Equilibrium shapes of a twist-bend nematic drop

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These notes supplement our paper Interfacial and morphological features of a twist-bend nematic drop, producing a number of analytical details of the mathematical model employed there to interpret the experimental observations of equilibrium shapes of a twist-bend nematic drop in two space dimensions. For the sake of continuity and completeness, some figures and equations are also reproduced here.

1 Equilibrium equations

Our starting point here is the energy functional

\[ F[r] := \int_0^L \left( 1 + \frac{1}{2} \omega \left[ (t \cdot n)^2 - c^2 \right] \right) ds, \]  

where \( L \) is the (undetermined) length of the curve \( \gamma \) bounding the drop, \( t \) is a unit tangent vector to \( \gamma \), and \( s \) is the corresponding arc-length co-ordinate, so that \( \gamma \) is described by the mapping \( s \mapsto r(s) \) and \( t = r' \), where a prime \( ' \) denotes differentiation with respect to \( s \).

Figure 1a illustrates an admissible shape for \( \gamma \), symmetric with respect to both axes \( x \) and \( y \), the former designating the orientation of \( n \). The area \( A \) enclosed by \( \gamma \) can be expressed in terms of \( r \) as

\[ A[r] := -\frac{1}{2} \int_0^L r \times t \cdot e_x ds, \]  

where \( e_x := e_x \times e_y \).

Constrained equilibrium for \( F \) requires that \( r \) makes the first variations \( \delta F \) and \( \delta A \) proportional to one another,

\[ \delta F = \lambda \delta A, \]  

where \( \lambda \) is a Lagrange multiplier, still to be determined.

The first variation \( \delta F \) is a functional, \( \delta F(r)[u] \), linear in the variation \( u \) of \( r \). Formally,

\[ \delta F(r)[u] := \frac{d}{ds} F[r_\varepsilon] \bigg|_{\varepsilon=0}, \]  

where \( r_\varepsilon := r + \varepsilon u \) and \( \varepsilon \) is a small, perturbation parameter. The perturbed curve \( \gamma_\varepsilon \) described by \( r_\varepsilon \) has unit tangent vector \( t_\varepsilon \) delivered by

\[ t_\varepsilon = t + \varepsilon (I - t \otimes t) u' + o(\varepsilon), \]  

where \( I \) is the identity tensor. Moreover, the local dilation ratio between lengths along \( \gamma_\varepsilon \) and lengths along \( \gamma \) is, to within first order in \( \varepsilon, 1 + \varepsilon \nu \cdot t' \). Thus, by letting \( n = e_x \) from (1) and (4) we obtain

\[ \delta F(r)[u] = \int_0^L \left\{ 2\omega \left[ (t \cdot e_x)^2 - c^2 \right] (I - t \otimes t) e_x + \left( 1 + \frac{1}{2} \omega \left[ (t \cdot e_x)^2 - c^2 \right] \right) t \right\} \nu ds. \]  

Similarly, we arrive at

\[ \delta A(r)[u] = \frac{1}{2} \int_0^L (\nu \cdot u - e_x \times r \cdot u') ds, \]  

where \( \nu := e_x \times t \) is the outer unit normal to \( \gamma \).

As shown in Fig. 1a, \( \gamma \) may possess a corner, that is a point, say at \( s = s_0 \), where the unit tangent \( t \) jumps from \( t^- \) to \( t^+ \) as \( s \) increases through \( s_0 \). If this is the case, splitting the integral in (7) into subintervals where \( t \) is continuous, allowing both \( u \) and \( u' \) to be everywhere continuous, and integrating by parts, we easily show that

\[ \delta A(r)[u] = \int_0^L \nu \cdot u ds. \]  

Contrariwise, proceeding just in the same way, we extract a jump contribution to \( \delta F(r) \) from every point of discontinuity for \( t \), which reads \( [f] \cdot u \), where

\[ f := 2\omega \left[ (t \cdot e_x)^2 - c^2 \right] (I - t \otimes t) e_x + \left( 1 + \frac{1}{2} \omega \left[ (t \cdot e_x)^2 - c^2 \right] \right) t \]  

and, as customary, for any discontinuous field \( \psi \) the jump \( [\psi] \) is defined by \( [\psi] := \psi^+ - \psi^- \), where \( \psi^+ \) and \( \psi^- \) are the right and left limits of \( \psi \) at the point of discontinuity.

Requiring (3) to be valid for arbitrary \( u \), by (6) and (8) we conclude that the equilibrium equation for the regular arcs of \( \gamma \), where \( t \) is continuous, is

\[ f' + \lambda \nu = 0, \]  

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while the equation
\[ \|f\| = 0 \]  \tag{11} \]
must hold at all corners, where \( t \) is discontinuous. These are precisely equations (8) and (9) in our main paper.

### 2 Equilibrium corners

In general, the equilibrium equations (10) and (11) are rather complicated. Symmetry may simplify them. In keeping with the experimental observations, we shall hereafter assume that \( \mathcal{C} \) has the two-fold symmetry displayed in Fig. 1 and that its corners may only occur on the symmetry axes.

For a corner on the \( y \) axis, \( t^- \) and \( t^+ \) satisfy
\[ t^+ \cdot e_x = t^- \cdot e_x, \quad t^+ \cdot e_y = -t^- \cdot e_y, \]  \tag{12} \]
and it can be shown that equation (11) reduces to
\[ 3 \omega \chi^2 - 2 \omega \epsilon^2 \chi - 2 - \omega \chi^4 = 0, \]  \tag{13} \]
where we have set \( \chi := (t \cdot e_x)^2 \). It can be easily proved that there is precisely one root of (13) in \([0, 1]\), which reads
\[ \chi = \chi_1(c, \omega) := \frac{1}{3} \left( \epsilon^2 + \sqrt{4 \epsilon^4 + \frac{6}{\omega}} \right), \]  \tag{14} \]
if and only if
\[ \omega \geq \omega_c^{(1)}(c) := \frac{2}{(1 - \epsilon^2)(3 + \epsilon^2)}. \]  \tag{15} \]
Otherwise, there is none and at equilibrium no corner can arise where \( \mathcal{C} \) meets the \( y \) axis. The inner corner angle \( \beta \) depicted in Fig. 1b is given by
\[ \beta = 2 \arcsin \sqrt{\chi_1}, \]  \tag{16} \]
where \( \chi_1 \) is as in (14); in particular, (16) implies that
\[ \lim_{c \to \infty} \beta(c, \omega) = 2 \arcsin c. \]  \tag{17} \]

Similarly, for a corner on the \( x \) axis,
\[ t^+ \cdot e_x = -t^- \cdot e_x, \quad t^+ \cdot e_y = t^- \cdot e_y \]  \tag{18} \]
and (11) reduces to
\[ 3 \omega \chi^2 - 2 \omega(c^2 + 2)\chi - (\omega \epsilon^4 - 4 \omega \epsilon^2 + 2) = 0. \]  \tag{19} \]
It can be easily proved that there is precisely one admissible root of (19), which reads
\[ \chi = \chi_2(c, \omega) := \frac{1}{3} \left( \epsilon^2 + 2 - \frac{2}{\sqrt{4(1 - \epsilon^2)^2 + 6 \omega}} \right), \]  \tag{20} \]
if and only if
\[ \omega \geq \omega_c^{(2)}(c) := \frac{2}{\epsilon^2(4 - \epsilon^2)}. \]  \tag{21} \]
Otherwise, there is none and at equilibrium no corner can arise where \( \mathcal{C} \) meets the \( x \) axis. The inner corner angle \( \alpha \) depicted in Fig. 1b is given by
\[ \alpha = 2 \arccos \sqrt{\chi_2}, \]  \tag{22} \]
where \( \chi_2 \) is as in (20); in particular, (22) implies that
\[ \lim_{c \to \infty} \alpha(c, \omega) = 2 \arccos c = 2 \vartheta, \]  \tag{23} \]
where \( \vartheta \) is the ideal cone angle.

The graphs of both \( \omega_c^{(1)} \) and \( \omega_c^{(2)} \) as functions of \( c \) are plotted in Fig. 2.
Lagrange multiplier now denotes differentiation with respect to \( x \).

We are only interested in finding the equilibrium arcs of \( \mathcal{C} \) in their Cartesian parametrization. The Euler-Lagrange equation associated with \( F^* \) is easily obtained and integrated once, leading to

\[
\Phi(y'; c, \omega) = \lambda x + b,
\]

where

\[
\Phi(u; c, \omega) := \frac{1}{2} \frac{1}{\sqrt{1 + u^2}} \left[ 2 - 3\omega + 2\omega c^2 + \omega c^4 \right] u
\]

and \( b \) is an arbitrary integration constant. Altering both \( x \) and \( y \) by the same factor, say \( \mu \), so as to produce a homothetic dilation (or contraction) of \( \mathcal{C} \) does not alter the left side of (26). Consequently, \( \lambda \) must be changed into \( \lambda/\mu \) for \( \mathcal{C} \) to remain an equilibrium curve. This shows that \( \lambda \) can be determined and the area constraint can be satisfied by simply rescaling any solution \( y = y(\xi) \) of (26) with \( \xi := \lambda x + b \). Similarly, since the differential equation (26) does not contain \( y \) explicitly, the constraint (25) can be satisfied by translating in space a solution.

Figure 3 illustrates a graphical argument to integrate (26). For an arbitrary \( \xi \), the light gray area represents the integral of \( y' \) in \( \xi \); such an area can be obtained by subtracting the dark gray area which represents the integral of \( \Phi \) in \( u \) from the whole area \( u\Phi(u) \) of the rectangle delimited by the coordinate lines through \((u, \xi)\). Thus, to within additive constants to be chosen so as to adjust the solution to the geometric constraint, a regular arc of \( \mathcal{C} \) can be represented in the parametric form

\[
y = Y(u; c, \omega) := u\Phi(u; c, \omega) - \Psi(u; c, \omega),
\]

\[
\xi = \Phi(u; c, \omega),
\]

where \( \Psi \) is the primitive of \( \Phi \) in \( u \). It is easily seen that, for a regular arc with \( x > 0 \) and \( y < 0 \) as shown in Fig. 1, \( Y \) can be given the following explicit representation

\[
Y(u; c, \omega) = -\frac{1}{2} \frac{1}{\sqrt{1 + u^2}} \left[ 2 + \omega - 2\omega c^2 + \omega c^4 \right] u + 2(2 + \omega - 3\omega c^2 + \omega c^4)u^2 + (2 - 4\omega c^2 + \omega c^4)u^4.
\]

With the aid of (27) and (29), by direct inspection one easily sees that the functions \( \Phi \) and \( Y \) enjoy the following properties.
As shown in Fig. 3, in region I a regular arc of $\mathcal{C}$ can meet a corner of the $y$ axis, whereas it meets none on the $x$ axis. These corners together with those on the $x$ axis, where $y' = u_M$, make the equilibrium shape of the drop resemble a diamond (see Fig. 17b in the main paper). Precisely, as above, one could try and extend an equilibrium regular arc of $\mathcal{C}$ also for $y' < u_m$, but again the lack of monotonicity of $\Phi$ for $0 < u < u_m$ is likely to bring $\mathcal{C}$ in the realm of metastability.

Figure 5 illustrates the typical graph of $\Phi$ against $u$ in region II of the phase diagram in Fig. 2. There are two values of $y'$, namely, $u_m$ and $u_M$, identified by (33) and (31), where an equilibrium regular arc of $\mathcal{C}$ can meet with corners on the two symmetry axes. Though characteristic of the whole region II, this specific graph was drawn for $c = \frac{\sqrt{2}}{2}$ and $\omega = \frac{1}{2}$.

Fig. 3: The plot of the function $\Phi$ against $u$ for $(c, \omega)$ in region I of the phase diagram in Fig. 2. The asymptote $\xi_\infty$ is delivered by (32); the single value $u_M$ of $y'$ where a regular arc of $\mathcal{C}$ may meet a corner on the $x$ axis is identified by (31). This specific plot, while typical of the whole region I, was obtained for $c = \frac{\sqrt{2}}{2}$ and $\omega = \frac{1}{2}$.

Fig. 4: The plot of the function $\Phi$ against $u$ for $(c, \omega)$ in region II of the phase diagram in Fig. 2. There are two values of $y'$, namely, $u_m$ and $u_M$ identified by (33) and (31), where an equilibrium regular arc of $\mathcal{C}$ can meet with corners on the two symmetry axes. Though characteristic of the whole region II, this specific graph was drawn for $c = \frac{\sqrt{2}}{2}$ and $\omega = 5$.

$$u_m := \sqrt{\frac{1}{\chi_1} - 1},$$

(33)

identifies the value of $y'$ where an equilibrium regular arc can meet a corner of the $y$ axis. These corners together with those on the $x$ axis, where $y' = u_M$, make the equilibrium shape of the drop resemble a diamond (see Fig. 17b in the main paper). Precisely, as above, one could try and extend an equilibrium regular arc of $\mathcal{C}$ also for $y' < u_m$, but again the lack of monotonicity of $\Phi$ for $0 < u < u_m$ is likely to bring $\mathcal{C}$ in the realm of metastability.

$$\rho(c, \omega) := \frac{\Phi(u_{\text{max}}; c, \omega)}{Y(u_{\text{min}}; c, \omega)},$$

(34)

By (28), for $\frac{\sqrt{2}}{2} \leq c \leq 1$, the aspect ratio $\rho$ of the extensions of the drop along $n$ and orthogonally to $n$ can be expressed as
Fig. 5: The plot of the function $\Phi$ against $u$ for $(c, \omega)$ in region III of the phase diagram in Fig. 2. $\Phi$ is monotonically increasing in the whole range $u \geq 0$, saturating at $\xi_\infty$, still given by (32).

As a consequence of (30), $\rho$ is easily seen to satisfy equation (16) in the main text.

where

$$u_{\text{max}} := \begin{cases} u_M & \text{in I } \cup \text{ II}, \\ \infty & \text{in III}, \end{cases} \quad u_{\text{min}} := \begin{cases} 0 & \text{in I } \cup \text{ III}, \\ u_m & \text{in II}. \end{cases}$$

(35)