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:

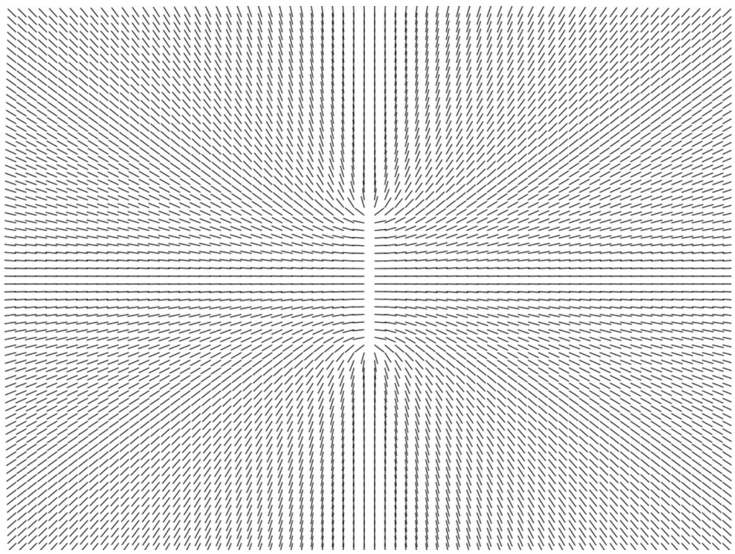
$$\begin{aligned} \begin{bmatrix} x' \\ y' \end{bmatrix} &= R^T(\alpha z) \begin{bmatrix} x \\ y \end{bmatrix} \\ &= \begin{bmatrix} \cos(\alpha z)\, x + \sin(\alpha z)\, y \\ -\sin(\alpha z)\, x + \cos(\alpha z)\, y \end{bmatrix} \end{aligned} \tag{7}$$

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

We begin by calculating the general Euler-Lagrange equation for the Frank free energy with all terms. This will simplify when we restrict the director to only polar-planar configurations. We do this one term at a time:

$$\begin{aligned}\delta(S^2) &= \int_\Omega 2S\,(\delta S)\;dV \\ &= \int_\Omega 2S\;(\nabla\cdot\delta\hat{\mathbf{n}})\;dV \\ &= -\int_\Omega 2\,(\nabla S)\cdot\delta\hat{\mathbf{n}}\,dV + \int_{\partial\Omega} 2\,(S\boldsymbol{\nu})\cdot\delta\hat{\mathbf{n}}\,dS\end{aligned} \tag{14}$$

$$\begin{aligned}\delta(T^2) &= \int_\Omega 2T\,(\delta T)\;dV \\ &= \int_\Omega 2T\,(\delta\hat{\mathbf{n}}\cdot(\nabla\times\hat{\mathbf{n}}) + \hat{\mathbf{n}}\cdot(\nabla\times\delta\hat{\mathbf{n}}))\;dV \\ &= \int_\Omega 4T\,(\nabla\times\hat{\mathbf{n}})\cdot\delta\hat{\mathbf{n}}\,dV - \int_{\partial\Omega} 2T\boldsymbol{\nu}\cdot(\hat{\mathbf{n}}\times\delta\hat{\mathbf{n}})\,dS\end{aligned} \tag{15}$$

where we have used the following identity[2]:

$$A\cdot(\nabla\times B) = -\nabla\cdot(A\times B) + B\cdot(\nabla\times A) \tag{16}$$

Also:

$$\begin{aligned}\delta\left|\mathbf{B}\right|^2 &= \int_\Omega 2\mathbf{B}\cdot(\delta\mathbf{B})\;dV \\ &= \int_\Omega 2\mathbf{B}\cdot(\delta\hat{\mathbf{n}}\times(\nabla\times\hat{\mathbf{n}}) + \hat{\mathbf{n}}\times(\nabla\times\delta\hat{\mathbf{n}}))\;dV \\ &= \int_\Omega 2\left[\delta\hat{\mathbf{n}}\cdot((\nabla\times\hat{\mathbf{n}})\times\mathbf{B}) + (\nabla\times\delta\hat{\mathbf{n}})\cdot(\mathbf{B}\times\hat{\mathbf{n}})\right]\;dV \\ &= \int_\Omega 2\left[\delta\hat{\mathbf{n}}\cdot((\nabla\times\hat{\mathbf{n}})\times\mathbf{B}) + \nabla\cdot(\delta\hat{\mathbf{n}}\times(\mathbf{B}\times\hat{\mathbf{n}})) + \delta\hat{\mathbf{n}}\cdot(\nabla\times(\mathbf{B}\times\hat{\mathbf{n}}))\right]\;dV \\ &= \int_\Omega 2\left[\nabla\times(\mathbf{B}\times\hat{\mathbf{n}}) + (\nabla\times\hat{\mathbf{n}})\times\mathbf{B}\right]\cdot\delta\hat{\mathbf{n}}\,dV + \int_{\partial\Omega} 2\left[\boldsymbol{\nu}\cdot(\delta\hat{\mathbf{n}}\times(\mathbf{B}\times\hat{\mathbf{n}}))\right]\;dS\end{aligned} \tag{17}$$

where we have used the following identities:

$$A\cdot(B\times C) = C\cdot(A\times B) = B\cdot(C\times A) \tag{18}$$

and

$$\nabla\cdot(A\times B) = (\nabla\times A)\cdot B - (\nabla\times B)\cdot A \tag{19}$$

And finally, we look at the Δ term:

$$\begin{aligned}
\delta\left(\Delta_{ij}\Delta_{ji}\right) &= \int_\Omega 2\Delta_{ij}(\delta\Delta_{ij})\,dV \\
&= \int_\Omega 2\Delta_{ij}\big[2\partial_i\delta n_j - 2\delta n_i\, n_k\partial_k n_j - 2n_i\delta n_k\partial_k n_j - 2n_i n_k\partial_k\delta n_j \\
&\qquad + \delta n_i n_j\partial_k n_k + n_i\delta n_j\partial_k n_k + n_i n_j\partial_k\delta n_k\big]\,dV \\
&= \int_\Omega 2\big[-2\Delta_{ij}\delta n_i\, n_k\partial_k n_j - 2\Delta_{ij}n_i\delta n_k\partial_k n_j + \Delta_{ij}\delta n_i n_j\partial_k n_k + \Delta_{ij}n_i\delta n_j\partial_k n_k \\
&\qquad 2\Delta_{ij}\partial_i\delta n_j - 2\Delta_{ij}n_i n_k\partial_k\delta n_j + \Delta_{ij}n_i n_j\partial_k\delta n_k\big]\,dV \\
&= \int_\Omega 2\big[-2\Delta_{kj}n_i\partial_i n_j - 2\Delta_{ij}n_i\partial_k n_j + \Delta_{kj}n_j\partial_i n_i + \Delta_{ik}n_i\partial_j n_j\big]\delta n_k\,dV \\
&\qquad + \int_\Omega 2\big[-2\partial_i\Delta_{ik} + 2\partial_j\left(\Delta_{ik}n_i n_j\right) - \partial_k\left(\Delta_{ij}n_i n_j\right)\big]\delta n_k\,dV \\
&\qquad + \int_{\partial\Omega} 2\big[2\Delta_{ij}\nu_i\delta n_j - 2\Delta_{ij}n_i n_k\nu_k\delta n_j + \Delta_{ij}n_i n_j\nu_k\delta n_k\big]\,dV
\end{aligned} \tag{20}$$

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:

$$\begin{aligned}
0 = &-\left(K_{11} - K_{24}\right)\nabla S \\
&+ 2\left(K_{22} - K_{24}\right)T\left(\nabla\times\hat{\mathbf{n}}\right) \\
&+ K_{33}\left[\nabla\times\left(\mathbf{B}\times\hat{\mathbf{n}}\right) + \left(\nabla\times\hat{\mathbf{n}}\right)\times\mathbf{B}\right] \\
&+ 4K_{24}\big[\Delta\cdot\hat{\mathbf{n}}\left(\nabla\cdot\hat{\mathbf{n}}\right) - \left(\hat{\mathbf{n}}\cdot\nabla\hat{\mathbf{n}}\right)\cdot\Delta - \left(\nabla\hat{\mathbf{n}}\right)\cdot\Delta\cdot\hat{\mathbf{n}} \\
&\quad - \nabla\cdot\Delta + \nabla\cdot\left(\hat{\mathbf{n}}\otimes\left(\hat{\mathbf{n}}\cdot\Delta\right)\right) - \tfrac{1}{2}\nabla\left(\hat{\mathbf{n}}\cdot\Delta\cdot\hat{\mathbf{n}}\right)\big]
\end{aligned} \tag{21}$$

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

$$\hat{\mathbf{n}}' = R(\alpha z)\begin{bmatrix}\cos\big(\theta(x', y')\big) \\ \sin\big(\theta(x', y')\big) \\ 0\end{bmatrix} \tag{22}$$

with

$$\begin{aligned}
x' &= \cos(\alpha z)x + \sin(\alpha z)y \\
y' &= -\sin(\alpha z)x + \cos(\alpha z)y
\end{aligned} \tag{23}$$

If we plug into eq. (21) 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 Simplified free energy

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:

$$\zeta = \frac{K - K_{22}}{K + K_{22}} \tag{24}$$

This gives:

$$K_{22} = K\,\frac{1-\zeta}{1+\zeta} \tag{25}$$

Then the simplified Euler-Lagrange equation is:

$$0 = -(1+\zeta)\nabla S + 2(1-\zeta)T\ \left(\nabla\times\hat{\mathbf{n}}\right) + (1+\zeta)\left[\nabla\times\left(\mathbf{B}\times\hat{\mathbf{n}}\right) + \left(\nabla\times\hat{\mathbf{n}}\right)\times\mathbf{B}\right] \tag{26}$$

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]

$$\begin{aligned} A \cdot (\nabla \times B) &= A_i \epsilon_{ijk} \partial_j B_k \\ &= \epsilon_{ijk} \left(\partial_j (A_i B_k) - B_k \partial_j A_i \right) \\ &= -\partial_j \left(\epsilon_{jik} A_i B_k \right) + B_k \epsilon_{kji} \partial_j A_i \\ &= -\nabla \cdot (A \times B) + B \cdot (\nabla \times A) \end{aligned} \tag{27}$$