Abstract

Recently it has been found that the structure of Skyrmions has a close analogy to that of fullerene shells in carbon chemistry. In this letter we show that this analogy continues further, by presenting a Skyrme field that describes a lattice of Skyrmions with hexagonal symmetry. This configuration, a novel ‘domain wall’ in the Skyrme model, has low energy per baryon (about 6% above the Faddeev-Bogomolny bound) and in many ways is analogous to graphite. By comparison to the energy per baryon of other known Skyrmions and also the Skyrme crystal, we discuss the possibility of finding Skyrmion shells of higher charge.
1 Introduction

Our recent work [1], involving numerical simulations of the full nonlinear field equations of the Skyrme model, has revealed that the structure of minimal energy multi-Skyrmions has a rich and fascinating complexity, where surfaces of constant baryon density are given by trivalent polyhedra with holes at the centre of each face. These structures are very reminiscent of those appearing in fullerene chemistry to describe closed shells of carbon atoms [8, 5], leading us to draw an analogy between Skyrmions and carbon chemistry.

More explicitly, the empirical Geometric Energy Minimization rule of ref. [1] states that, the baryon density isosurface of a charge $B$ Skyrmion is an almost spherical trivalent polyhedron with $4(B-2)$ vertices, $2(B-1)$ faces and $6(B-2)$ edges. For $B \geq 7$ the polyhedron comprises twelve pentagons and $2(B-7)$ hexagons, which is precisely the structure of a fullerene corresponding to a closed shell containing $4(B-2)$ carbon atoms. In particular, the $B = 7, 8$ and $9$ minimum energy configurations were seen to have the same structure as shell-like forms of $C_{20}, C_{24}$ and $C_{28}$ respectively [1, 5]. Motivated by this numerical work, a new approach to constructing Skyrme fields [6], based upon rational maps between Riemann spheres was developed. This has allowed a good mathematical understanding of some aspects of these Skyrmions and has also produced a Skyrme field of charge seventeen which has the structure of the most famous of the fullerenes, the $C_{60}$ Buckminsterfullerene. It too appears to be the minimal energy Skyrmion of this charge.

In considering very large fullerenes, where hexagons are dominant, the twelve pentagons may be viewed as defects, inserted into a flat hexagonal structure, in order to generate the required curvature necessary to close the shell. Energetically the optimum structure is an infinite hexagonal lattice, that is, a sheet of graphite; the most stable form of elemental carbon from the thermodynamic point of view. The reason that closed shells are preferred for a finite number of carbon atoms is that the penalty for introducing the pentagonal defects is not as severe as that incurred by having dangling bonds at the edges of a truncated graphite sheet. A prediction of the fullerene approach to Skyrmions is therefore that a Skyrme field should exist which represents a hexagonal lattice, that is, the analogue of graphite. Furthermore, although this configuration would have infinite energy, since it has infinite extent in two directions, its energy per baryon should be lower than that of any of the known finite energy Skyrmions. In the next section we shall verify this prediction and thus provide another piece of evidence in support of the similarities between fullerenes and Skyrmions.

For completeness, we include expressions for the Lagrangian of the Skyrme model, which in terms of the $su(2)$-valued right currents $R_\mu = (\partial_\mu U)U^\dagger$ is

$$
\mathcal{L} = -\frac{1}{2} \text{Tr}(R_\mu R^\mu) - \frac{1}{16} \text{Tr}([R_\mu, R_\nu][R_\mu, R_\nu]),
$$

where we have used scaled units of energy and length, and the baryon density $B$, whose spatial integral gives the integer-valued baryon number $B$, is given by

$$
B = -\frac{1}{24\pi^2} \epsilon_{ijk} \text{Tr}(R_i R_j R_k).
$$

(1.1)
As throughout this letter, we take latin indices to run over the spatial values 1, 2, 3. The corresponding Faddeev-Bogomolny bound on the energy $E$ is simply $E \geq |B| \times 12\pi^2$.

2 An ansatz with hexagonal symmetry

Following a suggestion of Atiyah, it has recently been proved by Jarvis \cite{Jarvis} that the space of SU(2) BPS monopoles is diffeomorphic to the space of equivalence classes of rational maps between Riemann spheres. These rational maps arise from the monopole as the scattering data of a linear operator when considered along all possible lines emanating from a chosen origin. Through the use of a new ansatz for Skyrme fields \cite{Skyrme}, it has been possible to use Jarvis rational maps to construct good approximations to the known minimum energy Skyrmions. The fact that Jarvis maps, being the scattering data along radial lines, are relevant reflects the feature that these Skyrmions are shell-like structures.

In this letter we are concerned with a two-dimensional lattice of Skyrmions, which is clearly not a shell-like configuration, making Jarvis maps inappropriate for this application. However, an older diffeomorphism of Donaldson \cite{Donaldson}, between SU(2) monopoles and based rational maps, is appropriate. These Donaldson maps arise as the scattering data of a linear operator considered along all lines in a chosen direction. This definition requires a decomposition of $\mathbb{R}^3$ into $\mathbb{R} \times \mathbb{C}$, which is exactly the situation for a lattice configuration, where the complex plane refers to the plane of the lattice and the real coordinate is the height above the lattice. To be precise, since we wish to consider an infinite lattice, the Donaldson map will not be rational, but instead is required to be merely meromorphic; which may be regarded as an infinite limit of a rational map.

A consideration of the ansatz introduced in ref.\cite{Skyrme}, together with the modifications discussed above, leads us to the following Skyrme field ansatz

$$U(x_1, x_2, x_3) = \exp\left(\frac{if}{1 + |W|^2} (W\tau_+ + \bar{W}\tau_- + (1 - |W|^2)\tau_3)\right), \quad (2.1)$$

where $\tau_i$ denote the Pauli matrices with $\tau_\pm = \tau_1 \pm i\tau_2$, $W \in \mathbb{C}P^1$ is a holomorphic function of $z = x_1 + ix_2$, and $f \in \mathbb{R}$ is a function of $x_3$.

The lattice occupies the $x_1x_2$ plane, in which we use the complex coordinate $z$. Thus from the above ansatz we see that the direction of the vector of pion fields is determined by the $\mathbb{C}P^1$ field $W$, given the position in the lattice, whereas the length of the vector of pion fields is determined by the profile function $f$, given the height above the lattice.

The next issue to address is that of the boundary conditions on the Skyrme field $U$ and hence on the functions $f$ and $W$. To have a periodic lattice there must exist complex constants $\Omega_1$ and $\Omega_2$ which are the fundamental periods of the lattice, that is,

$$U(z + n\Omega_1 + m\Omega_2, x_3) = U(z, x_3) \quad \forall n, m \in \mathbb{Z}. \quad (2.2)$$

Let $T^2$ denote the associated fundamental parallelogram, that is, the torus given by the region in the complex plane with vertices 0, $\Omega_1, \Omega_2, \Omega_1 + \Omega_2$ and opposite edges identified.
We can now restrict our analysis to the region of $\mathbb{R}^3$ given by $\mathbb{R} \times T^2$, with the field in the remaining regions determined by periodicity. Thus we see from our ansatz (2.1) that $W$ is required to be a holomorphic map $W : T^2 \mapsto \mathbb{C} \mathbb{P}^1$.

To consider the boundary conditions in the direction orthogonal to the plane of the lattice we need to recall our motivation. The lattice is being thought of as an infinite limit of the shell-like Skyrmions containing pentagons and hexagons. Thus, in approaching this limit, we imagine the lattice as being a part of the bottom of a larger and larger shell and hence below the lattice is the outside of the shell, where the Skyrme field tends to the vacuum, giving the boundary condition $\lim_{x_3 \to -\infty} U = 1_2$. However, above the lattice is the inside of the shell, where the Skyrme field is approaching the negative vacuum associated with the centre of the Skyrmion, so the appropriate boundary condition is $\lim_{x_3 \to +\infty} U = -1_2$. Note that this implies that our Skyrme lattice is a domain wall, separating regions of differing vacuum values. Examination of our ansatz (2.1) now reveals that the boundary conditions for the profile function $f(x_3)$ read

$$f(-\infty) = 0, \quad f(\infty) = \pi.$$  

(2.3)

To compute the baryon number and energy of the Skyrme field (2.1) in a fundamental section we shall follow the approach of ref.[6]. The strain tensor, defined as

$$D_{ij} = -\frac{1}{2} \text{Tr}(R_i R_j),$$

(2.4)

is symmetric and positive semi-definite. If it has eigenvalues $\lambda_1^2, \lambda_2^2, \lambda_3^2$ then the Skyrme energy density $\mathcal{E}$ and baryon density $\mathcal{B}$ are given by

$$\mathcal{E} = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_1^2 \lambda_2^2 + \lambda_2^2 \lambda_3^2 + \lambda_1^2 \lambda_3^2,$$

$$\mathcal{B} = \lambda_1 \lambda_2 \lambda_3 / 2\pi^2.$$  

(2.5) \hspace{1cm} (2.6)

For the ansatz (2.1) the strain in the direction normal to the lattice is orthogonal to the two strains in the directions of the lattice, which are equal. Therefore the $\lambda_i$ may be interpreted as the strains in the $x_i$ directions, making it is easy to show that

$$\lambda_3 = f', \quad \lambda_1 = \lambda_2 = 2J \sin f,$$

(2.7)

where we have defined the quantity

$$J = \frac{|\partial_z W|}{1 + |W|^2}.$$  

(2.8)

Substituting the expressions for the strains (2.7) into those for the energy and baryon density, we arrive at the result

$$\mathcal{E} = f'^2 + 8J^2(f'^2 + \sin^2 f) + 16J^4 \sin^4 f,$$

$$\mathcal{B} = \frac{2}{\pi^2} J^2 f' \sin^2 f.$$  

(2.9) \hspace{1cm} (2.10)
We now wish to use these densities to compute the energy $E$ and baryon number $B$ in a fundamental section of the lattice, by integrating over the region $x_3 \in (-\infty, \infty)$ and $(x_1, x_2) \in T^2$. To do this we note that since $W$ is a map $W : T^2 \mapsto \mathbb{C}P^1$, then it has an associated integer, $k$, which is its degree. Explicitly, $k$ is given by integrating over the torus the pullback under $W$ of the Fubini-Study area 2-form on $\mathbb{C}P^1$, which in this case gives

$$k = \frac{1}{\pi} \int_{T^2} J^2 \, dx_1 dx_2,$$  

since $W$ is a holomorphic function of $z$.

Using (2.11) it is now easy to see that the baryon number is equal to the degree $k$, since

$$B = \frac{2}{\pi^2} \int_{-\infty}^{\infty} f' \sin^2 f \, dx_3 \int_{T^2} J^2 \, dx_1 dx_2 = \frac{k}{\pi} \left[ f - \frac{1}{2} \sin 2f \right]_{-\infty}^{\infty} = k,$$  

where we have used the expression (2.11) and the boundary conditions (2.3).

In calculating the energy it will be useful to introduce a scale parameter $\mu$ by writing $u = x_3/\mu$ and setting $f(x_3) = g(u)$. Then, if $A$ is the area of the fundamental torus $T^2$, integrating the density (2.9) gives

$$E = \int_{-\infty}^{\infty} dx_3 \int_{T^2} dx_1 dx_2 \mathcal{E} = \frac{A}{\mu} E_1 + \frac{1}{\mu} E_2 + \mu E_3 + \frac{\mu}{A} E_4$$  

where the $E_i$’s are the following integrals over $u$

$$E_1 = \int_{-\infty}^{\infty} g^2 \, du,$$

$$E_2 = 8\pi k \int_{-\infty}^{\infty} g^2 \sin^2 g \, du,$$

$$E_3 = 8\pi k \int_{-\infty}^{\infty} \sin^2 g \, du,$$

$$E_4 = 16\mathcal{I} \int_{-\infty}^{\infty} \sin^4 g \, du.$$  

The only remaining dependence on the map $W$ is the quantity $\mathcal{I}$, which is defined as

$$\mathcal{I} = A \int_{T^2} J^4 \, dx_1 dx_2,$$  

and has the important property that it is independent of $A$.

The scale $\mu$ and area $A$ can now be determined, in terms of the $E_i$’s, by minimization of the energy (2.13). Requiring $\frac{\partial E}{\partial \mu} = \frac{\partial E}{\partial A} = 0$, gives the result

$$\mu = \sqrt{E_2/E_3}, \quad A = \sqrt{E_2 E_4/E_1},$$  

and hence a minimized energy of

$$E = 2(\sqrt{E_1 E_4} + \sqrt{E_2 E_3}).$$  

(2.17)
To proceed further we now need an explicit expression for the map $W(z)$. To obtain a holomorphic map from the torus, we take $W$ to be an elliptic function of $z$. Exactly which elliptic function to take is determined by the fact that we wish to construct a hexagonal lattice, so we require a fundamental period parallelogram which has a $60^\circ$ angle between the two fundamental periods. The appropriate elliptic function is the Weierstrass function $℘(z)$ satisfying

$$\wp^2 = 4(\wp^3 - 1), \quad (2.18)$$

which has real period $\Omega_1 = \Gamma(\frac{1}{6})\Gamma(\frac{1}{3})/(2\sqrt{3}\pi)$ and imaginary period given by $\Omega_2 = \Omega_1(1 + i\sqrt{3})/2$. From this we see that the period lattice is equilaterally triangular, and thus we have the desired $60^\circ$ angle. Obviously we can scale both the elliptic function and its argument and still retain the above desired property, hence we take

$$W(z) = c\wp(z/\alpha), \quad (2.19)$$

where $c$ and $\alpha$ are arbitrary real constants. Note that by the inclusion of the factor $\alpha$ we must now rescale the fundamental torus. Furthermore, for later computational purposes it is convenient to work with a rectangular fundamental torus, which is achieved by taking it to be the $T^2$ given by $(x_1, x_2) \in [0, \alpha\Omega_1] \times [0, \alpha\sqrt{3}\Omega_1]$. As this torus contains two fundamental parallelograms and the $\wp$-function has a double pole in each of these then, by counting preimages, we see that the degree of the map in this case is $k = 4$.

For a given $k$, the energy $E$ is minimized by minimizing the value of the integral $I$ defined in (2.15). This is clear since its only appearance is as a coefficient in front of the positive term $E_4$ in (2.14). Recall that $I$ is independent of the area $A$, and hence $\alpha$ since the two are simply related by

$$A = \sqrt{3}\alpha^2\Omega_1^2. \quad (2.20)$$

Computing $I$ for the one-parameter family of maps (2.19), given by varying $c$ for any fixed $\alpha$, we find that its minimum value is $I \approx 193$, which is attained when $c \approx 0.7$.

In order to continue with an analytical treatment we now make an ansatz for the profile function $g(u)$, which we shall see turns out to be a reasonably good choice. We choose the sine-Gordon kink profile function

$$g(u) = 2\arctan e^u, \quad (2.21)$$

which has the advantage that all the integrals in (2.14) can be performed exactly. The results are

$$E_1 = 2, \quad E_2 = 128\pi/3, \quad E_3 = 64\pi, \quad E_4 = 64I/3, \quad (2.22)$$

from which we find that the scale and area are

$$\mu = \sqrt{2/3}, \quad A = \frac{8}{3}\sqrt{I}, \quad (2.23)$$

and using (2.17) the energy is

$$E = 16\sqrt{2/3}(\sqrt{I} + 8\pi). \quad (2.24)$$
Recalling that \( B = k = 4 \) we thus compute that the energy per baryon is

\[
E/B = 1.076 \times 12\pi^2.
\]  

(2.25)

In discussing the energy of various configurations it will be useful to define \( \Delta \) to be the percentage excess over the Faddeev-Bogomolny bound i.e.

\[
\Delta = \left( \frac{E - 12\pi^2|B|}{12\pi^2|B|} \right) \times 100\%.
\]  

(2.26)

Thus, our ansatz for the lattice has \( \Delta_{\text{lat}} = 7.6\% \).

3 Skyrmion Architecture

In this section we discuss the accurately computed energies of various configurations, using a numerical relaxation of the full nonlinear Skyrme model. Using this information we speculate on the kinds of structures which may form for Skyrmions of high charge.

In the previous section we were able to compute an explicit Skyrme field which describes a lattice with a relatively small excess energy. However, some approximations were made, for example, the choice of the profile function (2.21) and so the energy of the true lattice will be lower than the ansatz value of \( \Delta_{\text{lat}} = 7.6\% \). To determine the true value, we take the ansatz field as a starting configuration in a numerical relaxation computation using the code described in detail in ref. [2]. The simulations were performed on a grid containing \( 100 \times 100 \times 58 \) points and periodic boundary conditions imposed in appropriate directions. The computation of the initial excess confirmed the value to be \( \Delta_{\text{lat}} = 7.6\% \) but after relaxation, which also involved some minor rescaling to be sure to obtain the minimum energy lattice, the excess of the true lattice was found to settle down to \( \Delta_{\text{lat}} = 6.1\% \).

In Fig.1 we display a surface of constant baryon density for the hexagonal lattice. The hexagonal structure is clearly visible, with the baryon density isosurface having a hole in the centre of each of the hexagonal faces. Note that the section of lattice we are considering contains exactly eight full hexagons and is of baryon number four, computed to be \( B = 3.84 \) on the discretized grid. The fact that each hexagon may be thought of as having baryon number one-half is the expected infinite limit of the polyhedron structure discussed in the introduction, where a charge \( B \) Skyrmion is found to have \( 2(B - 1) \) faces.

As mentioned in the introduction, the excess energy of the lattice is lower than that found for any finite charge Skyrmion. For a single Skyrmion the excess is \( \Delta_1 = 23\% \), whereas for the configurations up to charge nine the minimum excess occurs for \( B = 9 \) which has \( \Delta_9 = 9.8\% \). A relaxation of the charge seventeen buckyball configuration gives the smallest known value \( \Delta_{17} = 7.2\% \). Thus our results are all consistent with the fullerene picture of Skyrmions where, at least for Skyrmions of modest charge, the structure is a shell of pentagons and hexagons.

The fact that \( \Delta_{\text{lat}} \) is so low is encouraging for the possibility of Skyrmion shells at even higher charge, however it is not low enough to conclude that shell-like structures
continue indefinitely. This is because of the existence of the Skyrme crystal \([3, 3]\), which is a configuration that is periodic in all three space dimensions and consists of a crystal of half-Skyrmions. A Fourier series analysis \([3]\) approximates the energy excess of the crystal to be \(\Delta_{\text{cry}} = 3.8\%\) and a simple analytical formula exists which gives a good approximation to the fields of the Skyrme crystal \([3]\). Using this as an initial configuration in our relaxation scheme, we find a true energy for the Skyrme crystal of \(\Delta_{\text{cry}} = 3.6\%\). A surface of constant baryon density is shown in Fig.2. The half-Skyrmion structure of the crystal is evident and it is clear that this configuration is of a very different type to that of the lattice shown in Fig.1.

Naively, the fact that \(\Delta_{\text{cry}} < \Delta_{\text{lat}}\) suggests that there could be some value of the Skyrmion charge, \(B_{\text{crit}}\), at which the shell-like structures will be replaced by more three-dimensional configurations, but the details of how and when this might take place are unclear. However, a simple comparison of \(\Delta_{\text{cry}}\) and \(\Delta_{\text{lat}}\) measures the volume effect, but since these two values are not so different the crucial factor will be an area effect, which is associated with the fact that a finite portion of the Skyrme crystal needs to be smoothed off at the edges. One suitable candidate for completing the edge of the Skyrme crystal is a configuration like the face of the \(B = 4\) cubic Skyrmion. However, since this has an excess of \(\Delta_1 = 12\%\), quite a substantial piece of the crystal needs to be included before such a high penalty for its boundary could be accommodated. In contrast, a large shell structure only ever requires twelve pentagon defects and they can be included at a relatively small cost, as demonstrated by the \(B = 17\) buckyball with \(\Delta_{17} = 7.2\%\). All this suggests that even if the Skyrme crystal structure appears at some charge \(B_{\text{crit}}\) then this may well be very high.

Therefore, there is at least the possibility of a range of modest charges where other fullerene structures may exist. Other exotic possibilities include analogues of the bucky-tubes (long thin configurations comprised of spirals of hexagons with caps containing pentagons) and also shells inside shells.

If the above structure change to the Skyrme crystal does indeed occur then for \(B \geq B_{\text{crit}}\) then the fullerene analogy will be lost, since the Skyrme crystal is a configuration with valency six. However, it is possible that the known Skyrme crystal is not the minimum energy crystal structure. If, for example, a configuration exists with the structure of the diamond lattice, then the similarities with carbon atoms could be maintained. This is a four-valent lattice with tetrahedral symmetry, but would not be as simple as the tetrahedral lattice formed from individual Skyrmions in the nearest neighbour attractive channel, which relaxes to the cubically symmetric Skyrme crystal. However, it is a difficult task to investigate this possibility since a Skyrme field with the correct properties needs to be found before numerical simulations can be performed. Using the ideas from rational maps we were able to create a configuration to study the lattice and perhaps a similar technique could be employed to study other crystals.
4 Conclusions

We have introduced an ansatz for a Skyrme lattice with hexagonal symmetry and used it as an initial condition in a numerical relaxation of the full nonlinear equations of the Skyrme model. The result is further evidence to support the analogy between Skyrmions and fullerene shells in carbon chemistry.

Further work is required to address the issue of the structure of high charge Skyrmions. One approach is to collide Skyrmions, but it may also prove useful to use the Skyrme lattice, or at least a part of it. The interaction of two such lattices may shed some light on the subject of shell formation and it would also be interesting to study the scattering of Skyrmions off the lattice. These issues are currently under investigation.

Given the connection between Skyrmions, monopoles and rational maps, it seems likely that a similar lattice of monopoles will exist. In this letter we chose a specific elliptic function in our ansatz in order to obtain a hexagonal lattice. Other Skyrme fields can be obtained which correspond to different lattices by choosing other elliptic functions, though we expect them to have higher energy per baryon than the one considered here. However, in the monopole context all types of lattices would be on an equal footing since monopoles are BPS solitons. It would therefore be interesting to see if the Donaldson correspondence could be extended to infinite charge monopole lattices, with each characterized by an elliptic function.

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\(^1\)We have, in fact, also repeated the same procedure for a square lattice, which is quad-valent. The calculated excess \(\Delta \approx 6.8\%\), larger than that for the trivalent, hexagonal lattice, illustrating that the trivalent is more energetically favourable.
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**Figure Captions**

Fig. 1. Baryon density isosurface for the Skyrme lattice. The section displayed has baryon number four and contains effectively eight hexagons

Fig. 2. Baryon density isosurface for the Skyrme crystal. Each corner contains a half-skyrmion and the total baryon number shown is four. If the threshold for the isosurface were to be increased the corners would be connected by links of lower baryon density into a crystalline structure.
