Knots as Stable Soliton Solutions in a Three-Dimensional Classical Field Theory

Richard A. Battye[1] and P. M. Sutcliffe[2]
[1]*Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Silver Street, Cambridge, CB3 9EW, United Kingdom*
[2]*Institute of Mathematics, University of Kent at Canterbury, Canterbury, CT2 7NZ, United Kingdom*
(Received 16 September 1998)

We examine in detail recent claims that knotlike structures exist in a simple classical field theory which are stabilized by the Hopf charge. We present minimum energy configurations for charges one to eight generated numerically. It is found that the solutions exhibit a spectacular variety of behavior including closed loops, linked loops, and, most interestingly, knots. [S0031-9007(98)07755-2]

PACS numbers: 11.27.+d, 11.10.Lm

It has been suggested recently that knots might exist as stable soliton solutions in a simple three-dimensional classical field theory [1], opening up a wide range of possible applications in physics and beyond. We have reexamined and extended this work in some detail using a combination of analytic approximations and sophisticated numerical algorithms. Although most of the assertions made in the earlier work of Faddeev and Niemi [1] as to the structure of solitonic solutions are incorrect, the basic idea that complex soliton configurations exist in this model is sound. For charges between one and eight, we find solutions which exhibit a rich and spectacular variety of phenomena, including stable toroidal solitons with twists, linked loops, and also knots. The physical process which allows for this variety is the reconnection of stringlike segments.

The specific model under consideration is an O(3) variant of the Skyrme model [2] with Lagrangian density in $(3 + 1)$ dimensions given by [3]

$$\mathcal{L} = \partial_\mu \mathbf{n} \cdot \partial^\mu \mathbf{n} - \frac{1}{2}(\partial_\mu \mathbf{n} \times \partial_\nu \mathbf{n}) \cdot (\partial^\mu \mathbf{n} \times \partial^\nu \mathbf{n}), \tag{1}$$

where the field $\mathbf{n} = (n_1, n_2, n_3)$ takes values on the 2-sphere, that is, $\mathbf{n}^2 = 1$. The two parts to the Lagrangian are known as the sigma model and Skyrme terms, respectively, the latter being included to stabilize the solitons against radial scaling as in Derrick's theorem [4].

In order for a solution to have finite energy, the field must be fixed at spatial infinity, say $\mathbf{n}_\infty = (0, 0, 1)$, and hence the domain is compactified from $\mathbb{R}^3$ to S^3, so that at any fixed time we have a map $\mathbf{n}$: $S^3 \to S^2$. Therefore, each field configuration is characterized by a topological charge Q, since $\pi_3(S^2) = \mathbb{Z}$, which is known as the Hopf invariant. This can be defined formally in terms of the pullback of the area two-form ω on the target S^2. If $F = \mathbf{n}^*\omega$ is the pullback under $\mathbf{n}$ onto the domain, then it must be exact, $F = dA$, since the second cohomology group of the 3-sphere is trivial. One can then construct the Hopf charge by integrating the Chern-Simons term over $\mathbb{R}^3$,

$$Q = \frac{1}{4\pi^2} \int d^3x F \wedge A. \tag{2}$$

It can also be interpreted heuristically as the linking number between field lines, in contrast to other topological characteristics, such as baryon number in the Skyrme model, which are generally winding numbers. Since the preimage of a point on the target S^2 is a closed loop in $\mathbb{R}^3$, the preimages of any two distinct points will be linked exactly Q times. Just as in the case of other solitonic models, there exists a bound on the energy E of a configuration with charge Q [5]. However, the dependence is not linear but rather $E \geq c|Q|^{3/4}$ and $c = 16\pi^2 3^{3/8} \approx 238$.

Clearly, the equations of motion for this model are not analytically tractable, and hence a numerical approach is required. We have used a code originally designed to investigate Skyrmions in the O(4) version of the model [6–8] in three spatial dimensions on a discretized Cartesian grid, which can be trivially modified for the situation under consideration here. It was run on a Silicon Graphics Origin 2000 parallel supercomputer which now has 44 fast R10000 processors and 20 Gb of memory. We used spatial discretizations with 100^3 points and for the lower charges convergence was achieved in around 50 CPU hours, but the higher charge configurations took very much longer.

The basic minimization procedure is to create suitably random initial conditions with a specific Hopf charge, which are then evolved under the full equations of motion. The originally static initial conditions turn potential energy into kinetic energy as they evolve, and this kinetic energy is periodically removed when the potential energy begins to increase. A more detailed exposition of this method for locating minima in these models is given in Ref. [8]. The only technically difficult aspect is to produce initial conditions with a given Hopf charge which are devoid of any symmetries and are, hence, suitably random. This can be done in analogy to an approach used to construct Skyrme configurations.

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If $U(\mathrm{x})$ is a smooth SU(2) field with winding number B between two 3-spheres, which correspond to the compactified $\mathbb{R}^3$ and the group manifold of SU(2), then writing the components of U in terms of complex numbers Z_0 and Z_1 as

$$U = \begin{pmatrix} Z_0 & -\bar{Z}_1 \\ Z_1 & \bar{Z}_0 \end{pmatrix}, \tag{3}$$

where $|Z_0|^2 + |Z_1|^2 = 1$, one can construct an O(3) field from $\mathbf{n} = Z^\dagger \boldsymbol{\tau} Z$, where τ_j are the Pauli matrices and the column vector is $Z = (Z_0, Z_1)^T$. It is easy to see that the vector defined above has unit length and satisfies the boundary condition $\mathbf{n}(\infty) = \mathbf{n}_\infty$ if the original SU(2) field is the identity at spatial infinity. Furthermore, it can be shown that $Q = B$ [9], and so the problem is reduced to finding some appropriate Skyrme field configurations.

One can construct suitable Skyrme fields using the rational map approach [10]. In spherical polar coordinates (r, θ, ϕ), this involves specifying the angular distribution of the field using a rational function $R(z)$ with degree B of the complex variable $z = e^{i\phi}\tan(\theta/2)$, and a radial profile function $f(r)$, which satisfies the boundary conditions $f(0) = \pi$ and $f(\infty) = 0$. A particularly simple example is $R(z) = z^B$, which for $B = 1$ corresponds to a spherically symmetric hedgehog Skyrmion, and for $B > 1$ describes an axially symmetric toroidal field. Using the arguments above this allows us to construct an O(3) field with Hopf charge $Q = B$ which has only axial symmetry, since the Hopf projection breaks any spherical symmetry. Of course this is not particularly helpful from the point of view of the minimization procedure, but a simple modification to include nonsymmetric wiggles can remove all the symmetries and hence provide suitably random initial conditions. The precise map that we use for this is

$$R(z) = z^Q\left[1 + a\cos\left(\frac{m\phi^2}{2\pi}\right)\right], \tag{4}$$

which corresponds to a torus with $m \in \mathbb{Z}$ nonsymmetric wiggles of amplitude $a \in [0, 1)$.

We have relaxed the solutions for $Q = 1$ to 8, and we have displayed our results by plotting several interesting quantities in Fig. 1. The first is the preimage of the vector $(0, 0, -1)$, which defines the position of the soliton. In reality it is difficult to compute the locus of this preimage in the discretized domain, and hence we will plot isosurfaces of the vector $(0, 0, -1 + \epsilon)$, where $\epsilon \approx 0.2$ is small. This allows us to easily visualize the solitons position as the core of a tube rather than a single line. We will also explicitly display the linking number, thereby verifying the Hopf charge, by plotting in a similar way to the position the loci of two independent points $(0, -1, 0)$ and $(0, 0, -1)$. Finally, we also plot the isosurfaces of energy density. A more detailed discussion of the structure of each of the solitons is given in Ref. [11].

For both $Q = 1$ and 2 we see that the nonsymmetric initial conditions relax quickly back to the axially symmetric configurations which are well described by appropriate radial profile functions and the rational maps $R(z) = z$ and $R(z) = z^2$ for $Q = 1$ and $Q = 2$, respectively. In both cases the position of the soliton is a circle, but for $Q = 1$ the energy density is an axially symmetric lump which is localized at the origin, while for $Q = 2$ it is localized on a torus just inside the locus of the position. Upon examination of the linking structure, one can confirm the Hopf charge; the $Q = 1$ solution being linked once and the $Q = 2$ linked twice.

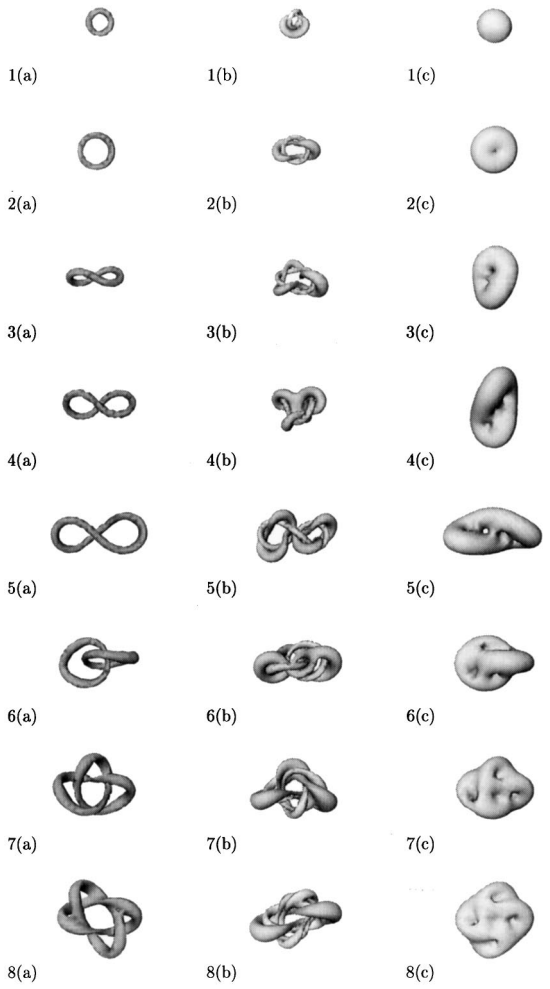

FIG. 1. For charges $Q = 1$ to $Q = 8$ we display the following quantities for the relaxed soliton solutions: (a) The position of the soliton; (b) the linking number of the field lines; (c) an energy density isosurface.

These two cases had previously been studied in Refs. [1,12] using an axially symmetric approach which reduces the problem effectively to two dimensions. We agree with both groups as to the structure of the $Q = 2$ solution, but in the case of $Q = 1$, where they disagree, we find agreement with Ref. [12]. Since our approach is completely general, using random initial conditions on a three-dimensional Cartesian grid with no symmetries, it is difficult to believe that our results could be misleading.

Therefore, this suggests that the numerical approach used in Ref. [1] is flawed.

We have also computed the total energy inside the discretized grid. Although there are some small systematic errors in making an absolute measurement of the total energy of the soliton since the grid is finite (see Ref. [11] for a detailed discussion), the relative values for different charges should yield important qualitative information. In particular, we find that our values for the energy of the $Q = 1$ and $Q = 2$ solitons, tabulated in Table I, are consistent with those of Ref. [12].

For $Q = 3$, 4, and 5 we find that the solutions are not axially symmetric and hence could not have been found using the methods employed in Refs. [1,12]. In each case the locus of the position sweeps out a closed loop which is twisted, the twists not being related to those in the initial conditions. The energy density isosurfaces are now not toroidal, being more reminiscent of pretzels with two, three, and four holes, respectively, but each one is also twisted to fit inside the locus of the position. Once again the Hopf charge can be verified by reference to the linking structure. We have also investigated toroidal configurations for these values of Q. As one might expect, if we use symmetric initial conditions the symmetry is preserved by the relaxation process, and hence we can make an estimate of the energies of these configurations. As shown in Table I, we find that energies of these symmetric saddle point solutions are larger than those for the minima which have twists. We should note that we found no evidence for the existence of a stable trefoil configuration for $Q = 3$, as suggested in Ref. [1]. We will discuss later why we believe that it is unlikely that such a configuration will exist.

Above $Q = 5$ there appears to be a dramatic change in the structure of the soliton solutions. At $Q = 6$ we see that the position of the soliton is no longer a single connected loop but consists of two linked disjoint loops. The fact that the position itself has linking number one makes the counting of the Hopf charge Q more subtle. In fact, a careful examination of the linking structure reveals that this configuration resembles two linked $Q = 2$ solitons. The Hopf charge is not simply additive in the case of a link since when a field line passes through the intersection it should be counted twice. Note that the energy density isosurface does not have the form of two linked loops but is concentrated in the region inside the position loops. For $Q = 7$ and $Q = 8$ even more exotic solutions are produced. It appears that the position of the $Q = 7$ soliton has the topology of a trefoil knot, while at $Q = 8$ the solution comprises of two $Q = 2$ solitons doubly linked. It should be emphasized that the solutions are relaxed from initial conditions which are perturbed tori, and hence the crossing—or reconnection—of field lines is a requisite. In Ref. [11] we discuss this process in detail and we present snapshots of the position during the relaxation process.

We should note that in any numerical relaxation procedure one can never be totally sure that the global minimum has been found, although as much as is possible has been done—random initial conditions and a fully three-dimensional algorithm. One way to increase confidence in numerical results is to establish rules dictating the structure of the solutions, which can in the end become predictive. In the case of O(4) Skyrmions, we suggested [7,8] the existence of a pattern in the solutions, which we called geometric energy minimization. In that case we had a very precise description of the structure of the solutions because they had point symmetries. Here, we have a more qualitative description of the solutions, but we can speculate on some general features of an energy minimization principle.

For linelike solitons reducing the length of the soliton will naively reduce the energy, but this must be balanced by an increase in gradient energy required to impose the correct linking of field lines in a reduced volume. For low charges it seems reasonable that the solutions be toroidal, with the twists distributed uniformly, but as the charge increases it appears that it is possible to reduce the length of string without a great cost in gradient energy by twisting the loop so that the links can be packed closer together. What happens for the higher charges is less well defined, but it is clear that having extra links in the position itself can reduce the number of links in each of the components, and hence also the length of string required. This is illustrated by the $Q = 6$ and $Q = 8$ solitons, which are composed of two $Q = 2$ solitons singly and doubly linked, respectively. The clear special case is $Q = 7$, the first structure where the position is actually knotted. We believe that the reason for this is symmetry; it would be impossible to distribute the links symmetrically into two components. This suggests that as the charge increases the number of linked possibilities will increase rapidly, with string reconnection being the mechanism by which one linked structure can metamorphose into another. Clearly, more work will be required to construct a more quantitative energy minimization principle.

TABLE I. Energy of the relaxed soliton and torus solutions for charges one to eight. Note that the difference in energies of the soliton and torus solutions for the first two charges is a reflection of the accuracy of our numerical computation of the energy.

Q	Soliton energy	Torus energy
1	504	505
2	835	836
3	1157	1181
4	1486	1542
5	1808	1974
6	1981	2361
7	2210	2600
8	2447	3050

It was suggested in Ref. [1] that the $Q = 3$ soliton had the topology of a trefoil knot, but our results clearly suggest that this is not the case. One could create such a configuration since it has the correct linking structure, but the energy minimization principle that we have discussed above explains why this is not likely to be the minimum energy configuration—the length of string required to have a knotted solution with $Q = 3$ is too long.

In conclusion, we have demonstrated numerically that a rich variety of fascinating closed, linked, and knotted configurations are generic in this model. It is possible to explain the nature of these solutions heuristically via a qualitative energy minimization principle based on the length of the string. The results we have presented are very much in keeping with the spirit of Ref. [1]. However, the details are very different, in particular the structure of the $Q = 1$ and $Q = 3$ solitons. This investigation will hopefully act as the basis for work on physical systems where this model may be applicable, in particular condensed matter [13] and particle physics [14].

Many thanks to Ludwig Faddeev, Jens Gladikowski, Meik Hellmund, Conor Houghton, Patrick Irwin, Nick Manton, Antti Niemi, Miguel Ortiz, Richard Ward, and Wojtek Zakrzewski for useful discussions. We acknowledge the use of the SGI Origin 2000 and Power Challenge at DAMTP in Cambridge supported by the HEFCE, SGI, PPARC, the Cambridge Relativity rolling grant and EPSRC Applied Mathematics Initiative Grant No. GR/K50641. The work of P. M. S. was supported by EPSRC Grant No. GR/L88320 and that of R. A. B. by Trinity College. We thank Paul Shellard for his tireless efforts to provide sufficient computational resources for projects such as this.

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