

Double helix director

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February 13, 2024

1 Selinger free energy

To investigate this system, we start with the Frank free energy as written by Selinger:

$$F = \frac{1}{2} (K_{11} - K_{24}) S^2 + \frac{1}{2} (K_{22} - K_{24}) T^2 + \frac{1}{2} K_{33} |\mathbf{B}|^2 + K_{24} \text{Tr} (\Delta^2) \quad (1)$$

with the following definitions for the distortion modes:

$$S = \nabla \cdot \hat{\mathbf{n}} \quad (2)$$

$$T = \hat{\mathbf{n}} \cdot (\nabla \times \hat{\mathbf{n}}) \quad (3)$$

$$B = \hat{\mathbf{n}} \times (\nabla \times \hat{\mathbf{n}}) \quad (4)$$

$$\begin{aligned} \Delta_{ij} = \frac{1}{2} [& \partial_i n_j + \partial_j n_i \\ & - n_i n_k \partial_k n_j - n_j n_k \partial_k n_i \\ & - \delta_{ij} \partial_k n_k + n_i n_j \partial_k n_k] \end{aligned} \quad (5)$$

2 Rotated system

We make two assumptions about the system: i) the z -dependence of the director corresponds to a rotation of a plane perpendicular to the cylindrical axis about the cylindrical axis by some angle αz , and ii) the director stays in a plane perpendicular to the cylindrical axis. We note that in an infinitely long cylindrical system, i) is true by translational symmetry. In this case, we may write:

$$\hat{\mathbf{n}} = R(\alpha z) [\cos \theta \quad \sin \theta \quad 0]^T \quad (6)$$

for some director angle θ as measured from the x -axis in the x - y -plane, and $R(z)$ a rotation about the z -axis and a function of z . We note that θ must be a function of x , y , and z , with the z -dependence corresponding to an *inverse* rotation of angle αz about the z -axis.¹ This gives:

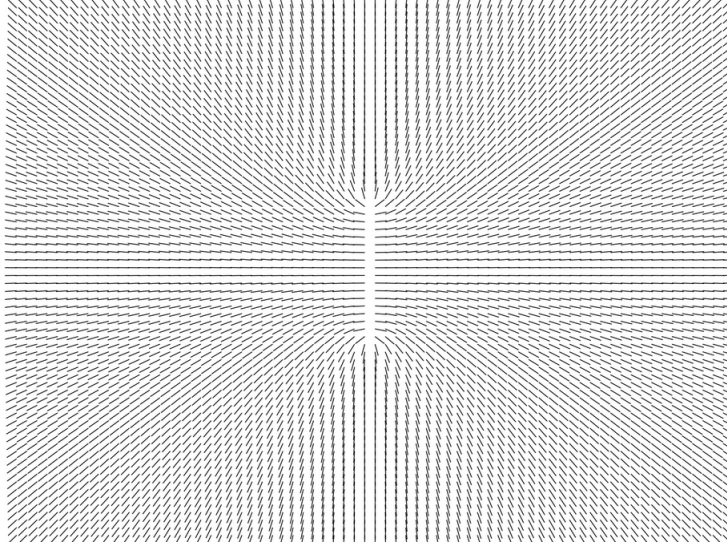
$$\begin{aligned} \begin{bmatrix} x' \\ y' \end{bmatrix} &= R^T(\alpha z) \begin{bmatrix} x \\ y \end{bmatrix} \\ &= \begin{bmatrix} \cos(\alpha z) x + \sin(\alpha z) y \\ -\sin(\alpha z) x + \cos(\alpha z) y \end{bmatrix} \end{aligned} \quad (7)$$

3 Rotated isotropic solution free energy

Taking θ to be the standard isotropic solution for two $+1/2$ disclinations gives:

$$\begin{aligned}\theta(x', y') &= \frac{1}{2} \tan^{-1} \left(\frac{y'}{x' - \frac{d}{2}} \right) + \frac{1}{2} \tan^{-1} \left(\frac{y'}{x' + \frac{d}{2}} \right) \\ &= \frac{1}{2} \tan^{-1} \left(\frac{-\sin(\alpha z) x + \cos(\alpha z) y}{\cos(\alpha z) x + \sin(\alpha z) y - \frac{d}{2}} \right) + \frac{1}{2} \tan^{-1} \left(\frac{-\sin(\alpha z) x + \cos(\alpha z) y}{\cos(\alpha z) x + \sin(\alpha z) y + \frac{d}{2}} \right)\end{aligned}\tag{8}$$

where here d is the disclination spacing. The result of plotting $\theta + \alpha z$ for $\alpha z = \pi/2$ gives the following rotated configuration:



One may explicitly calculate the free energy density for such a configuration. By symmetry, the free energy density at every z -value should be the same, so we evaluate at $z = 0$ to simplify the expressions. What we find is that (expectedly) only the twist and saddle splay terms depend on α . These give:

$$T^2(\alpha) = \alpha^2 f(x, y) \cos^4 \theta \tag{9}$$

$$|\Delta|^2(\alpha) = \alpha^2 f(x, y) + g(x, y) \tag{10}$$

with

$$f(x, y) = \frac{d^2 (d^2 - 4x^2 + 4y^2)^2}{(d^4 - 8d^2x^2 + 8d^2y^2 + 16x^4 + 32x^2y^2 + 16y^4)^2} \tag{11}$$

and $g(x, y)$ some function independent of α . Then the entire free energy goes as:

$$F = (K_{22} + (B - A)K_{24}) \alpha^2 + C \tag{12}$$

with

$$\begin{aligned}B &= \int_{\Omega} f(x, y) dV \\ A &= \int_{\Omega} f(x, y) \cos^4 \theta dV\end{aligned}\tag{13}$$

Clearly $B > A$ always, and so a twisted configuration will never be the minimum, at least for the configuration that we've written down.

4 Selinger Euler-Lagrange equation

To find the equilibrium state, we must minimize the Selinger free energy subject to the constraint that $\hat{\mathbf{n}}$ be a unit vector everywhere. The constraint can be written:

$$g(\mathbf{x}, \hat{\mathbf{n}}) = \hat{\mathbf{n}} \cdot \hat{\mathbf{n}} - 1 = 0 \quad (14)$$

Then the corresponding Lagrangian to be minimized is:

$$L = F - \lambda(\mathbf{x})g(\mathbf{x}, \hat{\mathbf{n}}) \quad (15)$$

The resulting functional derivative is is:

$$\delta L = \delta F - (2\lambda(\mathbf{x})\hat{\mathbf{n}}) \cdot \delta \hat{\mathbf{n}} \quad (16)$$

The resulting Euler-Lagrange equation then reads:

$$\frac{\delta F}{\delta \hat{\mathbf{n}}} = \lambda(\mathbf{x})\hat{\mathbf{n}} \quad (17)$$

where we have absorbed the factor of 2 into $\lambda(\mathbf{x})$ since it is arbitrary anyways. If we operate on both sides with $(I - \hat{\mathbf{n}} \otimes \hat{\mathbf{n}})$ we get the following:

$$(I - \hat{\mathbf{n}} \otimes \hat{\mathbf{n}}) \frac{\delta F}{\delta \hat{\mathbf{n}}} = \lambda(\mathbf{x}) [\hat{\mathbf{n}} - (\hat{\mathbf{n}} \cdot \hat{\mathbf{n}}) \hat{\mathbf{n}}] = 0 \quad (18)$$

where we have used the constraint on the left-hand side.

Below we calculate the functional derivative of F . This will simplify when we restrict the director to only polar-planar configurations. We do this one term at a time:

$$\begin{aligned} \delta(S^2) &= \int_{\Omega} 2S (\delta S) dV \\ &= \int_{\Omega} 2S (\nabla \cdot \delta \hat{\mathbf{n}}) dV \\ &= - \int_{\Omega} 2 (\nabla S) \cdot \delta \hat{\mathbf{n}} dV + \int_{\partial\Omega} 2 (S \boldsymbol{\nu}) \cdot \delta \hat{\mathbf{n}} dS \end{aligned} \quad (19)$$

$$\begin{aligned} \delta(T^2) &= \int_{\Omega} 2T (\delta T) dV \\ &= \int_{\Omega} 2T (\delta \hat{\mathbf{n}} \cdot (\nabla \times \hat{\mathbf{n}}) + \hat{\mathbf{n}} \cdot (\nabla \times \delta \hat{\mathbf{n}})) dV \\ &= \int_{\Omega} 4T (\nabla \times \hat{\mathbf{n}}) \cdot \delta \hat{\mathbf{n}} dV - \int_{\partial\Omega} 2T \boldsymbol{\nu} \cdot (\hat{\mathbf{n}} \times \delta \hat{\mathbf{n}}) dS \end{aligned} \quad (20)$$

where we have used the following identity²:

$$A \cdot (\nabla \times B) = -\nabla \cdot (A \times B) + B \cdot (\nabla \times A) \quad (21)$$

Also:

$$\begin{aligned} \delta |\mathbf{B}|^2 &= \int_{\Omega} 2\mathbf{B} \cdot (\delta \mathbf{B}) dV \\ &= \int_{\Omega} 2\mathbf{B} \cdot (\delta \hat{\mathbf{n}} \times (\nabla \times \hat{\mathbf{n}}) + \hat{\mathbf{n}} \times (\nabla \times \delta \hat{\mathbf{n}})) dV \\ &= \int_{\Omega} 2 [\delta \hat{\mathbf{n}} \cdot ((\nabla \times \hat{\mathbf{n}}) \times \mathbf{B}) + (\nabla \times \delta \hat{\mathbf{n}}) \cdot (\mathbf{B} \times \hat{\mathbf{n}})] dV \\ &= \int_{\Omega} 2 [\delta \hat{\mathbf{n}} \cdot ((\nabla \times \hat{\mathbf{n}}) \times \mathbf{B}) + \nabla \cdot (\delta \hat{\mathbf{n}} \times (\mathbf{B} \times \hat{\mathbf{n}})) + \delta \hat{\mathbf{n}} \cdot (\nabla \times (\mathbf{B} \times \hat{\mathbf{n}}))] dV \\ &= \int_{\Omega} 2 [\nabla \times (\mathbf{B} \times \hat{\mathbf{n}}) + (\nabla \times \hat{\mathbf{n}}) \times \mathbf{B}] \cdot \delta \hat{\mathbf{n}} dV + \int_{\partial\Omega} 2 [\boldsymbol{\nu} \cdot (\delta \hat{\mathbf{n}} \times (\mathbf{B} \times \hat{\mathbf{n}}))] dS \end{aligned} \quad (22)$$

where we have used the following identities:

$$A \cdot (B \times C) = C \cdot (A \times B) = B \cdot (C \times A) \quad (23)$$

and

$$\nabla \cdot (A \times B) = (\nabla \times A) \cdot B - (\nabla \times B) \cdot A \quad (24)$$

And finally, we look at the Δ term:

$$\begin{aligned} \delta(\Delta_{ij}\Delta_{ji}) &= \int_{\Omega} 2\Delta_{ij}(\delta\Delta_{ij}) dV \\ &= \int_{\Omega} 2\Delta_{ij} [2\partial_i\delta n_j - 2\delta n_i n_k \partial_k n_j - 2n_i \delta n_k \partial_k n_j - 2n_i n_k \partial_k \delta n_j \\ &\quad + \delta n_i n_j \partial_k n_k + n_i \delta n_j \partial_k n_k + n_i n_j \partial_k \delta n_k] dV \\ &= \int_{\Omega} 2[-2\Delta_{ij}\delta n_i n_k \partial_k n_j - 2\Delta_{ij}n_i \delta n_k \partial_k n_j + \Delta_{ij}\delta n_i n_j \partial_k n_k + \Delta_{ij}n_i \delta n_j \partial_k n_k \\ &\quad + 2\Delta_{ij}\partial_i \delta n_j - 2\Delta_{ij}n_i n_k \partial_k \delta n_j + \Delta_{ij}n_i n_j \partial_k \delta n_k] dV \\ &= \int_{\Omega} 2[-2\Delta_{kj}n_i \partial_i n_j - 2\Delta_{ij}n_i \partial_k n_j + \Delta_{kj}n_j \partial_i n_i + \Delta_{ik}n_i \partial_j n_j] \delta n_k dV \\ &\quad + \int_{\Omega} 2[-2\partial_i \Delta_{ik} + 2\partial_j (\Delta_{ik}n_i n_j) - \partial_k (\Delta_{ij}n_i n_j)] \delta n_k dV \\ &\quad + \int_{\partial\Omega} 2[2\Delta_{ij}\nu_i \delta n_j - 2\Delta_{ij}n_i n_k \nu_k \delta n_j + \Delta_{ij}n_i n_j \nu_k \delta n_k] dV \end{aligned} \quad (25)$$

For now, we assume that the boundaries are fixed so that the surface terms vanish. Putting all of these terms together gives the following Euler-Lagrange equation:

$$\begin{aligned} 0 = (I - \hat{\mathbf{n}} \otimes \hat{\mathbf{n}}) \Bigg[&-(K_{11} - K_{24}) \nabla S \\ &+ 2(K_{22} - K_{24}) T(\nabla \times \hat{\mathbf{n}}) \\ &+ K_{33} [\nabla \times (\mathbf{B} \times \hat{\mathbf{n}}) + (\nabla \times \hat{\mathbf{n}}) \times \mathbf{B}] \\ &+ 4K_{24} [\Delta \cdot \hat{\mathbf{n}} (\nabla \cdot \hat{\mathbf{n}}) - (\hat{\mathbf{n}} \cdot \nabla \hat{\mathbf{n}}) \cdot \Delta - (\nabla \hat{\mathbf{n}}) \cdot \Delta \cdot \hat{\mathbf{n}} \\ &\quad - \nabla \cdot \Delta + \nabla \cdot (\hat{\mathbf{n}} \otimes (\hat{\mathbf{n}} \cdot \Delta)) - \frac{1}{2} \nabla (\hat{\mathbf{n}} \cdot \Delta \cdot \hat{\mathbf{n}})] \Bigg] \end{aligned} \quad (26)$$

The idea here is to look at a general expression for a twisted planar configuration:

$$\hat{\mathbf{n}}' = R(\alpha z) \begin{bmatrix} \cos(\theta(x', y')) \\ \sin(\theta(x', y')) \\ 0 \end{bmatrix} \quad (27)$$

with

$$\begin{aligned} x' &= \cos(\alpha z)x + \sin(\alpha z)y \\ y' &= -\sin(\alpha z)x + \cos(\alpha z)y \end{aligned} \quad (28)$$

If we plug into eq. (26) and set $z = 0$ we will get a PDE in x and y . Imposing homeotropic boundary conditions gives us a minimum-energy configuration for a fixed α . Presumably we will have to solve this perturbatively with a regular and non-regular part. The non-regular part will have to be the two-defect configuration separated by a distance d . We may map out the free energy landscape for these two parameters, at the very least.

5 Bend-Splay Euler-Lagrange, as a check

To check our calculation, we just consider Bend-Splay terms. Taking $\epsilon = (K_{33} - K_{11})/(K_{33} + K_{11})$ gives:

$$(I - \hat{\mathbf{n}} \otimes \hat{\mathbf{n}}) \left[-(1 + \epsilon) \nabla S + (1 - \epsilon) [\nabla \times (\mathbf{B} \times \hat{\mathbf{n}}) + (\nabla \times \hat{\mathbf{n}}) \times \mathbf{B}] \right] = 0 \quad (29)$$

We calculate each term separately:

$$\nabla S - (\hat{\mathbf{n}} \cdot \nabla S) \hat{\mathbf{n}} \quad (30)$$

$$\hat{\mathbf{n}} \cdot \nabla \times (\mathbf{B} \times \hat{\mathbf{n}}) = \nabla \cdot (\hat{\mathbf{n}} \times (\mathbf{B} \times \hat{\mathbf{n}})) + (\nabla \times \hat{\mathbf{n}}) \cdot (\mathbf{B} \times \hat{\mathbf{n}}) \quad (31)$$

$$\begin{aligned} \hat{\mathbf{n}} \cdot [(\nabla \times \hat{\mathbf{n}}) \times \mathbf{B}] &= (\nabla \times \hat{\mathbf{n}}) \cdot (\mathbf{B} \times \hat{\mathbf{n}}) \\ &= (\nabla \times \hat{\mathbf{n}}) \cdot ((\hat{\mathbf{n}} \times (\nabla \times \hat{\mathbf{n}})) \times \hat{\mathbf{n}}) \\ &= (\nabla \times \hat{\mathbf{n}}) \cdot ((-\hat{\mathbf{n}} \cdot \nabla) \hat{\mathbf{n}} \times \hat{\mathbf{n}}) \end{aligned} \quad (32)$$

6 Simplified free energy

6.1 Free energy and Euler-Lagrange equation

For sake of ease, we assume $K_{24} = 0$ (in an infinite system we assume it does not matter) and $K_{11} = K_{33} = K$. We take ζ to be our twist elastic constant:

$$\zeta = \frac{K - K_{22}}{K + K_{22}} \quad (33)$$

This gives:

$$K_{22} = K \frac{1 - \zeta}{1 + \zeta} \quad (34)$$

Then the free energy is given by:

$$F = \int_{\Omega} (1 + \zeta) S^2 + (1 - \zeta) T^2 + (1 + \zeta) |\mathbf{B}|^2 dV \quad (35)$$

We may calculate each term explicitly for the planar director $\hat{\mathbf{n}} = [\cos \theta, \sin \theta, 0]$ with θ a function of (x, y, z) :

$$S = -\theta_x \sin \theta + \theta_y \cos \theta \quad (36)$$

$$T = -\theta_z \quad (37)$$

$$\mathbf{B} = \sin \theta (\theta_x \cos \theta + \theta_y \sin \theta) \hat{\mathbf{x}} - \cos \theta (\theta_x \cos \theta + \theta_y \sin \theta) \hat{\mathbf{y}} \quad (38)$$

So that:

$$S^2 = \theta_x^2 \sin^2 \theta + \theta_y^2 \cos^2 \theta - 2\theta_x \theta_y \sin \theta \cos \theta \quad (39)$$

$$T^2 = \theta_z^2 \quad (40)$$

$$|\mathbf{B}|^2 = \theta_x^2 \cos^2 \theta + \theta_y^2 \sin^2 \theta + 2\theta_x \theta_y \sin \theta \cos \theta \quad (41)$$

Calculating the free energy explicitly then gives:

$$F = \int_{\Omega} (1 + \zeta) |\nabla \theta|^2 + (1 - \zeta) \theta_z^2 dV \quad (42)$$

with $\nabla = \partial_x \hat{\mathbf{x}} + \partial_y \hat{\mathbf{y}}$ the two-dimensional gradient operator. The differential is:

$$\begin{aligned}\delta F &= 2 \int_{\Omega} (1 + \zeta) (\nabla \theta) \cdot (\nabla \delta \theta) + (1 - \zeta) \left(\frac{d\theta}{dz} \right) \left(\frac{d\delta \theta}{dz} \right) dV \\ &= 2 \int_{\Omega} (1 + \zeta) [\nabla \cdot (\delta \theta \nabla \theta) - (\nabla^2 \theta) \delta \theta] + (1 - \zeta) \left[\frac{d}{dz} \left(\delta \theta \frac{d\theta}{dz} \right) - \left(\frac{d^2 \theta}{dz^2} \right) \delta \theta \right] dV \\ &= \int_{\Omega} -2 \left[(1 + \zeta) \nabla^2 \theta + (1 - \zeta) \frac{d^2 \theta}{dz^2} \right] \delta \theta dV\end{aligned}\quad (43)$$

where we have assumed that the variation goes to zero at all the boundaries. Then the Euler-Lagrange equation reads:

$$(1 + \zeta) \nabla^2 \theta + (1 - \zeta) \frac{d^2 \theta}{dz^2} = 0 \quad (44)$$

6.2 Constant twist angular velocity configuration

We now consider a director given by:

$$\theta(x, y, z) = \theta(x', y') + \alpha z \quad (45)$$

where

$$\begin{aligned}x' &= \cos(\alpha z)x + \sin(\alpha z)y \\ y' &= -\sin(\alpha z)x + \cos(\alpha z)y\end{aligned}\quad (46)$$

We calculate this explicitly as follows:

$$\frac{\partial \theta}{\partial x} = \frac{\partial \theta}{\partial x'} \frac{\partial x'}{\partial x} + \frac{\partial \theta}{\partial y'} \frac{\partial y'}{\partial x} = \frac{\partial \theta}{\partial x'} \cos(\alpha z) - \frac{\partial \theta}{\partial y'} \sin(\alpha z) \quad (47)$$

so that

$$\frac{\partial^2 \theta}{\partial x^2} = \frac{\partial^2 \theta}{\partial x'^2} \cos^2(\alpha z) - 2 \frac{\partial^2 \theta}{\partial x' \partial y'} \cos(\alpha z) \sin(\alpha z) + \frac{\partial^2 \theta}{\partial y'^2} \sin^2(\alpha z) \quad (48)$$

similarly for y :

$$\frac{\partial^2 \theta}{\partial y^2} = \frac{\partial^2 \theta}{\partial x'^2} \sin^2(\alpha z) + 2 \frac{\partial^2 \theta}{\partial x' \partial y'} \cos(\alpha z) \sin(\alpha z) + \frac{\partial^2 \theta}{\partial y'^2} \cos^2(\alpha z) \quad (49)$$

Together this gives:

$$\nabla^2 \theta = \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} = \frac{\partial^2 \theta}{\partial x'^2} + \frac{\partial^2 \theta}{\partial y'^2} \quad (50)$$

so that it does not matter which plane we look at.

For the z -derivative we get:

$$\frac{\partial \theta}{\partial z} = \frac{\partial \theta}{\partial x'} \frac{\partial x'}{\partial z} + \frac{\partial \theta}{\partial y'} \frac{\partial y'}{\partial z} = \frac{\partial \theta}{\partial x'} \alpha y' - \frac{\partial \theta}{\partial y'} \alpha x' = -\alpha (\mathbf{x} \times \nabla) \theta \quad (51)$$

where $\mathbf{x} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}}$. The second derivative gives:

$$\begin{aligned}\frac{\partial^2 \theta}{\partial z^2} &= \frac{\partial^2 \theta}{\partial x' \partial z} \alpha y' + \frac{\partial \theta}{\partial x'} \alpha \frac{\partial y'}{\partial z} - \frac{\partial^2 \theta}{\partial y' \partial z} \alpha x' - \frac{\partial \theta}{\partial y'} \alpha \frac{\partial x'}{\partial z} \\ &= \frac{\partial^2 \theta}{\partial x'^2} \alpha^2 y'^2 - \frac{\partial^2 \theta}{\partial x' \partial y'} \alpha^2 y' x' - \frac{\partial \theta}{\partial x'} \alpha^2 x' + \frac{\partial^2 \theta}{\partial y'^2} \alpha^2 x'^2 - \frac{\partial^2 \theta}{\partial y' \partial x'} \alpha^2 x' y' - \frac{\partial \theta}{\partial y'} \alpha^2 y' \\ &= \alpha^2 (\mathbf{x} \times \nabla)^2 \theta\end{aligned}\quad (52)$$

³. The expression for energy then becomes:

$$F = \int_{\Omega} (1 + \zeta) |\nabla \theta|^2 + (1 - \zeta) \alpha^2 [(\mathbf{x} \times \nabla) \theta]^2 dV \quad (53)$$

and the Euler-Lagrange equation reads:

$$(1 + \zeta) \nabla^2 \theta + (1 - \zeta) \alpha^2 (\mathbf{x} \times \nabla)^2 \theta = 0 \quad (54)$$

We may decompose θ into $\theta_{\text{iso}} + \theta_c$ where $\theta_{\text{iso}} = \frac{1}{2}(\varphi_1 + \varphi_2)$ with φ_1, φ_2 the polar coordinates centered at $(\pm \frac{d}{2}, 0)$ and θ_c is a regular correction. Note that d is the spacing of the two $+1/2$ disclinations. Since $\nabla^2 \theta_{\text{iso}} = 0$ this gives the following linear equation for θ_c :

$$\left[(1 + \zeta) \nabla^2 + (1 - \zeta) \alpha^2 (\mathbf{x} \times \nabla)^2 \right] \theta_c = -(1 - \zeta) \alpha^2 (\mathbf{x} \times \nabla)^2 \theta_{\text{iso}} \quad (55)$$

6.3 Constant twist weak form

The $(\mathbf{x} \times \nabla)$ operator also has a nice product rule⁴. Also note that, in two dimensions, it has a nice integration formula⁵ Taking the inner product with some test function η then yields the following weak form:

$$(1 + \zeta) \langle \eta, \nabla^2 \theta_c \rangle + (1 - \zeta) \alpha^2 \langle \eta, (\mathbf{x} \times \nabla)^2 \theta_c \rangle = -(1 - \zeta) \alpha^2 \langle \eta, (\mathbf{x} \times \nabla)^2 \theta_{\text{iso}} \rangle \quad (56)$$

which finally yields:

$$\begin{aligned} & - (1 + \zeta) \langle \nabla \eta, \nabla \theta_c \rangle \\ & - (1 - \zeta) \alpha^2 \langle (\mathbf{x} \times \nabla) \eta, (\mathbf{x} \times \nabla) \theta_c \rangle = (1 - \zeta) \alpha^2 \langle (\mathbf{x} \times \nabla) \eta, (\mathbf{x} \times \nabla) \theta_{\text{iso}} \rangle \\ & \quad - (1 + \zeta) \langle \eta, \boldsymbol{\nu} \cdot \nabla \theta_c \rangle_{\partial \Omega} \\ & \quad - (1 - \zeta) \alpha^2 \langle \eta, (\mathbf{x} \times \boldsymbol{\nu}) (\mathbf{x} \times \nabla) \theta_c \rangle_{\partial \Omega} \end{aligned} \quad (57)$$

If we maintain Dirichlet boundary conditions, this becomes:

$$(1 + \zeta) \langle \nabla \eta, \nabla \theta_c \rangle + \alpha^2 (1 - \zeta) \langle (\mathbf{x} \times \nabla) \eta, (\mathbf{x} \times \nabla) \theta_c \rangle = -\alpha^2 (1 - \zeta) \langle (\mathbf{x} \times \nabla) \eta, (\mathbf{x} \times \nabla) \theta_{\text{iso}} \rangle \quad (58)$$

Additionally, we note that, in polar coordinates we have:

$$\frac{\partial \varphi}{\partial x} = -\frac{1}{r} \sin \varphi \quad (59)$$

$$\frac{\partial \varphi}{\partial y} = \frac{1}{r} \cos \varphi \quad (60)$$

This is true for polar coordinates centered at any origin. Then we also have that:

$$x = r_i \cos \varphi_i \pm \frac{d}{2} \quad (61)$$

$$y = r_i \sin \varphi_i \quad (62)$$

with $-$ for $i = 1$ and $+$ for $i = 2$. This implies:

$$r_i^2 = \left(x \mp \frac{d}{2} \right)^2 + y^2 \quad (63)$$

In that case:

$$\frac{\partial \varphi}{\partial x} = -\frac{y}{(x \mp \frac{d}{2})^2 + y^2} \quad (64)$$

$$\frac{\partial \varphi}{\partial y} = \frac{x \mp \frac{d}{2}}{(x \mp \frac{d}{2})^2 + y^2} \quad (65)$$

Putting this altogether we get:

$$(\mathbf{x} \times \nabla)\theta_{\text{iso}} = \frac{1}{2} \left[\frac{x^2 + y^2 + \frac{d}{2}x}{(x + \frac{d}{2})^2 + y^2} + \frac{x^2 + y^2 - \frac{d}{2}x}{(x - \frac{d}{2})^2 + y^2} \right] \quad (66)$$

For the boundary conditions, homeotropic anchoring demands that:

$$\theta|_{\partial\Omega} = \varphi \quad (67)$$

However, we have that:

$$\frac{1}{2} \left[\text{atan2} \left(y, x + \frac{d}{2} \right) + \text{atan2} \left(y, x - \frac{d}{2} \right) \right] \quad (68)$$

Hence, we must have:

$$\theta_c = \text{atan2} (y, x) - \frac{1}{2} \left[\text{atan2} \left(y, x + \frac{d}{2} \right) + \text{atan2} \left(y, x - \frac{d}{2} \right) \right] \quad (69)$$

6.4 Discussion of constant twist energy

In this section we more closely consider Eq. (53). We note that $|\nabla\theta|^2$ is minimized by θ_{iso} because it solves Laplace's equation. Further, $[(\mathbf{x} \times \nabla)\theta]^2 > 0$ always. Hence, for any $0 < \zeta < 1$ we have that:

$$(1 + \zeta) |\nabla\theta_{\text{iso}}|^2 \leq (1 + \zeta) |\nabla\theta|^2 \leq (1 + \zeta) |\nabla\theta|^2 + \alpha^2(1 - \zeta) [(\mathbf{x} \times \theta) \theta]^2 \quad (70)$$

with the first comparison an equality only when $\theta = \theta_{\text{iso}}$ by uniqueness of the solutions of Laplace's equation, and the second comparison an equality only when $\alpha = 0$ (or $(\mathbf{x} \times \nabla)\theta = 0$ which seems impossible for a configuration with two disclinations). This means that the minimizer is always $\theta = \theta_{\text{iso}}$ with $\alpha = 0$. Since $\zeta < 1$ always (lest we let $K_3 < 0$) this is always the case, and the director formalism will never produce a planar minimum energy configuration which has constant twist angular velocity.

6.5 Variable twist angular velocity

Here we assume a director configuration whose twist angular velocity α is a function of z . In this case, the x - and y -derivatives are unchanged, but the z derivatives vary considerably:

$$\frac{\partial\theta}{\partial z} = \frac{\partial\theta}{\partial x'}(\alpha + z\alpha')y' - \frac{\partial\theta}{\partial y'}(\alpha + z\alpha')x' \quad (71)$$

and then

$$\begin{aligned} \frac{\partial^2\theta}{\partial z^2} &= \frac{\partial^2\theta}{\partial x'^2}(\alpha + z\alpha')^2 y'^2 - \frac{\partial^2\theta}{\partial x'\partial y'}(\alpha + z\alpha')^2 y'x' + \frac{\partial\theta}{\partial x'}(2\alpha' + z\alpha'')y' - \frac{\partial\theta}{\partial x'}(\alpha + z\alpha')^2 x' \\ &\quad + \frac{\partial^2\theta}{\partial y'^2}(\alpha + z\alpha')^2 x'^2 - \frac{\partial^2\theta}{\partial y'\partial x'}(\alpha + z\alpha')^2 x'y' - \frac{\partial\theta}{\partial y'}(2\alpha' + z\alpha'')x' - \frac{\partial\theta}{\partial y'}(\alpha + z\alpha')^2 y' \end{aligned} \quad (72)$$

Finally we have:

$$\frac{\partial^2}{\partial z^2}\alpha z = \frac{\partial}{\partial z} [\alpha'z + \alpha] = \alpha''z + 2\alpha' \quad (73)$$

Notes

¹ Suppose $\mathbf{v}(\mathbf{x})$ is a vector field. Take L to be a linear transformation. We would like to act on \mathbf{v} by L in an *active* way. This means that, if L rotates a plane by some angle θ , then we are imagining taking \mathbf{v} (say on a piece of paper) and rotating the whole thing by the angle θ . There's two pieces to this: i) is that we must act on each of the vectors outputted by \mathbf{v} by L (again, think of rotating a vector field printed on a piece of paper). ii) is that, if we want to get the correct vector field at \mathbf{x} , we must actually sample \mathbf{v} at a point $L^{-1}\mathbf{x}$. This is because $L^{-1}\mathbf{x}$ is the point that will get mapped to \mathbf{x} by L .

2

$$\begin{aligned} A \cdot (\nabla \times B) &= A_i \epsilon_{ijk} \partial_j B_k \\ &= \epsilon_{ijk} (\partial_j (A_i B_k) - B_k \partial_j A_i) \\ &= -\partial_j (\epsilon_{jik} A_i B_k) + B_k \epsilon_{kji} \partial_j A_i \\ &= -\nabla \cdot (A \times B) + B \cdot (\nabla \times A) \end{aligned} \quad (74)$$

3

$$\begin{aligned} (\mathbf{x} \times \nabla)^2 &= \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \\ &= \left(x^2 \frac{\partial}{\partial y^2} - x \frac{\partial}{\partial x} - xy \frac{\partial}{\partial y} \frac{\partial}{\partial x} - y \frac{\partial}{\partial y} - yx \frac{\partial}{\partial x} \frac{\partial}{\partial y} + y^2 \frac{\partial}{\partial x^2} \right) \end{aligned} \quad (75)$$

4

$$\begin{aligned} (\mathbf{x} \times \nabla) (fg) &= \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) (fg) \\ &= x \left(g \frac{\partial f}{\partial y} + f \frac{\partial g}{\partial y} \right) - y \left(g \frac{\partial f}{\partial x} + f \frac{\partial g}{\partial x} \right) \\ &= g \left(x \frac{\partial f}{\partial y} - y \frac{\partial f}{\partial x} \right) + f \left(x \frac{\partial g}{\partial y} - y \frac{\partial g}{\partial x} \right) \\ &= g (\mathbf{x} \times \nabla) f + f (\mathbf{x} \times \nabla) g \end{aligned} \quad (76)$$

⁵ We first rewrite the operator as a divergence: $(\mathbf{x} \times \nabla)f = \nabla \cdot \mathbf{g}$ with $\mathbf{g} = f[-y \ x]^T$. Then we may explicitly calculate the integration formula using the divergence theorem:

$$\begin{aligned} \int_{\Omega} (\mathbf{x} \times \nabla) f \, dV &= \int_{\Omega} \nabla \cdot \mathbf{g} \, dV \\ &= \int_{\partial\Omega} (\hat{\nu} \cdot \mathbf{g}) \, dS \\ &= \int_{\partial\Omega} f (-\nu_x y + \nu_y x) \, dS \\ &= \int_{\partial\Omega} f (\mathbf{x} \times \hat{\nu}) \, dS \end{aligned} \quad (77)$$

Then the simplified Euler-Lagrange equation is:

$$0 = -(1 + \zeta) \nabla S + 2(1 - \zeta) T (\nabla \times \hat{\mathbf{n}}) + (1 + \zeta) [\nabla \times (\mathbf{B} \times \hat{\mathbf{n}}) + (\nabla \times \hat{\mathbf{n}}) \times \mathbf{B}] \quad (78)$$