\theta = \pi$ ($O_1$) and the point $O$ corresponding to the system ‘vacuum’, $\theta = 0$. Solutions for skyrmions within the cone phase are described by the lines connecting the skyrmion center ($O_1$) with the point $C$ corresponding to the cone phase (2). In figure 2(d) we indicate the magnetization trajectory along $\varphi = \psi_c + \pi/2$ direction.

The radial skyrmion energy density $e(\rho) = (2\pi L_0)^{-1} \int_0^{L_0} dz \int_0^{2\pi} d\varphi_0(\theta, \varphi)$ with positive exponentially decaying asymptotics (figure 3(a)) implies the attractive interaction between the skyrmions in the cone phase. Note that axisymmetric skyrmions in the saturated state of chiral magnets have a repulsive interskyrmion potential [13, 14, 17]. In figure 3(b) the reduced interaction energy between two asymmetric skyrmions, $E_{int}/E_0$, is plotted as a function of their separation distance for different values of the applied magnetic field ($E_0 = \int_0^{L_0} e(\rho) r d\rho$ is the total equilibrium energy of an isolated asymmetric skyrmion). The Lennard–Jones type potential profiles $E_{int}(r/L_0)$ show that the attractive interskyrmion coupling is characterized by a low potential barrier and a rather deep potential well establishing the equilibrium separation of skyrmions in the bound biskyrmion state (figure 3(c)).

In conclusion, regular solutions for isolated chiral skyrmions in the cone phase of cubic helimagnets have been derived by numerically solving the corresponding micromagnetic equations (5) and (6). These novel solitonic states are characterized by three-dimensional chiral modulations and an attractive interskyrmion potential. Similar skyrmionic states can arise in the cone phases admissible in uniaxial chiral ferromagnets with $C_n$ and $D_n$ symmetry [1, 3]. Axisymmetric skyrmions exist in the saturated phase of chiral ferromagnets as ensembles of repulsive isolated particles [4, 10, 14]. Our findings show that below the transition field into the cone phase, the axisymmetric skyrmions transform into asymmetric attractive solitons and may form biskyrmion and multiskyrmion states (clusters).

To date, no direct observations of isolated skyrmions or skyrmion clusters have been reported in the cone phases of chiral helimagnets. However, a few isolated observations such as a decomposition of a skyrmion lattice into cluster-like patterns [18] and the formation of skyrmionic droplets in MnSi plates [19], are in accord with our theoretical results and indicate possible directions for the investigation of this phenomenon.

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