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Forces on solid bodies immersed in nematic phases

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Abstract. A method is presented for finding, in the one-constant theory of nematics, the director field $\boldsymbol{u}$ that minimizes the free energy of a liquid crystal phase in contact with cylindrical or planar surfaces imposing appropriate boundary conditions on $\boldsymbol{u}$. The method is employed to find the resultant forces and moments acting on a long straight rod of radius ρ immersed in a nematic phase at distance d from a flat wall, under the assumption of strong-anchoring boundary conditions requiring $\boldsymbol{u}$ to be parallel to the rod axis at the rod surface and either (i) perpendicular or (ii) parallel to the wall at its surface. In both cases the net force on the rod tends to move it away from the wall. In case (ii) there is a torque on the rod tending to decrease the angle χ between the rod axis and the direction taken by $\boldsymbol{u}$ at the wall. The magnitude of this torque is proportional to $[\mathrm{sech}^{-1}(d/\rho)]^{-1}\chi$, which for large d/ρ is asymptotic to a slowly decreasing function of d/ρ, namely $[\ln(2d/\rho)]^{-1}\chi$. It also is shown that there are circumstances in which the method yields information about the forces acting between parallel rods in a nematic phase.

1. Preliminary observations

Consider a nematic phase $\mathcal{N}$ whose state is specified by giving a director field $\boldsymbol{u}$ with $|\boldsymbol{u}(\boldsymbol{m})| = 1$. As the interfaces between $\mathcal{N}$ and other phases or materials impose boundary conditions on $\boldsymbol{u}$, the total free energy of the phase $\mathcal{N}$ is affected by the relative position of bodies that may be immersed in it. It follows that a body immersed in a nematic phase can experience forces and torques that appear to arise from its interaction with other such bodies and the outer surfaces of that phase. Such forces have been put into evidence and quantified by physical experiments [1]. Our aim is to compute analytically these forces in simple configurations.

There is a theory of the transmission of stresses and torques through nematics; it was given in general formulation by Ericksen [2] and is elaborated with examples and references in the monograph of de Gennes [3]. We employ little of that theory here, because for the cases we consider the directions of resultant forces and moments on immersed bodies are evident from considerations of material symmetry, and hence the crucial step in the calculation of these resultants is finding the dependence of the equilibrium free energy of $\mathcal{N}$, Ψ_{eq}, on the bodies' position and orientation. In this study, emphasis is placed on the problem of finding a director field that truly minimizes free energy and the investigation of the uniqueness of that field.

We consider cases in which $\boldsymbol{u}$ is independent of z, i.e. $\boldsymbol{u} = \boldsymbol{u}(x, y)$, and we employ the one-constant theory of nematics in which w, the ratio of the free-energy density to the elastic constant k, is [4]

$$w = \tfrac{1}{2}|\nabla \boldsymbol{u}|^2. \tag{1}$$

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Although this case can appear quite restrictive, the analysis presented below sketches more realistic situations and permits us to do the calculations to the end. However, it is important to notice that probably no analytical result given here would survive if this approximation is dropped.

Thus, the problem of determining stable equilibrium states of $\mathcal{N}$ reduces to one of finding harmonic maps from a region Ω in $\mathbb{R}^2$ into the unit sphere S^2 that minimize the functional

$$W = W(\boldsymbol{u}) = \int_\Omega w \, \mathrm{d}x \, \mathrm{d}y \tag{2}$$

with $\boldsymbol{u}$ subject to conditions on the boundary $\partial\Omega$ of Ω. It is shown in [5] that when the energy is given by (1), and when both the domain and the boundary conditions are z-invariant, then the minimizers are also independent of z. Hence, we typically compute 3D situations.

We coordinate S^2 with a longitude θ and a latitude ϕ so that the Cartesian coordinates of $\boldsymbol{u}$ are given by

$$\begin{aligned} u^x &= \cos\phi\cos\theta \\ u^y &= \cos\phi\sin\theta \\ u^z &= \sin\phi \end{aligned} \tag{3}$$

and (1) takes the form

$$2w = |\nabla\phi|^2 + |\nabla\theta|^2 \cos^2\phi. \tag{4}$$

We take Ω to be a doubly connected open region in $\mathbb{R}^2$ whose boundary $\partial\Omega$ is the union of two disjoint curves Γ^a and Γ^b, and we consider strong anchoring boundary conditions of the following type. For three constants θ^0, ϕ^a, ϕ^b with θ^0 in $[0, 2\pi)$, ϕ^a and ϕ^b in $[-\pi/2, \pi/2]$, and $\phi^a \neq \phi^b$,

$$\begin{aligned} (\theta, \phi) &= (\theta^0, \phi^a) \qquad \text{on} \quad \Gamma^a \\ (\theta, \phi) &= (\theta^0, \phi^b) \qquad \text{on} \quad \Gamma^b. \end{aligned} \tag{5}$$

Our discussion rests on three observations.

Remark 1. *The minimizer $\boldsymbol{u}_*$ of W on the set $\mathcal{E}$ of functions $\boldsymbol{u}$ from Ω to S^2 that are in $H^1(\Omega; S^2)$ and obey (5) is unique. For the minimizer: $(\theta, \phi) = (\theta_*, \phi_*)$, where θ_* is a constant, i.e.*

$$\theta_* = \theta^0 \qquad \textit{in} \quad \Omega \tag{6}$$

and ϕ_* is the solution of the Dirichlet problem

$$\begin{aligned} \nabla^2\phi &= 0 \qquad \textit{in} \quad \Omega \\ \phi &= \phi^a \qquad \textit{on} \quad \Gamma^a \\ \phi &= \phi^b \qquad \textit{on} \quad \Gamma^b. \end{aligned} \tag{7}$$

The minimum value of $W(\boldsymbol{u})$ on $\mathcal{E}$ is

$$W_{min} = W(\boldsymbol{u}_*) = \tfrac{1}{2} \int_\Omega |\nabla\phi_*|^2 \, \mathrm{d}x \, \mathrm{d}y. \tag{8}$$

To verify the remark, note that the solution ϕ_* of (7) is unique, and, moreover if ϕ is a function in $H^1(\Omega; [-\pi/2, \pi/2])$ with $\phi_* = \phi$ on $\partial\Omega$, then

$$\int_\Omega |\nabla\phi|^2 \, \mathrm{d}x \, \mathrm{d}y > \int_\Omega |\nabla\phi_*|^2 \, \mathrm{d}x \, \mathrm{d}y \tag{9}$$

unless $\phi = \phi_*$ in Ω. For each $\boldsymbol{u}$ in $\mathcal{E}$, (4), (6) and (9) yield

$$
\begin{aligned}
2W(\boldsymbol{u}) &= \int_\Omega (|\nabla\phi|^2 + |\nabla\theta|^2 \cos^2\phi)\,\mathrm{d}x\,\mathrm{d}y \\
&\geqslant \int_\Omega |\nabla\phi|^2\,\mathrm{d}x\,\mathrm{d}y \\
&\geqslant \int_\Omega |\nabla\phi_*|^2\,\mathrm{d}x\,\mathrm{d}y = 2W(\boldsymbol{u}_*)
\end{aligned} \tag{10}
$$

where at least one of the two inequalities is strict unless θ is constant and ϕ equals ϕ_* on Ω.

Remark 2. *Let Ω_1 and Ω_2 be two conformally equivalent domains in $\mathbb{R}^2$, and let f be a conformal map from Ω_1 to Ω_2. Let h be a given bounded real-valued function on $\partial\Omega_2$, and let $\phi^{(2)}$ solve the problem*

$$
\begin{aligned}
\nabla^2\phi &= 0 \qquad \textit{in} \quad \Omega \\
\phi &= g \qquad \textit{on} \quad \partial\Omega
\end{aligned} \tag{11}
$$

with $\Omega = \Omega_2$ and $g = h$. Then (i) $\phi^{(1)} = \phi^{(2)} \circ f$ is the solution of (11) with $\Omega = \Omega_1$ and $g = h \circ f$, and (ii) $\phi^{(1)}$ and $\phi^{(2)}$ have the same Dirichlet energy, i.e.

$$
\tfrac{1}{2}\int_{\Omega_1} |\nabla\phi^{(1)}|^2\,\mathrm{d}x\,\mathrm{d}y = \tfrac{1}{2}\int_{\Omega_2} |\nabla\phi^{(2)}|^2\,\mathrm{d}x\,\mathrm{d}y. \tag{12}
$$

The conclusion (i) is well known; (ii) may be verified by direct calculation using the Cauchy–Riemann equations for f.

As we are concerned with cases in which Ω has connectivity two and hence is conformally equivalent to an annulus,

$$
A_\alpha^1 = \{(x, y) \in \mathbb{R}^2;\ \alpha^2 < x^2 + y^2 < 1\} \tag{13}
$$

with $0 < \alpha < 1$, our applications of remark 2 involve the solution of the model Dirichlet problem

$$
\begin{aligned}
\nabla^2\phi &= 0 \qquad \text{in} \quad A_\alpha^1 \\
\phi &= \phi^a \qquad \text{on} \quad \partial K_\alpha \\
\phi &= \phi^b \qquad \text{on} \quad \partial K_1
\end{aligned} \tag{14}
$$

where, for $\nu = \alpha$ and 1,

$$
K_\nu = \{(x, y);\ x^2 + y^2 = \nu^2\}. \tag{15}
$$

The solution ϕ_* of (14) is

$$
\phi_*(r) = (\phi^a - \phi^b)\frac{\ln r}{\ln\alpha} + \phi^b \tag{16}
$$

and yields

$$
\tfrac{1}{2}\int_{A_\alpha^1} |\nabla\phi_*|^2\,\mathrm{d}x\,\mathrm{d}y = \pi(\phi^a - \phi^b)^2[\ln(1/\alpha)]^{-1}. \tag{17}
$$

Thus, in view of remarks 1 and 2 we can assert the following.

Remark 3. *If Ω can be mapped conformally onto A_α^1, then the minimum value of W on $\mathcal{E}$ is*

$$
W(\boldsymbol{u}_*) = \pi[\ln(1/\alpha)]^{-1}\chi^2 \tag{18}
$$

with

$$
\chi = \phi^a - \phi^b. \tag{19}
$$

2. An immersed rod parallel to a planar wall

We consider here the net forces and torques that act on a solid cylindrical rod $\mathcal{R}$ of radius ρ that is immersed in a nematic phase $\mathcal{N}$ in such a way that each point on the axis of $\mathcal{R}$ lies at distance $d > \rho$ from a plane $\mathcal{P}$ that bounds $\mathcal{N}$. We take $\mathcal{P}$ to be the (x, z)-plane and $\mathcal{R}$ to be the set of points (x, y, z) in $\mathbb{R}^3$ with $x^2 + (y - d)^2 < \rho^2$. We suppose that the only bounding surfaces of $\mathcal{N}$ are $\mathcal{P}$ and the cylindrical surface of $\mathcal{R}$. Thus

$$\Omega = \{(x, y);\ y > 0, x^2 + (y - d)^2 > \rho^2\} \tag{20}$$

and $\partial\Omega = \Gamma^a \cup \Gamma^b$ with

$$\Gamma^a = \{(x, y);\ x^2 + (y - d)^2 = \rho^2\} \tag{21}$$

$$\Gamma^b = \{(x, y);\ y = 0\}. \tag{22}$$

We assume that the surface of the rod and the planar wall each impose a strong-anchoring boundary condition on $\boldsymbol{u}$.

We assume that at the rod surface $\boldsymbol{u}$ is parallel to the rod axis, which means that at that surface $(u^x, u^y, u^z) = (0, 0, 1)$, and $\boldsymbol{u}$ is at the north pole of S^2. In other words, on Γ^a the latitude ϕ of $\boldsymbol{u}$ is $\pi/2$ and the longitude θ is undefined.

As regards the planar wall $\mathcal{P}$, let us first assume that $\boldsymbol{u}$ is perpendicular to $\mathcal{P}$, i.e. that $(u^x, u^y, u^z) = (0, 1, 0)$ on Γ^b, so that we have

$$\begin{aligned} &\phi = \pi/2 \qquad \text{on} \quad \Gamma^a \\ &\phi = 0 \qquad \text{and} \qquad \theta = \pi/2 \qquad \text{on} \quad \Gamma^b. \end{aligned} \tag{23}$$

Clearly, in this case the minimizer of W on $\mathcal{E}$ has $\theta = \pi/2$ on all of Ω, and we may use equation (18) of remark 3 with $\chi = \pi/2$:

$$W(\boldsymbol{u}_*) = \frac{\pi^3}{4}[\ln(1/\alpha)]^{-1}. \tag{24}$$

When Ω is given by (20), the rational complex-variable function

$$\omega(\zeta) = \frac{\zeta - \mathrm{i}\sigma}{\zeta + \mathrm{i}\sigma} \qquad \zeta = x + \mathrm{i}y \tag{25}$$

with

$$\sigma = [d^2 - \rho^2]^{1/2} \tag{26}$$

conformally maps Ω onto the annulus A^1_α in such a way that the line Γ^b goes to the circle K_1, and the circle Γ^a goes to the circle K_α. In particular, the point $\omega = \alpha$ is the image of the point $\zeta = \mathrm{i}(d + \rho)$, i.e. $\alpha = \omega(\mathrm{i}d + \mathrm{i}\rho) = \rho/(d + \sigma)$, which yields

$$\alpha = \left[\frac{d - \sigma}{d + \sigma}\right]^{1/2} = \frac{s}{1 + (1 - s^2)^{1/2}} \qquad s = \frac{\rho}{d}. \tag{27}$$

For the boundary conditions (23), placement of (27) in (24) yields the following expressions for the equilibrium free energy of the phase $\mathcal{N}$ as a function Ψ_{eq} of s:

$$\begin{aligned} \Psi_{eq}(s) = kW(\boldsymbol{u}_*) &= \frac{1}{4}k\pi^3\left[\ln\left(\frac{1 + (1 - s^2)^{1/2}}{s}\right)\right]^{-1} \\ &= \frac{k\pi^3}{4}[\mathrm{sech}^{-1}(s)]^{-1}. \end{aligned} \tag{28}$$

It is clear that in this case there is no torque about the y-axis, but there is a force on $\mathcal{R}$ tending to increase d, i.e. tending to move the rod away from the surface $\mathcal{P}$, which we consider to be fixed. Indeed, the net force on $\mathcal{R}$ (per unit length of $\mathcal{R}$) has a component only in the y-direction and is

$$F = -\frac{\partial}{\partial d}\Psi_{eq}(\rho/d) = \frac{k\pi^3}{4d}(1-s^2)^{-1/2}[\text{sech}^{-1}(s)]^{-2}. \tag{29}$$

In the limit as $d \to \infty$ with ρ fixed,

$$\Psi_{eq} \sim \frac{k\pi^3}{4}[\ln(2d/\rho)]^{-1} \tag{30}$$

and

$$F \sim \frac{k\pi^3}{4d}[\ln(2d/\rho)]^{-2}. \tag{31}$$

Let us assume again that at the surface of $\mathcal{R}$ the director $\boldsymbol{u}$ is parallel to the axis of $\mathcal{R}$, i.e. to the z-axis, but now assume that at $\mathcal{P}$, i.e. at the (x, z)-plane, $\boldsymbol{u}$ is parallel to $\mathcal{P}$ and hence has $\theta = 0$. Each specification of ϕ at $\mathcal{P}$, i.e. of ϕ^b, now gives us an orientation, relative to the z-axis, for the preferred direction in the plane $\mathcal{P}$. Thus we assume that

$$\begin{aligned} &\phi = \phi^a = \pi/2 \qquad \text{on} \quad \Gamma^a \\ &\phi = \phi^b \qquad \text{and} \qquad \theta = 0 \qquad \text{on} \quad \Gamma^b \end{aligned} \tag{32}$$

and we note that

$$\chi = \frac{\pi}{2} - \phi^b \tag{33}$$

is now the angle between the axis of the rod and the preferred direction in the planar wall $\mathcal{P}$. For the minimizer $\boldsymbol{u}_*$ of W we here have $\theta = 0$ on all of Ω. The equations (25)–(27) hold again, but in place of (24) and (28), we have, by (18) and (27),

$$\Psi_{eq}(s, \chi) = kW(\boldsymbol{u}_*) = k\pi[\ln(1/\alpha)]^{-1}\chi^2 = k\pi[\text{sech}^{-1}(s)]^{-1}\chi^2 \tag{34}$$

with s again (ρ/d). For the force in the y-direction we have

$$F = -\frac{\partial}{\partial d}\Psi_{eq}(\rho/d, \chi) = \frac{\pi}{d}(1-s^2)^{-1/2}[\text{sech}^{-1}(s)]^{-2}\chi^2 \tag{35}$$

which is, of course, zero when the rod lies parallel to the preferred direction, i.e. when $\chi = 0$; F is a maximum, equal to the last expression on the right-hand side in (29), when the rod and the preferred direction are perpendicular, i.e. when $\chi = \pi/2$. The turning moment on the rod (which acts about the y-axis and tends to align the rod with the preferred direction) is the integral of m along the length of the rod, where m is given by

$$m = -\frac{\partial}{\partial \chi}\Psi_{eq}(s, \chi) = -2k\pi[\text{sech}^{-1}(s)]^{-1}\chi \tag{36}$$

and hence is proportional to χ and independent of z. The asymptotic forms of the equations (34)–(36) for the limit large (d/ρ) are

$$\Psi_{eq} \sim k\pi[\ln(2d/\rho)]^{-1}\chi^2 \tag{37}$$

$$F \sim \frac{k\pi}{d}[\ln(2d/\rho)]^{-2}\chi^2 \tag{38}$$

$$m \sim -2k\pi[\ln(2d/\rho)]^{-1}\chi. \tag{39}$$

It is interesting that when d is large compared with ρ, m decays slowly with increasing d.

3. Two parallel rods

We now consider two parallel cylindrical rods $\mathcal{R}^a$, $\mathcal{R}^b$, with radii ρ_a, ρ_b, which are immersed in a nematic with axial separation R and which have surfaces imposing different constant strong-anchoring boundary conditions on $\boldsymbol{u}$. Thus here

$$\Omega = \{(x, y); x^2 + y^2 > \rho_a^2, (x - R)^2 + y^2 > \rho_b^2\} \tag{40}$$

and $\partial\Omega = \Gamma^a \cup \Gamma^b$ with

$$\Gamma^a = \{(x, y); x^2 + y^2 = \rho_a^2\} = K_{\rho_a} \tag{41}$$

$$\Gamma^a = \{(x, y); (x - R)^2 + y^2 = \rho_b^2\}. \tag{42}$$

At the surface of $\mathcal{R}^a$, $\boldsymbol{u}$ is assumed to be parallel to the axis of $\mathcal{R}^a$, (i.e. to be parallel to the z-axis which means at the north pole of S^2) and hence has no defined longitude. At the surface of $\mathcal{R}^b$, $\boldsymbol{u}$ is assumed to be in the plane perpendicular to the axis of $\mathcal{R}^b$ (i.e. to be parallel to the (x, y)-plane which means on the equator of S^2) and to have a constant longitude θ^0. Therefore,

$$\begin{aligned} &\phi = \pi/2 \qquad \text{on} \quad \Gamma^a \\ &\phi = 0 \qquad \text{and} \qquad \theta = \theta^0 \qquad \text{on} \quad \Gamma^b \end{aligned} \tag{43}$$

and the minimizer of W on $\mathcal{E}$ has $\theta = \theta^0$ on all of Ω. Although we agree that these boundary conditions are not very physically realistic, they allow us to naturally extend our analysis to that case. Equation (18) with $\chi = \pi/2$, i.e. equation (24), holds again. To find the pertinent value of α we note that the domain Ω of (40) is conformally mapped into A_α^1 by the function

$$\omega(\zeta) = \frac{\sigma_2(\zeta - \sigma_1)}{\rho_a(\zeta - \sigma_2)} \qquad \zeta = x + \mathrm{i}y \tag{44}$$

with σ_1 and σ_2 obeying the equations

$$\sigma_1\sigma_2 = \rho_a^2 \qquad (R - \sigma_1)(R - \sigma_2) = \rho_b^2 \tag{45}$$

and with σ_2 chosen so that the formula

$$\alpha = \frac{\rho_b}{\rho_a}\left|\frac{\sigma_2}{R - \sigma_2}\right| \tag{46}$$

yields $\alpha = 1$. It follows from (44) that $\omega(\Gamma^a) = K_1$ and $\omega(\Gamma^a) = K_\alpha$.

We are interested in the limit in which the separation of the rods is large compared with their radii, i.e. in which

$$\beta = \left(\frac{\rho_a\rho_b}{R^2}\right)^{1/2} \ll 1. \tag{47}$$

In that limit (46) yields $\alpha = \beta^2 + \mathrm{O}(\beta^4)$, and hence, by remark 3,

$$\Psi_{eq} = \frac{k\pi^3}{4}[\ln(1/\alpha)]^{-1} \sim \frac{k\pi^3}{8}\left[\ln\left(\frac{R}{(\rho_a\rho_b)^{1/2}}\right)\right]^{-1}. \tag{48}$$

There is a net force on each rod tending to separate it from the other rod. This force of repulsion has a component only on the x-axis, and, for the limit of large separation, its magnitude per unit of rod length is

$$F = -\frac{\partial}{\partial R}\Psi_{eq} \sim \frac{k\pi^3}{8R}\left[\ln\left(\frac{R}{(\rho_a\rho_b)^{1/2}}\right)\right]^{-1}. \tag{49}$$

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References

[1] Poulin P, Cabuil V and Weitz D A 1997 *Phys. Rev. Lett.* **79** 4862
[2] Ericksen J L 1972 *Arch. Ration. Mech. Anal.* **9** 371
[3] de Gennes P G 1974 *The Physics of Liquid Crystal* (Oxford: Clarendon)
[4] Frank F C 1958 *Discuss. Faraday Soc.* **25** 1
[5] Bethuel F, Brezis H, Coleman B D and Hélein F 1992 *Arch. Ration. Mech. Anal.* **118** 149