Dzyaloshinskii offset explanation

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The differential equation governing an isolated disclination in $2D$ under bend-splay anisotropy is:

$$\frac{d^2\theta}{d\varphi^2} = \epsilon \left[\frac{d^2\theta}{d\varphi^2} \cos 2(\theta - \varphi) + \left(2\frac{d\theta}{d\varphi} - \left(\frac{d\theta}{d\varphi} \right)^2 \right) \sin 2(\theta - \varphi) \right] \tag{1}$$

with θ the director angle, φ the polar angle (as measured from the domain center), and ϵ the anisotropy parameter. Take $\theta_{\text{DZ}}(\varphi)$ to be the solution whose boundary condition gives a $+1/2$ disclination. Then consider the corresponding director configuration $\hat{\mathbf{n}}_{\text{DZ}} = (\cos\theta_{\text{DZ}}, \sin\theta_{\text{DZ}}, 0)$, and the corresponding Q-tensor configuration:

$$Q_{\text{DZ}} = S_0 \left(\hat{\mathbf{n}}_{\text{DZ}} \otimes \hat{\mathbf{n}}_{\text{DZ}} - I \right) \tag{2}$$

Here S_0 is the equilibrium value of the scalar order parameter for a uniaxial, uniform nematic configuration. If we initialize our system to this configuration in a circular domain of radius $20/\sqrt{2}$ and fix the boundary (i.e. impose Eq. (2) as a Dirichlet condition) then the disclination center[1] moves slightly to the right. Call this equilibrated configuration Q_{eq}, call the equilibrated disclination center $(x_{\text{eq}}, 0)$, and call (r', φ') the polar coordinates centered at $(x_{\text{eq}}, 0)$. Explicitly:

$$\varphi' = \text{atan2}(y, x - x_{\text{eq}}) \tag{3}$$

$$r' = \sqrt{(x - x_{\text{eq}})^2 + y^2} \tag{4}$$

We can schematically understand Q_{eq} with Fig. 1.

As the configuration relaxes, the yellow region remains unchanged from the initial configuration Q_{DZ} while the white region updates. The result of the white region updating is to move the disclination core to the red dot. As a representative example, we plot the director angle (calculated from Q_{eq}) as a function of φ' at several radii r' in Fig. 2.

The $r' = 10.0$ curve lies wholly in the unchanged region – we should compare to the initial Q_{DZ} configuration. To calculate the director angle from Q_{DZ} as a function of φ' along the $r' = 10.0$ curve, we must make a change of variables. Note that:

$$x = r' \cos\varphi' + x_{\text{eq}} \tag{5}$$

$$y = r' \sin\varphi' \tag{6}$$

so that:

$$\varphi = \text{atan2}(r' \sin\varphi', r' \cos\varphi' + x_{\text{eq}}) \tag{7}$$

Then the blue curve on our plot is given by:

$$\theta_{\text{DZ}}(\text{atan2}(r' \sin\varphi', r' \cos\varphi' + x_{\text{eq}})) \tag{8}$$

This matches with the red dotted curve, which indicates good agreement between Q_{DZ} and Q_{eq} in the yellow region.

[1] the point where $S = P$

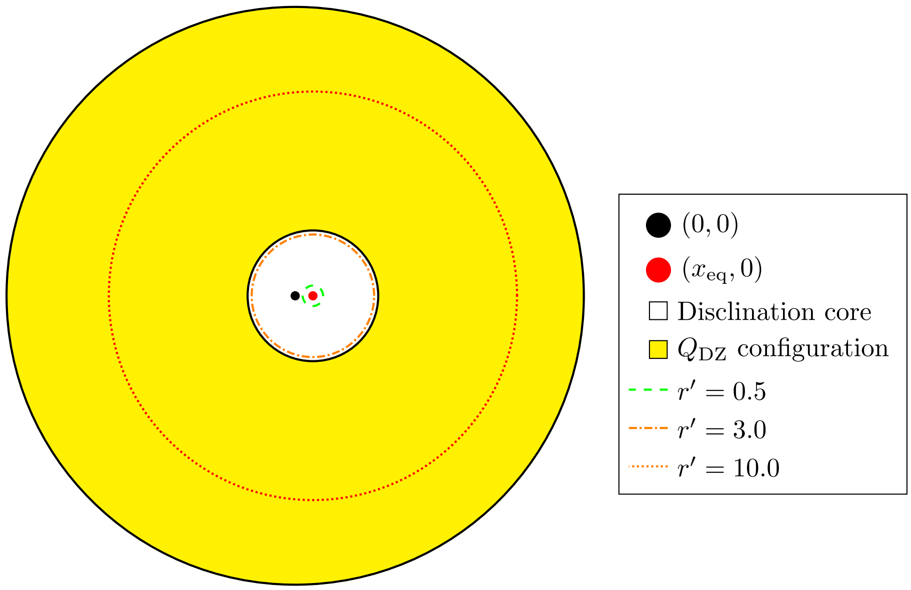

Figure 1

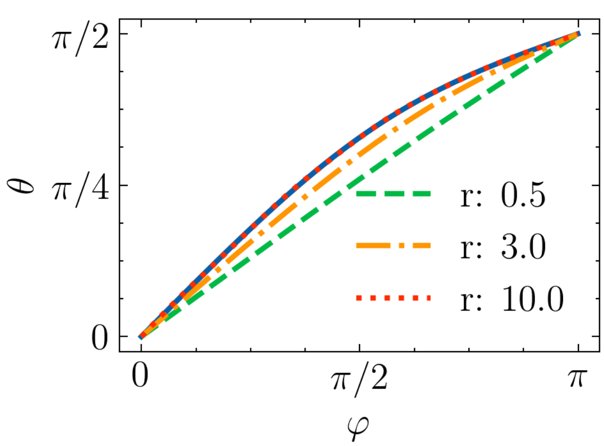

Figure 2