Far-field 3φ behavior

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1 Frank free energy in director angle

Frank free energy in two dimensions is given by:

$$F_n(\mathbf{n}, \nabla \mathbf{n}) = \int_\Omega \left[(1 - \epsilon) \left(\nabla \cdot \mathbf{n} \right)^2 + (1 + \epsilon) \left| \mathbf{n} \times \left(\nabla \times \mathbf{n} \right) \right|^2 \right] dV \tag{1}$$

with $\mathbf{n} = (\cos\theta, \sin\theta)$ and $\epsilon = (K_3 - K_1)/(K_3 + K_1)$. The splay term gives:

$$\begin{aligned} S &= \nabla \cdot \mathbf{n} \\ &= \partial_x \cos\theta + \partial_y \sin\theta \\ &= -\theta_x \sin\theta + \theta_y \cos\theta \end{aligned} \tag{2}$$

so that

$$S^2 = \theta_x^2 \sin^2\theta + \theta_y^2 \cos^2\theta - 2\theta_x\theta_y \cos\theta \sin\theta \tag{3}$$

For the bend term, we note:

$$\left(\nabla \times \mathbf{n} \right)_z = \theta_x \cos\theta + \theta_y \sin\theta \tag{4}$$

Then bend term itself gives:

$$\mathbf{B} = \sin\theta \left[\theta_x \cos\theta + \theta_y \sin\theta \right] \hat{\mathbf{i}} - \cos\theta \left[\theta_x \cos\theta + \theta_y \sin\theta \right] \hat{\mathbf{j}} \tag{5}$$

so that:

$$\left| \mathbf{B} \right|^2 = \theta_x^2 \cos^2\theta + \theta_y^2 \sin^2\theta + 2\theta_x\theta_y \cos\theta \sin\theta \tag{6}$$

Then we may rewrite the energy as follows:

$$F_n(\theta, \nabla\theta) = \int_\Omega \left[\left| \nabla\theta \right|^2 + \epsilon \left(\underbrace{-\theta_x^2 \sin^2\theta - \theta_y^2 \cos^2\theta + 2\theta_x\theta_y \cos\theta \sin\theta}_{\text{splay}} + \underbrace{\theta_x^2 \cos^2\theta + \theta_y^2 \sin^2\theta + 2\theta_x\theta_y \cos\theta \sin\theta}_{\text{bend}} \right) \right] \tag{7}$$

where the anisotropic terms are appropriately labeled.

2 Euler-Lagrange

For this, we consider each term separately:

$$\delta(\theta_x^2 \sin^2\theta) = 2\theta_x \sin^2\theta \left(\delta\theta \right)_x + 2\theta_x^2 \sin\theta \cos\theta \delta\theta \tag{8}$$

Then the corresponding term in the Euler-Lagrange equation is:

$$-2\theta_{xx} \sin^2\theta - \theta_x^2 \sin 2\theta \tag{9}$$

Similarly:

$$\delta(\theta_x^2 \cos^2\theta) = 2\theta_x \cos^2\theta\,(\delta\theta)_x - 2\theta_x^2 \cos\theta \sin\theta\delta\theta \tag{10}$$

so that the corresponding term in the Euler-Lagrange equation is:

$$-2\theta_{xx}\cos^2\theta + \theta_x^2 \sin 2\theta \tag{11}$$

Finally, we have:

$$\delta\left(2\theta_x\theta_y\cos\theta\sin\theta\right) = 2\theta_y\cos\theta\sin\theta\,(\delta\theta)_x + 2\theta_x\cos\theta\sin\theta\,(\delta\theta)_y - 2\theta_x\theta_y\sin^2\theta\delta\theta + 2\theta_x\theta_y\cos^2\theta\delta\theta \tag{12}$$

So that the corresponding Euler-Lagrange term is:

$$-2\theta_{xy}\sin 2\theta - 2\theta_y\theta_x\cos 2\theta \tag{13}$$

Given these, the Euler-Lagrange equation reads:

$$\begin{aligned}\nabla^2\theta = \epsilon\big[&\theta_{xx}\sin^2\theta + \theta_{yy}\cos^2\theta + \tfrac{1}{2}\left(\theta_x^2 - \theta_y^2\right)\sin 2\theta - \theta_{xy}\sin 2\theta - \theta_x\theta_y\cos 2\theta \\ &- \theta_{xx}\cos^2\theta - \theta_{yy}\sin^2\theta + \tfrac{1}{2}\left(\theta_x^2 - \theta_y^2\right)\sin 2\theta - \theta_{xy}\sin 2\theta - \theta_x\theta_y\cos 2\theta\big]\end{aligned} \tag{14}$$

with the first line corresponding to splay terms, and the second line bend terms.

3 Far-field behavior

The isotropic solution expands as follows:

$$\begin{aligned}\theta_{\text{iso}} &= q_1 \arctan\left(\frac{\sin\varphi}{\cos\varphi + \frac{1}{2}\frac{d}{r}}\right) + q_2 \arctan\left(\frac{\sin\varphi}{\cos\varphi - \frac{1}{2}\frac{d}{r}}\right) + \frac{\pi}{2} \\ &= -\frac{d(q_1 - q_2)}{2r}\sin\varphi + q_1\varphi + q_2\varphi + \frac{\pi}{2} + \mathcal{O}\left(\left(\frac{d}{r}\right)^2\right)\end{aligned} \tag{15}$$

Then, with $\frac{1}{2} = q_1 = -q_2$ we get that:

$$\theta_{\text{iso}} \approx -\frac{d}{2r}\sin\varphi + \frac{\pi}{2} \tag{16}$$

To get the Poisson equation in θ_c, we plug in θ_{iso} to the right-hand side of Eq. (14). Then, in the far-field limit, the rhs which are $\mathcal{O}(\theta^2)$ will drop out. This includes all terms with a factor of $\sin\theta$ or $\sin 2\theta$. Further, $\cos\theta \approx -1$ (where the sign is due to the $\pi/2$ term) so that the final Poisson equation reads:

$$\nabla^2\theta = \epsilon\left[-\theta_{yy} + \theta_{xx}\right] \tag{17}$$

The first term corresponds to splay, while the second term corresponds to bend. Calculated explicitly for the far-field θ_{iso} case, one gets:

$$\theta_{yy} = \frac{d\sin 3\varphi}{r^3} \tag{18}$$

$$\theta_{xx} = -\frac{d\sin 3\varphi}{r^3} \tag{19}$$

The right-hand side is exactly what we get in Eq. (27) in the manuscript.

4 Single disclination offset

To understand how the disclinations screen, consider the isotropic solution for a single disclination, but offset from the domain center by a distance $\pm d/r$. This reads:

$$\theta_{\text{iso, }1} = q \arctan\left(\frac{\sin\varphi}{\cos\varphi \pm \frac{1}{2}\frac{d}{r}}\right) \tag{20}$$

The expansion in d/r then reads:

$$\theta_{\text{iso, }1} = q\varphi \mp \frac{qd}{2r}\sin\varphi + \mathcal{O}\left(\left(\frac{d}{r}\right)^2\right) \tag{21}$$

If one plugs into the right-hand side of Eq. (14) and expands about d/r, then the result is as follows:

$$\nabla^2\theta_c = \epsilon\, f^q_{\text{DZ}}(\varphi) + \epsilon\, f^q_{\text{offset}}\left(\varphi, \frac{d}{r}\right) \tag{22}$$

Here f^q_{DZ} is the right-hand side of Eq. (14) with $q\varphi$ substituted for θ, while f^q_{offset} is the same, except with the first order term in Eq. (21) substituted for θ. If we were to solve with only $f^q_{\text{DZ}}(\varphi)$ for the right-hand side, then we would get the Dzyaloshinskii solution for charge q expanded to first order in ϵ. Additionally, the first order term of Eq. (21) is $(\pm)$ half the first order expansion of θ_{iso}.

This gives us some insight into where the 3φ behavior comes from. While the sum $f^{1/2}_{\text{DZ}} + f^{-1/2}_{\text{DZ}}$ does not cancel due to the nonlinear nature of the rhs of the Euler-Lagrange equation, it is true that $\frac{1}{2}\varphi - \frac{1}{2}\varphi = 0$. Hence, the fact that the isolated $1/2$ disclination goes as $\sin(\varphi)$ and the isolated $-1/2$ disclination goes as $\sin(3\varphi)$ is completely unrelated to the dipole far-field going as $\sin(3\varphi)$. Instead, we can understand this behavior as an equal contribution from either disclination, resulting from the fact that they are offset from the domain center in either direction.

5 Rewrite of bend term

Note that in two dimensions:

$$\mathbf{n}\cdot\nabla\mathbf{n} = (\theta_x\cos\theta + \theta_y\sin\theta)\left(-\sin\theta\hat{\mathbf{i}} + \cos\theta\hat{\mathbf{j}}\right) \tag{23}$$

so that:

$$|\mathbf{n}\cdot\nabla\mathbf{n}|^2 = \theta_x^2\cos^2\theta + \theta_y^2\sin^2\theta + 2\theta_x\theta_y\cos\theta\sin\theta \tag{24}$$

Hence, equivalent to the bend term.