Double helix director

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1 Selinger free energy

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

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

with the following definitions for the distortion modes:

$$S = \nabla \cdot \hat{\mathbf{n}} \tag{2}$$
$$T = \hat{\mathbf{n}} \cdot \left(\nabla \times \hat{\mathbf{n}}\right) \tag{3}$$
$$B = \hat{\mathbf{n}} \times \left(\nabla \times \hat{\mathbf{n}}\right) \tag{4}$$
$$\begin{aligned}\Delta_{ij} = \frac{1}{2}\big[&\partial_i n_j + \partial_j n_i \\ &- n_i n_k \partial_k n_j - n_j n_k \partial_k n_i \\ &- \delta_{ij} \partial_k n_k + n_i n_j \partial_k n_k\big]\end{aligned} \tag{5}$$

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:

$$\hat{\mathbf{n}} = R(\alpha z) \begin{bmatrix}\cos\theta & \sin\theta & 0\end{bmatrix}^T \tag{6}$$

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:

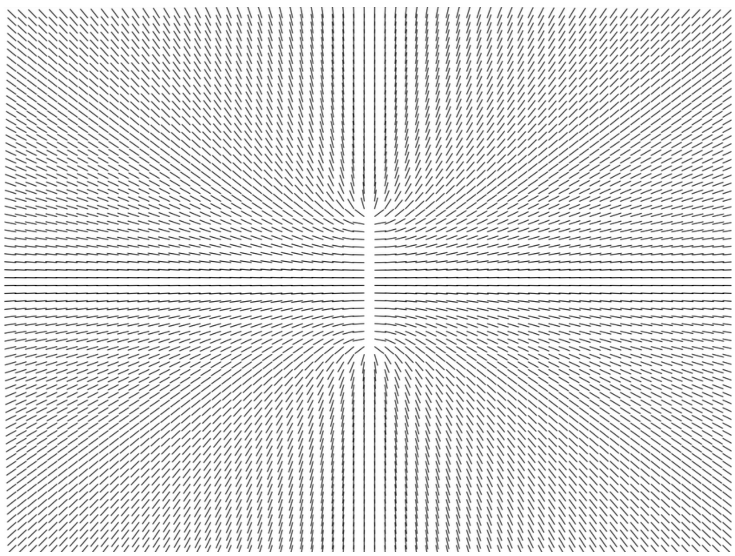
$$\begin{aligned}\begin{bmatrix}x' \\ y'\end{bmatrix} &= R^T(\alpha z) \begin{bmatrix}x \\ y\end{bmatrix} \\ &= \begin{bmatrix}\cos(\alpha z)\, x + \sin(\alpha z)\, y \\ -\sin(\alpha z)\, x + \cos(\alpha z)\, y\end{bmatrix}\end{aligned} \tag{7}$$

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

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

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

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

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:

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

Then the corresponding Lagrangian to be minimized is:

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

The resulting functional derivative is is:

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

The resulting Euler-Lagrange equation then reads:

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

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:

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

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:

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

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

where we have used the following identity[2]:

$$A \cdot (\nabla \times B) = -\nabla \cdot (A \times B) + B \cdot (\nabla \times A) \tag{21}$$

Also:

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

where we have used the following identities:

$$A \cdot (B \times C) = C \cdot (A \times B) = B \cdot (C \times A) \tag{23}$$

and

$$\nabla \cdot (A \times B) = (\nabla \times A) \cdot B - (\nabla \times B) \cdot A \tag{24}$$

And finally, we look at the Δ term:

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

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:

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

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

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

with

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

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:

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

We calculate each term separately:

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

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

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

6 Simplified free energy

6.1 Free energy and Euler-Lagrange equation

For sake of calculation, we rewrite the Frank free energy as:

$$F = \frac{1}{2} K_{11} S^2 + \frac{1}{2} K_{22} T^2 + \frac{1}{2} K_{33} \left|\mathbf{B}\right|^2 + \frac{1}{2} K_{24} P \tag{33}$$

with

$$P = \nabla \cdot \left[(\hat{\mathbf{n}} \cdot \nabla)\, \hat{\mathbf{n}} - \hat{\mathbf{n}}\, (\nabla \cdot \hat{\mathbf{n}}) \right] \tag{34}$$

the saddle splay term.

We take ζ to be our twist elastic constant:

$$\zeta = \frac{K - K_{22}}{K + K_{22}} \tag{35}$$

This gives:

$$K_{22} = K\, \frac{1-\zeta}{1+\zeta} \tag{36}$$

Then the free energy is given by:

$$F = \int_\Omega (1+\zeta) S^2 + (1-\zeta) T^2 + (1+\zeta) \left|\mathbf{B}\right|^2 + \frac{K_{24}}{K} P dV \tag{37}$$

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):

$$S = -\theta_x \sin\theta + \theta_y \cos\theta \tag{38}$$

$$T = -\theta_z \tag{39}$$

$$\mathbf{B} = \sin\theta\, (\theta_x \cos\theta + \theta_y \sin\theta)\, \hat{\mathbf{x}} - \cos\theta\, (\theta_x \cos\theta + \theta_y \sin\theta)\, \hat{\mathbf{y}} \tag{40}$$

So that:

$$
\begin{aligned}
S^2 &= \theta_x^2 \sin^2\theta + \theta_y^2 \cos^2\theta - 2\theta_x\theta_y \sin\theta\cos\theta && (41)\\
T^2 &= \theta_z^2 && (42)\\
|\mathbf{B}|^2 &= \theta_x^2 \cos^2\theta + \theta_y^2 \sin^2\theta + 2\theta_x\theta_y \sin\theta\cos\theta && (43)\\
P &= -\theta_{xy} + \theta_{yx} = 0 && (44)
\end{aligned}
$$

Calculating the free energy explicitly then gives:

$$
F = \int_\Omega (1+\zeta)\left|\nabla\theta\right|^2 + (1-\zeta)\,\theta_z^2 dV \tag{45}
$$

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

$$
\begin{aligned}
\delta F &= 2\int_\Omega (1+\zeta)\,(\nabla\theta)\cdot(\nabla\delta\theta) + (1-\zeta)\left(\frac{d\theta}{dz}\right)\left(\frac{d\delta\theta}{dz}\right) dV\\
&= 2\int_\Omega (1+\zeta)\left[\nabla\cdot(\delta\theta\nabla\theta) - \left(\nabla^2\theta\right)\delta\theta\right] + (1-\zeta)\left[\frac{d}{dz}\left(\delta\theta\frac{d\theta}{dz}\right) - \left(\frac{d^2\theta}{dz^2}\right)\delta\theta\right] dV\\
&= \int_\Omega -2\left[(1+\zeta)\nabla^2\theta + (1-\zeta)\frac{d^2\theta}{dz^2}\right]\delta\theta dV
\end{aligned} \tag{46}
$$

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

$$
(1+\zeta)\nabla^2\theta + (1-\zeta)\frac{d^2\theta}{dz^2} = 0 \tag{47}
$$

6.2 Constant twist angular velocity configuration

We now consider a director given by:

$$
\theta(x,y,z) = \theta(x',y') + \alpha z \tag{48}
$$

where

$$
\begin{aligned}
x' &= \cos(\alpha z)x + \sin(\alpha z)y\\
y' &= -\sin(\alpha z)x + \cos(\alpha z)y
\end{aligned} \tag{49}
$$

We calculate this explicitly as follows:

$$
\frac{\partial\theta}{\partial x} = \frac{\partial\theta}{\partial x'}\frac{\partial x'}{\partial x} + \frac{\partial\theta}{\partial y'}\frac{\partial y'}{\partial x} = \frac{\partial\theta}{\partial x'}\cos(\alpha z) - \frac{\partial\theta}{\partial y'}\sin(\alpha z) \tag{50}
$$

so that

$$
\frac{\partial^2\theta}{\partial x^2} = \frac{\partial^2\theta}{\partial x'^2}\cos^2(\alpha z) - 2\frac{\partial^2\theta}{\partial x'\partial y'}\cos(\alpha z)\sin(\alpha z) + \frac{\partial^2\theta}{\partial y'^2}\sin^2(\alpha z) \tag{51}
$$

similarly for y:

$$
\frac{\partial^2\theta}{\partial y^2} = \frac{\partial^2\theta}{\partial x'^2}\sin^2(\alpha z) + 2\frac{\partial^2\theta}{\partial x'\partial y'}\cos(\alpha z)\sin(\alpha z) + \frac{\partial^2\theta}{\partial y'^2}\cos^2(\alpha z) \tag{52}
$$

Together this gives:

$$
\nabla^2\theta = \frac{\partial^2\theta}{\partial x} + \frac{\partial^2\theta}{\partial y} = \frac{\partial^2\theta}{\partial x'} + \frac{\partial^2\theta}{\partial y'} \tag{53}
$$

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

For the z-derivative we get:

$$\frac{\partial\theta}{\partial z}=\frac{\partial\theta}{\partial x'}\frac{\partial x'}{\partial z}+\frac{\partial\theta}{\partial y'}\frac{\partial y'}{\partial z}=\frac{\partial\theta}{\partial x'}\alpha y'-\frac{\partial\theta}{\partial y'}\alpha x'=-\alpha\left(\mathbf{x}\times\nabla\right)\theta \tag{54}$$

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

$$\begin{aligned}\frac{\partial^2\theta}{\partial z^2}&=\frac{\partial^2\theta}{\partial x'\partial z}\alpha y'+\frac{\partial\theta}{\partial x'}\alpha\frac{\partial y'}{\partial z}-\frac{\partial^2\theta}{\partial y'\partial z}\alpha x'-\frac{\partial\theta}{\partial y'}\alpha\frac{\partial x'}{\partial z}\\&=\frac{\partial^2\theta}{\partial x'^2}\alpha^2 y'^2-\frac{\partial^2\theta}{\partial x'\partial y'}\alpha^2 y'x'-\frac{\partial\theta}{\partial x'}\alpha^2 x'+\frac{\partial^2\theta}{\partial y'^2}\alpha^2 x'^2-\frac{\partial^2\theta}{\partial y'\partial x'}\alpha^2 x'y'-\frac{\partial\theta}{\partial y'}\alpha^2 y'\\&=\alpha^2\left(\mathbf{x}\times\nabla\right)^2\theta\end{aligned} \tag{55}$$

[3]. The expression for energy then becomes:

$$F=\int_\Omega(1+\zeta)\left|\nabla\theta\right|^2+(1-\zeta)\alpha^2\left[\left(\mathbf{x}\times\nabla\right)\theta\right]^2dV \tag{56}$$

and the Euler-Lagrange equation reads:

$$(1+\zeta)\,\nabla^2\theta+(1-\zeta)\,\alpha^2\left(\mathbf{x}\times\nabla\right)^2\theta=0 \tag{57}$$

We may decompose θ into $\theta_{\text{iso}}+\theta_c$ where $\theta_{\text{iso}}=\frac{1}{2}\left(\varphi_1+\varphi_2\right)$ with φ_1,φ_2 the polar coordinates centered at $\left(\pm\frac{d}{2},0\right)$ 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:

$$\left[(1+\zeta)\nabla^2+(1-\zeta)\alpha^2\left(\mathbf{x}\times\nabla\right)^2\right]\theta_c=-(1-\zeta)\alpha^2\left(\mathbf{x}\times\nabla\right)^2\,\theta_{\text{iso}} \tag{58}$$

6.3 Constant twist weak form

The $(\mathbf{x}\times\nabla)$ operator also has a nice product rule[4]. Also note that, in two dimensions, it has a nice integration formula[5] Taking the inner product with some test function η then yields the following weak form:

$$(1+\zeta)\left\langle\eta,\nabla^2\theta_c\right\rangle+(1-\zeta)\alpha^2\left\langle\eta,\left(\mathbf{x}\times\nabla\right)^2\theta_c\right\rangle=-(1-\zeta)\alpha^2\left\langle\eta,\left(\mathbf{x}\times\nabla\right)^2\theta_{\text{iso}}\right\rangle \tag{59}$$

which finally yields:

$$\begin{aligned}&-(1+\zeta)\left\langle\nabla\eta,\nabla\theta_c\right\rangle\\&\quad-(1-\zeta)\alpha^2\left\langle\left(\mathbf{x}\times\nabla\right)\eta,\left(\mathbf{x}\times\nabla\right)\theta_c\right\rangle=(1-\zeta)\alpha^2\left\langle\left(\mathbf{x}\times\nabla\right)\eta,\left(\mathbf{x}\times\nabla\right)\theta_{\text{iso}}\right\rangle\\&\qquad\qquad-(1+\zeta)\left\langle\eta,\boldsymbol{\nu}\cdot\nabla\theta_c\right\rangle_{\partial\Omega}\\&\qquad\qquad-(1-\zeta)\alpha^2\left\langle\eta,\left(\mathbf{x}\times\boldsymbol{\nu}\right)\left(\mathbf{x}\times\nabla\right)\theta_c\right\rangle_{\partial\Omega}\end{aligned} \tag{60}$$

If we maintain Dirichlet boundary conditions, this becomes:

$$(1+\zeta)\left\langle\nabla\eta,\nabla\theta_c\right\rangle+\alpha^2(1-\zeta)\left\langle\left(\mathbf{x}\times\nabla\right)\eta,\left(\mathbf{x}\times\nabla\right)\theta_c\right\rangle=-\alpha^2(1-\zeta)\left\langle\left(\mathbf{x}\times\nabla\right)\eta,\left(\mathbf{x}\times\nabla\right)\theta_{\text{iso}}\right\rangle \tag{61}$$

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

$$\frac{\partial\varphi}{\partial x}=-\frac{1}{r}\sin\varphi \tag{62}$$

$$\frac{\partial\varphi}{\partial y}=\frac{1}{r}\cos\varphi \tag{63}$$

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

$$x = r_i \cos\varphi_i \pm \frac{d}{2} \tag{64}$$

$$y = r_i \sin\varphi_i \tag{65}$$

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

$$r_i^2 = \left(x \mp \frac{d}{2}\right)^2 + y^2 \tag{66}$$

In that case:

$$\frac{\partial\varphi}{\partial x} = -\frac{y}{(x \mp \frac{d}{2})^2 + y^2} \tag{67}$$

$$\frac{\partial\varphi}{\partial y} = \frac{x \mp \frac{d}{2}}{(x \mp \frac{d}{2})^2 + y^2} \tag{68}$$

Putting this altogether we get:

$$(\mathbf{x} \times \nabla)\theta_{\text{iso}} = \frac{1}{2}\left[\frac{x^2 + y^2 + \frac{d}{2}x}{\left(x + \frac{d}{2}\right)^2 + y^2} + \frac{x^2 + y^2 - \frac{d}{2}x}{\left(x - \frac{d}{2}\right)^2 + y^2}\right] \tag{69}$$

For the boundary conditions, homeotropic anchoring demands that:

$$\theta|_{\partial\Omega} = \varphi \tag{70}$$

However, we have that:

$$\frac{1}{2}\left[\text{atan2}\left(y, x + \tfrac{d}{2}\right) + \text{atan2}\left(y, x - \tfrac{d}{2}\right)\right] \tag{71}$$

Hence, we must have:

$$\theta_c = \text{atan2}\left(y, x\right) - \frac{1}{2}\left[\text{atan2}\left(y, x + \tfrac{d}{2}\right) + \text{atan2}\left(y, x - \tfrac{d}{2}\right)\right] \tag{72}$$

6.4 Discussion of constant twist energy

In this section we more closely consider Eq. (56). 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:

$$(1 + \zeta)\left|\nabla\theta_{\text{iso}}\right|^2 \leq (1 + \zeta)\left|\nabla\theta\right|^2 \leq (1 + \zeta)\left|\nabla\theta\right|^2 + \alpha^2(1 - \zeta)\left[(\mathbf{x} \times \theta)\,\theta\right]^2 \tag{73}$$

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 $K_33 < 0$) 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:

$$\frac{\partial\theta}{\partial z} = \frac{\partial\theta}{\partial x'}(\alpha + z\alpha')y' - \frac{\partial\theta}{\partial y'}(\alpha + z\alpha')x' \tag{74}$$

and then

$$\frac{\partial^2\theta}{\partial z^2} = \frac{\partial^2\theta}{\partial x'^2}(\alpha + z\alpha')^2 y'^2 - \frac{\partial^2\theta}{\partial x'\partial y'}(\alpha + z\alpha')^2 y'x' + \frac{\partial\theta}{\partial x'}(2\alpha' + z\alpha'')y' - \frac{\partial\theta}{\partial x'}(\alpha + z\alpha')^2 x'$$
$$+ \frac{\partial^2\theta}{\partial y'^2}(\alpha + z\alpha')^2 x'^2 - \frac{\partial^2\theta}{\partial y'\partial x'}(\alpha + z\alpha')^2 x'y' - \frac{\partial\theta}{\partial y'}(2\alpha' + z\alpha'')x' - \frac{\partial\theta}{\partial y'}(\alpha + z\alpha')^2 y' \tag{75}$$

Finally we have:

$$\frac{\partial^2}{\partial z^2}\alpha z = \frac{\partial}{\partial z}\left[\alpha' z + \alpha\right] = \alpha'' z + 2\alpha' \tag{76}$$

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]

$$\begin{aligned} A \cdot (\nabla \times B) &= A_i \epsilon_{ijk} \partial_j B_k \\ &= \epsilon_{ijk} \left(\partial_j (A_i B_k) - B_k \partial_j A_i\right) \\ &= -\partial_j \left(\epsilon_{jik} A_i B_k\right) + B_k \epsilon_{kji} \partial_j A_i \\ &= -\nabla \cdot (A \times B) + B \cdot (\nabla \times A) \end{aligned} \tag{77}$$

[3]

$$\begin{aligned} (\mathbf{x} \times \nabla)^2 &= \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \\ &= \left(x^2\frac{\partial}{\partial y^2} - x\frac{\partial}{\partial x} - xy\frac{\partial}{\partial y}\frac{\partial}{\partial x} - y\frac{\partial}{\partial y} - yx\frac{\partial}{\partial x}\frac{\partial}{\partial y} + y^2\frac{\partial}{\partial x^2}\right) \end{aligned} \tag{78}$$

[4]

$$\begin{aligned} (\mathbf{x} \times \nabla)(fg) &= \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)(fg) \\ &= x\left(g\frac{\partial f}{\partial y} + f\frac{\partial g}{\partial y}\right) - y\left(g\frac{\partial f}{\partial x} + f\frac{\partial g}{\partial x}\right) \\ &= g\left(x\frac{\partial f}{\partial y} - y\frac{\partial f}{\partial x}\right) + f\left(x\frac{\partial g}{\partial y} - y\frac{\partial g}{\partial x}\right) \\ &= g\,(\mathbf{x} \times \nabla)\,f + f\,(\mathbf{x} \times \nabla)\,g \end{aligned} \tag{79}$$

[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:

$$\begin{aligned} \int_\Omega (\mathbf{x} \times \nabla)\, f\, dV &= \int_\Omega \nabla \cdot \mathbf{g}\, dV \\ &= \int_{\partial\Omega} (\hat{\boldsymbol{\nu}} \cdot \mathbf{g})\, dS \\ &= \int_{\partial\Omega} f\,(-\nu_x y + \nu_y x)\, dS \\ &= \int_{\partial\Omega} f\,(\mathbf{x} \times \hat{\boldsymbol{\nu}})\, dS \end{aligned} \tag{80}$$

Then the simplified Euler-Lagrange equation is:

$$0 = -(1+\zeta)\nabla S + 2(1-\zeta)T\ (\nabla \times \hat{\mathbf{n}}) + (1+\zeta)\left[\nabla \times (\mathbf{B} \times \hat{\mathbf{n}}) + (\nabla \times \hat{\mathbf{n}}) \times \mathbf{B}\right] \tag{81}$$