Skyrmion Knots in Frustrated Magnets

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A magnetic Skyrmion is a stable two-dimensional nanoparticle describing a localized winding of the magnetization in certain magnetic materials. Skyrmions are the subject of intense experimental and theoretical investigation and have potential technological spintronic applications. Here we show that numerical computations of frustrated magnets predict that Skyrmions can be tied into knots to form new stable three-dimensional nanoparticles. These stable equilibria of twisted loops of Skyrmion strings have an integer-valued topological charge, known as the Hopf charge, that counts the number of particles. Rings are formed for low values of this charge, but for higher values it is energetically favorable to form links and then knots. This computational study provides a novel impetus for future experimental work on these nanoknots and an exploration of the potential technological applications of three-dimensional nanoparticles encoding knotted magnetization.

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Lord Kelvin initiated the study of knotted fields by proposing a vortex theory of atoms [1], where he envisaged vortex strings in the aether forming closed loops that would explain the distinct atomic species as a simple consequence of the existence of different types of knots and links. Over the past several years there has been a surge of interest in knotted fields, with a significant amount of theoretical research in addition to the physical realization of knots in many diverse systems, including hydrodynamics [2], optics [3], and liquid crystals [4], to name just a few examples. Here we investigate a nanoscale reincarnation of Kelvin's idea and provide numerical support for the existence of stable nanosize knots and links in a particular class of magnetic materials.

The lead character in our story is the magnetic Skyrmion, a two-dimensional topological soliton [5] that lives in a thin slice of a magnetic material and is characterized by the property that the direction of the local magnetization winds exactly once around the sphere of all possible directions. Magnetic Skyrmions were first obtained experimentally only a few years ago [6,7], but are now the subject of intense theoretical and experimental research, motivated by technological spintronic applications to information storage and logic devices [8]. The Skyrmion will play the role of the vortex in our modern reenactment of Kelvin's vision. The main idea is to liberate Skyrmions from their two-dimensional world to create fully three-dimensional stable topological solitons formed from closed loops of twisted Skyrmion strings.

The majority of current studies on Skyrmions involve a chiral ferromagnetic host. The existence of nanoscale Skyrmions in chiral ferromagnets, stabilized by the Dzyaloshinskii-Moriya interaction, was predicted by theoretical work [9] in the late 1980s, but it took two decades to obtain experimental confirmation [6,7]. Chiral ferromagnets are not inversion symmetric, so although they support Skyrmions they do not support anti-Skyrmions (where the magnetization again winds once around the sphere of all possible directions but this time with the opposite orientation). An alternative stabilization mechanism is provided by long-range dipolar interactions, which allows both Skyrmions and anti-Skyrmions, and these have been obtained experimentally [10] with a size of around 100 nm. Recent results [11–13] on Skyrmions in frustrated magnets show that these systems are capable of providing the richest phenomena. In addition to hosting both Skyrmions and anti-Skyrmions, there is an additional rotational degree of freedom that is frozen in other hosts. It is this new found flexibility that we exploit to obtain three-dimensional particles and knots.

We study a frustrated magnet in which there are competing nearest-neighbor ferromagnetic and higher-neighbor antiferromagnetic exchange interactions. We employ the continuum Ginzburg-Landau theory for these frustrated magnets, which has been shown [13] to successfully reproduce the properties of Skyrmions obtained from lattice computations. Within this approach the task is to solve for the spatial distribution of the direction of the magnetization $\mathbf{m}(\mathbf{r})$, where $\mathbf{m} = (m_1, m_2, m_3)$ is a vector of unit length and $\mathbf{r} = (x, y, z)$ is the spatial coordinate. Only the orientation of the magnetization varies as its magnitude can be taken to be equal to the constant saturation magnetization. The static equilibria are found by minimizing the Ginzburg-Landau energy for the frustrated magnet, which contains the following leading order terms [13]

$$E = \int \left(-\frac{I_1}{2}(\nabla \mathbf{m})^2 + \frac{I_2}{2}(\nabla^2 \mathbf{m})^2 + |\mathbf{H}| - \mathbf{H}\cdot\mathbf{m} \right) d^3 r, \qquad (1)$$

where the constants I_1 and I_2 are linear combinations of the nearest-neighbor ferromagnetic and higher-neighbor antiferromagnetic exchange constants, with the particular linear combinations depending upon the geometry of the atomic lattice. The final term is the Zeeman interaction with an external magnetic field $\mathbf{H}$, which is taken to lie along the third direction $\mathbf{H} = (0, 0, H)$.

For Skyrmions in frustrated magnets the crucial feature is that $I_1 > 0$ and $I_2 > 0$. The fact that the first term yields a negative contribution to the energy means that this term favors an increase in scale when considering the standard three-dimensional Derrick scaling argument, rather than the usual decrease in scale for a ferromagnet with $I_1 < 0$. We use scaled dimensionless units to set $I_1 = I_2 = 1$, so that the nanoscale sized Skyrmion has a size of order one in dimensionless units. When the background magnetic field is greater than the saturation field, $H \geq \frac{1}{4}$ in dimensionless units, the ground state is the fully polarized ferromagnetic state $\mathbf{m} = (0, 0, 1)$, aligned with $\mathbf{H}$. The inclusion of the constant term $|\mathbf{H}|$ in Eq. (1) makes use of the freedom to add a constant to the energy and is included so that the ground state $\mathbf{m} = (0, 0, 1)$ is defined to have zero energy. We consider isolated solitons embedded in this constant far field by taking the background magnetic field to be twice the saturation value, $H = \frac{1}{2}$. For simplicity we neglect anisotropy, but in fact anisotropy improves the stability of Skyrmions in frustrated magnets [12], so its inclusion should only strengthen the results of our findings.

The energy is computed using a finite difference approximation on large grids containing $150^3 - 200^3$ lattice points with a lattice spacing in the range 0.1–0.4. Periodic boundary conditions are imposed and derivatives are approximated by second order accurate finite differences. The energy is minimized by applying a leap-frog algorithm to evolve a second order dynamics in an auxiliary time with periodic removal of auxiliary kinetic energy [14]. We have verified that the results are stable to changes in the number of grid points and the lattice spacing.

The three-dimensional topology is provided by the Hopf charge [15] Q, which is an integer that counts the linking number of magnetization field lines (this being the appropriate topological generalization of the Skyrmion winding number in two dimensions). In detail, consider all the points in the material where the direction of the magnetization is equal to $\mathbf{m} = (0, 0, -1)$, which is exactly the opposite direction to the far field magnetization. In a three-dimensional medium this value of the magnetization will generically be attained on a closed curve in space (or potentially a collection of closed curves). This closed curve specifies the location of the Skyrmion string, as one of the characteristic features of the Skyrmion is that the magnetization at its center points in exactly the opposite direction to that of the far field. Now consider any other fixed direction for the magnetization, a convenient choice for visualization is to take $\mathbf{m} = [0, -(1/\sqrt{2}), -(1/\sqrt{2})]$, but any other direction will do just as well to compute the topology. This second direction will define a second closed curve in

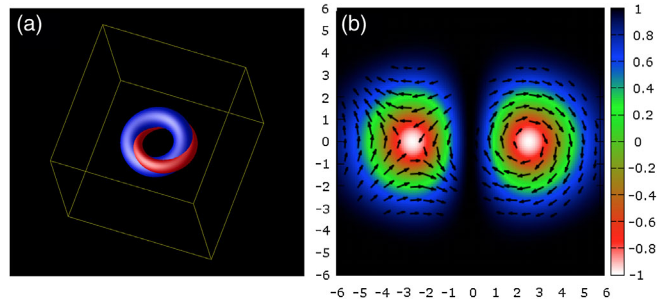

FIG. 1. The stable charge one soliton. (a) An isosurface (blue) enclosing the region of the magnetic material where the magnetization points in the direction $\mathbf{m} = (0, 0, -1)$, showing the location of the Skyrmion string. An isosurface (red) enclosing the region where $\mathbf{m} = [0, -(1/\sqrt{2}), -(1/\sqrt{2})]$ shows the twist of the Skyrmion string. This image clearly shows that the linking number, Q, is equal to 1. For scale, the outline of the displayed simulation box is a cube of side length 15 dimensionless units. (b) A cross section of the magnetization $\mathbf{m}$ in a plane containing the axis of rotational symmetry. The color represents the value of m_3 and the arrows are proportional to the two-component vector (m_1, m_2). This shows that the right-hand side of the cross section contains a Skyrmion and the left-hand side contains an anti-Skyrmion. Note that the color schemes in (a) and (b) are not related because they represent different quantities in the two figures.

the material by the same reasoning. The Hopf charge is the integer that counts the number of times these two closed curves are linked with each other. It is a mathematical theorem that this Hopf charge is topological [it does not change under any smooth deformation of the field $\mathbf{m}(\mathbf{r})$] and that its value does not depend upon the choice of the two particular fixed directions used to define the two closed curves. In other words, if two new directions are chosen then this will yield two new curves but the linking number will be unchanged.

A simple explicit example of a magnetization field with $Q = 1$ is given by

$$\mathbf{m}(\mathbf{r}) = \frac{4}{(\lambda^2 + r^2)^2} \begin{pmatrix} 2\lambda^2 xz - \lambda y(\lambda^2 - r^2) \\ 2\lambda^2 yz + \lambda x(\lambda^2 - r^2) \\ 2\lambda^2 z^2 - \lambda^2 r^2 + \frac{1}{4}(\lambda^2 - r^2)^2 \end{pmatrix}, \quad (2)$$

and has the topology of a circular Skyrmion string, with radius λ, lying in the plane $z = 0$ and twisted once. The above expression can be used as an initial field for a relaxation of the energy. The resulting stable equilibrium magnetization is displayed in Fig. 1. This ringlike charge one soliton consists of a closed circular Skyrmion string, where the Skyrmion is twisted once so that the first two components of the magnetization perform one full revolution as the circle is traversed. The characteristic winding of the Skyrmion is seen in cross section in the right half of the image in Fig. 1(b), where the Skyrmion string moves into the plane, and again in the left half of the image, where the Skyrmion string returns to the plane, but this time moving out of the plane so that it appears as an anti-Skyrmion in cross section. Applying random perturbations confirms that this static three-dimensional soliton solution with charge $Q = 1$ is stable. In our dimensionless units, the energy of this charge one solution is computed to be $E_1 = 280$, where this is the energy above the zero energy ground state given by the fully polarized ferromagnetic state $\mathbf{m} = (0, 0, 1)$, aligned with $\mathbf{H}$.

To study higher charge solutions ($Q > 1$) requires initial fields with any prescribed value of Q, as starting configurations for the energy minimizing the relaxation algorithm. Fortunately, there is a simple method [14] that uses complex polynomials to create initial rings with any value of Q, corresponding to a Skyrmion string twisted Q times. Furthermore, this method can also generate initial fields describing twisted Skyrmion strings that are knotted or linked, by using mathematical representations of knots and links in terms of the intersection of complex curves with the three sphere. All initial fields created using this method are first perturbed by a stretch along a random direction to break any potential symmetries of the initial field, to ensure a thorough test of the stability properties of the resulting static equilibria.

The results of the energy minimization computations reveal that stable ring equilibria, analogous to the $Q = 1$ ring, exist for higher values of the Hopf charge Q, with the Skyrmion string twisted Q times [the $Q = 3$ example is presented in Fig. 2(a)]. However, for $Q > 4$ the circular ring is unstable to a buckling instability that results in a stable buckled ring with lower energy [see Fig. 2(b) for the $Q = 6$ example]. The energies per unit Hopf charge E/Q, in units of the charge one energy E_1, are displayed as the black circles in Fig. 3 for these circular or buckled rings. For clarity, the $Q = 2$ energy, computed to be $E/Q = 0.73E_1$, is not shown on this plot.

The description of the topological Hopf charge in terms of a linking number reveals that a ring with charge Q_1 linked once with a ring with charge Q_2 yields a combined configuration with total Hopf charge equal to $Q = Q_1 + Q_2 + 2$, where the extra $+2$ is due to the linking of each ring once with the other. Initial fields of this type revert to stable rings under minimization of the energy for $Q \leq 6$, but for $Q = 7$ there is a stable link equilibrium with $Q_1 = 3$ and $Q_2 = 2$, presented in Fig. 2(c). Computations reveal that stable links exist for $Q \geq 7$ and the energy is lowest if the charge is distributed as equally as possible between the two components, so that $Q_1 = Q_2 = (Q - 2)/2$ if Q is even and $Q_1 = Q_2 + 1 = (Q - 1)/2$ if Q is odd. Furthermore, for $Q \geq 8$ these stable links have lower energy than the corresponding buckled rings. The energies of these links are displayed in Fig. 3 as the red squares.

If a Skyrmion string is twisted Q_1 times and tied into a trefoil knot before joining the ends then this yields a charge $Q = Q_1 + 3$, where the $+3$ results from the crossing number of the trefoil knot (the simplest nontrivial knot). Under minimization of the energy, initial fields of this type revert to stable rings for $Q < 7$ and to stable links for $Q = 7$, 8, 9. Remarkably, for $Q \geq 10$ stable trefoil knot equilibria are obtained with energies below the corresponding rings. Moreover, for $Q \geq 12$ these knot energies are also below those of the corresponding links. The knot energies are displayed in Fig. 3 as the blue triangles. The first stable trefoil knot is shown in Fig. 2(d), where 7 twists can be seen to contribute to the $Q = 10$ charge. A comparison of the energies of rings, links, and knots is presented in Fig. 3 and confirms the general conclusion that rings are formed for low values of the Hopf charge, but for

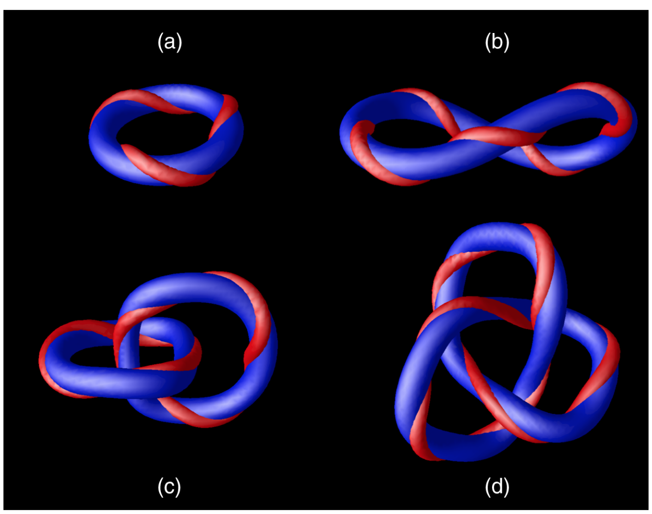

FIG. 2. Stable higher charge solitons. Isosurfaces enclosing the region of the magnetic material where the magnetization points in the directions $\mathbf{m} = (0, 0, -1)$ (blue) and $\mathbf{m} = [0, -(1/\sqrt{2}), -(1/\sqrt{2})]$ (red), for a selection of stable solitons: (a) the charge 3 circular ring, (b) the charge 6 buckled ring, (c) the charge 7 link with components of charge 3 and 2, (d) the charge 10 trefoil knot.

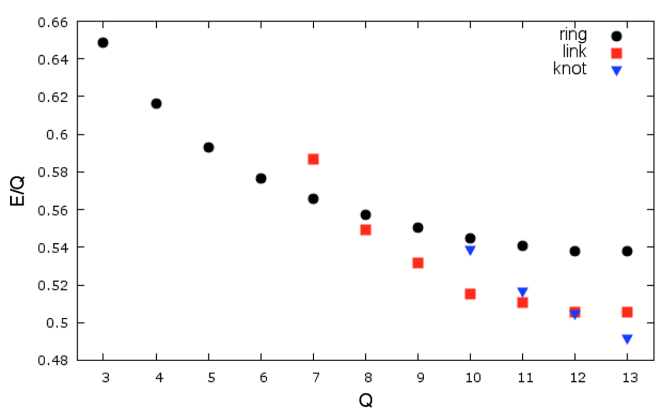

FIG. 3. Soliton energies. The energy per unit charge E/Q, in units of the charge one energy, for stable equilibria that take the form of circular or buckled rings (black circles), links (red squares), and knots (blue triangles).

higher values it is energetically favorable to form links and then knots.

Finally, we place our results in the context of previous work on Hopf solitons. The solitons presented here have a number of similarities to those in the mathematical Skyrme-Faddeev model, where stable knotted solitons were first conjectured to exist [16] and subsequently computed numerically [17,18]. Note that this is despite the fact that the term quadratic in derivatives has opposite sign in the two systems. Dynamical Hopf soliton rings exist [19,20] as solutions of the Landau-Lifshitz equations describing the evolution of the magnetization in a ferromagnetic material. These circular magnetic smoke rings drift along their symmetry axis but because they are dynamical they decay due to dissipation, unlike the static solitons considered here. Furthermore, the dynamical stabilization mechanism favors rings and not links or knots.

Several possible candidate materials have been suggested [11,12] as frustrated magnetic hosts for Skyrmions and significant experimental investigation is required to turn these possibilities into reality. The fact that the solitons are spatially localized in all directions within a constant far field ground state means that they are robust to changes in the system size and do not require the imposition of particular boundary conditions. It will certainly be a challenging task to engineer these complicated knotted structures but there are a number of recent exciting proposals for Skyrmions that could be adapted to this context. Examples include imprinting spatial structure in the magnetization field using optical vortex beams [21], using nanostructured templates formed from arrays of ferromagnetic nanorods [22], or seeding topological structures via nonmagnetic impurities [23]. Advanced magnetic imaging techniques for Skyrmions are rapidly developing, so the plethora of microscopy methods being investigated could allow the identification of the twist in a Skyrmion string that is the characteristic signature of these solitons.

In summary, the computational results presented in this Letter predict a zoo of exotic rings, links, and knots waiting to be discovered in the nanoscale world of frustrated magnets. We hope that the tantalizing prospect of a nanoscale resurrection of Kelvin's dream of knotted fields will provide a novel impetus for future work, together with an exploration of the potential technological applications of three-dimensional nanoparticles encoding knotted magnetization.

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[1] W. Thomson, Philos. Mag. Ser. 5 **34**, 15 (1867).
[2] D. Kleckner and W. T. M. Irvine, Nat. Phys. **9**, 253 (2013).
[3] M. R. Dennis, R. P. King, B. Jack, K. O'Holleran, and M. J. Padgett, Nat. Phys. **6**, 118 (2010).
[4] U. Tkalec, M. Ravnik, S. Čopar, S. Žumer, and I. Muševič, Science **333**, 62 (2011).
[5] N. S. Manton and P. M. Sutcliffe, *Topological Solitons* (Cambridge University Press, Cambridge, England, 2004).
[6] S. Muhlbauer, B. Binz, F. Jonietz, C. Pfleiderer, A. Rosch, A. Neubauer, R. Georgii, and P. Boni, Science **323**, 915 (2009).
[7] X. Z. Yu, Y. Onose, N. Kanazawa, J. H. Park, J. H. Han, Y. Matsui, N. Nagaosa, and Y. Tokura, Nature (London) **465**, 901 (2010).
[8] A. Fert, V. Cros, and J. Sampaio, Nat. Nanotechnol. **8**, 152 (2013).
[9] A. N. Bogdanov and D. A. Yablonskii, Sov. Phys. JETP **68**, 101 (1989).
[10] X. Yu, M. Mostovoy, Y. Tokunaga, W. Zhang, K. Kimoto, Y. Matsui, Y. Kaneko, N. Nagaosa, and Y. Tokura, Proc. Natl. Acad. Sci. U.S.A. **109**, 8856 (2012).
[11] T. Okubo, S. Chung, and H. Kawamura, Phys. Rev. Lett. **108**, 017206 (2012).
[12] A. O. Leonov and M. Mostovoy, Nat. Commun. **6**, 8275 (2015).
[13] S-Z. Lin and S. Hayami, Phys. Rev. B **93**, 064430 (2016).
[14] P. M. Sutcliffe, Proc. R. Soc. A **463**, 3001 (2007).
[15] M. F. Atiyah, *The Geometry and Physics of Knots* (Cambridge University Press, Cambridge, England, 1990).
[16] L. Faddeev and N. J. Niemi, Nature (London) **387**, 58 (1997).
[17] R. A. Battye and P. M. Sutcliffe, Phys. Rev. Lett. **81**, 4798 (1998).
[18] J. Hietarinta and P. Salo, Phys. Lett. B **451**, 60 (1999).
[19] N. R. Cooper, Phys. Rev. Lett. **82**, 1554 (1999).
[20] P. M. Sutcliffe, Phys. Rev. B **76**, 184439 (2007).
[21] H. Fujita and M. Sato, Phys. Rev. B **95**, 054421 (2017).
[22] N. Del-Valle, S. Agramunt-Puig, A. Sanchez, and C. Navau, Appl. Phys. Lett. **107**, 133103 (2015).
[23] S.-Z. Lin, S. Hayami, and C. D. Batista, Phys. Rev. Lett. **116**, 187202 (2016).