Linearizing Frank free energy minimization for two defects

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1 Deriving linearized Frank free energy minimization

We begin with the Euler-Lagrange equation for the Frank free energy in Cartesian coordinates:

$$\nabla^2\theta - \epsilon\left[\sin 2\theta\left(\theta_x^2 - \theta_y^2 - 2\theta_{xy}\right) + \cos 2\theta\left(\theta_{yy} - \theta_{xx} - 2\theta_x\theta_y\right)\right] = 0 \tag{1}$$

To do the perturbative expansion, rewrite as:

$$\nabla^2\theta = \epsilon f(\theta)$$

Expand θ as a singular part which is the solution to the isotropic problem, and a perturbative solution of the anisotropic equation:

$$\theta = \theta_{\text{iso}} + \epsilon\theta_c + \mathcal{O}(\epsilon^2)$$

Plugging in up to order ϵ yields:

$$\nabla^2\theta_{\text{iso}} + \epsilon\nabla^2\theta_c + \mathcal{O}(\epsilon^2) = \epsilon\left[f(\theta_{\text{iso}}) + f'(\theta_{\text{iso}})\epsilon\theta_c + \mathcal{O}(\epsilon^2)\right]$$

By definition, $\nabla^2\theta_{\text{iso}} = 0$ so we only have to calculate $f(\theta_{\text{iso}})$. The specific form for isomorph (a) is given by:

$$\theta_{\text{iso}} = q_1\varphi_1 + q_2\varphi_2 + \frac{\pi}{2} \tag{2}$$

where φ_1 and φ_2 are the polar angles relative to origins at the corresponding defect points (x_1, y_1) and (x_2, y_2). Note that in polar coordinates we have:

$$\begin{aligned}\frac{d}{dx} &= \cos\varphi\frac{\partial}{\partial r} - \frac{1}{r}\sin\varphi\frac{\partial}{\partial\varphi}\\ \frac{d}{dy} &= \sin\varphi\frac{\partial}{\partial r} + \frac{1}{r}\cos\varphi\frac{\partial}{\partial\varphi}\end{aligned} \tag{3}$$

The differential operators d/dx and d/dy are indifferent to a change in origin, so to evaluate $d\varphi_1/dx$ it suffices to calculate the quantity in Cartesian coordinates centered at defect 1. This is, of course, true for all the other polar differentials, so we get:

$$\begin{aligned}\frac{d\varphi}{dx} &= -\frac{1}{r}\sin\varphi\\ \frac{d\varphi}{dy} &= \frac{1}{r}\cos\varphi\end{aligned} \tag{4}$$

Calculating the rest of the differentials yields:

$$\begin{aligned}\frac{d^2\varphi}{dx^2} &= 2\frac{1}{r^2}\cos\varphi\sin\varphi = \frac{1}{r^2}\sin 2\varphi\\ \frac{d^2\varphi}{dy^2} &= -2\frac{1}{r^2}\sin\varphi\cos\varphi = -\frac{1}{r^2}\sin 2\varphi\\ \frac{d^2\varphi}{dx\,dy} &= \frac{1}{r^2}\left(\sin^2\varphi - \cos^2\varphi\right) = -\frac{1}{r^2}\cos 2\varphi\end{aligned} \tag{5}$$

Calculating the squared differential terms yields:

$$
\begin{aligned}
\left(\frac{d\theta_{\text{iso}}}{dx}\right)^2 &= q_1^2\left(\frac{d\varphi_1}{dx}\right)^2 + q_2^2\left(\frac{d\varphi_2}{dx}\right)^2 + 2q_1q_2\frac{d\varphi_1}{dx}\frac{d\varphi_2}{dx} \\
&= \frac{q_1^2}{r_1^2}\sin^2\varphi_1 + \frac{q_2^2}{r_2^2}\sin^2\varphi_2 + 2\frac{q_1q_2}{r_1r_2}\sin\varphi_1\sin\varphi_2 \\
\left(\frac{d\theta_{\text{iso}}}{dy}\right)^2 &= \frac{q_1^2}{r_1^2}\cos^2\varphi_1 + \frac{q_2^2}{r_2^2}\cos^2\varphi_2 + 2\frac{q_1q_2}{r_1r_2}\cos\varphi_1\cos\varphi_2 \\
\frac{d\theta_{\text{iso}}}{dx}\frac{d\theta_{\text{iso}}}{dy} &= q_1^2\frac{d\varphi_1}{dx}\frac{d\varphi_1}{dy} + q_2^2\frac{d\varphi_2}{dx}\frac{d\varphi_2}{dy} + q_1q_2\frac{d\varphi_1}{dx}\frac{d\varphi_2}{dy} + q_1q_2\frac{d\varphi_2}{dx}\frac{d\varphi_1}{dy} \\
&= -\frac{q_1^2}{r_1^2}\sin\varphi_1\cos\varphi_1 - \frac{q_2^2}{r_2^2}\sin\varphi_2\cos\varphi_2 - \frac{q_1q_2}{r_1r_2}\left(\sin\varphi_1\cos\varphi_2 + \sin\varphi_2\cos\varphi_1\right) \\
&= -\frac{q_1^2}{2r_1^2}\sin 2\varphi_1 - \frac{q_2^2}{2r_2^2}\sin 2\varphi_2 - \frac{q_1q_2}{r_1r_2}\sin\left(\varphi_1+\varphi_2\right)
\end{aligned} \tag{6}
$$

Using (5) and (6) we may simplify the factors in (1):

$$
\begin{aligned}
\theta_{\text{iso},x}^2 - \theta_{\text{iso},y}^2 - 2\theta_{\text{iso},xy} = &\frac{q_1^2}{r_1^2}\sin^2\varphi_1 + \frac{q_2^2}{r_2^2}\sin^2\varphi_2 + 2\frac{q_1q_2}{r_1r_2}\sin\varphi_1\sin\varphi_2 \\
&- \frac{q_1^2}{r_1^2}\cos^2\varphi_1 - \frac{q_2^2}{r_2^2}\cos^2\varphi_2 - 2\frac{q_1q_2}{r_1r_2}\cos\varphi_1\cos\varphi_2 \\
&+ 2\frac{q_1}{r_1^2}\cos 2\varphi_1 + 2\frac{q_2}{r_2^2}\sin 2\varphi_2 \\
= &- \frac{q_1^2}{r_1^2}\cos 2\varphi_1 - \frac{q_2^2}{r_2^2}\cos 2\varphi_2 - 2\frac{q_1q_2}{r_1r_2}\cos\left(\varphi_1+\varphi_2\right) \\
&+ 2\frac{q_1}{r_1^2}\cos 2\varphi_1 + 2\frac{q_2}{r_2^2}\sin 2\varphi_2 \\
= &\frac{q_1\left(2-q_1\right)}{r_1^2}\cos 2\varphi_1 + \frac{q_2\left(2-q_2\right)}{r_2^2}\cos 2\varphi_2 - 2\frac{q_1q_2}{r_1r_2}\cos\left(\varphi_1+\varphi_2\right)
\end{aligned} \tag{7}
$$

Additionally we can rewrite:

$$
\begin{aligned}
\theta_{\text{iso},yy} - \theta_{\text{iso},xx} - 2\theta_{\text{iso},x}\theta_{\text{iso},y} = &- \frac{q_1}{r_1^2}\sin 2\varphi_1 - \frac{q_2}{r_2^2}\sin 2\varphi_2 - \frac{q_1}{r_1^2}\sin 2\varphi_1 - \frac{q_2}{r_2^2}\sin 2\varphi_2 \\
&+ \frac{q_1^2}{r_1^2}\sin 2\varphi_1 + \frac{q_2^2}{r_2^2}\sin 2\varphi_2 + 2\frac{q_1q_2}{r_1r_2}\sin\left(\varphi_1+\varphi_2\right) \\
= &-\frac{q_1\left(2-q_1\right)}{r_1^2}\sin 2\varphi_1 - \frac{q_2\left(2-q_2\right)}{r_2^2}\sin 2\varphi_1 + 2\frac{q_1q_2}{r_1r_2}\sin\left(\varphi_1+\varphi_2\right)
\end{aligned} \tag{8}
$$

Finally, consider the angle addition formula:

$$
\sin\alpha\cos\beta - \sin\beta\cos\alpha = \sin(\alpha-\beta) \tag{9}
$$

Then, plugging the results above into (1) we get:

$$
\begin{aligned}
\nabla^2\theta_c = &\sin 2\theta_{\text{iso}}\left(\frac{q_1\left(2-q_1\right)}{r_1^2}\cos 2\varphi_1 + \frac{q_2\left(2-q_2\right)}{r_2^2}\cos 2\varphi_2 - \frac{q_1q_2}{r_1r_2}\cos\left(\varphi_1+\varphi_2\right)\right) \\
&+ \cos 2\theta_{\text{iso}}\left(-\frac{q_1\left(2-q_1\right)}{r_1^2}\sin 2\varphi_1 - \frac{q_2\left(2-q_2\right)}{r_2^2}\sin 2\varphi_1 + 2\frac{q_1q_2}{r_1r_2}\sin\left(\varphi_1+\varphi_2\right)\right) \\
= &\frac{q_1\left(2-q_1\right)}{r_1^2}\sin(2\theta_{\text{iso}}-2\varphi_1) + \frac{q_2\left(2-q_2\right)}{r_2^2}\sin(2\theta_{\text{iso}}-2\varphi_2) - \frac{q_1q_2}{r_1r_2}\sin(2\theta_{\text{iso}}-\varphi_1-\varphi_2)
\end{aligned} \tag{10}
$$

Note that, because each of the calculated quantities are only differentials of θ_{iso}, eq. (10) is agnostic to which 2-defect isomorph one is considering. Plugging in $\theta_{\text{iso}} = q_1\varphi_1 + q_2\varphi_2 + \pi/2$ for isomorph (a) gives:

$$\begin{aligned}\nabla^2\theta_c = &\frac{q_1\,(2-q_1)}{r_1^2}\sin(2(1-q_1)\varphi_1 - 2q_2\varphi_2) \\ &+ \frac{q_2\,(2-q_1)}{r_2^2}\sin(2(1-q_2)\varphi_2 - 2q_1\varphi_1) \\ &- \frac{q_1 q_2}{r_1 r_2}\sin((1-2q_1)\varphi_1 + (1-2q_2)\varphi_2)\end{aligned} \tag{11}$$

Plugging in $\theta_{\text{iso}} = q_1\varphi_1 + q_2\varphi_2$ for isomorph (b) just gives a minus sign for the right-hand side.

2 Boundary condition

Given that $\theta = \theta_{\text{iso}} + \epsilon\theta_c$, a physically relevant boundary condition for θ means a nontrivial boundary condition for θ_c. To this point, we note that if F is the Frank free energy, then a minimizer of the energy satisfies:

$$\begin{aligned} 0 &= \frac{\delta F}{\delta\theta} \\ \implies 0 &= \frac{\partial f}{\partial\theta} - \nabla\cdot\frac{\partial f}{\partial(\nabla\theta)}\end{aligned} \tag{12}$$

where f is the Frank free energy density. We call $\partial f/\partial(\nabla\theta)$ the configurational force. This is the analogue of the thing we take to have zero normal component in the case of the Q-tensor energy. We may calculate each term of the Frank free energy density explicitly:

Splay:

$$\begin{aligned}\frac{\partial(\partial_k n_k)^2}{\partial(\partial_i\theta)} &= \frac{\partial}{\partial(\partial_i\theta)}\left[\tfrac{1}{2}(\nabla\theta)^2 + \tfrac{1}{2}\cos 2\theta\left((\partial_y\theta)^2 - (\partial_x\theta)^2\right) - \sin 2\theta(\partial_x\theta)(\partial_y\theta)\right] \\ &= \partial_i\theta + \cos 2\theta\,(\delta_{iy}\partial_y\theta - \delta_{ix}\partial_x\theta) - \sin 2\theta\,(\delta_{ix}\partial_y\theta + \delta_{iy}\partial_x\theta)\end{aligned} \tag{13}$$

Bend:

$$\begin{aligned}\frac{\partial(\partial_k\partial_k n_j)^2}{\partial(\partial_i\theta)} &= \frac{\partial}{\partial(\partial_i\theta)}\left[\tfrac{1}{2}(\nabla\theta)^2 + \tfrac{1}{2}\cos 2\theta\left((\partial_x\theta)^2 - (\partial_y\theta)^2\right) + \sin 2\theta(\partial_x\theta)(\partial_y\theta)\right] \\ &= \partial_i\theta - \cos 2\theta\,(\delta_{iy}\partial_y\theta - \delta_{ix}\partial_x\theta) + \sin 2\theta\,(\delta_{ix}\partial_y\theta + \delta_{iy}\partial_x\theta)\end{aligned} \tag{14}$$

Then altogether this reads:

$$\frac{\partial f}{\partial(\partial_i\theta)} = 2\partial_i\theta - 2\epsilon\cos 2\theta\,(\delta_{iy}\partial_y\theta - \delta_{ix}\partial_x\theta) + 2\epsilon\sin 2\theta\,(\delta_{ix}\partial_y\theta + \delta_{iy}\partial_x\theta) \tag{15}$$

Call the extra term of the configurational stress arising from anisotropy:

$$C_i(\theta) = -\cos 2\theta\,(\delta_{iy}\partial_y\theta - \delta_{ix}\partial_x\theta) + \sin 2\theta\,(\delta_{ix}\partial_y\theta + \delta_{iy}\partial_x\theta) \tag{16}$$

so that

$$\frac{\partial f}{\partial(\partial_i\theta)} = 2\partial_i\theta + \epsilon 2C_i(\theta) \tag{17}$$

We substitute the perturbative expansion and then truncate terms of order $\mathcal{O}(\epsilon^2)$ to get:

$$\frac{\partial f}{\partial(\partial_i\theta)} \approx 2\partial_i\theta_{\text{iso}} + 2\epsilon\partial_i\theta_c + 2\epsilon C_i(\theta_{\text{iso}}) \tag{18}$$

Solving for the normal component of $\nabla\theta_c$ given the constraint of zero configurational stress gives:

$$\mathbf{n} \cdot \nabla\theta_c = -\frac{1}{\epsilon}\mathbf{n} \cdot \nabla\theta_{\text{iso}} - C_i(\theta_{\text{iso}}) \tag{19}$$

Call this g. Then Laplace's equation weak form reads:

$$\begin{aligned} &\left\langle \phi, \nabla^2\theta_c \right\rangle = \langle \phi, f \rangle \\ \implies &\langle \phi, \mathbf{n} \cdot \nabla\theta_c \rangle_{\partial\Omega} - \langle \nabla\phi, \nabla\theta \rangle = \langle \phi, f \rangle \\ \implies &\langle \nabla\phi, \nabla\theta \rangle = -\langle \phi, f \rangle + \langle \phi, g \rangle_{\partial\Omega} \end{aligned} \tag{20}$$

Hence, we must just integrate (19) along the boundary. Writing out (19) explicitly yields:

$$\begin{aligned} g = n_x \frac{1}{\epsilon}\left(\frac{q_1 \sin\varphi_1}{r_1} + \frac{q_2 \sin\varphi_2}{r_2}\right) - n_y \frac{1}{\epsilon}\left(\frac{q_1 \cos\varphi_1}{r_1} + \frac{q_2 \cos\varphi_2}{r_2}\right) \\ - n_x \left(\frac{q_1}{r_1}\sin((2q_1 - 1)\varphi_1 + 2q_2\varphi_2) + \frac{q_2}{r_2}\sin((2q_2 - 1)\varphi_2 + 2q_1\varphi_1)\right) \\ + n_y \left(\frac{q_1}{r_1}\cos((2q_1 - 1)\varphi_1 + 2q_2\varphi_2) + \frac{q_2}{r_2}\cos((2q_2 - 1)\varphi_2 + 2q_1\varphi_2)\right) \end{aligned} \tag{21}$$