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An exterior problem for liquid crystals



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Oseen-Frank theory

Free energy $I(\mathbf{n}) = \int_{\Omega} W(\mathbf{n}, \nabla \mathbf{n}) d\mathbf{x},$

$$2W(\mathbf{n}, \nabla \mathbf{n}) = K_1(\operatorname{div} \mathbf{n})^2 + K_2(\mathbf{n} \cdot \operatorname{curl} \mathbf{n})^2 + K_3|\mathbf{n} \wedge \operatorname{curl} \mathbf{n}|^2 \\ + (K_2 + K_4)(\operatorname{tr}(\nabla \mathbf{n})^2 - (\operatorname{div} \mathbf{n})^2).$$

$\mathbf{n}(\mathbf{x}) \in S^2$ (unit sphere) is the *director*.

2D case: $\mathbf{n}(\mathbf{x}) = (n_1(x_1, x_2), n_2(x_1, x_2), 0)$

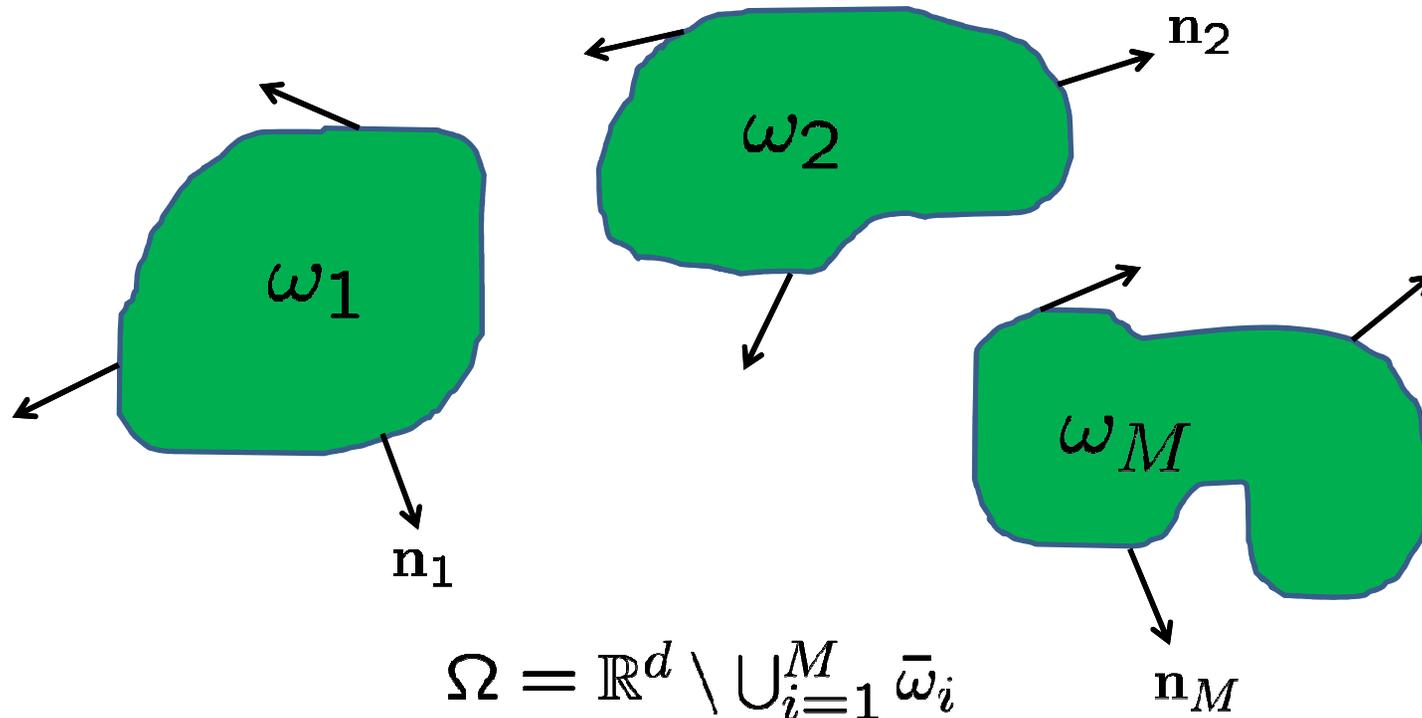
$$\operatorname{curl} \mathbf{n} = (0, 0, n_{2,1} - n_{1,2}), \quad \mathbf{n} \cdot \operatorname{curl} \mathbf{n} = 0$$

$$|\mathbf{n} \wedge \operatorname{curl} \mathbf{n}|^2 = |\operatorname{curl} \mathbf{n}|^2 = (n_{2,1} - n_{1,2})^2$$

$$\operatorname{tr}(\nabla \mathbf{n})^2 - (\operatorname{div} \mathbf{n})^2 = 0$$

Exterior problem for Oseen-Frank theory

$\omega_i \subset \mathbb{R}^d$ disjoint, bounded, open, with sufficiently smooth boundaries $\partial\omega_i$.



What can we say about equilibrium configurations \mathbf{n} in Ω satisfying the boundary conditions $\mathbf{n}|_{\partial\omega_i} = \mathbf{n}_i$, $i = 1, \dots, M$, in particular about their behaviour at ∞ ?

It would be nice to be able to handle the case $d = 3$ for general elastic constants and allow the ω_i to move. However we will assume that the ω_i are fixed, that $d = 2$, and that we are in the one-constant case

$$K_1 = K_2 = K_3 = 2, K_4 = 0.$$

Why is the one-constant $d = 2$ case so much simpler?

First, we can identify \mathbb{R}^2 with the complex plane \mathbb{C} , writing $z = x_1 + ix_2$ for $\mathbf{x} = (x_1, x_2)$, and identifying $\mathbf{n}(\mathbf{x})$ with

$$\tilde{\mathbf{n}}(z) = n_1(x_1, x_2) + in_2(x_1, x_2) = e^{i\Phi(\mathbf{x})}.$$

The Euler-Lagrange equation for the one-constant energy

$$I(\mathbf{n}) = \int_{\Omega} |\nabla \mathbf{n}|^2 dx,$$

$\mathbf{n} : \Omega \rightarrow S^2$, is the *harmonic map* equation

$$\Delta \mathbf{n} + |\nabla \mathbf{n}|^2 \mathbf{n} = \mathbf{0},$$

which is equivalent to

$$\Delta \tilde{\mathbf{n}} + |\nabla \mathbf{n}|^2 \tilde{\mathbf{n}} = ie^{i\Phi} \Delta \Phi = \mathbf{0},$$

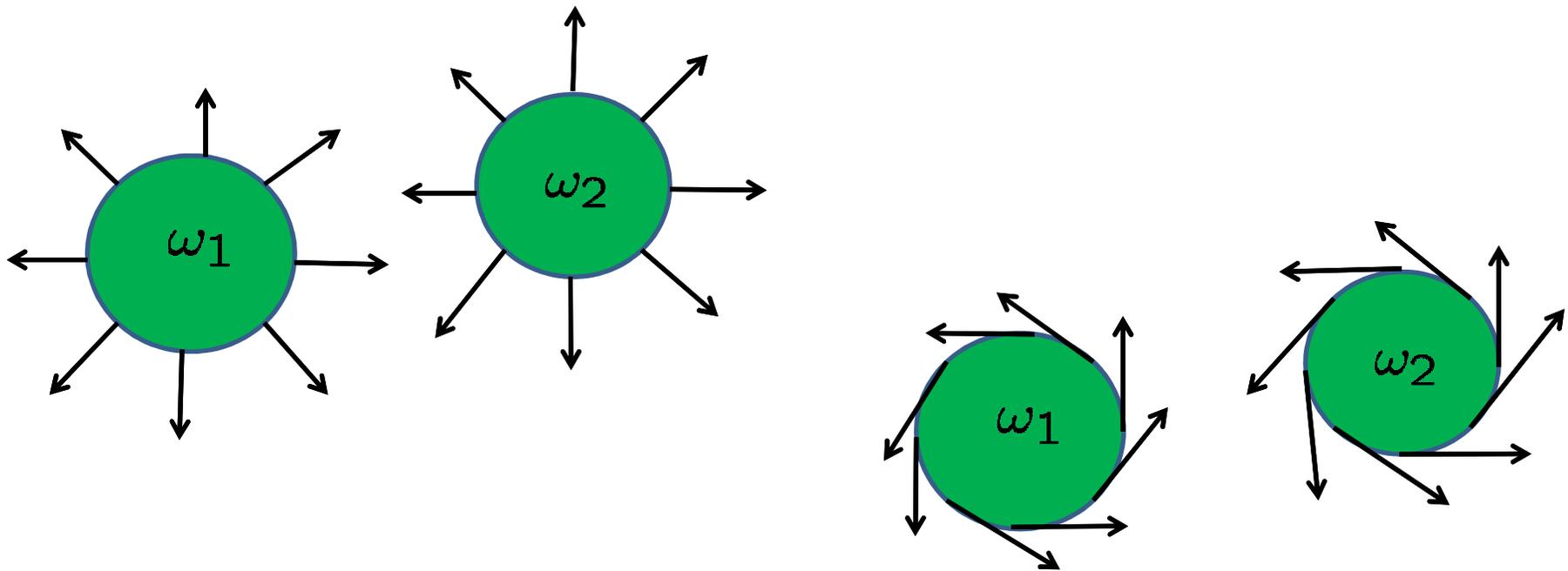
that is to the linear Laplace equation

$$\Delta \Phi = 0.$$

In particular, equilibrium solutions of locally finite energy are smooth (no defects).

Also, if $\tilde{n} = \tilde{n}(z)$, $\tilde{m} = \tilde{m}(z)$ are equilibrium solutions so is $\tilde{n}(z)\tilde{m}(z)$ as a product of complex numbers.

One interesting consequence is that any constant rotation, or rotation plus reflection, of an equilibrium is also an equilibrium.



In polar coordinates (r, θ) Laplace's equation $\Delta\Phi = 0$ becomes

$$\Phi_{ss} + \Phi_{\theta\theta} = 0,$$

where $s = \ln r$.

One solution is $\Phi = \theta$, giving the 2D hedgehog

$$e^{i\theta} = \frac{z}{|z|},$$

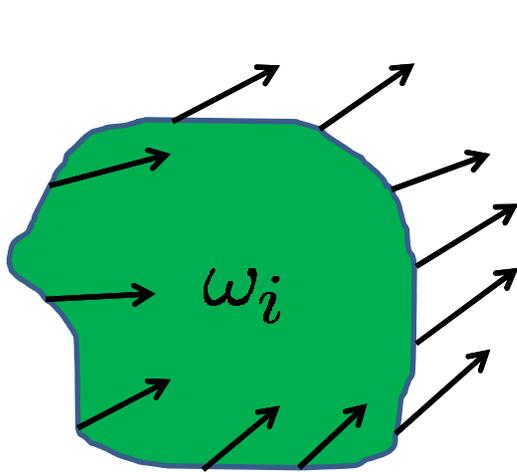
which has finite energy only for bounded domains not containing the origin.

Note that this solution, while solving Laplace's equation locally, is not a globally defined smooth solution due to the jump of 2π in θ as we circle the origin. How can this be remedied?

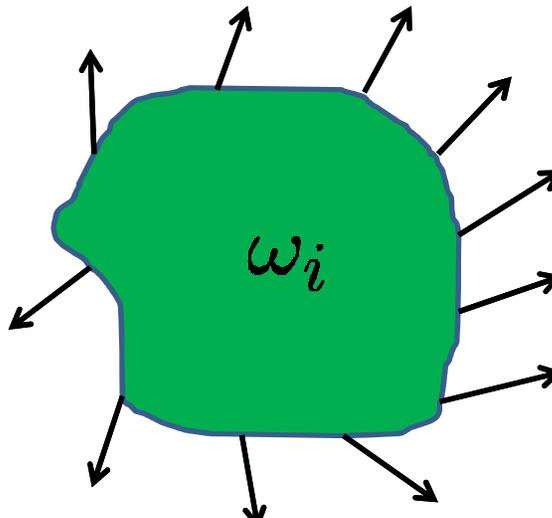
Definition of degree

If we smoothly parametrize $\partial\omega_i$ by $t \in [0, 2\pi)$, then can write $\mathbf{n}_i(t) = (\cos \Phi(t), \sin \Phi(t))$ with Φ smooth and define

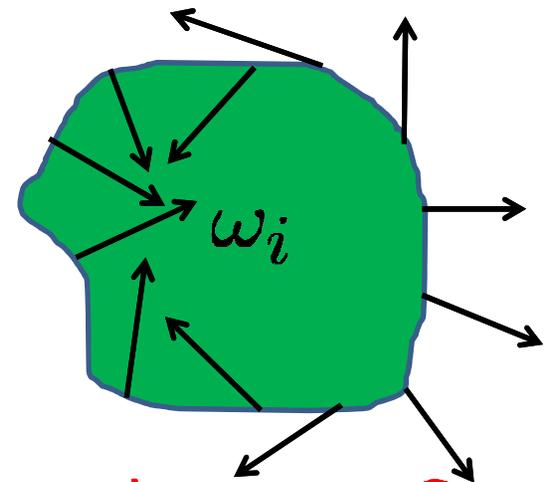
$$\begin{aligned} \deg \mathbf{n}_i &= \frac{1}{2\pi}(\Phi(2\pi) - \Phi(0)) \\ &= \frac{1}{2\pi} \int_0^{2\pi} \Phi'(t) dt. \end{aligned}$$



$\deg \mathbf{n}_i = 0$



$\deg \mathbf{n}_i = 1$



$\deg \mathbf{n}_i = 2$

Carbou's trick. Pick $\mathbf{a}_i \in \omega_i$, $i = 1, \dots, M$.

(For convenience we choose $\mathbf{a}_1 = \mathbf{0}$ to be the origin of polar coordinates.)

Let $d_i = \deg \mathbf{n}_i$. Then we can write any equilibrium solution $\tilde{\mathbf{n}}$ as

$$\tilde{\mathbf{n}}(z) = \left(\frac{z - \mathbf{a}_1}{|z - \mathbf{a}_1|} \right)^{d_1} \cdots \left(\frac{z - \mathbf{a}_M}{|z - \mathbf{a}_M|} \right)^{d_M} e^{i\varphi(z)},$$

where φ is a smooth solution of $\Delta\varphi = 0$ in Ω .

Rough proof:

$$\tilde{\mathbf{n}}(z) \left(\frac{z - \mathbf{a}_1}{|z - \mathbf{a}_1|} \right)^{-d_1} \cdots \left(\frac{z - \mathbf{a}_M}{|z - \mathbf{a}_M|} \right)^{-d_M}$$

is an equilibrium solution of degree zero.

Let $B_R = B(\mathbf{0}, R)$, so that $\cup_{i=1}^M \bar{\omega}_i \subset B_{R_0}$ for some R_0 , and

$$X = \{\mathbf{n} : \Omega \rightarrow S^2 : \int_{\Omega \cap B_R} |\nabla \mathbf{n}|^2 dx < \infty \text{ for all } R > R_0, \mathbf{n}|_{\partial \omega_i} = \mathbf{n}_i\}.$$

Let $k = \sum_{i=1}^M d_i$, where $d_i = \deg \mathbf{n}_i$.

X can be split into countably many *homotopy classes* (topologically distinct families of \mathbf{n} , so that director fields in two different homotopy classes cannot be continuously deformed one to the other). The different homotopy classes correspond to adding different multiples of 2π to the boundary values for φ on each $\partial \omega_i$.

Theorem. Let $k = \sum_{i=1}^M \deg \mathbf{n}_i$. There is a unique minimizer \mathbf{n}_C of

$$E(\mathbf{n}) = \int_{\Omega} \left(|\nabla \mathbf{n}|^2 - \frac{k^2}{|\mathbf{x}|^2} \right) d\mathbf{x},$$

in each homotopy class C , $\mathbf{n}_C : \bar{\Omega} \rightarrow S^1$ is a smooth harmonic map and

$$|\mathbf{n}_C(\mathbf{x}) - \mathbf{n}_C^\infty(\mathbf{x})| \leq \frac{C_0}{r},$$

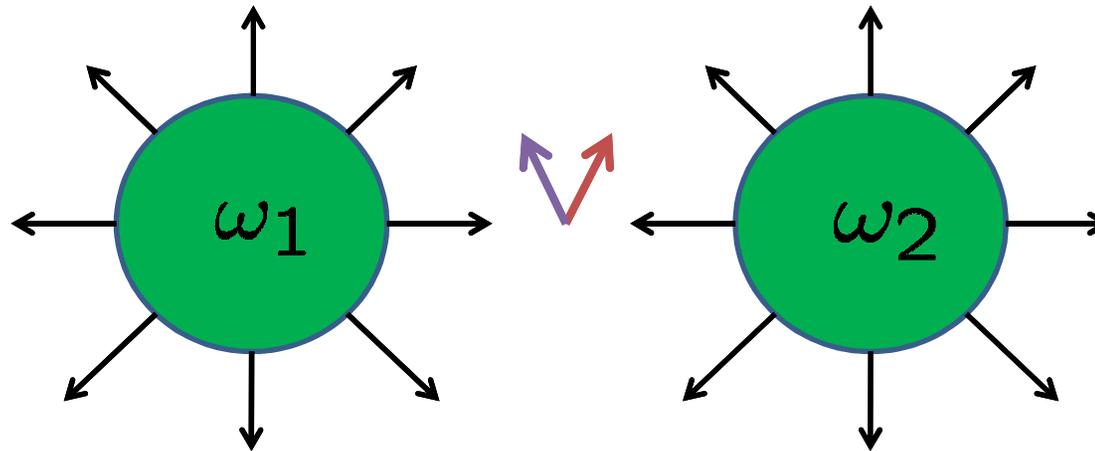
for some constant $C_0 > 0$, where

$$\mathbf{n}_C^\infty(\mathbf{x}) = (\cos(k\theta + \beta_C), \sin(k\theta + \beta_C))$$

and $\beta_C \in \mathbb{R}$. In each homotopy class C there is also a harmonic map $\hat{\mathbf{n}}_C$ with $E(\hat{\mathbf{n}}_C) = +\infty$.

Furthermore E attains a minimum \mathbf{n}^* in X , but \mathbf{n}^* is not in general unique.

Counterexample for uniqueness of \mathbf{n}^* .



Remarks

1. The nonuniqueness in this example might go away if we formulated everything in terms of *line-fields* $\mathbf{n} \otimes \mathbf{n}$. These can be handled by the trick of squaring $\tilde{\mathbf{n}}$, i.e. looking at the director field $\tilde{\mathbf{n}}^2$.
2. In the two-constant $d = 2$ case there can be radial solutions that are periodic in $\ln r$, so the asymptotic behaviour is much more complicated.