Disclination motion in the presence of a dipole

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1 Two dimensional free energy

The Q-tensor elastic free energy reads:

$$F_{\mathrm{el}} = L_1 \left(\partial_k Q_{ij}\right)^2 + L_2 \left(\partial_j Q_{ij}\right)^2 + L_3 Q_{lk} \left(\partial_l Q_{ij}\right)\left(\partial_k Q_{ij}\right) \tag{1}$$

The two-dimensional Q-tensor takes the form:

$$Q = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{12} & -Q_{11} \end{bmatrix} \tag{2}$$

Given that there are two free components, one may define a phase field ψ:

$$\psi = Q_{11} + iQ_{12} = Se^{i2\theta} \tag{3}$$

with S the scalar order parameter and θ the director angle as measured from the x-axis. Additionally, we may define a complex derivative:

$$\partial_z = \frac{1}{2}\left(\partial_x - i\partial_y\right) \tag{4}$$

and $\partial_{\overline{z}}$ its complex conjugate. Substituting into the free energy explicitly gives:

$$F_{\mathrm{el}} = 2L_1 \left|\nabla\psi\right|^2 + 4L_2 \left|\partial_z\psi\right|^2 + 4L_3 \left[\psi\left(\partial_z\psi\right)\left(\partial_z\overline{\psi}\right) + \overline{\psi}\left(\partial_{\overline{z}}\overline{\psi}\right)\left(\partial_{\overline{z}}\psi\right)\right] \tag{5}$$

with $\overline{\psi}$ the complex conjugate of the phase field, $\left|\nabla\psi\right|^2 = \partial_x\psi\partial_x\overline{\psi} + \partial_y\psi\partial_y\overline{\psi}$, and $\left|\cdot\right|^2$ the complex square. Taking the variation of this free energy gives the elastic contribution to the free energy:

$$-\frac{\delta F_{\mathrm{el}}}{\delta\overline{\psi}} = \left(8L_1 + 4L_2\right)\partial_z\partial_{\overline{z}}\psi + 4L_3\left[\overline{\psi}\left(\partial_{\overline{z}}^2\psi\right) + \psi\left(\partial_z^2\psi\right) + \left(\partial_z\psi\right)^2\right] \tag{6}$$

Nondimensionalizing in the same way as the Q-tensor gives:

$$-\frac{\delta F_{\mathrm{el}}}{\delta\overline{\psi}} = \left(4 + 2L_2\right)\partial_z\partial_{\overline{z}}\psi + 2L_3\left[\overline{\psi}\left(\partial_{\overline{z}}^2\psi\right) + \psi\left(\partial_z^2\psi\right) + \left(\partial_z\psi\right)^2\right] \tag{7}$$

2 Two dimensional equation of motion

The two-dimensional equation of motion reads:

$$\begin{aligned}\frac{\partial Q}{\partial t} = \kappa \mathbf{Q} - \mathbf{\Lambda} + \nabla^2 \mathbf{Q} \\ + \frac{L_2}{2}\left(\nabla\left(\nabla\cdot\mathbf{Q}\right) + \left[\nabla\left(\nabla\cdot\mathbf{Q}\right)\right]^T - \left(\nabla\cdot\left(\nabla\cdot\mathbf{Q}\right)\right)\mathbf{I}\right) \\ + \frac{L_3}{2}\left(2\nabla\cdot\left(\mathbf{Q}\cdot\nabla\mathbf{Q}\right) - \left(\nabla\mathbf{Q}\right):\left(\nabla\mathbf{Q}\right)^T + \tfrac{1}{2}\left|\nabla\mathbf{Q}\right|^2\mathbf{I}\right)\end{aligned} \tag{8}$$

Of course, we are only interested in the elastic portion. Explicitly substituting the $2D$ Q-tensor gives as above.

3 Disclination current

The disclination current is given by:

$$J = \partial_t \overline{\psi} \partial_{\overline{z}} \psi - \partial_t \psi \partial_{\overline{z}} \overline{\psi} \tag{9}$$

and the disclination velocity is just this quantity evaluated at the disclination center. We parameterize a test configuration of charge q which is embedded in nematic orientation field $\theta(z, \overline{z})$ near the disclination center as follows:

$$\psi = |z| \left(\frac{z}{\overline{z}}\right)^q e^{i2\theta} \tag{10}$$

We have assumed that the scalar order parameter decays linearly to zero at the core, that the test disclination director profile is as in the isotropic case (i.e. $q\varphi$) and that the director profile of the disclination superposes with the ambient orientation field. This is clearly a rough calculation, but the intention is to show that the change in the far-field disclination dipole due to anisotropy affects disclination motion in a measurable way.

Given that ψ evaluated at the core is zero, we consider terms in the equation of motion which only include gradients in ψ. The resulting current is explicitly given by:

$$\begin{aligned}J = \left(4 + 2L_2\right)\left[\left(\partial_z \partial_{\overline{z}} \overline{\psi}\right)\partial_{\overline{z}}\psi - \left(\partial_z \partial_{\overline{z}} \psi\right)\partial_{\overline{z}}\overline{\psi}\right] \\ + 2L_3\left[\left(\partial_{\overline{z}}\overline{\psi}\right)^2 \partial_{\overline{z}}\psi - \left(\partial_z \psi\right)^2 \partial_{\overline{z}}\overline{\psi}\right]\end{aligned} \tag{11}$$

For $q = +1/2$, Eq. (10) reduces to:

$$z e^{2i\theta} \tag{12}$$

Then we get:

$$J(z=0) = -i\left(8 + 4L_2\right)\partial_{\overline{z}}\theta - 2L_3 e^{i2\theta} \tag{13}$$

This may be written:

$$J(z=0) = \left(4 + 2L_2\right)\nabla^{\perp}\theta - 2L_3\left[\cos(2\theta)\hat{\mathbf{x}} + \sin(2\theta)\hat{\mathbf{y}}\right] \tag{14}$$

with $\nabla^{\perp} = \partial_y \hat{\mathbf{x}} - \partial_x \hat{\mathbf{y}}$. In polar coordinates it reads: $\nabla^{\perp}\theta = \frac{1}{r}\frac{\partial\theta}{\partial\varphi}\hat{\mathbf{r}} - \frac{\partial\theta}{\partial r}\hat{\boldsymbol{\varphi}}$.

For $q = -1/2$, Eq. (10) reduces to:

$$\overline{z}e^{2i\theta} \tag{15}$$

The result is:

$$J(z=0) = (4 + 2L_2)\,\nabla^{\perp}\theta \tag{16}$$