Solitonic Fullerene Structures in Light Atomic Nuclei

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The Skyrme model is a classical field theory which has topological soliton solutions. These solitons are candidates for describing nuclei, with an identification between the numbers of solitons and nucleons. We have computed numerically, using two different minimization algorithms, minimum energy configurations for up to 22 solitons. We find, remarkably, that the solutions for seven or more solitons have nucleon density isosurfaces in the form of polyhedra made of hexagons and pentagons. Precisely these structures arise, though at the much larger molecular scale, in the chemistry of carbon shells, where they are known as fullerenes.

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The Skyrme model [1] was first proposed in the early 1960s as a model for the strong interactions of hadrons, but it was set aside after the advent of quantum chromodynamics (QCD). Much later Witten [2] showed that it could arise as an effective description at low energies in the limit where the number of quark colors is large. Subsequent work [3] demonstrated that the single soliton solution (known as a Skyrmion) reproduced the properties of a nucleon to within an accuracy of around 30%, which is quite an achievement, given that there is, at present, no practical way of calculating the properties of nuclei from QCD via, for example, lattice gauge theory.

In order to study nuclei of a larger atomic number one first needs to compute the minimal energy configurations of multisolitons, since in the Skyrme model there is an identification between the numbers of solitons and nucleons. Here, we present the results of an extensive set of simulations using two very different approaches designed to compute the minimal energy solutions for up to 22 solitons. With a small number of caveats, these results establish an attractive analogy with fullerene cages familiar in carbon chemistry [4,5]. Although these classical solutions must first be quantized before a final comparison with experimental data can be performed it is expected that quantum corrections will be relatively small, since we are dealing with solitons, and so the classical solutions will contain important physically relevant information about the properties of nuclei.

The Skyrme model is defined in terms of an SU(2) valued field $U(\mathbf{x})$, with an associated static energy

$$E = \frac{1}{24\pi^2}\int\left\{\mathrm{Tr}(\partial_i U\,\partial_i U^{-1}) - \frac{1}{8}\,\mathrm{Tr}([(\partial_i U)U^{-1},(\partial_j U)U^{-1}]^2)\right\}d^3\mathbf{x}\,. \tag{1}$$

Note that the two physically relevant constants which would appear in front of each of the two terms in the most general version of (1) have, for convenience, been scaled out by an appropriate choice of energy and length units. For finite energy, we impose the boundary condition $U(\infty) = 1$, and pions are described by the usual quantum field theory treatment of fluctuations of the Skyrme field around this vacuum value, but nucleons arise in a very different manner, as classical soliton solutions.

The boundary condition implies a compactification of the domain, and therefore U is a map from compactified $\mathbb{R}^3 \sim S^3 \mapsto S^3$, since S^3 is the manifold of the target space, the group SU(2). Such mappings have nontrivial homotopy classes characterized by an integer valued winding number, which has the explicit representation

$$B = -\frac{\epsilon_{ijk}}{24\pi^2}\int \mathrm{Tr}[(\partial_i U)U^{-1}(\partial_j U)U^{-1}(\partial_k U)U^{-1}]\,d^3\mathbf{x}\,. \tag{2}$$

B, which stands for the baryon number or the number of nucleons, is often referred to as the topological charge and is the number of solitons in a given field configuration. A simple manipulation of Eqs. (1) and (2) allows one to deduce the Faddeev-Bogomolny (FB) bound $E \geq |B|$. Generically, a charge B field will have an energy density $\mathcal{E}$ [the integrand of (1)] and a baryon density $\mathcal{B}$ [the integrand of (2)] both of which consist of B well-separated lumps localized in space. However, as we discuss below, this is not the case for the minimal energy fields in which the solitons are close together.

The mathematical problem is to find, for each integer B, the field U which minimizes the energy (1) subject to the constraint (2). This can be addressed by numerical algorithms designed to minimize either a discretized version of the energy (1) or, equivalently, by solving a discretized version of the second-order field equations which follow from the variation of (1). This first approach is a very demanding computational exercise (see Ref. [6] for a detailed discussion), requiring the use of modern parallel supercomputers, but results for low charge ($B \leq 8$) were found using this method [7–10]. The results presented

here extend this numerical approach up to $B = 22$. In addition, we have applied a second, very different, technique to the construction of minimal energy solitons which not only allows us to have greater confidence that the numerical solutions we have constructed are indeed the global minima, but in addition provides a good analytic approximation to the numerical solutions, making it much easier to identify their structure and symmetries.

Our second approach makes use of the remarkable fact that minimal energy Skyrmions can be approximated by an ansatz involving rational maps between Riemann spheres [11], a result which we will further confirm. The Skyrme field is a map $U\colon \mathbb{R}^3 \mapsto S^3$, so it is not immediately obvious how to obtain such a map from rational maps which are between spheres $S^2 \mapsto S^2$. Briefly, the domain S^2 of the rational map is identified with concentric spheres in $\mathbb{R}^3$, and the target S^2 with spheres of latitude on S^3. To present the ansatz it is convenient to use spherical coordinates in $\mathbb{R}^3$, so that a point $\mathbf{x} \in \mathbb{R}^3$ is given by a pair (r, z), where $r = |\mathbf{x}|$ is the distance from the origin and z is a Riemann sphere coordinate, namely, $z = \tan[\theta/2]\exp[i\phi]$, where θ and ϕ are the normal spherical polar coordinates.

Now, let $R(z)$ be a degree B rational map; that is, $R = p/q$, where p and q are polynomials in z such that $\max[\deg(p), \deg(q)] = B$, with no common factors. Given such a rational map the ansatz for the Skyrme field is

$$U(r, z) = \exp\left[\frac{if(r)}{1 + |R|^2}\begin{pmatrix} 1 - |R|^2 & 2\bar{R} \\ 2R & |R|^2 - 1 \end{pmatrix}\right], \quad (3)$$

where $f(r)$ is a real profile function satisfying the boundary conditions $f(0) = \pi$ and $f(\infty) = 0$. This is determined by minimization of the Skyrme energy of the field (3) given a particular rational map R. The ansatz yields an exact solution for $B = 1$ and it was shown in Ref. [11] that for $2 \leq B \leq 8$, suitable maps exist for which the field (3) is a good approximation to the numerically computed solutions, in the sense that the symmetry is identical and the energy is only 1% or 2% above the numerically computed values.

Substituting the ansatz (3) into the energy (1) produces an energy function on the space of rational maps, which we denote by $\mathcal{I}(R)$, given by

$$\mathcal{I}(R) = \frac{1}{4\pi}\int\left(\frac{1 + |z|^2}{1 + |R|^2}\left|\frac{dR}{dz}\right|\right)^4 \frac{2i\, dz d\bar{z}}{(1 + |z|^2)^2}. \quad (4)$$

Therefore, our second approach to computing minimal energy Skyrmions is to search the (finite dimensional) parameter space of general degree B rational maps to find the one which minimizes $\mathcal{I}(R)$, using a powerful numerical minimization technique known as simulated annealing [12].

Clearly, this procedure is not guaranteed to find the minimum energy Skyrmion since the topography of the rational map space may be slightly different to that of the full nonlinear field theory, but as we shall see for the most part it works well, only encountering difficulties when there are two or more Skyrmion solutions, either saddle points or genuine local minima, with very similar energies. We use the first minimization technique as a check, and in the small number of cases where relaxing well-separated clusters consistently yield a different solution for a wide range of initial conditions, the symmetry of the Skyrmion solution is identified by eye from the baryon density isosurface, and an approximate rational map can then be found by relaxing in the rational map space restricted to have the correct symmetry. In such cases the values of $\mathcal{I}$ for the different solutions are usually very close [6].

The results of applying the two minimization techniques in this way are presented in Table I for $1 \leq B \leq 22$ and pictorially in Fig. 1 for $7 \leq B \leq 22$. In all but a small number of cases ($B = 10, 14, 16, 22$) we find that the minimum energy Skyrmion and that in the rational map space coincide. Furthermore, for each of these special cases, except $B = 14$, we were able to find a map with the same symmetry. For $B = 14$ we were prevented from finding a rational map approximation for the true minimum since its symmetry group, C_2, is a subgroup of that of the minimum energy rational map, D_2.

The baryon density isosurface can be associated with a polyhedron whose edges and vertices coincide with the regions in which the baryon density is localized. Examination of the solutions shows that, with the exception

TABLE I. A summary of the symmetries and energies of the Skyrmion configurations which we have identified as the minima. Included is the ionization energy (I_B)—that required to remove one Skyrmion—and the binding energy per Skyrmion ($\Delta E/B$)—that required to split the charge B Skyrmion into B charge one Skyrmions divided by the total number.

B	G	E/B	E_B	I_B	$\Delta E/B$
1	$O(3)$	1.2322	1.2322	0.0000	0.0000
2	$D_{\infty h}$	1.1791	2.3582	0.1062	0.0531
3	T_d	1.1462	3.4386	0.1518	0.0860
4	O_h	1.1201	4.4804	0.1904	0.1121
5	D_{2d}	1.1172	5.5860	0.1266	0.1150
6	D_{4d}	1.1079	6.6474	0.1708	0.1243
7	Y_h	1.0947	7.6629	0.2167	0.1375
8	D_{6d}	1.0960	8.7680	0.1271	0.1362
9	D_{4d}	1.0936	9.8424	0.1578	0.1386
10	D_3	1.0904	10.9040	0.1706	0.1418
11	D_{3h}	1.0889	11.9779	0.1583	0.1433
12	T_d	1.0856	13.0272	0.1829	0.1466
13	O	1.0834	14.0842	0.1752	0.1488
14	C_2	1.0842	15.1788	0.1376	0.1480
15	T	1.0825	16.2375	0.1735	0.1497
16	D_2	1.0809	17.2944	0.1753	0.1513
17	Y_h	1.0774	18.3158	0.2108	0.1548
18	D_2	1.0788	19.4184	0.1296	0.1534
19	D_3	1.0786	20.4934	0.1572	0.1536
20	D_{6d}	1.0779	21.5580	0.1676	0.1543
21	T_d	1.0780	22.6380	0.1522	0.1542
22	D_3	1.0766	23.6852	0.1850	0.1556

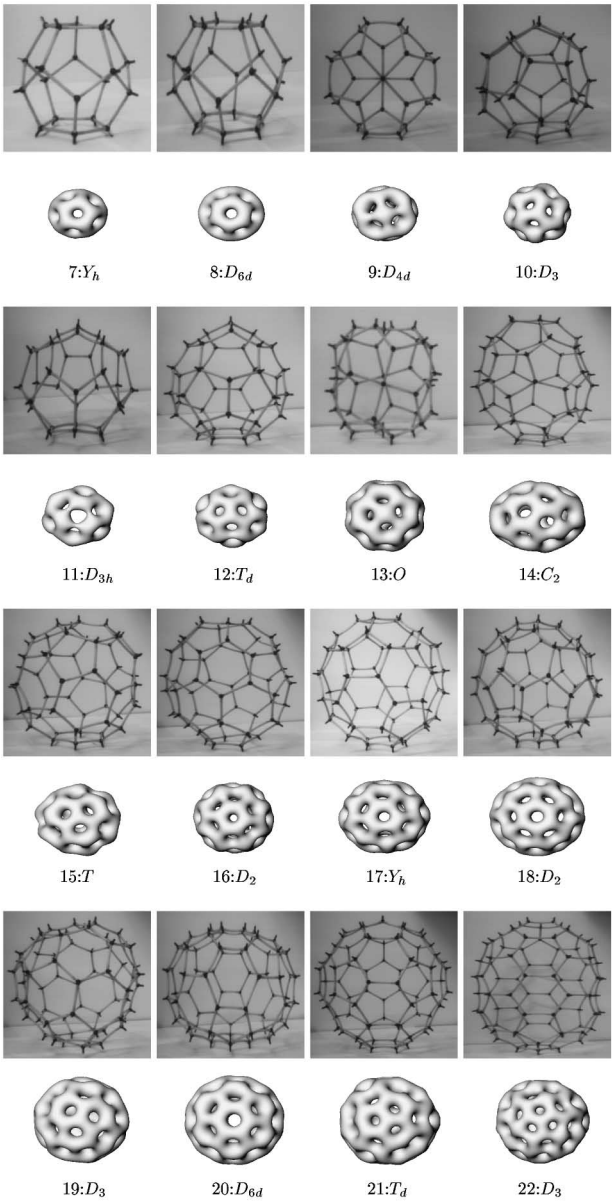

FIG. 1. The baryon density isosurfaces for the solutions which we have identified as the minima for $7 \leq B \leq 22$, and the associated polyhedral models. The isosurfaces correspond to $\mathcal{B} = 0.035$ and are presented to scale, whereas the polyhedra are not to scale.

of $B = 9$ and 13, the associated polyhedra are trivalent with $4(B - 2)$ vertices [the geometric energy minimization (GEM) rules] as predicted in Ref. [10], and for $B \geq 7$ they are comprised of 12 pentagons and $2(B - 7)$ hexagons. Such structures are common in a wide range of physical applications and have become a hot topic in carbon chemistry where they correspond to shells with carbon atoms placed at the vertices, the most famous being the icosahedrally symmetric Buckminsterfullerene C_{60} structure, which is also the traditional soccer ball design. For this reason we refer to such solutions as being of the fullerene type, with the prediction, spectacularly confirmed by our results in all cases except $B = 9$ and $B = 13$, that the polyhedron associated with the Skyrmion of charge B has a structure from the family of carbon cages for $C_{4(B-2)}$.

We had predicted in Ref. [10] that the Buckyball C_{60} configuration would be found for $B = 17$ and indeed an approximate rational map description was found in Ref. [11]. Here, we see that such a solution is the minimum energy solution of the full nonlinear field equations and in the rational map space. We see also that a large number of the other solutions have platonic symmetries which, from the mechanical point of view, implies the structure packs well. It would appear, therefore, that such structures may be preferred over less symmetric ones in the minimization procedure. We should note, however, that this is not always the case and rational maps with platonic symmetries can easily be found, for example, at $B = 9$, which do not give minima [6].

The polyhedra found for $B = 9$ and 13 do not obey the GEM rules nor are they of the fullerene type, since they contain four-valent links. They can, however, be related to a fullerene via the concept of symmetry enhancement, as follows. A very common structure within the fullerene polyhedra is two pentagons separated by two hexagons. If the edge which is common to the two hexagons is shrunk to have zero length, the four polygons then form a C_4 symmetric configuration containing a four-valent bond. For the case of $B = 9$, the polyhedron can be thought of as being created from a D_2 symmetric fullerene by the action of two such operations, and in the $B = 13$ case six operations can be used to convert another D_2 configuration into one with O symmetry. Empirically, we see that each symmetry enhancement operation appears to be accompanied by an equivalent one antipodally placed on the polyhedron, and single operations appear not to occur.

We have computed the energies of the solutions which are presented in Table I using the rational map ansatz to create initial conditions which are then relaxed under the action of the full nonlinear field equations. It should be noted that these values are (for $B > 1$) always a little less than the corresponding values computed solely within the rational map ansatz. On the discrete grid the computed value of the baryon number, $B_{\rm dis}$, is less than the corresponding integer B suggesting that the finite difference approximations used to compute the energy $E_{\rm dis}$ will underestimate the true energy. Moreover, in the initial conditions one must impose the boundary condition $U = 1$ at the edge of the box. By using a wide range of different grid sizes and spacing we have shown [6] that the value of $E_{\rm dis}/B_{\rm dis}$ can be computed accurately, and hence so can the true energy using the formula $E_B = B \times (E_{\rm dis}/B_{\rm dis})$. We claim that our determinations of $E_{\rm dis}/B_{\rm dis}$ are accurate in the absolute sense to within ± 0.001 and that the relative values are probably even more accurate.

We have also computed the ionization energy $I_B = E_{B-1} + E_1 - E_B$, which is the energy required

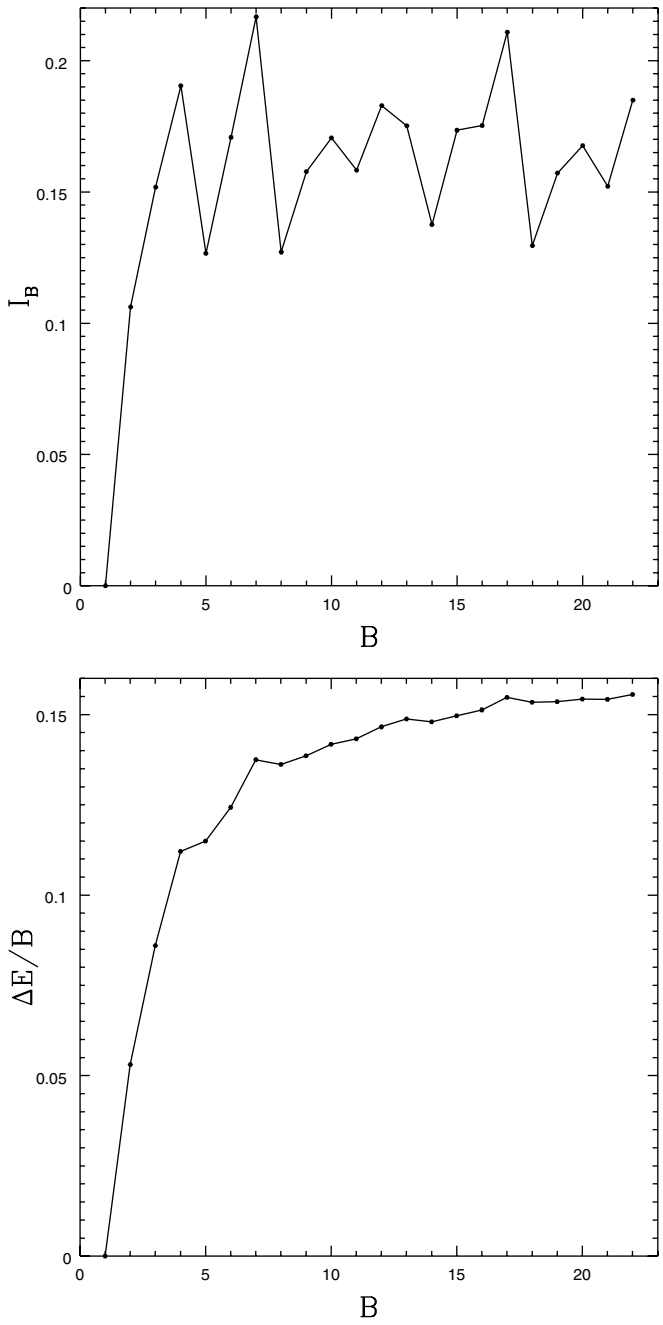

FIG. 2. On top the ionization energy I_B plotted against B. Notice that the most stable solutions are those with the most symmetry, $B = 4, 7, 17$, while the least stable are those with little symmetry $B = 5, 8, 14, 18$. On the bottom the binding energy per baryon $\Delta E/B$ plotted against B. We see that for large B the binding energy appears to level out at around 0.15–0.16 as one might expect in a simple model of nuclei.

to remove a single Skyrmion, and the binding energy per nucleon $\Delta E/B = E_1 - (E/B)$, which is the energy required to separate the solution into B well-separated Skyrmions divided by the total baryon number. These values are tabulated in Table I and are plotted against B in Fig. 2. The ionization energy is largest for the most symmetrical solutions $B = 4$, 7, and 17 and is least for those with little symmetry, $B = 5$, 8, 14, and 18, which is very much as one would expect. The binding energy appears to increase to an asymptotic value of around 0.15–0.16. This is a clear consequence of the FB bound since it is linearly related to E/B.

In fact, the value of E/B appears to have an asymptotic value which is around 6%–7% above the FB bound, compatible with the value obtained for a hexagonal lattice [13] which is the limit of an infinitely large fullerene (the analog of graphite in carbon chemistry). It is clear that an infinitely large shell is physically unlikely and that there probably exists a value B_* such that for $B > B_*$ the solutions no longer look like fullerene shells. In such a case the solutions are likely to begin to look more like portions cut from the infinite Skyrme crystal [14] whose E/B is only 4% above the FB bound. Another possibility is an intermediate state comprised of multiple shells [15], although all the known configurations of this kind have much larger values of E/B. We have definitely shown that $B_* > 22$ and we believe that the connection between Skyrmions, fullerenes, and rational maps will continue for much larger values of B.

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[1] T. H. R. Skyrme, Proc. R. Soc. London A **260**, 127 (1961).
[2] E. Witten, Nucl. Phys. **B223**, 422 (1983).
[3] G. S. Adkins, C. R. Nappi, and E. Witten, Nucl. Phys. **B228**, 552 (1983).
[4] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, and R. E. Smalley, Nature (London) **318**, 354 (1985).
[5] P. W. Fowler and D. E. Manolopoulos, *An Atlas of Fullerenes* (Clarendon Press, Oxford, 1995).
[6] R. A. Battye and P. M. Sutcliffe, "Skyrmions, Fullerenes and Rational Maps" (to be published).
[7] V. B. Kopeliovich and B. E. Stern, JETP Lett. **45**, 203 (1987).
[8] J. J. M. Verbaarschot, Phys. Lett. B **195**, 235 (1987).
[9] E. Braaten, S. Townsend, and L. Carson, Phys. Lett. B **235**, 147 (1990).
[10] R. A. Battye and P. M. Sutcliffe, Phys. Rev. Lett. **79**, 363 (1997).
[11] C. J. Houghton, N. S. Manton, and P. M. Sutcliffe, Nucl. Phys. **B510**, 507 (1998).
[12] P. J. M. van Laarhoven and E. H. L. Aarts, *Simulated Annealing: Theory and Applications* (Kluwer Academic Publishers, Dordrecht, The Netherlands, 1987).
[13] R. A. Battye and P. M. Sutcliffe, Phys. Lett. B **416**, 385 (1998).
[14] L. Castillejo, P. S. J. Jones, A. D. Jackson, J. J. M. Verbaarschot, and A. Jackson, Nucl. Phys. **A501**, 801 (1989).
[15] N. S. Manton and B. M. A. G. Piette, hep-th/0008110.