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Dilation sheath of smectic-A focal-conic singular lines

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We study the validity of the lamellae equidistance approximation within smectic-A focal conics. We show the existence of a lamellae dilation sheath surrounding the singular lines cores. The dilation is estimated using a perturbative model starting from the ideal focal-conic approximation. It is found to decay algebraically away from the singular lines cores, and its energy contributes to the total energy of the focal conic.

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Smectic-A liquid crystals are lamellar phases. They consist of piled liquid monolayers of rodlike molecules, which are oriented normally to the lamellae. The period $a_0 \sim 30$ Å compares with the molecular length. The smectic-A elastic distortions involve lamellae curvature

$$\sigma = \mathrm{div}\mathbf{n} \ , \tag{1}$$

where $\mathbf{n}$ is the normal to the lamellae (σ is also equal to the sum of the lamellae principal curvatures $1/R_1 + 1/R_2$), and lamellae dilation

$$e = \frac{a - a_0}{a_0} \ , \tag{2}$$

where a is the lamellae thickness. By "dilation," we intend both positive and negative thickness variations. The local energy density for large scale distortions is simply [1]

$$f = \tfrac{1}{2}K\sigma^2 + \tfrac{1}{2}Be^2 \ . \tag{3}$$

$(K/B)^{1/2} \equiv \lambda$ defines a characteristic length usually comparable with the lamellae thickness, i.e., *microscopic.* Minimization of (1) yields the smectic-A equilibrium equation

$$\mathrm{div}\{\lambda^2 \nabla_{\parallel}\sigma + e\mathbf{n}\} = 0 \ , \tag{4}$$

where $\nabla_{\parallel}\sigma = \nabla\sigma - (\nabla\sigma \cdot \mathbf{n})\mathbf{n}$ is the curvature gradient projected parallel to the lamellae. This equation, first obtained by Kleman and Parodi [2], is the *covariant* equation that generalizes the well-known de Gennes equation [3] valid only for quasiplanar layers. For a straightforward derivation of Eq. (4), see Ref. [4]. Smectics are frequently subject to external boundary constraints inducing large scale curvature $\sigma \sim 1/d$ (d is the sample thickness). Since curvature and dilation are not independent variables, some lamellae dilation arises even if the boundary conditions do not directly impose it. In the latter case, however, as long as $d \gg \lambda$, the dilation is extremely small ($\varepsilon \lesssim \lambda/d$; otherwise, it would exceed the curvature energy).

The usual theory of macroscopic smectic defects assumes that the interlayer distance is exactly constant [5], i.e., $e \equiv 0$. This implies that all the (curved) lamellae be strictly parallel and thus share a common curvature center locus. This locus, called the "focal" of the texture, is generally a pair of surfaces. The latter are singularities for the smectic piling, and because they are too energetic they degenerate to a pair of lines. The layers assume then the shape of the so-called Dupin's cyclides. The focal is a pair of an *ellipse* and a *hyperbola,* in perpendicular planes, the focus of one coinciding with the summit of the other. These ideal textures of parallel equidistant layers are called *focal conics* [5–7].

Real smectics show textures with pairs of singular ellipses and hyperbolas that look very similar to the above-described geometrical textures. However, the latter are not physical: $\frac{1}{2}Be^2$ alone is minimized ($e \equiv 0$) but not the total elastic energy density (3) (the layer shape is defined by the requirement that the focals degenerate to lines). As was proposed in Ref. [2], real focal conics should present a little dilation. From our previous energetic arguments, the latter must be very small as long as the curvature radiuses are macroscopic. However, the lamellae curvature diverges when approaching the singular lines. In this paper, we study the validity of the lamellae equidistance approximation in the vicinity of the ellipse and hyperbola singular lines. Note that our purpose is not to discuss a model for the singular lines cores, but to investigate the discrepancy between real and geometrical focal conics inside their bulk when approaching the lines cores.

Let us first define more precisely the *cores* of the singular lines. Extrapolating the focal-conic texture up to the ellipse and hyperbola lines leads to a divergence of the lamellae curvature and to a discontinuity of the lamellae orientation. This implies that the smectic will be highly distorted around these lines. The standard elastic energy (3) is no longer valid in these regions. One must consider, in addition, other distortions such as a tilt of the molecules with respect to the lamellae normal, the fusion of the smectic or nematic orders, etc. Accordingly, one should consider the tilt and fusion energies, the energies associated with the nematic bend, and twist distortions and higher-order smectic terms. It has been shown that these additional variables and energy terms are infinitesimal as soon as the scale of the distortions is larger than some corresponding coherence and penetra-

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tion lengths [1,8]. Far from second-order phase transitions, these lengths are $\sim\lambda$, i.e., comparable to a few molecular lengths. Consequently, the lines distortions will vanish exponentially outside a core of size $\sim\lambda$ centered on the singular lines. In principle, outside the cores, other terms such as the nematic constants K_{13} and K_{24} (saddle splay) should also be added to (3). However, they do not contribute to Eq. (4) since they are *surface terms* [9,10]. In other words, Eq. (4) can be considered as correct up to a distance of order a few λ from the lines cores.

Let us now define precisely the geometrical focal conics (of the first species [5]) and introduce the "confocal coordinates" (Fig. 1). The following parametrization and identities are taken from Ref. [11]. The ellipse ($\mathcal{E}$) and the hyperbola ($\mathcal{H}$), respectively, in the (x,y) and (x,z) planes, are parametrized by

$$\mathcal{E}: \begin{cases} x' = a\cos\phi \\ y' = b\sin\phi, \end{cases} \quad \mathcal{H}: \begin{cases} x'' = c\cosh u \\ z'' = b\sinh u, \end{cases} \tag{5}$$

where $c=(a^2-b^2)^{1/2}$. The lines EH joining a point of $\mathcal{E}$ to a point of $\mathcal{H}$ are called *generators*. The length of a segment $[E,H]$ is

$$L = a\cosh u - c\cos\phi > 0 \ . \tag{6}$$

The focal-conic texture is such that the normals to the lamellae are everywhere parallel to the generators. The surfaces perpendicular to the generators are called Dupin's cyclides; they are the lamellae of the geometrical focal conics. When the ellipse degenerates to a circle, the lamellae are simply concentric tori folded around the circle. The space is conveniently parametrized in coordinates $(\phi,u,r,)$, where (ϕ,u) defines a generator and r is a distance measured along the latter oriented from E to H. It is convenient to choose the origin of r such that Dupin's cyclides satisfy $r=$const. This is done by choosing an origin $O(\phi,u)$ different on each generator, such that O is prior to H and at a distance $a\cosh u$ (Fig. 1). We shall call such coordinates confocal coordinates. By construction, the geometrical focal conics satisfy

$$\mathbf{n}(\mathbf{r}) = \mathbf{e}_r \ , \qquad e(\mathbf{r}) = 0 \ . \tag{7}$$

The confocal coordinates are orthogonal with elementary arclengths

$$ds^2 = dr^2 + F^2 d\phi^2 + U^2 du^2 \ . \tag{8}$$

Let us now focus on the points that are within the segments $[E,H]$; they satisfy $c\cos\phi < r < a\cosh u$. Their distances (along the generators) to the singular lines are, respectively,

$$d_E = r - c\cos\phi > 0 \ , \qquad d_H = a\cosh u - r > 0 \ . \tag{9}$$

We have then $L = d_E + d_H$. The coefficients of the fundamental quadratic form (8) are given by [11]

$$F = b\frac{d_H}{L} \ , \qquad U = b\frac{d_E}{L} \ . \tag{10}$$

The differential operators appearing in Eq. (4) are thus given by [12]

$$\nabla g = \frac{\partial g}{\partial r}\mathbf{e}_r + \frac{1}{F}\frac{\partial g}{\partial \phi}\mathbf{e}_\phi + \frac{1}{U}\frac{\partial g}{\partial u}\mathbf{e}_u \ , \qquad \mathrm{div}\mathbf{h} = \frac{1}{FU}\left[\frac{\partial}{\partial r}(FUh_r) + \frac{\partial}{\partial \phi}(Uh_\phi) + \frac{\partial}{\partial u}(Fh_u)\right] \ . \tag{11}$$

Let us now show that geometrical focal conics are *not* a solution of the smectic equilibrium equation (4). We shall calculate $\mathrm{div}(\nabla_{\parallel}\sigma)$ in confocal coordinates, with $\sigma = \mathrm{div}\mathbf{e}_r$ [cf. Eqs. (1) and (7)]. Making use of Eqs. (9)–(11), we obtain

$$\sigma = \frac{1}{FU}\frac{\partial(FU)}{\partial r} = \frac{\partial}{\partial r}\ln(d_E d_H) = \frac{1}{d_E} - \frac{1}{d_H} \ , \tag{12}$$

which was expected since the ellipse and the hyperbola are the centers of curvature of the Dupin's cyclides. Since $(\mathbf{e}_\phi, \mathbf{e}_u)$ are parallel to the lamellae, we have simply

$$\nabla_{\parallel}\sigma = \frac{1}{F}\frac{\partial \sigma}{\partial \phi}\mathbf{e}_\phi + \frac{1}{U}\frac{\partial \sigma}{\partial u}\mathbf{e}_u \ . \tag{13}$$

Thus,

$$\mathrm{div}(\nabla_{\parallel}\sigma) = \frac{1}{FU}\left[\frac{\partial}{\partial \phi}\left[\frac{U}{F}\frac{\partial\sigma}{\partial\phi}\right] + \frac{\partial}{\partial u}\left[\frac{F}{U}\frac{\partial\sigma}{\partial u}\right]\right] \ . \tag{14}$$

Straightforward calculations yield then

$$\mathrm{div}(\lambda^2\nabla_{\parallel}\sigma) = \frac{\lambda^2 L^2}{b^2 d_E^2 d_H^2}\left[L + \frac{c^2\sin^2\phi}{d_E} - \frac{a^2\sinh^2 u}{d_H}\right] \ . \tag{15}$$

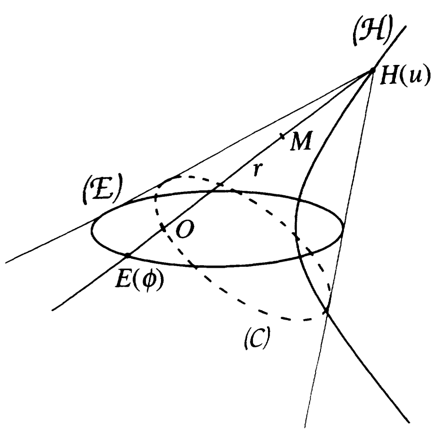

FIG. 1. A focal conic with its elliptical ($\mathcal{E}$) and hyperbolical ($\mathcal{H}$) singular lines. The smectic lamellae are Dupin's cyclides, satisfying $r=$const in the (ϕ,u,r) "confocal coordinates." The origin of r on each generator is defined geometrically by its intersection with circle ($\mathcal{C}$), the latter being the normal section of the revolution cone issuing from point $H(u)$ that passes through the minor axis of the ellipse.

This quantity does not vanish identically; therefore, geometrical focal conics do not satisfy Eq. (4).

Let us now consider a real focal conic. Since it closely resembles a geometrical focal conic, it should obey

$$\mathbf{n}(\mathbf{r})=\mathbf{e}_r+\delta\mathbf{n}(\mathbf{r}) , \quad e(\mathbf{r})=0+\varepsilon(\mathbf{r}) , \tag{16}$$

where $\delta\mathbf{n}$ and ε are small quantities (at least outside the cores). However, such equations do not define a unique texture. In principle, to solve the problem, one should express $\mathbf{n}$ and e as functions of a given texture (e.g., via the phase function of Ref. [2]). Then, Eq. (4) should be solved with the right boundary conditions. One faces then a difficult problem since Eq. (4) is not valid up to the (cores) boundaries. Nevertheless, it is possible to get some information about the lamellae dilation inside the focal-conic bulk. We shall use a perturbative model. A glance at (13) shows that within a geometrical focal conic, $\lambda^2\nabla_{\|}\sigma\equiv\lambda^2\nabla_{\|}(\mathrm{div}\mathbf{e}_r)$ is of order λ^2/d^2 and thus is infinitesimal well outside the cores since λ is a microscopic length. Therefore, to calculate the first-order approximation to ε, we can neglect in Eq. (4) the higher-order contribution to $\lambda^2\nabla_{\|}\sigma$ coming from $\delta\mathbf{n}$. Our perturbative approach will then consist in solving Eq. (4) with $\mathbf{n}$ and e given by Eqs. (16) where $\delta\mathbf{n}$ is set equal to zero:

$$\frac{\partial\varepsilon}{\partial r}+\varepsilon\,\mathrm{div}\mathbf{e}_r+\lambda^2\mathrm{div}[\nabla_{\|}(\mathrm{div}\mathbf{e}_r)]=0 . \tag{17}$$

Calling now

$$\xi=d_E , \quad L-\xi=d_H , \tag{18}$$

Eq. (17) becomes explicitly

$$\frac{\partial\varepsilon}{\partial\xi}+\varepsilon\left[\frac{1}{\xi}-\frac{1}{L-\xi}\right] =-\frac{\lambda^2L^2}{b^2\xi^2(L-\xi)^2}\left[L+\frac{c^2\sin^2\phi}{\xi}-\frac{a^2\sinh^2u}{L-\xi}\right] . \tag{19}$$

This equation is a first-order linear differential equation. The solution of its homogeneous part is $\mathrm{const}/[\xi(L-\xi)]$, and the complete solution is

$$\varepsilon(\xi)=\frac{\varepsilon_0L^2}{\xi(L-\xi)}-\frac{\alpha}{b^2}\frac{\ln\left[\dfrac{\xi}{L-\xi}\right]}{\dfrac{\xi}{\lambda}\dfrac{L-\xi}{\lambda}}+\frac{c^2\sin^2\phi}{b^2}\frac{L}{L-\xi}\frac{\lambda^2}{\xi^2} -\frac{a^2\sinh^2u}{b^2}\frac{L}{\xi}\frac{\lambda^2}{(L-\xi)^2} , \tag{20}$$

where

$$\alpha=L^2+c^2\sin^2\phi-a^2\sinh^2u$$

and ε_0 is a constant (depending on ϕ and u). As explained above, (20) is only valid outside cores of size $\sim\lambda$. We can admit that it works qualitatively well within, say, $\xi\in\,]3\lambda,L-3\lambda[$. Another limitation comes from the fact that the geometrical approximation for focal conics is not valid far above the ellipse plane as shown in Ref. [13]; therefore, we shall also keep u of order unity. Deep within the bulk of the focal conic ($\xi\sim L/2$), the dilation given by (20) is $\varepsilon\sim\varepsilon_0+O(\lambda^2/L^2)$. The validity of our perturbative model requires, therefore, $\varepsilon_0\ll 1$.

From (20), we see that the dilation becomes rather large close to the cores. Keeping only the terms that are dominant close to the ellipse, we are left with

$$\varepsilon\sim\varepsilon_0\frac{L}{\xi}+\frac{c^2\sin^2\phi}{b^2}\left[\frac{\lambda}{\xi}\right]^2 \quad (\xi\gtrsim 3\lambda) \tag{21}$$

and close to the hyperbola,

$$\varepsilon\sim\varepsilon_0\frac{L}{L-\xi}+\frac{a^2\sinh^2u}{b^2}\left[\frac{\lambda}{L-\xi}\right]^2 \quad (\xi\lesssim L-3\lambda) . \tag{22}$$

To ensure $\varepsilon<1$ close to the cores, we must assume $\varepsilon_0<\lambda/L$.

The two terms of Eqs. (21) or (22) have different physical origins. Let us come back to Eq. (4). It expresses the balance between the *dilation* and the *curvature* forces acting normally on the lamellae. It can be written as

$$\nabla e\cdot\mathbf{n}+e\sigma=-\mathrm{div}(\lambda^2\nabla_{\|}\sigma) , \tag{23}$$

which is term to term equivalent to Eq. (19). The *first* contribution in (21) and (22), coming from the homogeneous part of Eq. (19), results from the left hand side of Eq. (23). It simply traduces the "propagation" of an imposed dilation within the curved texture: Imagine, as an example, a system of concentric cylindrical layers submitted to an external dilation. Since there are no parallel curvature gradients, Eq. (23) reduces to its left hand side, i.e., to $\mathrm{div}(e\mathbf{n})=0$. Thus, in a sector of angle β limited between radii R_1 and R_2, this "propagation" reads $e_1R_1=e_2R_2$. It reflects the mechanical equilibrium of the sector under the action of dilation forces. ε_0 could be either imposed by the cores (which might somehow reduce in this way their energy) or by a mechanism of compensation between the two terms of (21) and (22). The *second* dilation term in (21) and (22) results from the bulk of the focal conic. Since it comes from the right hand side of Eq. (23), it is a reaction to the *curvature* forces arising from the *shape* of the lamellae (Dupin's cyclides). It sign is always *positive* and it vanishes on the summits of the ellipse and hyperbola singular lines. Close to the singular lines, it gives rise to a dilation energy $\sim\frac{1}{2}B(\lambda/d)^4$, d being the distance to the singular line. As $K=B\lambda^2$, it is comparable close to the lines to the curvature energy density $\sim\frac{1}{2}K(1/d)^2$.

In conclusion, we have shown that the usual lamellae equidistance approximation is not valid within the bulk of the focal conics around the singular lines. The latter have a coaxial structure: their core is surrounded by a *lamellae dilation sheath*. The corresponding dilation decreases *algebraically* away from the cores (whereas the distortions within the cores decreases exponentially).

The dilation sheath has mainly two contributions, as follows.

(i) The first is a short-range one, decreasing as $1/d^2$ (d is the distance to the cores), which is a reaction to the lamellae Dupin's cyclide shapes that give rise to curvature forces. This dilation is *positive* and large (close to unity) in the vicinity of the cores. It vanishes at the summits of the singular lines (and thus along the circle for a revolution focal conic). Its energy should compare both to the curvature and to the cores energies of the focal conic.

(ii) The second contribution is a long-range one, decreasing as $1/d$, whose sign and amplitude ε_0 cannot be determined within our perturbative model. It might be caused by the cores or appear to compensate the positive short-range dilation. In the latter case it would propagate a *negative* dilation far within the focal-conic bulk. Experimental studies of lamellae thicknesses could measure ε_0 and allow us to develop core models for the focal-conic singular lines.

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