Observing anisotropic defect core structure

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1 Computing single-defect core structure

To understand the defect core structure, we run a relaxation simulation for some anisortopy. For a uniaxial system, we may relate the Landau-de Gennes L_i parameters to the Frank-Oseen K_i parameters. This is given by:

$$K_{11} = 2L_1S^2 + L_2S^2 - \tfrac{2}{3}L_3S^3 \tag{1}$$
$$K_{22} = 2L_1S^2 - \tfrac{2}{3}L_3S^3 \tag{2}$$
$$K_{33} = 2L_1S^2 + L_2S^2 + \tfrac{4}{3}L_3S^3 \tag{3}$$

The splay-bend anisotropy parameter ϵ is given by:

$$\epsilon = \frac{K_{33} - K_{11}}{K_{33} + K_{11}} \tag{4}$$

Or, in terms of nondimensional Landau-de Gennes coefficients (that is, taking $L_i \to L_i/L_1$) we get:

$$\epsilon = \frac{L_3S}{2 + L_2 + \frac{1}{3}L_3S} \tag{5}$$