FAST TRACK COMMUNICATION

Skyrmion multi-walls

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Abstract

Skyrmion walls are topologically nontrivial solutions of the Skyrme system which are periodic in two spatial directions. We report numerical investigations which show that solutions representing parallel multi-walls exist. The most stable configuration is that of the square $N$-wall, which in the $N \to \infty$ limit becomes the cubically symmetric Skyrme crystal. There is also a solution resembling parallel hexagonal walls, but this is less stable.

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The Skyrme system, originally introduced as a model of nucleons, is an archetypal (3+1)-dimensional classical field theory admitting topological soliton solutions. Much is known about various types of skyrmion solutions, for example: isolated skyrmions in $\mathbb{R}^3$, up to relatively high charge [1–3]; a triply-periodic ‘Skyrme crystal’ [2, 4–6]; a doubly-periodic ‘Skyrme domain wall’ [7] and various types of singly-periodic ‘Skyrme chains’ [8].

The purpose of this communication is to investigate static $N$-wall solutions, i.e. the $N > 1$ generalization of the single-wall fields discussed in [7]. If one has two (or indeed $N$) well-separated parallel walls, then the force between them can be made attractive by a suitable relative orientation of the fields. So one expects there to be solutions representing $N$ walls bound together, although a priori the walls might merge together to form a single wall.

We investigate this by numerical minimization of the energy, and our main findings are as follows. There are two obvious shapes for a single wall, namely square and hexagonal, and it is known [7] that the latter has slightly lower energy than the former. If walls are allowed to attract, then they do not merge but remain identifiable as separate parallel walls. There is a stable bound configuration representing two parallel hexagonal walls, but this is not the lowest energy 2-wall state. For $N \geq 2$, the lowest energy state consists of $N$ parallel square walls (each one being a square array of half-skyrmions), and as $N \to \infty$ this approaches the Skyrme crystal.

The energy density of a static $SU(2)$-valued Skyrme field $U(x^i)$ on $\mathbb{R}^3$ is defined to be

$$ E := -\frac{1}{2} \text{tr}(L_i L_i) - \frac{1}{16} \text{tr}([L_i, L_j][L_i, L_j]) . $$

(1)
where $L_i = U^{-1} \partial U/\partial x^i$, and $x^i = (x, y, z)$ are the spatial coordinates. In what follows, let us write $U = \Phi_4 + i\Phi_1\sigma_j$, where $\sigma_j$ are the Pauli matrices, and the real 4-vector field $\Phi = (\Phi_1, \Phi_2, \Phi_3, \Phi_4)$ satisfies $\Phi \cdot \Phi = 1$.

In this communication, we deal with configurations which resemble $N$ walls or sheets, each parallel to the $xy$-plane: so the field is periodic in $x$ and $y$ (with periods $L_x$ and $L_y$, respectively) and satisfies the boundary condition

$$\Phi_4 \rightarrow \begin{cases} 1 & \text{as } z \rightarrow -\infty, \\ (-1)^N & \text{as } z \rightarrow \infty. \end{cases}$$

(2)

For $N = 1$, and more generally for $N$ odd, one has a domain wall which separates two vacuum regions, where $\Phi_4 = 1$ and $\Phi_4 = -1$, respectively; for $N$ even, one has the same vacuum on both sides of the multi-layered sheet. In the asymptotic region $|z| \gg 1$, the three fields $\Phi_j$ are small and they satisfy the Laplace equation, since the energy density reduces to $E \approx (\partial_i \Phi_j)^2$. Assuming (without loss of generality) that $L_y \geq L_x$, we see by separating variables that the leading behaviour as $|z| \rightarrow \infty$ is typically $\Phi_j \approx C \sin(\mu y) \exp(-\mu|z|)$, where $\mu = 2\pi/L_y$. In particular, the fields approach their asymptotic values exponentially quickly, with a scale determined by the larger of $L_x$ and $L_y$.

The topological charge $Q$ (over a single cell) is

$$Q = \int_{T^2 \times \mathbb{R}} Q \, dx \, dy \, dz,$$

(3)

where

$$Q = \frac{1}{24\pi^2} \sigma_{ijk} \text{tr}(L_i L_j L_k)$$

(4)

is the topological charge density. We claim that $Q$ is an integer. If $N$ is even, then (2) allows us to regard $\Phi$ as being defined, for topological purposes, on $T^2 \times S^1$, and then $Q$ equals the degree of $\Phi$. If $N$ is odd, then it is not quite so obvious why $Q$ is an integer, but it follows from the theorem in the appendix of [8]. The energy $E$ is defined to be

$$E := \frac{1}{12\pi^2} \int_{T^2 \times \mathbb{R}} E \, dx \, dy \, dz,$$

(5)

and it satisfies the usual Faddeev bound $E \geq Q$.

In what follows, we describe $N$-wall configurations which were found by numerical minimization of the energy functional $E$. We used a first-order finite-difference scheme for $E$, with the spatial points $(x, y, z)$ being represented by a rectangular lattice having lattice spacing $h$, and we applied conjugate-gradient minimization. The lattice error in $E$ goes like $h^2$, and we extrapolated the finite-$h$ results for both $E$ and $Q$ to $h = 0$. The extrapolated value of $Q$ then gives a measure of the remaining error, which for the situations described below turns out to be less than 0.2%. The boundary condition (2) was modelled by imposing $\Phi_4 = 1$ at $z = -L_z/2$ and $\Phi_4 = (-1)^N$ at $z = L_z/2$. As remarked above, the walls are exponentially localized in $z$, and so as long as $L_z$ is taken to be large enough, there is no discernable finite-size effect; a value of $L_z = 10 + 2N$ turns out to be sufficient for this. In each case, we adjusted the periods $L_x$ and $L_y$ to their optimal size, meaning that the energy-per-cell is made as small as possible. Numerical minima were randomly perturbed and then re-minimized, as a test of their stability. As initial configurations we used the same sort of 'rational map ansatz' as in [7], involving a Weierstrass elliptic function of $x + iy$ (the lemniscatic form to get square symmetry, and the equianharmonic form to get hexagonal symmetry), together with a suitable profile function $f(z)$ satisfying $f(-L_z/2) = 0$ and $f(L_z/2) = N\pi$.

The results are consistent with the anticipated general principle that the lowest-energy configurations are arrays of half-skyrmions. For an $N$-wall, we expect that each fundamental
Figure 1. Energy densities of the square 1-wall, square 2-wall and hexagonal 2-wall, and plot of the energy $\tilde{E}$ for the square $N$-wall ($1 \leq N \leq 5$) and hexagonal $N$-wall ($1 \leq N \leq 2$).
(This figure is in colour only in the electronic version)

Table 1. Energy $\tilde{E}$ and cell size $L$ for the square $N$-wall.

| $N$ | $\tilde{E}$ | $L$ |
|-----|-------------|-----|
| 1   | 1.068       | 4.25|
| 2   | 1.053       | 4.47|
| 3   | 1.048       | 4.54|
| 4   | 1.046       | 4.58|
| 5   | 1.044       | 4.61|

cell will contain a multiple of $4N$ half-skyrmions, and therefore its topological charge $Q$ will be a multiple of $2N$; this indeed turns out to be the case. As mentioned above, the walls do not merge, but retain their identity; the location of each wall can be determined by looking at the locus where $\Phi_4 = 0$.

The simplest case to describe is the square one, with $L_y = L_x = L$; our results for $1 \leq N \leq 5$ are summarized in table 1, which gives the energy-per-charge $\tilde{E}$, and the optimal value of $L$, for each $N$. Pictures of the $N = 1$ and $N = 2$ cases are presented in figure 1, together with a plot of the energy data in table 1. Let us first comment on the data. The normalized energy $\tilde{E}$ of the square $N$-wall is surprisingly close to having a $1/N$-dependence (although there is no obvious reason why this should be so), and extrapolating on this basis gives $\tilde{E} \approx 1.039$ in the $N \to \infty$ limit. This is very close to the energy of the (triply-periodic) Skyrme crystal, a cubic array in which each fundamental cube contains eight half-skyrmions:
its energy-per-charge, computed using the method described above, is $E = 1.038$. Further support for the claim that the square $N$-wall tends to the Skyrme crystal as $N \to \infty$ comes from looking at the symmetries of the field $\Phi$. These include, for example, the translations

$$
\begin{align*}
x &\mapsto x + \frac{1}{2}L_x \Rightarrow (\Phi_1, \Phi_2, \Phi_3, \Phi_4) \mapsto (\Phi_1 - \Phi_2, \Phi_3, \Phi_4), \\
y &\mapsto y + \frac{1}{2}L_y \Rightarrow (\Phi_1, \Phi_2, \Phi_3, \Phi_4) \mapsto (\Phi_1 - \Phi_2, -\Phi_3, \Phi_4), \\
z_p &\mapsto z_{p+1} \Rightarrow (\Phi_1, \Phi_2, \Phi_3, \Phi_4) \mapsto (\Phi_1, -\Phi_2, -\Phi_3, -\Phi_4),
\end{align*}
$$

where the third translation (in $z$) denotes moving from the $p$th wall to the $(p+1)$st wall. These are exactly the same as the translation symmetries of the Skyrme crystal [2]. The values for the optimal cell length $L = L_x = L_y$ are consistent with their approaching $L = 4.7$ as $N \to \infty$, this being the cell size of the Skyrme crystal (and similarly the distance between each parallel pair of walls is approximately $4.7/2$, as one would expect).

Each three-dimensional plot in figure 1 is an isosurface of the energy density $E$, namely where $E$ equals 0.6 times its maximum value. For the square case, the plots are over four fundamental cells. One clearly sees square arrays of half-skyrmions. Observe that, for $N = 2$, the half-skyrmions are aligned in the $z$-direction; the same is true for $N > 2$.

Let us turn now to the case of hexagonal symmetry. For ease of computation, we follow the same scheme as in [7], namely taking $L_y = \sqrt{3}L_x$ and fitting two fundamental parallelograms into the corresponding rectangle. Each such rectangle, of each wall, contains eight half-skyrmions, as is seen in the hexagonal 2-wall picture of figure 1. For $N = 1$, the energy of the hexagonal arrangement is $\hat{E} \approx 1.062$, less than that of the corresponding square case [7], but for $N \geq 2$, the hexagonal arrangement is less efficient than the square one, and (depending on the values of $L_x$ and $L_y$) it is either a local minimum of the energy functional or it is unstable. There is a local minimum hexagonal 2-wall solution with energy $\hat{E} \approx 1.055$, which is only very slightly (less than 0.2%) higher than that of the square 2-wall. Its energy density is depicted in figure 1; one feature to note is that the two walls are not aligned in the $z$-direction, but are offset. If $L_x$ and $L_y$ are allowed to change so that the relation $L_y = \sqrt{3}L_x$ no longer holds, then this solution becomes unstable and changes into the square 2-wall.

An isolated skyrmion of charge $Q \geq 3$ typically has a polyhedral shell structure, analogous to carbon fullerenes, and it may be viewed as constructed from a section of the hexagonal 1-wall (graphene), with the insertion of defects to create a spherical shell [2, 7]. There has also been an investigation [9] of the possibility of constructing skyrmions as multi-walled spherical shells, with the ‘shell material’ consisting of a double or triple wall. For the cases that were examined in [9], either the walls coalesced, or one obtained a structure which resembled a shell-like part of the Skyrme crystal. The findings reported above are consistent with this; in particular, multiple hexagonal walls appear to be rather unstable, and therefore unsuitable for constructing shells. But it does raise the possibility of stable high-charge skyrmions constructed as shells of square multi-wall material, or equivalently as hollow chunks of Skyrme crystal, and this would be worth investigating further.

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