
Publisher's PDF, also known as Version of record

Link to published version (if available): 10.1103/PhysRevLett.121.237801

Link to publication record in Explore Bristol Research
PDF-document
Woven Nematic Defects, Skyrmions, and the Abelian Sandpile Model

Thomas Machon
H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, United Kingdom

Gareth P. Alexander
Department of Physics and Centre for Complexity Science, University of Warwick, Coventry, CV4 7AL, United Kingdom

(Received 8 August 2018; published 3 December 2018; corrected 4 December 2018)

We show that a fixed set of woven defect lines in a nematic liquid crystal supports a set of nonsingular topological states which can be mapped on to recurrent stable configurations in the Abelian sandpile model or chip-firing game. The physical correspondence between local skyrmion flux and sandpile height is made between the two models. Using a toy model of the elastic energy, we examine the structure of energy minima as a function of topological class and show that the system admits domain wall skyrmion solitons.

DOI: 10.1103/PhysRevLett.121.237801

The interplay of periodicity and topology can lead to particularly rich phenomenology, as evidenced by both electronic [1] and mechanical systems [2]. In the liquid crystal literature, blue phases with their networks of defect lines provide a classic example [3]. Many other periodic topological structures, typically stabilized through surface geometry and topology have been found in liquid crystalline systems, with strong analogies to chiral magnetic systems [4]. Following early work on effective interactions between colloids in liquid crystals [5,6] regular arrays of defects and colloids were found [7], with similar techniques being used to create large systems of periodic [8], entangled and knotted defect lines [9,10]. Defect arrays have also been created by immersing sheets with regular arrays of punctures into a liquid crystal host [11], or with arrays of toron excitations [12] as well as in numerical studies in cholesterics [13]. We note that similar topological distortions can also be generated using the Hopf invariant [14,15].

In this Letter we study topological physics in a periodic system of a different kind: skyrmions in nematic liquid crystals entangled with a fixed lattice of woven defect lines (Fig. 1). We note that systems containing arrays of skyrmions have been studied numerically in cholesterics [16] and experimentally in skyrmion bags [17]. We show that the topologically allowed transitions between different skyrmion configurations in a fixed lattice of defects can be expressed in terms of a simple set of allowed hopping moves for skyrmion charge. By considering these allowed moves as an equivalence relation, we show there is a duality between topological classes of skyrmions on such a lattice and stable recurrent states of the Abelian sandpile model on a graph associated to the defect lattice. Physically, one identifies sandpile height with local skyrmion charge in the lattice and the allowed skyrmion hopping moves correspond directly to generalized collapses in the Abelian sandpile model. Mathematically this result can be thought of in the context of correspondences between the recurrent states of the Abelian sandpile model and graph Laplacians [18], between graph Laplacians and rooted spanning trees (via the matrix-tree theorem), between rooted spanning trees and branched double covers [19], and between branched double covers and nematic defect topology [20,21]. Motivated by the analogy with sandpile height,
we construct a toy model for the energetics of these states. We investigate the structure of ground states in each topological class for a $3 \times 3$ square lattice. We then consider the toy model in the case of large systems which exhibits soliton structures consisting of lines of skyrmions. In a physical realization of the system we have in mind, the defect lines could be inclusions, fibers, or colloids, which simulate disclination lines in the surrounding nematic texture in a similar manner to the imprinting of defect lines in the blue phases using polymers [22], or in the creation of colloids that either mimic disclination lines [23] or have other desired topological properties [24–26]. An alternative route to the generation of such structures may be through micropatterned substrates, which can be used to generate freestanding networks of twist disclination lines [27].

Skyrmions appear as topological distortions in nematic liquid crystals and have an integer charge, $q$. The skyrmion flux through a surface $\Sigma$ may be computed via an integral of the topological charge density in terms of the unit magnitude director field $\mathbf{n}$ as

$$ q = \frac{1}{8\pi} \int_\Sigma dA_I \epsilon_{ijk} \epsilon_{abc} n_a \partial_j n_b \partial_k n_c, $$

(1)

which is an integer if $\Sigma$ is closed. There are two important observations that one can make from Eq. (1). The first is that measuring skyrmion charge is done via a surface integral, so that skyrmions naturally live on surfaces. Therefore, if the skyrmion charge is localized to a region on a given surface then in three dimensions the skyrmion charge becomes confined to a tubelike object. The second observation is that under the action of the nematic inversion symmetry $\mathbf{n} \rightarrow -\mathbf{n}$, $q \rightarrow -q$, so that locally skyrmion charge is only defined up to sign. Mathematically, this represents the action of the fundamental group $\pi_1({\mathbb R}P^2)$ on $\pi_2({\mathbb R}P^2)$, where $\mathbb{RP}^2 = S^2/(x \sim -x)$ is the nematic ground state manifold [29,30].

Consider a skyrmion in a fixed defect array $L$ such as the square woven lattice of Fig. 1. For a skyrmion in a free system, there is a translational symmetry so the skyrmion may move around [31]. In the lattice of defects there are not only geometric but topological obstructions for the skyrmion to move around the lattice. As we show below, skyrmions may only move around the lattice according to generalizations of the hopping rule shown in Fig. 1. These hopping rules originate in the interaction between skyrmions and line defects [30] and its relation to the $q \rightarrow -q$ and $\mathbf{n} \rightarrow -\mathbf{n}$ symmetry. Around a nematic disclination line the director field is nonorientable—as can be seen in the typical $\pm 1/2$ profiles. Tracking $\mathbf{n}$ along a circuit around a disclination line one finds that it realizes the transformation $\mathbf{n} \rightarrow -\mathbf{n}$. This changes the charge of the skyrmion. More exotic topological aspects of nematics can be understood in a similar manner [20,21]. A way of visualizing this is as follows: If a pair of point defects are nucleated in a nematic, then a skyrmion distortion is created that connects them [4,14]. Consider now dragging one of the point defects along a path that entangles several line defects and then meets back up and annihilates with the original defect, leaving behind a skyrmion entangled with the disclination lattice. Up to smooth deformations of the texture there are a finite number of topologically inequivalent ways that this may occur, indexed by a twisted cohomology group [21] and from the perspective of algebraic topology the distinct topological states of skyrmions entangled with a fixed set of disclination lines are given by elements in the set

$$ H^2({\mathbb R}^3 \setminus L; \mathbb{Z}^o) $$

(2)

where $H^2({\mathbb R}^3 \setminus L; \mathbb{Z}^o)$ is the twisted cohomology group with coefficient system $\mathbb{Z}^o$ given by the integers along with the map $\gamma: \pi_1({\mathbb R}^3 \setminus L) \rightarrow \mathbb{Z}_2$ which sends each meridian of $L$ to $-1 \in \mathbb{Z}_2$. If the disclination line is a knot or link, then the size of this cohomology group is a knot invariant, the knot determinant, which is equal to the Alexander polynomial evaluated at $-1$ [20,21].

Our goal is to study the possible ways of entangling skyrmions with a fixed lattice of woven defect lines such as the one shown in Fig. 1, given by Eq. (2). Mathematically this amounts to studying topological equivalence classes of textures, i.e., free homotopy classes of maps [29] $[\Omega, \mathbb{RP}^2]$ where $\Omega = {\mathbb R}^3 \setminus L$, where $L$ is the defect set. Important, this means that all the results presented here assume that no other defects interact with the system; our classification holds only as long as no additional defects are created and the topology of the defect set does not change. As discussed above, the defect lines in the array may be thought of as generated by inclusions, and we assume that the boundary conditions are such that the director field $\mathbf{n}$ is free on the surface of the defect lines (up to topological class).

To compute Eq. (2) for a set of line defects $L$ such as the ones shown in Fig. 1 one first draws a checkerboard surface $\Sigma$ for $L$, as shown in Fig. 2, which is related to the surfaces arising through the use of the Pontryagin-Thom construction [14]. One then writes a basis $\{\alpha\}$ of cycles on $\Sigma$ and a
dual basis of cycles in $\mathbb{R}^3 \setminus \Sigma$, which are bases for the homology groups $H_1(\Sigma; \mathbb{Z})$ and $H_1(\mathbb{R}^3 \setminus \Sigma; \mathbb{Z})$, respectively. These bases satisfy the condition

$$\text{Lk}(\alpha_i, \beta_j) = \delta_{ij},$$

as illustrated in Fig. 2, where the vertical $\beta$ cycles meet up at infinity. From a physical perspective, $\beta_{ij}$ represents skyrmion flux through the site $(i, j)$, the $\alpha$ cycles encode the topological information about how this skyrmion flux can be moved around the defect lattice. As drawn in Fig. 2, $\Sigma$ is orientable, and one can consider the push-offs, $p^\pm \alpha_{ij}$ of cycles on $\Sigma$ in either the positive or negative direction, which can be expressed as linear combinations of cycles in $\{\beta\}$. In the case of Fig. 2 it is readily shown that

$$p^+ \alpha_{ij} = -\beta_{i+1,j} - \beta_{i-1,j} + 2\beta_{ij},$$

$$p^- \alpha_{ij} = -\beta_{i,j+1} - \beta_{i,j-1} + 2\beta_{ij},$$

The group $H^2(\mathbb{R}^3 \setminus \mathcal{L}; \mathbb{Z}^\omega)$ is then given by integer combinations of the $\beta_{ij}$ along with the equivalence relations given by $p^+ \alpha_{ij} = -p^- \alpha_{ij}$ for each $(i, j)$. Considered as a linear map, we have $p^+ + p^- = -\nabla_\Lambda^2$, the graph Laplacian of a black graph, $\Lambda$, of $\mathcal{L}$ (Fig. 1(a)). This defines the equivalence relation on the possible sets of skyrmion fluxes, and consequently the topologically distinct ways of entangling skyrmions with this array are given by integer-valued functions $\psi: \Lambda \rightarrow \mathbb{Z}$, with two functions equivalent if they differ by any integer-valued function $f$ in the image of the graph Laplacian, $f = \nabla_\Lambda^2 g$, so that

$$\psi \sim \psi + \nabla_\Lambda^2 g.$$  

Finally, accounting for the $\mathbf{n} \rightarrow -\mathbf{n}$ symmetry leads to an identification of $\psi$ with $-\psi$. The set of states thus has the structure of $\tilde{G}_\Lambda / \mathbb{Z} \cong \mathbb{Z}^\Lambda / \nabla_\Lambda^2 \mathbb{Z}$. For a finite lattice, we may write

$$\tilde{G}_\Lambda = \mathbb{Z} \oplus G_\Lambda,$$

where $G_\Lambda$ is a finite Abelian group and $\mathbb{Z}$ measures the charge of the entire lattice taken as a single object. Although here we focus on the square woven lattice shown in Fig. 1, other lattices are possible and described by the same general framework. For example, one can take the kagome lattice, considered as families of straight lines, and make the vertices alternating over and under crossings; $\Lambda$ is then the honeycomb lattice.

The group $G_\Lambda$ is known as the sandpile group for the lattice $\Lambda$, its order is given by $\det(\nabla_\Lambda^2)'$, where $\langle \nabla_\Lambda^2 \rangle'$ is the Laplacian matrix with a single row and column removed. In statistical mechanics it indexes stable recurrent states in the Abelian sandpile model [32] or chip-firing games [33, 34]. The Abelian sandpile model (see Ref. [35] for a review) on a square lattice $\Lambda$ associates to each lattice $i$ site a non-negative height $h_i$. Sites with $h_k \geq 4$ are termed unstable and collapse according to the rule

$$h_i \rightarrow h_i - (\nabla_\Lambda^2)_{ij} \delta_{jk},$$

The dynamics of the model is specified by incrementing $h$ at a random site by one, and then collapsing sites until the system is stable. To ensure this process terminates on a finite lattice, one designates a node as the sink which may not collapse.

In a seminal paper [18] Dhar showed that the set of recurrent stable configurations of this system are given by the sandpile group, $G_\Lambda$. The analogy between Eqs. (6) and (8) is clear. In the sandpile model, the function $h$ represents sandpile height at each lattice site. We are therefore motivated to consider $\psi$ as an analogous field, measuring local skyrmion charge. While such an equivalence is not strictly possible from a topological perspective, as $\psi$ is not a topological invariant (skyrmions are extended objects and cannot be rigorously localized in general), it is likely that a physical realization of this system would display sufficient structural regularity for $\psi$ to be defined in an ad hoc manner. There is some subtlety originating in the $x \sim -x$ symmetry of the nematic. This can be alleviated [21] by choosing a branch cut, realized as a spanning surface for the defect array (as shown by the grey surface in Fig. 2), after which the director field may be oriented, and a signed field $\psi$ may be defined. Note that in our system, $\psi$ can take all integer values rather than non-negative as in the case of $h$. Equation (6) then becomes an algebraic description of the allowed rules for moving skyrmion charge around the lattice. In the sandpile model, the presence of the sink node ensures that the state space is finite, we can enforce a similar condition by demanding the total charge in the defect array is zero, so that $\sum h = 0$. In a physical system this can be enforced by anchoring conditions at the boundary of the cell containing the defect array, for example. In this case, the number of states is finite, and the connection to the sandpile model further allows us to estimate the number of topological states for a square lattice of size $N$. In this case, one may show that the size of the group (and hence the number of topological states) scales as $|G_\Lambda| \sim e^{N^2}$, where

$$s = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \log(2 - \cos \theta_1 - \cos \theta_2) d\theta_1 d\theta_2$$

is the entropy per site in the sandpile model [18] as well as 2D phantom polymers at their critical point [36].

We now consider a system realizing these topological states. We assume that the configuration can be labeled by a function $\psi: \Lambda \rightarrow \mathbb{Z}$ describing the local skyrmion charge at each lattice site. We then wish to give an expression for the elastic energy of the configuration with a given $\psi$. This depends on the director field configuration $\mathbf{n}$. The nematic is symmetric under $\mathbf{n} \rightarrow -\mathbf{n}$, whereas the skyrmion charge
changes sign, so that any expression for the energy of the system must be symmetric under \( \psi \rightarrow -\psi \). If we assume that the director field is in a local elastic energy minimum at each lattice site, then to lowest order we might try to write down a coarse-grained energy for the system as a function of the topological charge:

\[
F = \frac{K}{2} \sum_{i \in \Lambda} \psi_i^2, \tag{10}
\]

where \( K \) is an energy scale. Given Eq. (10), it is natural to ask for the ground state configuration within each topological class. An explicit representative for each state may be obtained from the Smith normal form [37], \( P^{-1} \nabla_3^2 Q = M \), where \( M \) is diagonal. Let \( \tau_i \) denote the \( i \)th invariant factor of \( \nabla_3^2 \), then given a group element

\[
\phi = (\phi_1, \ldots, \phi_n) \in \bigoplus_{i=1}^n \mathbb{Z}_{\tau_i}, \tag{11}
\]

a function \( \psi : \Lambda \rightarrow \mathbb{Z} \) representing the class \( \phi \) can be written as \( \tilde{P}^T \phi \), where \( \tilde{P}^T \) consists of the columns of \( P^T \) corresponding to the nontrivial elementary divisors. In general we may therefore write configurations in the form

\[
\psi = \tilde{P}^T \phi + \nabla_3^2 \chi, \tag{12}
\]

where \( \chi : \Lambda \rightarrow \mathbb{Z} \) is an arbitrary integer-valued function. To minimize the energy in a given topological state, we choose \( \chi \) in Eq. (12) that minimizes Eq. (10) for a given \( \phi \).

If \( \nabla_3^2 \) is the Laplacian integral then the ground states for each topological class may be found easily. The \( 3 \times 3 \) lattice (as shown in Fig. 1(a)) is the largest Laplacian integral square lattice and so will serve as our example. In this case \( G_3 = \mathbb{Z}_8 \oplus \mathbb{Z}_{24} \), so without the nematic symmetry there are 192 topological states. Accounting for the nematic and lattice symmetries reduces this to 42. Equation (12) gives \( \phi = (a, b) \), with \( a \in \mathbb{Z}_8 \) and \( b \in \mathbb{Z}_{24} \). In general, there is ground state degeneracy for a given \( \phi \). Figure 3 shows the 12 lowest energy configurations for the state \( \phi = (0, 4) \), with energy 6, the highest ground state energy and degeneracy of any state on the \( 3 \times 3 \) lattice. Note there are configurations in this class with \( |\psi| \leq 1 \), and this is true for all classes on the \( 3 \times 3 \) lattice. Skyrmions are typically observed with charge \( \pm 1 \) and one may ask whether it is possible to use the topology of the defect lattice to create higher order charges. Mathematically, this is equivalent to asking whether

\[
m_\Lambda(\phi) = \inf_{\chi} \| \tilde{P}^T \phi + \nabla_3^2 \chi \|_\infty \tag{13}
\]

is equal to 1. For an arbitrary knotted or linked defect array this is not true [20,21], as evidenced by the (4, 4) torus link. More generally computing \( m_\Lambda(\phi) \) is related to the shortest lattice vector problem in the \( \infty \) norm which is known to be NP hard [38]. On probabilistic grounds it’s likely that \( m_\Lambda(\phi) = 1 \), the number of configurations with \( |\psi| \leq n \) and \( \sum \psi = 0 \) is equal to the \( |\Lambda|^{th} \) central \( (2n + 1)^{st} \) multinomial coefficient. In particular, for \( n = 1 \), the central trinomial coefficients, \( T_{|\Lambda|} \), may be written in terms of Legendre polynomials as

\[
T_{|\Lambda|} = (-3)^{|\Lambda|/2} P_{|\Lambda|}((3)^{-1/2}) \sim \frac{3^{|\Lambda|+1/2}}{2 \sqrt{2|\Lambda|}}. \tag{14}
\]

As \( \ln 3 > s \) [Eq. (9)], there are far more configurations with \( |\psi| < 1 \) than there are topological classes.

Moving beyond these small-scale systems, one can instead consider a large system of the type shown in Fig. 1; a similar experimental system can be seen in Ref. [11]. On a general \( N \times N \) lattice any state may be deformed, via moves of the form Eq. (6), so that it has support only on the boundary of the lattice. This can be done iteratively by setting \( \psi \) to zero on successive Moore boundaries of an \( n \times n \) sublattice, beginning with \( n = 1 \). As such, in the infinite limit, the structure of the sandpile group becomes irrelevant, and the properties of the system are determined fully by the local move rules [39]. We may thus write \( \psi = \nabla_3^2 \chi \) in this case so the energy becomes

\[
F = \frac{K}{2} (\nabla_3^2 \chi, \nabla_3^2 \chi), \tag{15}
\]
where $\chi$ is an arbitrary integer valued function related to the physically observable field $\phi$ by $\phi = \nabla^2 \chi$. The ground states of Eq. (15) are given by the kernel of $\nabla^2$ which in particular includes the constant functions, $\chi = c$. The system therefore admits domain wall skyrmion solitons at the interface between $\chi = c_1$ and $\chi = c_2$, as indicated in Fig. 4 [40].

It is a pleasure to acknowledge useful conversations with B. G. Chen. T. M. would like to acknowledge funding from the NSF through Grant No. DMR-1262047.

[39] Computing the Green’s function in the infinite case is an amusing exercise, the integer-valued requirement means that one must break the $D_3$ symmetry of the lattice. In particular, one may choose the Green’s function such that it has support on a cone in $\mathbb{Z}^2$, with its values determined by the integer part of the resistance between appropriate points on an infinite lattice of unit magnitude resistors.
[40] While thermal properties of Eq. (15) are not directly relevant to the liquid crystalline system, simple Monte Carlo simulations of the equilibrium model with Eq. (15) as a Hamiltonian suggest the existence of a Kosterlitz-Thouless type transition involving the proliferation of such domain wall solitons which consist of lines of $\pm 1$ skyrmions, stabilized by the fixed defect array.

Corrections: A misspelling introduced in the abstract during the production process has been fixed.