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

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Colbert-Kelly | Analysis of a G-L Energy |
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)
- \( \varepsilon \) - coherence length which can depend on temperature \( (\xi(T)) \)/diffuse interface/core radius
When in equilibrium, the order parameter $u$ minimizes $E_\varepsilon$. Taking variations of $u$, the following must be satisfied

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

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

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: \(u_\varepsilon = \tanh\left(\frac{x}{\sqrt{2}\varepsilon}\right)\) 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

1. Ginzburg-Landau (GL) Functional
2. Introduction to Liquid Crystals (LCs)
3. Effects of Defects in Liquid Crystals
4. The Generalized GL Functional
5. References
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

\[ n = \cos(\vartheta)v + \sin(\vartheta)c \]

\[ |n| = |c| = |v| = 1 \]
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

\[ p \parallel n \times v \implies p \perp c \]

The elastic energy contribution from the polarization field is described as

\[ \int_{\Omega} \nabla \cdot p \, dx = \int_{\partial \Omega} p \cdot \nu \, d\sigma \]

where \( \nu \) is the outer unit normal vector on \( \partial \Omega \).
Want $\int_{\partial \Omega} p \cdot \nu \, d\sigma$ to be as negative as possible.

$\Rightarrow \quad p = -\alpha \nu, \; \alpha \in \mathbb{R}_+ \; \text{on} \; \partial \Omega$

$\Rightarrow \quad c \parallel \tau \; \text{on} \; \partial \Omega$

Introducing boundary values model effect of spontaneous polarization.
The resulting framework becomes minimizing

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

\[ u = (u_1, u_2), \quad |u| = 1 \]

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

splay and bend constants \( k_1, k_2 > 0, \ k_1 \neq k_2 \) to incorporate electrostatic contribution from \( \mathbf{p} \).

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

for \( \text{deg } g := d > 0 \).
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We study instead

\[
J_\varepsilon(u) = \frac{1}{2} \int_\Omega k_1 (\text{div } u)^2 + k_2 (\text{curl } u)^2 + \frac{1}{2\varepsilon^2} (1 - |u|^2)^2 \, dx \\
= \int_\Omega j_\varepsilon(u, \nabla u) \, dx
\]

where  

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

where \(g\) is smooth on \(\partial\Omega\), \(|g| = 1\), and \(\text{deg } g = d > 0\).
Set $k = \min(k_1, k_2)$.

\[
k_1 (\text{div } u)^2 + k_2 (\text{curl } u)^2
\]

\[
= k_1 |\nabla u|^2 + (k_2 - k_1) (\text{curl } u)^2 + 2k_1 \det \nabla u
\]

\[
= k_2 |\nabla u|^2 + (k_1 - k_2) (\text{div } u)^2 + 2k_2 \det \nabla u
\]

If $k = k_1$, all constants in second line are positive and if $k = k_2$, all constants in third line are positive.
Splay Configuration

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

\[ \nabla \times u_s = 0 \implies (\nabla \cdot u_s)^2 = |\nabla u_s|^2 = \frac{1}{|x|^2} \text{ for } x \neq 0 \]
Bend Configuration

\[ u_b = \pm \frac{x^t}{|x|} = \pm \left(-x_2, x_1\right) = \pm i \frac{x}{|x|} \]

\[ \text{div} \ u_b = 0 \implies (\text{curl} \ u_b)^2 = |\nabla u_b|^2 = \frac{1}{|x|^2} \text{ for } x \neq 0 \]
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 $J_\varepsilon$ in the set of admissible functions. Then from our construction

$$J_\varepsilon(u_\varepsilon) \leq J_\varepsilon(\tilde{u}_\varepsilon) \leq k\pi d \log\left(\frac{1}{\varepsilon}\right) + C_1$$
Now, note that \( k \int_\Omega \det \nabla u \, dx = k \pi d \) for all \( u \) in the set of admissible functions. Hence, if \( k = k_1 \),

\[
\int_\Omega k_1 (\text{div} \, u)^2 + k_2 (\text{curl} \, u)^2 \, dx \\
= \int_\Omega k |\nabla u|^2 + (k_2 - k) (\text{curl} \, u)^2 + 2k \det \nabla u \, dx \\
= \int_\Omega k |\nabla u|^2 + (k_2 - k) (\text{curl} \, u)^2 \, dx + 2k \pi d \\
\geq \int_\Omega k |\nabla u|^2 \, dx
\]
\[ J_\varepsilon(u_\varepsilon) \geq \frac{1}{2} \int_\Omega k |\nabla u_\varepsilon|^2 + \frac{1}{2\varepsilon^2} (1 - |u_\varepsilon|^2)^2 \, dx \]

\[ \geq k \pi d \log \left( \frac{1}{\varepsilon} \right) - C_2 \]

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

$$\Rightarrow \quad \int_{B_1} (1 - |v|^2)^2 \, dy \leq C_3$$
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 \( \mathcal{L} u = -k_1 \nabla (\nabla \cdot u) + k_2 \nabla \times (\nabla \times u) \), then for \( v \) defined on \( B_1 \) solves

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

\[ \Rightarrow \]

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

where \( C_4 \) does not depends on \( x_0 \), giving the estimates.
\[ J_\varepsilon(u_\varepsilon) \leq k\pi d \log \left( \frac{1}{\varepsilon} \right) + C_1 \]
\[ J_\varepsilon(u_\varepsilon) \geq k\pi d \log \left( \frac{1}{\varepsilon} \right) - C_2 \]
\[ \frac{1}{\varepsilon^2} \int_{\Omega} (1 - |u_\varepsilon|^2)^2 \, dx \leq C_3 \]
\[ \|u_\varepsilon\|_{C(\overline{\Omega}), \varepsilon\|\nabla u_\varepsilon\|_{C(\overline{\Omega})} \leq C_4 \]

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

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

where \( a_j \in \Omega, a_l \neq a_j \) for \( l \neq j \) and \( h \in H^1(\Omega) \) for some subsequence \( \varepsilon_\ell \rightarrow 0 \); convergence is strong in \( L^2 \) and weakly \( H^1_{loc}(\overline{\Omega} \setminus \{a_1, \ldots, a_d\}) \).
Because \( \{u_\epsilon\} \) are minimizers to \( J_\epsilon \), we obtain stronger convergence, i.e. \( u_\epsilon \rightharpoonup u^* \) in \( C^\alpha_{\text{loc}}(\Omega \setminus \{a_1, \ldots, a_d\}) \) and \( C^m_{\text{loc}}(\Omega \setminus \{a_1, \ldots, a_d\}) \). Furthermore \( |u_\ell| \to 1 \) uniformly 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 $a_j$

\[
\Omega = (\Omega \setminus \bigcup_{j=1}^d B_\rho(a_j)) \cup (\bigcup_{j=1}^d B_\rho(a_j) \setminus B_{r_\varepsilon}(a_j)) \cup (\bigcup_{j=1}^d B_{r_\varepsilon}(a_j))
\]

$\varepsilon \ll r_\varepsilon = o(1)$
The function \( u_\star = \prod_{j=1}^{d} \frac{x-a_j}{|x-a_j|} e^{ih(x)} \) satisfies

\[
\begin{align*}
\int_{\Omega} k_1 |\nabla h|^2 + (k_2 - k_1)(\text{curl } u_\star)^2 \, dx < \infty & \quad \text{if } k = k_1 \\
\int_{\Omega} k_2 |\nabla h|^2 + (k_1 - k_2)(\text{div } u_\star)^2 \, dx < \infty & \quad \text{if } k = k_2
\end{align*}
\]
\[ \frac{x - a_j}{|x - a_j|} = e^{i\theta_j(x)}, \quad x \neq a_j \]
Fix \( a_n \). Then set \( \phi_n = \sum_{j \neq n} \theta_j + h \). Then we have

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

The constant \( C \) does not depend on \( \rho \).
\[
\begin{cases}
\frac{1}{|\partial B_\rho(a_n)|} \int_{\partial B_\rho(a_n)} \phi_n \, dx \to m_n\pi & \text{for some } m_n \in \mathbb{Z} \text{ if } k = k_1 \\
\frac{1}{|\partial B_\rho(a_n)|} \int_{\partial B_\rho(a_n)} \phi_n \, dx \to \frac{\pi}{2} + m_n\pi & \text{for some } m_n \in \mathbb{Z} \text{ if } k = k_2.
\end{cases}
\]

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

\[u_*(\rho y + a_n) \to \begin{cases}
\pm y & \text{if } k = k_1 \\
\pm iy & \text{if } k = k_2
\end{cases}\]

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 $\tilde{v}_\ell$. 

\[ r_\varepsilon \quad \rho \]
Let \( a = (a_1, \ldots, a_d) \), for simplicity, let \( k = k_1 \). Then we can write

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

Using the constructed test function, we can show

\[
\lim_{\ell \to \infty} \left( J_{\epsilon_{\ell}} (u_{\ell}) - k\pi d \ln \left( \frac{1}{\epsilon_{\ell}} \right) \right) = kW(a) + H(a, k_1, k_2) + d\gamma
\]

where \( a \) minimizes \( kW(b) + H(b, k_1, k_2) \), \( b \in \Omega^d \).
\[ G_b = \sum_{n=1}^{d} \ln(|x - b_n|), \]

\[ W(b) = \frac{1}{2} \int_{\partial \Omega} 2G_b(\partial_\tau g \times g) - (\partial_\nu G_b)G_b \, d\sigma + \pi d \]

\[ - \sum_{m \neq n} \pi \ln(|b_n - b_m|) \]

and

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

\[ H(b, k_1, k_2) := \min_{\phi} \mathcal{H}(b, \phi, k_1, k_2) \]

\[ v = \prod_{j=1}^{d} \frac{x - b_j}{|x - b_j|} e^{i\phi(x)} \]
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Thank you!