Coupled quasimonopoles in chiral magnets

Gideon P. Müller, Filipp N. Rybakov, Hannes Jónsson, Stefan Blügel, and Nikolai S. Kiselev

1Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany
2Science Institute and Faculty of Physical Sciences, University of Iceland, 107 Reykjavík, Iceland
3Department of Physics, RWTH Aachen University, 52056 Aachen, Germany
4Department of Physics, KTH—Royal Institute of Technology, SE-10691 Stockholm, Sweden
5Ural Federal University, Ekaterinburg 620002, Russia

(Received 1 May 2019; revised manuscript received 18 February 2020; accepted 30 March 2020; published 4 May 2020)

Magnetic singularities, also known as magnetic monopoles or Bloch points, represent intriguing phenomena in nanomagnetism. We show that a pair of coupled Bloch points—a dipole string—may appear as a stable state in cubic chiral magnets. Analysis of the thermodynamic stability of such objects in the interior of crystals and in geometrically confined systems is presented. Employing advanced Monte Carlo simulations, we reveal an effect of spontaneous nucleation of dipole strings with characteristic size on the order of the helix pitch at temperature close to the paramagnetic phase transition. Such behavior of chiral magnets at elevated temperature drastically distinguishes them from ordinary ferromagnets and may provide a significant contribution to the topological Hall effect even in the absence of skyrmions.

DOI: 10.1103/PhysRevB.101.184405

I. INTRODUCTION

Point singularities in magnets [1,2] are topologically non-trivial objects known as Bloch points (BPs) [3] or hedgehogs and recently have become commonly referred to as quasimonopoles or monopoles [4,5]. Within the classical continuum magnetic approach, such a singularity is a point where the magnetization vector \( \mathbf{M}(r) \) suffers a discontinuity, but there is, nevertheless, no divergence in the energy [2]. Contrary to the hypothetical Dirac monopole, the magnetic flux through the surface surrounding a magnetic singularity is equal to zero. Nevertheless, noticeable similarity between these objects does exist. For instance, similar to the Dirac string stretching from a magnetic monopole, a magnetic singularity can be considered as an origin of a skyrmion string [4,6] representing vortex strings in the magnetization vector field. Typically, skyrmion strings are observed as singularity-free magnetic textures stretching throughout the entire sample between free edges. Of particular interest are the systems where skyrmion strings can end with point singularities within the crystal [7]. Earlier it has been proven both theoretically [8] and experimentally [9] that the configuration, known as a chiral bobber, where one end of a skyrmion string goes to a surface while another one ends with a point singularity inside the sample, can be stable in an isotropic chiral magnet.

Another possible scenario corresponds to the case when both ends of the string represent point singularities with opposite topological charge [6] (see Ref. [3] for the definition of topological charge for point singularities). Textures of this type are known under different names such as the dipole string (DS) [6], skyrmion string [10], magnetic globule [11], toron [12], or monopole-antimonopole pair [13] in spin systems and as the pipe [14] or toron [15] in liquid crystals. Here, we use the name dipole string introduced by Ostlund in Ref. [6], which, to the best of our knowledge is the first work where this type of spin textures was studied.

In bulk crystals of ordinary Heisenberg ferromagnets, DSs cannot be statically stable and collapse via shrinking and mutual annihilation of the two Bloch points [6]. In bulk crystals of chiral magnets, an isolated DS remains unstable; however, depending on material parameters it either shrinks and disappears or expands into an infinite skyrmion tube [12]. It is worth mentioning that the existence of statically stable isolated DSs in bulk crystals of chiral magnets, as claimed in Ref. [12], is not confirmed by our studies [16]. On the other hand, in Ref. [12] the authors pointed out that the stability of a DS can be achieved in a thin film of a chiral magnet when the singularities are located in the vicinity of opposite surfaces of the film. In this case, the mechanism of stabilization for a pair of quasimonopoles is similar to that of a coupled pair of chiral bobbers situated near opposite surfaces of the film [17]. A more sophisticated scheme for stabilization of such a configuration in a thin disk of a chiral magnet has been suggested in Ref. [13]. The disk has to be covered by additional magnetic layers coupled to a chiral magnet via exchange interaction and has strong perpendicular anisotropy. These artificial interfaces serve to pin the spins perpendicular to the interface on the top and bottom surfaces of the sample. The analog of such artificial confinement has been used for the stabilization of exotic textures in liquid crystals squeezed between glass plates where the surfaces are treated to align the molecules along the normal [15].

We present in this paper results showing that the stability of such a coupled pair of quasimonopoles does not in general
require geometric confinement but can be achieved even within the interior of chiral magnets favoring skyrmions [18], such as MnSi [19], FeGe [20], Fe$_{1-x}$Co$_x$Si [21], and some other Si- and Ge-based metallic alloys and insulating magnets such as Cu$_2$OSeO$_3$ [22] and alloys of β-Mn-type Co-Zn-Mn [23]. Furthermore, we consider different mechanisms for the stabilization of coupled quasimonopoles in geometrically confined systems beyond thin films. We also study the thermodynamic properties of such magnetic textures at elevated temperature by means of advanced Monte Carlo simulations.

II. MODEL

The energy of the simulated system is described by an extended Heisenberg model for an isotropic chiral magnet defined by the following Hamiltonian [24]:

$$E = -J \sum_{\langle ij \rangle} \mathbf{n}_i \cdot \mathbf{n}_j - \sum_{\langle ij \rangle} \mathbf{D}_{ij} \cdot (\mathbf{n}_i \times \mathbf{n}_j) - \mu_s B_{ext} \sum_i \mathbf{n}_i, \quad (1)$$

where $\mathbf{n}_i = \mu_i / \mu_s$ is the unit vector of the magnetic moment at lattice site $i$, $\langle ij \rangle$ denote the summation over all nearest-neighbor pairs once, $J$ is the Heisenberg exchange constant, $\mathbf{D}_{ij}$ is the Dzyaloshinskii-Moriya vector defined as $\mathbf{D}_{ij} = D r_{ij}$ with the scalar constant $D$ and the unit vector $\mathbf{r}_{ij}$ pointing from site $i$ to site $j$, and $B_{ext}$ is an external magnetic field. In order to keep the generality of the results presented below, as well as consistency with earlier studies, the size of the simulation domain is always given in terms of reduced units with respect to $L_D = 2\pi a J / D$—the lowest period of a spin spiral in the continuous limit ($J \gg D$), where $a$ is the cubic lattice constant (for details see Appendix A). Note that in cubic chiral magnets, for instance, in alloys of Mn$_{1-x}$Fe$_x$Si and Mn$_{1-x}$Fe$_x$Ge, $L_D$ may vary from a few nanometers up to a few hundred nanometers depending on composition $x$ [25]. An external magnetic field is always given with respect to $B_D = D^2 / (\mu_s J)$—the critical field at which the bulk system reaches the field polarized ferromagnetic state.

It is known that this model (1) has predictive power and describes well fundamental properties of chiral magnets. The dipolar interactions can be added when quantitative agreement with experiments is required [9,26].

To estimate the stability of the magnetic states discussed in this paper we performed spin dynamics relaxation based on the Landau-Lifshitz-Gilbert equation of motion and the calculation of minimum-energy paths with the geodesic nudged elastic band method [27]. These calculations, as well as the visualization of the isosurfaces, have been performed with the Spirit framework [28]. For very large systems we used a direct energy minimization with the nonlinear conjugate gradients method and finite temperature simulations with the Monte Carlo method implemented for the NVIDIA CUDA architecture [29]. The latter allowed us to perform simulations for systems of large sizes $\approx (10L_D)^3$ with $L_D \sim 30a$, composed of $\approx 10^7$ lattice sites.

III. DIPOLE STRING IN THE VICINITY OF MAGNETIC INHOMOGENEITIES

Figure 1 shows a magnetic texture of a DS, which is composed of two coupled singularities with a skyrmionic core between them. Note that due to the presence of discontinuities such an object cannot be classified by the Hopf invariant [30].

Despite the trivial topology of the DS [6], at certain conditions the annihilation of the BPs can be associated with a large energy barrier which makes the DS stable. For instance, as shown in Fig. 1, a cluster of DSs can be stabilized due to confinement effects. Our numerical analysis shows that DSs have the tendency to repel each other (for details see Appendix B). The isolated DS within the conical or ferromagnetic phase collapses because there is no energy barrier that could prevent the annihilation of the two BPs. Below, we show that a single DS can be stabilized in the interior of a crystal due to its coupling to textures representing defects or distortions of the ground state.

For a moderately strong external magnetic field, $B_{ext} < B_D$, the global energy minimum for (1) corresponds to the conical state—a helical spin spiral with $\mathbf{k} \parallel \mathbf{B}_{ext}$ and a magnetization tilted towards the direction of $\mathbf{B}_{ext}$. In practice, magnetic textures are often distorted or contain various defects or inclusions, i.e., localized magnetic structures that differ from the ground-state texture. A prime example of such an inclusion in the conical phase is the skyrmion tube (SKT) [17,31]. Figure 2(a) shows an isolated SKT in the conical phase with distinctive modulations in the isosurfaces. The states shown in Figs. 2(b)–2(d) represent stable configurations of DSs of varying size coupled to the SKT. The minimum-energy path between these configurations is shown in Fig. 2(e). It was calculated using the geodesic nudged elastic band method [27] implemented in the Spirit framework [28]. In order to keep the results as transferable as possible between different materials, the energy is given in units of $J^2 / D$, which is proportional to the unique product of powers of micromagnetic constants, namely, $M_s B_D L_D^7$ ($M_s$ is the saturation magnetization), the dimension of which is in units of joule. The minimum-energy path clearly shows the presence of an energy barrier between
Fig. 2. (a)–(d) Stable three-dimensional spin configurations representing inclusions in the conical phase in a bulk sample of an isotropic chiral magnet. The inclusions are composed of a skyrmion tube and a dipole string of varying size coupled thereto. (e) A minimum-energy path between the elongated dipole string coupled to a skyrmion tube as shown in (d) and the isolated skyrmion tube shown in (a) calculated using periodic boundary conditions in all three directions for $B_{\text{ext}} = 0.45B_D$ with $L_D = 20a$. The magnetic states corresponding to the intermediate local minima are shown in (b) and (c). For the magnetic states at the saddle points marked as hollow circles, see Fig. S1 in Supplemental Material [32]. (f)–(h) Examples of dipole strings coupled to a skyrmion tube in a cube of side length $9L_D$. Single or multiple dipole strings, including elongated ones, may be coupled to the same skyrmion tube.

The intermediate configurations, indicating that the DS attached to the SkT indeed represents a metastable state that cannot be destroyed by small excitations. The distance $d_{BP}$ between the poles of the elongated DSs is quantized with a pitch $\sim L_D$, while the lowest-energy state always corresponds to the state with the smallest $d_{BP} < L_D$ as in Fig. 2(b), which may vary slightly with the value of the applied field. The energy of such a coupled state increases approximately linearly with $d_{BP}$ and tends to the energy of two coupled infinitely long skyrmion tubes. It has been shown recently that such coupled states appear due to the attractive interaction between skyrmion tubes at $B_{\text{ext}} < B_D$ [31,33,34]. A single SkT can host a number of DSs coupled to it. Examples of such states are shown in Figs. 2(f)–2(h).

Edge dislocations represent another type of inclusion that can appear within a conical phase. They belong to the family of native defects emerging in striplike states in magnetism [35] and beyond [36]. We find that an edge dislocation can provide stability for the DS in the interior of the crystal as shown in Fig. 3. We find that the range in magnetic field strength where an isolated DS coupled to an edge dislocation is stable includes at least $0.31B_D$ to $0.83B_D$.

Note that ordinary periodic or open boundary conditions cannot be applied in the case presented in Fig. 3 due to the broken symmetry of the spin texture. This can be clearly seen in the cross sections shown in Figs. 3(c)–3(h). Both the $x$ and $z$ direction cannot be treated with periodic boundary conditions.

In order to calculate physically correct states of a bulk crystal, but with nonperiodic boundary conditions, a special scheme was applied. In the $y$ direction periodic boundary conditions are applied. In the $x$ direction, the spins at the boundary layers are pinned according to the analytical solution of the conical state for the corresponding applied magnetic field determined by the polar angle $\theta = \arccos(B_{\text{ext}}/B_D)$ and the azimuthal angle $\varphi = 2\pi z/L_D + \varphi_0$. In order to enforce the stability of the dislocation within the simulated domain, the values of $\varphi_0$ on the left and right boundary of the domain ($x_{\text{min}}$ and $x_{\text{max}}$) are set to be different with $\Delta\varphi_0 = \pi$. The infinite continuation in the $z$ direction is achieved by the following method. In ordinary periodic boundary conditions the upward neighbors for spins in the endmost upper layer, $z = z_{\text{max}}$, are the spins in the endmost lower layer with $z = z_{\text{min}}$. Contrary to this, in our implementation, the spins in the layer with $z = z_{\text{max}} - L_D$ play the role of upward neighbors for the endmost upper layer. Correspondingly for the endmost lower layer, $z = z_{\text{min}}$, the downward neighboring spins are in the layer with $z = z_{\text{min}} + L_D$. This enables the calculation of a single defect line in the striplike phase, as shown in Fig. 3. From the above it is clear that the size of the simulated domain along the $z$ axis, $L_z$, has to be a multiple of $L_D$. Moreover, $L_z$ should
be large enough to host at least a few periods of the spin spiral and material parameters have to be chosen such that \( L_D = N a \), where \( N \) is an integer and \( a \) is the lattice parameter. In our simulations we used \( L_c = 8L_D \) and \( L_z = 32a \), meaning 256 lattice sites along the \( z \) axis. For consistency, we used the same number of lattice sites in the other directions, \( L_x = L_y = L_z \).

**IV. DIPOLE STRINGS IN NANOWIRES**

The results presented in the previous sections clearly show that inclusions and inhomogeneities typically occurring in the conical phase, such as SkTs and edge dislocations, can provide stability to DSs in the interior of crystals. On the other hand, to observe the nanoscale textures of the DS in an experimental setup at reduced temperature, the size of the sample plays an important role. Below we show that for samples of finite size the stability of DSs is naturally provided by coupling with edge modulations inherent in chiral magnets [37–39].

Figure 4(a) shows a diagram of magnetic states calculated for a long nanowire as function of the width \( W \) in an external magnetic field applied along its main axis. We find a surprisingly wide range of applied field strength and nanowire width where a single DS remains stable. When the applied field approaches \( B_{\text{ext}} = B_D \) the conical phase is suppressed. Similar to chiral bobbers, the saturation of the conical phase at high magnetic field limits the stability of the DS and leads to its collapse. Similar to the case of a DS attached to an edge dislocation in a bulk crystal, the upper bound for the stability of the DS is \( B_{\text{ext}} \approx 0.86B_D \) and remains nearly constant for \( W/L_D > 2 \), but decreases as the wire is made thinner. There is also a lower limiting field below which the DS disappears via the escape of the BPs from the system through the free edges. The value of the lower bounding field decreases gradually with increasing width, \( W \), of the wire. We estimate the critical width of the nanowire to be \( W \approx 10L_D \), above which the DS may remain stable even at zero magnetic field.

Over the whole range where the DS is stable, its energy is higher than that of the conical phase. Within this range, there is a region where the energy density of a single SkT along the wire is lower than that of the conical phase, meaning that it represents the ground state of the system [40]. Outside this region, the SkT remains stable up to high \( B_{\text{ext}} \) [see the gray curve in Fig. 4(a)]. Note, in the spin-lattice model the critical field of the skyrmion collapse is defined by the ratio of internal coupling parameters, \( J/D \), while in the continuum limit the collapse does not occur even if \( B_{\text{ext}} \to \infty \) [41].

Figure 4(b) shows the dependence of the total energy of the SkT and DS as a function of the length \( L \) of the wire with respect to the ground state which for the chosen parameters corresponds to the conical phase with edge modulations. Since the SkT occupies the whole volume of the wire, its energy increases linearly with \( L \). On the other hand, the energy of the DS as a three-dimensional (3D) localized state remains approximately constant. The presence of a DS introduces local distortion to the ground state. In the calculations with periodic boundary conditions and finite \( L \), the energy of the DS may somewhat deviate from the self-energy of the DS when \( L \to \infty \) (dashed line). The distortions introduced by the SkT and DS in the nanowire are visualized in Figs. 4(c)
FIG. 4. (a) Phase diagram of magnetic states in a nanowire of width $W$ and an external magnetic field $B_{\text{ext}}$ applied along the wire. The red region corresponds to a single SkT ground state, while the stability range for the SkT is denoted by the solid gray line (open circles). The blue region corresponds to the stability of the isolated dipole string. Note, $W/L_D \to \infty$ denotes the limiting case of a semi-infinite crystal with a single surface representing a flat boundary between the crystal and vacuum. The DS, in this scenario, remains stable with an equilibrium position near that boundary. The symbol $\times$ indicates the parameter values chosen for (b)–(f). (b) The self-energy of the DS, $E_{\text{DS}}$, and the SkT, $E_{\text{SkT}}$, with respect to the energy of the conical ground state, $E_{\text{cone}}$, as function of the length, $L$, of the nanowire. The horizontal dashed line represents the self-energy of the DS in an infinitely long nanowire, $E_{\text{DS}} \approx 19.5J^2/D$, estimated using special boundary conditions as used for Fig. 3 in Sec. III. (c) and (d) illustrate isosurfaces ($\theta = 90^\circ$) of the SkT and DS, respectively. The presence in isosurfaces of a stripelike pattern indicates the modulations of magnetization near the free edges. (e, f) The minimum-energy path calculated for $W = 2.25L_D$ and $B_{\text{ext}} = 0.43B_D$, describing the transition from an infinite skyrmion tube (I) to an isolated dipole string (IV) and then to the conical state with edge modulations (V). More intermediate states are shown for $W = 2L_D$ and $B_{\text{ext}} = 0.45B_D$ in Fig. S2 in Supplemental Material [32]. For the costly computations of the minimum-energy paths in (e) and (f) we set $L_D = 20a$, while for (a)–(d) we use $L_D = 30a$, explaining the $\approx 20\%$ difference of energies in (b) and (f).

and 4(d), where edge modulations have distinctly different periodicity. Noticeably, such behavior of the self-energy of the SkT and DS applies to a broad range of parameter values. In particular, for any $B_{\text{ext}}$ and any $W/L_D$ where the DS is stable, and the ground state is the conical phase with edge modulations [the blue region in Fig. 4(a)], there is always a certain critical $L$ above which the DS is lower in energy than the SkT. This can lead to a transition from SkT to DS.

To illustrate the possibility of such a transition, we calculated the minimum-energy path from a homogeneous SkT (I) to a single DS (IV) and then to the conical state with edge modulations (V). In Figs. 4(e) and 4(f) we show only those parts of the minimum-energy path which remain approximately invariant as the length of the nanowire is varied. The path between states (III) and (IV) depends on the length of the nanowire and is therefore not shown. There is a barrier on this stretch of path, and then the energy gradually drops while SkTs with one end, which are located above and below the DS, move to the opposite ends of the wire (see also Fig. S2 in Supplemental Material [32]). Thereby, for a sufficiently long wire, $L \gg L_D$, and appropriate value of $B_{\text{ext}}$ the condition $E_{(I)} \gg E_{(IV)}$ will be satisfied. The energy barrier of $\approx 2J^2/D$ for the collapse of the DS is of the same order of magnitude as the energy barrier for the chiral bobber estimated with the same method in Ref. [8]. On the other hand, the height of the energy barrier is not the only factor determining the stability of localized states [42]. The preexponential factor in the Arrhenius expression for the lifetime, reflecting the relative entropy of the transition state and the initial state, also needs to be evaluated. The estimation of the lifetime of the metastable states depicted in Fig. 4(e) is a topic of future studies.
V. DIPOLE STRINGS AT HIGH TEMPERATURE

In the previous sections we discuss the case of DS stability at zero temperature, \( T = 0 \). The self-energy of the DS, \( E \), in this case, may take relatively high values. Nevertheless, at high temperature the free energy of the DS, \( F = E - TS \), can be significantly reduced due to the contribution of the entropy, \( S \). The purpose of this section is to provide clear evidence of this fact and illustrate the spontaneous appearance of DSs at high temperature, \( T \sim T_c \), which we observe in our simulation. The results presented in this section are not intended to be a comprehensive answer to the question where DSs can be observed, but rather are clear evidence of the fact that the DSs may play a significant role in the thermodynamic properties of chiral magnets.

This section is organized as follows. First, we provide calculated energy values of the DS in comparison to a chiral bobber in the frame of the model. We also make an estimate of these quantities for the B20-type alloys such as MnSi and FeGe. After that, we discuss some aspects of realistic, large-scale Monte Carlo simulations. Then, we present an advanced approach for the visualization and analysis of highly fluctuating textures in Monte Carlo simulations employing forward and inverse fast Fourier transform (FFT) of 3D vector fields. By means of this approach, we estimate the critical temperature in our model and illustrate the behavior of the system near the critical temperature. In the two last subsections, we demonstrate the effect of skyrmion lattice melting and provide clear evidence for the emergence of dipole strings as a state representing a dynamic array of fluctuating lumps at high temperature. In order to emphasize the latter effect, we compare the behavior of the chiral magnet to the pure Heisenberg model of a ferromagnet.

A. From the Heisenberg model to the model of chiral magnets

The model of chiral magnets used in this paper can be also called a frustrated Heisenberg model by which we here mean the presence of Dzyaloshinskii-Moriya interaction (DMI). This model is widely used for simulations of B20-type cubic chiral magnets such as MnSi and FeGe. This model, of course, is a significant simplification and fundamentally unable to describe a number of effects like canting \([43]\), magnetism from itinerant electrons, etc. Nevertheless, it is believed \([21,24]\) that this simplified model is suitable for describing the basic properties of isotropic chiral magnets.

For most of the B20-type cubic chiral magnets the period of the helical modulations in the ground state is typically substantially larger than the lattice constant: \( L_{D,MnSi} = 18 \text{ nm}, L_{D,FeGe} = 70 \text{ nm} \), and \( a_{\text{MnSi}} = 0.456 \text{ nm}, a_{\text{FeGe}} = 0.469 \text{ nm} \) \([44,45]\). Even in the rough approximation assuming that the internode distance in the model (1) effectively corresponds to the lattice constant of a B20-type crystal, in accordance with (A1) and (A2), the appropriate value for the DMI constant \( D \) should be \( \approx 0.16J/D \) and \( \approx 0.04J/\alpha \) for MnSi and FeGe, respectively. In other words, the constant \( D \) is expected to be relatively small compared to the exchange constant \( J \). Therefore, it is reasonable to expect that such a slightly frustrated mode should inherit many key properties of the primary Heisenberg model to which we also refer as the \( D = 0 \) model. In particular, it is expected that the phase transition from the ordered to the paramagnetic state should occur in close vicinity of the temperature \( T_{2}^{\beta=0} \), corresponding to the second-order phase transition between the ordered state and the paramagnetic state in the primary Heisenberg model. Note, this critical temperature has been previously calculated with high accuracy \([46,47]\) and equals \( T_{2}^{\beta=0} = 1.443J/k_B \). Moreover, it is worth emphasizing that there is clear evidence of the fact that monopoles play a significant role at temperatures near \( T_c \), even in the \( D = 0 \) model \([48,49]\). For instance, it was shown that their appearance in 3D Heisenberg-like ferromagnets has an impact on the anomalous Hall effect \([10,50]\). In the previous Secs. III and IV, we have shown that the presence of DMI can lead to the coupling of such monopoles into dipole strings. In accordance with the above, it is of special interest to study how the appearance of such coupled monopoles may affect the system near the critical temperature.

First, let us estimate the typical energy of the DS in a moderate magnetic field. In the sections above the energies of the states are given in units of \( J^2/D \) while here it will be convenient to present the energies in units of \( J \), because the critical temperature is expected to be near the value \( J/k_B \). By using (A2) one can write the following simple relation:

\[
\frac{J^2}{D} = \frac{L_D}{2\pi a} J \approx 0.16 \left( \frac{L_D}{a} \right) J \tag{2}
\]

In Table I we present the energies of the DS, \( E_{DS} \), as well as the chiral bobber \([8]\), \( E_{cha} \), for comparison.

| Texture       | \( B_{ext} = 0.35B_D \) | \( B_{ext} = 0.4B_D \) | \( B_{ext} = 0.45B_D \) |
|---------------|-----------------|-----------------|-----------------|
| Dipole string | 2.2             | 2.0             | 1.9             |
| Chiral bobber | 0.69            | 0.66            | 0.40            |

For material parameters of MnSi, we estimate a value of \( L_D/a \approx 40 \), which corresponds to the energy of a dipole string \( E_{DS} \approx 80J \). At first sight, the expected influence of such an energetically expensive excitation on the thermodynamic properties should be negligible. However, at high temperature, the free energy of such a particle can decrease significantly due to the contribution of entropy.

B. Finite temperature Monte Carlo simulations for bulk chiral magnets

The Monte Carlo simulations with a reasonably small ratio of \( D/J \) and as a result a realistically large value of \( L_D \) must be performed on quite large 3D lattices composed of a few hundred lattice sites per each of the three directions. This requires a lot of computational resources even for a model including only nearest neighbors. We solve this problem by means of parallel calculations on a GPU. It is worth explaining the choice of this approach, because many alternative approaches can be found in the literature.

One of the first Monte Carlo simulations for the Hamiltonian (1) in three dimensions was reported in Ref. \([51]\). One of the important results reported in this paper clearly shows...
that for a large DMI constant, \( D/J \approx 0.73 \) for any temperature \( 0 \leq T \leq T_c \), there is always a finite range of external magnetic field where a lattice of infinitely long skyrmion tubes represents the ground state of the system. A similar result is known for the two-dimensional (2D) model, where flat chiral skyrmions remain thermodynamically stable in a wide range of temperature, in both the continuum micromagnetic limit [18] and the spin-lattice model [24].

On the other hand it is known that, in the continuum limit of the 3D model (1), i.e., small ratios of \( D/J \), the skyrmion lattice loses its thermodynamic stability—even for \( T \to 0 \). Indeed, in the micromagnetic model of a bulk isotropic chiral magnet, the energies of isolated skyrmion tubes, as well as the skyrmion lattice, are always higher than that of the conical phase [52]. Earlier, it was also shown that in the framework of the Landau theory for phase transitions the lattice of skyrmion tubes is not stable near the critical temperature, at least when the leading terms of expansion are taken into account [53]. The studies of the stability of a skyrmion lattice at finite temperature are motivated to a large extent by experimental observation of an anomalous phase appearing near the critical temperature in a narrow range of temperature and external field [54–58]. It is commonly accepted to refer to this phase as the A phase, where “A” stands for “anomalous.”

An unusual approach to resolve the above-mentioned discrepancy between the results of Monte Carlo simulations and experimental observation has been suggested in the same work by Buhrandt and Fritz [51] (see also Ref. [4]). According to their approach one has to add additional interactions with spins located next to nearest neighbors in the 100-type directions. The corresponding constants of these interactions, \( J' \) and \( D' \), are selected such as to compensate (minimize) the influence of the discrete lattice on the magnetic textures which are assumed to be continuous. In the limit \( T = 0 \), this method indeed guarantees accuracy. In particular, following this approach one can increase the accuracy of the calculations performed on relatively small grids and large ratios \( D/J \), obtaining results closer to those of large grids and small ratios \( D/J \). The latter means that one can achieve a better agreement between the spin-lattice model and the micromagnetic model. Remarkably, this approach allows one to outperform the standard finite difference scheme used in most micromagnetic

FIG. 5. Snapshots of direct and filtered magnetic textures in Monte Carlo simulations after full thermalization are shown. The snapshots correspond to different temperature values given in units of \( \mu_B J/k_B \); 1.29, 1.32, 1.36, and 1.48. In these simulations periodical boundary conditions are applied in all three directions. The top row of images corresponds to a nonfrustrated Heisenberg ferromagnet (DMI constant \( D = 0 \)). The bottom row corresponds to the case of a chiral magnet with a DMI constant of \( D = 0.2J \). In both cases, the external magnetic field \( \mu_B B_{\text{ext}} = 0.016J \) is applied along the vertical \( z \) axis. Note, in the case of a chiral magnet, this field value corresponds to 0.48\( B_0 \). The first two images in both rows for \( T = 1.29 \) illustrate the noisy spin texture before filtering and the clean one after filtering. Note that in the case of the chiral magnet the modulations along the vertical \( z \) axis are noisy but visible. Noticeably, for identical filtering parameters, the reasonably large excitations—after filtering—can be seen only above the critical temperature, \( T_c^{\text{pure}} \) in the case of the pure Heisenberg magnet, while in the case of the chiral magnet the same rate of excitations can be seen even below the critical temperature (compare the last image in the top row for \( T = 1.48 \) and the second image in the bottom row for \( T = 1.29 \)). Isolated, “long-lived” dipole strings can be observed at \( T = 1.29 \), although their concentration is low; see red arrow. At \( T = 1.32 \), a high concentration of “long-lived” dipole strings can be observed. Surprisingly, dipole strings can also be observed above \( T_c \); see the image in the bottom row for \( T = 1.36 \). However, in this case, the dipole strings on average have a slightly smaller size. They are nucleated more often but also decay within fewer Monte Carlo iterations. When the perturbations are very strong (the rightmost snapshot in the bottom row), it is quite difficult to confidently distinguish dipole strings from other “lumps.” This state has more similarities with the dipole strings-free case (\( D = 0 \)) at higher temperature, \( T > 1.5 \) (not shown in the figure). One may conclude that the emergence of dipole strings is mainly enhanced for \( T \sim T_c \).
the three field components, that is, the 3D real-to-complex The algorithm consists of three steps: (1) 3D FFT of each of the idea behind this approach is in the spirit of image denoising. For instance, in some classical models, it was shown that similar competing interactions may significantly affect the system and shift it towards the Lifshitz point [61]. Taking this into account we performed our Monte Carlo simulations directly for the Hamiltonian (1), i.e., with nearest neighbors only. We use a large lattice size ($N = 160^3$) and a small ratio of $D/J = 0.2$. Such a small $D/J$ results in a helix period $L_D$ of about $32a$ and makes the model more realistic and comparable to the case of MnSi. On each Monte Carlo step we used a standard Metropolis algorithm, implemented for massively parallel GPU architectures [29].

C. Advanced approach for analysis of highly fluctuating spin textures at high temperature

A natural obstacle for the analysis of spin systems at high temperature is that of fluctuations which prevent the proper identification of spin textures by means of simple visualization. Here, we discuss an advanced approach allowing us to identify a variety of textures based on Fourier transforms as a very valuable tool for the analysis of fluctuating periodical structures [51]. Note, it is assumed that the size of the spin textures is significantly larger than the lattice constant. The idea behind this approach is in the spirit of image denoising. The algorithm consists of three steps: (1) 3D FFT of each of the three field components, that is, the 3D real-to-complex FFT applied to $n_x$, $n_y$, and $n_z$; (2) spectrum filtering, that is, zeroing of amplitudes of highly oscillating harmonics—the critical period of such suppressed harmonics is a configurable parameter; and (3) inverse 3D FFTs, that is, the 3D complex-to-real inverse FFT applied to each of the three spectra.

After the processing we get a new vector field $\mathbf{f}$ which can then be visualized, for instance, by showing only those spins in real space for which $\pi_x < 0$ (see Fig. 5 and see movie 1 in Supplemental Material [32]). This method removes the highly oscillating components and allows one to see extended textures if they exist at a given temperature. To speed up the processing of such data, we took into account the Hermitian properties of the arrays obtained from real numbers by FFT. We also used 2D denoising in the same manner for cross sections of our rectangular domain to be able to identify helicoidal ordering.

Movie 1 in Supplemental Material [32] demonstrates how the filtering works. In the first minute, a stable solution is considered. It is obtained by direct minimization with periodic boundaries in $x$ and $y$ directions and open boundaries in the $z$ direction. One can see a cluster of chiral bobbers on the top surface, a single DS and skyrmion tube in the volume, and isolated chiral bobbers on the bottom surface (several periods of the surface spiral [17] are also visible on the bottom surface). At the 40th second, the Metropolis algorithm is launched for approximately 500 iterations (by one iteration we mean applying the Metropolis routine to all spins in the system once). Such a number of iterations at a temperature $T = 1.28$ is not enough to destroy such a state, but the system becomes very noisy. After that, the action of the two- and three-dimensional filters is demonstrated. It helps to very clearly identify the presence of all those objects (skyrmion tube, chiral bobbers, and DS) in the system, which were seen before the temperature was applied.

D. Critical temperature estimation

There are a few approaches to determine the critical temperature in Monte Carlo simulations. The most widely used one is the temperature dependencies of specific heat, susceptibility, and/or Binder cumulant. However, for systems with the ground state characterized by long-periodic modulations, the size of the simulated domain should be extremely large—at least several times larger than the period of the modulations. Even for a GPU-parallelized Monte Carlo simulation, it represents quite a challenging problem.

Here, we estimate the critical temperature of the system at zero field by tracing the effect of spontaneous symmetry breaking. We start with the 3D Heisenberg model ($D = 0$) with periodic boundary conditions in all three directions. We start with a fully random distribution of the spin directions and then perform approximately $10^5$ steps to achieve thermal stabilization. We clearly observe that for a temperature of $T \leq 1.44$ the system exhibits spontaneous symmetry breaking, meaning it possesses a constant magnetization component (for each of the projections). On the other hand, for temperatures $T \geq 1.45$, after thermalization, each component of the magnetization fluctuates around zero. Therefore, for the case of the pure Heisenberg model, we obtained a good agreement ($1.44 < T^c < 1.45$) with the well-known result $T^c = 1.443$ [46,47].

For $D \neq 0$, we estimated $T_c$ at $B_{\text{ext}} = 0$ as the temperature above which the system loses its helical order. Here, we started with a period-optimized helicoid (five periods along the $z$ axis) and checked whether the helical order remains the same after complete thermalization. By means of this approach, we found that at $B_{\text{ext}} = 0$ the system loses its helical order in the range of $1.34 < T_c < 1.35$.

E. Melting the skyrmion lattice

Due to the time-consuming nature of these calculations, we considered a narrow temperature range, $1.28 \leq T \leq 1.48$, and one value of the external magnetic field, $B_{\text{ext}} = 0.4B_D = 0.016$, which is known from continuum theory to be the most energetically favorable for skyrmions in thick films [17,62]. In this part of the calculations, we first prepared a well-relaxed lattice of skyrmion strings as an initial guess for the Monte Carlo runs. We also made independent runs, reducing the size of the lattice in the $x$ direction from 160 to 138, so as to optimize the aspect ratio and get a slight benefit for a triangular lattice. Remarkably, we were not able to stabilize the lattice of skyrmion strings at this magnetic field within the temperature range. In particular, in the case of periodic boundary conditions along all three directions, the skyrmion lattice melts.
We performed the same simulations with open boundary conditions along the $z$ direction, which corresponds to a thick film with a thickness of $t = 5L_D$. Note, in the limit of $T \to 0$, the lattice of skyrmion strings is a global energy minimum for such a film due to a chiral surface twist effect [17]. Nevertheless, even in this case the skyrmion lattice decays. Movie 2 in Supplemental Material [32] demonstrates the full process of melting at $T = 1.29$ for such a thick film.

Interestingly, in the case of a film, after thermalization, the top and bottom surfaces are occupied by chiral bobbers, regardless of the initial state. Thus, the entropy contribution to the free energy of a particle exceeds the potential energy $E_{CCB} \sim 20J$, and such a near-surface state becomes a global minimum. Note that the spontaneous nucleation of chiral bobbers at high temperature has also been reported in independent studies for cubic samples [63].

F. Emergence of dipole strings at high temperature

By carefully examining structures at high temperature, we found an interesting phenomenon. Movie 3 in Supplemental Material [32] demonstrates the Metropolis iterations after completion of thermal stabilization at $T = 1.32$. Thermal fluctuations lead to the nucleation of dipole strings, their perturbations, drift, and annihilation. For comparison, movie 4 in Supplemental Material [32] demonstrates the case of $D = 0$ at $T = 1.48$. On one hand, after filtering with identical parameters, both systems clearly show the appearance of some “short-lived” excitations in the form of flashes over the whole volume of the simulated domain. On the other hand, in the case of $D \neq 0$ shown in movie 3 in Supplemental Material, there are a lot of obviously more long-lived and more volumetric excitations which we identified with our FFT filtering tool as dipole strings. Note, we use a slightly higher temperature for the case $D = 0$ because not even the previously mentioned short-lived excitations appear at $T = 1.32$ and for the same filtering parameters one would see no excitations at all.

Remarkably, we observe the emergence of dipole strings not only below but also above $T_c$ (see Fig. 5). Thereby, one may conclude that dipole strings at temperature about $T_c$ are an essential part of the most probable states of the thermodynamic ensemble for the considered moderate external field value. We hope that this phenomenon, when studied more thoroughly, will help explain a number of experimental anomalies observed inside and near the A-phase region in helimagnets [58,64,65].

VI. CONCLUSIONS

In conclusion, we have shown that in a wide class of isotropic chiral magnets a three-dimensionally localized state composed of a pair of Bloch points or quasimonopole and antimonopole can be stable. By calculating minimum-energy paths, we have shown that a finite-energy barrier protects such dipole strings from collapsing. In the interior of a crystal, a dipole string remains stable when it is located near a defect line of the conical phase or is coupled to a skyrmion tube. We have shown that for a wide range in magnetic field strength and parameter values, in both extended and confined systems, dipole strings can be stable.

The effect of spontaneous appearance of dipole strings at high temperature, $T \sim T_c$, revealed by advanced Monte Carlo simulations, suggests that dipole strings may play a significant role in the thermodynamic and transport properties of chiral magnets.

In order to experimentally confirm the existence of dipole strings, the most promising avenue seems to be the partial or full reconstruction of the 3D magnetic configuration inside a crystal using some magnetic imaging technique, such as off-axis electron holography [39,66], the x-ray magnetic circular dichroism photoemission electron microscopy [67], or x-ray vector nanotomography [68] (see also Appendix C). According to recent studies, it is expected that stable magnetic textures containing singularities may also be confirmed with spin- and magnetotransport measurements [38,69,70].

ACKNOWLEDGMENTS

We thank I. Maccari, D. Weston, and E. Babaev for discussions. G.P.M. and H.J. acknowledge funding from the Icelandic Research Fund (Grant No. 185405-051). The work of F.N.R. was supported by Swedish Research Council Grants No. 642-2013-7837, No. 2016-06122, and No. 2018-03659; by the Göran Gustafsson Foundation for Research in Natural Sciences and Medicine; and by Olle Engkvists Stiftelse. S.B. acknowledges funding from Deutsche Forschungsgemeinschaft (DFG) through SPP 2137 “Skyrmionics” Grant No. BL 444/16-1, the Collaborative Research Center SFB 1238

![Graph](Image)
(Project No. C01), and the DARPA TEE program through MIPR Grant No. HR001831554 from DoI. The work of N.S.K. was supported by Deutsche Forschungsgemeinschaft (DFG) via SPP 2137 “Skyrmionics” Grant No. KI 2078/1-1.

APPENDIX A: EQUILIBRIUM PERIOD OF THE SPIN SPIRAL

In accordance with the results of Ref. [24], the equilibrium period of the spin spiral (for $B_{ext} = 0$) in a discrete model (1)

$$L_D^{(discrete)} = 2\pi a/ \arctan(D/J). \quad (A1)$$

Because, for the vast majority of materials, spin-orbit interactions are relatively weak, $D \ll J$, it is convenient to use the approximate formula

$$L_D = 2\pi aJ/D, \quad (A2)$$

which is simultaneously exact in the continuum theory [71] for which the considered Hamiltonian (1) is equivalent to a finite-difference scheme of second-order accuracy. So, for example, if $L_D = 20a$, then the relative mismatch of the periods is $\approx 3\%$. For $L_D = 32a$ the mismatch is only $\approx 1\%$.

APPENDIX B: NONEQUILIBRIUM LATTICES COMPOSED OF DIPOLE STRINGS

To investigate the stability of lattices of dipole strings we performed a systematic study for various symmetries: simple cubic, body-centered cubic, face-centered cubic, tetragonal, and hexagonal close-packed lattices, where dipole strings are located at the vertices of the lattice. For each of these cases, we estimated the dependencies of the energy of the fully relaxed state as a function of the unit-cell size. This paper aimed to find a configuration which represents a global or local minimum with an equilibrium unit-cell size. According to our calculations, none of the studied lattice symmetries provides a stable configuration for the dipole string lattice. In most of the cases, the energy continuously decays with increasing cell size in any of the directions. Above a critical size, when the interaction between the dipole strings is getting weak, the dipole strings collapse. Only in a few exceptional cases the variation of the unit-cell size leads to the appearance of a minimum on the energy dependence, as shown in Fig. 6 (blue line) for an hcp lattice of dipole strings. Nevertheless, the variation of the size of the unit cell in another dimension leads to the decay of the energy and always ends up with the collapse of the dipole strings. Thereby, we conclude that, most likely, dipole strings cannot form a lattice with an equilibrium period, at least with the symmetries mentioned above. However, a stable lattice of limited size is possible, under suitable boundary conditions such as, for example, free boundaries of the sample.

APPENDIX C: CHAINS OF SKYRMIONS, BOBBERS, AND DIPOLE STRINGS ON A RACETRACK

The transmission electron microscopy (TEM) is a well-established technique for magnetic imaging. In a standard TEM setup, the directions of the electron beam and the external magnetic field coincide while the projection plane—the plane of the image—is perpendicular to this direction. Thereby, a more appropriate regime for magnetic imaging with TEM is the regime when the magnetic field is perpendicular to the nanowire or nanostripe. In this section, we show that the stability of the DSs in this regime is also accessible. Moreover, we show that in this case the DSs may coexist with other localized objects as skyrmion tubes and chiral bobbers. To illustrate this we performed micromagnetic simulations [29] taking into account demagnetizing fields and using material constants for FeGe [9]. Namely, the exchange stiffness $A = 4.75 \text{ pJ m}^{-1}$, Dzyaloshinskii-Moriya interaction constant $D = 0.853 \text{ mJ m}^{-2}$, and saturation magnetization $M_s = 384 \text{ kA m}^{-1}$. We calculated the equilibrium state of a $2000 \times 120 \times 120$-nm strip with randomly distributed skyrmions, top/bottom bobbers, and dipole strings (see Fig. 7). The discretization size was $2 \text{ nm}$. The magnitude of the transverse magnetic field was chosen equal to $300 \text{ mT}$.

The equilibrium chains considered here may possibly find application in storage devices. Interestingly, the existence of four types of particles increases the theoretical data density. However, nearby dipole strings strongly push apart. Also, if one places the top and bottom bobber one after another, they can approach each other, forming a coupled pair [8]. Thus, some natural restrictions may be imposed on the sequence and the real gain in data density will be smaller than 2.

[1] E. Feldtkeller, Z. Angew. Phys. 19, 530 (1965).
[2] W. Döring, J. Appl. Phys. 39, 1006 (1968).
[3] A. P. Malozemoff and J. C. Slonczewski, Magnetic Domain Walls in Bubble Materials (Academic, New York, 1979).
[4] P. Milde, D. Köhler, J. Seidel, L. M. Eng, A. Bauer, A. Chacon, J. Kindervater, S. Mühlbauer, C. Pfeifer, S. Buhrandt, and C. Schütte, Science 340, 1076 (2013).
We dispute the following statement on page 7 of Ref. [12]:

“A. O. Leonov and K. Inoue, Phys. Rev. B 121, 014406 (2014).”

[12] A. O. Leonov and K. Inoue, Phys. Rev. B 121, 014406 (2014).
[61] T. Garel and S. Doniach, J. Phys. C 13, L887 (1980).

[62] A. O. Leonov, Y. Togawa, T. L. Monchesky, A. N. Bogdanov, J. Kishine, Y. Kousaka, M. Miyagawa, T. Koyama, T. Akimitsu, T. Koyama, K. Harada, S. Mori, D. McGrouther, R. Lamb, M. Krajnak, S. McVitie, R. L. Stamps, and K. Inoue, Phys. Rev. Lett. 117, 087202 (2016).

[63] J. Waters, T. Sluckin, D. Kramer, H. Fangohr, and O. Hovorka, lecture delivered at the DPG Spring Meeting, Berlin, Germany, March 2018.

[64] A. E. Petrova and S. M. Stishov, Phys. Rev. B 91, 214402 (2015).

[65] N. M. Chubova, E. V. Moskvin, V. A. Dyad’kin, Ch. Dewhurst, S. V. Maleev, and S. V. Grigor’ev, J. Exp.: Theor. Phys. 125, 789 (2017).

[66] P. A. Midgley and R. E. Dunin-Borkowski, Nat. Mater. 8, 271 (2009).

[67] S. Da Col, S. Jamet, N. Rougemaille, A. Locatelli, T. O. Mentes, B. S. Burgos, R. Afid, M. Darques, L. Cagnon, J.-C. Toussaint, and O. Fruchart, Phys. Rev. B 89, 180405(R) (2014).

[68] C. Donnelly, M. Guizar-Sicairos, V. Scagnoli, S. Gliga, M. Holler, J. Raabe, and L. J. Heydermann, Nature (London) 547, 328 (2017).

[69] H. Du, J. P. DeGrave, F. Xue, D. Liang, W. Ning, J. Yang, M. Tian, Y. Zhang, and S. Jin, Nano Lett. 14, 2026 (2014).

[70] M. Redies, F. R. Lux, J.-P. Hanke, P. M. Buhl, G. P. Müller, N. S. Kiselev, S. Blügel, and Y. Mokrousov, Phys. Rev. B 99, 140407(R) (2019).

[71] I. E. Dzyaloshinskii, Sov. Phys. JETP 20, 665 (1965).