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Metastable nematic hedgehogs

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Abstract. For nematic liquid crystals, we study the local stability of a radial hedgehog against biaxial perturbations. Our analysis employs the Landau–de Gennes functional to describe the free energy stored in a ball, whose radius is a parameter of the model. We find that a radial hedgehog may be either unstable or metastable, depending on the values of the elastic constants. For unstable hedgehogs, we give an explicit expression for the radius of the ball within which the instability manifests itself: it can be interpreted as the size of the biaxial core of the defect; it is of the same order of magnitude as the radius of the disclination ring predicted by Penzenstadler and Trebin's model. The metastable hedgehogs predicted by our model are the major novelty of the paper. They tell us that we may also expect truly uniaxial point defects, whose core contains no biaxial structure.

1. Introduction

Hedgehog is the figurative name often given to a special defect exhibited by several ordered media; it is a point defect surrounded by a radially symmetric structure. For uniaxial nematic liquid crystals, the structure around a hedgehog is the unit field $\boldsymbol{n}$ representing the orientation of the optic axis; it is radial relative to the defect, as in polar spherical coordinates the field $\boldsymbol{e}_r$ is relative to the origin. Figure 1 makes this idea clearer.

Strictly speaking, this is a *radial* hedgehog. In studying orientational transitions in nematic droplets, Lavrentovich and Terent'ev [1] observed a different structure around a point defect, with a lower degree of symmetry, being axisymmetric instead of radially symmetric. They called this type of hedgehog *hyperbolic* and compared its stability to that of the radial one. Here we content ourselves with studying only the local stability of radial hedgehogs.

The classical Frank's theory for uniaxial nematics posits the following free-energy density per unit volume

$$\sigma_F = k_1(\operatorname{div}\boldsymbol{n})^2 + k_2(\boldsymbol{n}\cdot\operatorname{curl}\boldsymbol{n})^2 + k_3|\boldsymbol{n}\wedge\operatorname{curl}\boldsymbol{n}|^2 + (k_2+k_4)(\operatorname{tr}(\nabla\boldsymbol{n})^2 - (\operatorname{div}\boldsymbol{n})^2) \tag{1.1}$$

where k_1 to k_4 are material constants subject to the inequalities

$$2k_1 > k_2 + k_4 \qquad k_3 > 0 \qquad |k_4| < k_2 \tag{1.2}$$

put forward by Ericksen in [2] to ensure that σ_F is positive definite.

Within Frank's theory the stability of a hedgehog has been extensively studied, especially in the mathematical literature of the last few years. Brezis *et al* [3] first proved that when $k_1 = k_2 = k_3 = k$ and $k_4 = 0$, that is, when (1.1) reduces to

$$\sigma_F = k|\nabla\boldsymbol{n}|^2 \tag{1.3}$$

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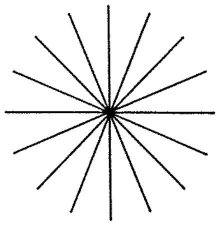

Figure 1. Radial hedgehog.

the free energy stored in a ball subject to the radial boundary condition for $\boldsymbol{n}$ attains its minimum on the radial hedgehog placed at the centre, whatever the radius of the ball. Surprisingly enough, when Frank's constants k_1, k_2 and k_3 are not all equal to one another, the radial hedgehog need not be the energy minimizer in a ball as above. This conclusion, which is due to the work of Hélein [4], Cohen and Taylor [5] and Kinderlehrer and Ou [6], is briefly recalled in section 4 below; it warns us, who will employ Landau–de Gennes theory, to consider properly the role played by *all* elastic constants in determining both stable and unstable hedgehogs.

Our analysis will have a local nature. We allow for moderate biaxial alterations of the order parameter tensor $\boldsymbol{Q}$ about the uniaxial radial hedgehog placed at the centre of a ball $\mathcal{B}_R$, whose radius R is treated as a parameter. We regard $\mathcal{B}_R$ as the core of the hedgehog, inside which a biaxial structure may or may not be present: it will be thought of as if it were removable by local surgery from the surrounding, mostly uniaxial, environment. Such an interpretation of $\mathcal{B}_R$ will become evident in section 5, where we describe the class of admissible biaxial variations of the radial hedgehog; there we prescribe the principal axis of $\boldsymbol{Q}$ to be the triad of unit vectors in the frame of spherical coordinates, while the eigenvalues of $\boldsymbol{Q}$ are left free to vary in the interior of $\mathcal{B}_R$, as well as on its boundary. Thus, the eigenvectors of $\boldsymbol{Q}$ preserve the radial symmetry of the uniaxial configuration, whereas its eigenvalues may break it.

The variational analysis is presented in sections 6 and 7, and summarized in the phase diagram illustrated in section 8 for all admissible values of the elastic constants in the Landau–de Gennes free-energy functional. The main outcome of this study is that a uniaxial hedgehog, already stable against uniaxial variations, can be either stable or unstable against biaxial variations in $\mathcal{B}_R$, depending on R and on the value of the elastic constants. When unstable, it is so only for R less than a critical value R_c, which we determine explicitly. When stable, it is so irrespective of the value of R. We interpret R_c as the size of the core within which a stable biaxial structure may develop, whose details elude our local analysis. When the hedgehog is stable, we cannot appreciate even a faint trace of such a biaxial structure, as there is no eigenmode that makes the second variation of the energy vanish. We move one step further, asserting that in the case of stable hedgehogs such a core structure fails to exist. It is as if there were two types of hedgehog, one with a core structure and the other without.

Here *stability* is to be properly meant as *local* stability. Furthermore, locally stable hedgehogs should indeed be called *metastable*, as proven by the various studies on the formation of a ring disclination from a hedgehog. They have been neatly summarized in a recent paper [7], where an attempt is also made to resolve the differences in the various theoretical models, by resorting to a Monte Carlo simulation. The outcomes of this simulation, however, are not conclusive, as they do predict the formation of a ring disclination, but with a radius of the order of the nematic coherence length, in contrast to the prediction of Penzenstadler and Trebin's model [8], which estimates a radius larger than

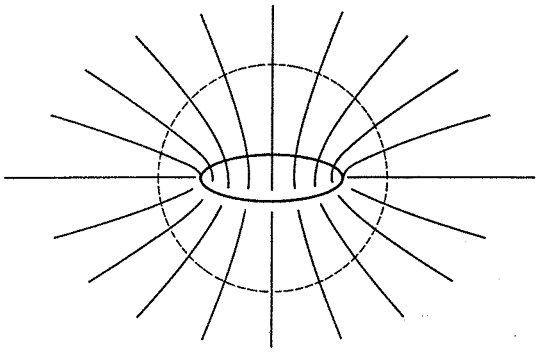

Figure 2. Ring disclination. Both the ring and the polar axis consist of uniaxial states, with scalar order parameters opposite in sign.

this by at least one order of magnitude.

On the other hand, Penzenstadler and Trebin's model appears to be the best theoretical model available, being based on a fine estimate of the free energy in a class of biaxial orientations that mimic the structure surrounding a ring disclination, which indeed is no longer viewed as a singularity for the optic axis, as was the case in Mori and Nakanishi's model [9]. Following Lyuksyutov [10], Penzenstadler and Trebin regard the ring as being composed of uniaxial states with optic axis tangent to it and negative scalar order parameter. The liquid crystal is again uniaxial along the axis orthogonal to the plane of the ring, where the orientation is parallel to the same axis and the scalar order parameter is positive; all around the ring there are biaxial states. Figure 2 illustrates schematically a ring disclination.

In the class of fields employed in [8] the radially uniaxial orientation is recovered at infinity as an asymptotic boundary condition; thus, the eigenvectors of the order parameter tensor $\boldsymbol{Q}$ vary in space together with its eigenvalues. In this class the radial hedgehog is obtained from the scaling that shrinks the uniaxial ring to its centre; as this limiting case is approached, the energy stored within the ring increases, and so it is little surprise that the total energy achieves its minimum away from it. The energy is minimized for a specific value of the scaling parameter, which then determines the equilibrium radius of the ring.

From a variational perspective, such a result amounts to saying that there is a path emanating from the radial hedgehog in the chosen admissible class of fields, along which the energy first decreases: this is enough to conclude that the radial hedgehog is *unstable*, though a deeper analysis would be required to make sure that the ring determined from this argument is indeed the absolute minimizer. More importantly, in approaching the hedgehog, the fields of [8] fail to be close to it in any classical norm, as we show in some detail in section 9. Thus, this peculiar instability of the radial hedgehog might indeed mask a metastability, which can be revealed by a local stability analysis.

Here our study focuses, as it were, on the reverse side of Penzenstadler and Trebin's model. We restrict our attention to *small* biaxial perturbations of the radial uniaxial hedgehog, exploring its *incipient* instability. We find it to be metastable for certain values of the elastic constants in the Landau–de Gennes free-energy functional. We think of metastable hedgehogs as having no biaxial core. This brings to mind the picture proposed by Schopohl and Sluckin in [11], which, apart from an isotropic point at the centre of the hedgehog, exhibits a truly uniaxial core.

In sections 2 and 3 below we prepare the way to the linearized analysis outlined in the subsequent sections. Finally, in section 9 we compare our study to the former ones, and in section 10 we present our main conclusions.

2. Landau–de Gennes free energy

We will describe a liquid crystal by means of a second-order tensor $\boldsymbol{Q}$ proportional to the *alignment tensor* employed in [16]; more details about the definition of $\boldsymbol{Q}$ can be found, for example, in section 1.3 of [12]. $\boldsymbol{Q}$ is a traceless and symmetric tensor whose eigenvalues q_i satisfy the condition

$$-\tfrac{1}{3} \leqslant q_i \leqslant \tfrac{2}{3}\,. \tag{2.1}$$

This tensor, usually referred to as the *order tensor*, represents biaxial configurations when its eigenvalues are all distinct, while it represents uniaxial states when two eigenvalues coincide. In the latter case $\boldsymbol{Q}$ is usually cast thus:

$$\boldsymbol{Q} = s_0(\boldsymbol{n} \otimes \boldsymbol{n} - \tfrac{1}{3}\boldsymbol{I}) \tag{2.2}$$

where the unit vector $\boldsymbol{n}$ stands for the optic axis and the scalar $s_0 \in [-\frac{1}{2}, 1]$ is known as the *scalar order parameter*, or *degree of orientation*. Isotropy occurs when $\boldsymbol{Q} = \boldsymbol{0}$.

Our aim is to study the following free-energy functional

$$\mathcal{F} := \int_{\mathcal{B}} (f_{el} + \sigma)\, \mathrm{d}V$$

where f_{el} is the elastic free-energy density and σ is an internal potential. The integration domain $\mathcal{B}$ represents the region occupied by the liquid crystal and, at this stage, its boundary $\partial\mathcal{B}$ may be taken to be of class C^2. We devote this section to the description of f_{el} deferring a full treatment of the internal potential to the next section. We express the elastic term following Landau–de Gennes theory which yields

$$f_{el} := L_1|\nabla\boldsymbol{Q}|^2 + L_2(\operatorname{div}\boldsymbol{Q})^2 + L_3 I_3\,. \tag{2.3}$$

In Cartesian components I_3 has the following expression:

$$I_3 := Q_{ij,k}Q_{ik,j}$$

where the sum over repeated indices is understood and $Q_{ij,k} := \partial Q_{ij}/\partial x_k$. This term contributes a surface energy depending only on the trace of $\boldsymbol{Q}$ on $\partial\mathcal{B}$ since the following formula holds:

$$\int_{\mathcal{B}} I_3\,\mathrm{d}V = \int_{\mathcal{B}} (\operatorname{div}\boldsymbol{Q})^2\,\mathrm{d}V + \int_{\partial\mathcal{B}} \boldsymbol{Q}\cdot\{\nabla_{\mathrm{s}}(\boldsymbol{Q}\boldsymbol{\nu}) - \boldsymbol{Q}\nabla_{\mathrm{s}}\boldsymbol{\nu} - \operatorname{div}_{\mathrm{s}}\boldsymbol{Q}\otimes\boldsymbol{\nu}\}\,\mathrm{d}A\,. \tag{2.4}$$

Here $\boldsymbol{\nu}$ is the outer normal to $\partial\mathcal{B}$ and the subscript 's' refers to the surface version of both operators ∇ and div, according to the definition:

$$\nabla_{\mathrm{s}}\boldsymbol{f}(p) := \nabla\boldsymbol{f}(p)\boldsymbol{E}_{\mathrm{s}}(p)$$
$$(\operatorname{div}_{\mathrm{s}}\boldsymbol{f})(p) := \operatorname{tr}(\nabla_{\mathrm{s}}\boldsymbol{f}(p))$$

where p is a point on $\partial\mathcal{B}$, $\boldsymbol{E}_{\mathrm{s}} := \boldsymbol{I} - \boldsymbol{\nu}\otimes\boldsymbol{\nu}$ is the projector on the tangent plane in p to $\partial\mathcal{B}$ and $\boldsymbol{f}$ is a vector field of class C^1 on $\partial\mathcal{B}$.

When $\boldsymbol{Q}$ is uniaxial as in (2.2), L_1, L_2 and L_3 reduce to Frank's constants through the following relations:

$$k_1 = k_3 = (2L_1 + L_2 + L_3)s_0^2 \tag{2.5a}$$
$$k_2 = 2L_1 s_0^2 \tag{2.5b}$$
$$k_4 = L_3 s_0^2\,. \tag{2.5c}$$

It is to be noted that Landau–de Gennes theory leads to the equality $k_1 = k_3$ which would fail to apply to many real substances. There have been several attempts to overcome this difficulty with Landau–de Gennes theory; they all rely on adding new terms to the energy density in (2.3) that depend on higher powers of $\boldsymbol{Q}$. The most systematic study of the consequences resulting from these higher terms is [13]. Following this line of thought, however, leads to a considerable increase in the number of elastic constants. Here, to keep things simple, we will adopt the original Landau–de Gennes theory, and so equality (2.5*a*) will hereafter be held true. As shown by (2.5*c*), the constant L_3 is directly related to k_4, which introduces a surface term in Frank's energy, whose integral over $\mathcal{B}$ can be made into an integral on $\partial\mathcal{B}$, precisely as in (2.4). Another surface term, originally introduced in Frank's energy by Nehring and Saupe [18], has recently received much attention in a still open debate (cf e.g. [19, 20]). Also this term, universally called the k_{13}-term, has its analogue in the theory we employ here, but we omit it because it would bring in f_{el} the second gradient of $\boldsymbol{Q}$, and so disregarding the higher-order terms listed in [13] would be no longer justified.

We end this section by recasting Ericksen's inequalities for Frank's constants (1.2) in terms of L_1, L_2 and L_3:

$$2L_1 + 2L_2 + L_3 > 0 \tag{2.6a}$$

$$2L_1 + L_2 + L_3 > 0 \tag{2.6b}$$

$$-2L_1 < L_3 < 2L_1 \tag{2.6c}$$

$$L_1 > 0\,. \tag{2.6d}$$

Inequalities (2.6), which are assumed to hold throughout this paper, are less restrictive than those expressing the requirement that the free-energy density in (2.3) be positive definite. Moreover, it is easily shown that they are not all independent, as (2.6*b*) follows from (2.6*a*) and (2.6*c*).

3. Lyuksyutov's constraint

In this section we focus attention on the internal potential σ, which in Landau–de Gennes theory is given the form

$$\sigma(\boldsymbol{Q}) := a\,\mathrm{tr}\,\boldsymbol{Q}^2 - b\,\mathrm{tr}\,\boldsymbol{Q}^3 + c(\mathrm{tr}\,\boldsymbol{Q}^2)^2 \qquad b > 0 \tag{3.1}$$

where tr denotes the trace. The function expressing $\sigma(\boldsymbol{Q})$ is often a severe obstacle in finding an explicit solution to variational problems for $\mathcal{F}$: we present an argument, originally due to Lyuksyutov [10] and recovered in this form by Penzenstadler and Trebin [8], which reduces to a single term the formula for σ.

This method rests upon the observation that constants a and c in (3.1) are much greater than b, so that the term $\mathrm{tr}\,\boldsymbol{Q}^3$ can be viewed as a perturbation. As a first step, a minimization of $a\,\mathrm{tr}\,\boldsymbol{Q}^2 + c(\mathrm{tr}\,\boldsymbol{Q}^2)^2$ is performed, yielding

$$Q_0^2 := (\mathrm{tr}\,\boldsymbol{Q}^2) = -\frac{a}{2c} > 0$$

for the minimizer. Then, $\sigma = -b\,\mathrm{tr}\,\boldsymbol{Q}^3$ is inserted in the free-energy functional and attention is confined to the order tensors $\boldsymbol{Q}$ satisfying the condition

$$\mathrm{tr}\,\boldsymbol{Q}^2 = Q_0^2\,. \tag{3.2}$$

We will conform to this formulation writing (3.2) as

$$\mathrm{tr}\,\boldsymbol{Q}^2 = \tfrac{2}{3}s_0^2 \tag{3.3}$$

since a uniaxial configuration like (2.2) has $\operatorname{tr} \boldsymbol{Q}^2 = \frac{2}{3}s_0^2$. Thus, we can write $\mathcal{F}$ in the form

$$\mathcal{F}[\boldsymbol{Q}] = \int_{\mathcal{B}} \{L_1|\nabla \boldsymbol{Q}|^2 + L_2(\operatorname{div} \boldsymbol{Q})^2 + L_3 I_3 - b \operatorname{tr} \boldsymbol{Q}^3\} \, \mathrm{d}V \tag{3.4}$$

subject to (2.1), (3.3) and

$$\boldsymbol{Q} = \boldsymbol{Q}^{\mathrm{T}} \tag{3.5a}$$

$$\operatorname{tr} \boldsymbol{Q} = 0\,. \tag{3.5b}$$

Hereafter, having in mind a hedgehog, the region $\mathcal{B}$ will be the ball $\mathcal{B}_R$ with its centre at the singular point, whose radius R is to be treated as a parameter, since we seek the critical value R_c within which the biaxial structure would be preferred energetically.

4. Local uniaxial stability

Before turning to the study of $\mathcal{F}$ in $\mathcal{B}_R$, it seems appropriate to give an account of a theorem first proved by Cohen and Taylor [5], which establishes a relation among Frank's constants ensuring that a hedgehog is locally stable in a class of uniaxial perturbations altering the optic axis only in a spherical region surrounding the defect. It states that the radial hedgehog is locally stable against these variations if and only if Frank's constants satisfy the inequality

$$8(k_2 - k_1) + k_3 > 0 \tag{4.1}$$

which, translated into the language of Landau–de Gennes theory, reads as

$$2L_1 - 7(L_2 + L_3) > 0\,. \tag{4.2}$$

From now on, we take it as satisfied.

Inequality (4.1) has an interesting story. That its reverse causes a radial hedgehog to become unstable against uniaxial perturbations had already been proved by Hélein [4]; his proof was constructive, based on an explicit example. Conversely, Cohen and Taylor's proof that (4.1) suffices to ensure stability is quite involved; a simpler proof has recently been given by Kinderlehrer and Ou [6].

5. Admissible class

So far, we have imposed on $\boldsymbol{Q}$ some restrictions arising both from the general theory and from the particular problem under study, but to obtain an explicit expression for $\mathcal{F}$ we also need a representation formula for the order tensor. Hence, we consider only tensors that can be cast in the following form:

$$\boldsymbol{Q} = s_r(r, \vartheta)\boldsymbol{e}_r \otimes \boldsymbol{e}_r + s_\vartheta(r, \vartheta)\boldsymbol{e}_\vartheta + s_\varphi(r, \vartheta)\boldsymbol{e}_\varphi \otimes \boldsymbol{e}_\varphi \tag{5.1}$$

where $(\boldsymbol{e}_r, \boldsymbol{e}_\vartheta, \boldsymbol{e}_\varphi)$ is the local frame associated with polar spherical coordinates (r, ϑ, φ). This class includes both uniaxial and biaxial configurations; besides, it has two important features that are worth noting: the eigenvalues of $\boldsymbol{Q}$ are independent of the longitude φ, while at each point the eigenvectors are members of the orthonormal triad $(\boldsymbol{e}_r, \boldsymbol{e}_\vartheta, \boldsymbol{e}_\varphi)$. The former property amounts to requiring that the admissible configurations be symmetric about the polar axis. The latter property provides a more drastic restriction, as it requires the eigenvectors of $\boldsymbol{Q}$ to preserve the radial symmetry of the hedgehogs. Both requirements help in keeping calculations simple (though not too simple) and allow us to capture many details of the phenomenon we aim to describe. They seem even more justified in the light of the attitude taken here of looking just for the incipient instability of a radial hedgehog,

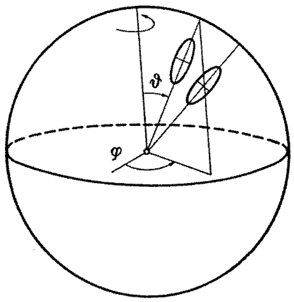

Figure 3. A pictorial description of the order tensor $\boldsymbol{Q}$ belonging to the admissible class. The ellipsoids represent the eigenvectors of $\boldsymbol{Q}$ through their principal axes while their semi-axes are proportional to the eigenvalues of $\boldsymbol{M}$.

which we expect to break its symmetry as little as possible. Figure 3 shows a schematic of the configurations described by (5.1). $\boldsymbol{Q}$ is represented through ellipsoids: their principal axes are along its eigenvectors, while their semi-axes are proportional to the eigenvalues of $\boldsymbol{M} := \boldsymbol{Q} + \frac{1}{3}\boldsymbol{I}$.

We are now in a position to express conditions (2.1), (3.3) and (3.5) in terms of the eigenvalues of $\boldsymbol{Q}$; while (3.5*a*) is obviously verified, (3.5*b*) and (3.3) lead, respectively, to the following relations:

$$s_r + s_\vartheta + s_\varphi = 0 \qquad s_r^2 + s_\vartheta^2 + s_\varphi^2 = \tfrac{2}{3}s_0^2 \tag{5.2}$$

which represent a circumference in the eigenvalues space. If we transform the triple $(s_r, s_\vartheta, s_\varphi)$ into $(s_r', s_\vartheta', s_\varphi')$ according to the formulae

$$\begin{aligned} s_r &= \frac{1}{\sqrt{3}}s_r' - \frac{2}{\sqrt{6}}s_\vartheta' \\ s_\vartheta &= \frac{1}{\sqrt{3}}s_r' + \frac{1}{\sqrt{6}}s_\vartheta' - \frac{1}{\sqrt{2}}s_\varphi' \\ s_\varphi &= \frac{1}{\sqrt{3}}s_r' + \frac{1}{\sqrt{6}}s_\vartheta' + \frac{1}{\sqrt{2}}s_\varphi' \end{aligned} \tag{5.3}$$

then the circumference is represented in a simpler way as

$$s_r' = 0 \qquad (s_\vartheta')^2 + (s_\varphi')^2 = \tfrac{2}{3}s_0^2$$

or, by introducing the angle ψ in $]-\pi, \pi]$ as

$$s_r' = 0 \qquad s_\vartheta' = -\sqrt{\tfrac{2}{3}}s_0 \cos\psi \qquad s_\varphi' = \sqrt{\tfrac{2}{3}}s_0 \sin\psi \tag{5.4}$$

so that the eigenvalues of $\boldsymbol{Q}$ can be given as functions of ψ only:

$$s_r = \frac{2}{3}s_0 \cos\psi \qquad s_\vartheta = -\frac{2}{3}s_0 \cos\left(\psi - \frac{\pi}{3}\right) \qquad s_\varphi = -\frac{2}{3}s_0 \cos\left(\psi + \frac{\pi}{3}\right) \tag{5.5}$$

where s_0 is taken as *positive*.

Equations (5.5) show that $\psi = 0, \pi$, $\psi = \frac{\pi}{3}, -\frac{2\pi}{3}$, and $\psi = \frac{2\pi}{3}, -\frac{\pi}{3}$ describe, respectively, uniaxial configurations along $\boldsymbol{e}_r$, $\boldsymbol{e}_\vartheta$, and $\boldsymbol{e}_\varphi$; they differ, though, by the sign of the scalar order parameter: it is positive for $\psi = 0, \frac{2\pi}{3}$, and $-\frac{2\pi}{3}$, whereas it is negative for $\psi = \frac{\pi}{3}, \pi$, and $-\frac{\pi}{3}$. Finally, on considering condition (2.1), it can be shown that the set of admissible states in the $(s_\vartheta', s_\varphi')$-plane should be confined to the region within the equilateral triangle drawn in figure 4.

The origin coincides with the centre of the triangle and represents the isotropic state since $\boldsymbol{Q}$ there vanishes. The medians describe uniaxial configurations; in particular, the radial hedgehogs lie on the s_ϑ'-axis ($\psi = 0$). The circumference expressing Lyuksyutov's

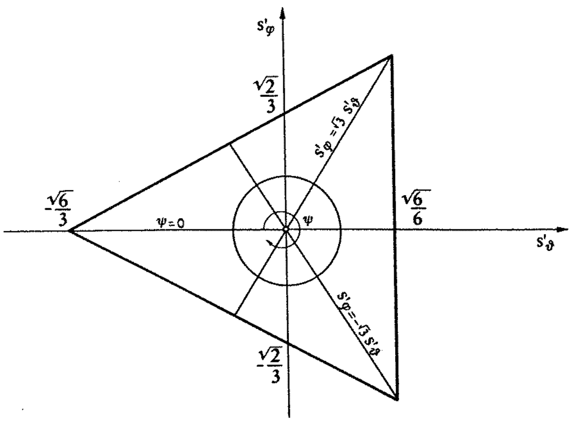

Figure 4. Admissible states. The region inside the equilateral triangle represents configurations compatible with the properties of $\boldsymbol{Q}$. Lyuksyutov's constraint corresponds to the circumference drawn in the picture.

constraint is contained in the interior of the triangle until s_0 is less than $\frac{1}{2}$; when $s_0 = \frac{1}{2}$, it becomes tangent to it with all contact points lying on the uniaxial lines, while, when $s_0 = 1$, it circumscribes the triangle. The fact that the circumference could partially escape the admissible triangle will not invalidate our analysis, since this employs only a small arc on the constraint, about the point $\psi = 0$, which corresponds to a radially uniaxial configuration with positive scalar order parameter. There always is such an arc falling within the admissible triangle, provided $s_0 < 1$. Since $s_0 = 1$ would make $\boldsymbol{Q}$ in (2.2) the order tensor of a perfectly aligned uniaxial nematic, excluding this case, has no physical relevance.

6. Azimuthal variation

Hereafter the centre of $\mathcal{B}_R$ will be the origin of the polar spherical coordinates introduced above. With the aid of the representation formula (5.1), after some calculations mainly based on the formulae in subsection 2.3.3 of [12], we obtain

$$|\nabla \boldsymbol{Q}|^2 = \frac{4s_0^2}{9}\left\{\frac{3}{2}|\nabla\psi|^2 + \frac{6}{r^2}\left(\frac{1}{2} + \cos^2\psi + \cot^2\vartheta\sin^2\psi\right)\right\}$$

$$(\operatorname{div}\boldsymbol{Q})^2 = \frac{4s_0^2}{9}\left\{\left(\frac{3}{r}\cos\psi - \sin\psi\,\nabla\psi\cdot\boldsymbol{e}_r\right)^2 + \left(\sin\left(\frac{\pi}{3}-\psi\right)\nabla\psi\cdot\boldsymbol{e}_\vartheta + \frac{1}{r}\sqrt{3}\cot\vartheta\sin\psi\right)^2 + \sin^2\left(\frac{\pi}{3}+\psi\right)(\nabla\psi\cdot\boldsymbol{e}_\varphi)^2\right\}$$

$$\operatorname{tr}\boldsymbol{Q}^3 = \frac{4s_0^3}{9}\frac{1}{2}\cos\psi(1 - 4\sin^2\psi)$$

$$\boldsymbol{Q}\cdot\{\nabla_{\rm s}(\boldsymbol{Q}\boldsymbol{\nu}) - \boldsymbol{Q}\nabla_{\rm s}\boldsymbol{\nu} - \operatorname{div}_{\rm s}\boldsymbol{Q}\otimes\boldsymbol{\nu}\} = -\frac{4s_0^2}{9}\frac{1}{R}\left\{\frac{9}{2} - 3\sin^2\psi\right\}$$

the latter formula being computed on the boundary of $\mathcal{B}_R$. Then, inserting these expressions in (3.4) we reduce $\mathcal{F}$ to a functional of ψ:

$$\frac{9}{4s_0^2}F[\psi] := 2\pi\int_0^R \mathrm{d}r\, r^2 \int_0^\pi \mathrm{d}\vartheta\,\sin\vartheta\left\{L_1\left[\frac{3}{2}\left(\psi_{,r}^2 + \frac{1}{r^2}\psi_{,\vartheta}^2\right) + \frac{6}{r^2}\left(\frac{1}{2} + \cos^2\psi + \sin^2\psi\cot^2\vartheta\right)\right] + (L_2 + L_3)\left[\left(\frac{3}{r}\cos\psi - \psi_{,r}\sin\psi\right)^2\right.\right.$$

$$+\frac{1}{r^2}\left(\psi_{,\vartheta}\sin\left(\frac{\pi}{3}-\psi\right)+\sqrt{3}\sin\psi\cot\vartheta\right)^2\Bigg]-bs_0\cos\psi\left(\frac{1}{2}-2\sin^2\psi\right)\Bigg\}$$
$$-2\pi RL_3\int_0^\pi\sin\vartheta\left\{\frac{9}{2}-3\sin^2\psi\right\}\mathrm{d}\vartheta \tag{6.1}$$

where, to comply with (5.1), ψ is a smooth function of r and ϑ only, and $\psi_{,r}$ and $\psi_{,\vartheta}$ denote its partial derivatives. The presence in (6.1) of terms with $\cot\vartheta$ requires the following conditions on ψ to make the energy finite:

$$\psi(r,0)=\psi(r,\pi)=0 \qquad \forall r\in[0,R]\,. \tag{6.2}$$

We note that the surface term in (2.3) plays a role too, since we impose no conditions on the eigenvalues, but satisfying Lyuksyutov's constraint; we will return to this point in section 9 on making comparisons with other approaches to the problem.

In the spirit of Cohen and Taylor's theorem (see section 4), we do not try to solve the Euler–Lagrange equation of (6.1), but we study the effects on the radial configuration $\psi=0$ of a perturbation chosen in a suitable class. Thus, we first consider variations of the following kind:

$$\psi(u)=\varepsilon\nu(u)$$

where $u:=\cos\vartheta$, and ν is a function of class $C^2(-1,1)$, which are called the *azimuthal* variations because they depend only on ϑ. At the lowest order in ε, we obtain

$$F[\varepsilon\nu]=F[0]+\frac{8\pi}{3}s_0^2\varepsilon^2F_2[\nu]+\mathrm{o}(\varepsilon^2) \tag{6.3}$$

where F_2 is essentially the second variation of F at $\psi=0$ in the above class. To compute F_2, we express (6.1) in terms of u with the aid of (6.2) and an integration by parts:

$$F_2[\nu]=\int_{-1}^1\mathrm{d}u\Big\{\tfrac{1}{2}\big(L_1+\tfrac{1}{2}(L_2+L_3)\big)(1-u^2)(\nu')^2+2\big(L_1+\tfrac{1}{2}(L_2+L_3)\big)\frac{u^2\nu^2}{1-u^2}$$
$$+\big[\tfrac{1}{4}bs_0R^2-2L_1-\tfrac{5}{2}(L_2+L_3)+L_3\big]\nu^2\Big\} \tag{6.4}$$

where use has also been made of the end-point conditions for ν,

$$\nu(1)=\nu(-1)=0 \tag{6.5}$$

inherited from (6.2). In (6.4), as below in this section, a prime denotes differentiation with respect to u. The equilibrium equation for $F_2[\nu]$ is

$$((1-u^2)\nu')'+\left(2\Gamma-\frac{4}{1-u^2}\right)\nu=0 \tag{6.6}$$

where, by (2.6*b*),

$$\Gamma:=\frac{1}{L_1+\frac{1}{2}(L_2+L_3)}\big(-\tfrac{1}{4}bs_0R^2+4L_1+\tfrac{5}{2}L_3+\tfrac{7}{2}L_2\big). \tag{6.7}$$

It follows from the maximum principle that when $\Gamma<2$ the only solution of (6.6) satisfying (6.5) is $\nu=0$. To see this, suppose for a contradiction that ν is positive somewhere in $]-1,1[$. Thus, there is at least one point u_0 in $]-1,1[$ where ν attains its maximum: being $\nu(u_0)>0$, $\nu'(u_0)=0$, and $\nu''(u_0)<0$, it follows from equation (6.6) that u_0 must satisfy

$$\frac{2}{1-u_0^2}<\Gamma\,.$$

Were $\Gamma < 2$, there would be no u_0 satisfying this inequality, and so no solution of (6.6) and (6.5) taking positive values in $]-1, 1[$. The same argument works with trivial adjustments in case ν would take negative values.

Equation (6.6) is known as *Legendre equation* and an analysis based on the properties of the associated Legendre functions (see pp 998 and ff of [14]) shows that a non-trivial bounded solution of (6.6) subject to (6.5) exists whenever 2Γ may be written as the product of two consecutive integers and this, in turn, leads to the conclusion that the first acceptable eigenvalue is $\Gamma = 3$. Accordingly, we require $\Gamma \geqslant 3$, obtaining

$$\frac{bs_0 R^2}{4} \leqslant L_1 + 2L_2 + L_3 \,. \tag{6.8}$$

Since both b and s_0 are positive, condition (6.8) is satisfied for no value of R if $L_1+2L_2+L_3 \leqslant 0$, and so we conclude that in this case the hedgehog is locally stable against the kind of biaxial perturbations considered here. On the other hand, if $L_1+2L_2+L_3 > 0$, our analysis proves the existence of an instability for the hedgehog in the region $R \leqslant R_c$, where

$$R_c := \frac{2}{\sqrt{bs_0}}\sqrt{L_1 + 2L_2 + L_3}\,. \tag{6.9}$$

In terms of Frank's constants, the requirement that $L_1 + 2L_2 + L_3 > 0$ becomes

$$k_4 < 2k_1 - \tfrac{3}{2}k_2 \tag{6.10}$$

which is compatible with Ericksen's inequalities.

We have thus selected, among all values of Frank's constants satisfying Eriksen's inequalities, those which allow the liquid crystal to gain energy by escaping into the biaxial phase. Moreover, it is worth noting that (6.10) implies that such a biaxial structure should exist when k_4, the surface-like constant of Frank's theory, does not exceed an upper bound, given in terms of k_1 and k_2.

The existence of a critical radius should be interpreted as the sign that the radial hedgehog exhibits a biaxial core: when the critical radius fails to exist, the core ceases to be biaxial. An estimate of R_c for MBBA gives $R_c \approx 10^2$ Å, in substantial agreement with the results of [8].

7. Radial variation

We explore in this section the stability of a radial hedgehog against biaxial perturbations in a broader class. While the azimuthal variations do not depend on the radial coordinate, those now being considered do; thus, we call them the *radial* variations. In the incipient instability of a hedgehog they should reveal a more complex biaxial structure, as one spiralling about the centre of the defect. The competition between these unstable modes and those considered above will be analysed in section 8.

We set $\psi(r, u) := \varepsilon\nu(r, u)$ with $\nu(r, -1) = \nu(r, 1)\ \forall r \in [0, R]$. Again, the second variation F_2 is obtained from (6.1) and (6.2) via two integrations by parts, but now attention should be paid to the fact that ν need not vanish for $r = R$, because the ball $\mathcal{B}_R$ is thought of as if it were isolated from the surrounding hedgehog through an ideal surgery:

$$F_2[\nu] := \int_0^R \mathrm{d}r \int_{-1}^1 \mathrm{d}u \big\{ \tfrac{1}{2} L_1 r^2 \nu_{,r}^2 + \tfrac{1}{2}\big(L_1 + \tfrac{1}{2}(L_2 + L_3)\big)(1-u)^2 \nu_{,u}^2$$

$$+2\big(L_1 + \tfrac{1}{2}(L_2+L_3)\big)\frac{u^2\nu^2}{1-u^2} + \tfrac{3}{4} b s_0 r^2 \nu^2 - \big(2L_1 + \tfrac{3}{2}(L_2+L_3)\big)\nu^2 \big\}$$

$$-RL_2 \int_{-1}^1 \mathrm{d}u \nu^2(R,u)\,. \qquad (7.1)$$

The equilibrium equations for F_2 are

$$L_1(r^2\nu_{,r})_{,r} + \big(L_1 + \tfrac{1}{2}(L_2+L_3)\big)((1-u^2)\nu_{,u})_{,u} = \big(L_1 + \tfrac{1}{2}(L_2+L_3)\big)\frac{4u^2\nu}{1-u^2}$$

$$+\tfrac{3}{2} b s_0 r^2 \nu - 2\big(2L_1 + \tfrac{3}{2}(L_2+L_3)\big)\nu \qquad (7.2a)$$

$$\tfrac{2L_2}{L_1}\nu(R,u) = R(\nu_{,r})|_{r=R} \qquad (7.2b)$$

where the latter expresses the natural boundary condition for ν. If we seek a solution of (7.2) in the form $\nu(r,u) = \rho(r)w(u)$, then (7.2*a*) splits into two eigenvalue problems, while (7.2*b*) gives rise to a boundary condition on ρ:

$$(r^2\rho')' - \frac{3b}{2L_1}s_0 r^2 \rho - \lambda\rho = 0 \qquad \frac{2L_2}{L_1}\rho(R) = R\rho'(R) \qquad (7.3)$$

$$((1-u^2)w')' - \frac{4u^2}{1-u^2}w - \mu w = 0 \qquad w(-1) = w(1) = 0 \qquad (7.4)$$

with λ and μ satisfying the following relation:

$$(\lambda - 2)L_1 + (\mu + 6)(L_1 + \tfrac{1}{2}(L_2+L_3)) = 0\,. \qquad (7.5)$$

In equations (7.3) and (7.4) a prime denotes differentiation with respect to r and u, respectively. Equation (7.4) has the same structure as (6.6), since it can also be written in the form

$$((1-u^2)w')' + \left((4-\mu) - \frac{4}{1-u^2}\right)w = 0\,.$$

Thus the analysis already performed can be repeated *verbatim*, obtaining non-trivial solutions for (7.4) only when μ is not positive and such that $4-\mu$ is the product of consecutive integers; hence, the first eigenvalue occurs for $\mu = -2$.

If we define $y(x) := \rho(Rx)$, we can write (7.3) thus:

$$(x^2y')' - (\beta x^2 + \lambda)y = 0 \qquad (7.6a)$$

$$y'(1) = \frac{2L_2}{L_1}y(1) \qquad (7.6b)$$

with

$$\beta := \frac{3bs_0}{2L_1}R^2 > 0. \qquad (7.6c)$$

Here a prime clearly denotes differentiation with respect to x. It follows from the general theory of singular differential equations that a solution of (7.6*a*), bounded as $x \to 0^+$, exists only if $\lambda \geqslant 0$ and it can be represented as a power series everywhere convergent in $\mathbb{R}^+$ (see, for example, theorem 4.3 of [15]):

$$y(x) = x^\alpha \sum_{k=0}^\infty c_k x^k \qquad (7.7)$$

with $c_0 = 1$ and $\alpha := -\frac{1}{2} + \frac{1}{2}\sqrt{1+4\lambda} \geqslant 0$. The coefficients c_k are determined on substitution of (7.7) into (7.6*a*), which yields the recursive formulae:

$$2nc_{2n}(2n + \sqrt{1+4\lambda}) = \beta c_{2n-2} \qquad c_{2n+1} = 0 \qquad \text{for} \quad n = 1, 2, \ldots . \tag{7.8}$$

As to limit condition (7.6*b*), we note that, by (7.7),

$$y'(1) - \alpha y(1) = \sum_{n=1}^{\infty} 2nc_{2n} . \tag{7.9}$$

The series on the right-hand side of (7.9) can be estimated by appeal to (7.8):

$$2nc_{2n} < \frac{\beta}{2 + \sqrt{1+4\lambda}} c_{2n-2} .$$

Hence,

$$\sum_{n=1}^{\infty} 2nc_{2n} < \frac{\beta y(1)}{2 + \sqrt{1+4\lambda}}$$

so that

$$\frac{y'(1)}{y(1)} < \alpha + \frac{\beta}{2 + \sqrt{1+4\lambda}} . \tag{7.10}$$

This inequality provides a lower bound on the values of β for which there is a non-trivial solution for (7.6):

$$\beta > \left(\frac{2L_2}{L_1} - \alpha\right)(2\alpha + 3) . \tag{7.11}$$

Moreover, since c_k are all positive, by (7.9) we also have

$$\frac{2L_2}{L_1} = \frac{y'(1)}{y(1)} > \alpha \tag{7.12}$$

and so a non-trivial solution of (7.6) exists only if $L_2 > 0$, since L_1 is positive by (2.6*d*). Making use of (7.8) and (7.9), we may write (7.6*b*) in a more expressive way:

$$\sum_{n=0}^{\infty} b_n \beta^n = 0 \tag{7.13}$$

with

$$b_n = \frac{2n + \alpha - \frac{2L_2}{L_1}}{h_n} \qquad \text{for} \quad n = 0, 1, 2, \ldots$$
$$h_0 = 1 \qquad h_n = 2n(2n + 1 + 2\alpha)h_{n-1} \qquad \text{for} \quad n = 1, 2, \ldots .$$

By equation (7.5), all these coefficients also depend on the elastic constants through the eigenvalue λ.

Finding a non-trivial solution to problem (7.6) amounts to finding a root of (7.13). Through (7.6*c*), this determines the critical radius for a radial variation, which depends on the elastic constants in an intricate way. Whether this variation actually prevails over the azimuthal ones in activating an unstable mode is discussed in the following section.

8. Phase diagram

We can combine the results of the preceding sections in a diagram illustrating the local stability of the hedgehog, for all admissible values of Landau–de Gennes constants. To this end we introduce the dimensionless quantities ξ and η defined as

$$\xi := \frac{L_2}{L_1} \qquad \eta := \frac{L_3}{L_1}\,. \tag{8.1}$$

Hereafter, in dealing with radial variations, we restrict our attention to the lowest eigenvalue λ_1 obtained from (7.5) by setting $\mu = -2$:

$$\lambda_1 := -2\frac{L_1 + L_2 + L_3}{L_1} = -2(\xi + \eta + 1)\,.$$

Thus, the azimuthal component w of a possibly unstable radial mode is precisely the same as the first unstable azimuthal mode. It is now to be determined whether the higher degree of freedom in a radial variation can change the picture drawn from the azimuthal stability analysis in section 6. A solution of (7.6*a*) exists only if $\lambda_1 \geqslant 0$, that is in the half-plane

$$\xi + \eta + 1 \leqslant 0\,. \tag{8.2}$$

Condition (7.12) can be stated as

$$\eta > -(2\xi^2 + 2\xi + 1) \tag{8.3}$$

which applies only for $\xi > 0$.

On the other hand, as shown in section 6, an azimuthal instability happens if and only if $L_1 + 2L_2 + L_3 > 0$, that is whenever

$$1 + 2\xi + \eta > 0\,. \tag{8.4}$$

Moreover, in seeking biaxial instabilities of a hedgehog, we should make sure that it is locally stable against uniaxial variations, requiring, by (4.2), that

$$2 - 7(\xi + \eta) > 0\,. \tag{8.5}$$

Finally, Ericksen's inequalities (2.6*a*), (2.6*c*) and (2.6*d*) read as

$$2 + 2\xi + \eta > 0 \qquad -2 < \eta < 2\,. \tag{8.6}$$

Collecting all these inequalities, we obtain the regions in the (ξ, η)-plane outlined in figure 5.

In region $\mathcal{M}$ the hedgehog is locally stable against all biaxial variations hitherto considered, while in $\mathcal{V}_a$ only the azimuthal unstable modes are allowed. Region $\mathcal{V}_r$ is divided into two parts by the line $1 + 2\xi + \eta = 0$ (broken in figure 5): below it, only radial unstable modes may arise, whereas above it, the two types of unstable mode compete one against the other. We decide which one prevails by comparing the critical radii of both.

Since $\xi \leqslant 1$ in $\mathcal{V}_r$, the coefficients b_n appearing in (7.13) are positive for all $n \geqslant 1$, so that the function $f(\beta) := \sum_{n=1}^{\infty} b_n \beta^n$ is monotonically increasing and equation (7.13), written in the form

$$\frac{2L_2}{L_1} - \alpha = f(\beta) \tag{8.7}$$

assures us that, if $2L_2/L_1 > \alpha$, there is a unique value of β allowing for a non-trivial solution of (7.6). Furthermore, we show that the radial instability prevails over the azimuthal one everywhere in $\mathcal{V}_r$, as it is excited at greater values of the critical radius. Let β_m be the lower bound for β given by $\beta_m := (2\xi - \alpha)(\alpha + 3)$ (see (7.11)) and let β_a be the critical value of β in the azimuthal case, corresponding to (6.9) through the definition of β in (7.6*c*):

$$\beta_a := 6(1 + 2\xi + \eta)\,. \tag{8.8}$$

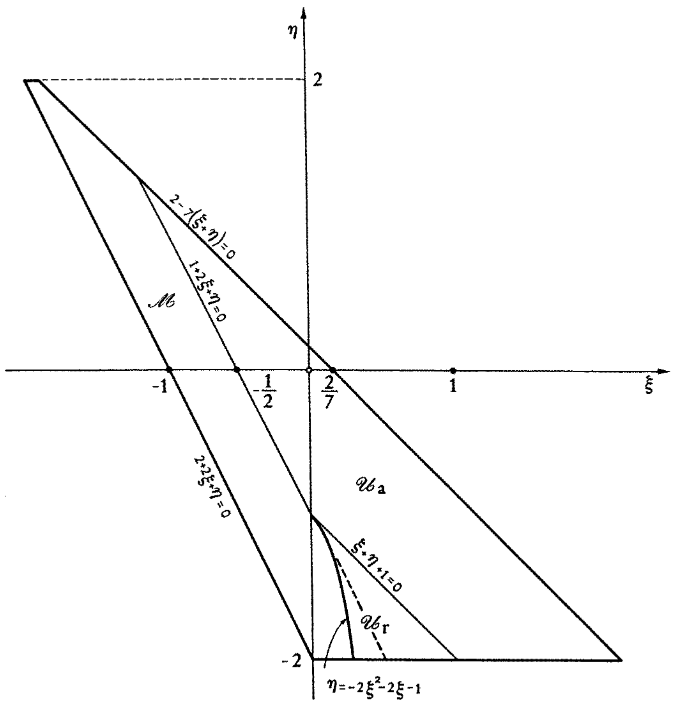

Figure 5. Phase diagram. It illustrates how the instability of the radial hedgehog depends on the elastic constants.

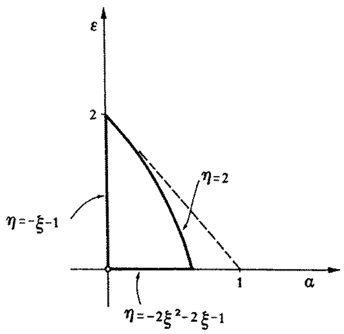

Figure 6. Region $\mathcal{V}_r$, after the change of coordinates $(\xi, \eta) \to (\varepsilon, \alpha)$.

If we express the value of α corresponding to the lowest eigenvalue λ_1 as a function of ξ and η:

$$\alpha(\xi, \eta) = -\tfrac{1}{2} + \tfrac{1}{2}\sqrt{-7 - 8\xi - 8\eta} \tag{8.9}$$

and define $\varepsilon(\xi, \eta) := 2\xi - \alpha(\xi, \eta)$, by the change of variables

$$\xi = \tfrac{1}{2}(\varepsilon + \alpha) \qquad \eta = -\tfrac{1}{8}((2\alpha + 1)^2 + 7 + 4(\varepsilon + \alpha))$$

we transform $\mathcal{V}_r$ into the region delimited by the new coordinate axes and the parabola $\varepsilon = 2 - 2\alpha - \alpha^2$, as sketched in figure 6.

Hence, $\beta_m - \beta_a = \alpha(2\varepsilon + 3\alpha)$ is clearly positive in the admissible region, except for $\alpha = 0$ where it vanishes. The desired conclusion then follows from the inequalities $\beta > \beta_m \geqslant \beta_a$.

Remark 1. As an aside, we observe that the region delimited by the lines $\eta = -2$, $\xi = 0$ and the parabola $\eta = -(2\xi^2 + 2\xi + 1)$ is stable not only for the lowest eigenvalue λ_1 but for

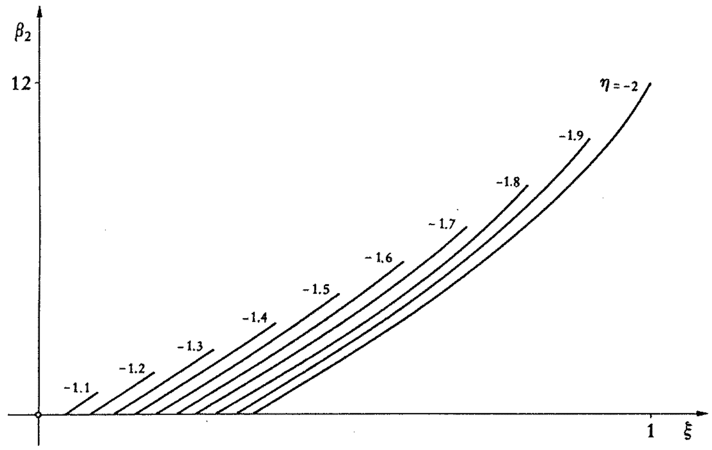

Figure 7. The curves show the behaviour of the quadratic approximation to β in $\mathcal{V}_r$ for different values of η.

all other eigenvalues as well. In fact, this region in the (ξ, η)-plane is characterized by the inequality $2\xi < \alpha_1$, with α_1 the value of α corresponding to λ_1. Since α is a monotonically increasing function of λ, we have $2\xi < \alpha_i$ for all $i \geqslant 1$, where α_i is α computed for the ith eigenvalue; thus, by (7.12), only the trivial solution of (7.6) survives here.

Unlike the azimuthal unstable mode, we have no explicit expression for the critical radius that excites the radial mode; nevertheless, we can use equation (7.13) to determine β, and then R_c, with the desired accuracy. To grasp the qualitative behaviour of β in $\mathcal{V}_r$ it suffices to consider the quadratic approximation to the function f in (8.7), which leads us to

$$\beta = \beta_2(\xi, \eta) := \frac{-b_1 + \sqrt{b_1^2 - 4b_0 b_2}}{2b_2} \tag{8.10}$$

where

$$b_0 := \alpha - 2\xi \qquad b_1 := \frac{2 + \alpha - 2\xi}{2(3 + 2\alpha)} \qquad b_2 := \frac{4 + \alpha - 2\xi}{8(3 + 2\alpha)(5 + 2\alpha)}\,.$$

The curves in figure 7 are sections of the graph of $\beta = \beta_2(\xi, \eta)$ for several selected values of η, viewed from the plane $\eta = -2$.

The straight line $1 + \xi + \eta = 0$ in figure 5 represents the locus where the radial unstable mode, prevailing in $\mathcal{V}_r$, is replaced by the azimuthal mode. It is interesting to note that this transition between the two modes happens with a discontinuity in the critical radius. Indeed, a direct computation shows the existence of a jump between β_a, expressed by (8.8), and β_2:

$$\beta_a - \beta_2 = 6\xi - \frac{5[2\xi - 2 + \sqrt{\frac{4}{5}(5 + 2\xi - \xi^2)}]}{2 - \xi}\,. \tag{8.11}$$

We close this section with yet another remark about higher modes.

Remark 2. Condition $2L_2/L_1 > \alpha$ implies the existence of non-trivial solutions of (7.6) also for eigenvalues λ other than λ_1. For any given value of the elastic constants, only a finite number n^* of coefficients b_n are negative. Equation (7.13) can be written as $\sum_{n=0}^{n^*} -b_n\beta^n = \sum_{n=n^*+1}^{\infty} b_n\beta^n$, where both sides are monotone, convex functions. As

$\beta \to +\infty$, the left-hand side goes to infinity more slowly than the right-hand one, and it takes a positive value at $\beta = 0$. This suffices to conclude that there is precisely one value of β satisfying (7.13), as claimed.

9. Comparison with previous studies

In this section we put our work in the same perspective as other studies on the fine structure of point defects in nematics. Our main term of comparison is Penzenstadler and Trebin's paper [8], often cited above. They show that a radial hedgehog is always unstable since its energy exceeds that of a non-singular ring disclination. Their analysis is nonlinear, though confined within a narrow class of biaxial orientations: the admissible order tensors are represented by the formula

$$\boldsymbol{Q}^{\lambda} := \sqrt{\tfrac{3}{2}}\,Q_0\big[A^{\lambda}(r,\vartheta)\big(\boldsymbol{e}_r \otimes \boldsymbol{e}_r - \tfrac{1}{3}\boldsymbol{I}\big) + B^{\lambda}(r,\vartheta)\big(\boldsymbol{e}_z \otimes \boldsymbol{e}_z - \tfrac{1}{3}\boldsymbol{I}\big)\big] \tag{9.1}$$

where the unit vector $\boldsymbol{e}_z$ lies along the polar axis in a spherical coordinate system, and the functions A^{λ} and B^{λ} are given the special form

$$A^{\lambda}(r,\vartheta) = \frac{r^2}{\sqrt{r^4 + \lambda^2 r^2(3\cos^2\vartheta - 1) + \lambda^4}} \qquad B^{\lambda}(r,\vartheta) = \frac{\lambda^2}{r^2}A^{\lambda}(r,\vartheta) \tag{9.2}$$

where λ is a positive parameter with the physical dimensions of a length. The functions in (9.2) are such that

$$\lim_{r\to\infty} A^{\lambda}(r,\vartheta) = 1 \qquad \lim_{r\to 0^+} A^{\lambda}(r,\vartheta) = 0$$
$$\lim_{r\to\infty} B^{\lambda}(r,\vartheta) = 0 \qquad \lim_{r\to 0^+} B^{\lambda}(r,\vartheta) = 1 \qquad \text{for all } \lambda > 0$$

so that away from the origin $\boldsymbol{Q}^{\lambda}$ approaches the radial hedgehog, whereas at the origin it represents the uniaxial orientation along the polar axis. On the other hand, in the limit as $\lambda \to 0^+$, B^{λ} vanishes everywhere, while A^{λ} is equal to 1, so that $\boldsymbol{Q}^{\lambda}$ tends to the radial hedgehog. With this choice of A^{λ} and B^{λ} the class of admissible fields in (9.1) is a one-parameter family: the energy attains its minimum for $\lambda = \lambda_0 > 0$, which represents the equilibrium radius of the ring; the estimate of λ_0 for a typical nematic liquid crystal such as MBBA turns out to be $\lambda_0 \approx 250$ Å.

The eigenvectors of $\boldsymbol{Q}^{\lambda}$ differ everywhere from the triad $(\boldsymbol{e}_r, \boldsymbol{e}_{\vartheta}, \boldsymbol{e}_{\varphi})$, but on the equatorial plane $\vartheta = \frac{\pi}{2}$; nevertheless, $\boldsymbol{e}_{\varphi}$ is an eigenvector of $\boldsymbol{Q}^{\lambda}$ for all values of ϑ. To compute the angle ψ^{λ} that represents the eigenvalues of $\boldsymbol{Q}^{\lambda}$ as ψ defined in (5.4) represents those of $\boldsymbol{Q}$ in (5.1), we compare the eigenvalue of $\boldsymbol{Q}^{\lambda}$ relative to $\boldsymbol{e}_{\varphi}$, that is $-\frac{1}{3}(A^{\lambda} + B^{\lambda})\sqrt{\frac{3}{2}}Q_0$, to the corresponding eigenvalue of $\boldsymbol{Q}$, as given by (5.5*c*): by (3.2) and (3.3), we conclude that

$$\psi^{\lambda} = \arccos\left(\frac{A^{\lambda} + B^{\lambda}}{2}\right) - \frac{\pi}{3} \tag{9.3}$$

where the cosine function is inverted onto the interval $[0, \pi]$. It is easily seen that ψ^{λ} vanishes at the origin and that

$$\psi^{\lambda}(r,\vartheta) \geqslant \psi^{\lambda}\left(r, \frac{\pi}{2}\right) \qquad \text{for all } r > 0 \quad \text{and} \quad \vartheta \in [0, \pi]$$

so that ψ^{λ} attains its minimum on the equatorial plane; a direct computation then shows that

$$\min \psi^{\lambda} = \psi^{\lambda}\left(\lambda, \frac{\pi}{2}\right) = -\frac{\pi}{3} \tag{9.4}$$

in agreement with the uniaxial nature of the ring. Equation (9.4) also shows that, for small λ, $\boldsymbol{Q}^{\lambda}$ cannot be regarded as a small biaxial perturbation of the radial hedgehog, for which $\psi \equiv 0$, and this explains why metastable hedgehogs escape Penzenstadler and Trebin's analysis.

There is a further aspect under which our analysis is different from theirs. Here the surface-like elastic constant L_3 affects the critical radius, as is clear for example in (6.9), while the formula for λ_0 in [8] depends only on L_1 and L_2. The reason is that here the core of the defect has a free spherical interface, and no boundary condition is enforced, neither on it nor at infinity, as done in [8].

Recently, the predictions of [8] have been confirmed by a numerical simulation of the energy minimizers in a droplet subject to a radially uniaxial boundary condition [16]. In these calculations Landau–de Gennes energy is employed, but both L_2 and L_3 in (2.3) are set equal to zero. On the phase diagram in figure 5, this choice of elastic constants would correspond to the origin. Since it falls within the region where the unstable azimuthal mode manifests itself, the simulations of [16] agree with our analysis. It would be interesting to explore, through the same numerical algorithm, the other regions in the above phase diagram.

More than twenty years ago, Candau *et al* observed a radial hedgehog in a droplet, which exhibited a small twisted region in its core. When viewed between crossed polarizers, the arms of the extinction cross were twisted as well. 'When rotating the polarizer and analyser together, the extinction arms rotate the same way. This demonstrates the radial nature of the configuration of the liquid crystal within the droplet' (cf [17], p 287). To our knowledge, similar observations have not been reported again for nematics. A qualitative explanation might be provided within our model through the hedgehogs falling in the region $\mathcal{V}_r$ of the phase diagram in figure 5, where the effective unstable mode is radial, rather than azimuthal, and the core is larger in size.

10. Conclusions

The local stability analysis of radial hedgehogs proposed in this paper has shown that some are metastable against biaxial variations in a rather wide class. The core of these hedgehogs fails to possess a biaxial fine structure: it should be adequately described by the model first proposed by Schopohl and Sluckin [11], which is formulated within the theory of uniaxial nematics with only a scalar order parameter. Among the locally unstable hedgehogs, we distinguish two categories, depending on the values of the elastic constants. In the one category, the core of the defect should develop a biaxial equilibrium structure with the ring described in [8], while in the other the core should be larger in size and its biaxial structure more complex, with some spiral feature, like that suggested by the observations of [17].

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