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Half-Integer Point Defects in the Q-Tensor Theory of Nematic Liquid Crystals

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Abstract We investigate prototypical profiles of point defects in two-dimensional liquid crystals within the framework of Landau–de Gennes theory. Using boundary conditions characteristic of defects of index $k/2$, we find a critical point of the Landau–de Gennes energy that is characterised by a system of ordinary differential equations. In the deep nematic regime, b^2 small, we prove that this critical point is the unique global minimiser of the Landau–de Gennes energy. For the case $b^2 = 0$, we investigate in greater detail the regime of vanishing elastic constant $L \to 0$, where we obtain three explicit point defect profiles, including the global minimiser.

Keywords Nonlinear elliptic PDE system · Singular ODE system · Stability · Vortex · Liquid crystal defects

1 Introduction

Defect structures are among the most important and visually striking patterns associated with nematic liquid crystals. These are observed when passing polarised light through a liquid crystal sample and are characterised by sudden, localised changes in the intensity and/or polarisation of the light (Chandrasekhar and Ranganath 1986; Gennes 1974). Understanding the mechanism that generates defects and predicting

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their appearance and stability is one of the central objectives of any liquid crystal theory.

The mathematical characterisation of defects depends on the underlying model (Ericksen 1990; Gennes 1974; Kléman 1983; Virga 1994). In the Oseen–Frank theory, nematic liquid crystals are described by a vector field $\mathbf{n}$ defined on a domain $\Omega \subset \mathbb{R}^d$ taking values in $\mathbb{S}^{d-1}$ ($d = 2, 3$), which describes the mean local orientation of the constituent particles. Defects correspond to discontinuities in $\mathbf{n}$ Chandrasekhar and Ranganath (1986), Kléman and Lavrentovich (2006), Virga (1994) and may be classified topologically. For example, for planar vector fields in two-dimensional domains (i.e., $d = 2$ above), point defects may be characterised by the number of times $\mathbf{n}$ rotates through 2π as an oriented circuit around the defect is traversed. For nonpolar nematic liquid crystals, $\mathbf{n}$ and $-\mathbf{n}$ are physically equivalent; in this case, it is more appropriate to regard $\mathbf{n}$ as taking values in $\mathbb{RP}^{d-1}$ rather than $\mathbb{S}^{d-1}$. The classification of point defects in two dimensions then allows for both integer and half-integer indices $k/2$, $k \in \mathbb{Z}$ (Ball and Zarnescu 2011; Chandrasekhar and Ranganath 1986; Kléman and Lavrentovich 2006), as $\mathbf{n}$ is constrained to turn through a multiple of π rather than 2π on traversing a circuit. Prototypical examples of such defects are shown in Figs. 1, 2, 3 and 4.

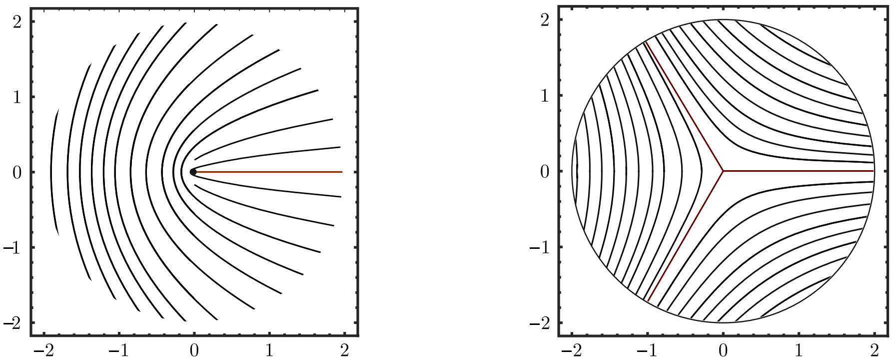


Fig. 1 Defects of index $\frac{1}{2}$ (*left*) and $-\frac{1}{2}$ (*right*)

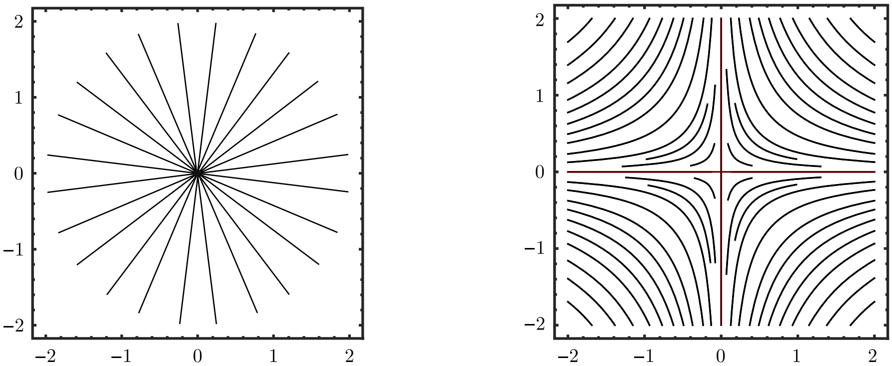


Fig. 2 Defects of index 1 (*left*) and −1 (*right*)

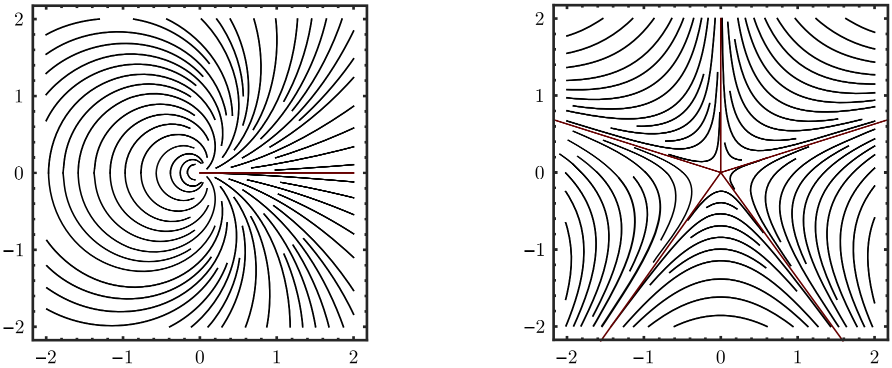


Fig. 3 Defects of index $\frac{3}{2}$ (*left*) and $-\frac{3}{2}$ (*right*)

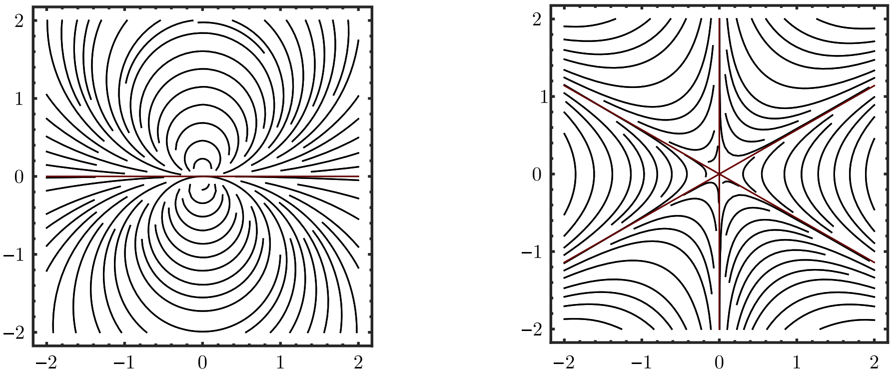


Fig. 4 Defects of index 2 (*left*) and −2 (*right*)

A deficiency of the Oseen–Frank theory is that point defects in two dimensions, which are observed experimentally, are predicted to have infinite energy; moreover, the theory does not allow for half-integer indices [see Ball and Zarnescu (2011), Gennes (1974)]. These shortcomings are addressed by the more comprehensive Landau–de Gennes Q-tensor theory Gennes (1974). In this theory, the order parameter describing the liquid crystal system takes values in the space of Q-tensors (or 3×3 traceless symmetric matrices),

$$\mathscr{S}_0 \stackrel{\text{def}}{=} \left\{ Q \in \mathbb{R}^{3\times 3},\ Q = Q^t,\ \text{tr}(Q) = 0 \right\}.$$

Equilibrium configurations of liquid crystals correspond to local minimisers of the Landau–de Gennes energy, which in its simplest form is given by

$$\mathcal{F}[Q] \stackrel{\text{def}}{=} \int_\Omega \left\{ \frac{L}{2}|\nabla Q(x)|^2 - \frac{a^2}{2}\text{tr}(Q^2) - \frac{b^2}{3}\text{tr}(Q^3) + \frac{c^2}{4}\left(\text{tr}(Q^2)\right)^2 \right\} dx. \quad (1.1)$$

Here $Q \in \mathscr{S}_0$, $L > 0$ is the elastic constant, and $a^2, c^2 > 0$, $b^2 \geq 0$ are material parameters which may depend on temperature [for more details see Gennes (1974)].

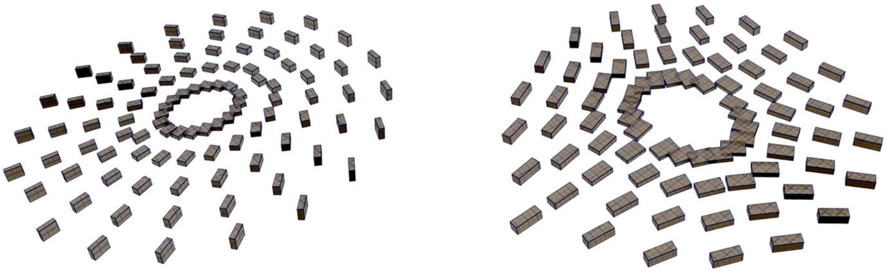


Fig. 5 Q-tensor defect of index $\frac{1}{2}$ (*left*) and $-\frac{1}{2}$ (*right*)

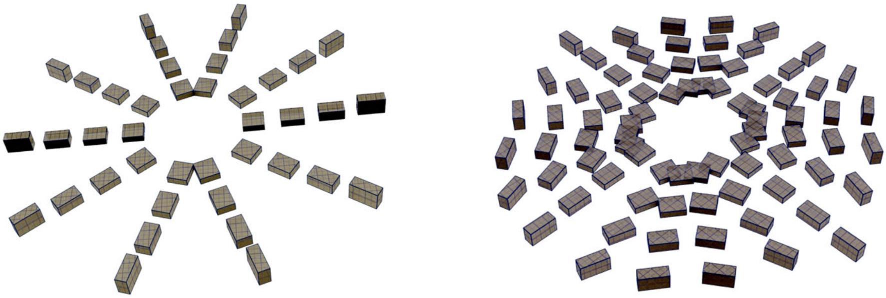


Fig. 6 Q-tensor defect of index 1 (*left*) and -1 (*right*)

One can visualise Q-tensors as parallelepipeds whose axes are parallel to the eigenvectors of $Q(x)$ with lengths given by the eigenvalues (Copara et al. 2013).[1] Figure 5 displays defects of index $\pm\frac{1}{2}$ using this representation, and Fig. 6 displays defects of index ± 1.[2]

This paper is a rigorous study of point defects in liquid crystals in two-dimensional domains using Landau–de Gennes theory. We investigate equilibrium configurations in the disc $\Omega = \{(x, y) : x^2 + y^2 < R\}$ subject to boundary conditions characteristic of prototypical defects, namely that on $\partial\Omega = \{(R\cos\phi, R\sin\phi)\}$, Q is proportional to

$$Q_k = \left(n \otimes n - \frac{1}{3}I\right), \ n = \left(\cos(\tfrac{k}{2}\phi), \sin(\tfrac{k}{2}\phi), 0\right).$$

We first introduce an ansatz

$$Y = u(r)\sqrt{2}\left(n(\varphi) \otimes n(\varphi) - \frac{1}{2}I_2\right) + v(r)\sqrt{\frac{3}{2}}\left(e_3 \otimes e_3 - \frac{1}{3}I\right), \tag{1.2}$$

[1] The careful reader will note that $\mathrm{tr}(Q) = 0$ implies that the eigenvalues cannot all be positive. In order to obtain positive lengths for the axes, we add to each eigenvalue a sufficiently large positive constant (we assume the eigenvalues of Q are bounded).

[2] The figures represent the numerically computed solutions of (3.7), (3.8) for $k = \pm 1, \pm 2$.

and note that Y satisfies the Euler–Lagrange equations (2.6) for the Landau–de Gennes energy (1.1) provided that (u, v) satisfies a system of ODEs given by (3.7), (3.8). It follows that for all parameters L, a, b, c, the ansatz Y is a critical point of the energy.

Next, we show that for every $k \in \mathbb{Z}$, the critical point Y is actually the unique global minimiser of the energy (1.1) in the low-temperature regime, i.e. for b^2 sufficiently small. Equivalently, in this regime, Y describes the unique ground-state configuration for a two-dimensional index-k point defect. In general, it is very difficult to find a global minimiser of a nonconvex energy. In this case we can deal with the nonlinearity using properties of the defect profile (u, v) and the Hardy decomposition trick Ignat et al. (2013). Similar ideas to prove global minimality are used in Shirokoff et al. (2015) for a problem in diblock copolymers.

In the case $b^2 = 0$, we also study the regime of vanishing elastic constant $L \to 0$ [see the appendix of Nguyen and Zarnescu (2013) for a discussion of the physical relevance of this regime] and show that it leads to a harmonic map problem for Y. We find three explicit solutions—two biaxial and, for even k, one uniaxial—and show that one of the biaxial solutions is the unique global minimiser of (1.1). The uniaxial critical point is analogous to the celebrated "escape in third dimension" solution of Cladis and Kléman (1992, 1972).

The profile and stability of liquid crystal defects have been extensively studied in the mathematics literature (Bauman et al. 2012; Bethuel et al. 1992; Biscari and Virga 1997; Canevari 2015; Fatkullin and Slastikov 2009; Golovaty and Montero 2013; Henao and Majumdar 2012; Ignat et al. 2014, 2015, 2013; Kralj et al. 1999; Gartland and Mkaddem 1999). Let us briefly mention a few papers which bear directly on the present work. In Kralj et al. (1999) the problem of investigating equilibria of liquid crystal systems in cylindrical domains (effectively 2D discs) was studied numerically for the Landau–de Gennes model under homeotropic boundary conditions (i.e. $k = 2$ above), subject to the so-called Lyuksyutov constraint $\mathrm{tr}(Q^2) = a^2/c^2$. The authors compare three different solutions of this model corresponding to "planar positive", "planar negative" and "escape in third dimension". They numerically explore the energies of these solutions and find a crossover between the "planar negative" and "escape in third dimension" solutions depending on the parameters b and L. For $b = 0$, the "planar negative" solution is found to have lower energy than the other two.

In recent papers Ignat et al. (2013, 2014, 2015) the radially symmetric 3D point defect, the so-called melting hedgehog, was studied within the framework of Landau–de Gennes theory. The authors investigate the profile and stability of the defect as a function of the material constants a^2, b^2, c^2. In particular, it is shown that for a^2 small enough the melting hedgehog is locally stable, while for b^2 small enough it is unstable. We utilise some ideas introduced in the liquid crystal context in these papers to derive our present results.

The paper is organised as follows: The mathematical formulation of the problem is given in Sect. 2. In Sect. 3 we introduce an ansatz Y satisfying boundary conditions characteristic of a point defect of index $k/2$, and show that Euler–Lagrange equations simplify from a system of PDEs to a system of two ODEs. We establish the existence of a solution of this system of ODEs, and thereby prove the existence of a critical point of the Landau–de Gennes energy.

In Sect. 4 we study qualitative properties of the solution in the infinitely low-temperature regime, i.e. for $b^2 = 0$. We study separately the case of fixed $L > 0$ and the limit $L \to 0$. The main result for fixed L is that for all $k \in \mathbb{Z}$, Y is the unique global minimiser of the Landau–de Gennes energy over $H^1(\Omega, \mathscr{S}_0)$. Thus, for b^2 sufficiently small, Y describes the unique ground state for point defects in 2D liquid crystals. In the limit $L \to 0$, we derive the corresponding harmonic map problem and explicitly find three solutions—two biaxial and, for even k, one uniaxial. We show that one of the biaxial solutions, Y_-, is the unique global minimiser of the Dirichlet energy. Section 5 contains a discussion of the results and an outlook on further work.

2 Mathematical Formulation of the Problem

We consider the following Landau–de Gennes energy functional on a two-dimensional domain $\Omega \subset \mathbb{R}^2$,

$$\mathcal{F}[Q] \stackrel{\text{def}}{=} \int_\Omega \frac{1}{2}|\nabla Q(x)|^2 + \frac{1}{L} f(Q)\, dx, \quad Q \in H^1(\Omega; \mathscr{S}_0). \tag{2.1}$$

Here $L > 0$ is a positive elastic constant, $\mathscr{S}_0$ denotes the set of Q-tensors defined by

$$\mathscr{S}_0 \stackrel{\text{def}}{=} \{Q \in \mathbb{R}^{3\times3},\ Q = Q^t,\ \text{tr}(Q) = 0\}$$

and the bulk energy density $f(Q)$ is given by

$$f(Q) = -\frac{a^2}{2}|Q|^2 - \frac{b^2}{3}\text{tr}(Q^3) + \frac{c^2}{4}|Q|^4,$$

where $a^2, c^2 > 0$ and $b^2 \geq 0$ are material parameters and $|Q|^2 \stackrel{\text{def}}{=} \text{tr}(Q^2)$.

We are interested in studying critical points and local minimisers of the energy (2.1) for $\Omega = B_R$, where $B_R \subset \mathbb{R}^2$ is the disc of radius $R < \infty$ centred at 0, such that Q satisfies boundary conditions corresponding to a point defect at 0 of index $k/2$. Specifically, we define

$$Q_k(\varphi) = \left(n(\varphi) \otimes n(\varphi) - \frac{1}{3}I\right), \tag{2.2}$$

where

$$n(\varphi) = \left(\cos\left(\frac{k}{2}\varphi\right), \sin\left(\frac{k}{2}\varphi\right), 0\right), \quad k \in \mathbb{Z} \setminus \{0\}, \tag{2.3}$$

and I is the 3×3 identity matrix. The boundary condition is then taken to be

$$Q(x) = s_+ Q_k(\varphi) \quad \text{for all } x \in \partial B_R, \tag{2.4}$$

where $x = (R\cos\phi, R\sin\phi)$ and

$$s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}. \tag{2.5}$$

The value of s_+ is chosen so that $s_+ Q_k$ minimises $f(Q)$. Critical points of the energy functional satisfy the Euler–Lagrange equation:

$$L\Delta Q = -a^2 Q - b^2\left[Q^2 - \frac{1}{3}|Q|^2 I\right] + c^2 Q|Q|^2 \text{ in } B_R, \quad Q = s_+ Q_k \text{ on } \partial B_R, \tag{2.6}$$

where the term $b^2\frac{1}{3}|Q|^2 I$ accounts for the constraint $\mathrm{tr}(Q) = 0$.

3 Existence of Special Solutions

In general, it is difficult to find critical points of the Landau–de Gennes energy. However, due to symmetry we are able to find a special class of solutions of the Euler–Lagrange Eq. (2.6).

We consider the following ansatz, expressed in polar coordinates $(r, \varphi) \in (0, R) \times [0, 2\pi]$:

$$Y(r, \varphi) = u(r)F_n(\varphi) + v(r)F_3, \tag{3.1}$$

where

$$F_n(\varphi) \stackrel{\text{def}}{=} \sqrt{2}\left(n(\varphi) \otimes n(\varphi) - \frac{1}{2}I_2\right), \quad F_3 \stackrel{\text{def}}{=} \sqrt{\frac{3}{2}}\left(e_3 \otimes e_3 - \frac{1}{3}I\right), \tag{3.2}$$

$n(\varphi)$ is given by (2.3) and $I_2 = e_1 \otimes e_1 + e_2 \otimes e_2$ (e_i denotes the standard basis vectors in $\mathbb{R}^3$). It is straightforward to check that $|F_n|^2 = |F_3|^2 = 1$ and $\mathrm{tr}(F_n F_3) = 0$, so that Q_k may be expressed as

$$Q_k(\varphi) = \frac{1}{\sqrt{2}}F_n(\varphi) - \frac{1}{\sqrt{6}}F_3.$$

It follows that $Y(r, \phi)$ satisfies the boundary conditions (2.4) provided

$$u(R) = \frac{1}{\sqrt{2}}s_+, \quad v(R) = -\frac{1}{\sqrt{6}}s_+. \tag{3.3}$$

Remark 3.1 For $k = 2$, $Y(r, \varphi)$ satisfies hedgehog boundary conditions (see Fig. 6, left), while for $k = \pm 1$, Y satisfies boundary conditions corresponding to a defect of index $\pm\frac{1}{2}$ (Chandrasekhar and Ranganath 1986; Kléman and Lavrentovich 2006). The $-\frac{1}{2}$-defect is also called a Y-defect because of its shape (see Fig. 5, right).

We would like to show that the ansatz (3.1) satisfies the Euler–Lagrange Eq. (2.6) provided $u(r)$ and $v(r)$ satisfy a certain system of ODEs. It is straightforward to check that

$$\Delta Y = \left(u''(r) + \frac{u'(r)}{r} - \frac{k^2 u(r)}{r^2}\right) F_n(\varphi) + \left(v''(r) + \frac{v'(r)}{r}\right) F_3 \tag{3.4}$$

and

$$Y^2 = -\sqrt{\frac{2}{3}} uv F_n(\varphi) + \frac{1}{\sqrt{6}}\left(-u^2 + v^2\right) F_3 + \frac{1}{3}|Y|^2 I, \quad |Y|^2 = u^2 + v^2. \tag{3.5}$$

Substituting (3.1), (3.4) and (3.5) into (2.6) we obtain

$$\begin{aligned} &\left(u''(r) + \frac{u'(r)}{r} - \frac{k^2 u(r)}{r^2}\right) F_n(\varphi) + \left(v''(r) + \frac{v'(r)}{r}\right) F_3 \\ &\quad = \frac{1}{L}\left(-a^2 u + \sqrt{\frac{2}{3}} b^2 uv + c^2 u\left(u^2 + v^2\right)\right) F_n(\varphi) \\ &\qquad + \frac{1}{L}\left(-a^2 v - \frac{1}{\sqrt{6}} b^2 \left(-u^2 + v^2\right) + c^2 v\left(u^2 + v^2\right)\right) F_3. \end{aligned} \tag{3.6}$$

Taking into account that the matrices $F_n(\varphi)$, F_3 are linearly independent for any $\varphi \in [0, 2\pi]$, we obtain the following coupled system of ODEs for $u(r)$ and $v(r)$:

$$\begin{aligned} u'' + \frac{u'}{r} - \frac{k^2 u}{r^2} &= \frac{u}{L}\left[-a^2 + \sqrt{\frac{2}{3}} b^2 v + c^2\left(u^2 + v^2\right)\right], \\ v'' + \frac{v'}{r} &= \frac{v}{L}\left[-a^2 - \frac{1}{\sqrt{6}} b^2 v + c^2\left(u^2 + v^2\right)\right] + \frac{1}{\sqrt{6}L} b^2 u^2, \quad r \in (0, R). \end{aligned} \tag{3.7}$$

Boundary conditions at $r = 0$ follow from requiring Y to be a smooth solution of (2.6), while boundary conditions at $r = R$ are given by (3.3), as follows:

$$u(0) = 0, \; v'(0) = 0, \quad u(R) = \frac{1}{\sqrt{2}} s_+, \quad v(R) = -\frac{1}{\sqrt{6}} s_+. \tag{3.8}$$

In order to show the existence of a solution Y of (2.6) of the form (3.1), we need to establish the existence of a solution of the system of ODEs (3.7)–(3.8). We do this using methods of calculus of variations. Substituting the ansatz (3.1) into the Landau–de Gennes energy (2.1), we obtain a reduced 1D energy functional corresponding to the system (3.7),

$$\mathscr{E}(u,v)=\int_0^R\left[\frac{1}{2}\left((u')^2+(v')^2+\frac{k^2}{r^2}u^2\right)-\frac{a^2}{2L}(u^2+v^2)+\frac{c^2}{4L}\left(u^2+v^2\right)^2\right]r\mathrm{d}r$$
$$-\frac{b^2}{3L\sqrt{6}}\int_0^R v(v^2-3u^2)\,r\mathrm{d}r. \tag{3.9}$$

The energy $\mathscr{E}$ is defined on the admissible set

$$S=\left\{(u,v):[0,R]\to\mathbb{R}^2\,\middle|\,\sqrt{r}u',\sqrt{r}v',\frac{u}{\sqrt{r}},\sqrt{r}v\in L^2(0,R),\ u(R)=\frac{s_+}{\sqrt{2}},\right.$$
$$\left.v(R)=-\frac{s_+}{\sqrt{6}}\right\}. \tag{3.10}$$

Theorem 3.2 *For every $L>0$ and $0<R<\infty$, there exists a global minimiser $(u(r),v(r))\in[C^\infty(0,R)\cap C([0,R])]\times[C^\infty(0,R)\cap C^1([0,R])]$ of the reduced energy (3.9) on S, which satisfies the system of ODEs (3.7) – (3.8).*

Proof It is straightforward to show that $\mathscr{E}(u,v)\geq -C$ for all $(u,v)\in S$. Therefore, there exists a minimising sequence (u_m,v_m) such that

$$\lim_{m\to\infty}\mathscr{E}(u_m,v_m)=\inf_S\mathscr{E}(u,v).$$

Using the energy bound, we obtain that $(u_m,v_m)\rightharpoonup(u,v)$ in $[H^1((0,R);r\,\mathrm{d}r)\cap L^2((0,R);\frac{\mathrm{d}r}{r})]\times H^1((0,R);r\,\mathrm{d}r)$ (perhaps up to a subsequence). Using the Rellich–Kondrachov theorem and the weak lower semicontinuity of the Dirichlet energy term in $\mathscr{E}$, we obtain

$$\liminf_{m\to\infty}\mathscr{E}(u_m,v_m)\geq\mathscr{E}(u,v),$$

which establishes the existence of a minimiser $(u,v)\in S$. Since (u,v) is a minimiser of $\mathscr{E}$ on S, it follows that (u,v) satisfies the Euler–Lagrange Eqs. (3.7). Then the matrix-valued function $Y:B_R(0)\to\mathscr{S}_0$ defined as in (3.1) is a weak solution of the PDE system (2.6), and thus is smooth and bounded on B_R [see for instance Majumdar and Zarnescu (2010)]. Since F_3 is a constant matrix we have that $v(r)=\mathrm{tr}(YF_3)\in C^\infty(0,R)\cap L^\infty(0,R)$. Similarly F_n is smooth on $B_R\setminus\{0\}$ hence $u(r)=\mathrm{tr}(YF_n)\in C^\infty(0,R)\cap L^\infty(0,R)$.

Furthermore, since $u\in H^1((0,R);r\,\mathrm{d}r)\cap L^2((0,R);\frac{\mathrm{d}r}{r})$ we have for any $[a,b]\subset(0,R]$ that $u\in H^1([a,b])$ hence continuous. Moreover, we have:

$$u^2(b)-u^2(a)=2\int_a^b u'(s)u(s)\,\mathrm{d}s\leq\left(\int_a^b|u'(s)|^2\,s\mathrm{d}s\right)^{\frac{1}{2}}\left(\int_a^b|u(s)|^2\,\frac{\mathrm{d}s}{s}\right)^{\frac{1}{2}}.$$

Hence, taking into account that the right-hand side of the above tends to 0 as $|b-a|\to 0$ we get that u is continuous up to 0 so $u\in C([0,R])\cap L^2((0,R);\frac{\mathrm{d}r}{r})$ and therefore $u(0)=0$.

Using the Euler–Lagrange equations for v, we obtain

$$v'(r) = \frac{1}{r}\int_0^r g(u, v)\, s\, \mathrm{d}s, r > 0$$

where $g(u, v) = \frac{v}{L}\left[-a^2 - \frac{1}{\sqrt{6}}b^2 v + c^2\left(u^2 + v^2\right)\right] + \frac{1}{\sqrt{6}L}b^2 u^2$. It follows that $\lim_{r\to 0} v'(r) = 0$. Using again the equation for v at $r = R$, we get that $v \in C^1([0, R])$. □

Remark 3.3 Using maximum principle arguments, it is possible to show [see Majumdar and Zarnescu (2010)]

$$|Y|^2 = u^2 + v^2 \leq \frac{2}{3}s_+^2.$$

4 The Case $b = 0$: Properties of Y

In this section we concentrate on the problem (3.7) for the case $b^2 = 0$. In this case, the bulk energy $f(Q)$ becomes the standard Ginzburg–Landau potential (that is, a double well potential in $|Q|^2$). We are then able to show that there is a unique global minimiser (u, v) of the energy (3.9) and that this minimiser satisfies $u > 0$ and $v < 0$ on $(0, R]$.

Lemma 4.1 *Let* $L > 0$, $0 < R < \infty$, $b^2 = 0$. *Let* (u, v) *be a global minimiser of* (3.9) *over the set* S *defined in* (3.10). *Then:*

1. $u > 0$ *on* $(0, R]$.
2. $v < 0$ *and* $v' \geq 0$ *on* $[0, R]$.

Proof We define $\tilde{u} := |u|$ and $\tilde{v} := -|v|$. We note that since $b^2 = 0$, $(\tilde{u}, \tilde{v})$ is a global minimiser of $\mathscr{E}$ on S. It follows from Theorem 3.2 that $\tilde{u} \in C^\infty(0, R) \cap C([0, R])$, $\tilde{v} \in C^\infty(0, R) \cap C^1([0, R])$ and that $(\tilde{u}, \tilde{v})$ satisfies the Euler–Lagrange Eqs. (3.7) and boundary conditions (3.8) with $b^2 = 0$.

Suppose for contradiction that $\tilde{u}(r_0) = 0$ for some $r_0 \in (0, R)$. Since $\tilde{u}$ is smooth and nonnegative, it follows that $\tilde{u}'(r_0) = 0$. On the other hand, the unique solution of the initial-value problem for the second-order regular ODE satisfied by $\tilde{u}$ (for given, fixed $\tilde{v}$):

$$\tilde{u}'' + \frac{\tilde{u}'}{r} - \frac{k^2\tilde{u}}{r^2} = \frac{\tilde{u}}{L}\left[-a^2 + c^2\left(\tilde{u}^2 + \tilde{v}^2\right)\right]$$

on (r_0, R) with initial conditions $u(r_0) = u'(r_0) = 0$ is given by $\tilde{u} \equiv 0$ identically. But this contradicts the fact that $\tilde{u}(R) = \frac{s_+}{\sqrt{2}} > 0$. Therefore, $\tilde{u} > 0$ on $(0, R)$, and since $u(R) > 0$, it follows that $u > 0$ on $(0, R]$.

A similar argument shows that $v < 0$ on $(0, R]$, which then allows us to establish that $v' \geq 0$ on $(0, R)$. Indeed, from the Euler–Lagrange equation for v, it follows that

$$v'(r) = \frac{1}{r}\int_0^r \frac{v}{L}\left[-a^2 + c^2(u^2+v^2)\right] s\,\mathrm{d}s.$$

From Remark 3.3, we get that $u^2 + v^2 \leq \frac{a^2}{c^2}$, which together with the preceding yields

$$v' \geq 0 \text{ on } [0, R].$$

Since $v(R) < 0$, it follows that $v(0) < 0$, so that $v < 0$ on $[0, R]$. □

Proposition 4.2 *Let $L > 0$, $0 < R < \infty$, $b^2 = 0$. There exists a unique solution of* (3.7)*,* (3.8) *in the class of solutions satisfying $u > 0$, $v < 0$ on $(0, R)$.*

Proof Existence follows from Theorem 3.2 and Lemma 4.1. To prove uniqueness, we use the approach of Brezis and Oswald Brezis and Oswald (1986). Suppose that (u, v) and (ξ, η) satisfy (3.7) with $u, \xi > 0$ and $v, \eta < 0$ on $(0, R)$.

We obtain

$$\frac{\Delta_r u}{u} - \frac{\Delta_r \xi}{\xi} = \frac{1}{L}\left(c^2(u^2+v^2) - c^2(\xi^2+\eta^2)\right), \tag{4.1}$$

$$\frac{\Delta_r v}{v} - \frac{\Delta_r \eta}{\eta} = \frac{1}{L}\left(c^2(u^2+v^2) - c^2(\xi^2+\eta^2)\right), \tag{4.2}$$

where $\Delta_r u = u'' + \frac{u'}{r}$. Multiplying the first equation by $\xi^2 - u^2$ and the second equation by $\eta^2 - v^2$, and then adding the two, we obtain

$$\left(\frac{\Delta_r u}{u} - \frac{\Delta_r \xi}{\xi}\right)(\xi^2 - u^2) + \left(\frac{\Delta_r v}{v} - \frac{\Delta_r \eta}{\eta}\right)(\eta^2 - v^2) = -\frac{c^2}{L}(u^2+v^2-\xi^2-\eta^2)^2.$$

Multiplying by r, integrating over $[0, R]$ and taking into account that $u(R) = \xi(R)$, $v(R) = \eta(R)$, we obtain

$$\int_0^R \left\{\left[(u/\xi)'\xi\right]^2 + \left[(\xi/u)'u\right]^2 + \left[(v/\eta)'\eta\right]^2 + \left[(\eta/v)'v\right]^2\right\} r\,\mathrm{d}r$$
$$+ \int_0^R \frac{c^2}{L}(u^2+v^2-\xi^2-\eta^2)^2\, r\,\mathrm{d}r = 0.$$

This implies $u(r) = k_1\xi(r)$ and $v(r) = k_2\eta(r)$ for some $k_1, k_2 \in \mathbb{R}$ and every $r \in [0, R]$. Therefore, due to the boundary conditions, we obtain $k_1 = k_2 = 1$, and the proof is finished. □

Now we are ready to investigate the minimality of the solution of the Euler–Lagrange Eq. (2.6) introduced in Sect. 3 with respect to variations $P \in H_0^1(B_R, \mathscr{S}_0)$. We show that for $b^2 = 0$, the solution Y given by (3.1) is the unique global minimiser of energy (2.1).

Theorem 4.3 *Let $b^2 = 0$ and let Y be given by (3.1) with (u, v) the unique global minimiser of the reduced energy (3.9) in the set S (defined in (3.10)). Then Y is the unique global minimiser of the Landau–de Gennes energy (2.1) in $H^1(B_R; \mathscr{S}_0)$.*

Proof We take $P \in H_0^1(B_R; \mathscr{S}_0)$ and compute the difference in energy between $Y+P$ and Y,

$$\mathcal{F}(Y + P) - \mathcal{F}(Y) = \mathcal{I}[Y](P, P) + \frac{1}{L} \int_{B_R} \frac{c^2}{4} (|P|^2 + 2\,\mathrm{tr}(Y P))^2, \tag{4.3}$$

where

$$\mathcal{I}[Y](P, P) = \frac{1}{2} \int_{B_R} |\nabla P|^2 + \frac{1}{2L} \int_{B_R} |P|^2 \left(-a^2 + c^2|Y|^2\right) \tag{4.4}$$

, and we have used the fact that Y satisfies (2.6) in order to eliminate the first-order terms in P. Thus, it is sufficient to prove that $\mathcal{I}[Y](P, P) \geqslant C\|P\|_{L^2}$ for every $P \in H_0^1\,(B_R(0), \mathscr{S})$.

To investigate (4.4) we use a Hardy trick (see, for instance Ignat et al. (2013)). From Lemma 4.1, we have that $v < 0$ on $[0, R]$. Therefore, any $P \in H_0^1(B_R, \mathscr{S}_0)$ can be written in the form $P(x) = v(r)U(x)$, where $U \in H_0^1(B_R, \mathscr{S}_0)$. Using Eq. (3.7) for v, we have the following identity

$$v\Delta v = \frac{v^2}{L} \left(-a^2 + c^2|Y|^2\right)$$

and therefore

$$\mathcal{I}[Y](P, P) = \frac{1}{2} \sum_{i,j} \int_{B_R} |\nabla v(|x|)U_{ij}(x) + v(|x|)\nabla U_{ij}(x)|^2 + \Delta v(|x|)v(|x|)U_{ij}^2(x). \tag{4.5}$$

Integrating by parts in the second term above, we obtain

$$\sum_{i,j} \int_{B_R} \Delta v\, v\, U_{ij}^2 = -\sum_{i,j} \int_{B_R} |\nabla v|^2 U_{ij}^2 + 2\nabla v \cdot \nabla U_{ij}\, v\, U_{ij}.$$

It follows that

$$\mathcal{I}[Y](P, P) = \frac{1}{2} \int_{B_R} v^2\, |\nabla U|^2.$$

Using the fact that $0 < c_1 \le v^2 \le c_2$ (see Lemma 4.1) and the Poincaré inequality, we obtain

$$\mathcal{I}[Y](P, P) \ge C \int_{B_R} |P|^2.$$

From (4.3), it follows that

$$\mathcal{F}(Y+P) - \mathcal{F}(Y) \geq C\|P\|_{L^2}^2, \tag{4.6}$$

therefore Y is the unique global minimiser of the energy $\mathcal{F}$. □

Remark 4.4 It is straightforward to use the continuity of the solutions (u, v) with respect to the parameter b^2 to show that for b^2 small enough, the solution (u_b, v_b) of (3.7)–(3.8) found in Theorem 3.2 generates a global minimiser Y of the energy (2.1).

4.1 Limiting Case $L \to 0$

Next we consider the limit $L \to 0$. We define the energy

$$\mathscr{E}_L(u, v) = \int_0^R \left[\frac{1}{2}\left((u')^2 + (v')^2 + \frac{k^2}{r^2}u^2 \right) + \frac{c^2}{4L}\left((u^2+v^2) - \frac{a^2}{c^2} \right)^2 \right] r\,\mathrm{d}r.$$

For $b = 0$, $\mathscr{E}_L$ coincides with the reduced energy (3.9) up to an additive constant. We also define the following space:

$$H = \left\{ (u, v) : [0, R] \to \mathbb{R}^2 \mid \sqrt{r}u', \sqrt{r}v', \frac{u}{\sqrt{r}}, \sqrt{r}v \in L^2(0, R) \right\}.$$

Lemma 4.5 *In the limit $L \to 0$ the following statements hold:*

1. *If $(u_L, v_L) \in S$ (see (3.10)) and $\mathscr{E}_L(u_L, v_L) \leq C$, then $(u_L, v_L) \rightharpoonup (u, v)$ in H (perhaps up to a subsequence). Moreover, $(u, v) \in S$ and $u^2(r) + v^2(r) = \frac{a^2}{c^2}$ a.e. $r \in (0, R)$.*
2. *$\mathscr{E}_L$ Γ-converges to $\mathscr{E}_0$ in S , where*

$$\mathscr{E}_0(u, v) = \begin{cases} \int_0^R \frac{1}{2}\left((u')^2 + (v')^2 + \frac{k^2}{r^2}u^2 \right) r\,\mathrm{d}r & \text{if } u^2+v^2 = \frac{a^2}{c^2}, \\ \infty & \text{otherwise.} \end{cases} \tag{4.7}$$

Proof The first statement follows from the energy estimate $\mathscr{E}_L(u_L, v_L) \leq C$.

Next we show the Γ-convergence result. To do this we must check the following:

- for any $(u_L, v_L) \in S$ such that $(u_L, v_L) \to (u, v)$ in S, we have that

$$\liminf_{L\to 0} \mathscr{E}_L(u_L, v_L) \geq \mathscr{E}_0(u, v);$$

- for any $(u, v) \in S$, there exists a sequence $(u_L, v_L) \in S$ such that

$$\limsup_{L\to 0} \mathscr{E}_L(u_L, v_L) = \mathscr{E}_0(u, v).$$

The first part of the Γ-convergence result follows from the lower semicontinuity of the Dirichlet term in the energy $\mathscr{E}_L$ and the penalisation of the potential. To prove the second part, we note that for any $(u, v) \in S$, we may take the recovery sequence $(u_L, v_L) = (u, v)$, for which the lim sup equality is clearly satisfied. □

Next we show that the global minimiser of $\mathscr{E}_0$ defines the unique global minimiser of a certain harmonic map problem.

Theorem 4.6 *Let $0 < R < \infty$. There exist exactly two critical points of $\mathscr{E}_0$ over the set S defined in (3.10). These are explicitly given by the following formulae:*

$$
\begin{aligned}
u_-(r) &= 2\sqrt{2}s_+ \frac{R^{|k|}r^{|k|}}{r^{2|k|}+3R^{2|k|}}, \quad v_-(r) = \sqrt{\frac{2}{3}}s_+ \frac{r^{2|k|}-3R^{2|k|}}{r^{2|k|}+3R^{2|k|}},\\
u_+(r) &= 2\sqrt{2}s_+ \frac{R^{|k|}r^{|k|}}{3r^{2|k|}+R^{2|k|}}, \quad v_+(r) = \sqrt{\frac{2}{3}}s_+ \frac{R^{2|k|}-3r^{2|k|}}{3r^{2|k|}+R^{2|k|}}
\end{aligned}
\tag{4.8}
$$

with s_+ given by (2.5) with $b^2 = 0$. If we define

$$Y_\pm = u_\pm F_n + v_\pm F_3,$$

then Y_- is the unique global minimiser and Y_+ is a critical point of the following harmonic map problem:

$$\min\left\{\int_{B_R}\frac{1}{2}|\nabla Q|^2 \,\middle|\, Q\in H^1(B_R,\mathscr{S}_0),\ Q(R)=Q_k,\ |Q|^2=\frac{2}{3}s_+^2 \text{ a.e. in } B_R\right\}. \tag{4.9}$$

Proof The constraint $u^2 + v^2 = \frac{a^2}{c^2}$ may be incorporated through the substitution

$$u = \sqrt{\frac{2}{3}}s_+\sin\psi, \quad v = -\sqrt{\frac{2}{3}}s_+\cos\psi, \tag{4.10}$$

where $\psi : (0, R] \to \mathbb{R}$. In terms of ψ, the energy $\mathscr{E}_0$ is given up to a multiplicative constant by

$$\mathscr{E}_0[\psi] = \frac{1}{2}\int_0^R \left(r\psi'^2 + \frac{k^2}{r}\sin^2\psi\right) \mathrm{d}r. \tag{4.11}$$

Critical points of $\mathscr{E}_0$ satisfy the Euler–Lagrange equation

$$\left(r\psi'\right)' = \frac{k^2}{r}\sin\psi\cos\psi \tag{4.12}$$

and therefore belong to $C^\infty(0, R)$. From (3.3) and (4.10), ψ satisfies the boundary condition $\psi(R) = \frac{\pi}{3} + 2\pi j$ for $j \in \mathbb{Z}$. Without loss of generality, we may take $j = 0$ [since ψ and $\psi + 2\pi j$ correspond to the same (u, v)]. Therefore, we may take the boundary condition as

$$\psi(R) = \frac{\pi}{3}. \tag{4.13}$$

The Euler–Lagrange Eq. (4.12) may be integrated to obtain the relation

$$\frac{1}{2}r^2\psi'^2 - \frac{k^2}{2}\sin^2\psi = -\frac{k^2}{2}\alpha \tag{4.14}$$

for some constant $\alpha \leq 1$. We claim that $\alpha = 0$. First, we note that $\alpha < 0$ would imply that $r^2\psi'^2$ is bounded away from zero, which is incompatible with $\mathscr{E}_0[\psi]$ being finite. Next, $\alpha = 1$ would imply that $\sin^2\psi = 1$ identically, which is incompatible with the boundary condition (4.13). It follows that $0 \leq \alpha < 1$. If $\alpha > 0$, we may define $x(t) = \psi(\exp t)$ for $t \in (-\infty, \ln R)$. Then $\frac{1}{2}\dot{x}^2 = \frac{k^2}{2}\left(\sin^2 x - \alpha\right)$. It is an elementary result (the simple pendulum problem) that $x(t)$ is periodic with period T (we omit the explicit expression for T); this implies that $\psi\left(e^{-T}r\right) = \psi(r)$. In addition, $A := \int_\tau^{\tau+T}\sin^2 x\, dt$ is strictly positive and independent of τ; in terms of ψ, this implies that

$$\int_{e^{-nT}R}^{R} \frac{\sin^2\psi}{r}\,\mathrm{d}r = nA$$

for $n \in \mathbb{N}$. It follows that $u^2/r = \frac{2}{3}s_+^2\sin^2\psi/r$ is not square-integrable, which is incompatible with $\mathscr{E}_0[\psi]$ being finite. Thus we may conclude that $\alpha = 0$.

We claim now that any solution of (4.12) satisfies either $r\psi'(r) = |k|\sin\psi$ or $r\psi'(r) = -|k|\sin\psi$ on the whole interval $(0, R)$. For suppose $\chi(r)$ is a smooth solution of (4.12), and that for some point $r_0 \in (0, R)$ we have that $r_0\chi'(r_0) = |k|\sin\chi(r_0)$. Then regarding (4.12) as a *regular* second-order ODE on $(0, R)$, we have that the *initial-value problem* (4.12) with initial conditions $\psi(r_0) = \chi(r_0)$, $\psi'(r_0) = \frac{|k|}{r_0}\sin\chi(r_0)$ has a unique smooth solution on $(0, R)$, namely the one satisfying the first-order equation $\chi'(r) = \frac{|k|}{r}\sin\chi(r)$ on $(0, R)$, which proves our claim.

Solving the first-order separable ODEs and applying the boundary conditions (4.13), we obtain exactly two solutions $\psi_\pm$ satisfying

$$\tan\frac{\psi_\pm(r)}{2} = \frac{1}{\sqrt{3}}\left(\frac{r}{R}\right)^{\mp|k|}.$$

These correspond via (4.10) to (4.8).

It is straightforward to check using the definition of $Y_\pm$ and (3.4) that

$$\Delta Y_\pm = -\frac{3}{2s_+^2}|\nabla Y|^2 Y_\pm,\ |Y_\pm|^2 = \frac{2}{3}s_+^2,\ Y_\pm(R,\varphi) = Q_k(\varphi).$$

Therefore, $Y_\pm$ are critical points of the harmonic map problem (4.9).

Next, we show that Y_- is the unique global minimiser of the harmonic map problem (4.9). Take $P \in H_0^1(B_R; \mathscr{S}_0)$ such that $|Y_- + P|^2 = \frac{2}{3}s_+^2$. Then

$$\frac{1}{2}\int_{B_R}|\nabla(Y_- + P)|^2 - \frac{1}{2}\int_{B_R}|\nabla Y_-|^2 = \frac{1}{2}\int_{B_R}|\nabla P|^2 + 2\sum_{ij}\nabla[Y_-]_{ij}\cdot\nabla P_{ij}.$$

Integrating by parts and using the Euler–Lagrange equation for Y_-, we obtain

$$\frac{2}{3}s_+^2\int_{B_R}\sum_{ij}\nabla[Y_-]_{ij}\cdot\nabla P_{ij}=\int_{B_R}|\nabla Y_-|^2\,\mathrm{tr}(Y_-P).$$

Using the fact that $|P|^2=-2\,\mathrm{tr}(Y_-P)$, we obtain

$$\frac{1}{2}\int_{B_R}|\nabla(Y_-+P)|^2-\frac{1}{2}\int_{B_R}|\nabla Y_-|^2=\frac{1}{2}\int_{B_R}|\nabla P|^2-\frac{3}{2s_+^2}|\nabla Y_-|^2|P|^2.$$

The fact that Y_- is harmonic implies that

$$\Delta v_-=-\frac{3}{2s_+^2}\,v_-|\nabla Y_-|^2,$$

and we have that $v_-<0$ on $[0,R]$. Therefore

$$\frac{1}{2}\int_{B_R}|\nabla(Y_-+P)|^2-\frac{1}{2}\int_{B_R}|\nabla Y_-|^2=\frac{1}{2}\int_{B_R}|\nabla P|^2+\frac{\Delta v_-}{v_-}|P|^2$$

Using the decomposition $P=v(r)U$ and applying the Hardy decomposition trick in exactly the same way as in the proof of Theorem 4.3, we obtain

$$\frac{1}{2}\int_{B_R}|\nabla(Y_-+P)|^2-\frac{1}{2}\int_{B_R}|\nabla Y_-|^2\geq C\|P\|_{L^2}^2$$

Therefore Y_- is unique global minimiser of harmonic map problem (4.9). □

Remark 4.7 It is straightforward to check that in the limit $L\to 0$, the Γ-limit of the Landau–de Gennes energy

$$\mathscr{F}(Q)=\frac{1}{2}\int_{B_R}|\nabla Q|^2+\frac{c^2}{4L}\left(|Q|^2-\frac{2}{3}s_+^2\right)^2$$

is exactly the harmonic map problem (4.9).

Remark 4.8 For k even, there is another explicit solution of the harmonic map problem (4.9). Let

$$U=s_+\left(m\otimes m-\frac{1}{3}I\right),\tag{4.15}$$

where

$$m(r,\phi)=\left(\frac{2R^{\frac{k}{2}}r^{\frac{k}{2}}}{R^k+r^k}\cos\left(\frac{k\phi}{2}\right),\frac{2R^{\frac{k}{2}}r^{\frac{k}{2}}}{R^k+r^k}\sin\left(\frac{k\phi}{2}\right),\frac{R^k-r^k}{R^k+r^k}\right).$$

We note that U is *uniaxial* (i.e., two of its eigenvalues are equal). It is straightforward to show that U is a critical point of the harmonic map problem (4.9). Computing energies of Y_+, Y_- and U explicitly, we obtain

$$\mathscr{E}_D(Y_-) = \frac{2}{3}|k|\pi s_+^2 < 2|k|\pi s_+^2 = \mathscr{E}_D(Y_+) = \mathscr{E}_D(U),$$

where $\mathscr{E}_D(Q) = \frac{1}{2}\int_{B_R} |\nabla Q|^2$ is the Dirichlet energy.

Remark 4.9 The harmonic map (4.15) is an example of a more general construction. Let $\zeta = x + iy$, and let $f(\zeta)$ be meromorphic. Let

$$m(x, y) = \frac{\left(2\mathrm{Re}\, f, 2\mathrm{Im}\, f, 1 - |f|^2\right)}{1 + |f|^2}.$$

Then it is straightforward to show that m defines an S^2-valued harmonic map (note that $|m| = 1$), and that $U := \sqrt{3/2}(m \otimes m - \frac{1}{3}I)$ defines an S^4-valued harmonic map. The example (4.15) is obtained by taking $f = (\zeta/R)^{k/2}$, which corresponds to the boundary conditions (2.4).

Remark 4.10 The results of (Bauman et al. 2012) imply that for $|k| > 1$ and $b^2 > 0$, the global minimiser Y of a reduced energy in the limit $L \to 0$ approaches a harmonic map different from Y_-. In that case, the limiting harmonic map has $|k|$ isolated defects of index $\mathrm{sgn}(k)/2$.

5 Conclusions and Outlook

We have found a new highly symmetric equilibrium solution Y of the Landau–de Gennes model, relevant for the study of liquid crystal defects of the form (3.1). This solution is valid for all values of parameters a, b, c, elastic constant L and index k. The properties of this solution can be explored by investigating the system of ordinary differential Eqs. (3.7) – (3.8).

We have provided a detailed study of solution Y in the deep nematic regime when the material parameter b^2 is small enough (see Kralj et al. 1999; Mkaddem and Gartland 2000) for a discussion on the physical relevance of this regime). In this case we have shown that Y is a global minimiser of the Landau–de Gennes energy, provided (u, v) is a global minimiser of the energy (3.9). In this sense, we have constructed the unique ground state of the 2D point defect, and linked its study to analysing solutions of the ordinary differential Eqs. (3.7) –(3.8).

In the limiting case $L \to 0$ for $b^2 = 0$, we have obtained for all k two explicit defect profiles Y_- and Y_+ (see Fig. 7), defined in Theorem 4.6. The global minimiser Y is equal to Y_-. For even k, we obtain a third explicit profile U (see Fig. 9) defined in Remark 4.8. It is straightforward to compute the eigenvalues of $Y_\pm$ and U (see Fig. 8),

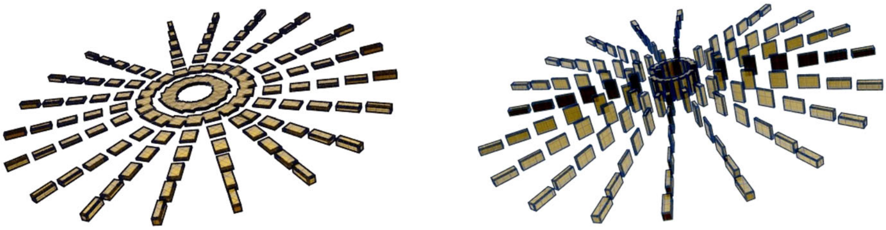


Fig. 7 Y_- (*left*) and Y_+ (*right*) defects for of strength 1

Fig. 8 Eigenvalues of 1-strength defects: Y_- (*solid*), Y_+ (*dashed*), U (*dotted*)

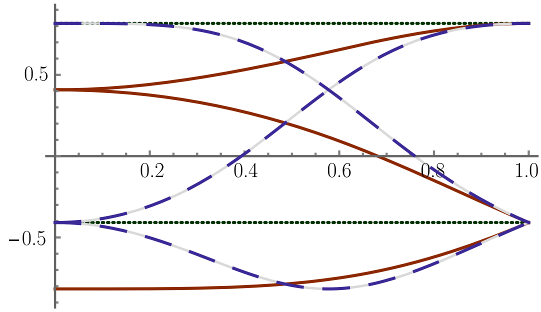
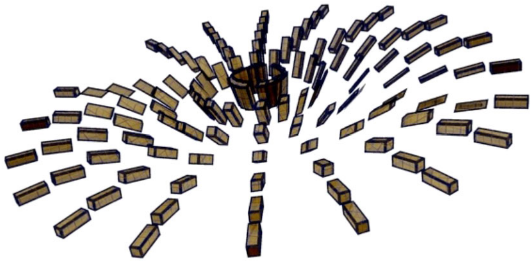


Fig. 9 Uniaxial defect of strength 1



$$\lambda_1^{\pm} = \sqrt{\frac{2}{3}} v^{\pm}(r), \quad \lambda_2^{\pm} = -\frac{u^{\pm}}{\sqrt{2}} - \frac{v^{\pm}}{\sqrt{6}}, \quad \lambda_3^{\pm} = \frac{u^{\pm}}{\sqrt{2}} - \frac{v^{\pm}}{\sqrt{6}}, \tag{5.1}$$

$$\lambda_1^U = \lambda_2^U = -\frac{1}{3}, \quad \lambda_3^U = \frac{2}{3}. \tag{5.2}$$

It is clear that the global minimiser $Y_-(r)$ is always biaxial except for points $r = 0$ and $r = R$, while the critical point Y_+ is uniaxial at 0, R and the point of intersection of λ_1^+ and λ_2^+. Moreover, it is clear that λ_3 is the smallest eigenvalue. The structure of the defect profile Y_+ bears a resemblance to the three-dimensional *biaxial torus* profile (Mkaddem and Gartland 2000). However, whereas the biaxial torus is a candidate for the ground state in three dimensions, in this two-dimensional setting Y_+ has higher energy than Y_-, at least in the small-L regime. The profile U is always uniaxial and its energy coincides with the energy of Y_+ (Fig. 9).

It is a very interesting and challenging task to find the ground state and universal profile of the 2D defect for general parameters a, b, c, L. We are planning to tackle this problem in the future.

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