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Theory of orientational modes at a nematic–solid interface
When do surface modes appear?

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Orientational modes at a solid–nematic interface with Rapini–Papoular boundary conditions are analysed in the framework of continuum nematodynamics, including the coupling of the director and fluid velocity. In the case of planar orientation, a surface mode appears in addition to the ordinary bulk modes, if the coupling between the director and fluid velocity, governed by the Leslie coefficient μ_2, is large enough. The dispersion relation for the surface mode exhibits two distinctive regimes as μ_2 increases. In a realistic situation, the relaxation rate of the surface mode is several times slower than that of the corresponding bulk mode.

1. Introduction

In a recent paper we have analysed the spectrum of light scattered from a nematic liquid crystal in contact with a solid surface [1]. The incoming light wave was considered to be confined to a thin layer close to the surface through the use of the evanescent wave of the light totally reflected from the solid–nematic interface [2, 3, 4]. The nematic liquid crystal was described solely in terms of the director field, so that the influence of the fluid velocity was neglected. In this case no orientational surface modes appear, the usual bulk orientational fluctuations being only slightly perturbed at the surface. The main effect on the evanescent light scattering spectrum is due to the non-conservation of the perpendicular component of the wavevector. The resulting expression for the scattered field correlation function is rather complicated and depends also on the surface anchoring interaction. In most experimental situations, however, the difference between the evanescent wave scattered field correlation function and the ordinary, single exponential bulk one is rather small.

In the present paper we are extending the analysis to include also the coupling between the director and the fluid velocity fields. This extension was initially dictated by the need to have a more accurate calculation of the scattered light correlation function. It is well known that the correction of the effective viscosity in the case of bend motion is quite large due to the fluid backflow effect [5]. The effective viscosity changes by a factor of up to about three in typical nematics as the wavevector direction changes form perpendicular to the director (splay or twist mode), where there is no backflow, to parallel to the director (bend mode), where the backflow is strong.

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As we will show in this paper, close to the solid surface the inclusion of the fluid velocity has a more remarkable consequence than just changing the effective viscosity. An orientational surface mode appears in certain situations if the coupling between the fluid velocity and the director is strong enough. The characteristic of the surface modes is that their amplitude decays exponentially in the direction perpendicular to the surface [6]. It is interesting to note that in the absence of the coupling to fluid velocity, the nature of the usual Rapini–Papoular [7] surface interaction is such that the surface modes are not possible.

The inclusion of the fluid velocity adds a degree of freedom to the problem and another independent boundary condition for the velocity. The result is that close to the surface, the fluid can no longer follow the motion of the director which effectively increases the viscous drag on the director. This both modifies the bulk waves at the surface and introduces an additional slower surface orientational mode with relaxation rate depending on the component of the wavevector parallel to the surface.

The starting point of the analysis will be the continuum equations of nemato-dynamics together with the appropriate boundary conditions [8]. We will first show how the surface mode appears and then briefly discuss how the bulk modes are modified.

2. Basic equations

The most interesting situation occurs when the nematic director is parallel to the surface along the x direction (planar orientation) and the director fluctuations $\delta\mathbf{n}$ are perpendicular to the plane of unperturbed director $\mathbf{n}$ and the normal to the surface which is along the z direction. This corresponds to the twist–bend branch of the bulk modes. In this case the y component v of the fluid velocity is coupled to $\mathbf{n}$. Let Θ be the small angle that $\mathbf{n}$ makes with the x axis. From the equations of nematodynamics we have

$$K_3\frac{\partial^2\Theta}{\partial x^2}+K_2\frac{\partial^2\Theta}{\partial z^2}-\mu_2\frac{\partial v}{\partial x}=\gamma\frac{\partial\Theta}{\partial t}, \tag{1}$$

$$\eta_c\frac{\partial^2 v}{\partial x^2}+\eta_a\frac{\partial^2 v}{\partial z^2}+\mu_2\frac{\partial^2\Theta}{\partial t\partial x}=0, \tag{2}$$

where K_i are the Franck elastic constants, μ_2 is the Leslie coefficient coupling orientation and flow, $\eta_{a,b,c}$ are the Miesowicz viscosities and γ is the rotational viscosity. The boundary conditions are

$$\frac{\partial\Theta}{\partial z}(x,0)=\frac{\omega}{K_2}\Theta(x,0) \tag{3}$$

and

$$v(x,0)=0. \tag{4}$$

Here ω is the anchoring strength. We seek solution to equations (1)–(3) of the form

$$\Theta=\theta(z)\exp(iq'x)\exp(-t/\tau) \tag{5}$$

and

$$v=u(z)\exp(iq'x)\exp(-t/\tau). \tag{6}$$

There are very many parameters in the problem and to see which combinations of them are essential we introduce dimensionless combinations

$$a=\frac{K_3}{K_2},\quad b=\frac{\eta_c}{\eta_a},\quad c=\frac{\mu_2^2}{\eta_a\gamma},\quad r=\frac{\gamma K_2}{\tau\omega^2},\quad q=q'\frac{K_2}{\omega},\tag{7}$$

and a new dimensionless independent variable $s=\omega/K_2 z$.

In order that the pure bend viscosity be positive, c must be smaller than b. All three materials parameters, a, b, and c are, in most nematics, somewhat larger than one. In 5CB, for example, $a=2{\cdot}6$, $b=3{\cdot}1$, and $c=2{\cdot}5$, and unless otherwise specified we will be using these values in our numerical examples. As c is proportional to η_2^2, it is a direct measure of the magnitude of the coupling between the director and fluid velocity.

Putting equations (5), (6) and (7) into equations (1) and (2) and eliminating u, we get the following equation for θ:

$$\frac{d^4\vartheta}{ds^4}-[(a+b)q^2-r]\frac{d^2\vartheta}{ds^2}+q^2[abq^2-(b-c)r)]\vartheta=0.\tag{8}$$

The boundary conditions become

$$\frac{d\theta}{ds}(0)-\theta(0)=0,\tag{9}$$

$$\frac{d^2\vartheta}{ds^2}(0)-(aq^2-r)\vartheta(0)=0.\tag{10}$$

θ must also be finite at infinity.

The roots of the characteristic polynomial of equation (8) can be considered to be functions of the relaxation parameter r. At r smaller than

$$r_-=(a-b+2c-2\surd[c(a-b+c)])q^2,$$

all roots are real, with two being positive and two negative. At $r_-<r<r_+$, where

$$r_+=(a-b+2c+2\surd[c(a-b+c)])q^2,$$

all four roots are complex, with two of them having a negative real part. In these two regions a surface mode may exist, as we will show in the next section. When $r>r_+$, there are either four imaginary roots or two imaginary and one real positive and one real negative root. In this region we get the bulk mode, which is slightly modified at the surface. Its dispersion relation, as will be shown, remains unperturbed.

3. Surface mode

As noted above, at $r<r_+$, there exist two roots of the characteristic equation of equation (8) with negative real parts, so we can construct a solution to equations (8), (9) and (10) in the form

$$\theta=A\exp(-\kappa_1 s)+B\exp(-\kappa_2 s),\tag{11}$$

where the real parts of κ_1 and κ_2 are positive. A solution of the form (11) which also satisfies the boundary conditions represents a coupled orientational–flow surface mode.

The boundary conditions (9) and (10) give

$$A(\kappa_1+1)+B(\kappa_2+1)=0,\tag{12}$$

$$A[\kappa_1^2-(aq^2-r)]+B[\kappa_2^2-(aq^2-r)]=0.\tag{13}$$

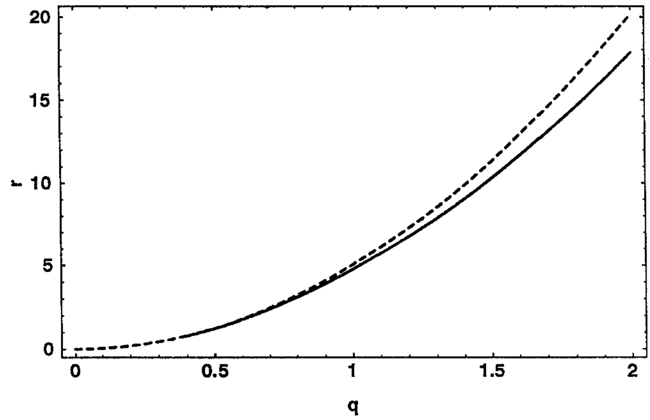

Figure 1. The dispersion relation for the surface mode (solid curve) and for the bulk mode (dashed) at $q_\perp = 0$ for $c = 1{\cdot}5$, $a = 2{\cdot}6$ and $b = 3{\cdot}1$.

κ_1 and κ_2 are roots of the characteristic polynomial and must therefore satisfy

$$\kappa_1^2\kappa_2^2 = abq^4 - (b-c)q^2r)] = 0 \tag{14}$$

and

$$\kappa_1^2 + \kappa_2^2 = (a+b)q^2. \tag{15}$$

For a non-trivial solution of equations (12) and (13), the determinant of this system must be zero. Also, κ_1 and κ_2 must not be equal. With this and equations (14) and (15) we get

$$\kappa_1\kappa_2 + (\kappa_1\kappa_2) + aq^2 - r = 0. \tag{16}$$

Equation (16) is an implicit dispersion relation connecting r and q for the surface mode. Using explicit expressions for κ_1 and κ_2, we can put it in the form

$$q = \frac{\surd\{a + b - (r/q^2) + 2\surd[ab - (b-c)]\}}{(r/q^2) - a - \surd[ab - (b-c)(r/q^2)]}. \tag{17}$$

In order for this expression to have a physical meaning, q must be real. This condition determines the exact form of the dispersion relation which depends also on the magnitude of the coupling parameter c. Three cases can be distinguished.

(1) $c < \frac{4}{3}(b^2/b + 3a)$. In the case of very small coupling parameter, q is not real for any value of r/q^2 and the surface mode does not exist.

(2) $\frac{4}{3}(b^2/3b + 3a) < c < (b^2/a + b)$. q is real and positive for r/q^2 lying between p_1 and p_2, where

$$p_1 = \tfrac{1}{2}\{2a - b + c + \surd[(2a - b + c)^2 + 4a(b-a)]\}$$

and

$$p^2 = \frac{ab}{b-c}.$$

In this interval, q attains a finite minimum value at $r/q^2 = p^2$, which means that the surface wave only appears at a finite value of q. At this value of q, the surface mode splits off the bulk mode dispersion relation. Figure 1 shows the dispersion relation for

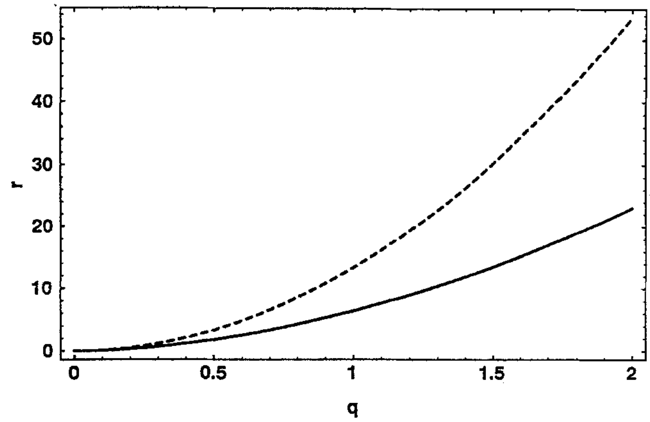

Figure 2. The dispersion relation for the surface mode (solid curve) and for the bulk mode (dashed) at $q_\perp = 0$ for $c = 2{\cdot}5$, $a = 2{\cdot}6$ and $b = 3{\cdot}1$.

the bulk mode with no perpendicular component of the wavevector $q_\perp$ and for the surface mode, calculated numerically from equation (17).

(3) $c > (b^2/a + b)$. In this case, valid for example in 5CB, q is real and positive for $p_1 > r/q^2 < r_+/q^2$. At $r = r_+$, $q = 0$ so that the surface mode exists at any value of q. Figure 2 shows the dispersion relation, calculated numerically, for the surface mode, again with the bulk mode at $q_\perp = 0$ for comparison.

From the figures, it is seen that the surface mode is always slower than the bulk one. When c is small, the difference between the relaxation times of the surface mode and bulk mode for wavevector q ($q_\perp = 0$ for the bulk mode) is also quite small and the surface mode may be difficult to detect experimentally. When c has a value above 2, which is usual in most nematics, the surface mode is slower by a factor of up to 3 for typical values of a and b.

4. Bulk mode

As stated in the Introduction, the surface waves are characterized by exponentially decaying spatial dependence in the direction perpendicular to the surface. Oscillating spatial form represents bulk modes, which may be modified at the surface, but have a plane wave form away from the surface. When $r > r_+$, at least two of the roots of the characteristic polynomial of equation (8) are imaginary and the solutions of equations (8), (9) and (10) represent bulk modes. Their exact form close to the surface again depends on the value of the coupling parameter c.

(1) $c < (b^2/a + b)$. In this case, two roots are imaginary and two are always real, one of them negative, so that the bulk solution has the form of a plane wave reflecting from the surface, plus an exponentially decaying term at the surface

$$\theta = A\exp(i\beta s) + B\exp(-i\beta s) + C\exp(-\kappa s). \tag{18}$$

We now have three constants to satisfy the boundary conditions and so β can have any value. The characteristic equation becomes simply the well-known dispersion relation for the bulk nematic twist–bend mode

$$r = q^2\frac{(\beta^2 + aq^2)(\beta^2 + b^2)}{\beta^2 + (b - c)q^2} \tag{19}$$

or, putting in the meaning of a, b, c, and q and setting $q_\perp = \beta\omega/K_2$,

$$\frac{1}{\tau} = \frac{q_\perp^2 K_2 + q^2 K_3}{\gamma - (\mu_2^2 q^2/\eta_a q_\perp^2 + \eta_c q^2)}, \tag{20}$$

which is the familiar form [8].

(2) $c > (b^2/a + b)$. In the case of strong coupling between the director and flow, the bulk solution is somewhat more complicated. For r only a little larger than r_+, all the roots are imaginary and the solution has the form

$$\theta = A\exp(i\beta s) + B\exp(-i\beta s) + C\exp(i\beta' s) + D\exp(-i\beta' s), \tag{21}$$

which simply represents two reflecting plane waves with different wavevectors (q, β) and (q, β') having the same relaxation rate. β can again have any value and the characteristic equation gives the same bulk dispersion relation (19) or (20). The boundary conditions give two relations between the amplitudes A, B, C, and D. β' is also determined through equations (14) or (15), connecting the roots of the characteristic equation.

When β (or r/q^2) becomes too large, β' becomes imaginary and the solution switches back to the form (18). This slightly complicated behaviour is a consequence of the simple fact that the bulk dispersion relation (19) has a minimum at a finite value of β for $c > (b^2/a + b)$, so that for a certain range of r, there are two values of β giving the same relaxation rate.

5. Discussion

We have shown that the equations of nemato-dynamics predict a surface mode at a solid–nematic interface when the director is parallel to the surface. This mode, with bend–twist polarization is slower than the usual bulk bend–twist mode with the same tangential component of the wavevector. Both the appearance of the mode and its slowness are the consequences of the boundary condition requiring that the fluid velocity at the surface is zero. The coupling between the director and flow is particularly strong for the bend mode, and as the fluid cannot move close to the surface, the surface mode can be pictured as a pure rotational bend motion, without the accompanying fluid backflow. This makes the effective viscosity larger and so the surface mode is slower than the bulk one.

Up to now we have only discussed the bend–twist mode and the director parallel to the surface. Keeping the same surface orientation, the splay–bend mode, where the director deviation $\delta\mathbf{n}$ is in the x–z plane, is also possible. In this case, the situation is more complicated because both x and z components of the fluid velocity are coupled to the director through the Leslie coefficients μ_2 and μ_3. Usually μ_3 is much smaller than μ_2. So, while we have not made a detailed analysis of this case, we expect that a surface mode with bend–splay orientation also exists and behaves similarly to the bend–twist mode.

The situation is different for the case of the director perpendicular to the surface. The bulk mode with the wavevector tangential to the surface, that is in the x direction, is either pure twist for $\delta\mathbf{n}$ perpendicular to the x–z plane or pure splay for $\delta\mathbf{n}$ along x. Pure twist is not coupled to the fluid flow and pure splay is coupled only weakly through μ_3. The corresponding surface wave, if it would exist, would also be predominantly of the twist or splay type and so at most weakly coupled to the fluid flow. But we have seen that in the case of weak coupling the surface mode does not exist. This qualitative argument is also borne out by a calculation similar to the one presented above, in which an implicit relation between the relaxation parameter r and surface wavenumber q has no real, physically admissable solution for the range of parameters found in real nematics. So, in the case of the director perpendicular to the surface, we do not expect a surface wave to exist. This is also the case that was analysed by Papanek in a more complicated slab geometry [9].

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References

[1] Copic, M., Park, C., and Clark, N. A., 1992, *Molec. Crystals liq. Crystals*, **222,** 111.
[2] Lan, K. H., Ostrovsky, N., and Sornette, D., 1986, *Phys. Rev. Lett.*, **57,** 17.
[3] Allain, C., Ausserre, D., and Rondelez, F., 1985, *Phys. Rev. Lett.*, **54,** 1948.
[4] Selser, J. C., Rotschild, K. J., Swalen, J. D., and Rondelez, F., 1982, *Phys. Rev. Lett.*, **48,** 1960.
[5] Orsay Liquid Crystal Group, 1971, *Molec Crystals Liq. Crystals*, **13,** 187.
[6] Ingard, K. U., 1988, *Fundamentals of Waves and Oscillations* (Cambridge University Press).
[7] Rapini, A., and Papoular, M., 1969, *J. Phys., Paris, Colloq.*, **30,** C4.
[8] de Gennes, P. G., and Prost, J., 1993, *The Physics of Liquid Crystals* (Clarendon Press), Chap. 5.
[9] Papanek, J., 1990, *Molec. Crystals liq. Crystals*, **179,** 139.