Linearizing Frank free energy minimization for two defects

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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):

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

Additionally we can rewrite:

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

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.