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Skyrmion crystals and their symmetries

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We discuss the phase diagram of Skyrmion crystals as a function of both density and pressure. The use of symmetry properties of the various phases and of Fourier expansions tailored to fit these symmetries facilitates our discussion. A simple cubic arrangement of half-Skyrmions is, almost everywhere, the lowest-energy phase. At very high densities the simple cubic phase undergoes a transition to a body-centered-cubic crystal of half-Skyrmions. The transition to a crystal of Skyrmions at low densities, that was previously suggested, is not accessible thermodynamically. A first-order phase transition leading to a phase separation occurs before the previous transition can be reached.

I. INTRODUCTION

The Skyrme[1] model describes nucleons as solitons in a nonlinear theory of π mesons. In quantum chromodynamics, when the number of colors becomes infinite it was argued that baryons are indeed solitons in a mesonic theory.[2] The phenomenological applications of the Skyrme model thus involve a double approximation, changing N_c, the number of colors, from infinity to three, and using a theory containing only pions as a low-energy approximation for a more complicated meson theory. In spite of these rather severe approximations, the model has been shown to give a reasonable description of single-nucleon properties[3] and of meson-baryon scattering.[4]

In this paper we deal with the properties of nuclear matter in the Skyrme model. In the classical approximation Skyrmions attract each other at large separations. At zero temperature, where all kinetic energy can be neglected, this attraction will cause the ground state to be a crystal. A numerical calculation to determine the whole structure of the ground state turns out to be too difficult. Thus the usual approach is to assume a crystal symmetry and to perform a numerical solution using this symmetry as a constraint. We do not know of a simple way to guess the symmetry of the ground state. Only approximate arguments based on the nature of the long-range interactions between Skyrmions have served as guidelines for finding the symmetry of the ground state. This symmetry is described by a group that includes elements of space groups and isospin transformations.

The first guess for the crystal symmetry was made by Klebanov[5] who was the first to investigate this subject. He arranged Skyrmions on a simple cubic lattice and showed that the Skyrmions could be rotated so that every Skyrmion is attracted by its six nearest neighbors.[6] This served as a starting point for a numerical relaxation procedure. Wüst, Brown, and Jackson[7] have investigated the Klebanov lattice as a function of the baryon density. They showed that, at densities close to the minimum of the energy, the ground state does not resemble a crystal of Skyrmions. If the density is decreased below its value at the minimal energy a first-order phase transition was claimed to occur and the low-density lattice resembles a crystal of Skyrmions. These results were confirmed by Walhout[8] who also investigated finite-temperature effects and quantum fluctuations in this model. Jackson, Wirzba, and Castillejo[9] have investigated the low-density phase transition of Ref. 7 by discussing the interactions of two Skyrmions on a hypersphere. A physical description of this phase transition was provided by Goldhaber and Manton.[10] They argued that at low densities the crystal may be viewed as an arrangement of Skyrmions whereas the high-density phase may be described as a crystal of half-Skyrmions. These authors suggest that in the high-density region, the simple cubic lattice of Skyrmions becomes a body-centered lattice of half-Skyrmions. While the half-Skyrmion crystal was arrived at by considering the Klebanov lattice, it will be shown to have a much wider range of validity. Other symmetries also have an energy minimum which is well described by a lattice of half-Skyrmions.

The Klebanov lattice, yields an energy per baryon of 1.08 (the units of energy will be discussed in Sec. II). In the same units the energy has a lower bound of 1.0. The symmetry of this lattice at the minimum of the energy, as obtained at first was very close to the Goldhaber-Manton suggestion.[5,7,8] Two recent papers[11,12] confirmed that the lowest-energy state of the Klebanov lattice does indeed have the half-Skyrmion structure.

It has been shown later that the Klebanov symmetry of the ground state does not yield the lowest energy. Jackson and Verbaarschot[11] have shown that starting with a cubic lattice of Skyrmions and an isospin rotation different from the one used by Klebanov a lower ground-state energy can be obtained. This state has a tetragonal symmetry. In the units used above, the energy of their arrangement is 1.07. At low densities in this symmetry, as in the Klebanov arrangement, each Skyrmion has six nearest neighbors, all in the maximum attraction

configuration. The tetragonal symmetry has an extra advantage over the Klebanov ansatz of improving the next-to-nearest-neighbor attraction.

In a recent paper[12] we have shown that a configuration with even lower energy exists. At low density, in this configuration, Skyrmions are arranged in a face-centered-cubic lattice,[13] and each Skyrmion has 12 nearest neighbors all in the maximum attraction configuration. This symmetry has also been discovered by Castillejo, Jones, Jackson, Vebaarschot, and Jackson[14] who also discuss the phase diagram of Skyrmion crystals. In this symmetry the ground-state energy is 1.038. The energy minimum is reached in a high-density phase, which can be described as a simple cubic lattice of half-Skyrmions.

We cannot prove that the new lattice is indeed the lowest-energy of classical nuclear matter in the Skyrme model. The fact that this energy is only 3.8% above the lower bound which cannot be reached[1] suggests to us that this is very likely.

In this paper we investigate the phase structure of the Skyrmion crystal including the new symmetry configuration that was described in Refs. 12 and 14. The phase diagram of the crystal is studied as a function of density and as a function of pressure. At very high densities the new, simple cubic crystal of half-Skyrmions undergoes a first-order phase transition to the body-centered lattice of half-Skyrmions investigated previously. At densities below those of the minimum of the energy the system becomes thermodynamically unstable. As we increase the volume the crystal undergoes a first-order phase transition that leads to a phase separation. Part of the system remains at the density which minimizes the energy, and part of the volume is empty. Technically this is due to the fact that the energy per unit cell of the crystal is not a convex function of the energy. Thus the phase transition between a crystal of half-Skyrmions to a crystal of Skyrmions that was investigated in Refs. 5–11 and 14 is not accessible, it appears on a thermodynamically unstable branch of the phase diagram. A sign of this instability is that near the region of transition dP/dV is positive corresponding to a negative compressibility, and clearly the pressure cannot increase as the volume increases. Earlier calculations did not identify this instability since they calculated the energy of a single unit cell, where surface energies cannot be neglected and phase separation does not occur.

Our method for dealing with the numerical problem of finding the lowest-energy configuration once the symmetry is assumed has already been outlined;[12] it is an adaptation of methods used in condensed-matter physics.[15] We expand the field in a Fourier-type series that is consistent with the assumed crystal symmetry. We then use the expansion coefficients as variational parameters to find the minimum of the energy. This turns out to be a rapidly convergent expansion. The first term alone gives an energy within 3% of the minimum. Five terms suffice to determine the minimum to a fraction of 1%. This method has some clear advantages over the usual lattice calculations. Since we use a Fourier expansion we can perform integrations very accurately and it is easier to obtain the energy with a higher accuracy than in the usual grid methods, while the correct baryon number is assured by construction. Since we are using a variational method, our results can serve as upper bounds.

The program of our paper is as follows. In Sec. II we review the Skyrme model and define the units used in this paper. Section III is devoted to the symmetries of various crystals used as ground states and to the Fourier expansions used. Section IV contains a description of the variational procedure for obtaining ground-state energies, the numerical results, and a discussion of their physical interpretation. Conclusions are presented in Sec. V.

II. THE SKYRME MODEL

In the SU(2)-invariant Skyrme model, the order parameter is a unitary two-dimensional matrix U. Alternatively this matrix may be described by a four-vector n^α that satisfies

$$\sum_\alpha n^\alpha n^\alpha = 1 \ . \tag{1}$$

The energy of a time-independent state in this model is given by

$$E=\int d^3x \left[\frac{F_\pi^2}{8} \sum_{\alpha,i} (\partial_i n^\alpha)^2 + \frac{1}{4e^2} \sum_{\alpha,\beta,i,j} (\partial_i n^\alpha \partial_j n^\beta - \partial_i n^\beta \partial_j n^\alpha)^2 \right] , \tag{2}$$

where F_π and e are parameters to be fitted. This is a nonlinear σ model with a fourth-order term added to stabilize the soliton.[1] In what follows it is convenient to use the notation $n^\alpha=(\sigma,\pi_1,\pi_2,\pi_3)$. The interaction in Eq. (2) is invariant under the global chiral O(4) that rotates the components of n^α. We will use mainly isospin rotations which act as an O(3) rotation on π_i.

It is convenient to rescale the coordinates by

$$x_{\text{new}} = \frac{F_\pi e}{\sqrt{2}} x_{\text{old}} \tag{3}$$

and the energy by

$$E_{\text{new}} = \frac{e}{3\pi^2\sqrt{2}F_\pi} E_{\text{old}} \ . \tag{4}$$

In these units the energy of a time-independent solution is given by

$$E=\frac{1}{24\pi^2}\int d^3x \left[\sum_{\alpha,i} (\partial_i n^\alpha)^2 + \sum_{\alpha,\beta,i,j} (\partial_i n^\alpha \partial_j n^\beta - \partial_i n^\beta \partial_j n^\alpha)^2 \right] . \tag{5}$$

The baryon number in this model corresponds to the topological charge. It is given in the above units by[1]

$$B=\frac{1}{12\pi^2}\int d^3x \, \epsilon_{ijk}\epsilon_{\alpha\beta\gamma\delta} n^\alpha \partial_i n^\beta \partial_j n^\gamma \partial_k n^\delta \ . \tag{6}$$

The above units are chosen so the energy is bounded by[1]

$$E \geq B \ . \tag{7}$$

The above inequality cannot be saturated, for flat space, unless n^α is a constant everywhere and then both E and B vanish.[1] An identical inequality holds, locally, for the energy density and the baryon density. The energy of a single Skyrmion[1] ($B=1$) in our units is $E=1.23$.

The interaction of two Skyrmions has been studied in this model by considering a state that is a product of two single baryon solutions.[6] In this product ansatz which is reliable for large separations, but has difficulties at short separations,[16] the maximum attraction is when one of the solutions is rotated in isospin by an angle π around an axis perpendicular to the axis separating the two Skyrmions.[6]

As a starting point in constructing the ground state of the Skyrmion crystal one uses the maximum attraction configuration described above. The low-density configuration is conjectured to resemble a set of Skyrmions arranged on a lattice, and rotated in isospin so that as many Skyrmions as possible are in the maximum attraction configuration. This arrangement of Skyrmions serves to determine the symmetry of the lattice. Such an argument is only intuitive, since the minimum of the energy does not appear in the low-density configuration, where the ground state resembles a crystal of Skyrmions, but rather at a high-density phase where the picture of distinguishable Skyrmions is not valid. The high-density phase was conjectured to be a crystal of half-Skyrmions.[10] Although this conjecture was not recognized in the first numerical calculations, it turns out to be correct for all the symmetries studied so far.[11,12,14] As will be shown later, only the high-density phase is physical, whereas the low-density phase which plays a major role in our intuitive picture and in guessing the lowest-energy state, is not accessible thermodynamically.

III. CRYSTAL SYMMETRIES

In this section we describe various crystal configurations that were suggested for the ground state of Skyrmion matter and describe their symmetries. We also discuss the Fourier-type expansion that we use and obtain the relations among Fourier coefficients for each symmetry. Such relations are selection rules appropriate to the symmetries investigated.

In order to classify the symmetries of the Skyrmionic crystal one has to go beyond the standard list of space groups.[17] Space groups involve symmetry operations which are due to translations and rotations in three-dimensional space alone. The baryon density and the energy density of a Skyrmion crystal can be classified by these space groups. The Skyrme field n^α will have symmetry elements which involve simultaneous space transformations and O(4) transformation acting on the internal degrees of freedom n^α. These new symmetries are analogous to generalized space groups.[18] We are not aware of a complete classification of such groups or of a standard nomenclature.

In the discussion that follows we will refer to various symmetries by the standard name of the space group which describes the symmetry of the component σ. Note that σ has a larger symmetry than the space group; this is a black and white symmetry involving sign reversal of σ. The symmetry of the complete fields n^α will be defined by listing a set of transformations which serve as generators of the symmetry. All symmetry operations can be obtained by repeated application of the generators.

Once we have defined the symmetry of a configuration we proceed by expanding n^α in a Fourier-type series that is consistent with the crystal symmetry. Using a Fourier series for the field n^α is not convenient because it is a unit vector. We prefer to expand an unnormalized vector $\bar{n}^\alpha$ in a Fourier series and then define n^α by

$$n^\alpha = \frac{\bar{n}^\alpha}{(\bar{n}^\beta \bar{n}^\beta)^{1/2}} \ , \tag{8}$$

where summation over β is implied. This normalization procedure will not ruin the symmetry we impose, since n^α has the same symmetry as $\bar{n}^\alpha$. To use this expansion one has to make sure that there is no point where all components of $\bar{n}^\alpha$ vanish. There is no worry that such a point will accidentally arise in our numerical search procedure. In the vicinity of such a point derivatives of n^α will be very large and these will give rise to very large energies. We will return to discuss such points and their physical significance when we discuss our variational procedure in Sec. VI.

We will discuss four crystal symmetries. Our notation for the crystal symmetries are those of Ref. 17.

(A) The Klebanov low-density configuration. This is a simple cubic lattice of Skyrmions, where σ is invariant under the space group $P_{n\bar{3}}$.

(B) The Goldhaber-Manton high-density version of the Klebanov structure. This is a bcc lattice of half-Skyrmions, where σ is invariant under the space group $P_{n\bar{3}m}$.

(C) The new low-density structure. This is an fcc lattice of Skyrmions where σ is invariant under the space group $F_{m\bar{3}m}$.

(D) The new high-density structure. This is a simple cubic lattice of half-Skyrmions where σ is invariant under the space group $P_{m\bar{3}m}$.

Consider a point in space $x_i=(x,y,z)$, where the field is given by $n^\alpha=(\sigma,\pi_1,\pi_2,\pi_3)$. We define the symmetry of the crystal by a set of operations which involve a change in x_i and an associated change in n^α. The changes of x_i are translations by an amount L, rotations, and reflections. The changes in n^α are reflections and O(4) transformations.

The symmetry of configuration (A) is defined by the following transformations:

(A1) $x_i=(-x,y,z)$ and $n^\alpha=(\sigma,-\pi_1,\pi_2,\pi_3)$,

(A2) $x_i=(y,z,x)$ and $n^\alpha=(\sigma,\pi_2,\pi_3,\pi_1)$,

(A3) $x_i=(x+L,y,z)$ and $n^\alpha=(\sigma,-\pi_1,\pi_2,-\pi_3)$.

Symmetry (A1) is a reflection in real space coupled with a reflection operation on n^α. Relation (A2) is a simultaneous rotation around a threefold axis in both spaces. Relation (A3) is a translation by L along the x axis coupled by a rotation by π around the 2 axis in isospin.

Thus, if there is a Skyrmion centered at (0,0,0) there will be a second one at $(L,0,0)$ and it will be rotated by π around the 2 axis. The two Skyrmions will be in a maximum attraction configuration. For symmetry reasons there will be Skyrmions at all corners of the cubic lattice and all nearest neighbors will be attractive in the low-density limit.

Using the definitions of the energy and the baryon density, Eqs. (5) and (6), and the symmetry (A3) we can see that these densities are invariant under a translation by L. The same definitions when combined with the symmetry (A1) show that the baryon and energy densities are invariant under inversions. The densities will thus have a unit cell of size L, but the unit cell of the fields will be $2L$. Each cube of size L has Skyrmions at all its corners, each contributing $\frac{1}{8}$ to the baryon number of the cube. The cell of size L thus has one unit of baryon number and the cell of size $2L$ eight units.

The symmetry of the high density, Goldhaber-Manton[9] structure (B) has three generators (B1), (B2), and (B3) which are identical to (A1), (A2), and (A3), respectively. It has an extra symmetry:

$$\text{(B4) } x_i=(L/2-z,L/2-y,L/2-x)$$
$$\text{and } n^\alpha=(-\sigma,\pi_2,\pi_1,\pi_3) .$$

This transformation involves a rotation by π around an axis going through the points $(0,L/4,L/2)$ and $(L/2,L/4,0)$ and an O(4) transformation.

In this symmetry, half-Skyrmions with σ near -1 are centered at the points where Skyrmions were located in the low-density phase. Half-Skyrmions with σ near $+1$ are located at the centers of cubes, e.g., at the point $(L/2,L/2,L/2)$. This structure is a body-centered-cubic lattice of half-Skyrmions. Both the density and field unit cells of this structure are identical to those of low-density limit (A).

The new structure (C) at low densities has two generators (C1) and (C2) that are identical to (A1) and (A2). It also has the additional generators

$$\text{(C3) } x_i=(x,z,-y) \text{ and } n^\alpha=(\sigma,\pi_1,\pi_3,-\pi_2) ,$$

$$\text{(C4) } x_i=(x+L,y+L,z) \text{ and } n^\alpha=(\sigma,-\pi_1,-\pi_2,\pi_3) .$$

The symmetry (C3) is associated with a rotation around a fourfold axis in space, combined with an isospin rotation. The symmetry (C4) is associated with a translation from the corner of a cube to the center of a face combined with an O(3), isospin rotation acting on π_i. This is a rotation by an angle of π around an axis perpendicular to the face of the cube.

The unit cell of the baryon and energy densities for this symmetry are identical to those of n^α, all have the size $2L$. If the center of a Skyrmion is located at (0,0,0) then symmetry (C4) will make sure that the face centers such as $(L,L,0)$ also contain the center of a Skyrmion and the isospin rotation of (C4) will cause them to be in the maximal attraction configuration. It can be seen that the Skyrmions at $(0,L,L)$ and $(L,L,0)$ which are also nearest neighbors are in the maximum attraction configuration. Thus the symmetry (C) has the advantage that each Skyrmion is surrounded by 12 nearest neighbors all in the maximum attraction configuration, rather than six such neighbors in symmetry (A). The unit cell of size $2L$ has Skyrmions in all corners each contributing $\frac{1}{8}$ unit of baryon number, and Skyrmions at the centers of the faces that contribute $\frac{1}{2}$ unit each. The total baryon number in each unit cell is therefore four units.

Symmetry (D), which has the lowest energy, is a half-Skyrmion version of the fcc lattice (C). Three of its generators (D1), (D2), and (D3) are identical to (C1), (C2), and (C3), respectively. The additional symmetry appearing here is given by

$$\text{(D4) } x_i=(x+L,y,z) \text{ and } n^\alpha=(-\sigma,-\pi_1,\pi_2,\pi_3) .$$

The symmetry (D4) is a translation combined with an O(4) rotation by π in the σ,π_1 plane. The symmetry (C4), which remains one of the crystal symmetries of this structure, can be obtained by combining two transformations of the type (D4).

In this symmetry we note that at the origin, $x_i=0$, where $\pi_i=0$ we may take without loss of generality $\sigma=-1$ and the field in this vicinity will resemble that in the center of a Skyrmion. The symmetries (D1), (D2), and (D4) imply that $\sigma=0$ on any surface $x_i=\pm L/2$. A cube containing the origin and bounded by these surfaces contains half a Skyrmion with $\sigma<0$. Because of relation (D4), $\sigma=1$ at $(L,0,0)$. Near this point we put the second type of half-Skyrmions, with $\sigma>0$. Thus the crystal may be viewed as an "antiferromagnetic" arrangement of half-Skyrmions, each filling a cube of size L. The symmetry operations above ensure that the two types of half-Skyrmions are appropriately rotated in isospin so that the fields are smooth and the energy is minimal.

In this symmetry the densities have a unit cell of size L but the fields have a unit cell twice this size: namely, $2L$. To see the baryon content of each unit cell we take the unit cell with boundaries $x_i=\pm L/2$. As discussed above such a cell contains half a unit of baryon number. The unit cell of the fields has size $2L$ and contains four units of baryon number exactly as in the structure (C).

The four symmetries which we discussed share the property that the low-density symmetry is a subgroup of the high-density symmetry: (A) is a subgroup of (B) and (C) is a subgroup of (D). Phase transitions between (A) and (B) and between (C) and (D) are allowed according to Landau and Lifshitz[19] to be of second order. Whether such phase transitions actually occur depends on the energetics of the problem. This will be discussed in Sec. IV.

The next stage is to expand the unnormalized vector $\bar{n}^\alpha$ in a Fourier series. Because the symmetries discussed above have two common transformations (A1) and (A2), all symmetries will have an expansion of the type

$$\bar{\pi}^1=\sum_{h,k,l}\alpha_{hkl}\sin(h\pi x/L)\cos(k\pi y/L)\cos(l\pi z/L) \quad (9)$$

and

$$\bar{\sigma}=\sum_{a,b,c}\beta_{abc}\cos(a\pi x/L)\cos(b\pi y/L)\cos(c\pi z/L) . \quad (10)$$

π^2 and π^3 are obtained from π^1 by using the symmetry operation (A2). The further constraints imposed on the expansion coefficients α and β may be read off by imposing the symmetry relations on Eqs. (9) and (10).

The symmetries impose the following constraints on the expansion coefficients. For symmetry (A): (Ai) h and k are odd, m is even; (Aii) a, b, and c are even; (Aiii) $\beta_{abc}=\beta_{bca}=\beta_{cab}$.

For symmetry (B) which has symmetry (A) as a subgroup, there are three relations (Bi), (Bii), and (Biii) which are identical to (Ai), (Aii), and (Aiii). In addition two more relations hold: (Biv) $\alpha_{hkl}=-(-1)^{(h+k+l)/2}\alpha_{khl}$; (Bv) $\beta_{abc}=-(-1)^{(a+b+c)/2}\beta_{bac}$.

Symmetry (C) has two types of solutions: (Ci) h is odd; k and l are even; a, b, and c are odd. Or (Cii) h is even; k and l are odd; a, b, and c are even.

Symmetry (D) which has (C) as a subgroup, has a single constraint (Di) which is identical to (Ci).

The symmetries discussed in this section, and the Fourier expansions based on them, will serve in the next section as a basis for calculating the energies and the phase diagram of the Skyrmion crystal.

IV. CALCULATION AND RESULTS

Our calculation of the energy of a Skyrmion crystal proceeds in two stages. First we assume that the ground state is a periodic crystal where it is only necessary to calculate the energy of a single unit cell. After this calculation is done it turns out that the energy is not a convex function of the density; this fact signals the onset of a thermodynamic instability. In such a region a phase separation occurs, where different parts of the system obey different symmetries. In the second stage we proceed to obtain the phase diagram of the system by a standard Maxwell construction. Previous calculations have disregarded the phase separation signaled by a nonconvex energy and have not used a Maxwell construction. Since they calculated the energy of a single unit cell where surface effects are dominant they did not observe the phase separation numerically.

In the first stage we calculate the energy of a single unit cell for each symmetry. This is done by performing a variational calculation using the parameters α_{hkl} and β_{abc} as variables. This procedure replaces the usual calculation where space is discretized and the values of n^α on the grid are calculated. The advantages of our method are (1) symmetries are easily incorporated into the calculation, (2) the integrals involved in the calculation of the energy can be computed with high accuracy, while correctness of the baryon number is automatic, (3) rather than solving a differential equation we employ a simple program searching for a minimum, (4) it turns out that the series in question are rapidly convergent and only a small number of parameters is needed, and (5) it is easy to perform a variation without changing the baryon number.

As a starting point for our search procedure we use the lowest nonvanishing terms in the Fourier expansion. Because of the derivatives appearing in the definition of the energy each component will contribute terms proportional to the squares or higher powers of the momenta. Thus high Fourier components will be suppressed.

The baryon density of the solution as given in Eq. (6) is proportional to the Jacobian of the transformation between the hypersphere $S3$ described by n^α and the $R3$ space of the coordinates x_i. The total baryon number of the solution is equal to the number of times the solution covers the hypersphere of unit radius. Because of Eq. (8) the number of times n^α covers the unit sphere is equal to the number of times $\bar{n}^\alpha(x)$ wraps around the origin: namely, the point $\bar{n}^\alpha(x)=0$. When the functional dependance of $\bar{n}^\alpha$ on x is simple enough the winding number is easy to determine by direct inspection or by plotting $\bar{n}^\alpha$. This can be done at the beginning of our variational calculation when we take as a starting point the lowest Fourier components allowed by the symmetry under consideration. As we proceed by varying the functional of the solution we do not want the baryon number to change. A smooth variation of n^α cannot change the baryon number. The auxiliary variables $\bar{n}^\alpha$ are not normalized so that a smooth change in them can result in a discontinuous change in the baryon number. This can happen when under the variation the surface of the solution goes through a point where $\bar{n}^\alpha(x)=0$, and the origin moves from the inside of the surface to the outside or vice versa. There is no danger of this happening when we minimize the energy, since near such a point Eq. (8) will force n^α to be rapidly varying and the energy of such a configuration will be very large. Nevertheless, we calculate the baryon number of our solution as a check of the calculation and find it to be consistent with the symmetry result to five significant figures. This serves as a check on our calculation and on the accuracy of our integration routines.

The auxiliary variables $\bar{n}^\alpha$ that we have introduced are not uniquely determined. The variables n^α are invariant under any transformation of the type

$$\bar{n}^\alpha \rightarrow \Phi \bar{n}^\alpha , \tag{11}$$

where Φ is an arbitrary nonvanishing function of the coordinates. This lack of uniqueness does not cause difficulties. Since we deal with a truncated Fourier series for $\bar{n}^\alpha$, the continuous set of degenerate minima turns, in this case, into a shallow minimum. No difficulties were encountered in finding this minimum numerically. In discussing the numerical analysis involved in finding the solution to symmetry (D) we will show how the freedom of choosing Φ can actually be used to facilitate the analysis. Other symmetries were analyzed using a constant Φ.

Our analysis[12] of symmetries (A) and (B) was motivated by an attempt to verify numerically the Goldhaber-Manton[10] conjecture. Earlier numerical calculations[5,7,8] did not produce a ground state having the symmetry (B) that is implied by this conjecture. The calculation of the minimal energy of symmetry (B) started with the lowest Fourier components $\alpha_{110}=1$ and β_{200}. Only four extra terms in the Fourier expansion were needed to obtain an energy of 1.08. The terms needed were α_{130}, β_{222}, α_{114}, and α_{330}. The first two of the new terms are about 4% as compared with the leading terms, while the last two are

about 0.2%. All higher terms are insignificant. The small size of the higher coefficients proves the rapid convergence of the Fourier expansion we are using. Adding to our search procedure coefficients allowed by symmetry (A) but forbidden by symmetry (B) did not improve the energy of the solution. This shows that symmetry (B) does indeed describe the symmetry of the local minimum of the energy.

Our results concerning the (B) phase agree with those of Ref. 11. The energy obtained this way is lower than the energy of phase (A) but the energy difference is very small. The minimum energy is obtained for a lattice size $L=5.55$ and the energy at the minimum is $E=1.078$. We have not pursued the study of the complete density dependance of the energy; this has been discussed in Refs. 11 and 14.

To analyze the Skyrmion configurations that belong to symmetry (D) we again start with the lowest nonvanishing Fourier components, α_{100} and β_{111}. Without loss of generality we may take $\alpha_{100}=1$, then by varying β_{111} we obtain $E=1.07$. The convergence of the series is so rapid that even the lowest term in the expansion suffices to give a lower energy than the minimum of configuration (B). Two variational procedures are open for this case. The first is straightforward: namely, expanding both $\bar{\sigma}$ and $\bar{\pi}$ in Fourier components and minimizing. A second way is to make use of a convenient rescaling function Φ from Eq. (11). We pick this function so that $\bar{\sigma}$ is exactly given by the lowest Fourier component:

$$\bar{\sigma}=\cos(\pi x/L)\cos(\pi y/L)\cos(\pi z/L)\ ; \tag{12}$$

thus only the parameters α_{hkl} remain as variational parameters. Such a choice of Φ is not generally possible. Since Φ is nonvanishing we must know the zeros of $\bar{\sigma}$ in order to pick a parametrization such as Eq. (12). For symmetry (D) these zeros are determined by symmetry considerations, and thus automatically included in Eq. (12). We have compared calculations with and without using Eq. (12); the energies obtained in both ways are equal within numerical accuracy. The advantage of using Eq. (12) is that the variational function contained less parameters thus simplifying the numerical analysis.

The energy at minimum obtained this way is

$$E=1.038\ . \tag{13}$$

This is the lowest-energy configuration obtained so far. While we do not have a proof that this is indeed the global minimum of the energy, the fact that this configuration is so close to the lower bound makes this very likely. The lattice size for the minimal energy configuration is $L=4.71$. The baryon density of this configuration is given in Fig. 1. The baryon density is high at the corners of the cube of size L where the centers of the half-Skyrmions are located; the density is also large on the links connecting these points. On the lines parallel to the links and going through the centers of the faces the baryon density vanishes because of symmetry reasons. This can be seen by combining the expressions of the fields n^{α} for this symmetry with the expression for the baryon density. The energy density for this configuration

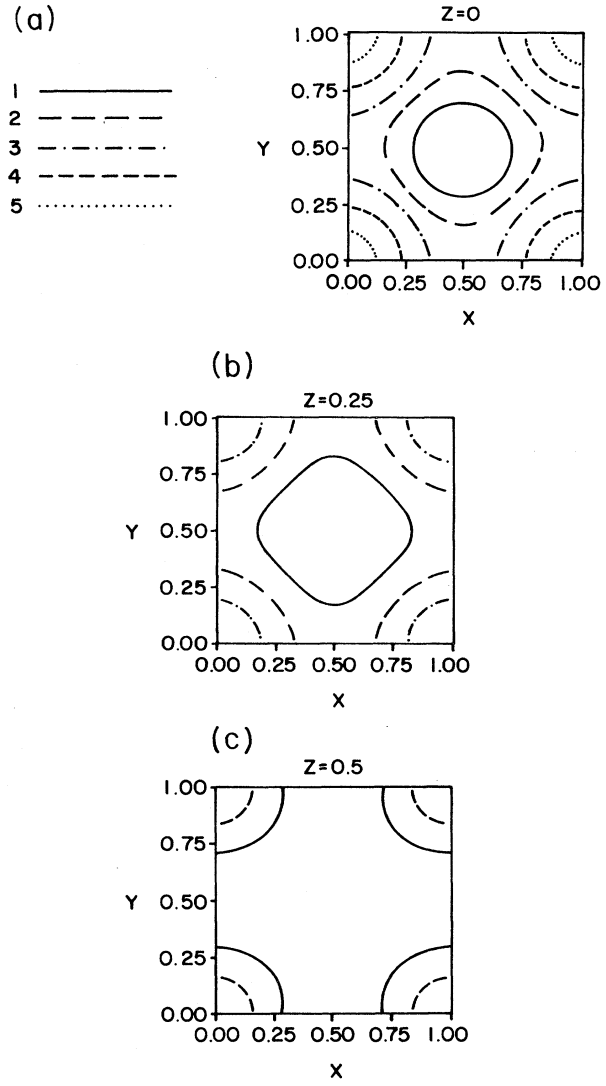

FIG. 1. The baryon density of the minimum-energy configuration. Cuts of the baryon density in x-y plane at (a) $z=0$, (b) $z=L/4$, and (c) $z=L/2$. The density at $z=3L/4$ is identical to that of (b) because of symmetry. Contours are in units of 0.01, baryons per unit L^3, axes are in units of L.

is almost identical to the baryon density. This should not come as a surprise since the energy density bounded below by the baryon density and its integral is only larger by 3.8% than the baryon number.

The average baryon density of symmetry (D) is lower by about 18% than that of symmetry (B). The distances between the centers of nearest half-Skyrmions in the simple cubic lattice of (D) are almost identical to the distance in the bcc lattice of half-Skyrmions in symmetry (B), in fact they differ only by 2%. We thus learn that the half-Skyrmions behave essentially like almost rigid objects. The difference in densities between the two configurations is mainly due to the higher density of the fcc as compared with the simple cubic, a geometric effect.

The energy per baryon of a single unit cell of the Skyrmion crystal was calculated as a function of the lattice

parameter L. For symmetry (D) it is well approximated by the expression

$$E=0.1056L+0.0412+2.3505/L \ . \tag{14}$$

The energy of a single unit of the Skyrmion crystal having symmetry (B) was given by Jackson and Verbaarschot:[11]

$$E=0.0952L+0.0188+2.939/L \ . \tag{15}$$

Using the energies per unit cell we can now study the phase diagram of Skyrmion matter.

In comparing the two configurations one must note that symmetry (B) contains eight units of baryon number per unit cell while symmetry (D) contains only four. In order to compare the two configurations at equal baryon density one should take

$$L_{(B)}={}^3\sqrt{2}L_{(D)} \ . \tag{16}$$

Figure 2 shows a comparison between the energies of the two phase, as a function of the lattice parameter L, but with phase (B) normalized according to Eq. (16) so that the comparison of the energies is at equal baryon densities. Figure 3 shows the same energies plotted as a function of the volume $V=L^3$, where again Eq. (16) has been used so that equal volumes correspond to equal densities. There are three conclusions to be drawn from this diagram.

(i) The ground state of Skyrmion matter obeys symmetry (D).

(ii) For V or L to the right of the minimum, namely, at lower densities, a phase separation occurs. As we increase the volume and decrease the density, it is advantageous for the system to separate into a phase we have denoted by S, where part of the system remains at the density that corresponds to the minimum of the energy and the rest is empty. In Figs. 2 and 3 the stable branches of the phase diagram are drawn as solid lines and the unstable lines are dashed.

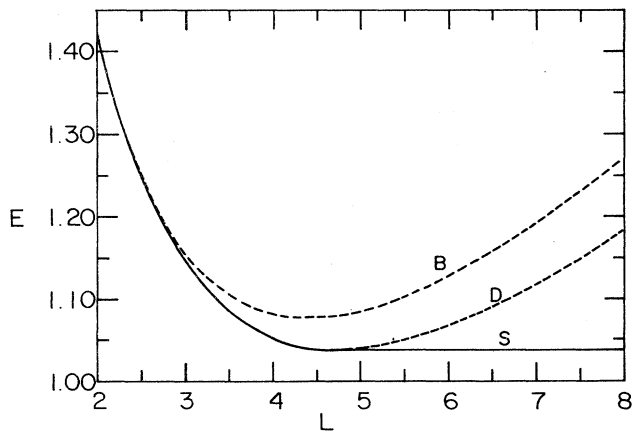

FIG. 2. The energies of phases (B) and (D) and (S) as a function of lattice size. The lattice size has been normalized so that the configurations appear at equal density. The solid lines correspond to stable phases, the dashed lines to unstable phases.

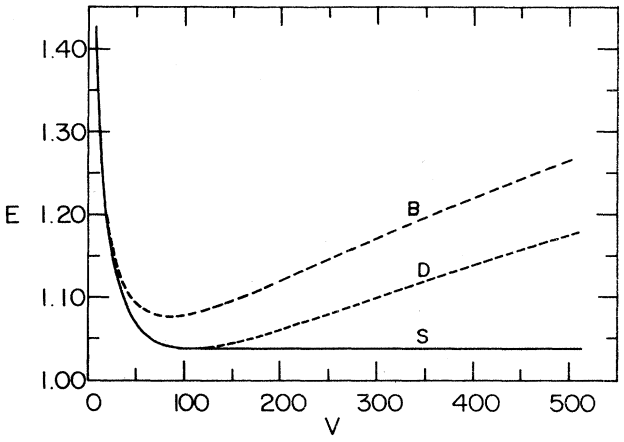

FIG. 3. The energies of phases (B) and (D) and (S) as a function of volume of the unit cell, normalized so that the configurations appear at equal density. The solid lines correspond to stable phases, the dashed lines to unstable phases.

(iii) At very high densities, phases (B) and (D) intersect causing a first-order phase transition. This transition cannot be seen from Figs. 2 and 3; a better resolution figure to show this will be presented.

The two phase transitions appearing will be elaborated next.

Since we are dealing with Skyrmion matter at zero temperature, we can translate the volume dependance of the energy into pressure dependance by using

$$P=-\frac{\partial E}{\partial V} \ . \tag{17}$$

In dealing with the low-density phase transition we observe that the S phase in Figs. 2 and 3 is a result of a thermodynamic instability. At infinite L or V the energy is that of separated Skyrmions, $E=1.23$ in our units. The line S is therefore the straight-line tangent to line D that joins the minimum to the point at infinity. We have thus used the standard Maxwell construction we are supposed to use when the diagram is not convex. Figure 4 shows the phase diagram where we have plotted P vs V. In this diagram we have included only the phases (D) and (S); again the unstable branch is a dashed line. Along the line D beyond the phase transition from D to S the pressure becomes negative; this is also obvious from Fig. 3 since the energy increases as the volume increases. There is no simple way in which we can exert such negative pressure. The Coulomb interaction in nuclear matter could be the source of negative pressure; unfortunately just because of this interaction nuclear matter in bulk prefers to undergo β decay giving rise to neutron stars. The point M on Fig. 4 denotes the minimum of the pressure. The point T denotes the phase transition between a crystal of Skyrmions and a crystal of half-Skyrmions that was previously investigated. We conclude that at the transition point dP/dV is positive and this corresponds to negative compressibility clearly indicating that the phase transition is not on a metastable branch but on an unstable branch of the diagram. Skyrmion matter there-

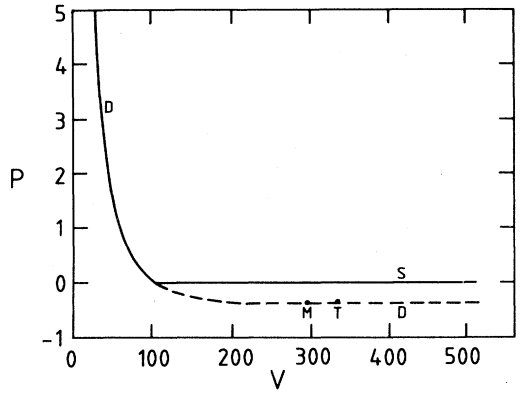

FIG. 4. P vs V diagram of phases (D) and (S). Note that the pressure along curve D gets negative. M denotes the minimal pressure, T denotes the point where a transition to phase (C) would have taken place if phase separation did not occur. Also note that at point T the compressibility is negative.

fore does not undergo a second-order phase transition[14] at T but a first-order transition at much lower volume.

A second phase transition occurs at much lower volume, namely, at higher pressure and density. This is a transition between symmetry (B) and (D). The energy differences between two phases is too small to be seen in Fig. 3. Figure 5 shows an enlarged region of Fig. 3 where we can clearly see that the lines B and D intersect. This is again a first-order transition, and the energy is not a convex function of volume. A common tangent to the two curves is drawn through the points a and b, according to the standard Maxwell construction, and on this line the system is in a mixture of two separated phases D

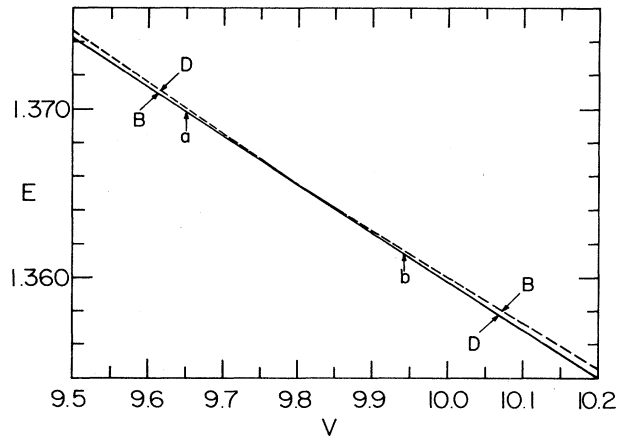

FIG. 5. Enlarged drawing showing the phase transition at high density. Above the transition D has the lowest energy, below the transition phase (B) is lower in energy. The Maxwell construction is achieved by drawing a common tangent to the two curves, a straight line joining points a and b.

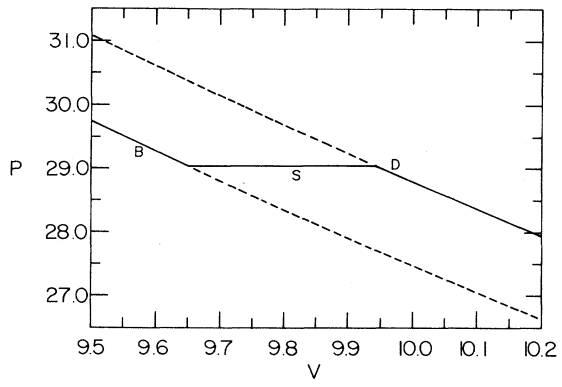

FIG. 6. P vs V diagram in the region of the high-pressure transition.

and B. Along this line the pressure is constant as is seen in the P vs V plot in Fig. 6. It should be emphasized that this phase transition appears at very high density and pressure and that the energy differences between phase (B) and (D) are very small. The existence of this phase transition may be strongly influenced by extra terms in the Lagrangian, a point which we have not investigated.

V. CONCLUSIONS

In this paper we have investigated nuclear matter in the Skyrme model at the classical limit, neglecting quantum corrections. We have investigated the lowest-energy phase, a simple cubic lattice of half-Skyrmions. This phase obeys a symmetry which we have denoted by D, which is a Skyrmionic generalization of the crystallographic space group $P_{m\bar{3}m}$.

This phase remains the lowest-energy phase over a large range of densities. At the minimum of the energy a first-order phase transition occurs and the transition to a crystal of Skyrmions rather than a crystal of half-Skyrmions[14,20] is unphysical. At high density there is a first-order transition to the phase which we have denoted by B, a bcc arrangement of half-Skyrmions, a Skyrmionic generalization of the crystallographic space group $P_{n\bar{3}m}$.

The half-Skyrmion picture of Goldhaber and Manton[10] turns out to be a very reliable description of Skyrmion matter at high density. It describes well all high-density phases, even those that were not known when the suggestion was made. In addition it provides a way to understand the difference in density between the various phases. The half-Skyrmions turn out to be rather rigid objects which retain their size in different phases.

In this paper our treatment was restricted to the classical limit of Skyrmion matter. When quantum corrections are included, they will certainly play a major role and modify the results. The kinetic energy inherent in the quantum-mechanical analysis will modify the crystal into a liquid. We have not attempted an analysis of the quantum effects in order to see what properties of the Skyr-

mion solid remain in the quantum state. Drawing on the experience with standard liquid-solid transitions we may assume that even in a liquid short-range order reminiscent of the solid phase is retained.

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