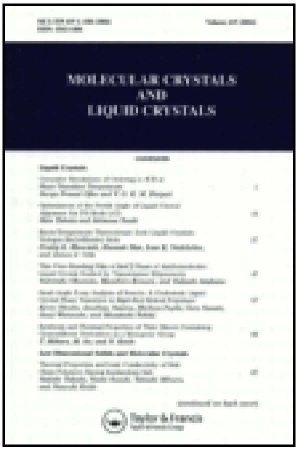

Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

Generalized Young-Laplace Equation for Nematic Liquid Crystal Interfaces and its Application to Free-Surface Defects

Alejandro D. Rey [a]

[a] Department of Chemical Engineering, McGill University, 3610 University Street, Montreal, Quebec, Canada, H3A 2B2

Version of record first published: 24 Sep 2006

To cite this article: Alejandro D. Rey (2001): Generalized Young-Laplace Equation for Nematic Liquid Crystal Interfaces and its Application to Free-Surface Defects, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 369:1, 63-74

To link to this article: http://dx.doi.org/10.1080/10587250108030009

Mol. Cryst. Liq. Cryst., Vol. 369, pp. 63-74
Reprints available directly from the publisher
Photocopying permitted by license only

Generalized Young-Laplace Equation for Nematic Liquid Crystal Interfaces and its Application to Free-Surface Defects

ALEJANDRO D. REY*

Department of Chemical Engineering, McGill University, 3610 University Street, Montreal, Quebec, Canada H3A 2B2

(Received May 16, 2000)

This paper uses the classical theories of liquid crystal physics to formulate the Young-Laplace equation of capillary hydrostatics for interfaces between viscous isotropic (I) fluids and nematic liquid crystals (NLC's). The equation provides an expression of pressure jumps across interfaces and determines the geometry of the interface. In addition, the force balance equation at a capillary point or line singularity containing a nematic surface defect is also derived from first principles. It is shown that the areal pressure balance and the line or point force balance equations provide a complete set to determine the geometry of an interface containing a defect. A new expression for the Peach-Koehler force for surface defects is developed. The contribution of the surface Peach-Koehler force to areal pressure balances is also identified. The equations are applied to solve for the interfacial geometry of a NLC whose free-surface contains a point defect. Consistency of the new approach developed in this paper with previously presented results is demonstrated.

Keywords: Young-Laplace equation; nematic liquid crystals; capillarity singularity; free-surface defects; interfacial geometry

1. INTRODUCTION

The determination of interfacial shapes and free-surface reliefs is a fundamental problem in interfacial science, and it plays a role in phenomena such as wetting, spreading, surface waves, nucleation, coagulation [1]. In static conditions the determination of the interfacial geometry is usually found by either the minimization of the total surface energy or equivalently by using the normal stress boundary condition, known as the Young-Laplace equation. On the other hand,

* Corresponding Author: e-mail: inaf@musicb.mcgill.ca Tel: (514) 398–4196 Fax: (514) 398–6678

under dynamic conditions the normal stress boundary condition is the only available method. In liquid crystalline interfaces under static conditions all the effort has been devoted to the free-energy method, but not much attention has been directed to the stress boundary condition approach. The details of this method and its application to nematic droplets has been given by Virga [2]. This methodology is effective to determine complex shapes and it is readily extended to non-equilibrium conditions. The rest of this paper restricts the discussion to static conditions.

General interfacial theories for NLC/I interfaces have been presented in the literature [3–14], but the complete and specific form for the Young-Laplace equation, necessary for a better understanding of interfacial phenomena in liquid crystalline materials, has apparently not yet been given and analyzed. For a recent review, see reference 3. A number of technological and scientific applications involving nematic interfaces can be found in the literature [3,14,15].

The normal stress boundary condition involving nematic liquid crystals involves a number of elastic effects that are absent in isotropic viscous fluids. For NLC, bulk energies contain gradient (Frank elasticity), gravitational, and magnetic contributions [16], and surface energies contain anchoring and gradient (splay-bend) contributions [3]. Thus the stress boundary conditions will generally be a force balance originating from these five energies. As shown below, the generalized Young-Laplace equation is a compact and clear expression of this balance. To apply the Young-Laplace equation the director field that defines the orientation in the NLC must be known or solved for, using the equations of nematostatics [16].

A characteristic of NLC is the display of disclination and point defects in the bulk, interfaces, and free surfaces [16]. In the latter case, capillarity interacts with the nematic orientation field, giving rise to specific free-surface reliefs [16,17]. An example of periodic free-surface pattern formation arises in NLC's with a free-surface subjected to magnetic fields, or thin films supported by a solid with hybrid orientation boundary conditions at the solid and free-surface [17,18]. The system displays a periodic array of point defects arranged in an hexagonal lattice, and the surface relief displays a corresponding lattice of pimples and dimples, whose characteristic length scale is in the micron size scale. The periodic surface pattern is easily detected by optical means. Although the problem has been solved using the free energy minimization method, in this paper we show the alternative method using the nematic Young-Laplace equation, showing how this approach may be used to determine interfacial and free-surface geometries in the presence of several free-energies.

Capillary systems with singularities arise in diverse interfacial systems, such as pinching in pendant droplets, and corner singularites in grain-boundaries [18]. In the problem described above, an array of free-surface point defects, at the location of the defect we have a double capillary-orientation singularity. This kind of problems are characteristic of liquid crystalline materials and in the past [16,17,18] they have been alnalyzed with the free energy method. The presence of a capillary singularity, such as a cusp, has been analyzed for isotropic [19] and liquid crystalline materials [9] using the edge boundary condition corresponding to the areal normal-stress boundary condition. More specifically, the corner or cone angle in a cusp is determined by a force balance involving the surface stress tensor. For NLC the surface stress tensor involves anchoring [20,21] and saddle-splay contributions. For the problem at hand, a free-surface defect at a capillary singularity, the interfacial force balance must include the Peach-Koehler force [22,23,24] acting on the free-surface defect. In this paper we show how to formulate force balances at double capillary-orientation singularities.

The objectives of this paper are: (1) to present the generalized Young-Laplace equation for nematic free-surfaces and its boundary condition, (2) to apply these eqations to the case of a free-surface defect in a nematic liquid crystal film, (3) to provide an alternative method to determine interfacial and free-energy geometries that can be extended to non-equilibrium cases.

The organization of this paper is as follows. Section 2 presents the well-known free enrgies in NLC's. Section 3 presents the generalized Young-Laplace equation for interfaces between NLC's and viscous isotropic fluids. A discussion of the different components of the nematic surface stress tensor is included. The identity of all the terms appearing in the Young-Laplace equation is discussed. Section 4 presents the force balance equation that applies to capillary-orientation singularities, such as a surface disclination line on an edge or a point defect on a cusp. The Peach-Koehler stress tensor that gives the force acting on a surface defect is formulated. Section 5 uses the two equation formulated in this paper, the Young-Laplace equation and the force balance at a double-capillary-oirentation singularity, to analyse the interfacial geometry of a free-surface point defect. Section 6 gives the conclusions.

2. LIQUID CRYSTAL FREE ENERGIES

Consider the interphase between an isotropic viscous fluid and a uniaxial rod-like nematic liquid crystal. The system is isothermal, and both phases are incompressible. The interphase is assumed to be elastic. Assume that a NLC occupies region R^n, and that an isotropic viscous fluid region R^i. The NLC structure is given by the director **n**, which is a unit vector representing the average molecular orientation. The orientation of the interface between the NLC/I regions is characterized by a unit normal **k**, directed from R^n into R^i. The total free energy of the NLC is given by:

$$F = F_{el} + F_{an} + F_{is} + F_g + F_m \tag{1}$$

where F_{el} is the elastic, F_{an} the anchoring, F_{is} the isotropic free energy, F_g the gravitional, and F_m the magnetic energy. The elastic free energy F_{el}, also known as Frank energy, contains long range gradient contributions and is given by:

$$F_{el} = \int f_b \, dV + \int f_s \, dS \tag{2}$$

where the bulk f_b and surface f_s gradient free energy densities are [3,9]:

$$f_b = \frac{1}{2}K_{11}(\nabla \cdot \mathbf{n})^2 + \frac{1}{2}K_{22}(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + \frac{1}{2}K_{33}|\mathbf{n} \times \nabla \times \mathbf{n}|^2 \quad \text{(3a,b)}$$
$$f_s = \frac{1}{2}(K_{22} + K_{24})\mathbf{h} \cdot \mathbf{g}; \quad \mathbf{h} = (\mathbf{n} \cdot \nabla_s)\mathbf{n} - \mathbf{n}(\nabla_s \cdot \mathbf{n})$$

where $\{K_{ii}\}$; ii=11,22,33,24, are the splay, twist, bend, and saddle-splay (Frank) constants, and **h** is the surface gradient energy density vector. The anchoring energy F_{an} arises from deviations of the director from the preferred orientation, or easy axis [9]:

$$F_{an} = \int \gamma_{an} dS; \quad \gamma_{an} = \frac{C}{2}(\mathbf{n} \cdot \mathbf{k})^2 \quad \text{(4a,b)}$$

where γ_{an} is the anchoring energy density, known as the Rapini-Papoular energy;[2] for C>0 (C<0) the preferred orientation is tangential (normal) to the interface. The isotropic free energy F_{is} is the surface integral of the usual isotropic interfacial tension γ_{is}. The total surface free energy density γ is thus the sum of isotropic, anchoring, and gradient, contributions:

$$\gamma = \gamma_{is} + \gamma_{an} + f_s \tag{5}$$

The director-dependent magnetic free-energy density f_m is given by:

$$f_m = -\frac{1}{2}\chi_a(\mathbf{n} \cdot \mathbf{H})^2 \tag{6}$$

where χ_a is the anisotropic magnetic susceptibility and **H** is the magnetic field. The gravitational free energy density is: $f_g = \rho\tau$, where ρ is the mass density, and τ the gravitational potential.

3. THE YOUNG-LAPLACE EQUATION FOR NEMATIC INTERFACES

The interfacial stress boundary condition at the NLC/I interface is expressed by [1]:

$$-\mathbf{k} \cdot (\mathbf{T}^i - \mathbf{T}^n) = \nabla_s \cdot \mathbf{t} \tag{7}$$

where $T^{i/n}$ is the total stress tensor in the two bulk phases, and **t** is the surface stress tensor. The bulk stress tensors are given by [9]:

$$\mathbf{T}^i = -p^i\mathbf{I}; \quad \mathbf{T}^n = -(p^n + f_m + f_g + f_b)\mathbf{I} + \mathbf{T}^E; \quad \mathbf{T}^E = -\frac{\partial f_b}{\partial \nabla \mathbf{n}} \cdot (\nabla \mathbf{n})^T \tag{8a,b,c}$$

where $p^{i/n}$ are the hydrostatic pressures, $\mathbf{T}^E$ is the Ericksen stress tensor, $(\nabla\mathbf{n})^T_{ij} = \nabla_j n_i$. The surface stress tensor **t** for the NLC/I is given by the sum of the normal (tension) stresses $\mathbf{t}^N$, the bending stresses $\mathbf{t}^B$ [11], and distortion stresses $\mathbf{t}^D$:

$$\mathbf{t}^N = \gamma\mathbf{I}_s; \quad \mathbf{t}^B = -\mathbf{I}_s \cdot \frac{\partial \gamma}{\partial \mathbf{k}}\mathbf{k}; \quad \mathbf{t}^D = -\mathbf{I}_s \cdot \frac{\partial \gamma}{\partial \nabla_s \mathbf{n}} \cdot (\nabla_s \mathbf{n})^T \tag{9a,b}$$

The surface normal stresses $\mathbf{t}^N$ are the usual tension stresses (t^N_{11}, t^N_{22}) present in all fluid interfaces; here 1 and 2 refer to directions of an orthonormal surface base coordinate system[1]. The asymmetric bending stress tensor $\mathbf{t}^B$ has no analogue in three dimensions, and only have 13 and 23 components (t^B_{13}, t^B_{23}) Bending stresses are proprtional to the anchoring coefficient C and to the splay-bend modulus K_{22}+K_{24}. The asymmetric distortion stress tensor $\mathbf{t}^D$ is the analogue to the bulk Ericksen stress $\mathbf{T}^E$ and contains normal (t^D_{11}, t^D_{22}) and shear components (t^D_{12}, t^D_{21}). Surface distorion stresses are proprtional to the splay-bend modulus K_{22}+K_{24}. In the absence of curvature, only forces arising from the divergence of the bending stresses $(\nabla_s \cdot \mathbf{t}^B_s)$ act along the unit normal **k**. Thus the presence of finite anchoring and surface gradient energy produces normal forces to the interface.

To obtain the Young-Laplace equation for NLC/I interfaces we substitute eqns. (8,9) into equation (1) and project the result along **k**, and find:

$$p^i - p^n = -(f_m + f_g + f_b) + \mathbf{kk} : \left(\frac{\partial f_b}{\partial \nabla \mathbf{n}} \cdot (\nabla \mathbf{n})^T\right) + 2H\gamma - \nabla_s \cdot \left(\mathbf{I}_s \cdot \frac{\partial \gamma}{\partial \mathbf{k}}\right) \tag{10}$$

where H = $-\nabla_s.\mathbf{k}/2$ is the mean curvature. The excess pressure or "pressure jump" is a function of the bulk free energy f_b, the Ericken stress $\mathbf{T}^E$, the surface free energy density γ, and the surface stress tensor **t**. An important observation is the terms contributed by the saddle-splay energy f_s are of the same functional form as those from anchoring energy. In terms of the nematic free energies given in eqns. (4,5,6), the Young-Laplace equation becomes:

$$p^i - p^n = -(f_m + f_g + f_b) + \mathbf{kk} : \left(\frac{\partial f_b}{\partial \nabla \mathbf{n}} \cdot (\nabla \mathbf{n})^T\right) + 2H(\gamma_{is} + \gamma_{an}) \tag{11}$$

$$\gamma'_{an}[2H(\mathbf{n}\cdot\mathbf{k}) + \nabla_s \cdot \mathbf{n}] - \gamma''_{an}[\mathbf{kn} : \nabla_s\mathbf{n} - \mathbf{nn} : \mathbf{b}] -$$

$$\left(\frac{K_{22} + K_{24}}{2}\right)\{\nabla\mathbf{n} : \nabla_s\mathbf{n} - (\nabla\cdot\mathbf{n})(\nabla_s\cdot\mathbf{n}) + (\mathbf{n}\nabla_s) : (\nabla\mathbf{n})^T - (\mathbf{n}\cdot\nabla_s)(\nabla\cdot\mathbf{n})\}$$

where γ'_{an}=C (**n.k**), γ''_{an}=C, $\mathbf{b}=\nabla_s\mathbf{k}$, and $\mathbf{nn:b}=\Sigma\Sigma n_i n_j b_{ji}$.

The distinguishing feature of the nematic interface in comparison with an isotropic interface is brought forth by analysis of the Young-Laplace equation. We find that in constrast to isotropic interfaces, the nematic interface is characterized by an internal length λ =γ/K, where K is an average Frank elastic constant. Accordingly, bulk and surface nematic distortions couple to interfacial curvature, such that when the internal length scale is much bigger than the external (system size,) scale, curvature is preferred to nematic distortions. On the other extreme, when the internal length scale is much smaller than the external scale, flat interfaces with nematic distortions are energetically favorable. Equation (10) provides a framework to design and interpret experiments aimed at creating surface roughening and patterning using nematic distortions.

4. FORCE BALANCE EQUATIONS FOR CAPILLARY-ORIENTATION SINGULARITIES

The generalized Young-Laplace equation is an areal stress balance equation, whose solution requires a boundary condition. Typically, the bounday condition is the specification of the contact angle. For a two-phase system, and in the absence of a defect, the force balance at a capillary singularity is simply the balance between the two corresponding surface stress tensors:

$$v^1 \cdot \mathbf{t}(\mathbf{k}^1) + v^2 \cdot \mathbf{t}(\mathbf{k}^2) = 0 \qquad (12)$$

where the $v^{1,2}$ are the unit surface vectors pointing away from the point or edge, and the $\mathbf{k}^{1,2}$ are unit normals to the two interfaces at the point or edge. Figure 1 shows a capillary singularity with a non-singular director field, at which eqn.(12) holds. In this case, at the singularity the unit normal is not defined since $\mathbf{k}^1$ and $\mathbf{k}^2$ are distinct. This case occurs in the presence of weak anchoring, when the director surface orientation is not fixed. Thus for this case we have a capillary singularity with a non-singular director field.

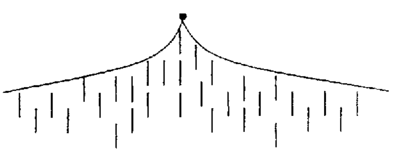

FIGURE 1 Schematic of a capillary singularity with a non-singular director field. At the capillary singularity the force balance equation is given in terms of the surface stress tensor. This situation arises in the presence of weak director anchoring

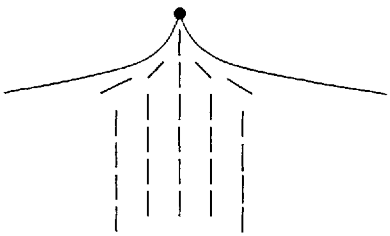

FIGURE 2 Schematic of a capillary-orientation singularity. At the capillary singularity there is also a nematic defect. For a capillary singularity corresponding to an edge the nematic defect is a disclination line. For a capillary singularity corresponding to a cusp the neamtic defect is a point defect. The double capillary-orientation singularity arises with strong director anchoring

The presence of a nematic surface defect in conjunction with a capillary singularity is shown in Fig. 2. In this case the unit normal and the director are simultaneously undefined. The presence of this double singularity occurs when the director surface orientation is fixed with respect to the surface unit normal. This double singularity is denoted here by capillary-orientation singularity. The presence of an interfacial orientational defect introduces an additional force in eqn.(12), known as the Peach-Koehler force Φ:

$$\nu^1 \cdot \mathbf{t}(\mathbf{k}^1) + \nu^2 \cdot \mathbf{t}(\mathbf{k}^2) + \Phi = 0 \tag{13}$$

In the case of planar director anchoring, when $\mathbf{n}.\mathbf{k}^1 = \mathbf{n}.\mathbf{k}^2 = 0$, the surface stress tensor appearing in eqn.(13) reduces to $\mathbf{t}=\mathbf{t}^N$. Peach-Koehler forces in NLC acting on defects located in the bulk have been discussed in the literature [22,23,24]. For example when a defect is embedded in an orientation inversion wall created by a magnetic field, the Peach-Koehler force is twice the surface tension (magneto-elastic energy per unit area) of the wall and is directed along the imposed magnetic field, such that if the defect moves in that specific direction the director field left behind has uniform orientation parallel to the imposed magnetic field [24]. When the defect is at a free-surface and arises by the imposition of a magnetic field normal to the surface, the Peach-Koehler forces are also given by the magneto-elastic energy per unit area and are directed normal to the surfaces whose intersection defines the defect. The geometry or the interfaces and the corresponding director field for the case of planar fixed director anchoring is defined in Fig. (2). In this case we can write the total Peach-Koehler force Φ as:

$$\Phi = \nu^1 \cdot \Psi(\mathbf{k}^1) + \nu^2 \cdot \Psi(\mathbf{k}^2);$$

$$\Psi(\mathbf{k}^1) = \nu^1\mathbf{k}^1 \int_{-\infty}^{0} (\mathrm{f_b} + \mathrm{f_m})\,\mathrm{dz}; \quad \Psi(\mathbf{k}^2) = \nu^2\mathbf{k}^2 \int_{-\infty}^{0} (\mathrm{f_b} + \mathrm{f_m})\,\mathrm{dz} \tag{14, a,b,c}$$

where z is measured in a direction normal to the interface, ψ is the surface Peach-Koehler tensor, and all vector quantities are evaluated at the singularity.

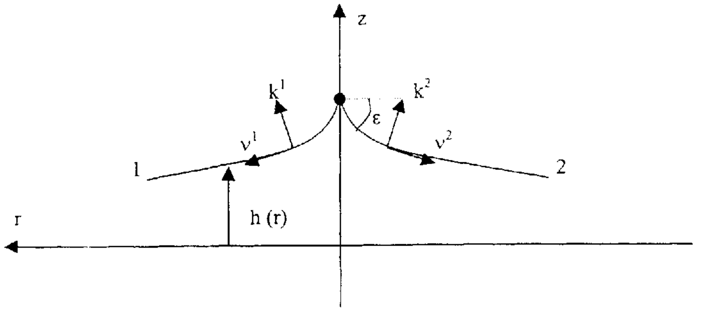

FIGURE 3 Schematic of the geometry and coordinate system for a capillary-point defect singularity. The adopted coordinate system is cylindrical (r,φ,z), since there is axial symmtery. The distance from the undisturbed height to the free-surface is h (r). The director orientation at the surface is fixed and tangential. The double singularity is located at (r=0). The tangential vector away from the singularity are ν^1, ν^2, and the corresponding unit normals are $\mathbf{k}^1$,$\mathbf{k}^2$

Now we recall that the surface stress tensor contributes to a force at a capillary singularity equal to the projections of the surface stress tensors along the intersecting surfaces: $\Sigma \upsilon^i.\mathbf{t}^i$, while at a surface it contributes to a capillary pressure equal to the normal projection of the surface divergence of the surface stress tensor: $(\nabla_s.\mathbf{t}).\mathbf{k}$. In a similar way, the surface Peach-Koehler tensor contributes to a nematic pressure equal to:

$$p^n = (\nabla_s \cdot \mathbf{\Psi}) \cdot \mathbf{k} \tag{15}$$

$$p^n = (\nabla_s \cdot \nu) \int_{\infty}^{0} (f_b + f_m)\, dz \tag{16}$$

A surface disclination line gives no contribution, since the surface divergence of the unit tangent vector is zero: $(\nabla_s.\nu) = 0$. On the other hand for a surface point defect, we find using a cylindrical coordinate system (r, φ,z) the additional pressure is finite and given by:

$$(\nabla_s \cdot \Psi) \cdot \mathbf{k} = (\nabla_s \cdot \nu) \int_{-\infty}^{0} (f_b + f_m)\, dz$$

$$= \frac{1}{\sqrt{1+h'^2}} \frac{1}{r} \frac{d}{dr} \left(\frac{r}{\sqrt{1+h'^2}} \right) \int_{-\infty}^{0} (f_b + f_m)\, dz \tag{17}$$

where h'=dh/dr, and h (r) is the height of the free-surface measured from the undistorterd interface. When $h' \ll 1$ this equation representing the hydrostatic pressure p^n simplifies to:

$$p^n = (\nabla_s \cdot \Psi) \cdot \mathbf{k} = \frac{1}{r} \int_{-\infty}^{0} (f_b + f_m)\, dz \tag{18}$$

Thus the concept of the Peach-Koehler force in bulk nematic defects is also applicable to interfacial defects, such that forces on surface defects contribute to pressures on the underlying interfaces. The hydrostatic pressure is given by the projected surface divergence of the surface Peach-Koehler tensor (eqn.(18)), and the force at a surface defect is given by the projected surface Peach-Koehler tensor (eqn.(14a)).

5. FREE-SURFACE DEFECT IN NEMATIC LIQUID CRYSTALS UNDER A MAGNETIC FIELD

As an example of the use of the Young-Laplace equation (10) and the surface Peach-Koehler force (14a), we analyze the existence of a single free-surface point defect in the presence of a magnetic field and gravity. This case has been analyzed using the minimization of the free-energy and its results have been confirmed experimentally. The present discussion gives an alternative view that may be useful in other geometries and non-static conditions. The geometry is defined in Fig. (3), and we follow the director field analysis provided in the literature [18]. We shall adopt the one constant approximation: $K_{11}=K_{22}=K_{33}=K$. The undisturbed nematic surface is located at z=0, and the NLC lies in the region z<0. A magnetic field H is applied along the z-axis and far from the interfaces the director **n** is parallel to H, while at the free-surface the director is parallel to the surface. The application of H causes a displacement h (r). The director field is: **n** (r,φ,z)= (sinθ,0, cos θ). The total bulk magneto-elastic free energy density is:

$$f_m + f_g = \frac{K}{2\xi^2}\left(\xi^2\left(\frac{\partial\theta}{\partial z}\right)^2 + \sin^2\theta\right) \tag{19}$$

where ξ is the magnetic coherence length, $\xi = \sqrt{K/\chi_a}/H$. Minimization of the total magneto-elastic energy with θ ($z \to -\infty$) = 0 leads to:

$$\xi^2\left(\frac{\partial\theta}{\partial z}\right)^2 = \sin^2\theta \tag{20}$$

The total magneto-elastic energy per unit area is then:

$$\int_{-\infty}^{0} (f_b + f_m)\, dz = \frac{K}{\xi} \qquad (21)$$

For the present geometry and tangential director boundary conditions the Young-Laplace equation becomes:

$$p^i - p^n = -(f_m + f_g + f_b) + \mathbf{kk} : \left(\frac{\partial f_b}{\partial \nabla \mathbf{n}} \cdot (\nabla \mathbf{n})^T \right) + 2H(\gamma_{is}) \qquad (22)$$

Furthermore using equation (20) we find that:

$$-(f_m + f_b) + \mathbf{kk} : \left(\frac{\partial f_b}{\partial \nabla \mathbf{n}} \cdot (\nabla \mathbf{n})^T \right) = 0 \qquad (23)$$

simplifying eqn.(22) to:

$$p^i - p^n = -f_g + 2H(\gamma_{is}) \qquad (24)$$

For the present geometry: $f_g = \rho g h$, and for $h' \ll 1$ the curvature 2H is:

$$2H = \frac{1}{r}\frac{d}{dr}(rh') \qquad (25)$$

The capillary pressure p^n is given:

$$p^n = (\nabla_s \cdot \Psi) \cdot \mathbf{k} = \frac{1}{r} \int_{-\infty}^{0} (f_b + f_m)\, dz = \frac{1}{r}\left(\frac{K}{\xi}\right) \qquad (26)$$

Neglecting the constant ambient pressure, we finally find the shape equation for h(r):

$$-\frac{1}{r}\left(\frac{K}{\xi}\right) = -\varrho\, gh + \frac{1}{r}\frac{d}{dr}(rh')\gamma_{is} \qquad (27)$$

Introducing the capillary length $\lambda=(\gamma_{is}/\rho g)^{1/2}$, the equation becomes identical to that found by the energy method [18]:

$$-\frac{1}{r}\left(\frac{K}{\xi\gamma_{is}}\right) = -\frac{h}{\lambda^2} + \frac{1}{r}\frac{d}{dr}(rh') \qquad (28)$$

To find the boundary condition for this equation we use the force balance equation (13) at the singularity:

$$t^1\gamma_{is} + t^2\gamma_{is} + \Phi = \mathbf{0}; \quad \Phi = \mathbf{k}^1\frac{K}{\xi} + \mathbf{k}^2\frac{K}{\xi} \qquad (29)$$

Taking the projection of this equation with the unit vector along z we get:

$$-2\gamma_{is}\sin\varepsilon + 2\frac{K}{\xi}\cos\varepsilon = 0 \qquad (30)$$

which defines the angle ε of the singularity with the horizontal (r) direction:

$$\tan\varepsilon = \frac{K}{\gamma_{is}\xi} \qquad (31)$$

which for $\varepsilon \ll 1$ reduces to $\varepsilon = K/(\gamma_{is}\,\xi)$. The angle ε is given by the ratio of the two surface energies and although it was just stated in the literature [16,18], the method developed in this paper provides another derivation. The solution of eqns.(28) is found in [18] and is quoted here for completeness:

$$h(r) = \lambda\varepsilon \int_0^{\pi/2} d\beta \exp(-r\cos\beta/\lambda) \qquad (32)$$

The Young-Laplace equation offers a simple and direct way to compute interfacial geometries. In the case of capillary-orientation singularities, application of the force balance equation at the singularity determines the shape of the singularity, also in a direct maner. The concept of Peach-Koehler force already used in describing forces in bulk defects, proves useful in analyzing surface defects.

6. CONCLUSIONS

The determination of interfacial geometry is important in variety of multiphase and capillary problems. In systems involving nematic liquid crystal phases the static interfacial geometry can be determined using free energy minimization or by the direct use of the generalized Young-Laplace equation. The latter is a normal stress balance equation in which all the bulk and surface free energies appear as contributions to stresses. This method of surface relief and interfacial geometry determination in the future can be extended to treat dynamic problems, such as wetting and surface waves.

The boundary conditions needed to solve the Young-Laplace equation is a force balance equation involving the surface stress tensor. For nematics the surface stress tensor contains tension, bending, and distortion stresses. In the presence of a capillary singularity such as an edge or a cusp with weak director anchoring the force balance only involves the surface stress tensor. On the other hand when the capillary singularity is also an orientation singularity, such as a disclination line on an edge or a point defect on a cusp, the force balance also contains the surface Peach-Koehler force acting on a defect. In this paper we have identified the nature of the surface Peach-Koehler force acting on a surface defect by formulating a surface Peach-Koehler stress tensor. In addition, we have shown that the surface divergence of the Peach-Koehler stress tensor gives rise to an hydrostatic pressure acting on the underlying surface on which the defect is located. The complete interfacial stress balance and point force balance formulation was applied to the case of a free-surface point defect in a nematic liquid crystal, and the results were shown to be consistent with those found by the energy method.

The framework developed here is general and can be applied to nematic interfacial problems in any geometry, containg capillary and/or orientation singularities.

Acknowledgements

Financial support of the Natural Sciences and Engineering Research Council (NSERC) of Canada is gratefully acknowledged.

References

[1] D. A. Edwards, H. Brenner, D.T. Wasan, Interfacial Transport Processes and Rheology (Butterworth, MA, 1991).
[2] E.G. Virga, Arch. Rational Mech. Anal., **107**, 371, 1989.
[3] H. Yokoyama, "Handbook of Liquid Crystal Research", edited by P.J. Collins and J.S. Patel (Oxford University Press, New York), Chapter 6, 179, 1997.
[4] T.J. Sluckin, and A. Poniewierski, in Fluid Interfacial Phenomena, edited by C.A. Croxton, (Wiley, Chichester), Chap. 5, 1986.
[5] A.K. Sen and D.E. Sullivan, Phys. Rev A., **35**, 1391 (1987).
[6] M.A. Osipov, and S. Hess, J. Chem. Phys., **99**, 4181 (1993).
[7] C. Papenfuss and W. Muschik, Mol. Cryst. Liq. Cryst., **262**, 561, 1995.
[8] J.L. Ericksen, in Advances in Liquid Crystals, G.H. Brown ed. (Academic, New York, 1979), vol. 4, p. 1.
[9] E.G. Virga, Variational Theories for Liquid Crystals (Chapman Hall, London 1994).
[10] J.T. Jenkins and P.J. Barrat, Appl. Math., **27**, 111 (1974).
[11] A.D. Rey, J. Chem. Phys., **110**, 9769 (1999).
[12] G. Barbero and G. Durand, in Liquid Crystals in Complex Geometries, G.P. Crawford and S. Zumer eds (Taylor and Francis, London 1996), pp 21–52.
[13] W.J.A. Goosens, Mol. Cryst. Liq. Cryst., **124**, 305 (1985).
[14] A.A. Sonin, Freely Suspended Liquid Crystalline Films, (John Wiley, New York), (Oxford University Press, London), 1993.
[15] A.A. Sonin, "The Surface Physics of Liquid Crystals" (Gordon and Breach Publishers, Amsterdan, 1995).
[16] P.G. de Gennes and J. Prost, The Physics of Liqid Crystals, 2^{nd} edn (Oxford University Press, London, 1993).
[17] N.V. Madhusudana and K.R. Sumathy, Mol. Cryst. Liq. Cryst., **129**, 137, 1985.
[18] M.J. Stephen and J.P. Straley, Rev. Mod. Phys., **46**, 617, 1974.
[19] M.E. Gurtin, Thermomechanics of Evolving Phase Boundaries in the Plane, Oxford Science Publication, Oxford, pp. 94, 1993.
[20] A.D. Rey, J. Chem. Phys., 2000.
[21] A.D. Rey, Mol. Cryst. Liq. Cryst., **338**, 197, 2000.
[22] J.D. Eshelby, Phil. Mag. A **42**, 403, 1980.
[23] G.A. Maugin and C. Trimarco, Int. J. Engng Sci., **33**, 1663, 1995.
[24] A.D. Rey, Liq. Cryst., **7**, 315, 1990.