Analysis of a Ginzburg-Landau Type Energy Model for Smectic C* Liquid Crystals with Defects

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Applied and Computational Mathematics Division Seminar Series
National Institute of Standards and Technology

May 28, 2013

Outline

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GL functional is defined as

$$E_\varepsilon(u) = \frac{1}{2}\int_\Omega |\nabla u|^2 + \frac{1}{2\varepsilon^2}(1-|u|^2)^2\,dx$$

- Introduced in study of phase transition problems in superconductivity (also used in superfluids and mixture of fluid states)
- u - complex order parameter (condensate wave function/concentration/vector field orientation)
- ε - coherence length which can depend on temperature ($\xi(T)$)/diffuse interface/core radius

When in equilibrium, the order parameter u minimizes E_ε. Taking variations of u, the following must be satisfied

$$\delta E_\varepsilon = \int_\Omega [-\Delta u - \frac{1}{\varepsilon^2} u(1-|u|^2)]\delta u \, dx = 0$$

$\Longrightarrow$

$$-\Delta u = \frac{1}{\varepsilon^2} u(1-|u|^2)$$

Ex: $u_t = u + tv$, $\delta E_\varepsilon = \frac{dE_\varepsilon}{dt}(u+tv)|_{t=0}$, $\delta u = v$

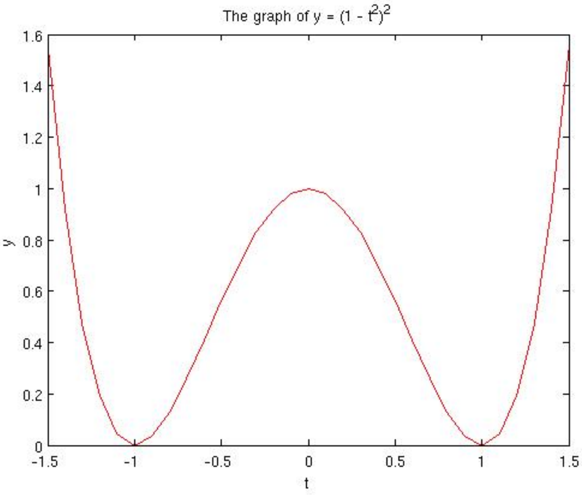
Example in 1D

The Euler-Lagrange (E-L) equation in 1D then becomes

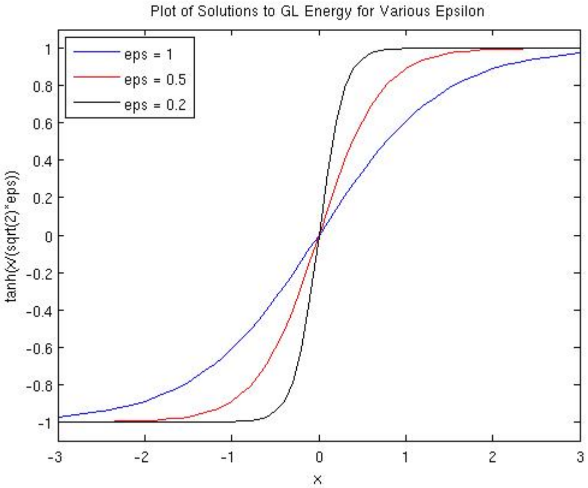
$$-u_{xx} - \frac{1}{\varepsilon^2}u(1-u^2) = 0$$

Solution: $u_\varepsilon = \tanh(\frac{x}{\sqrt{2}\varepsilon})$ given the boundary conditions $u(0) = lim_{|x|\to\infty} u_x(x) = 0$.

The function $y = (1 - t^2)^2$ (Two-well potential in 1D)



Plot of solutions for various epsilons



Outline

What are LCs

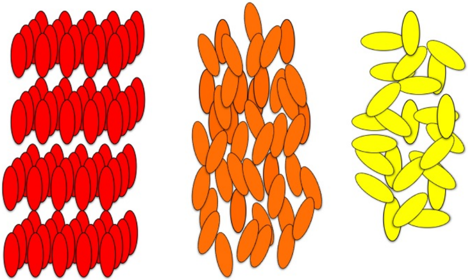


Figure: The molecular orientation of different states of matter. Left - Solid, Middle - Liquid Crystal, Right - Isotropic Liquid

Types of LCs

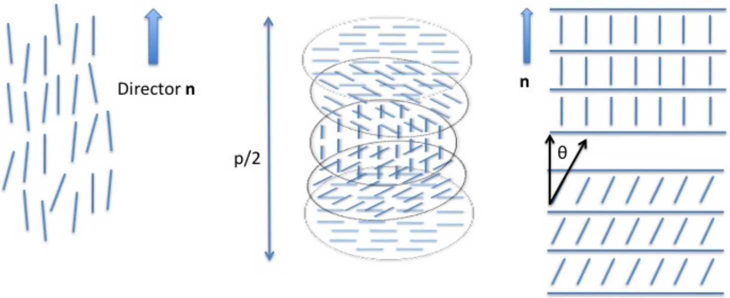


Figure: Arrangement of Molecules in particular LCs. Left - Nematic LCs, Middle - Cholesteric (Chiral Nematic) LCs, Right - Smectic LCs

Smectic C* Liquid Crystal Molecular Orientation

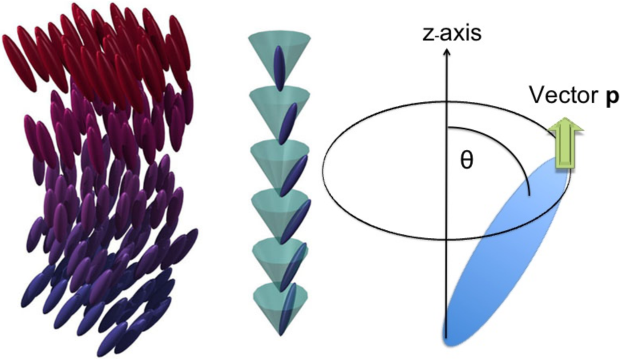
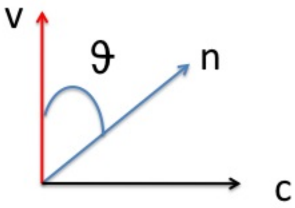


Figure: Left Two Figures Source: http://barrett-group.mcgill.ca/teaching/liquid_crystal/LC03.htm

Director Projection onto Plane



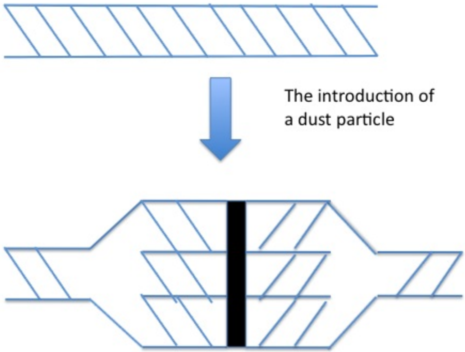
c : c-director

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

$n = \cos(\vartheta)v + \sin(\vartheta)c$

Outline

Introducing a dust particle



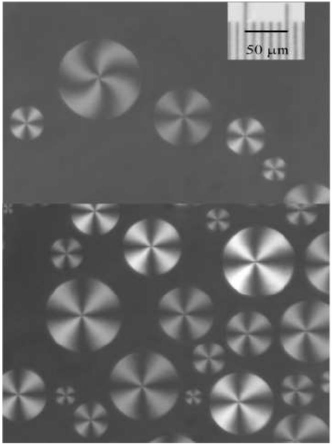
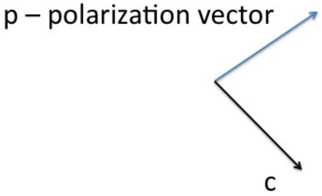


Figure: The effect of impurity ions on a thin film Smectic C* liquid crystal[LPM]

Energy Described over Smectic C* Liquid Crystals

- Consists of elastic energy, anchoring energy at domain boundary, and anchoring energy at boundary of defect core
- Energy from core boundary negligible.
- Anchoring energy at domain boundary results from polarization field.

Effect of polarization field



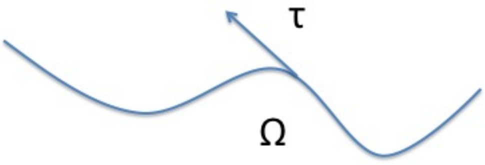
$$\mathbf{p} \| \mathbf{n} \times \mathbf{v} \implies \mathbf{p} \perp \mathbf{c}$$

The elastic energy contribution from the polarization field is described as

$$\int_{\Omega} \nabla \cdot \mathbf{p}\, dx = \int_{\partial\Omega} \mathbf{p} \cdot \nu \, d\sigma$$

where ν is the outer unit normal vector on $\partial\Omega$

Want $\int_{\partial\Omega} \mathbf{p} \cdot \nu \, d\sigma$ to be as negative as possible.
$\implies$ $\mathbf{p} = -\alpha\nu$, $\alpha \in \mathbb{R}_+$ on $\partial\Omega$
$\implies$ $\mathbf{c} \| \tau$ on $\partial\Omega$



Introducing boundary values model effect of spontaneous polarization.

The resulting framework becomes minimizing

$$\int_{\Omega} k_1(\text{div } u)^2 + k_2(\text{curl } u)^2 \, dA$$

$$u = (u_1, u_2), |u| = 1$$

$$\text{div } u = \partial_{x_1} u_1 + \partial_{x_2} u_2, \quad \text{curl } u = \partial_{x_1} u_2 - \partial_{x_2} u_1$$

splay and bend constants $k_1, k_2 > 0$, $k_1 \neq k_2$ to incorporate electrostatic contribution from **p**.

$$\{u \in H^1(\Omega) : |u(x)| = 1 \text{ for } x \in \Omega \text{ and } u = g \text{ on } \partial\Omega\} = \emptyset$$

for deg $g := d > 0$.

Outline

We study instead

$$\begin{aligned} J_\varepsilon(u) &= \frac{1}{2}\int_\Omega k_1(\operatorname{div} u)^2 + k_2(\operatorname{curl} u)^2 + \frac{1}{2\varepsilon^2}(1-|u|^2)^2\,dx \\ &= \int_\Omega j_\varepsilon(u,\nabla u)\,dx \end{aligned} \tag{1}$$

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

where g is smooth on $\partial\Omega$, $|g| = 1$, and $\deg g = d > 0$

Set $\underline{k} = \min(k_1, k_2)$.

$$\begin{aligned} & k_1(\text{div } u)^2 + k_2(\text{curl } u)^2 \\ & = k_1|\nabla u|^2 + (k_2 - k_1)(\text{curl } u)^2 + 2k_1 \det \nabla u \\ & = k_2|\nabla u|^2 + (k_1 - k_2)(\text{div } u)^2 + 2k_2 \det \nabla u \end{aligned}$$

If $\underline{k} = k_1$, all constants in second line are positive and if $\underline{k} = k_2$, all constants in third line are positive.

Splay Configuration

$$u_s = \pm \frac{x}{|x|} = \pm \frac{(x_1, x_2)}{|x|}$$

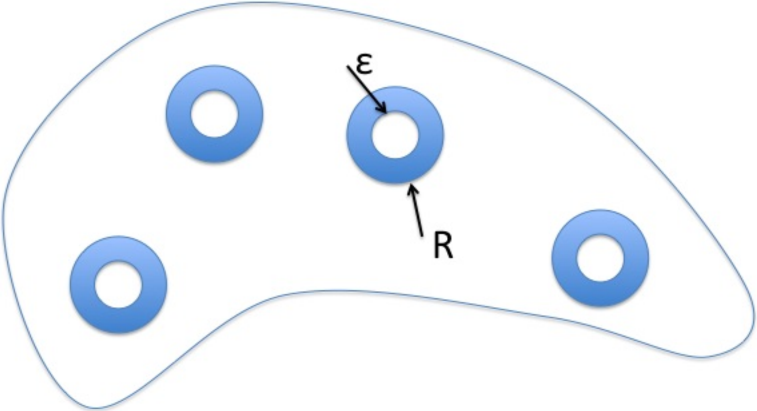
$$\text{curl } u_s = 0 \implies (\text{div } u_s)^2 = |\nabla u_s|^2 = \frac{1}{|x|^2} \text{ for } x \neq 0$$

Bend Configuration

$$u_b = \pm\frac{x^t}{|x|} = \pm\frac{(-x_2, x_1)}{|x|} = \pm i\frac{x}{|x|}$$

$$\text{div } u_b = 0 \implies (\text{curl } u_b)^2 = |\nabla u_b|^2 = \frac{1}{|x|^2} \text{ for } x \neq 0$$

Choose $b_1, \ldots, b_d$, fix $R > 0$ and define a particular test function $\tilde{u}_\varepsilon$.



Let $u_\varepsilon \in H^1_g(\Omega;\mathbb{R}^2)$ be a minimizer to J_ε in the set of admissible functions. Then from our construction

$$J_\varepsilon(u_\varepsilon) \leq J_\varepsilon(\tilde{u}_\varepsilon) \leq \underline{k}\pi d \log(\frac{1}{\varepsilon}) + C_1$$

Now, note that $\underline{k}\int_\Omega \det \nabla u\, dx = \underline{k}\pi d$ for all u in the set of admissible functions. Hence, if $\underline{k} = k_1$,

$$\begin{aligned}
&\int_\Omega k_1(\operatorname{div}\, u)^2 + k_2(\operatorname{curl}\, u)^2\, dx \\
&= \int_\Omega \underline{k}|\nabla u|^2 + (k_2 - \underline{k})(\operatorname{curl}\, u)^2 + 2\underline{k}\det \nabla u\, dx \\
&= \int_\Omega \underline{k}|\nabla u|^2 + (k_2 - \underline{k})(\operatorname{curl}\, u)^2\, dx + 2\underline{k}\pi d \\
&\geq \int_\Omega \underline{k}|\nabla u|^2\, dx
\end{aligned}$$

$$J_\varepsilon(u_\varepsilon) \geq \frac{1}{2}\int_\Omega \underline{k}|\nabla u_\varepsilon|^2 + \frac{1}{2\varepsilon^2}(1-|u_\varepsilon|^2)^2\,dx$$
$$\geq \underline{k}\pi d \log(\frac{1}{\varepsilon}) - C_2$$

The last inequality is due to the work of Bethuel, Brezis, and Helein [BBH] and Struwe [St]

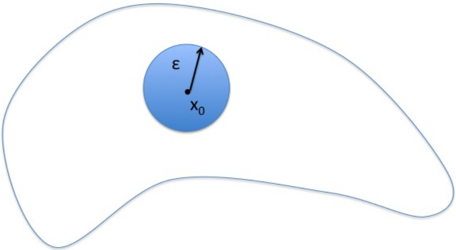
With the two inequalities, we obtain the following estimate

$$\frac{1}{\varepsilon^2}\int_\Omega (1-|u_\varepsilon|^2)^2\,dx \leq C_3$$

From the above inequality, we can show

$$\|u_\varepsilon\|_{C(\overline{\Omega})}, \varepsilon\|\nabla u_\varepsilon\|_{C(\overline{\Omega})} \leq C_4$$

for $0 < \varepsilon < 1$.



Define $v(y) = u_\varepsilon(\varepsilon y + x_0)$, $x_0 \in \overline{\Omega}, y \in B_1(0) := B_1$.
$\Longrightarrow$

$$\int_{B_1} (1 - |v|^2)^2 \, dy \leq C_3$$

E-L Equations

$$-k_1\nabla(\nabla\cdot u)+k_2\nabla\times(\nabla\times u)=\frac{1}{\varepsilon^2}u(1-|u|^2)$$

Identifying $\mathscr{L}u=-k_1\nabla(\nabla\cdot u)+k_2\nabla\times(\nabla\times u)$, then for v defined on B_1 solves

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

$\implies$

$$\|v\|_{C^1(B_{1/2})}\leq C_4$$

where C_4 does not depends on x_0, giving the estimates.

- $J_\varepsilon(u_\varepsilon) \leq \underline{k}\pi d \log(\frac{1}{\varepsilon}) + C_1$
- $J_\varepsilon(u_\varepsilon) \geq \underline{k}\pi d \log(\frac{1}{\varepsilon}) - C_2$
- $\frac{1}{\varepsilon^2}\int_\Omega (1-|u_\varepsilon|^2)^2\,dx \leq C_3$
- $\|u_\varepsilon\|_{C(\overline{\Omega})}, \varepsilon\|\nabla u_\varepsilon\|_{C(\overline{\Omega})} \leq C_4$

With these estimates, using the Structure and Compactness results of Lin [L], we obtain a family $\{u_\varepsilon\}$ of functions that satisfy the following:

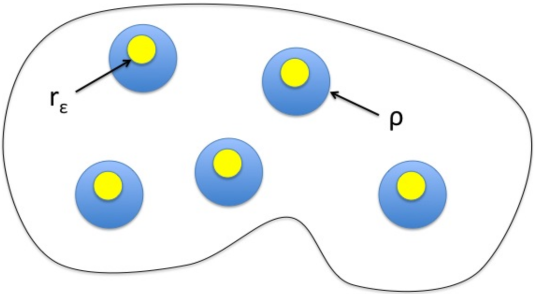
$$u_{\varepsilon_\ell}(x) \to u_*(x) := \prod_{j=1}^{d} \frac{x-a_j}{|x-a_j|} e^{ih(x)}$$

where $a_j \in \Omega$, $a_l \neq a_j$ for $l \neq j$ and $h \in H^1(\Omega)$ for some subsequence $\varepsilon_\ell \to 0$; convergence is strong in L^2 and weakly $H^1_{loc}(\overline{\Omega} \setminus \{a_1, \ldots, a_d\})$.

Because $\{u_\varepsilon\}$ are minimizers to J_ε, we obtain stronger convergence, i.e. $u_{\varepsilon_\ell} \to u_*$ in $C^\alpha_{loc}(\overline{\Omega} \setminus \{a_1, \ldots, a_d\})$ and $C^m_{loc}(\Omega \setminus \{a_1, \ldots, a_d\})$. Furthermore $|u_\ell| \to 1$ uniformily away from $\{a_1, \ldots, a_d\}$.

This gives us information away from the cores but not much about defects or what is occurring near them.

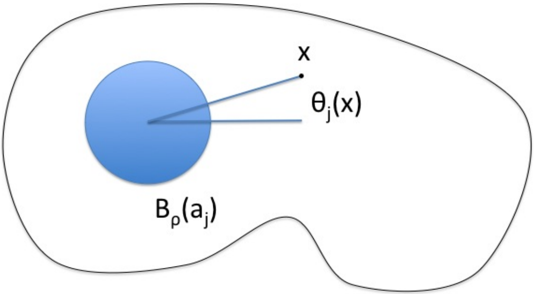
We analyzing the canonical map $u_*(x)$ for x near each defect a_j



$\Omega = (\Omega \setminus \cup_{j=1}^{d} B_\rho(a_j)) \cup (\cup_{j=1}^{d} B_\rho(a_j) \setminus B_{r_\varepsilon}(a_j)) \cup (\cup_{j=1}^{d} B_{r_\varepsilon}(a_j)))$
$\varepsilon << r_\varepsilon = o(1)$

The function $u_* = \prod_{j=1}^{d} \frac{x-a_j}{|x-a_j|} e^{ih(x)}$ satisfies

$$\begin{cases} \int_\Omega k_1|\nabla h|^2 + (k_2 - k_1)(\text{curl } u_*)^2 \, dx < \infty & \text{if } \underline{k} = k_1 \\ \int_\Omega k_2|\nabla h|^2 + (k_1 - k_2)(\text{div } u_*)^2 \, dx < \infty & \text{if } \underline{k} = k_2 \end{cases}$$



$$\frac{x - a_j}{|x - a_j|} = e^{i\theta_j(x)}, x \neq a_j$$

Fix a_n. Then set $\phi_n = \sum_{j \neq n} \theta_j + h$. Then we have

$$\begin{cases} \displaystyle\int_{B_\rho(a_n)} \frac{\sin^2(\phi_n)}{|x-a_n|^2}\,dx \leq C & \text{if } \underline{k} = k_1 \\ \displaystyle\int_{B_\rho(a_n)} \frac{\cos^2(\phi_n)}{|x-a_n|^2}\,dx \leq C & \text{if } \underline{k} = k_2. \end{cases}$$

The constant C does not depend on ρ.

$$\begin{cases} \frac{1}{|\partial B_\rho(a_n)|} \int_{\partial B_\rho(a_n)} \phi_n \, dx \to m_n \pi & \text{for some } m_n \in \mathbb{Z} \text{ if } \underline{k} = k_1 \\ \frac{1}{|\partial B_\rho(a_n)|} \int_{\partial B_\rho(a_n)} \phi_n \, dx \to \frac{\pi}{2} + m_n \pi & \text{for some } m_n \in \mathbb{Z} \text{ if } \underline{k} = k_2. \end{cases}$$

In terms of the limit function, the above limit implies that

$$u_*(\rho y + a_n) \to \begin{cases} \pm y & \text{if } \underline{k} = k_1 \\ \pm i y & \text{if } \underline{k} = k_2 \end{cases}$$

in $L^2(\partial B_1)$ as $\rho \to 0$. Hence, one pattern has less energy than the other in either case. ($k_2 < k_1 \implies$ bend pattern has less energy than splay pattern)

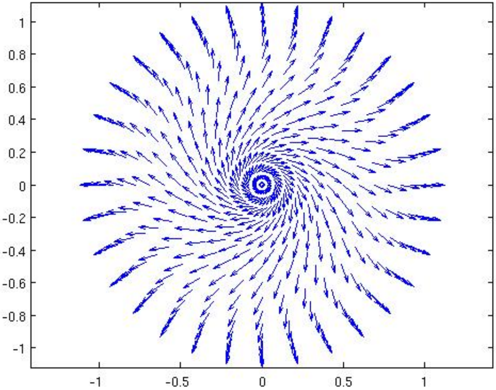


Figure: $g = e^{i\theta}, k_2 < k_1$

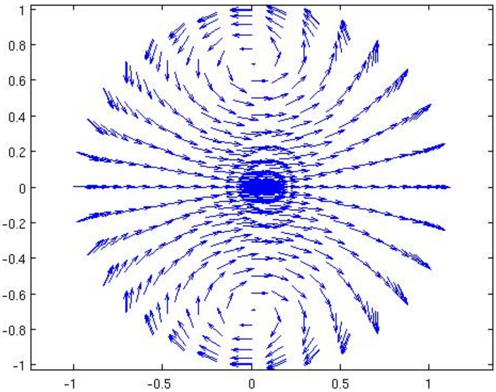
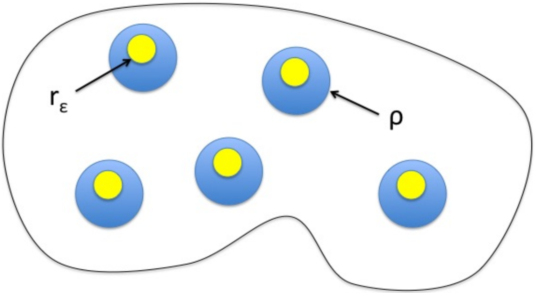


Figure: $g = e^{2i\theta}, k_2 < k_1$

Now we want to show that these locations minimize the energy over the domain. Again, construct the proper test function $\tilde{v}_\ell$



Let $\mathbf{a} = (a_1, \ldots, a_d)$, for simplicity, let $\underline{k} = k_1$. Then we can write

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

Using the constructed test function, we can show

$$\lim_{\ell\to\infty}\left(J_{\varepsilon_\ell}(u_\ell) - \underline{k}\pi d \ln\left(\frac{1}{\varepsilon_\ell}\right)\right) = \underline{k}W(\mathbf{a}) + H(\mathbf{a}, k_1, k_2) + d\gamma$$

where $\mathbf{a}$ minimizes $\underline{k}W(\mathbf{b}) + H(\mathbf{b}, k_1, k_2)$, $b \in \Omega^d$.

$G_{\mathbf{b}} = \sum_{n=1}^{d} \ln(|x - b_n|)$,

$$W(\mathbf{b}) = \frac{1}{2}\int_{\partial\Omega} 2G_{\mathbf{b}}(\partial_\tau g \times g) - (\partial_\nu G_{\mathbf{b}})G_{\mathbf{b}}\, d\sigma + \pi d - \sum_{m \neq n} \pi \ln(|b_n - b_m|)$$

and

$$\mathscr{H}(\mathbf{b}, \phi, k_1, k_2) = \frac{1}{2}\int_{\Omega} k_1 |\nabla\phi|^2 + (k_2 - k_1)(\text{curl } v)^2\, dx \text{ if } \underline{k} = k_1$$

$$H(\mathbf{b}, k_1, k_2) := \min_{\phi} \mathscr{H}(\mathbf{b}, \phi, k_1, k_2)$$

$$v = \prod_{j=1}^{d} \frac{x - b_j}{|x - b_j|} e^{i\phi(x)}$$

Outline

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Thank you!