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Energy Considerations for Parabolic Cyclides in SmA Liquid Crystals

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For Dupin cyclides in the SmA liquid crystal phase, Kleman and Lavrentovich [1] found that increasing the saddle-splay constant \bar{K} caused the minimum of the total elastic energy to occur at a decreased value of the eccentricity e , close to unity. We extend this work to the parabolic cyclides and present an analytical expression for the total elastic energy that is finite over a suitable range of values for the latus rectum, conventionally denoted in this context by -4ℓ (>0). The length of the latus rectum characterises the parabolic focal conic structure analogously to the eccentricity of the Dupin cyclide focal conics. We demonstrate that the total energy is minimised at a particular value of ℓ . It is further observed that the usual saddle-splay elastic term acts independently of ℓ and that varying the value of \bar{K} does not affect the actual value of ℓ at which the minimum of the elastic energy occurs.

Keywords: parabolic cyclides; smectic A liquid crystals

INTRODUCTION

Recently, Kleman and Lavrentovich [1] analysed the change in the total elastic energy of a family of Dupin cyclides as values of the eccentricity e varied within the range $0 \leq e < 1$. They found that generally the energy W could attain a minimum only for some value of e close to 1, and that increasing the saddle-splay elastic constant forced a corresponding decrease in the value of e at which this minimum occurred. Here, it will be shown that there is a similar behaviour for families of parabolic cyclides, where the length of the common latus rectum

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of the confocal parabolas controls the occurrence of the minimum value of the relevant energy W .

The description of parabolic cyclide surfaces is based upon two confocal parabolas in mutually perpendicular planes, with the vertex of one parabola passing through the focus of the other. As considered in [1] for the case of Dupin cyclides, both splay and saddle-splay energy terms will be included in the elastic energy for a family of equidistantly spaced parabolic cyclide surfaces.

THE PARABOLIC CYCLIDE

Following Forsyth [2], we describe the two confocal parabolas in Cartesian coordinates by

$$y^2 = 4\ell(x + \ell), \quad z = 0, \quad (1)$$

$$z^2 = -4\ell x, \quad y = 0, \quad (2)$$

where ℓ is assumed to be a fixed non-zero real constant, -4ℓ being the latus rectum of parabola (2). The general Cartesian equation of a parabolic cyclide surface as stated by Stewart, Leslie, and Nakagawa [3], may then be written as

$$x(x^2 + y^2 + z^2) + (x^2 + y^2)(\ell - \mu) - z^2(\ell + \mu) - (x - \mu + \ell)(\ell + \mu)^2 = 0 \quad (3)$$

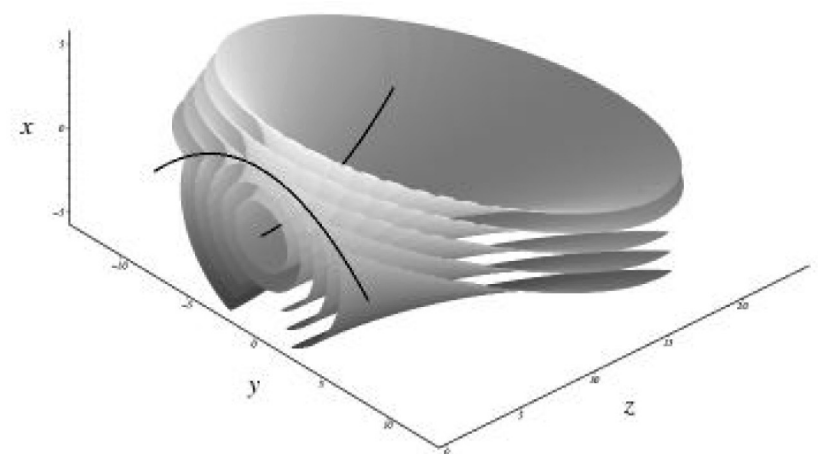
where μ is a real parameter. We parametrise Eq. (3) as [3],

$$\left. \begin{aligned} x &= [\mu(\theta^2 + t^2 - 1) + \ell(t^2 - \theta^2 - 1)](1 + \theta^2 + t^2)^{-1}, \\ y &= 2t[\ell(\theta^2 + 1) + \mu](1 + \theta^2 + t^2)^{-1}, \\ z &= 2\theta(\ell t^2 - \mu)(1 + \theta^2 + t^2)^{-1}, \end{aligned} \right\} \quad (4)$$

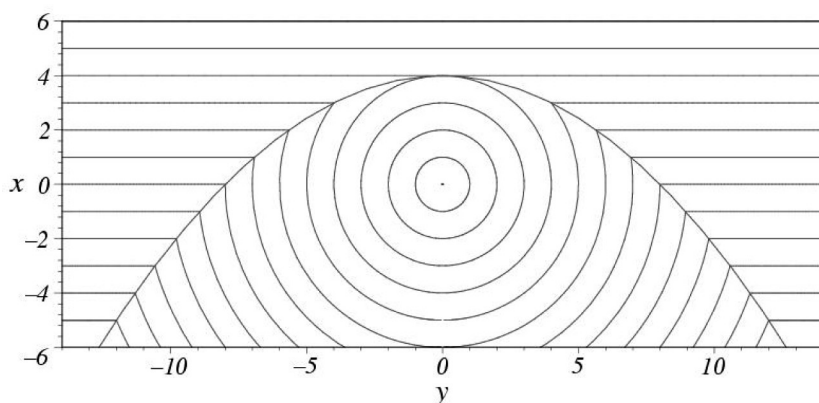
for $-\infty < \theta < \infty$ and $-\infty < t < \infty$. For fixed μ , varying θ and t in (4) maps out one complete cyclide surface. Continuing this process for different values of μ gives parallel layers of cyclides as shown in Figure 1. Transforming the (x, y, z) system (4) to the (μ, θ, t) coordinate system we introduce the following scale factors [3]

$$\left. \begin{aligned} L &= 1, \\ M &= 2|\ell t^2 - \mu|/(1 + \theta^2 + t^2), \\ N &= 2|\ell(\theta^2 + 1) + \mu|/(1 + \theta^2 + t^2), \end{aligned} \right\} \quad (5)$$

such that the absolute value of the Jacobian of the transformation is $J = LMN$.



(a)



(b)

FIGURE 1 Parts of equally spaced parabolic cyclide surfaces are shown in the upper illustration. The lower illustration shows a cross-section of the upper figure in the plane $z = 0$ (which corresponds to $\theta \equiv 0$).

ELASTIC ENERGY

The total elastic energy of a family of parabolic cyclide surfaces is defined as the integral over the volume of the energy density f which, in the SmA phase, takes the form [1,4]

$$f = \frac{1}{2}K(\nabla \cdot \mathbf{a})^2 + \overline{K} \nabla \cdot ((\nabla \cdot \mathbf{a})\mathbf{a}), \quad (6)$$

where the usual liquid crystal director coincides with the unit normal \mathbf{a} to the cyclide surfaces, and K and \bar{K} are the splay and saddle-splay elastic constants, respectively. For the particular surfaces that will be encountered below, it proves convenient to introduce the positive parameter $p = -\ell$ since ℓ (which may be any real number) will take negative values in the description that follows. The elastic energy can then be expressed as

$$W = \int fJ \, dt \, d\theta \, d\mu = W_1 + W_2, \quad (7)$$

where we have introduced

$$\begin{aligned} W_1 &= \frac{1}{2}K \int \frac{4}{(1 + \theta^2 + t^2)^2} \left(\left| \frac{lt^2 - \mu}{l(\theta^2 + 1) + \mu} \right| + \left| \frac{l(\theta^2 + 1) + \mu}{lt^2 - \mu} \right| - 2 \right) dt \, d\theta \, d\mu \\ &= \frac{1}{2}K \int \frac{4}{(1 + \theta^2 + t^2)^2} \left(\frac{pt^2 + \mu}{p(\theta^2 + 1) - \mu} + \frac{p(\theta^2 + 1) - \mu}{pt^2 + \mu} - 2 \right) dt \, d\theta \, d\mu, \end{aligned} \quad (8)$$

$$W_2 = -8\bar{K} \int \frac{1}{(1 + \theta^2 + t^2)^2} dt \, d\theta \, d\mu. \quad (9)$$

THE W_1 AND W_2 ENERGIES

Notice that there are no parabolic line defects present in the region described by $-pt^2 < \mu < p(\theta^2 + 1)$, as can be seen from (8). Henceforth, to ensure that the integrals in (8) are finite and that the volume we are considering excludes defects, we restrict $0 < \mu < p$. We then evaluate W over the finite volume that excludes the parabolic line defects (essentially over a fixed number of smectic layers) by restricting μ such that $r_c < \mu < R_c$, where $0 < r_c < R_c < p$.

Energy W_1 can be rewritten as

$$W_1 = \frac{1}{2}K \int P_1(P_2 + P_3 - 2) \, dt \, d\theta \, d\mu, \quad (10)$$

where

$$P_1 = \frac{4}{(1 + \theta^2 + t^2)^2}, \quad P_2 = \frac{pt^2 + \mu}{p(\theta^2 + 1) - \mu}, \quad P_3 = \frac{p(\theta^2 + 1) - \mu}{pt^2 + \mu}.$$

The P_1P_2 term in (10) may be expressed as, with $x = t/(1 + \theta^2)^{1/2}$ and $\hat{\mu} = \mu/p$,

$$\begin{aligned}
& \int P_1 P_2 dt d\theta d\mu \\
&= 16p \int_{r_c/p}^{R_c/p} \int_0^\infty \int_0^\infty \frac{(\theta^2 + 1)x^2 + \hat{\mu}}{(\theta^2 + 1 - \hat{\mu})(\theta^2 + 1)^{3/2}(1 + x^2)^2} dx d\theta d\hat{\mu}, \\
&= 4\pi p \int_{r_c/p}^{R_c/p} \int_0^\infty \frac{\theta^2 + \hat{\mu} + 1}{(\theta^2 + 1 - \hat{\mu})(\theta^2 + 1)^{3/2}} d\theta d\hat{\mu} \\
&= 4\pi p \int_{r_c/p}^{R_c/p} \left(-2 \frac{\sin^{-1}(\sqrt{1 - \hat{\mu}})}{\sqrt{1 - \hat{\mu}}\sqrt{\hat{\mu}}} + \frac{\pi}{\sqrt{1 - \hat{\mu}}\sqrt{\hat{\mu}}} - 1 \right) d\hat{\mu} \\
&= 4\pi p \left[2 \left(\sin^{-1}(\sqrt{1 - \hat{\mu}}) \right)^2 + \pi \sin^{-1}(2\hat{\mu} - 1) - \hat{\mu} \right]_{r_c/p}^{R_c/p}.
\end{aligned} \tag{11}$$

Similarly, we integrate the $P_1 P_3$ term in (10) to give

$$\begin{aligned}
& \int P_1 P_3 dt d\theta d\mu \\
&= 16p \int_{r_c/p}^{R_c/p} \int_0^\infty \int_0^\infty \frac{\theta^2 + 1 - \hat{\mu}}{(1 + \theta^2 + t^2)^2(t^2 + \hat{\mu})} dt d\theta d\hat{\mu} \\
&= 4\pi p \int_{r_c/p}^{R_c/p} \int_0^\infty \left(-\frac{3}{(1 + \theta^2)^{3/2}} \right. \\
&\quad \left. + 2 \frac{(1 + \theta^2)^{3/2} - \hat{\mu}^{3/2}}{(1 + \theta^2 - \hat{\mu})(1 + \theta^2)^{3/2}\sqrt{\hat{\mu}}} \right) d\theta d\hat{\mu} \\
&= 4\pi p \int_{r_c/p}^{R_c/p} \left(\frac{2 \sin^{-1}(\sqrt{1 - \hat{\mu}})}{\sqrt{1 - \hat{\mu}}\sqrt{\hat{\mu}}} - 1 \right) d\hat{\mu} \\
&= 4\pi p \left[-2 \left(\sin^{-1}(\sqrt{1 - \hat{\mu}}) \right)^2 - \hat{\mu} \right]_{r_c/p}^{R_c/p}.
\end{aligned} \tag{12}$$

Finally, the P_1 term in (10), which also appears in energy W_2 , may be written as

$$\begin{aligned}
& \int P_1 dt d\theta d\mu = 16p \int_{r_c/p}^{R_c/p} \int_0^\infty \int_0^\infty \frac{1}{(\theta^2 + 1)^{3/2}(1 + x^2)^2} dx d\theta d\hat{\mu} \\
&= 4\pi p \int_{r_c/p}^{R_c/p} \int_0^\infty \frac{1}{(\theta^2 + 1)^{3/2}} d\theta d\hat{\mu} \\
&= 4\pi p \int_{r_c/p}^{R_c/p} d\hat{\mu} = 4\pi(R_c - r_c).
\end{aligned} \tag{13}$$

TOTAL ELASTIC ENERGY

Therefore, the final expression for the total elastic energy $W = W_1 + W_2$, valid for $p > 10 \mu\text{m}$ is, from (7)–(13):

$$W = 2K\pi p \left\{ \pi \left[\sin^{-1} \left(\frac{2R_c}{p} - 1 \right) - \sin^{-1} \left(\frac{2r_c}{p} - 1 \right) \right] - 4 \left(1 + \frac{\bar{K}}{K} \right) \left(\frac{R_c}{p} - \frac{r_c}{p} \right) \right\}. \quad (14)$$

Notice that, when expanded, the final term in (14) is linear in $R_c - r_c$ and independent of p , therefore the value of the latus rectum that minimises the energy is unaffected by the choice of saddle-splay elastic constant \bar{K} . This energy, as a function of p , is shown in Figure 2 for $r_c = 0.1 \mu\text{m}$, $R_c = 10 \mu\text{m}$ and $p > 10 \mu\text{m}$.

Inner core radius r_c and the difference $p - R_c$ can be thought of as measures of the distances between the finite number of smectic layers we consider and the two parabolic defects. However, from Figure 2 it is clear that for given core radii lengths, the critical value of p (or of the latus rectum) does not correspond to a value that forces symmetry on the system, i.e., if p_c is the minimising value of p then in Figure 2 we observe that $p_c - R_c \neq r_c$.

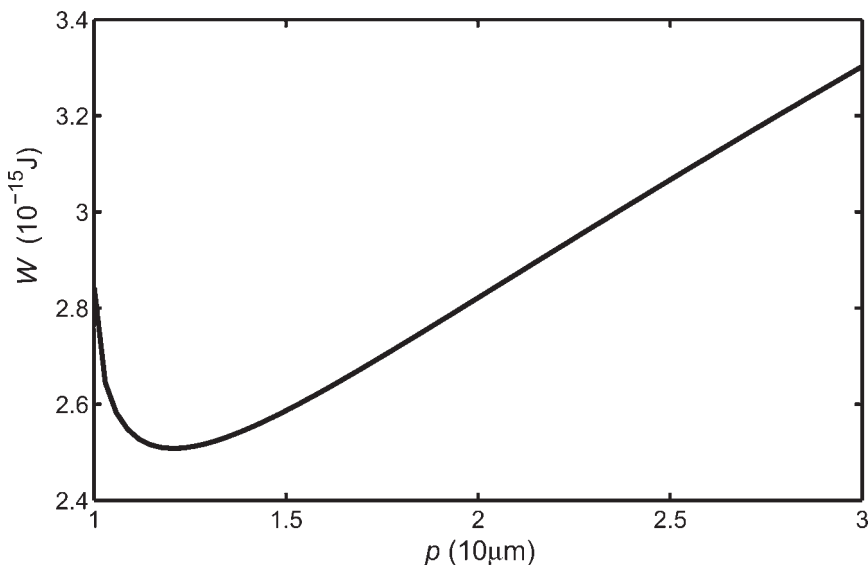


FIGURE 2 The energy of parabolic cyclide (14) for $\bar{K} = -5 \times 10^{-12} \text{ N}$, $K = 5 \times 10^{-12} \text{ N}$, $r_c = 0.1 \mu\text{m}$, and $R_c = 10 \mu\text{m}$.

DISCUSSION

We have shown that the minimum energy for a fixed number of parabolic cyclide surfaces in SmA is dependent upon the latus rectum, $-4\ell = 4p$, of the underlying confocal parabolic structure. The key result is given by Eq. (14), which has been plotted in Figure 2 for the physical parameters shown in the Caption. More recent work has demonstrated qualitatively similar features for any suitably restricted values of R_c .

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