Theory of elastic interaction between axially symmetric 3D skyrmions in confined chiral nematic liquid crystals and in skyrmion bags

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ABSTRACT

We study axially symmetrical 3D skyrmionic particles (torons, Hopfions) in a thin homeotropic cell filled with a cholesteric liquid crystal. We show that a small 3D skyrmion asymptotically can be presented as a particle with six multipole moments. In this case, the odd moments – dipole, octupole and the fifth-order moments – are helicoidal moments, generated by chirality. And even moments – quadrupole, hexadecapole and sixth order moments – have the usual form, as colloidal particles in nematics. Thus, we find the exact analytical solution for the far field director configuration around the 3D skyrmion and the exact analytical expression for the elastic interaction potential between 3D skyrmions in a homeotropic cell with thickness $L$. We show that it has an exponential decay length equal $\lambda_{SS} = L/n$. The comparison with the experiment allows us to recover approximately one set of multipole coefficients for the small 3D skyrmion. We also describe the expansion of the skyrmion bag analytically depending on the number $N$ of anti-skyrmions in it and obtain an agreement with the experiment. Along the way, we determined the director field and the elastic interaction potential between chiral axially symmetric colloidal particles in the unlimited nematic and in the homeotropic cell, taking into account higher order elastic terms.

1. Introduction

Skyrmions are topological solitons, built from configurations of various fields with chirality.

Originally, Skyrme built an effective Lagrangian entirely in meson fields (pions), and baryons – as fermions – could emerge from that Lagrangian as solitons...
Skyrmions were predicted and observed in quantum
Hall systems [5–7]. Later, Bose–Einstein condensates
with spin degrees of freedom were shown to accommodate
Skyrmions [8–11]. As well, great attention has been
paid to Skyrmions in noncentrosymmetric ferromagnets
[12–18] with the presence of Dzyaloshinskii–
Moriya spin-orbit interaction, such as MnSi [7,13,14] and
Fe1−xCoxSi [15,16]. Chiral magnetic skyrmions are
now considered as promising objects for applications in
magnetic data storage technologies and in the emerging
spin transport electronics (spintronics), because local
twisted magnetic structures coupled to electric or spin
currents could be used to manipulate electrons and their
spins [17,18]. Theoretical aspects of skyrmions in chiral
magnets were investigated in [19–30].

Recently, LC skyrmions have been realised as micron-sized
solitons in a chiral nematic material confined between two parallel substrates and they attracted
great research interest [31–58].

It is not a secret that 3D skyrmions in liquid crystals
are similar to ordinary particles. On the other hand, the behaviour of colloidal particles in liquid crystals is a very
interesting topic [59–64]. Novel anisotropic elastic interactions between colloidal particles lead to the formation
of various structures and even colloidal 2D and 3D quasicrystals [65–77]. The theoretical aspects of the
behaviour of colloidal particles in nematic liquid crystals
are studied in [78–91], and the theoretical description
of 2D and 3D colloidal quasicrystals is given in [92–94].

In this paper, we will try to bridge the gap between
3D skyrmions and colloidal particles in liquid crystals.
We will look at the skyrmion as a colloidal particle and
consider the interaction between skyrmions as an elastic
interaction between colloidal particles. This can be done
exactly outside the core of the skyrmion, beyond the
region with strong director deformations. Then the
director distribution can be accurately determined analytically and the elastic interaction potential between 3D
skyrmion particles can be calculated exactly. We

consider skyrmions with axial symmetry in a
homeotropic cell of thickness $L$ with strong boundary
conditions, when the director looks vertically at the
surfaces of the bounding planes. It turns out that the
chirality of the liquid crystal manifests itself in the birth
of chiral multipole coefficients $a_i^j$, which are absent
in ordinary colloidal particles in the nematic. Usually, colloidal particles in nematics have only zero-helicity mul-
tipole coefficients $a_i^1$. And then it turns out that the 3D
skyrmion in the region of weak deformations can be
described as a set of multipoles: zero $a_i^0$ and chiral $a_i^j$.

We consider in more detail the case of 3D skyrmion
particles that are symmetric in shape with respect to the
median horizontal plane $z = L/2$ and consider only the
helicity $q = \pi/2$. We also restrict ourselves to multipole
moments up to the sixth order inclusively. Then we
obtain the interaction potential between 3D skyrmions
and find the multipole coefficients from agreement with
experiment.

Along the way, we determine the director field in the
unlimited nematic around a chiral axially symmetric
colloidal particle, taking into account higher order elastic
terms, and also find the elastic interaction potential
between such particles with multipole moments of
orders $l = 1 \div 6$.

Next, we apply our results to 3D skyrmions in the
skyrmion bag. As the number $N$ of skyrmions in the bag
increases, the distance between them gets larger. We
find an approximate analytical formula for the distance
between skyrmions as a function of the number $N$ of
skyrmions in the bag and cell thickness $L$, which also
agrees with the experiment.

2. 3D skyrmions as a colloidal particle: a new
perspective

In this work, we will not take into account the influence
of an electric or magnetic field. Elastic Frank free energy
of the nematic liquid crystal is presented in the form:

$$F_{\text{bulk}} = \int dV \left[ \frac{K_1}{2} (\text{div} \mathbf{n})^2 + \frac{K_2}{2} (\mathbf{n} \times \mathbf{q}_0 + \mathbf{q}_0)^2 + \frac{K_3}{2} (\mathbf{n} \times \text{rot} \mathbf{n})^2 \right],$$

with $K_1, K_2, K_3$ being elastic constants for splay, twist
and bend deformations respectively. In this paper we
will use the one-constant approximation $K = K_1 = K_2 = K_3$, so that the free of the system is
equal to:

$$F_{\text{bulk}} = \frac{K}{2} \int dV \left[ (\text{div} \mathbf{n})^2 + (\mathbf{n} \times \mathbf{q}_0)^2 + (\mathbf{n} \times \text{rot} \mathbf{n})^2 \right],$$
where $K$ is the elastic constant and $q_0 = 2\pi/p$ is the wavenumber of the cholesteric helix in the ground state, and $p$ is the pitch of the helix at which the director completes a revolution of $2\pi$. The chiral term $Kq_0 n \cdot \nabla n$ arises due to the presence of chiral molecules in which there is no inversion centre. We consider the geometry when a cholesteric liquid crystal or a nemato-cholesteric mixture is placed into a homeotropic cell with a thickness $L$ of the order of the helix pitch $L/p \approx 1$. We will assume that rigid boundary conditions $n \cdot z$ are fixed on the cell boundaries.

In such systems, there can arise axially symmetric 3D solitons (torons, hopfions), which for generalisation we will call 3D skyrmions (or simply skyrmions) in a liquid crystal, although usually in the condensed matter physics the word 'skyrmion' refers to a 2D soliton shown in Figure 1. Due to the homeotropic boundary conditions, the director far from the skyrmion tends to the equilibrium distribution of $n_0 \cdot z$ in the entire space. Regardless of the shape, size and other parameters of the 3D skyrmion, the director field deformations decay with distance from the skyrmion and eventually become small, $n(r)$ approximately $(n_x, n_y, 1)$, where $|n_\mu| \ll 1$, $n_0 = (0, 0, 1)$ is the ground state, $\mu = \{x, y\}$ hereinafter. We will consider just this zone, where the deformation is already small. Assuming $|n_\mu| \approx \epsilon$ one can easily obtain that up to $\epsilon^2$ chiral term $n \cdot \nabla n = \partial_x(n_x n_y) - 2 n_x \partial_x n_y + \partial_y n_y - \partial_y n_x$. In this paper, we consider exclusively axially symmetric skyrmions. Obviously, for axially symmetric skyrmions, the space volume integral of this distribution equals zero $\int n \cdot \nabla n \cdot dV = 0$, i.e. far from such a skyrmion, a cholesteric liquid crystal in a homeotropic cell can be considered as a nematic. That is a very important point!

Thus, far from the skyrmion the bulk free energy takes a simple harmonic form

$$F_{\text{bulk}} = \frac{K}{2} \int dV \nabla n_\mu \cdot \nabla n_\mu,$$

where repeated $\mu$ implies summation over $x$ and $y$, i.e. $(\nabla n_\mu)^2 = (\nabla n_x)^2 + (\nabla n_y)^2$. The Euler-Lagrange equations for $n_\mu$ are of the Laplace type

$$\Delta n_\mu = 0. \quad (4)$$

### 2.1. Colloidal particles with chirality in the unlimited nematic liquid crystal

Now, for clarity, we will temporarily digress from the LC cell under consideration and see what axially symmetric solutions can arise in an unlimited space. That is, suppose that there is some small axially symmetric particle in the unlimited nematic liquid crystal.

In the paper [90] it was shown that the solution of the Laplace equation for axially symmetric particles has the form:

$$n_\mu = \sum_{l=1}^{N} a_l (-1)^l \partial_\mu \partial_z^{l-1} \frac{1}{r} \quad (5)$$

where $a_l$ is the multipole moment of the order $l$ and $2^l$ is the multipolarity; $N$ - is the maximum possible order without anharmonic corrections. In this case $n_x \propto \cos(\varphi)$ and $n_y \propto \sin(\varphi)$ with $\varphi$ being the polar angle. But this result is valid only in the absence of twisting around the particle. For example particles with a hyperbolic hedgehog, a Saturn-ring configuration, boojums or hexadecapole particles in [91] capture the formula (5). Index $l$ is the standard index in spherical harmonics $Y_{lm}(\theta, \varphi)$ and expansion (5) is equivalent to

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Figure 1. (Colour online) Schematic representation of a 2D skyrmion. The director makes a full turn by $\pi$ when moving from the center to the periphery. Here a) top view and b) side view.
the expansion on functions $Y_{lm}(\theta, \phi)/r^{l+1}$ with $l \geq 1$ and $m = 1$ or $m = -1$ [95].

In order to find the energy of the system: particle(s) + LC, it is necessary to introduce some effective free energy functional $F_{\text{eff}}$ [90], so that its Euler-Lagrange equations would have the above solutions (5). In the one constant approximation with Frank constant $K$ the effective functional has the form:

$$F_{\text{eff}} = K \int d^3 x \left\{ \frac{(V n_\mu)^2}{2} - 4\pi \sum_{l=1}^{N} A_l(x) \partial_\mu \partial_z^{-l-1} n_\mu \right\}$$

(6)

which brings Euler-Lagrange equations:

$$\Delta n_\mu = 4\pi \sum_{l=1}^{N} (-1)^{l} \partial_\mu \partial_z^{-l-1} A_l(x)$$

(7)

where $A_l(x)$ are multipole moment densities in the point $x = (x, y, z)$, $\mu = x, y$ and repeated $\mu$ means summation on $x$ and $y$ like $\partial_\mu n_\mu = \partial_x n_x + \partial_y n_y$. For the infinite space the solution has the known form:

$$n_\mu(x) = \int d^3 x' \frac{1}{|x-x'|} \sum_{l=1}^{N} (-1)^l \partial_\mu \partial_z^{-l-1} A_l(x')$$

(8)

If we consider $A_l(x) = a_l \delta(x)$ this really brings solution (5). This means that effective functional (6) correctly describes the interaction between the particle and LC.

Consider $N_p$ particles in the NLC, so that $A_l(x) = \sum_i a_l^i \delta(x-x_i)$, $i = 1 \div N_p$. Then substitution (8) into $F_{\text{eff}}$ (6) brings: $F_{\text{eff}} = U_{\text{self}} + U_{\text{interaction}}$ where

$$U_{\text{self}} = \sum_i U^{\text{self}}_i$$

and $U^{\text{self}}_i$ is the divergent self energy.

Interaction energy $U_{\text{interaction}} = \sum_{i<j} U^{\text{int}}_{ij}$. Here $U^{\text{int}}_{ij}$ is the elastic interaction energy between $i$ and $j$ particles in the unlimited NLC:

$$U^{\text{int}}_{ij} = 4\pi K \sum_{l=0}^{N} a_l^i a_l^j (-1)^l \frac{1}{r^{l+1}} P_{l+1}(\cos \theta)$$

(9)

Here unprimed quantities $a_l^i$ are used for particle $i$ and primed $a_l^j$ for particle $j$, $r = |x_i-x_j|$, $\theta$ is the angle between $r$ and $z$ and we used the relation $P_l(\cos \theta) = (-1)^l \frac{1}{\sqrt{2\pi}} \partial_\theta^l \frac{1}{z}$ for Legendre polynomials $P_l$. This is the general expression for the elastic interaction potential between axially symmetric colloidal particles in the unlimited NLC when taking into account the high order elastic terms [90].

But what will happen if there is still helical twisting or circular cutting around the particle? In such a more general case, the axisymmetric solution has the property $n_\mu^x \propto \cos(\varphi + y)$ and $n_\mu^y \propto \sin(\varphi + y)$ with $\varphi$ being the polar angle and $y$ being the helicity number. This means that the director field $n^y$ can be presented in the form $n^y = (n_x^y, n_y^y, 1) = (\varphi, \cos \psi y, \sin \psi y, 1)$ with $\psi = \varphi + y$. So helicity $y$ is the angle between the horizontal projection of the director $n^y$ and polar angle $\varphi$. Then such a more general axially symmetric solution with helicity $y$ can be represented as a linear combination of solutions (5) in the form:

$$n_x^y = \sum_{l=1}^{N} a_l^y (-1)^l (\cos \psi \partial_z^{-l-1} - \sin \psi \partial_z^{-l-1}) \frac{1}{r}$$

(10)

$$\cos(\varphi + y)$$

$$n_y^y = \sum_{l=1}^{N} a_l^y (-1)^l (\sin \psi \partial_z^{-l-1} + \cos \psi \partial_z^{-l-1}) \frac{1}{r}$$

(11)

$$\sin(\varphi + y)$$

and the most general axially symmetric solution is the sum over all possible helicities $y$:

$$n_x^y = \sum_{y} n_x^y$$

$$= \sum_{y} (-1)^l (\sum_y a_l^y \cos \psi \partial_z^{-l-1} - \sum_y a_l^y \sin \psi \partial_z^{-l-1}) \frac{1}{r}$$

(12)

$$n_y^y$$

$$= \sum_{y} n_y^y$$

$$= \sum_{y} (-1)^l (\sum_y a_l^y \sin \psi \partial_z^{-l-1} + \sum_y a_l^y \cos \psi \partial_z^{-l-1}) \frac{1}{r}$$

(13)

Actually this means that the total director field can be presented in the form $n = \sum_y n^y = (\theta(x) \cdot \cos \psi(x), \theta(x) \cdot \sin \psi(x), 1) = (\sum_y \theta, \cos \psi_y, \sum_y \theta \sin \psi_y, 1)$. Inasmuch as $\psi_y = \varphi + y$ and $\theta_y = \theta_y(\rho, z)$ depends on the $(\rho, z)$ of the point $x$ in cylindrical coordinates $(\rho, \varphi, z)$, we can tell that the total angle $\psi(x)$ depends on the point $x = (\rho, \varphi, z)$. When we make summation over all possible helicities $y$ we mean that it can be either series on discrete $y$ or even integration on continuous $y$. In pure 2D skyrmion (see Figure 1) the most stable configuration is $\psi = \varphi + \pi/2$ [22]. In 3D case the authors of [33,34] made assumptions $\theta = \theta(\rho, z)$ and $\psi = \varphi$ and came to the same result $\psi = \varphi + \pi/2$. We go beyond that approximation below and use a combination of solutions with $\psi_0^x = \varphi$ and $\psi_{n/2}^x = \varphi + \pi/2$ and make the total angle $\psi(x)$ non-uniform. We think that another values of helicity $y \neq 0, \pi/2$ are possible as well for some 3D solitons [58], but we do not take them into account.
If we introduce such a pair of orthogonal vectors
\[ \vec{A}_l^\pm = \left( \sum_i a_i^l \cos \gamma, -\sum_i a_i^l \sin \gamma \right) \]
and
\[ \vec{A}_l^\mp = \left( \sum_i a_i^l \sin \gamma, \sum_i a_i^l \cos \gamma \right) = \left( -a_i^l, a_i^l \right), \] and \( \vec{A}_l \cdot \vec{A}_l^\mp = 0 \)
for each multipole order \( l \), then a more general axially symmetric solution with helicities can be presented as a linear combination of solutions (5) in the form:

\[ n_\mu = \sum_{l=1}^{N} \frac{(-1)^l A_{1}^{\mu\alpha} \partial_\alpha \partial_{l-1} \frac{1}{r}}{r} \]  
(14)

Let’s analyse the quantities \( A_{1}^{\mu\alpha} \). In the paper [92] the authors collected multipole moments for various axially symmetrical colloidal particles without helicity in the nematic liquid crystal. For such particles \( A_{1}^{\mu\alpha} \) are diagonal matrices \( A_{1}^{\mu\alpha} = a_i \delta_{\mu\alpha} \). In other words, for such particles \( a_i^l = a_i \) and \( a_i^l = 0 \). For example, a spherical particle with a volume is described by three numbers \( (a_2, a_4, a_6) = (-0.36R^3, -0.023R^3, -0.0018R^3) \), where \( R \) is the radius of the particle; a polystyrene microspheres with conically degenerate boundary conditions has coefficients \( (a_2, a_4, a_6) = (-0.017R^3, -0.092R^3, 0.003R^3) \); and a colloidal sphere with hyperbolic hedgehog has coefficients \( (a_1, a_2, a_3) = (2.04R^2, -0.72R^3, 0.157R^4) \) with \( R \) being the radius of the particle [92]. But \( a_i^l \neq 0 \) for 3D skyrmion particles or for colloidal particles with helicity, and we proceed to such cases.

If we introduce such multipole moment densities \( A_{1}^{\mu\alpha}(\mathbf{x}) = A_{1}^{\mu\alpha} \delta(\mathbf{x}) \), then the free energy functional (6) will be rewritten as:

\[ F_{eff} = K \int d^3 x \left\{ \frac{(\nabla n_\mu)^2}{2} - 4\pi \sum_{l=1}^{N} A_{1}^{\mu\alpha}(\mathbf{x}) \partial_\alpha \partial_{l-1} n_\mu \right\} \]  
(15)

This functional correctly describes the interaction between a liquid crystal and an axially symmetric particle with chirality since its Euler-Lagrange equation is:

\[ \Delta n_\mu = 4\pi \sum_{l=1}^{N} (-1)^{l-1} \partial_\alpha \partial_{l-1} A_{1}^{\mu\alpha}(\mathbf{x}) \]  
(16)

and for the infinite space it has the known solution:

\[ n_\mu(\mathbf{x}) = \int d^3 x' \frac{1}{|\mathbf{x} - \mathbf{x}'|} \sum_{l=1}^{N} (-1)^l \partial_\alpha \partial_{l-1} A_{1}^{\mu\alpha}(\mathbf{x}') \]  
(17)

which coincides with (14).

If we consider \( N_p \) particles with helicity in the NLC, so that \( A_{1}^{\mu\alpha}(\mathbf{x}) = \sum_i A_{1}^{\mu\alpha}(\mathbf{x} - \mathbf{x}_i) \), \( i = 1 \div N_p \). Then substitution (16) into \( F_{eff} \) (15) brings: \( F_{eff} = U^{self} + U^{interaction} \) where \( U^{self} = \sum_i U_i^{self} \), here \( U_i^{self} \) is the divergent self energy.

Interaction energy \( U^{interaction} = \sum_{i<j} U_{ij}^{int} \). Here \( U_{ij}^{int} \) is the elastic interaction energy between \( i \) and \( j \) particles in the unlimited NLC:

\[ U_{ij}^{int} = 4\pi K \sum_{l=1}^{N} \left( a_i^l a_j^l \right)^x + a_i^l a_j^l (-1)^l \frac{(l + 1)!}{r^{l+1}} P_{l+1}(\cos \theta) \]  
(18)

Here unprimed quantities \( (a_i^l, a_j^l) \) are used for particle \( i \) and primed \( (a_i^l', a_j^l') \) for particle \( j \), \( r = |\mathbf{x} - \mathbf{x}_j| \), \( \theta \) is the angle between \( \mathbf{r} \) and \( \mathbf{z} \). In general case:

\[ a_i^l a_j^{l'} + a_j^{l'} a_i^l = \sum_{\gamma \gamma'} a_i^l a_j^{l'} \gamma \gamma' \cos(y - y') \]  
(19)

with summation over all possible helicities \( y \) for every multipole order \( l \). Actually in general case helical twisting of the molecules on the particle’ surface can produce different helicities and different multipole coefficients \( a_i^l \). But we do not need to know all \( a_i^l \), as it is sufficient to know only two coefficients \( (a_i^l, a_j^l) \) for each \( l \) to determine the director field: \( (a_i^l, a_j^l) = (\sum_i a_i^l \cos \gamma, -\sum_i a_i^l \sin \gamma) \).

When helicity or spiral cutting on the surface is absent, only \( a_i^l = a_i \) remain.

Expression (18) is the general expression for the elastic interaction potential between axially symmetric helical colloidal particles in the unlimited NLC with taking into account the high order elastic terms.

### 2.2. 3D skyrmion as a colloidal particle with chirality in confined nematic liquid crystal

In the case of confined NLC it means the replacement of \( r = \frac{1}{x-x'} \) with Green’s function \( G(\mathbf{x}, \mathbf{x}') \) (see [85,86]), which satisfies equation \( \Delta G(\mathbf{x}, \mathbf{x}') = -4\pi \delta(\mathbf{x} - \mathbf{x}') \) for \( \mathbf{x}, \mathbf{x}' \in \mathbf{V} \) (\( \mathbf{V} \) is the volume of the bulk NLC) and \( G(\mathbf{x}, s) = 0 \) for any \( s \) of the bounding surfaces \( \Sigma \). Then director field in any point \( \mathbf{x} \) inside the cell is defined as:

\[ n_\mu(\mathbf{x}) = \int d^3 x' G(\mathbf{x}, \mathbf{x}') \sum_{l=1}^{N} (-1)^l \partial_\alpha \partial_{l-1} A_{1}^{\mu\alpha}(\mathbf{x}') \]  
(20)

Then formula (9) for the confined NLC has the form:

\[ U_{ij}^{int\, confined} = -4\pi K \sum_{l=1}^{N} \left( a_i^l a_j^l \right)^x + a_i^l a_j^l \partial_\alpha \partial_{l-1} \gamma \gamma' \cos(y - y') \]  
(21)

The first most important dipole term in the general case has the form:
\[ U_{ij, \text{dipole}}^{\text{int, confined}} = -4\pi K (a_i^x a_j^x + a_i^y a_j^y) \partial_y \partial_y G(x_i, x_j') = -4\pi K \sum_{y' \neq y} a_i^y a_j^y \cos(y - y') \partial_y \partial_y G(x_i, x_j') \]

(22)

Formula (21) gives the most general expression for the elastic interaction energy between any axially symmetric colloidal particles with helicity or between 3D skyrmions in the homeotropic cell with thickness \( L \).

Now we can return to the consideration of one skyrmion (toron, hopfion) inside a homeotropic cell with thickness \( L \). In the general case, it is described by \( 2N \) numbers \( (a_i^x, a_i^y) \) - multipole moments, \( l = 1 \div N \). But symmetry considerations make it possible to reduce the number of these coefficients. First, below we will restrict ourselves to cases with helicity \( y = 0 \) and \( y = \pi/2 \) (for example, we will not consider hopfions with \( y = \pi/4 \)). Then all coefficients \( a_i^0 \) and \( a_i^{y/2} \) can be non-zero. For instance, for any axially symmetric 3D solitons with an asymmetric shape with respect to the median plane \( z = L/2 \) or similar particles (for example, a dipole particle with a hyperbolic hedgehog in a homeotropic cell with a cholesteric at \( L/p \approx 1 \)), all the coefficients \( a_i^0 \) and \( a_i^{y/2} \) are different from zero.

Secondly, it can be shown (we will not give a proof of this here) that if a 3D soliton has a symmetric shape with respect to the middle of the cell \( z = L/2 \), then only even coefficients \( a_i^0 \) and odd coefficients \( a_i^{y/2} \) remain. Thus, for \( y \)-symmetric 3D solitons, only \( N \) non-zero numbers remain. In this paper, we will consider only terms up to \( N = 6 \) and will consider only such 3D skyrmions that have symmetrical shape with respect to the median plane \( z = L/2 \). Then only odd helical coefficients \( (a_1^{y/2}, a_2^{y/2}, a_3^{y/2}) \) - chiral dipole, chiral octupole and chiral moment of the order 5 - will be nonzero. And also there will be even nonzero coefficients \( (a_0^0, a_0^{y/2}, a_0^{3y/2}) \) - ordinary quadrupole moment, hexadecapole moment and sixth order moment. For example, such moments are present in particles with boojums [90] and in hexadecapole colloids [91]. So a 3D skyrmion of symmetrical shape, with respect to the median plane \( z = L/2 \) can be described by 6 numbers \( (a_1^{y/2}, a_2^{y/2}, a_3^{y/2}, a_0^0, a_0^{y/2}, a_0^{3y/2}) \) or by 12 vectors: \( \vec{A}_1^y = (0, -a_1^{y/2}) \); \( \vec{A}_1^x = (a_1^{y/2}, 0) \); \( \vec{A}_2^y = (a_2^{y/2}, 0) \); \( \vec{A}_2^x = (0, a_2^{y/2}) \); \( \vec{A}_3^y = (0, -a_3^{y/2}) \); \( \vec{A}_3^x = (a_3^{y/2}, 0) \); \( \vec{A}_4^y = (0, a_4^0) \); \( \vec{A}_4^x = (a_4^0, 0) \); \( \vec{A}_5^y = (a_5^{y/2}, 0) \); \( \vec{A}_5^x = (0, a_5^{y/2}) \); \( \vec{A}_6^y = (a_6^{y/2}, 0) \); \( \vec{A}_6^x = (0, a_6^{y/2}) \).

Let’s consider a 3D skyrmion, which has a symmetrical shape with respect to the median plane \( z = L/2 \), and which is located at the centre of a homeotropic cell at the point \( x_0 = (0, 0, L/2) \). Then the director field (20) at large distances from the skyrmion centre is described by the formula

\[ n_\rho(x) = \sum_{l=1}^{N=6} A_{l \mu} \partial_\mu \partial_\rho G(x, x') |_{x'=-(0,0,L/2)} \]

(23)

The Green function for the homeotropic cell can be taken from electrodynamics [96]:

\[ G(x, x') = \frac{4}{L} \sum_{n=1}^{\infty} \frac{\sin(n\pi/2)\sin(n\pi x/L)K_0(n\rho x/L)}{n\pi/2 \sin(n\pi L/L)} \]

(24)

where \( \rho = \sqrt{(x-x')^2 + (y-y')^2} \) is the horizontal projection of the distance between particles and \( z \in [0, L] \) and \( K_0 \) is modified Bessel function.

Then the director field at an arbitrary point \( x \) with coordinates \( (\rho, \phi, z) \) inside the cell can be written as:

\[ n_\rho(x) = \frac{4}{L} \cos(\phi + \pi/2) \sum_{n=1,3,5,}^{\infty} \sin(n\pi/2)\sin(n\pi z/L)K_1(n\rho x/L) \]

\[ \left[ a_4^{\pi/2}(n\pi/2 - a_3^{\pi/2}(n\pi/2)^3 + a_5^{\pi/2}(n\pi/2)^5 \right] + \]

\[ + \frac{4}{L} \cos(\phi) \sum_{n=2,4,6,}^{\infty} \cos(n\pi/2)\sin(n\pi z/L)K_1(n\rho x/L) \]

\[ \left[ a_2^{\pi/2}(n\pi/2)^2 - a_4^{\pi/2}(n\pi/2)^4 + a_6^{\pi/2}(n\pi/2)^6 \right] \]

(25)

\[ n_\phi(x) = \frac{4}{L} \sin(\phi + \pi/2) \sum_{n=1,3,5,}^{\infty} \sin(n\pi/2)\sin(n\pi z/L)K_1(n\rho x/L) \]

\[ \left[ a_4^{\pi/2}(n\pi/2 - a_3^{\pi/2}(n\pi/2)^3 + a_5^{\pi/2}(n\pi/2)^5 \right] + \]

\[ + \frac{4}{L} \sin(\phi) \sum_{n=2,4,6,}^{\infty} \cos(n\pi/2)\sin(n\pi z/L)K_1(n\rho x/L) \]

\[ \left[ a_2^{\pi/2}(n\pi/2)^2 - a_4^{\pi/2}(n\pi/2)^4 + a_6^{\pi/2}(n\pi/2)^6 \right] \]

(26)

Let \( d \) be the diameter of a skyrmion in the symmetry plane \( z = L/2 \) and we will introduce the dimensionless \( \sigma = d/L \). If we introduce dimensionless multipole moments \( (b_1, b_2, b_3, b_4, b_5, b_6) \), then the coefficients can be represented as \( (a_1^{y/2}, a_2^{y/2}, a_3^{y/2}) = (b_1d^2, b_2d^4, b_3d^6) \) and \( (a_0^0, a_0^{y/2}, a_0^{3y/2}) = (b_2d^3, b_4d^5, b_6d^7) \). Then, in the Cartesian coordinate system, the director field at any point \( x \) with coordinates \( (x, y, z) \) can be represented as:
\[ n_x(x) = -\frac{4y}{\rho} \sum_{n=1.35..}^{\infty} \sin(n\pi/2) \sin(n\pi L) K_1(n\pi L) \]
\[ [b_1(n\pi\sigma) - b_3(n\pi\sigma)^3 + b_5(n\pi\sigma)^5] + \]
\[ + \frac{4x}{\rho} \sum_{n=2.46..}^{\infty} \cos(n\pi/2) \sin(n\pi L) K_1(n\pi L) \]
\[ [b_2(n\pi\sigma)^2 - b_4(n\pi\sigma)^4 + b_6(n\pi\sigma)^6] \tag{27} \]

\[ n_y(x) = \frac{4x}{\rho} \sum_{n=1.35..}^{\infty} \sin(n\pi/2) \sin(n\pi L) K_1(n\pi L) \]
\[ [b_1(n\pi\sigma) - b_3(n\pi\sigma)^3 + b_5(n\pi\sigma)^5] + \]
\[ + \frac{4y}{\rho} \sum_{n=2.46..}^{\infty} \cos(n\pi/2) \sin(n\pi L) K_1(n\pi L) \]
\[ [b_2(n\pi\sigma)^2 - b_4(n\pi\sigma)^4 + b_6(n\pi\sigma)^6] \tag{28} \]

where \( \rho = \sqrt{(x-x')^2 + (y-y')^2} \). The formulas (27) and (28) define an analytical description of the director field for any axially symmetric skyrmion (3D soliton) outside its strong deformation region, provided that it has a symmetric shape with respect to \( z = L/2 \) and it has no chirality other than \( \gamma = \pi/2 \). That is, different 3D skyrmionic particles (torons, Hopfions) will differ only in sets of coefficients \( b_1, b_2, b_3, b_4, b_5, b_6 \).

Consider now the interaction between two identical 3D skyrmionic particles. Since they are in the centre, then \( z = z' = L/2 \) and let \( \rho \) be the distance between them. Then the general formula (21) gives the following interaction potential:
\[ U_{ij}^{\text{int.confined}} = U_{ij}^{\text{helical}} + U_{ij}^{\text{shape}} \tag{29} \]

\[ U_{ij}^{\text{helical}} = 16\sigma K_d \sum_{n=1.35..}^{\infty} K_0\left(\frac{n\pi L}{L}\right) \cdot |b_1(n\pi\sigma)|^2 \]
\[ -2b_1 b_3(n\pi\sigma)^4 + 2b_1 b_3(n\pi\sigma)^6 + \]
\[ + b_3^2(n\pi\sigma)^6 - 2b_3 b_5(n\pi\sigma)^8 + b_5^2(n\pi\sigma)^{10} \tag{30} \]

\[ U_{ij}^{\text{shape}} = 16\sigma K_d \sum_{n=2.46..}^{\infty} K_0\left(\frac{n\pi L}{L}\right) \cdot |b_2(n\pi\sigma)|^4 \]
\[ -2b_2 b_4(n\pi\sigma)^6 + 2b_2 b_4(n\pi\sigma)^8 + \]
\[ + b_4^2(n\pi\sigma)^8 - 2b_4 b_6(n\pi\sigma)^{10} + b_6^2(n\pi\sigma)^{12} \tag{31} \]

Since the function \( K_0(x) \) has the asymptotic \( K_0(x) \approx e^{-x} \sqrt{\frac{x}{2\pi}} \) for big \( x \), we see that the interaction potential between 3D skyrmions in the homeotropic cell with thickness \( L \), has exponential decay length equal \( \lambda_{SS} = L/\pi \). This result is new for 3D skyrmions, but that is not a surprise, as usual colloidal dipole particles have the same decay length [85]. In the paper [40], the authors obtained similar functional dependency for dipole-dipole interaction between 2D skyrmions. Still, they did not find the decay length equal \( \lambda_{SS} = L/\pi \) as a function of the cell thickness.

It can be seen that the potential consists of two parts: the first one that depends on the chirality \( U_{ij}^{\text{helical}} \) and has the leading dipole-dipole interaction. The second part depends on the envelope shape of the 3D soliton \( U_{ij}^{\text{shape}} \) and has the leading quadrupole-quadrupole interaction. That is a new thing. As far as we know, this is a principally new result for 3D skyrmions. Almost all analytical investigations before made an assumption that \( \psi = \psi(\varphi) \) and they came to the configuration \( \psi = \varphi + \pi/2 \) with the dipole moment. We found the solution which has nonuniform \( \psi(x) \) and contains the quadrupole moment and higher multiple moments as well.

The set of coefficients \( b_1, b_2, b_3, b_4, b_5, b_6 \) is found either from the asymptotics of the exact 3D soliton or by fitting the experimental interaction potential and/or director distribution. Using the relation \( K_0'(x) = -K_1(x) \) we find an expression for the force of interaction between two identical 3D skyrmions (or between two identical spiral particles of a symmetric shape with respect to \( z \)):
\[ F_{ij} = F_{ij}^{\text{helical}} + F_{ij}^{\text{shape}} \tag{32} \]

\[ F_{ij}^{\text{helical}} = 16\sigma K \sum_{n=1.35..}^{\infty} K_1\left(\frac{n\pi L}{L}\right) \cdot |b_1^2(n\pi\sigma)^3 - 2b_1 b_5(n\pi\sigma)^5 + \]
\[ + 2b_1 b_3(n\pi\sigma)^7 + b_3^2(n\pi\sigma)^7 - 2b_3 b_5(n\pi\sigma)^9 + b_5^2(n\pi\sigma)^{11} \] \tag{33} \]

\[ F_{ij}^{\text{shape}} = 16\sigma K \sum_{n=2.46..}^{\infty} K_1\left(\frac{n\pi L}{L}\right) \cdot |b_2^2(n\pi\sigma)^5 - 2b_2 b_4(n\pi\sigma)^7 + \]
\[ + 2b_2 b_6(n\pi\sigma)^9 + b_4^2(n\pi\sigma)^9 - 2b_4 b_6(n\pi\sigma)^{11} + b_6^2(n\pi\sigma)^{13} \] \tag{34} \]

In the work [39] the force of interaction between LC skyrmions with diameter \( d = 6.7 \mu m \) in a cell with thickness \( L = 10 \mu m \) and average elastic constant \( K = 12.1 \mu N \) was experimentally measured. As a result of the fitting (see Figure 2), we found that one set of coefficients can be approximately represented as \( (b_1, b_2, b_3, b_4, b_5, b_6) = (0.17, -0.06, -0.003, 0.0005, 0.0013, -0.00052) \). We want to stress out that the quadrupole moment \( b_2 \), the octupole moment \( b_3 \), the hexadecapole moment \( b_4 \) and higher moments \( b_5 \) and \( b_6 \) are very important for the
fitting of the experimental data on close distances. As far as we know, all these moments were absent in previous papers on 3D skyrmions.

In Figure 3 it is shown the director field distribution with the same coefficients \((b_1, b_2, b_3, b_4, b_5, b_6)\) according to formulas (27,28) on the spheroidal surface with radius 0.6 \(L\) with first three terms in the series (calculations were made in Mathematica 12).

It is clearly seen that odd helical coefficients \((b_1, b_3, b_5)\) define the helicity of the director field while even coefficients \((b_2, b_4, b_6)\) define the envelope shape of the director field.

3. Behaviour of 3D skyrmions in a skyrmion bag

Figure 4 schematically shows a skyrmion bag with anti-skyrmions. The blue colour schematically shows the orientation of the director downwards at an angle \(\pi\), and the white colour shows it upwards at an angle 0. Thus, the orientation of the director inside the small skyrmions is opposite to the orientation inside the large skyrmion bag, and therefore they can be called anti-skyrmions, although in fact they are ordinary skyrmions.

The black colour shows the area where the director lies approximately in the horizontal plane at an angle \(\pi/2\). It was found in [39] that the distance between skyrmions in a bag increases with the number \(N\) of skyrmions in the bag. Let’s try to explain this.

It is natural to assume that the energy of the skyrmion bag itself is proportional to its circumference \(E_{\text{bag, self}} = 2\pi R a > 0\), where \(R\) is the radius of the skyrmion bag (the radius of the large black circle in Figure 4), and \(a\) is the linear energy density. Inside the skyrmion bag, the skyrmions repel each other and organise a quasi-hexagonal lattice with a distance \(2r\) between the centres and the unit cell area \(S_{\text{skyrmion}} = 2\sqrt{3} r^2\).

Then \(\pi R^2 \approx N S_{\text{skyrmion}}\) and \(r = \frac{\sqrt{3} R}{\sqrt{2N}\sqrt{3}}\). Each skyrmion interacts with 6 neighbours and then its interaction energy is \(6U(2r)/2 = 3U(2r)\), where \(U(2r) = a K_0(2\pi r)\) is the interaction potential between two skyrmions \((a = 16\pi^3 K d b_1^2 (d/2)^3)\) with \(d\) being diameter of the small skyrmion (small black circles in Figure 4) and \(b_1\) is the dipole multipole coefficient. We left here only the first most important dipole term from the formula (29). Then the total energy of the skyrmion bag with \(N\) skyrmions inside becomes:

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Figure 2. (Colour online) The interaction force between 3D skyrmions in \(pN\). Comparison between analytical expression (32) with \((b_1, b_2, b_3, b_4, b_5, b_6) = (0.17, -0.06, -0.003, 0.0005, 0.0013, -0.00052)\) and experiment. Experimental points were taken from [39].

Figure 3. (Colour online) Director field according to formulas (27,28) on the spheroidal surface with radius 0.6 \(L\) with first three terms in the series. \(a\) Calculation with coefficients \((b_1, b_2, b_3, b_4, b_5, b_6) = (0.17, -0.06, -0.003, 0.0005, 0.0013, -0.00052)\). \(b\) Calculation with odd helical coefficients only \((b_1, b_2, b_3, b_4, b_5, b_6) = (0.17, 0, -0.003, 0, 0.0013, 0)\). \(c\) Calculation with even 'shape' coefficients only \((b_1, b_2, b_3, b_4, b_5, b_6) = (0, -0.06, 0, 0.0005, 0, -0.00052)\). Calculations were made in Mathematica 12.
Then introducing the equation:

\[ x = \frac{2\pi R}{L \sqrt{2N \sqrt{3}}} \]

The equilibrium condition \( \frac{\partial}{\partial R} E_{\text{bag}, N} = 0 \) leads to the equation:

\[ \frac{aL \sqrt{2\sqrt{3}}}{3a\sqrt{N\pi}} = K_1 \left( \frac{2\pi^3/2R}{L \sqrt{2N \sqrt{3}}} \right) \]

Using the asymptotics \( K_1(x) \approx e^{-x} \sqrt{\frac{4}{2\pi}} \) for big \( x \) and introducing the dimensionless variable \( x = \frac{2\pi R}{L \sqrt{2N \sqrt{3}}} \) we can get such a relationship between different pairs \( (N_1, x_1) \) and \( (N_2, x_2) \):

\[ x_2 - x_1 + \frac{1}{2} \ln \left( \frac{x_2}{x_1} \right) = \frac{1}{2} \ln \left( \frac{N_2}{N_1} \right) \]

Suppose we know from the experiment the distance \( x_1 \) for one skyrmion bag with \( N_1 \) skyrmions inside. Then it is required to define \( x_2 \) for any other \( N_2 \). First, consider the case when \( |\ln(N_2/N_1)| < 1 \). Then we introduce \( \epsilon = \frac{x_2}{x_1} - 1 \) and expand Equation (37) to \( \epsilon^2 \). As a result, we get the following solution for the size \( r_2 \) of one elementary cell of the bag with \( N_2 \) skyrmions:

\[ r_2 = r_1 + r_1 \cdot \left( 1 + \frac{4\pi r_1}{L} \sqrt{1 + \frac{4\pi r_1}{L}} - 2 \ln \left( \frac{N_2}{N_1} \right) \right) \]

and the distance between two nearest skyrmions will be \( 2r_2 \). It is known from the experiment [39] that \( r_1 = 6.2 \mu m \) for the bag \( S_{13} \) with \( N_1 = 13 \) and \( L = 10 \mu m \). Then we get the normalised curve \( r_2(N_2) \) in Figure 4(b).

It can be seen that it describes quite well the experimental points for different numbers of (anti) skyrmions. In the same way we can find how the bag radius \( R \) depends on \( N \) using (38) and \( r = \frac{\sqrt{2\pi R}}{L \sqrt{2N \sqrt{3}}} \). Then the bag radius \( R_2 \) with \( N_2 \) skyrmions can be defined via the bag radius \( R_1 \) with \( N_1 \) skyrmions:

\[ R_2 = \sqrt{\frac{N_2}{N_1}} R_1 \]

\[ = \left[ 2 + \frac{4\pi^3/2R_1}{L \sqrt{2N_1 \sqrt{3}}} \right] - \left[ 1 + \frac{4\pi^3/2R_1}{L \sqrt{2N_1 \sqrt{3}}} \right]^2 - 2 \ln \left( \frac{N_2}{N_1} \right) \]

One can also get the theoretical asymptotics for \( N_2 \gg N_1 \), then:

\[ r_2 = r_1 + \frac{L}{4\pi} \ln \left( \frac{N_2}{N_1} \right) \]

And the correspondent dependence of the bag radius \( R \):

\[ R_2 = \sqrt{\frac{N_2}{N_1}} R_1 \]

\[ = \frac{N_2}{N_1} R_1 + \frac{L \sqrt{2\pi \sqrt{3}}} {4\pi^3/2} \ln \left( \frac{N_2}{N_1} \right) \]

4. Conclusion

In this paper, we tried to bridge the gap between 3D skyrmions and colloidal particles in liquid crystals. We looked at a 3D skyrmion in a cholesteric homeotropic cell as a colloidal particle and considered the interaction between 3D skyrmions as an elastic interaction between colloidal particles. This can be done exactly outside the core of the skyrmion, beyond the region with strong
director deformations. Then the director distribution can be accurately determined analytically and the elastic interaction potential between 3D skyrmion particles can be calculated exactly. We considered skyrmions with axial symmetry in a homeotropic cell of thickness $L$ with strong boundary conditions, when the director looks vertically at the surfaces of the bounding planes. It turns out that the chirality of the liquid crystal manifests itself in the birth of chiral multipole coefficients $a_l^\gamma$, which are absent in ordinary colloidal particles in the nematic. Usually, colloidal particles in nematics have only zero-helicity multipole coefficients $a_l^0$. And then we show that the 3D skyrmion in the region of weak deformations can be described as a set of multipoles: zero $a_l^0$ and chiral $a_l^\gamma$. But we do not need to know all $a_l^0$, as it is sufficient to know only two coefficients $(a_l, a_l^\gamma)$ for each $L$ to determine the director field: $(a_l, a_l^\gamma) = \left( \sum_{\gamma} a_l^\gamma \cos \gamma, - \sum_{\gamma} a_l^\gamma \sin \gamma \right)$.

We have considered in more detail the case of 3D skyrmion particles which have symmetrical shape with respect to the median plane $z = L/2$ and consider only the helicity $\gamma = \pi/2$. We also limited ourselves to multipole moments up to the sixth order inclusively. Then we obtained the interaction potential between 3D skyrmions and found the multipole coefficients to be in agreement with the experiment. We found that 3D skyrmions have not only the dipole moment, but the quadrupole moment $b_2$, the octupole moment $b_3$, the hexadecapole moment $b_4$ and higher moments $b_5$ and $b_6$, which all are very important for the fitting of the experimental repulsion between 3D skyrmions on close distances. As far as we know, all these moments were absent in previous papers on 3D skyrmions. Only dipole moment and dipole interaction were taken into account. As well we find exact analytical expression for the elastic interaction potential between 3D skyrmions in a homeotropic cell with thickness $L$ and show that it has exponential decay length equal $\lambda_{SS} = L/\pi$.

Next, we applied our results to 3D skyrmions in a skyrmion bag. As the number of skyrmions $N$ in the bag increases, the distance between them gets larger as well. We have found an approximate analytical formula for the distance between skyrmions depending on the number of $N$ skyrmions in the bag, which also agrees with experiment.

Along the way, we determined the director field around a chiral axially symmetric colloidal particle in the unlimited nematic liquid crystal and in the confined homeotropic cell, taking into account higher order elastic terms with orders $l = 1 \div 6$. In general case it can have as well a double set of multipoles: zero $a_l^0$ and chiral $a_l^\gamma\pi/2$ for $l = 1 \div 6$. We also have found the elastic interaction potential between such particles.

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