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Equilibria of a discrete Landau–de Gennes theory for nematic liquid crystals

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Abstract We study equilibria of a discrete version of the Landau–de Gennes energy functional for nematic liquid crystals. We consider the regime of small intersite coupling and present necessary and sufficient conditions for the continuation of equilibria of the decoupled Landau–de Gennes system. We also identify a class of small coupling Landau–de Gennes equilibria that correspond to equilibria of a discretized Oseen–Frank energy. The theory is presented for the case of 2×2 Q-tensors and for the one-elastic-constant energy functionals in finite lattices and graphs. We also present some immediate consequences of the continuation theory to Landau–de Gennes and Oseen–Frank gradient dynamics in the small intersite coupling limit. The results rely on continuation and symmetry arguments and are also related to the construction of breather solutions of discrete nonlinear Schrödinger equations near the anticontinuous limit, a problem arising in photonics.

1 Introduction

We study static configurations of a discretized Landau–de Gennes energy functional in the regime of small intersite coupling, and their relation to static configurations of an analogous discrete Oseen–Frank energy functional. The two discretized functionals are defined in graphs and we restrict our attention to one-elastic-constant models. The main results presented in the paper are necessary and sufficient conditions for the continuation of equilibria of the decoupled Landau–de Gennes discrete theory. As a corollary we show that, in the limit of vanishing intersite coupling, there is a class of Landau–de Gennes equilibria with limiting configurations that are Oseen-Frank equilibria. We also give criteria for the continuation of Oseen–Frank equilibria to Landau–de Gennes equilibria with small intersite coupling.

The Oseen–Frank and Landau–de Gennes continuum theories are commonly used models for nematic liquid crystals [8,16]. The two theories describe the nematic liquid crystal by different quantities and the Landau–de Gennes theory can be thought of as a generalization of the Oseen–Frank theory that includes biaxiality, spatial variations of the order parameter, and more general singular-like structures [8,27]. The motivation for the present work are mathematical results of Majumdar and Zarnescu [17] for 3-D domains and 3×3 Q-tensors showing that, as the coupling constant vanishes, the minimizers of the Landau–de Gennes energy have limits that are Oseen–Frank minimizers. The convergence is in $W^{1,2}(D)$, $D\subset\mathbf{R}^3$ the domain, and is uniform away from the vicinity of singularities of the Oseen–Frank minimizers.

The present work examines a somewhat different but related problem in a simpler discrete setting, drawing on an analogy with the notion of the "anticontinuous limit" of breather solutions of discrete nonlinear Schrödinger (DNLS) equations [13], and using variants of the implicit function theorem [4,29] and symmetry arguments. The main relevant results are by Pelinovsky, Kevrekidis and Frantzeskakis [23,24], see also [25], and extend results of MacKay and Aubry [14] on the continuation of isolated breather solutions. We show that in the case of the 2×2 Q-tensor the reduction argument of [25] leads to necessary and sufficient conditions for the continuation of Oseen–Frank equilibria to Landau–de Gennes equilibria for small coupling constant. The equation for Oseen–Frank equilibria appears as the lowest order bifurcation (or reduced) equation for the continued solutions. A more physical interpretation of these results is that, for small intersite coupling, the extra component of the Q-tensor that appears in the Landau–de Gennes theory is determined by an equation for the component described by the Oseen–Frank theory.

The computations used in the proofs also imply that the Oseen–Frank gradient flow is an approximation of the dynamics on a stable normally hyperbolic invari-

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ant manifold [9,11,30] of the Landau–de Gennes gradient flow. This means that as the system relaxes to an equilibrium we should see a faster decay of the extra Landau–de Gennes components and then a slower approach to the equilibrium that can be described by Oseen–Frank components. We note that the relevance of the anticontinuous limit to equilibria of discrete parabolic problems is well known, see [5]. The present problem has additional geometric structure due to the higher dimension of the target space and symmetries.

The discrete theory concerns finite lattices and graphs, and splits into two cases, for sets with and without (a discrete analogue of a) boundary, respectively. The case without boundary has an additional global $SO(2)$ symmetry that leads to degenerate equilibria. Immediate extensions of our results to the infinite lattice are expected for some unstable solutions. The continuation of the more interesting stable configurations on infinite lattices is possible but not immediate. We have also obtained generalizations for the 3×3 Q-tensor case using a similar ideas. The geometry of the anticontinuous limit equilibria is more involved [15,18] and the verification of the smooth nondegeneracy conditions used in the proofs requires longer computations. We plan to present that case elsewhere. The main contribution of the present work is to show the application of the continuation ideas to discrete liquid crystal equations in the simplest setting that is also of physical interest [21]. The 2×2 case also makes the connection to the DNLS problem immediate: the dimensionality of the target space is the same and the structure of the quadratic functional leads to the bifurcation equation of [23,24]. We note that we have only considered discretizations of the Landau–de Gennes and Oseen–Frank functional with equal elastic constants. This is a widely used simplification of the two theories [1,10,17,22,27]. Extensions to more general Landau–de Gennes and Oseen–Frank functionals are discussed in the last section.

A fuller comparison of our results to the original continuous problem requires further analysis and the consideration of examples. One question is the analogue of singularities in the discrete problems, we remark on this in the last section.

The paper is organized as follows. In Sect. 2, we define the Landau–de Gennes and Oseen–Frank functionals and state the main results for the 2×2 Q-tensor. In Sect. 3, we present the proofs. In Sect. 4, we remark on possible extensions.

2 Discrete Landau–de Gennes system and anticontinuous limit

The Landau–de Gennes theory for nematic liquid crystals is a system of partial differential equations for the Q-tensor, a $q\times q$ symmetric traceless real matrix-valued function defined on a domain $D\subset\mathbf{R}^d$. The domain D is the domain occupied by the liquid crystal, and the matrix $Q(x)$, $x\in D$, describes the orientation of the nematic liquid crystal at a point $x\in D$, see [8,21,27] for more details. In the present work, we present results for the $q=2$ case. This case is also of great physical relevance, as it can be occur in domains of dimension $d=1,2,3$.

The equations for static configurations in D are obtained by extremizing the Landau–de Gennes energy functional

$$\mathcal{F}_{LG}(Q)=\int_D\left(\frac{L}{2}|\nabla Q|^2+f_B(Q)\right),\tag{1}$$

where $|\nabla Q|^2=\sum_{i,j=1}^q\sum_{k=1}^d(\partial_{x_k}Q_{i,j})^2$, and

$$f_B(Q)=-\frac{a^2}{2}\mathrm{tr}(Q^2)-\frac{b^2}{3}\mathrm{tr}(Q^3)+\frac{c^2}{4}(\mathrm{tr}(Q^2))^2.\tag{2}$$

L, a, b, c are positive constants that describe the state and elastic properties of the material, see [18,21,27]. The Dirichlet problem is obtained by varying over configurations with fixed boundary values of Q at ∂D.

A related simpler model for nematic liquid crystals is the Oseen–Frank theory [16], where the orientation of the liquid crystal is described by a unit vector field $\mathbf{n}\in S^{q-1}$ defined on the domain $D\in\mathbf{R}^d$. The equations are obtained by extremizing the Oseen–Frank functional

$$\mathcal{F}_{OF}(\mathbf{n})=\int_D|\nabla\mathbf{n}|^2,\tag{3}$$

where $|\nabla\mathbf{n}|^2=\sum_{k=1}^d\sum_{i=1}^q(\partial_{x_k}\mathbf{n}_i)^2$. The Dirichlet problem is obtained by varying over configurations with fixed boundary values of $\mathbf{n}$ at ∂D.

The Oseen–Frank description is more intuitive as it describes molecules with a preferred direction of alignment ($\mathbf{n}$, $-\mathbf{n}$ represent the same orientation [21]). The Q-tensor includes more information, and the Landau–de Gennes theory can describe the isotropic–nematic phase transition, spatial variations of a nematic order parameter, and biaxiality [8,27]. Temperature effects can be included in the parameters, e.g. the negative sign in the quadratic part of f_B describes a material below the critical temperature for the isotropic–nematic transition.

The functionals (1), (3) are commonly studied special cases of the respective Landau–de Gennes and Oseen–Frank functionals [1,18,22,27]. The general cases of (1), (3) include three elastic parameters, see, e.g. [27]. In the case of $d=3$, $q=2$, (3) is obtained from the Oseen–Frank energy [7] using equal values for the elastic (splay, bend and twist) parameters. In the case $d=q=3$, we obtain (3) by assuming equal elastic parameters and by adding to the Oseen–Frank energy a divergence term [10]. Also, the Oseen–Frank functional (3) and its generalizations can be obtained from the general versions of the first term of (1) using the "uniaxial approximation" (or Ansatz), see [19,27]. The results below are a mathematical justification of this approximation for the $q = 2$ discrete case in the vanishing coupling limit. Extensions to the more general Landau–de Gennes functionals are discussed briefly in the last section.

The gradient flows of $-\mathcal{F}_{LG}$, $-\mathcal{F}_{OF}$ describe relaxation to equilibria, and can be coupled to other continuum theories, e.g. electromagnetism, and fluid flow [7,21]. Discrete versions of the above systems are used in numerical computation [6,20] and are also relevant to studies at the nano-scale, e.g. colloids [27].

The present study was motivated by the question of the limit of energy minimizing static configurations of (1) as $L \to 0^+$ [17], i.e. the elastic constant is small compared to the parameters in f_B, see [26] for the physical relevance of this limit. We will address this and related questions in a discrete version of the theory, using instead continuation ideas, especially the extension of the anticontinuous limit of [2,14] to problems with degeneracy in the decoupled limit [23,24].

In the discrete version of the Landau–de Gennes theory, Q will a function on a discrete set $\overline{G}$. We assume that $\overline{G}$ has the structure of a graph, that is a pair $(\overline{G}, c)$ defined by the discrete set $\overline{G}$ and a function $c : \overline{G} \times \overline{G} \to \{0, 1\}$ satisfying $c(n, n) = 0$, $\forall n \in \overline{G}$, and $c(n, m) = c(m, n)$, $\forall n, m \in G$. The matrix c is the *connectivity matrix* of the graph, with $c(n, m) = c(m, n) = 1$ (0) representing sites n, m that are connected (not connected).

We further consider a set $\partial G \subset \overline{G}$, and let $G = \overline{G} \setminus \partial G$.

In applications to numerical solution of the Landau–de Gennes system in domains $D \subset \mathbf{R}^d$, G and ∂G will be discrete analogues of D and the boundary ∂D respectively. The use of graphs allows for more variety, e.g. lattices on more general manifolds, domains with holes, and discretization of branched manifolds, see, e.g. Fig. 1. The first two graphs (from left) represent discretizations of the circle and the interval respectively, in the third graph indicates branching and more varied boundaries.

We will thus consider two versions of the discrete theory, where (i) the discretized functional is defined on functions on $\overline{G}$, and (ii) the discretized functional is defined on functions on G. In the second case the values at ∂G are fixed and play the role of boundary values.

Let Sym_0^q denote the set of symmetric traceless $q \times q$ real matrices. Also, given $A \subset \overline{G}$ we let $X(A)$ denote the set of functions $f : A \to \mathrm{Sym}_0^q$. We have $X(\overline{G}) \approx \mathbf{R}^{d_q|A|}$ Given A_1, A_2 disjoint subsets of $\overline{G}$ such that $A_1 \cup A_2 = \overline{G}$, we have $X(\overline{G}) = X(A_1) \times X(A_2)$, and we may write $\overline{Q} \in X(\overline{G})$ as $\overline{Q} = [Q_1, Q_2]$ with $Q_j \in X(A_j)$.

The first discrete version of $\mathcal{F}_{LG}$ we consider will have the form

$$\overline{\mathcal{F}} = L\overline{\mathcal{F}}_2 + \overline{\mathcal{F}}_4, \tag{4}$$

with $\overline{\mathcal{F}}_2$, $\overline{\mathcal{F}}_4 : X(\overline{G}) \to \mathbf{R}$ defined by

$$\overline{\mathcal{F}}_2(\overline{Q}) = \frac{1}{4} \sum_{n,m \in \overline{G}} c(n, m)|\overline{Q}(n) - \overline{Q}(m)|^2, \tag{5}$$

where $|M|^2 = \sum_{i,j=1}^q M_{i,j}^2$, and

$$\overline{\mathcal{F}}_4(\overline{Q}) = \sum_{n \in \overline{G}} f_B(\overline{Q}(n)), \tag{6}$$

with f_B as in (2). The set Sym_0^q is a real linear space of dimension $d_q = \frac{q(q-1)}{2} - 1$ and $X(\overline{G})$ is a linear space of dimension $|\overline{G}|d_q$. The functionals $\overline{\mathcal{F}}_2$, $\overline{\mathcal{F}}_4$ are real analytic.

Equilibria are critical points of $\overline{\mathcal{F}}$ in $X(\overline{G})$ and satisfy $\nabla\overline{\mathcal{F}}(\overline{Q}) = 0$. The gradient flow is $\dot{Q} = -\nabla\overline{\mathcal{F}}(\overline{Q})$. The phase space is $X(\overline{G}) \approx \mathbf{R}^{d_q|\overline{G}|}$.

To define the discrete analogue of equations with Dirichlet boundary data, we consider (a nonempty) $\partial G \subset \overline{G}$, and choose a function $Q_b : \partial D \to \mathrm{Sym}_0^q$. Let $G = \overline{G} \setminus \partial G$. We have $X(\overline{G}) = X(G) \times X(\partial G)$. Then the second discretized version of $\mathcal{F}_{LG}$ will have the form

$$\mathcal{F} = L\mathcal{F}_2 + \mathcal{F}_4, \tag{7}$$

with $\mathcal{F}_2$, $\mathcal{F}_4 : X(G) \to \mathbf{R}$ defined by

$$\mathcal{F}_2(Q, Q_b) = \overline{\mathcal{F}}_2([Q, Q_b]), \quad \mathcal{F}_4(Q, Q_b) = \overline{\mathcal{F}}_4([Q, Q_b]), \tag{8}$$

with $\overline{\mathcal{F}}_2$, $\overline{\mathcal{F}}_4$ as in (5), (6), respectively. The functions $\mathcal{F}_2$, $\mathcal{F}_4$ are real analytic.

Equilibria are critical points of $\mathcal{F}$ in $X(G)$ and satisfy the equations $\nabla_Q\mathcal{F}(Q, Q_b) = 0$. The gradient flow is $\dot{Q} = -\nabla_Q\mathcal{F}(Q, Q_b)$. The phase space is $X(G) \approx \mathbf{R}^{d_q|G|}$. The function Q_b represents Dirichlet data at ∂G.

We consider the problem of continuation of $L = 0$ solutions in the discrete setting. To state our main results we consider first the discrete critical point equations for $L = 0$. At $L = 0$ the equations for the critical points of $\overline{\mathcal{F}}$, $\mathcal{F}$

at different sites decouple and it suffices to study solutions of the d_q equations

$$\nabla f_B(Q) = 0, \tag{9}$$

with $Q \in \mathrm{Sym}_0^q$.

The solutions for cases $q = 2$, 3 are well-known [15,18]. We focus on the case $q = 2$, where $d_q = 2$.

Proposition 1 *The set of critical points of f_B in $Sym_0^2 \approx \mathbf{R}^2$ is the union of the following disjoint sets: (i) the origin $\{0\}$, and (ii) an embedded manifold $\Sigma^2 \approx S^1$. The infimum of f_B in Sym_0^2 is attained at the points of Σ^2.*

The critical points of $\overline{\mathcal{F}}_4$, $\mathcal{F}_4$ are, therefore, maps from $\overline{G}$, G, respectively, to either Σ^2 or the origin. We classify them according to their support.

Denote the 1-torus (i.e. the circle S^1) by $\mathbf{T}$. Then the set of maps from $\overline{G}$ to $\{0, \Sigma^2\}$ and support in U is

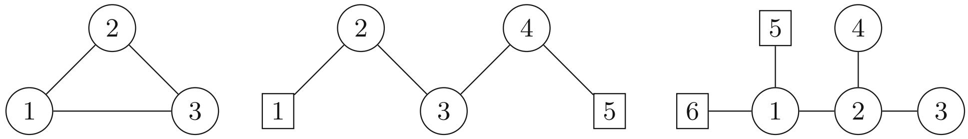

Fig. 1 Examples of graphs with and without boundaries. Circles represent interior points. Squares represent boundary points, where the value of Q is fixed

denoted by $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$. By Proposition 1, $\mathcal{C}_0(\overline{\mathcal{F}}_4, U) \approx \mathbf{T}^{|U|}$. Similarly, the set of maps from G to $\{0, \Sigma^2\}$ and support in U is denoted by $\mathcal{C}_0(\mathcal{F}_4, U)$. By Proposition 1, $\mathcal{C}_0(\overline{\mathcal{F}}_4, U) \approx \mathbf{T}^{|U|}$. The sets $\mathcal{C}(\mathcal{F}_4, U)$, $U \subset G$, are independent of the choice of the boundary data.

Note that given two different subsets U, V of $\overline{G}$ with nonempty union, the corresponding sets $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$, $\mathcal{C}_0(\overline{\mathcal{F}}_4, V)$ are disjoint. A similar statement holds for manifolds of critical points of $\mathcal{F}_4$.

The main question we address is which of the $L = 0$ equilibria can be continued to solutions of the $L > 0$ problem. We will present necessary and sufficient conditions.

We note that the most interesting case is the continuation of critical points that are minima of $\overline{\mathcal{F}}_4$, and $\mathcal{F}_4$. We will see that this corresponds to critical points in $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$, with $U = \overline{G}$, and $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$ with $U = G$, respectively All other critical points will be shown to be unstable under $-\nabla\overline{\mathcal{F}}_4$, $-\nabla\mathcal{F}_4$, respectively. Their continuation is also expected to be unstable. We include them because they may be of dynamical interest. Also the continuation argument is the same for all choices of U.

We first state the results for the case without boundaries. The discretized functional $\overline{\mathcal{F}}$ then has a global $SO(2)$ symmetry defined in the next section. A consequence is that the critical points of $\overline{\mathcal{F}}$ are not isolated.

Lemma 1 *Let $q = 2$, then every critical point of $\overline{\mathcal{F}}$ belongs to a circle of critical points of $\overline{\mathcal{F}}$.*

We first state a (necessary) condition that must be satisfied by a one parameter family $Q(L)$, $L \in [0, \epsilon_0)$, of critical points of $\overline{\mathcal{F}} = L\overline{\mathcal{F}}_2 + \overline{\mathcal{F}}_4$ that is continued from a $L = 0$ critical point that belongs to $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$.

Proposition 2 *Let $q = 2$. Let $Q(L) \in Sym_0^q$ be a critical point of $\overline{\mathcal{F}} = L\overline{\mathcal{F}}_2 + \overline{\mathcal{F}}_4$, for every $L \in [0, \epsilon_0]$. Assume also that $Q(L)$ is C^1 in $[0, \epsilon_0]$ and that there exists $U \subset \overline{G}$ such that $Q(0) \in \mathcal{C}_0(\overline{\mathcal{F}}_4, U)$. Then $Q(0)$ is a critical point of $\overline{\mathcal{F}}_2$, restricted to $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$.*

Thus, the continued branches must be critical points of the quadratic functional $\overline{\mathcal{F}}_2$, restricted to the $|U|$-torus $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$. The equation for these critical points will be referred to as the reduced (or bifurcation equation) at $L = 0$. Note that the assumed critical points belong to circles of critical points. This fact is not essential for stating the necessary condition.

The second result states that satisfying the bifurcation equation at $L = 0$ is also a sufficient condition for continuation, provided an additional nondegeneracy condition is also satisfied.

A manifold M of critical points of $\overline{\mathcal{F}}$ is *nondegenerate* if for every $Q \in M$ the nullspace of $\nabla^2\overline{\mathcal{F}}(Q)$ has dimension $\dim(M)$.

We then show that nondegenerate solutions of the bifurcation equation at $L = 0$ can be continued to circles of equilibria of the $L \neq 0$ problem.

Proposition 3 *Let $q = 2$. Let U be a nonempty subset of $\overline{G}$. Suppose that $\mathcal{S}_0$ is a nondegenerate circle of critical points of $\overline{\mathcal{F}}_2$, restricted to $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$. Then there exists $L(\psi_0) > 0$ and a unique one-parameter real analytic family $\mathcal{S}(L)$, $|L| < L(\psi_0)$, of circles of critical points of $\overline{\mathcal{F}}(Q) = L\overline{\mathcal{F}}_2(Q) + \overline{\mathcal{F}}_4(Q)$, for all $L \in [0, L(\psi_0))$, that also satisfies $\mathcal{S}(0) = \mathcal{S}_0$.*

The results for the discrete problem with boundary are similar. In this case the energy $\mathcal{F}$ does not have the global $SO(2)$ symmetry. This is due to the presence of boundary data, specifically pairwise interaction terms in $\mathcal{F}_2$ involving a site in the "interior" G and the "boundary" ∂G. As the boundary values are kept fixed, we can not apply the symmetry to them. A consequence of the lack of this symmetry is that critical points of $\mathcal{F}$ can be isolated.

The first statement is a necessary condition for branches $Q(L)$, $L \in [0, \epsilon_0)$, of critical points of $\mathcal{F} = L\mathcal{F}_2 + \mathcal{F}_4$ that are continued from $L = 0$ critical points.

Proposition 4 *Let $q = 2$. Let $Q_b : \partial G \to Sym_0^2$. Let $Q(L) \in Sym_0^2$ by a critical point of $\mathcal{F} = L\mathcal{F}_2(Q, Q_b) + \mathcal{F}_4(Q, Q_b)$, for every $L \in [0, \epsilon_0]$. Assume also that $Q(L)$ is C^1 in $[0, \epsilon_0]$ and that there exists a nonempty $U \subset G$ such that $Q(0) \in \mathcal{C}_0(\mathcal{F}_4, U)$. Then $Q(0)$ is a critical point of $\mathcal{F}_2$ restricted to $\mathcal{C}_0(\mathcal{F}_4, U)$.*

The equation for the critical points of $\mathcal{F}_2$ restricted on the $|U|$-torus $\mathcal{C}_0(\mathcal{F}_4, U)$ is the bifurcation or reduced equation at $L = 0$. We note here that the boundary conditions will appear in the bifurcation equations through the pairwise couplings between sites of G and ∂G.

Nondegenerate solutions of the bifurcation or reduced equation at $L = 0$ can also be continued to equilibria of the $L = 0$ functional. Nondegeneracy here means nondegeneracy of the Hessian of the reduced functional $\mathcal{F}_2$ restricted to $\mathcal{C}_0(\mathcal{F}_4, U)$ at the critical point.

Proposition 5 *Let $q = 2$. Let U be an nonempty subset of G Also let $Q_b : \partial G \to Sym_0^2$. Suppose that ψ_0 is a nondegenerate critical point of $\mathcal{F}_2(\cdot, Q_b)$, restricted to $\mathcal{C}_0(\mathcal{F}_4, U)$. Then there exists $L(\psi_0) > 0$ and a unique one-parameter real analytic family $Q(L, \psi_0)$, $|L| < L(\psi_0)$ satisfying (i) $Q = Q(L, \psi_0)$ is a critical point of $\mathcal{F}(Q, Q_b) = L\mathcal{F}_2(Q, Q_b) + \mathcal{F}_4(Q, Q_b)$, for all $L \in [0, L(\psi_0))$, and (ii) $Q(0; \psi_0) = Q_0$.*

A subcase of special interest is that of $U = G$, with the image Q_b in Σ^2.

The above connect the continuation of the anticontinuous limit solutions to properties of critical points of the $\overline{\mathcal{F}}_2$, and $\mathcal{F}_2$ restricted to the $|U|$-tori $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$, and $\mathcal{C}_0(\mathcal{F}_4, U)$, respectively. The corresponding bifurcation equations at $L = 0$ are guaranteed to have solutions precisely because of the variational structure. However, finding these solutions and verifying the nondegeneracy conditions is a nontrivial problem and will in most cases require numerical computation. A few explicit solutions are known from studies of the discrete vortices of the DNLS [23], and this is due to the fact that the bifurcation equations of the present problem coincide with ones seen in the DNLS problem. This becomes clear in the next section.

The continuation results allow us to determine the solutions of the $L = 0$ problem that can be continued for $L \neq 0$ by solving equations for the variables parametrizing sets of the $L = 0$ equilibria, i.e. the $|U|$-tori. It should be emphasized that the $L \neq 0$ solutions have additional components. These components are given by a function that is defined on the $|U|$-tori. The existence of this function is described in Lemma 3 in the next section.

The continuation results above do not depend on the sign of L. The range $L < 0$ is not physical, but the observation underlines the methods used in the proofs. (The sign of L will affect the stability of the gradient flows.) We will not address the stability of continued solutions in detail here. The stability in the directions on the $|U|$-tori requires a detailed analysis. These directions belong to the kernel of the linearization around these equilibria at $L = 0$. In all other directions we see persistence of stable and unstable directions as we vary L. Thus unstable $L = 0$ equilibria that can be continued remain unstable.

In the special case where $U = \overline{G}$ (for $\overline{\mathcal{F}}_2$) and $U = G$ and $Q_b \in \Sigma^2$ (for $\mathcal{F}_2$), these critical points coincide with critical points of a suitable discretization of the Oseen–Frank functional. The discretization of Oseen–Frank energy follows along the lines of the discretization of the Landau–de Gennes energy above, and is given in the next section, see (36), (37).

Proposition 6 *Let $q = 2$. (i) Let $U = \overline{G}$. Then critical points of the function $\overline{\mathcal{F}}_2$, restricted to $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$ are in a one-to-one correspondence with critical points of suitable discretization of the Oseen–Frank functional on functions on $\overline{G}$, see (36). (ii) Let $U = \overline{G}$, and consider a Q_b with values in Σ^2. Then critical points of the function $\mathcal{F}_2$, restricted to $\mathcal{C}_0(\mathcal{F}_4, U)$ are in a one-to-one correspondence with critical points of a suitable discretization of the Oseen–Frank functional on functions on G that also depends on Q_b, see (37).*

Thus, the equilibria of the decoupled Landau–de Gennes energy that satisfy the necessary continuation condition are Oseen–Frank equilibria. Following the observation for arbitrary U, the continued Landau–de Gennes $L \neq 0$ equilibria have additional components that are however a function of the Oseen–Frank variables. This function is constructed in Lemma 3. Comparing with [23], we see that the equation for Oseen–Frank equilibria is the bifurcation equation for the continuation of DNLS breathers.

The calculations used to prove the above imply the existence of normally hyperbolic submanifolds of the Landau–de Gennes flow. We use the definition of normal hyperbolicity in [30].

Proposition 7 *Let $q = 2$. Let $r \geq 1$. (i) Let U be a subset of $\overline{G}$. Then set $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$ is r-normally hyperbolic under the flow of $-\nabla\overline{\mathcal{F}}_4$. Let $U^c = \overline{G} \setminus U$. Every point of $\mathcal{C}_0(\overline{\mathcal{F}}_4, U_1)$ has $2|U^c|$ unstable directions, and $|U|$ stable directions. (ii) Let $Q_b : \partial G \to Sym_0^q$. Let U be a subset of G. Then set $\mathcal{C}_0(\mathcal{F}_4, U)$ is r-normally hyperbolic under the flow of $-\nabla_Q\overline{\mathcal{F}}_4(Q; Q_b)$. Let $U^c = G \setminus U$. Every point of $\mathcal{C}_0(\overline{\mathcal{F}}_4, U_1)$ has $2|U^c|$ unstable directions, and $|U|$ stable directions.*

The appearance of normal hyperbolicity is a consequence of the gradient structure of the flow, the dimensionality of the target space, and the additional local $SO(2)$ symmetry of the $L = 0$ problem.

The role of normal hyperbolicity in this problem can be explored further. A first consequence of normal hyperbolicity at $L = 0$ that all the invariant sets $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$ and $\mathcal{C}_0(\mathcal{F}_4, U)$ persist for $|L|$ sufficiently small, see e.g. [30]. In the case of empty U^c, and $L > 0$, the Landau–de Gennes gradient flow on the invariant manifold is a deformed version of the Oseen–Frank flow. In addition we can argue that the $L \neq 0$ critical points of the continuation results above must belong to the $L \neq 0$ perturbed invariant manifolds. Note that in the case $L = 0$ the invariant set of the Landau–de Gennes flow is stable only for $U = G$, $U^c = \emptyset$. This also implies linear instability of the continued equilibria for $U^c \neq \emptyset$. These considerations also explain why extensions to the case of infinite lattices with empty U^c are not immediate. We further comment on this point in the last section.

3 Continuation of anticontinuous limit solutions, bifurcation equation, and Oseen–Frank model

In this section, we present proofs of the results. The proofs of Propositions 2, 4 (necessary conditions) and 3, 5 (sufficient conditions) follow along the lines of [25]. We here present somewhat extended versions, with some added details. The main step is Lemma 3, allowing us to reduce the equation for critical points of $\overline{\mathcal{F}}$, $\mathcal{F}$ for small $|L|$ to an equation for the angular variables along the $L = 0$ critical points. This is the bifurcation (or reduced) equation. The argument uses the implicit function theorem, see [4], ch. 4, for the real analytic version. The reduced equation we present here is global, i.e. valid on the whole $|U|$-torus. We also emphasize that in the case without boundaries the function giving us the other components is equivariant under the global $SO(2)$ symmetry. The necessary conditions for continuation follow by examining the structure of the bifurcation equation at $L = 0$. The sufficient conditions follow from the implicit function theorem and symmetry considerations for the $L = 0$ bifurcation equation.

Proposition 6, connecting the bifurcation equation to discrete Oseen–Frank equilibria in the case of empty U^c, follows from a straightforward computation. We include the connection to the the bifurcation equation for DNLS breathers [23,24]. Also, Proposition 7 follows from the definition of normal hyperbolicity (that we do not include), see [30], pp. 20–22.

The first step is an analysis of the critical points of f_B of (2), and of the $L = 0$ critical points of $\overline{\mathcal{F}}$, $\mathcal{F}$. Considering f_B, we write the Q-tensor as

$$Q = \begin{bmatrix} q_1 & q_2 \\ q_2 & -q_1 \end{bmatrix}, \tag{10}$$

we then have by (2)

$$f_B(Q) = -a^2(q_1^2 + q_2^2) + c^2(q_1^2 + q_2^2)^2. \tag{11}$$

Using polar coordinates $q_1 = r\cos\psi$, $q_2 = r\sin\psi$, and $f_B(Q) = -a^2r^2 + c^2r^4$.

Therefore, the set of critical points of f_B in Sym_0^2 consists of (i) the origin, (ii) the set (circle) of points

$$r = \frac{a}{\sqrt{2}c}, \quad \psi \in [0, 2\pi). \tag{12}$$

Lemma 2 *The critical sets of f_B in Sym_0^2 are nondegenerate. At the origin we have $\nabla^2 f_B(0) = -2a^2 I$, I the 2×2 identity. At the circle (12) we have $f_B''(\frac{a}{\sqrt{2}c}) = 4a^2$. The other entries of the Hessian in polar coordinates vanish on this set.*

Proof The statements follow from (11). □

Proof of Proposition 1 (i): We immediately have the critical points of the statement, with Σ^2 the circle (12). By (11), f_B is coercive and by Lemma 2 the infimum of f_b is attained on Σ^2. □

Thus any solution $\overline{Q}$ of $\nabla\overline{\mathcal{F}}_4 = 0$ is specified by a set $U \subset \overline{G}$, and a function $\Theta : U \to \mathbf{T}$, and is given by

$$\begin{aligned} r(n) &= \frac{a}{\sqrt{2}c}, \quad \psi(n) = \Theta(n), \quad n \in U; \\ \overline{Q}(n) &= 0, \quad n \in U^c, \end{aligned} \tag{13}$$

where $U^c = \overline{G} \setminus U$.

Similarly, any solution Q of $\nabla_Q \mathcal{F}_4(Q; Q_b) = 0$ is specified by a set $U \subset G$, and a function $\Theta : U \to \mathbf{T}$, and is given by

$$\begin{aligned} r(n) &= \frac{a}{\sqrt{2}c}, \quad \psi(n) = \Theta(n), \quad n \in U; \\ Q(n) &= 0, \quad n \in U^c, \end{aligned} \tag{14}$$

where $U^c = G \setminus U$. Here the static solution is also determined by the boundary data Q_b.

Note that, considering the linear stability of critical points (13), (14) under the flows $-\nabla\overline{\mathcal{F}}_4, -\nabla_Q\mathcal{F}_4(Q; Q_b)$, respectively, every point in U^c leads to two unstable directions. Continuations of $L = 0$ equilibria (13), (14) with nonempty U^c will also be unstable by standard perturbation arguments for symmetric matrices [12].

To study of critical points of $\overline{\mathcal{F}}$ and $\mathcal{F}$, we may use different coordinate systems for the target space Sym_0^2 at each site n of $\overline{G}$ and G respectively. We refer to the coordinates q_1, q_2 of (10) as *Cartesian* coordinates. The coordinates r, θ above will be referred as *polar* coordinates. The polar and Cartesian coordinate systems are diffeomorphic in the vicinity of the circle of (12).

To prove the results we parametrize a neighborhood of the tori $\mathbf{T}^{|U|}$ of $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$, $\mathcal{C}_0(\mathcal{F}_4, U)$ in $X(\overline{G})$, $X(G)$, respectively, using mixed polar-Cartesian coordinates

$$\psi(n) \in \mathbf{R}, \quad \rho(n) \in V, \quad n \in U, \tag{15}$$

with V an open interval in $\mathbf{R}$, and

$$x(n) \in \mathbf{R}^2, \quad n \in U^c, \tag{16}$$

where $U^c = \overline{G} \setminus U$ or $G \setminus U$.

The variable $\psi(n)$ belongs to $\mathbf{R}$, which covers $\mathbf{T}$ at the site $n \in U$. The $\rho(n)$ parametrize the directions that are transverse to the circle $\mathbf{T}$ on the plane. We are interested in the critical points of functions on $\mathbf{R}^{|U|} \times V^{|U|} \times \mathbf{R}^{2|U^c|}$ that are 2π-periodic in the first $|U|$ variables $\psi(n)$, $n \in U$.

In particular, let $\mathcal{G}$ be either $\overline{\mathcal{F}}$ or $\mathcal{F}$ with U, U^c defined as above for each case. Then $\mathcal{G}$ is a real-valued function on $\mathbf{R}^{|U|} \times V^{|U|} \times \mathbf{R}^{2|U^c|}$ that is 2π-periodic on each variable $\psi(n)$, $n \in U$.

Configurations in $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$ or $\mathcal{C}_0(\mathcal{F}_4, U)$ are of the form $[\psi \mathrm{mod}(2\pi), \rho_0, 0]$, with $\psi \in \mathbf{R}^{|U|}$. The vector ρ_0 can be the origin, i.e. choosing V to an interval around the radius $a/\sqrt{2}c$ in (13) or (14). We can then write any $Q \in X(\overline{G})$, $X(G)$ in the neighborhood of the sets $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$, $\mathcal{C}_0(\mathcal{F}_4, U)$ respectively as $[\psi \mathrm{mod}(2\pi), \rho, x]$, $\psi \in \mathbf{R}^{|U|}$, $\rho \in V^{|U|}$, $x \in \mathbf{R}^{2|U^c|}$.

We let

$$g_n = \partial_{\psi_n}\mathcal{G}, \quad n \in U; \tag{17}$$

$$h_n = \partial_{\rho_n}\mathcal{G}, \quad n \in U; \tag{18}$$

$$f_n^j = \partial_{x_n^j}\mathcal{G}, \quad n \in U^c, \quad j = 1, 2. \tag{19}$$

Denoting the corresponding vectors by $g \in \mathbf{R}^{|U|}$, $h \in \mathbf{R}^{|U|}$, $f \in \mathbf{R}^{2|U^c|}$, and letting $z = [\rho, x] \in V^{|U|} \times \mathbf{R}^{2|U^c|}$, we let

$$\begin{aligned} F_\psi(\psi, z, L) &= g(\psi, z, L), \\ F_z(\psi, z, L) &= [h(\psi, z, L), f(\psi, z, L)]. \end{aligned} \tag{20}$$

Both F_ψ, F_z are 2π-periodic in each variable $\psi(n)$, $n \in |U|$.

Then critical points of $\mathcal{G}$ in the vicinity of $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$ (for $\mathcal{G} = \overline{\mathcal{F}}$) or $\mathcal{C}_0(\mathcal{F}_4, U)$ (for $\mathcal{G} = \mathcal{F}$) are solutions of

$$F_\psi(\psi, z, L) = 0, \quad F_z(\psi, z, L) = 0. \tag{21}$$

This follows form the fact that polar-Cartesian coordinate system is nonsingular in the neighborhood of the sets $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$ (for $\mathcal{G} = \overline{\mathcal{F}}$) and $\mathcal{C}_0(\mathcal{F}_4, U)$ (for $\mathcal{G} = \mathcal{F}$).

We note that $\overline{\mathcal{F}}$ is invariant under the global $SO(2)$ action

$$\overline{Q}(m) \mapsto A\overline{Q}(m)A^T, \quad m \in \overline{G}, \tag{22}$$

where A is an arbitrary special orthogonal 2×2 matrix. Let A be rotation by an angle ϕ. In the region where the polar-Cartesian system is defined, this action has the form $\psi(j) \mapsto \psi(j) + 2\phi$, $\rho(j) \mapsto \rho(j)$ at the sites $j \in U$, and $x(j) \mapsto A^2 x(j)$ at the sites $j \in U^c$.

Proof of Lemma 1 By a standard argument the image of any critical point of $\overline{F}$ under (22), $A \in SO(2)$ arbitrary, is also a critical point of $\overline{F}$. Also the orbit of any point under the action (22), $A \in SO(2)$ arbitrary, is a circle. □

Lemma 3 *Let $q = 2$, and let $\mathcal{G} = \overline{\mathcal{F}}$ or $\mathcal{F}$. (i) There exists $L_0 > 0$ such that for every $\psi \in \mathbf{R}^{|U|}$ and $L \in (-L_0, L_0)$ there exists a unique $z(\psi, L) \in V^{|U|} \times \mathbf{R}^{2|U^c|}$ satisfying*

$$F_z(\psi, z(\psi, L), L) = 0. \tag{23}$$

The solution $z(\psi, L)$ is 2π-periodic in each $\psi(n)$, $n \in |U|$, real analytic in ψ, $\forall \psi \in \mathbf{R}^{|U|}$, and L, $\forall L \in (-L_0, L_))$, and satisfies $z(\psi, 0) = z_0 = [\rho_0, 0]$. (ii) In the case where $\mathcal{G} = \overline{\mathcal{F}}$, $z(\psi, L) = [x(\psi, L), \rho(\psi, L)]$ has the following equivariance property, $\forall L \in (-L_0, L_0)$: let $\tilde{\psi}(j) = \psi(j) + \phi$, $j \in |U|$, ϕ an arbitrary real. Let A be the matrix of rotation by $\phi/2$ on the plane. Then $z(\tilde{\psi}, L) = [\tilde{x}, \tilde{\rho}]$, where $\tilde{x}(j) = Ax(j)$, $\forall j \in U^c$, and $\tilde{\rho}(j) = \rho(j)$, $\forall j \in U$.

Proof (i) Fix $\psi \in \mathbf{R}^{|U|}$. The solution of $F_z(\psi, z, 0)$ is $z_0 = [\rho_0, 0]$. We first want to show that there is a unique one-parameter family $z(\psi, L)$, $L \in (-\epsilon, \epsilon)$ for some $\epsilon > 0$ satisfying $F_z(\psi, z(\psi, L), L) = 0$. We want to apply the implicit function theorem, and we first need to check that the derivative $D_z F_z(\psi, z_0, 0)$ of F_z with respect to z at $L = 0$ is invertible. We have

$$D_z F_z(\psi, z_0, 0) = \begin{bmatrix} \nabla^2_\rho \mathcal{G}(\psi, z_0, 0) & 0 \\ 0 & \nabla^2_x \mathcal{G}(\psi, z_0, 0) \end{bmatrix}. \tag{24}$$

The block-diagonal structure is due to the fact that the z and ρ components come from uncoupled sites in U^c, U, respectively. Similarly, by lack of coupling between the sites at $L = 0$ it suffices to examine f_B at its critical points.

We consider first the origin. Using (10), (11), and Lemma 2,
we have

$$\nabla^2_x \mathcal{G}(\psi, z_0, 0) = -2a^2 I, \tag{25}$$

with I the $2|U^c| \times 2|U^c|$ identity. For the sites of U, we have by Lemma 2

$$\nabla^2_\rho \mathcal{G}(\psi, z_0, 0) = 4a^2 I, \tag{26}$$

with I the $|U| \times |U|$ identity.

Combining (24), (25), (26), $D_z F_z(\psi, z_0, 0)$ is nonsingular. The function F_z is real analytic in z and L in the vicinity of $z = z_0$ and $L = 0$, and we can apply the analytic implicit function theorem, see, e.g. [4], to obtain the one-parameter family of solutions $z(\psi, L)$ of $F_z = 0$, $|L| < \epsilon$. Furthermore, $z(\psi, 0) = z_0$. The statement holds for arbitrary ψ and by the 2π-periodicity of F_z in the variables $\psi(n)$, $n \in |U|$, $z(\psi, L)$ is also 2π-periodic in the $\psi(n)$, $\forall n \in |U|$. By the compactness of $\mathbf{T}^{|U|}$ we may choose $\epsilon = L_0$ independent of ψ. Since F_z is also real analytic in ψ, the implicit function theorem with ψ as a parameter implies that z is also real analytic in ψ.

To show (ii), we claim that by the global $SO(2)$ symmetry of $\overline{\mathcal{F}}$, applying (22) to each site, A rotation by $\phi/2$, to a solution $[\psi, z]$, $z = [\rho, x]$, of the second equation of (21), we obtain another solution $[\tilde{\psi}, \tilde{z}]$ of the second equation of (21), where $\tilde{\psi}(j) = \psi(j) + \phi$, $\forall j \in |U|$, $\tilde{z} = [\tilde{\rho}, \tilde{x}]$, $\tilde{\rho}(j) = \rho(j)$, $\forall j \in |U|$, $\tilde{x}(j) = Ax(j)$, $\forall j \in U^c$.

By uniqueness of the solution for each ψ, assuming $|L| < L_0$, we must then have $\tilde{z}(\psi, L) = z(\tilde{\psi}, L)$, which implies the statement.

To see the claim, consider a smooth functional $\mathcal{L}$ in $\mathbf{R}^m = V_1 \times V_2$, $V_j = \mathbf{R}^{m_j}$, and a diffeomorphism h in $\mathbf{R}^m$ such that $\mathcal{L} \circ h = \mathcal{L}$ in $\mathbf{R}^m$. Assume also that $h = [h_1, h_2]$, where the h_j are diffeomorphisms in V_j, $j = 1, 2$. Let $q = [q_1, q_2]$, and assume $D_2 \mathcal{L}(q_1, q_2) = 0$, then by the chain rule

$$D_2(\mathcal{L} \circ h)(q) = D_2 \mathcal{L}(h(q)) D h_2(q_2). \tag{27}$$

On the other hand, by $\mathcal{L} \circ h = \mathcal{L}$ in $\mathbf{R}^m$, and q a solution of $D_2 \mathcal{L} = 0$ we have

$$D_2(\mathcal{L} \circ h)(q) = D_2(\mathcal{L})(q) = 0.$$

Then the fact that $D h_2(q_2))$ is nonsingular and (27) imply $D_2 \mathcal{L}(h_1(q_1), h_2(q_2)) = 0$. The claim follows by letting $\psi \in V_1$, $z \in V_2$, and $h_1(\psi) = \tilde{\psi}$, $h_2(z) = \tilde{z}$. □

We remark that in the case $\mathcal{G} = \mathcal{F}$, F_z and F_ψ also depend on the boundary values Q_b. This parameter does not affect the linearization around the $L = 0$ solution, but does affect the size of the perturbation for $L \neq 0$. Since the perturbation includes terms arising from the coupling terms $\overline{\mathcal{F}}_2$, $\mathcal{F}_2$, we expect that in near $\psi \in \mathbf{T}^{|U|}$ with larger difference between $Q(n) \in \Sigma^2$

at neighboring sites the interval of L for which we can continue is expected to become smaller. These details of the problem are glossed over by compactness, but are worth examining further in examples. (As in [17] we may want to assume that Q_b takes values in Σ^2.) Another hidden parameter is the set G, e.g. a larger graph would affect the size of the $L \neq 0$ perturbation. Here a relevant question is the behavior as we refine a grid that approximates a domain.

By Lemma 3, for L sufficiently near the origin, solutions of (21) are determined by solutions of the first equation of (21) with $z(\psi, L)$ a solution of the second equation of (21). Thus, the problem is reduced to solving the the reduced (or bifurcation) equation

$$g(\psi, z(\psi, L), L) := F_\psi(\psi, z(\psi, L), L) = 0, \quad \psi \in \mathbf{T}^{|U|}. \tag{28}$$

Given a solution ψ of the reduced equation, the components ρ, x of the critical equilibrium are given by $z(\psi, L)$.

Note also that a local version of the reduction lemma above is also possible. In such a version the interval of L will depend on the point $\psi \in \mathbf{T}^{|U|}$ around which we apply the implicit function theorem. The reduced equation is again (28) but can be valid for a larger interval of L. This may be of interest for further study. The constant $L_0 > 0$ of Lemma 3 exists by compactness, but also takes into account the worst case scenario from configurations that may not be near interesting solutions of the reduced equations.

The continuation conditions are obtained by the bifurcation equation at $L = 0$. The proof also implies that the bifurcation equation has a variational structure.

Proof of Propositions 2, 4 Let

$$\mathbf{g}(\psi, L) := g(\psi, z(\psi, l), L), \tag{29}$$

g as in (28), then by (17), and Eq. (23) for $z(\psi, L)$, we have

$$\mathbf{g}(\psi, L) = \nabla_\psi \mathcal{G}(\psi, z(\psi, L), L). \tag{30}$$

Letting also $\mathcal{G}_2$ be $\overline{\mathcal{F}}_2$ or $\mathcal{F}_2$ (for Propositions 2, 4, respectively) we see that since both $\mathcal{F}_4$ and $\overline{\mathcal{F}}_4$ are independent of the angular variables ψ, (30) is

$$\mathbf{g}(\psi, L) = \nabla_\psi L \mathcal{G}_2(\psi, z(\psi, L)). \tag{31}$$

By the real analyticity of the functions z and $\mathcal{G}$, we can expand $\mathbf{g}$ in powers of L as

$$\mathbf{g}(\psi, L) = \sum_{k=1}^{\infty} L^k \mathbf{g}_k(\psi), \quad |L| < L_0. \tag{32}$$

The lowest order term is

$$\mathbf{g}_1(\psi) = \nabla_\psi \mathcal{G}_2(\psi, z(\psi, 0)) = \nabla_\psi \mathcal{G}_2(\psi, z_0). \tag{33}$$

By the hypothesis of Propositions 2, 4, and Lemma 3, we have a branch $\psi(L)$, $L \in [0, \epsilon_0)$, of solutions of $\mathbf{g}(\psi(L), L) = 0$, and, therefore,

$$L^{-1}\mathbf{g}(\psi(L), L) = 0, \quad \forall L \in (0, \epsilon_0). \tag{34}$$

Taking the limit $L \to 0^+$, and using (32), (33), we have that $\Theta = \psi(0)$ satisfies

$$\mathbf{g}_1(\Theta) = \nabla_\psi \mathcal{G}_2(\Theta, z_0) = 0. \tag{35}$$

Using the definition of z_0, see Lemma 3, and the Q-tensors defined by (13), (14), we have the statements of Propositions 2, 4, respectively. ◻

We now give sufficient conditions for the continuation of solutions of (35) to solutions of (28) for L sufficiently near the origin. By the periodicity in the variables $\psi(j)$, $j \in |U|$, Eq. (35) always has solutions, the critical points of $\mathcal{G}_2$ on $\mathbf{T}^{|U|}$.

The difference between Propositions 3 and 5 is that in the first the problem has an extra $SO(2)$ symmetry under the global rotation $\psi(j) \mapsto \psi(j) + \phi$, $j \in U$, ϕ an arbitrary real. In particular, the invariance of $\overline{\mathcal{F}}_2 : X(\overline{G}) \to \mathbf{R}$ under (22), and the equivariance of $z(\psi, L)$ under the global rotation from Lemma 3, imply that $\overline{\mathcal{F}}_2(\psi, z(\psi, L))$ is also invariant under $\psi(j) \mapsto \psi(j) + \phi$, $j \in U$, ϕ an arbitrary real, for all $|L| < L_0$. Thus all critical points of $\overline{\mathcal{F}}_2(\psi, z_0)$, $\psi \in \mathbf{T}^{|U|}$, belong to circles, the orbits of any critical point by the global rotation.

Proof of Proposition 3 By Lemma 3 and (31), to find critical points of $\overline{\mathcal{F}}$, $|L| < L_0$, it suffices to find critical points of the functional $\mathcal{E}(\psi, L) = \overline{\mathcal{F}}_2(\psi, z(\psi, L))$, $|L| < L_0$, defined for $\psi \in \mathbf{T}^{|U|}$, i.e. z is known. We want to show the existence of critical points of $\mathcal{E}(\cdot, L)$ for $|L|$ sufficiently small by continuing critical points of $\mathcal{E}(\cdot, 0) = \overline{\mathcal{F}}_2(\cdot, z_0)$. By Lemma 3 the functional $\mathcal{E}(\psi, L)$ is real analytic and invariant under the global rotation $\psi(j) \mapsto \psi(j) + \phi$, $j \in U$, ϕ an arbitrary real, $\forall |L| < L_0$.

By the definition of nondegeneracy, the Hessian of $\overline{\mathcal{F}}_2(\cdot, z_0)$ has a one-dimensional nullspace, along the orbit of the global rotation. We use a local cooordinate system in the neighborhood of circles of critical points of $\overline{\mathcal{F}}_2(\cdot, z_0)$. These circles are parallel to the diagonal in $\mathbf{T}^{|U|}$. For example, using the variables $\varphi = [\varphi(1), \dots, \varphi(|U|)]$ defined by $\varphi = M\psi$, M an orthogonal matrix such that

$$\varphi(1) = \frac{1}{\sqrt{|U|}}[\psi(1) + \cdots + \psi(|U|)],$$

we see that $\mathcal{E}(M\varphi, L)$, is independent of φ_1, $\forall |L| < L_0$. We apply the implicit function theorem to continue uniquely in the neighborhood of nondegenerate critical points $\phi^\perp = [\phi(2), \dots, \phi(|U|)]$ of $\overline{\mathcal{F}}_2(M\phi, z_0)$. For each such $\phi^\perp$ we have a unique real analytic branch of solutions $\phi^\perp(L)$, L sufficiently near the origin, with $\phi^\perp(0) = \phi^\perp$. The value of the variable $\phi_1 \in$

$[0, 1/\sqrt{m}2\pi)$ parametrizing the circle of critical points is arbitrary and we thus have a circle of critical points of $\mathcal{E}(\cdot, L)$ in $\mathbf{T}^{|U|}$. □

Proof of Proposition 5 In this case, a nondegenerate critical point is an isolated critical point. Also the Hessian of $\mathcal{F}_2(\cdot, z_0)$ at such a point is nonsingular. The statement follows from the implicit function theorem. □

We now show the connection between the reduced functionals appearing in the bifurcation equation and discretized Oseen–Frank functionals. In the case without boundary, we discretize the Oseen–Frank functional $\mathcal{F}_{OF}$ of (3) by

$$\overline{\mathcal{F}}_{OF}(\overline{\mathbf{n}}) = \frac{1}{2} \sum_{n,m \in \overline{G}} c(n,m)|\overline{\mathbf{n}}(n) - \overline{\mathbf{n}}(m)|^2, \quad \overline{\mathbf{n}} : \overline{G} \to \mathbf{T}. \tag{36}$$

In the case where the domain has a boundary, we consider configurations $\overline{n} = [\mathbf{n}, \mathbf{n}_b]$, $\mathbf{n} : G \to \mathbf{T}$, with given boundary values $\mathbf{n}_b : \partial G \to \mathbf{T}$. The discretized Oseen–Frank functional will be then defined by

$$\mathcal{F}_{OF}(\mathbf{n}) = \overline{\mathcal{F}}_{OF}([\mathbf{n}, \mathbf{n}_b]). \tag{37}$$

Proof of Proposition 6 (i) Equation (35) is the equation for critical points of $\mathcal{F}_2$, see (5), over configurations

$$\overline{Q}(m) = \frac{a}{\sqrt{2}c} \begin{bmatrix} \cos\psi(m) & \sin\psi(m) \\ \sin\psi(m) & -\cos\psi(m) \end{bmatrix}, \tag{38}$$

for all sites $m \in \overline{G}$. In expression (5) for $\overline{\mathcal{F}}_2$, we have sums of $|\overline{Q}(n) - \overline{Q}(m)|^2$, n, $m \in \overline{G}$, and we compute

$$|\overline{Q}(n) - \overline{Q}(m)|^2 = \frac{2a^2}{c^2} \left(1 - \cos(\psi(n) - \psi(m))\right), \tag{39}$$

for all $n, m \in \overline{G}$. Consider also the discretized Oseen–Frank functional $\overline{\mathcal{F}}_{OF}$ of (36) with $\mathbf{n}(k) = [\cos\phi(k), \sin \phi(k)]$, for all $k \in \overline{G}$. We compute

$$|\mathbf{n}(n) - \mathbf{n}(m)|^2 = 2 - 2\cos(\phi(n) - \phi(m)), \tag{40}$$

for all $n, m \in \overline{G}$.

Comparing (5), (36) and (39), (40), the functionals $\overline{\mathcal{F}}_2$ and $\overline{\mathcal{F}}_{OF}$ are the same, modulo constants, and the relation $\phi(m) = \psi(m)$, for all $m \in \overline{G}$.

(ii) We use the discretized functional (37) with $\mathbf{n}(k) = [\cos\phi(k), \sin\phi(k)]$, for $k \in G$, similarly for the sites of ∂G. Thus, all pairwise interactions are as in (i), and the calculation is the same. □

The connection with the DNLS equation arises by noting that the analogue of $\overline{\mathcal{F}}_2$, restricted on $|U|$-tori is the quadratic energy functional

$$H_2 = \sum_{n,m \in \overline{G}} |A(n) - A(m)|^2,$$

restricted to the set of all $A(n) = re^{i\phi(n)}$, $\phi(n) \in \mathbf{R}$, if $n \in U$, and $A(n) = 0$ if $n \in U^c$, see, e.g. [25]. The restricted functional, denoted by h_2, is then

$$\begin{aligned} h_2 &= \sum_{n,m \in U} |A(n) - A(m)|^2 \\ &= r^2 \sum_{n,m \in U} [2 - 2\cos(\phi(n) - \phi(m)]. \end{aligned}$$

We thus recover the pairwise interactions of the discrete Oseen–Frank functional. We observe that pairwise interactions between sites in U and U^c contribute a constant term that is omitted. Similar observations apply to the case with boundary, in that case we have additional quadratic coupling between sites of G and ∂G.

Proof of Proposition 7 (i) This is immediate from Lemma 2 and the definition of r-normal hyperbolicity, see [30], p. 20-22. The dimension of $\mathcal{C}_0(\overline{\mathcal{F}}_4, U)$ is $|U|$. Each site $n \in U^c$ contributes two unstable directions. Each site $n \in U$ contributes one stable direction. (ii) The dimension of $\mathcal{C}_0(\mathcal{F}_4, U)$ is $|U|$. Each site $n \in U^c$ contributes two unstable directions. Each site $n \in U$ contributes one stable direction. □

4 Discussion

We have presented necessary and sufficient conditions for the continuation of anticontinuous limit static solutions of a discretized Landau–de Gennes functional in lattices and graphs. The construction is related to the question of continuation of breather solutions of discrete NLS equations, with some obvious differences due to the presence of boundary values, and the parabolic nature of the liquid crystal problem.

We have examined the case of 2×2 Q-tensor case for the equal constant theories. These simplifications are models of physical interest, e.g. in the experimental devices described in [1,22]. The resulting bifurcation equation is the equation for continuation of the DNLS breathers. We have also remarked that in the case where U^c non-empty the $L = 0$ and continued solutions are linearly unstable. This means that the immediate extension of the breather machinery to the continuation of finite support $L = 0$ solutions in infinite domain, as in [14,23–25], is less interesting in the nematic liquid crystal problem. Possible extensions to infinite lattices can use similar ideas, see, e.g. [3], but we need to define reasonable notions of boundary conditions. This seems possible in some domains, e.g. infinite strips. The global reduction Lemma 3 also used the compactness of the finite dimensional tori, the argument an infinite torus will require some uniform estimate of the perturbation. Another option is to use a local reduction statement to study the continuation of particular Oseen–Frank equilibria.

Also of interest is the behavior of the continuation arguments as we approximate a compact planar domain by finer grids. The discrete problem in a fixed graph does not include a precise notion of dislocations or other singularities of the continuous theories. We expect however that the discrete analogue of singularities are large differences between neighboring sites. We noted that such large differences increase the size of the perturbation and decrease the interval of L in the continuation statements. These observations can be made quantitative, this is left for future work. We note that graphs provide a simple way to approximate more general sets where these questions are relevant, such as intervals joined at one or several points. The dependence of static configurations on the boundary values is another interesting problem.

We note that we have extended some of the results of the paper for the discrete Landau–de Gennes functional with a 3×3 Q-tensor. That case has some complications that are hidden from the present work and are related to the structure of the critical set of f_B [15,18]. An additional difficulty is that the coordinate system used to find the critical points is singular at all nontrivial critical points. We have used an alternative coordinate system to show that the nontrivial critical sets are nondegenerate in a smooth sense, and that the ideas of the present paper also go through. These results will be presented in a separate manuscript.

More general Landau–de Gennes theories include models with three elastic constants [19,27]. These terms replace the term $|\nabla Q|^2$ of (1). Restriction of the generalized Landau–de Gennes energies to the uniaxial critical sets of f_B yields the well known general Oseen–Frank energies with splay, bend and twist parameters, see, e.g. [27] for the relation between the Landau–de Gennes and Oseen–Frank elastic parameters in the 3×3 case. In the discrete theory presented, the main property we use is the nondegeneracy of the critical sets of the $L = 0$ Landau–de Gennes energy. This is a property of the onsite term f_B in (1) and the results apply to more general intersite coupling energies. For instance, Lemma 3 (i) and the proof of Proposition 4 only use regularity properties of the coupling and are applicable to discrete versions of more general Landau–de Gennes coupling energies, assuming that the elastic constants vanish maintaining fixed ratios, e.g. $L_j = L\lambda_j$, $j = 1$, 2, 3, with $L \to 0^+$, see the notation of [27]. The $L = 0$ reduced equation involves the λ_j and is a necessary condition for the continuation of the anticontinuous limit equilibria. We thus have an analogue of Proposition 4 for more general discretized Landau–de Gennes coupling terms, e.g. the ones in [27]. Proposition 7 (i) on normal hyperbolicity also applies to these functionals. Necessary conditions for the continuation of anticontinuous limit equilibria require more care. The necessary condition for the case with boundary, being a nondegenerate solution of the $L = 0$ reduced equation, see Proposition 5, also applies to the general discretized Landau–de Gennes coupling terms of [27]. The case of graphs without boundary requires more care because of the role of symmetries in the arguments and the fact that some generalized Landau–de Gennes couplings have less symmetry away from the anticontinuous limit equilibria. Equivariance of the reduced equation for static solutions, as well as (nonvacuous) sufficient conditions for continuation of anticontinuous limit equilibria are not immediate and must be examined in more detail. The problem can be also examined by considering continuation from the equal elastic parameter case away from the anticontinuous limit. We plan to address some of these problems in future work.

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