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Liquid crystals and geodesics

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Abstract. — Since a unit vector \( \mathbf{n} \) is a point on the unit sphere, any one-dimensional liquid crystal configuration \( \mathbf{n}(z) \), \( a \leq z \leq b \), generates a path on the unit sphere. In order to see what configurations are stable, we map the unit sphere onto a surface \( G \) having the property that equilibrium configurations of a nematic liquid crystal map into geodesic lines on the surface (geodesics). The shape of the surface depends on the elastic constant ratios \( k_1/k_3 \) and \( k_2/k_3 \); it is a sphere when all three constants are equal. A picture or model of the surface for a particular material is helpful in visualizing the equilibrium configurations that correspond to prescribed boundary conditions \( \mathbf{n}(a) \) and \( \mathbf{n}(b) \), and in studying their energy and stability. For example, a configuration \( \mathbf{n}(z) \) is in stable equilibrium if and only if the path on \( G \) is a curve of least length among nearby curves having the same end points, and arc length \( ds \) on \( G \) is proportional to \( dz \). The physical interpretation of the proportionality of \( ds \) to \( dz \) is that the elastic free energy density of the liquid crystal is a constant, independent of \( z \).

1. Introduction. — The equilibrium equations of liquid crystals are satisfied by both stable and unstable states. Although it is important to know whether a state is stable, it is not always obvious whether a solution represents a stable state. For example, Porte and Jadot [1] found a critical value of the tilt angle at the surface of a liquid crystal cell at which a 180° twisted configuration transforms into a nontwisted configuration. Beyond the critical angle, both nontwisted and 180° twisted states satisfy the equilibrium equations, but it is not easy to show whether only one or both states are stable. The equilibrium equations are the conditions for the energy integral to be stationary. The mathematical conditions for such a stationary value to be a minimum (stable state) are cumbersome to apply. Therefore, it is important to have another way of looking at the stability problem.

Fortunately, there is an analogy with a rubber band stretched over a tall, but perfectly smooth and slippery mountain. If properly placed, the rubber band stretched over the top may be in equilibrium, but if the mountain is tall enough and its diameter thin enough, a sidewise push would make the rubber band slip off the summit and assume a shorter path going around the mountain instead of over it. This is a perfect analogy to the twisted-nontwisted instability described by Porte and Jadot [1]. The stability conditions depend on the shape of the mountain. It remains to find the shape of the « mountain » for nematic liquid crystals. The shape must be such that stable equilibrium configu-
rations have the shortest paths. After this shape is determined, one can see which equilibrium states are stable.

We will describe the configuration of a liquid crystal by a smoothly varying unit vector field \( \mathbf{n} \), the liquid crystal director. As additional assumptions we suppose that the liquid crystal lies between the planes \( z = a \) and \( z = b \), and that \( \mathbf{n} \) is a function of \( z \) alone and not of other space coordinates. \( \mathbf{n}(z) \) thus describes a path on the unit sphere as \( z \) varies from \( a \) to \( b \). Possible equilibrium configurations \( \mathbf{n}(z) \) are those which are stationary for free energy.

Corresponding to a given free energy function for the liquid crystal, we show how to map the unit sphere and associated paths into another surface \( G \) such that for fixed director orientations at the boundary \( \mathbf{n}(a) \) and \( \mathbf{n}(b) \):

1. \( \mathbf{n}(z) \) is an equilibrium configuration if and only if the path on \( G \) is a geodesic and the arc length \( ds \) of the path on \( G \) is a constant multiple of \( dz \).

2. \( \mathbf{n}(z) \) is a stable equilibrium configuration if and only if it is an equilibrium configuration whose path on \( G \) has less length than all other nearby curves with the same end points.

A curve on \( G \) is a geodesic if and only if every sufficiently small arc is the shortest path between its end points [2]. According to this definition, a geodesic (like an equilibrium configuration) provides a stationary value, not necessarily a minimum. The problem of determining the stability is now seen as the problem of deciding whether a given geodesic path is shorter than all other nearby curves with the same end points. The boundary conditions \( \mathbf{n}(a) \) and \( \mathbf{n}(b) \) at the upper and lower surfaces of a liquid crystal cell correspond to a pair of points on the surface \( G \), and equilibrium configurations to geodesic lines joining the points. A geodesic line may be pictured as the curve assumed on a slippery surface by a rubber band stretched between the boundary points. Stability is determined by whether the rubber band, pinned at its end points, can slip off the « mountain » without being stretched.

The surface \( G \) is readily constructable from the elastic constant ratios \( k_1/k_3 \) and \( k_2/k_3 \). It is then usually easy to use \( G \) to discover the possible equilibrium configurations, to estimate their energy, and to analyse their stability properties.

The present paper derives the differential equations for the surface \( G \). A companion paper discusses its shape and the application to stability problems, such as the one treated by Porte and Jadot [1].

2. Terminology and notation. — We shall map the unit sphere onto another surface of revolution \( G \) called the geodesic surface by the mapping

\[
R = R(\theta), \quad Z = Z(\theta), \quad \Phi = \Phi
\] (2.1)

where \( \theta, \Phi \) are spherical polar coordinate angles with \( \theta \) measured from the \( z \) axis and \( \Phi \) the azimuth angle, and where \( R, Z, \) and \( \Phi \) are the radial, axial, and angle coordinates of a cylindrical coordinate system.

A configuration \( \mathbf{n}(z) \), alias \( \theta(z), \Phi(z) \) generates a path on the unit sphere and the geodesic surface. An equilibrium configuration generates a solution path on the unit sphere and the geodesic surface. Our goal is to determine the mapping functions \( R(\theta), Z(\theta) \) such that the solution paths on the geodesic surface are geodesic lines.

3. Equilibrium configurations. — A nematic liquid crystal has an elastic energy density [1]

\[
f_k(\theta, \Phi, \Theta) = \frac{1}{2} k_3 [\Phi^2 f(\theta) + \Phi^2 g(\theta)], \quad (3.1)
\]

\[
k_3 f(\theta) = k_1 \sin^2 \theta + k_3 \cos^2 \theta, \quad (3.2)
\]

\[
k_3 g(\theta) = \sin^2 \theta (k_2 \sin^2 \theta + k_3 \cos^2 \theta). \quad (3.3)
\]

Here \( \Theta = d\theta/dz \) and \( \Phi = d\Phi/dz \). The positive constants \( k_1, k_2, \) and \( k_3 \) are the elastic constants for splay, twist, and bend, respectively. Equilibrium configurations have \( \theta(z), \Phi(z) \) such that the configuration energy per unit area

\[
F = \int f_k \, dz \quad (3.4)
\]

is stationary. The Euler equations for this stationary value problem are [4]

\[
- \frac{\partial f_k}{\partial \Phi} + \frac{d}{dz} \left[ \frac{\partial f_k}{\partial \Phi} \right] = 0, \quad (3.5)
\]

\[
- \frac{\partial f_k}{\partial \Theta} + \frac{d}{dz} \left[ \frac{\partial f_k}{\partial \Theta} \right] = 0. \quad (3.6)
\]

Since \( f_k \) does not depend on \( \Phi \), equation (3.5) yields

\[
\Phi \, g(\theta) = c = \text{constant}. \quad (3.7)
\]

Equations (3.7) and (3.6) can be used to show that

\[
f_k = p_0 = \text{constant}. \quad (3.8)
\]

Equilibrium configurations are characterized by the first-order differential equations (3.7) and (3.8).

4. Geodesic lines on a surface of revolution. — Let the surface of revolution be specified by (2.1). The differential arc length \( ds \) on the surface of revolution satisfies

\[
ds^2 = dR^2 + dZ^2 + R^2 d\Phi^2. \quad (4.1)
\]

A configuration \( \theta(z), \Phi(z) \) on the unit sphere generates a path on the surface of revolution that has

\[
\left[ \frac{ds}{dz} \right]^2 = [R^2 + Z^2] \theta^2_z + R^2 \Phi^2_z. \quad (4.2)
\]

Here the primes denote derivatives with respect to \( \theta \).
We introduce the abbreviation
\[ p(\theta, \phi, \theta, \phi) = \left( \frac{ds}{dz} \right)^2. \] (4.3)

A geodesic line connecting two points on the surface is a path that gives a stationary value of the distance
\[ s = \int p^{1/2} \, dz \] (4.4)
between the two points. The Euler equations for this stationary value problem have the form (3.5) and (3.6) with \( f_k \) replaced by \( p^{1/2} \). The first equation yields
\[ \frac{R^2 \phi_2}{ds/dz} = c = \text{constant}, \] (4.5)
after which it is found that the second equation yields nothing new, being satisfied identically. This means that as long as (4.5) is satisfied, \( ds/dz \) can be an arbitrary function of \( z \), which becomes understandable upon writing (4.4) as \( \int ds \) rather than \( \int (ds/dz) \, dz \) [5].

Equation (4.5) is equivalent to Clairaut’s theorem [7]
\[ R^2 \frac{d\phi}{ds} = R \sin \alpha = c, \] (4.6)
where \( \alpha \) is the angle between a geodesic line and the local meridian. The geodesic lines are characterized by (4.5) or (4.6).

It is important for our purpose to note that the geodesic lines can also be found by seeking stationary values of the integral of \( (ds/dz)^2 \):
\[ \frac{p}{dz} = \int p \, dz. \] (4.7)
The Euler equations for this problem are like (3.5) and (3.6) with \( f_k \) replace by \( p \). The results already given in (3.7) and (3.8) now yield
\[ R^2 \Phi_2 = C = \text{constant}, \] (4.8)
\[ p = p_0 = \text{constant}. \] (4.9)
For the stationary values of (4.7), \( ds/dz \) is constant, not an arbitrary function of \( z \) as it was in (4.4). The resulting paths, however, are the same geodesic lines, for from (4.8) and (4.9), one can form
\[ \frac{R^2 \phi_2}{ds/dz} = \frac{C}{p_0^{1/2}} = c = \text{constant}, \] (4.10)
which is the same as (4.5) or (4.6).

5. The geodesic surface. — 5.1 Equations defining the surface. — Having proved that the geodesic lines can be obtained by seeking stationary values of (4.7), the integral of \( (ds/dz)^2 \), we can obtain the geodesic surface by choosing \( R(\theta) \) and \( Z(\theta) \) such that \( (ds/dz)^2 \) is proportional to the elastic energy density \( f_k \). We set
\[ p = 2f_k/k_3. \] (5.1)

Then, by comparison of (4.2) and (3.1),
\[ R^2 = g(\theta), \quad (R^2 + Z^2) = f(\theta), \quad \Phi = \varphi. \] (5.2)

Equations (5.2) define the desired mapping of the unit sphere onto the geodesic surface, a surface having the property that the paths which correspond to equilibrium configurations are geodesic lines. This is true because (3.4) is stationary for the equilibrium configurations, (4.7) is stationary for the geodesics, and (5.1) makes one integral a constant times the other.

Since \( g(\theta) \) is positive for \( \theta \) between 0 and \( \pi \) with \( g(0) = g(\pi) = 0 \), our geodesic surface defined by (5.2) will exist and be a topological sphere provided \( f(\theta) = [g'(\theta)]^2/4 g(\theta) = [Z'(\theta)]^2 \) is also positive between 0 and \( \pi \).

From (5.2) and (3.2)-(3.3), an explicit differential equation for \( Z(\theta) \) may be expressed as
\[ [Z'(\theta)]^2 = 1 - a_1 \sin^2 \theta - \frac{\cos^2 \theta(1 - 2 a_2 \sin^2 \theta)^2}{(1 - a_2 \sin^2 \theta)} \] (5.3)
where
\[ a_1 = 1 - k_1/k_3, \quad a_2 = 1 - k_2/k_3. \] (5.4)
We take \( Z(\pi/2) = 0 \) in the integration of (5.3).

5.2 The case of equal elastic constants. — The shape of the geodesic surface depends on the elastic constant ratios \( k_1/k_3 \) and \( k_2/k_3 \). That the surface is a sphere in the case of equal elastic constants is easily proved. When \( k_1 = k_2 = k_3 \), \( f(\theta) \equiv 1 \) and \( g(\theta) = \sin \theta \) so that the integrand in (3.4) is
\[ f_k = \frac{1}{2} k_3 [\theta^2_z + \phi^2_2 \sin^2 \theta]. \] (5.5)

In spherical coordinates, the square of the differential arc length on the surface of a sphere of radius \( r \) is
\[ ds^2 = r^2 (d\theta^2 + d\phi^2 \sin^2 \theta). \] (5.6)
Hence, a path on the sphere has
\[ (ds/dz)^2 = r^2 (\theta^2_z + \phi^2_2 \sin^2 \theta) = 2 r^2 f_k/k_3. \] (5.7)
Since \( (ds/dz)^2 \) on the sphere is a constant times \( f_k \), minimization of the energy (3.4) is equivalent to finding the shortest paths on the sphere by minimizing (4.7).

It follows that in the case of equal elastic constants, the geodesic surface is a sphere. The paths on the sphere that correspond to equilibrium configurations are simply great circles. The effect of different elastic constants on the shape of the geodesic surface is discussed in the following paper [8].
5.3 Relation of Energy to Distance on the Geodesic Surface. — Because of (3.8) and (5.1), we know that the value of ds/dz is constant along the path on the geodesic surface that corresponds to an equilibrium configuration. Hence, for such a path,

$$\frac{ds}{dz} = \frac{s}{z_2 - z_1}$$  \hspace{1cm} (5.8)

where $s$ is the dimensionless path length on the geodesic surface that corresponds to the length $z_2 - z_1$ in the configuration. It follows that the integral $P$ becomes

$$P = \int_{z_1}^{z_2} \left[ \frac{ds}{dz} \right]^2 dz = \frac{ds}{dz} \int ds = \frac{s^2}{z_2 - z_1}. \hspace{1cm} (5.9)$$

But it follows from (5.1) that $P = 2F/k_3$. Hence the elastic energy per unit area of an equilibrium configuration is

$$F = \frac{k_3 s^2}{2(z_2 - z_1)}. \hspace{1cm} (5.10)$$

What about the energy of nonequilibrium configurations? Clearly, that, too, is given by (5.10) if ds/dz is constant along the path on the geodesic surface. Now the same path (graph on the surface) can be generated by any number of nonequilibrium configurations, obtained by simultaneously varying the $z$ dependence of $\theta$ and $\varphi$ without changing the relation between them. Of all these configurations that belong to the same path, the one with ds/dz constant (i.e., $f_k =$ constant) has minimum energy [9]. Hence, the energy of nonequilibrium configurations is greater than or equal to (5.10), with the equality holding when the $z$ dependence is adjusted to obtain minimum energy for the prescribed path, i.e., the equality holds when ds/dz is constant along the path on the geodesic surface, which means that the energy density $f_k$ is constant throughout the configuration.

The stretched rubber band analogy brings out two aspects of stable equilibrium configurations of liquid crystals: (1) the relation between $\theta$ and $\varphi$ must be right to give the shortest path on the geodesic surface, and (2) the energy density $f_k$ must be constant. A nonequilibrium configuration is like a rubber band constrained somewhere other than at the end points. The minimum energy for any path is obtained when there are only lateral constraints so that the stretch is constant along the length. For any path (even the shortest one) a higher energy can be obtained if the rubber band is pinched up so that the stretch is not constant along the length.

5.4 Condition for a Real Geodesic Surface. — It is interesting to note that there is a domain of positive $(k_1/k_3, k_2/k_3)$ for which $[Z'(\theta)]^2$, given by (5.3), is negative for some interval of $\theta$. In this case, a real geodesic surface fails to exist for all $\theta$.

By algebraic manipulation, equation (5.3) can be put in the form

$$[Z'(\theta)]^2 = \sin^2 \theta[- a_1 + M(\theta)],$$

$$M(\theta) \equiv 4 a_2 \cos^2 \theta + \frac{1 - a_2}{1 - a_2 \sin^2 \theta}. \hspace{1cm} (5.11)$$

where $a_1$ and $a_2$ are as in (5.4). The condition that the geodesic surface be real for all $\theta$ is $a_1 \leq M(\theta)$. With the abbreviation

$$y \equiv (k_2/k_3)^{1/2} \hspace{1cm} (5.12)$$

we find that $M(\theta)$ has an extremum of 1 at $\cos \theta = 0$ if $y \neq 0$, an extremum of $4 - 3y^2$ at $\sin \theta = 0$, and, if $0 \leq y \leq 1/2$, a minimum of

$$M_{\text{min}} = 4y(1 - y). \hspace{1cm} (5.13)$$

when

$$\sin^2 \theta = (1 - y^2)/(1 - y^2). \hspace{1cm} (5.14)$$

The condition $a_1 \leq 1$ reduces to $k_1/k_3 \geq 0$, which is no restriction at all for positive elastic constants. The condition $a_1 \leq 4 - 3y^2$ leads to

$$k_1/k_3 \geq 3(k_2/k_3 - 1). \hspace{1cm} (5.15)$$

The condition $a_1 \leq M_{\text{min}}$ leads to

$$k_1/k_3 \geq 1 - 2(k_2/k_3)^{1/2}. \hspace{1cm} (5.16)$$

Figure 1 shows the region of elastic constants (5.15) and (5.16) for which the geodesic surface is real for all $\theta$. 

![Fig. 1. — Condition for a real geodesic surface. The geodesic surface is real for all $\theta$ when the elastic constants fall below the upper line (5.15) and above the lower curve (5.16).](image)
As far as is known, the elastic constants for all nematic liquid crystals satisfy the inequalities (5.15) and (5.16), giving a geodesic surface that is real for all \( \theta \). However, we have not discovered any physical requirement that this should be so.

6. Conclusion. — We have defined a surface [by (2.1) and (5.2)] with the property that one-dimensional equilibrium configurations \( \theta(z), \phi(z) \) of a nematic liquid crystal map into geodesic lines of the surface. We call this surface the geodesic surface of the nematic liquid crystal. The energy of an equilibrium configuration, given by (5.10), is proportional to the square of its path length on the geodesic surface. Furthermore, the energy of any configuration is also related to its path length on the geodesic surface by (5.10) when the \( z \) dependence is arranged to minimize the energy with the path fixed. The shape of the geodesic surface depends on the elastic constants. For equal elastic constants, \( k_1 = k_2 = k_3 \), it is a sphere. The geodesic surface is useful in picturing the equilibrium configurations that correspond to prescribed boundary conditions and in discussing their energy and stability. Some examples are elaborated in a companion paper [8].

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References


[2] LYUSTERNIK, L. A., Shortest Paths-Variational Problems. Translated by P. Collins and Robert B. Brown (MacMillan Company, New York) 1964, p. 48. This definition is equivalent to the other common definitions as a path whose principal normal coincides everywhere with the normal to the surface, or as a path of zero geodesic curvature [3].


[5] It is obvious that the \( z \) dependence, or parametrization has nothing to do with the geodesics on a surface. Although it suits our purpose to specify a path (i.e., graph, or set of points) on the surface by a pair of functions \( \theta(z), \phi(z) \), only the relation between \( \theta \) and \( \phi \) is essential to the path. Related to this point is the fact that a configuration \( \theta(z), \phi(z) \) determines a path, but the path (graph) does not, without the \( z \) dependence, determine a configuration. Although the terms path, curve (and even geodesic) are advantageously used in the specialized literature [6] to include the parametrization, these terms are used in this footnote to mean merely the graph or set of points on the surface. A parametrized path (i.e., path including the \( z \) dependence) does, of course, determine a configuration.


