Analysis of Defects in Minimizers for a Planar Frank Energy

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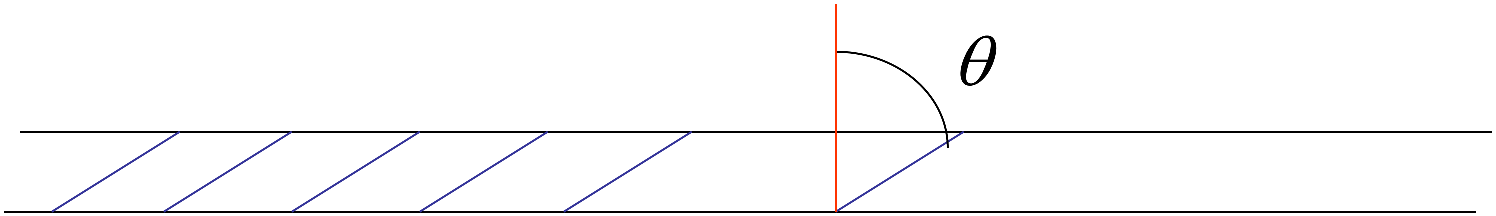
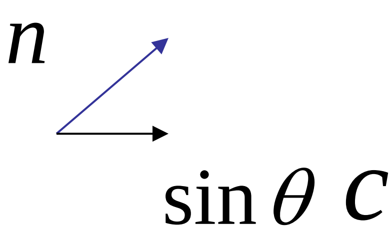
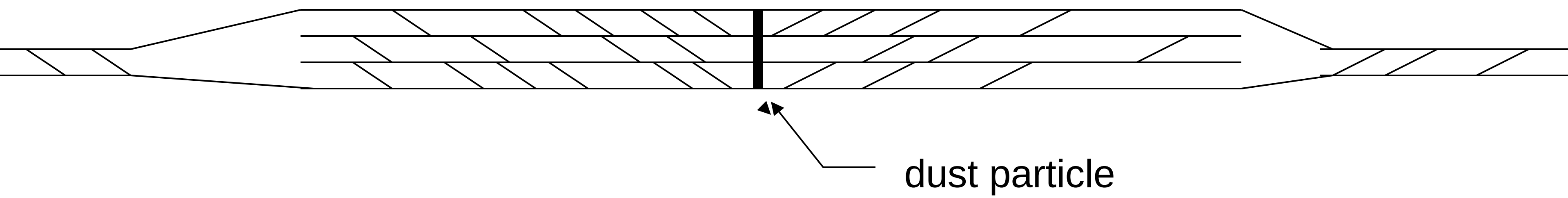
I. Defects in smectic C^* films

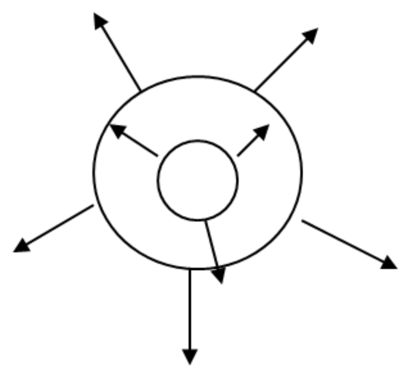




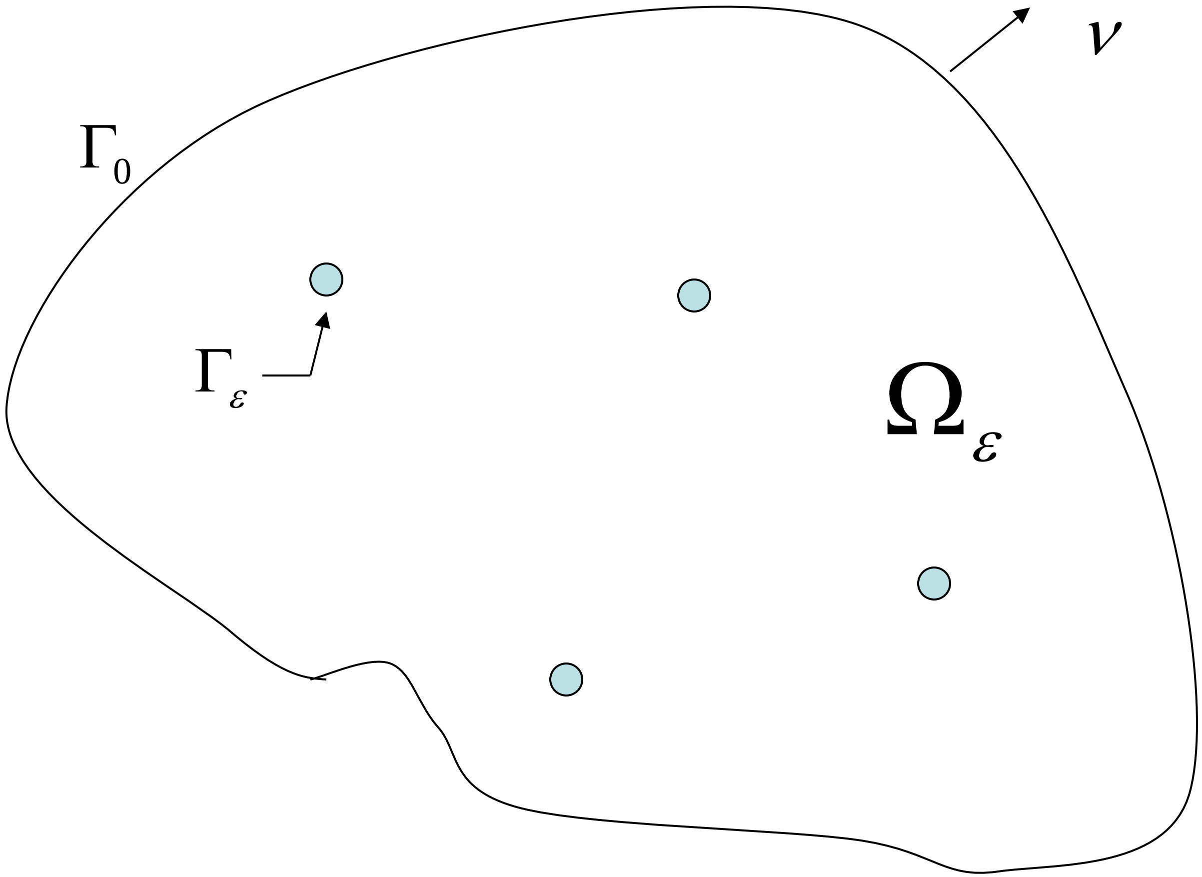
$$|n| = |c| = 1$$



Here c is a vector field rather than a line field.
The defects that form will have degree ± 1 rather than $\pm\frac{1}{2}$.



$$\Gamma_{\varepsilon,i} = \partial B_\varepsilon(a_i)$$



$$
\begin{aligned}
E_\varepsilon(c) &= \int_{\Omega_\varepsilon} [k_1 (div\, c)^2 + k_2 (curl\, c)^2] dx + \\
&\int_{\Gamma_\varepsilon} \sigma_\varepsilon(c,\nu) ds + \int_{\Gamma_0} \sigma_0(c,\nu) ds
\end{aligned}
$$

$$
\begin{aligned}
c &= (c_1, c_2), \quad |c| = 1 \\
div\, c &= \partial_{x_1} c_1 + \partial_{x_2} c_2 \text{ and } curl\, c = \partial_{x_1} c_2 - \partial_{x_2} c_1
\end{aligned}
$$

splay and bend constants $k_1, k_2 > 0$

$$
\int_{\Gamma_\varepsilon} \sigma_\varepsilon(c,\nu) ds \equiv \text{ anchoring energy at the particle surface}
$$

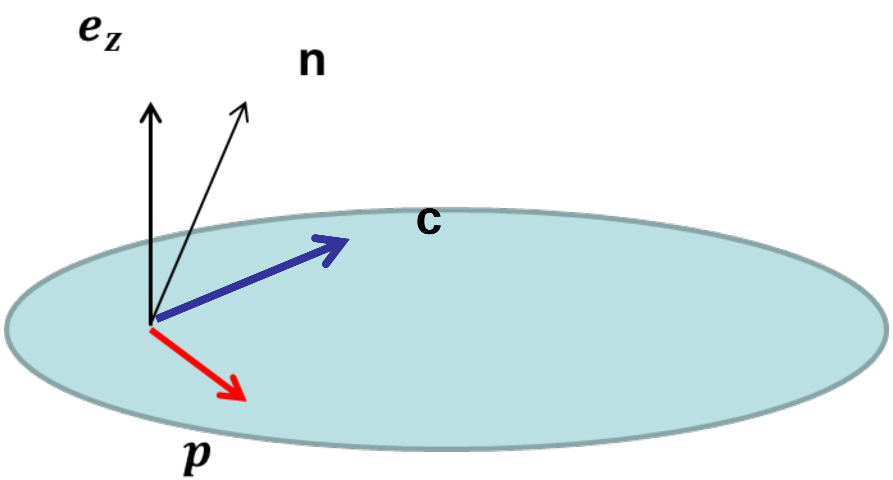
In the case of SmC^* islands the energy

$$
\int_{\Gamma_0} \sigma_0(c,\nu) ds
$$

is due to polar splay.

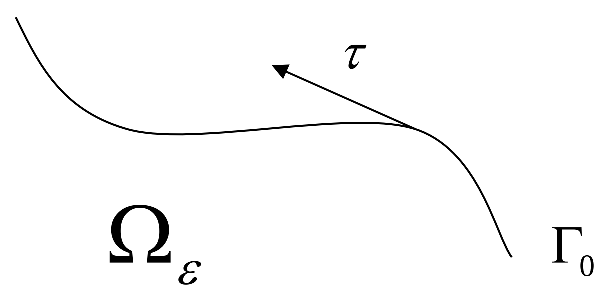
In a C^* material the polarization field satisfies

$$p \parallel n \times e_z$$



$$
\begin{aligned}
\text{Elastic Polar Energy} &= \\
\sigma \int_{\Omega_\varepsilon} div\, p\, dx &= \sigma \int_{\Omega_\varepsilon} curl\, c\, dx \\
&= \int_{\Gamma_\varepsilon} \sigma\, c \cdot \tau\, ds + \int_{\Gamma_0} \sigma\, c \cdot \tau\, ds
\end{aligned}
$$

$$
\int_{\Gamma_0} \sigma_0(c, \nu) ds \equiv \int_{\Gamma_0} \sigma\, c \cdot \tau\, ds
$$



In this case the weak anchoring condition

$$\int_{\Gamma_0} \sigma_0(c,\nu) ds \equiv \int_{\Gamma_0} \sigma\, c \cdot \tau\, ds$$

should be as negative as possible. We replace this with the strong anchoring condition

$$c = \pm\tau \text{ on } \Gamma_0.$$

We also assume the anchoring energy on Γ_ε is negligible.

The problem becomes minimize

$$E_\varepsilon(c) \quad = \quad \int_{\Omega_\varepsilon} [k_1(div\, c)^2 + k_2(curl\, c)^2]dx$$

among $\{c \in H^1(\Omega_\varepsilon) : |c(x)| = 1 \text{ for } x \in \Omega_\varepsilon, \text{ and } c = g \text{ on } \Gamma_0\}$.

One has to vary both the defect locations $\{B_\varepsilon(a_l)\}$, and the texture $c(x)$ defined on $\Omega_\varepsilon = \Omega \setminus \bigcup_l B_\varepsilon(a_l)$ to do this.

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Textural transformations in islands on free standing smectic-C^* liquid crystal films

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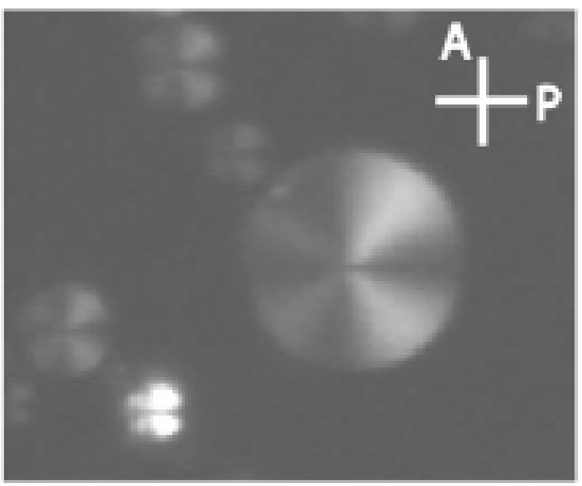
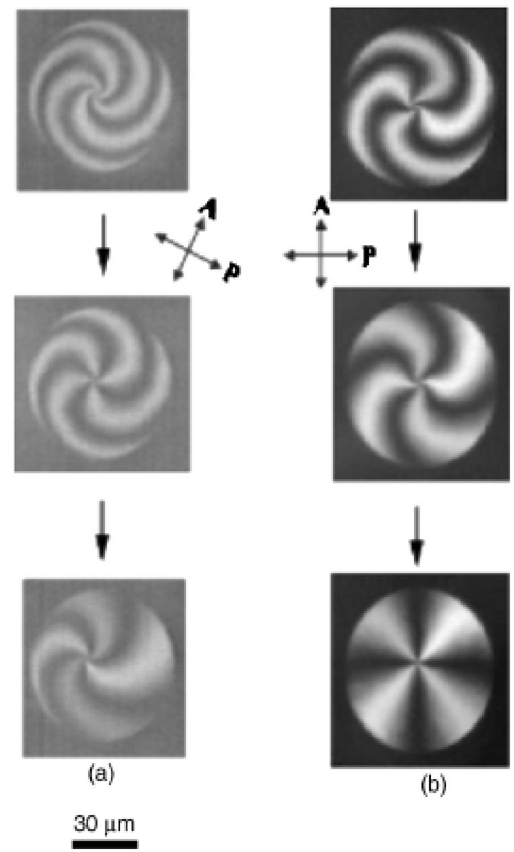




Polarization has a large electrostatic contribution.

Lee-Pelcovits-Meyer

Electrostatic Energy due to p:

$$\mathcal{E}_{el}(p) = k_e l \int_\Omega (div\, p)^2\, dx = k_{el} \int_\Omega (curl\, c)^2\, dx$$

Add this into the Frank energy by replacing k_2 with

$$k_{eff} = k_2 + k_{el} \gg k_2$$

We study a relaxed Frank energy instead.

Energy:

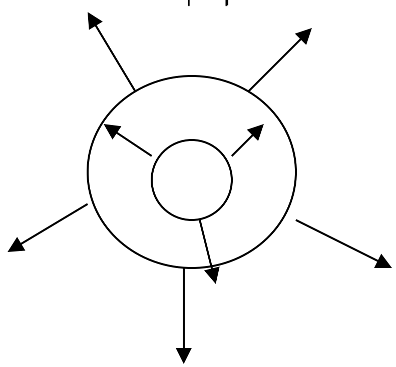
$$\mathcal{E}_\varepsilon(c) = \frac{1}{2}\int_\Omega [k_1(div\, c)^2 + k_2(curl\, c)^2 + \frac{1}{2\varepsilon^2}(1-|c|^2)^2]dx$$

$$c \in H^1_g(\Omega) = \{c \in H^1(\Omega;\mathbb{R}^2) : c = g \text{ on } \partial\Omega\}$$

where $g \in H^1(\partial\Omega), |g| = 1,$ and $\deg g = d > 0.$

SPLAY

$$c_s = \frac{\mathbf{x}}{|\mathbf{x}|}$$

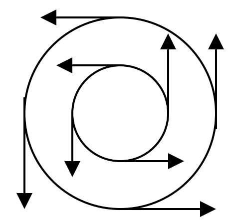


$$curl\, c_s = 0$$

For $\mathbf{x} \neq 0$ $\quad |\nabla c_s|^2 = (div\, c_s)^2$

BEND

$$c_b = \frac{\mathbf{x}^t}{|\mathbf{x}|} = i\frac{\mathbf{x}}{|\mathbf{x}|}$$



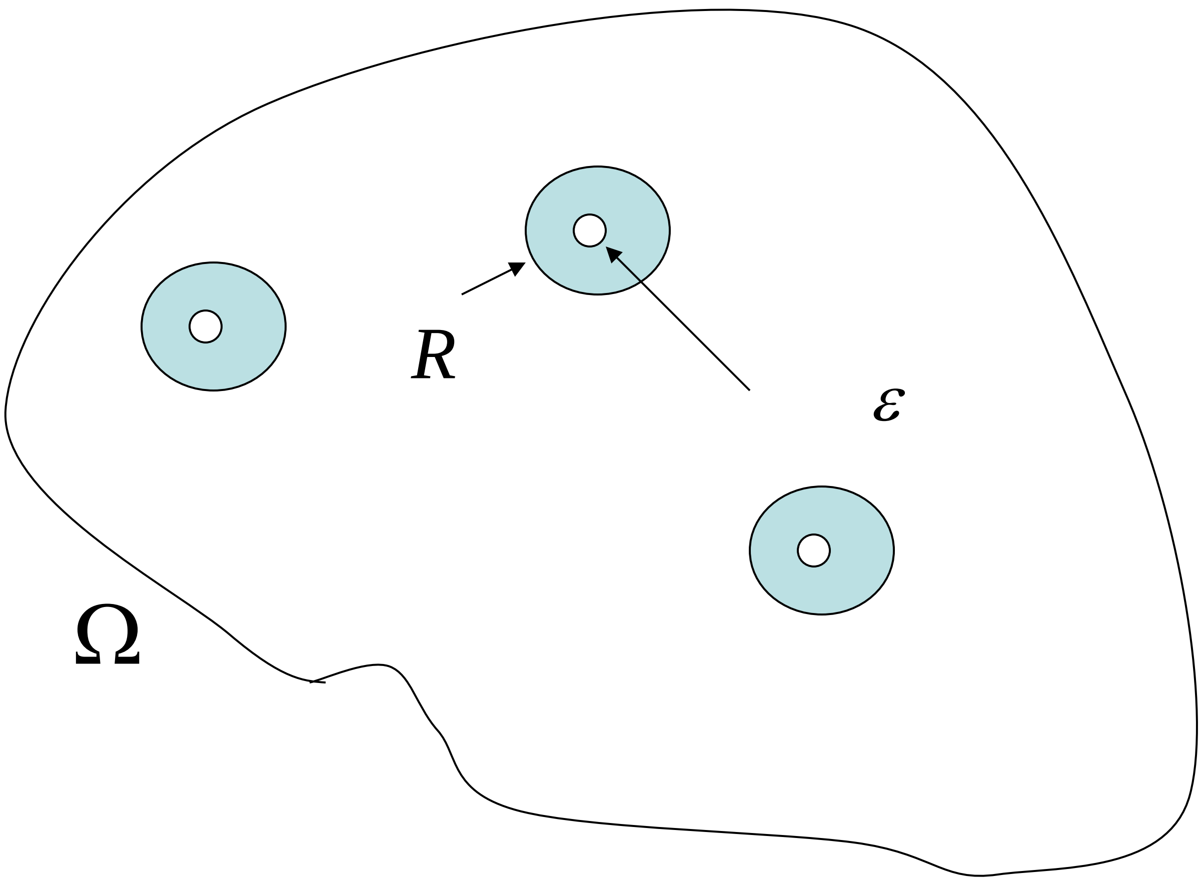
$$div\, c_b = 0$$

$$|\nabla c_b|^2 = (curl\, c_b)^2$$

Set $\underline{k} = min(k_1, k_2)$ and $\mathbf{b} = \{b_1, ..., b_d\}$.

Test functions:

Let $\tilde{c}_\varepsilon = c_s$ in $B_R(b_j) \setminus B_\varepsilon(b_j)$ if $\underline{k} = k_1$
and $\tilde{c}_\varepsilon = c_b$ in $B_R(b_j) \setminus B_\varepsilon(b_j)$ if $\underline{k} = k_2$.
Assume $\tilde{c}_\varepsilon$ is extended smoothly to $\overline{\Omega} \setminus \cup_{j=1}^{j=d} B_R(b_j)$
so that $\tilde{|}\tilde{c}_\varepsilon| = 1$ and $\tilde{c}_\varepsilon \in H^1_g(\Omega)$.



Let $\{c_\varepsilon\}$ be minimizers to $\mathcal{E}_\varepsilon(v)$ for $v \in H^1_g(\Omega)$.

Then

$$\mathcal{E}_\varepsilon(c_\varepsilon) \leq \mathcal{E}_\varepsilon(\tilde{c}_\varepsilon) \leq \pi \underline{k} d\, log(\frac{1}{\varepsilon}) + M_1$$

Next

$$\begin{aligned} k_1 (div\, c)^2 &\quad + k_2 (curl\, c)^2 \\ = k_1 |\nabla c|^2 &\quad + (k_2 - k_1)(curl\, c)^2 + k_1\, det \nabla c \\ = k_2 |\nabla c|^2 &\quad + (k_1 - k_2)(div\, c)^2 + k_2\, det \nabla c. \end{aligned}$$

Assume that $\underline{k} = k_1$.
So that

$$k_1(div\, c_\varepsilon)^2 + k_2(curl\, c_\varepsilon)^2 = \underline{k}|\nabla c_\varepsilon|^2 + (k_2 - \underline{k})(curl\, c_\varepsilon)^2 + \underline{k}\, det\nabla c_\varepsilon.$$

Now

$$\int_\Omega det\nabla c_\varepsilon\, dx = \pi d \text{ and } k_2 - \underline{k} \geq 0$$

.
So

$$\int_\Omega \underline{k}|\nabla c_\varepsilon|^2\, dx \leq \int_\Omega k_1(div\, c_\varepsilon)^2 + k_2(curl\, c_\varepsilon)^2\, dx$$

and we see

$$\pi\underline{k}d\, log(\frac{1}{\varepsilon}) - M_2 \leq \frac{1}{2}\int_\Omega [\,\underline{k}|\nabla c_\varepsilon)|^2 + \frac{1}{2\varepsilon^2}(1 - |c_\varepsilon)|^2)^2\,]dx - M_2 \leq \mathcal{E}_\varepsilon(c_\varepsilon)$$

Assume that $\underline{k} = k_1$.
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$$\pi\underline{k}d\, log(\frac{1}{\varepsilon}) - M_2 \leq \frac{1}{2}\int_\Omega [\,\underline{k}|\nabla c_\varepsilon)|^2 + \frac{1}{2\varepsilon^2}(1 - |c_\varepsilon)|^2)^2\,]dx - M_2 \leq \mathcal{E}_\varepsilon(c_\varepsilon)$$

lower bound from BBH

From these estimates (after Struwe) we find

$$\frac{1}{\varepsilon^2}\int_\Omega (1-|c_\varepsilon|^2)^2 dx \leq M_3.$$

To see this we have

$$\mathcal{E}_\varepsilon(c_\varepsilon) \leq \pi \underline{k} d \, log(\frac{1}{\varepsilon}) + M_1$$

$$\frac{1}{2}\int_\Omega [k_1(div\, c)^2 + k_2(curl\, c)^2 + \frac{1}{2\varepsilon^2}(1-|c|^2)^2] dx =$$

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$$\frac{1}{2}\int_\Omega [k_1(div\, c)^2 + k_2(curl\, c)^2 + \frac{1}{2\varepsilon^2}(1-|c|^2)^2] dx$$

$$\mathcal{E}_{2\varepsilon}(c_\varepsilon) + \frac{3}{8\varepsilon^2}\int_\Omega (1-|c_\varepsilon|^2)^2 dx =$$

$$\pi \underline{k} d\, log(\frac{1}{2\varepsilon}) + \frac{3}{8\varepsilon^2}\int_\Omega (1-|c_\varepsilon|^2)^2 dx - M_2 \leq$$

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$$\pi \underline{k} d\, log(\frac{1}{\varepsilon}) + \frac{3}{8\varepsilon^2}\int_\Omega (1-|c_\varepsilon|^2)^2 dx - M_2' =$$

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$$\mathcal{E}_\varepsilon(c_\varepsilon) \leq \pi \underline{k} d\, log(\frac{1}{\varepsilon}) + M_1$$

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The estimate

$$\frac{1}{\varepsilon^2}\int_\Omega (1-|c_\varepsilon|^2)^2 dx \le M_3.$$

implies

$$(*) \qquad ||c_\varepsilon||_{C(\overline{\Omega})},\ \varepsilon||\nabla c_\varepsilon||_{C(\overline{\Omega})} \le M_4$$

To see this we dilate

$$v(y) = c_\varepsilon(\varepsilon y + x_0).$$

Then

$$\int_{B_1(0)} (1-|v|^2)^2 dy \le M_3'$$

$$\int_{B_1(0)} (1 - |v|^2)^2 dy \leq M_3'$$

We see that v solves a semi-linear elliptic system with a uniform estimate on it's right side:

$$\mathcal{L}v = v(|v|^2 - 1).$$

This implies

$$||v||_{C^1(B_{\frac{1}{2}})} \leq M_4,$$

and gives

$$||c_\varepsilon||_{C(\overline{\Omega})}, \, \varepsilon||\nabla c_\varepsilon||_{C(\overline{\Omega})} \leq M_4$$

The two estimates:

$$\frac{1}{2}\int_{\Omega}[\,\underline{k}|\nabla c_{\varepsilon})|^2+\frac{1}{2\varepsilon^2}(1-|c_{\varepsilon})|^2)^2\,]dx-M_1\le\mathcal{E}_{\varepsilon}(c_{\varepsilon})\le\pi\underline{k}d\,log(\frac{1}{\varepsilon})+M_1$$

also imply that to a significant degree, the structure of minimizers for $\mathcal{E}_{\varepsilon}$ is equivalent to that for the G–L energy

$$G_{\varepsilon}(v)=\frac{1}{2}\int_{\Omega}[\underline{k}|\nabla v|^2+\frac{1}{2\varepsilon^2}(1-|v|^2)^2]dx.$$

$\{c_{\varepsilon}\}$ is a family of ”low energy states” for G_{ε}.

Structure and Compactness results for low energy states (Lin). Assume that Ω is simply connected.

Given $\{c_\varepsilon\}$ there exists a subsequence $\varepsilon_l \to 0$,
$\mathbf{a} = (a_1, ..., a_d) \in \Omega^d$ for which $a_l \neq a_j$ if $l \neq j, 1 \leq l, j \leq d$,
and a function $h(x) \in H^1(\Omega)$ so that

$$c_{\varepsilon_l}(x) \to c^*(x) \equiv \Pi_{j=1}^d \frac{(x - a_j)}{|x - a_j|} e^{ih(x)}$$

strongly in $L^2(\Omega)$ and weakly in $H^1_{loc}(\overline{\Omega} \setminus \{a_1, ...a_d\})$.

Since $\{c_{\varepsilon_l}\}$ are minimizers for $\mathcal{E}_\varepsilon$ and not simply low energy states we get stronger convergence

Theorem 1. $c_{\varepsilon_l} \to c^*$ in $C^\alpha_{loc}(\overline{\Omega} \setminus \{a_1..., a_d\})$ and $C^m_{loc}(\Omega \setminus \{a_1..., a_d\})$ for $0 < \alpha < 1$ and $m \in \mathbb{N}$.

Furthermore

$$\frac{(1 - |c_{\varepsilon_l}|^2)}{\varepsilon_l} \to 0 \quad \text{in} \quad L^2_{loc}(\overline{\Omega} \setminus \{a_1..., a_d\}).$$

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Furthermore

$$\frac{(1 - |c_{\varepsilon_l}|^2)}{\varepsilon_l} \to 0 \quad \text{in} \quad L^2_{loc}(\overline{\Omega} \setminus \{a_1 ..., a_d\}).$$

This together with $\varepsilon|\nabla c_\varepsilon| \leq M$ implies that $|c_\varepsilon|$ converges uniformly to 1 away from $\{a_1, ... a_d\}$.

Idea of proof for H^1 convergence:

Let $\overline{B} \in \Omega \setminus \{a_1, ..., a_d\}$,

$$e(u) = \begin{cases} k_1|\nabla u|^2 + (k_2 - k_1)(\text{curl } u)^2 & \text{if } \underline{k} = k_1 \\ k_2|\nabla u|^2 + (k_1 - k_2)(\text{div } u)^2 & \text{if } \underline{k} = k_2, \end{cases}$$

and

$$\mathcal{E}(u; D) = \int_D e(u).$$

Then $\mathcal{E}(c^*; B) \leq \liminf_{\varepsilon \to 0} \mathcal{E}_\varepsilon(c_\varepsilon; B)$.

If there is a gap then we can adjust c^* to show that $\{c_\varepsilon\}$ are not minimizers.
Then $\mathcal{E}(c^*; B) = \lim_{\varepsilon \to 0} \mathcal{E}_\varepsilon(c_\varepsilon; B)$

Then $||c_\varepsilon||_{H^1(B)} \to ||c^*||_{H^1(B)}$.

It follows that $c_\varepsilon \to c^*$ in H^1.

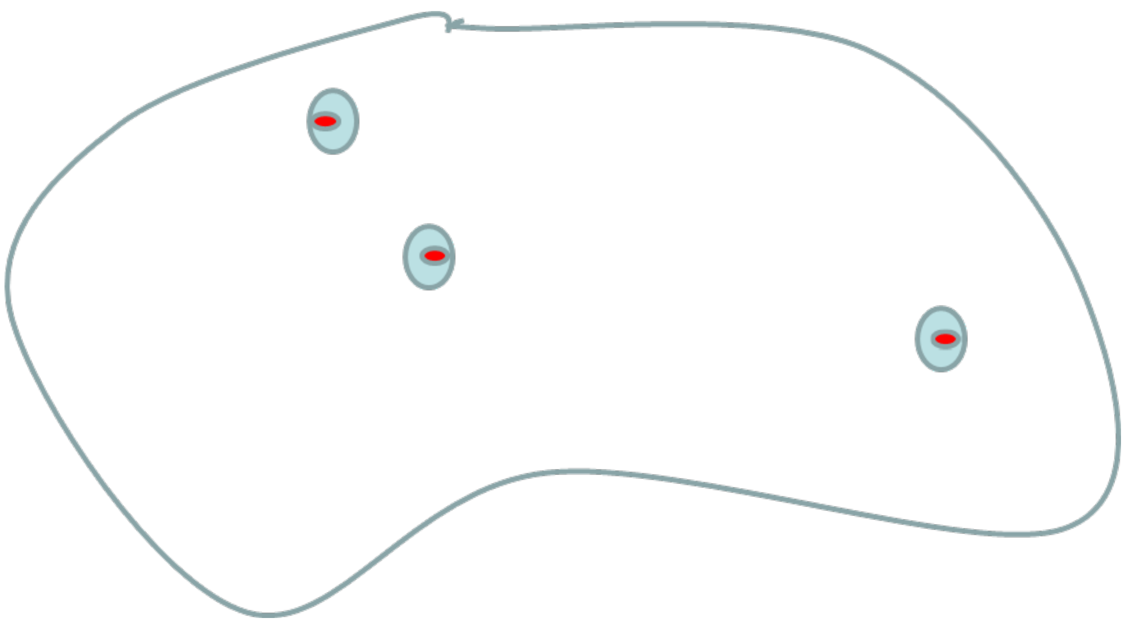
To prove higher regularity one uses that $f(t) = (1 - t^2)^2$ is convex near $t = 1$ and that $|c^*|$ is uniformly close to 1.
to show

$$||c_\varepsilon||_{H^k_{loc}(\Omega\setminus\{a_1,\ldots,a_d\})} \text{ estimates for } k \geq 2$$

We can separate Ω into three regions:

1. $\Omega \setminus \bigcup_{m=1}^{d} B_\rho(a_m)$ outer region,
2. $\bigcup_{m=1}^{d} B_\rho(a_m) \setminus B_{r_\varepsilon}(a_m)$, $\varepsilon \ll r_\varepsilon = o(1)$ near the cores,
3. $\bigcup_{m=1}^{d} B_{r_\varepsilon}(a_m)$ cores

Theorem 1 takes care of the outer region.



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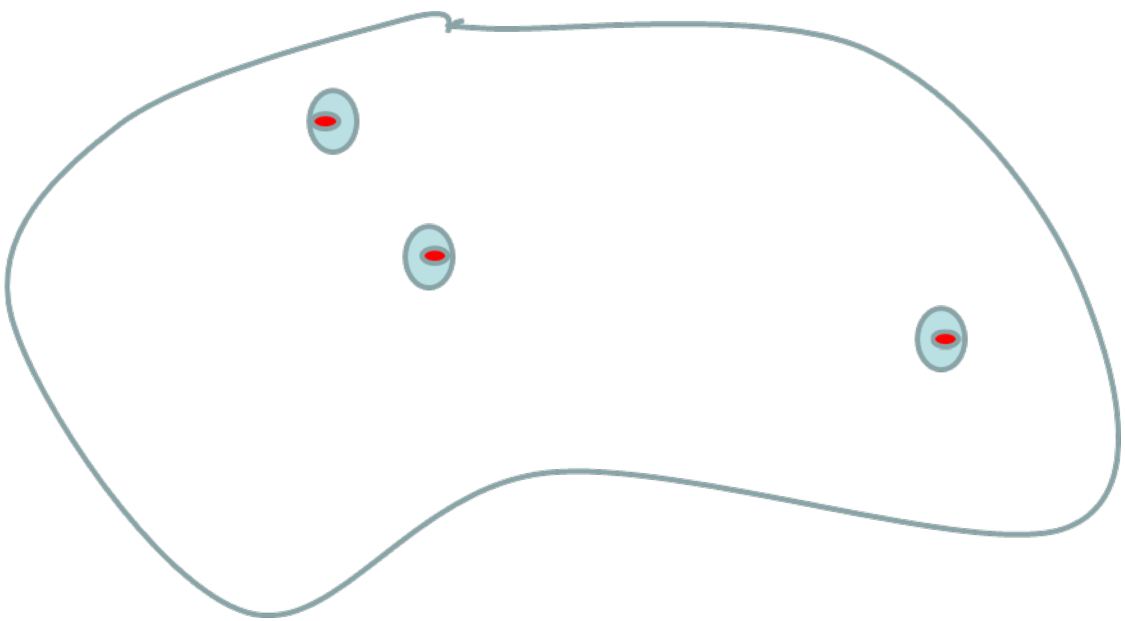
This approach says little about the cores.



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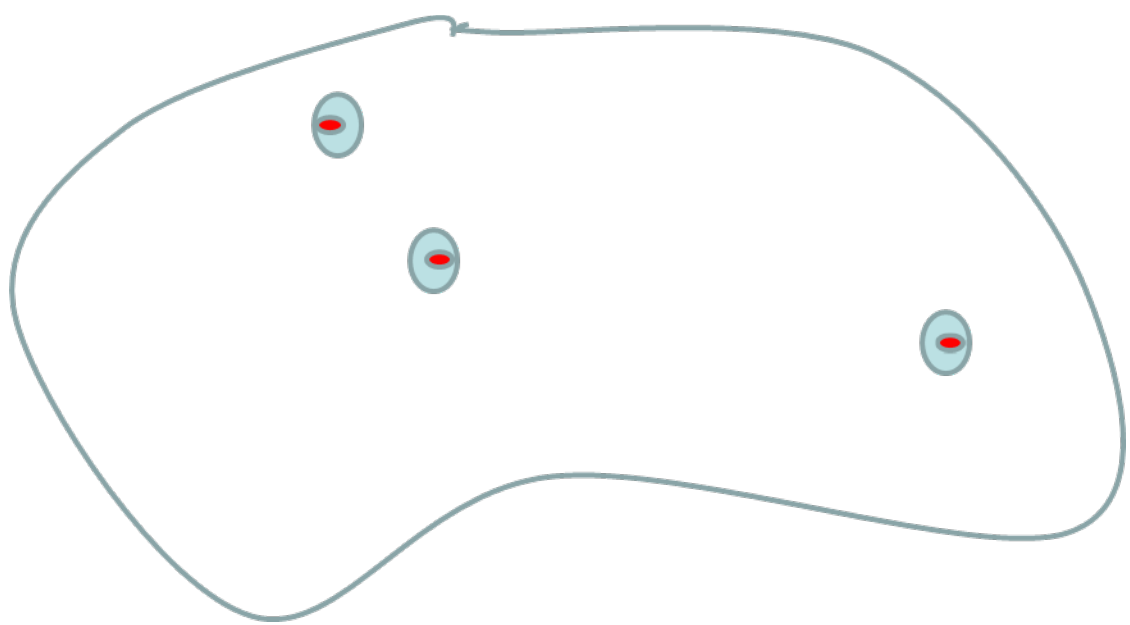
Theorem 1 takes care of the outer region.
This approach says little about the cores.
To treat the region near the cores we study $c^*(x)$ for x near the $\{a_m\}$.



In the case for the GL functional the limiting solution is

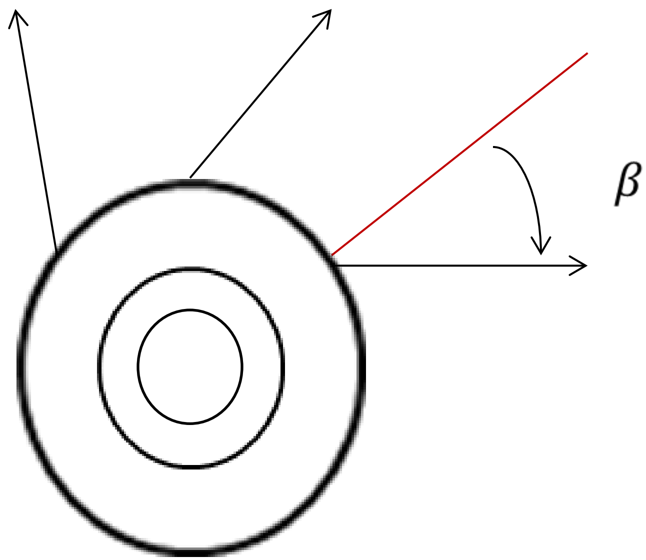
$$v^*(x) = \Pi_{j=1}^{d} \frac{(x-a_j)}{|x-a_j|} e^{ih(x)}$$

where $\Delta h = 0$ in Ω.

$$v^*(x) \to \frac{(x-a_l)}{|x-a_l|} (\Pi_{j\neq l} \frac{(a_l-a_j)}{|a_l-a_j|} e^{ih(a_l)}) = \frac{(x-a_l)}{|x-a_l|} e^{i\beta} \text{ as } x \to a_l$$

.

$$v^*(\rho y + a_l) \to y e^{i\beta} \text{ for } y \in \partial B_1$$



For our case

$$c^*(x) = \Pi_{j=1}^{d} \frac{(x - a_j)}{|x - a_j|} e^{ih(x)}$$

We have

$$\int_\Omega [|\nabla h|^2 + (curl\, c^*)^2] dx < \infty \quad \text{if } \underline{k} = k_1,$$
$$\int_\Omega [|\nabla h|^2 + (div\, c^*)^2] dx < \infty \quad \text{if } \underline{k} = k_2.$$

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We have

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$$\int_\Omega [|\nabla h|^2 + (div\, c^*)^2] dx < \infty \qquad \text{if } \underline{k} = k_2.$$

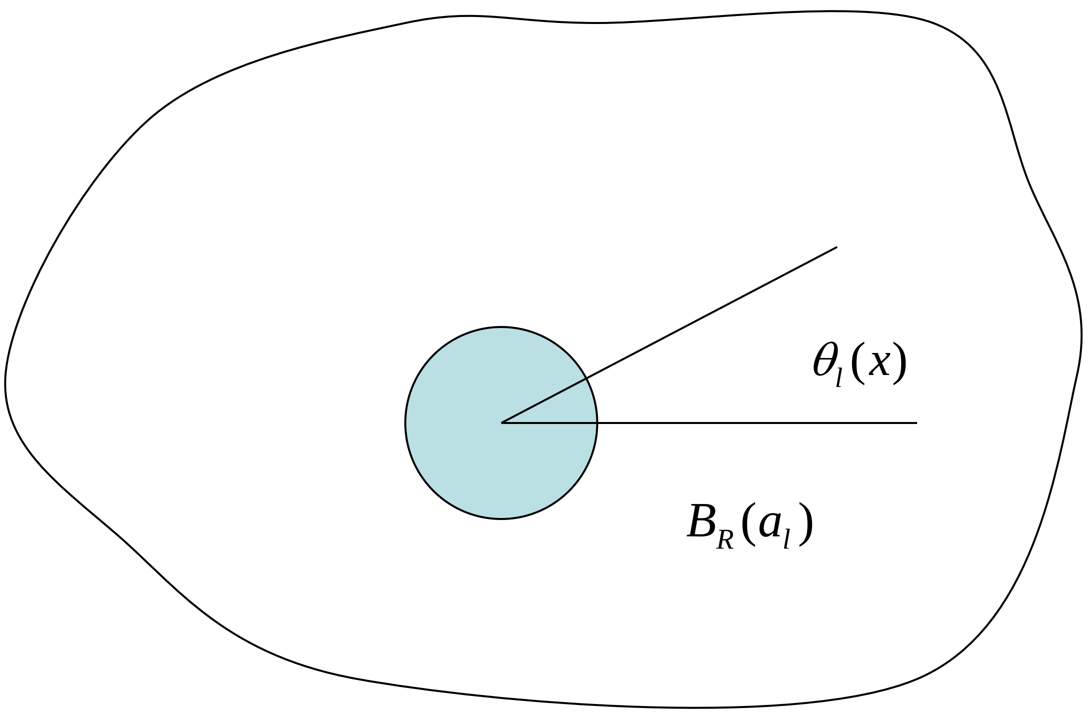
To determine

$$\lim_{r \to 0} h(ry + a_l) \quad \text{in} \quad L^2(\partial B_1)$$

it suffices to examine

$$\lim_{r \to 0} ⨍_{\partial B_r(a_l)} h\, ds.$$

$$\frac{x-a_l}{|x-a_l|} = e^{i\theta_l(x)}.$$



Fix a_l and set $f(x) = \sum_{j \neq l} \theta_j(x) + h(x)$.

Then $c^*(x) = \frac{(x-a_l)}{|x-a_l|} e^{if(x)}$ and

$$\int_{B_R(a_l)} \frac{(\sin f(x))^2}{|x-a_l|^2} dx \leq \int_\Omega (curl\, c^*)^2 dx + M < \infty \text{ if } \underline{k} = k_1,$$

$$\int_{B_R(a_l)} \frac{(\cos f(x))^2}{|x-a_l|^2} dx \leq \int_\Omega (div\, c^*)^2 dx + M < \infty \text{ if } \underline{k} = k_2.$$

We have $⨍_{\partial B_r(a_l)} f\, ds \approx$ const for $\frac{\overline{r}}{2} \leq r \leq \overline{r}$

Fix a_l and set $f(x) = \sum_{j \neq l} \theta_j(x) + h(x)$.

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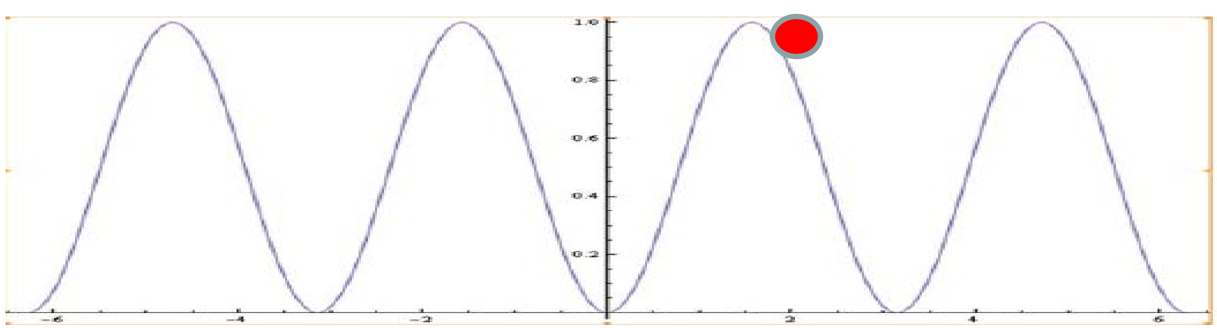
We have $\fint_{\partial B_r(a_l)} f\, ds \approx \text{const}$ for $\frac{\overline{r}}{2} \leq r \leq \overline{r}$



It follows that

$$\lim_{r\to 0} \fint_{\partial B_r(a_l)} f\,ds = n\pi \text{ for some } n \in \mathbb{Z} \text{ if } \underline{k} = k_1$$

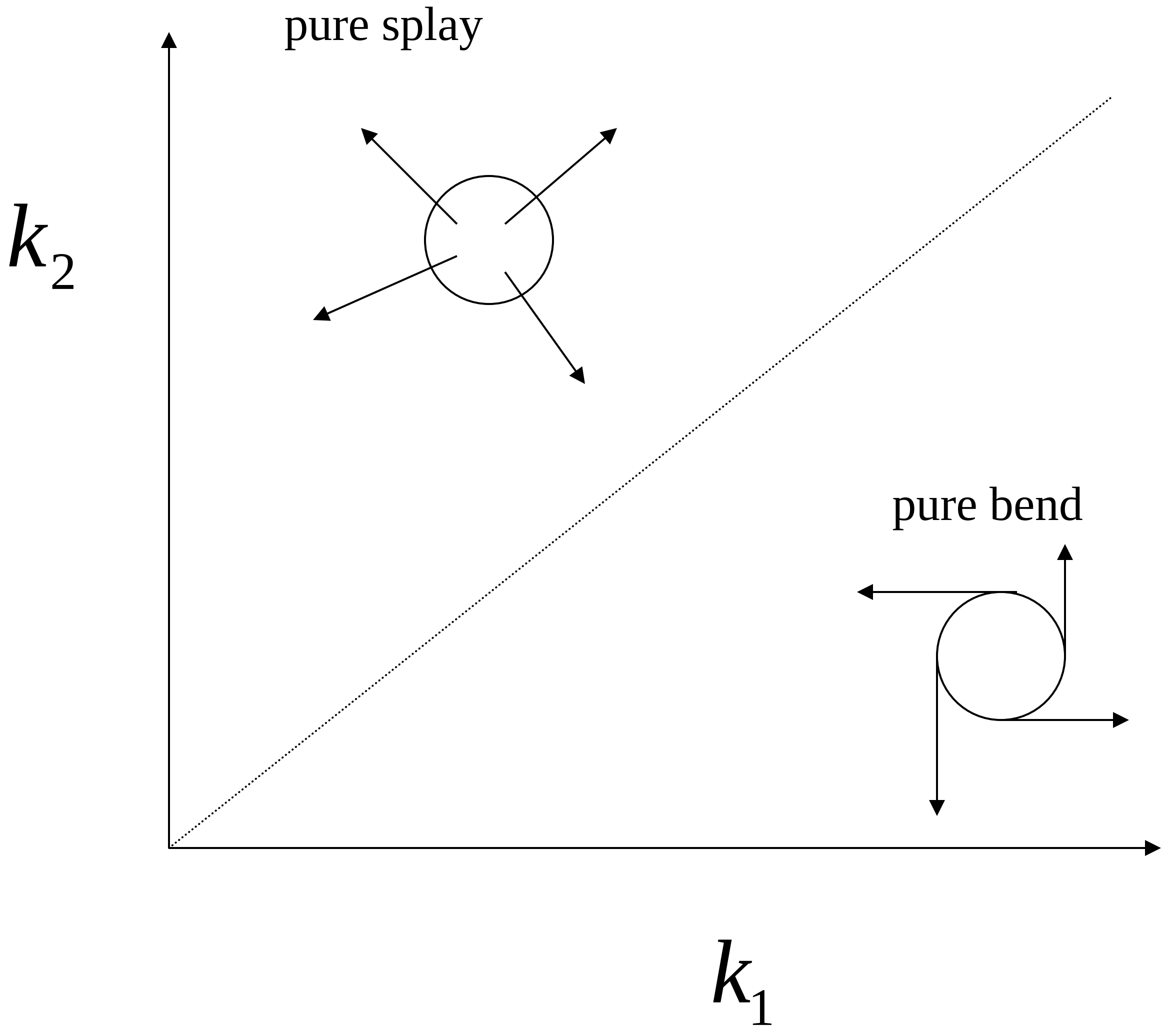
and

$$\lim_{r\to 0} \fint_{\partial B_r(a_l)} f\,ds = \frac{\pi}{2} + n\pi \text{ for some } n \in \mathbb{Z} \text{ if } \underline{k} = k_2.$$

In terms of $\mathbf{c}^*$ this implies that

$$\mathbf{c}^*(\rho\mathbf{y} + a_n) \to \begin{cases} \pm\mathbf{y} & \text{if } k_2 > k_1 \\ \pm i\mathbf{y} & \text{if } k_1 > k_2 \end{cases}$$

in $L^2(\partial B_1(0))$ as $\rho \to 0$. Thus if $k_2 > k_1$ then $\mathbf{c}^*$ has a pure splay pattern near each defect and if $k_1 > k_2$ then $\mathbf{c}^*$ asymptotically has a pure bend pattern near each a_n.


pure splay
k_2
pure bend
k_1

$$
\begin{aligned}
\mathcal{E}_\varepsilon(c) &= \frac{1}{2}\int_\Omega [k_1(div\, c)^2 + k_2(curl\, c)^2 \\
&\quad + \frac{1}{2\varepsilon^2}(1-|c|^2)^2]dx
\end{aligned}
$$

Assume $k_1 < k_2$. So a splay pattern has less energy than a bend pattern.

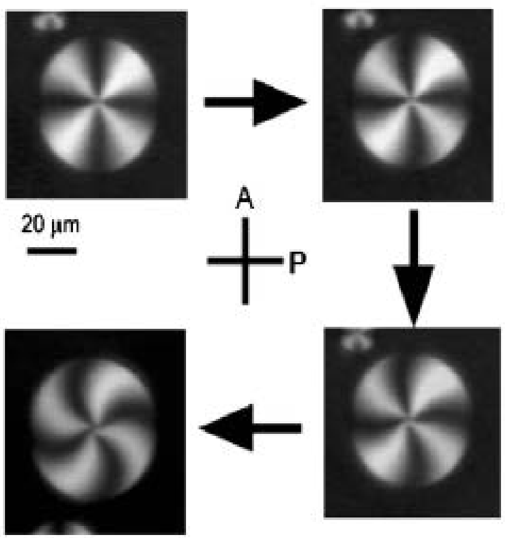
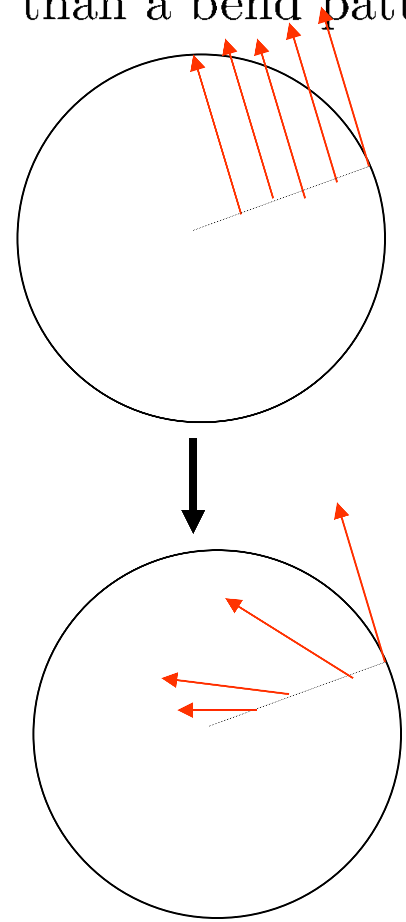


FIG. 4. Transformation of a pure bend island into a reversing spiral island. It took around 30 min.



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Modeling dipolar and quadrupolar defect structures generated by chiral islands in freely suspended liquid crystal films

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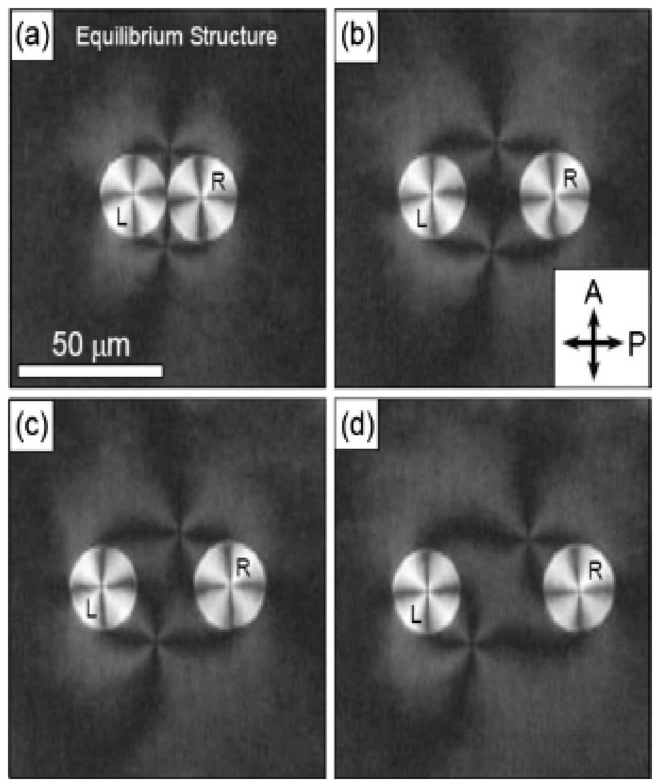
A. Pattanaporkratana,[4,5] C. S. Park,[4] J. E. Maclennan,[4] and N. A. Clark[4]



Theorem 2. Assume that $\underline{k} = k_1$. So that

$$k_1(div\, c)^2 + k_2(curl\, c)^2 = \underline{k}|\nabla c|^2 + (k_2 - \underline{k})(curl\, c)^2 + \underline{k}\, det\nabla c.$$

Then

$$\lim_{\varepsilon_l \to 0}\{\mathcal{E}_{\varepsilon_l}(c_{\epsilon_l}) - \pi \underline{k} d \ln \frac{1}{\varepsilon_l}\} = \mathfrak{W}(\mathbf{a}) + d\gamma + \delta$$

where $\mathbf{a}$ minimizes $\mathfrak{W}(\mathbf{b})$ for $\mathbf{b} \in \Omega^d$.

$$
\begin{aligned}
\mathfrak{W}(\mathbf{b}) \quad = \quad & \inf_{z\in\mathfrak{A}_g}\Bigg\{\underline{k}\Bigg(-\pi\sum_{\ell\neq j}\log|b_\ell - b_j| + \frac{1}{2}\int_{\partial\Omega} R\partial_\nu R ds \\
& - \int_{\partial\Omega} z\partial_\tau R ds + \frac{1}{2}\int_\Omega |\nabla z|^2 dx\Bigg) \\
& +(k_2 - \underline{k})\int_\Omega (curl\, u*)^2 dx\Bigg\}
\end{aligned}
$$

such that

$u^* = \Pi_{j=1}^d \frac{(x-b_j)}{|x-b_j|} e^{iz(x)}$, $R = \sum_{j=1}^d \ln(|x-b_j|)$,

and

$\mathfrak{A}_g = \{z \in H^1(\Omega) : u^* = g \text{ on } \partial\Omega\}$.

$$\mathfrak{W}(\mathbf{b}) = \inf_{z\in\mathfrak{A}_g}\Bigg\{\underline{k}\Bigg(-\pi\sum_{\ell\neq j}\log|b_\ell - b_j| + \frac{1}{2}\int_{\partial\Omega} R\partial_\nu R ds$$

$$-\int_{\partial\Omega} z\partial_\tau R ds + \frac{1}{2}\int_\Omega |\nabla z|^2 dx\Bigg)$$

$$+(k_2 - \underline{k})\int_\Omega (curl\, u*)^2 dx\Bigg\}$$

Reduced energy for G-L

such that

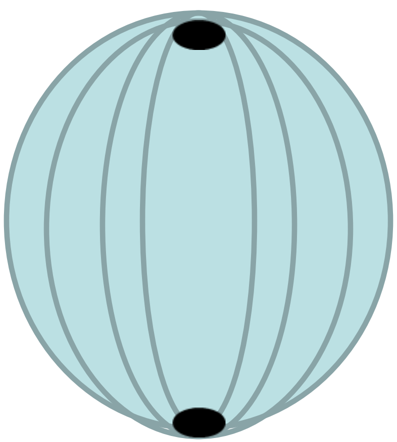
$u^* = \Pi_{j=1}^d \frac{(x-b_j)}{|x-b_j|} e^{iz(x)}$
and

$\mathfrak{A}_g = \{z \in H^1(\Omega) : u^* = g \text{ on } \partial\Omega\}.$

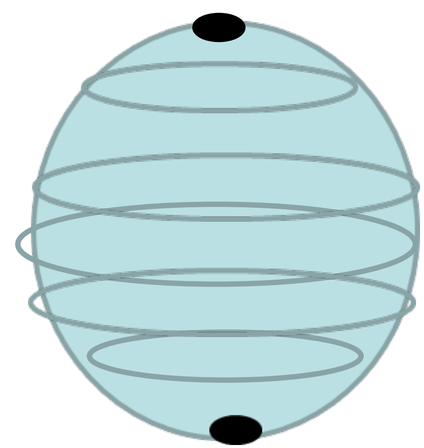
Vitelli-Nelson

Tilted molecules on spherical shells.

$k_1 < k_2$



$k_1 > k_2$



Giomi, Bowick, Ma, Majumdar
Tilted Molecules on Nanoparticles

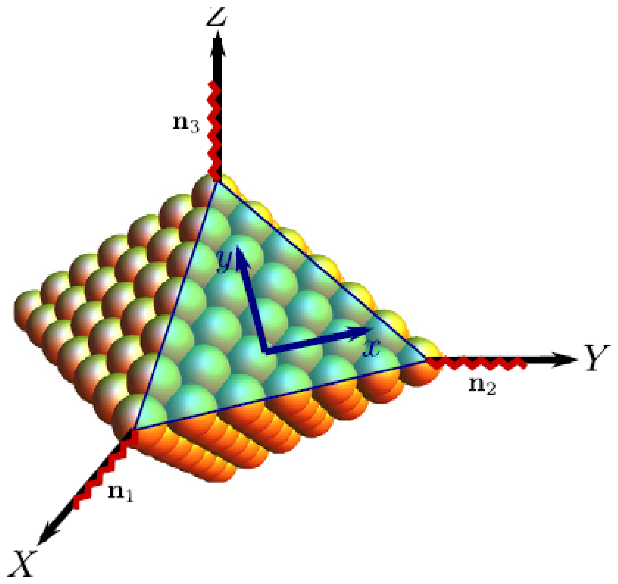


Fig. 4: (Colour on-line) Schematic of an octahedral nanoparticle with the chains oriented at the vertices of a single triangular face as prescribed by the continuous model.