Some Mathematical Analysis of Molecules in Ferroelectric Liquid Crystals

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Outline

Liquid Crystal Phases

Liquid Crystal is a state of matter between liquid and solid.

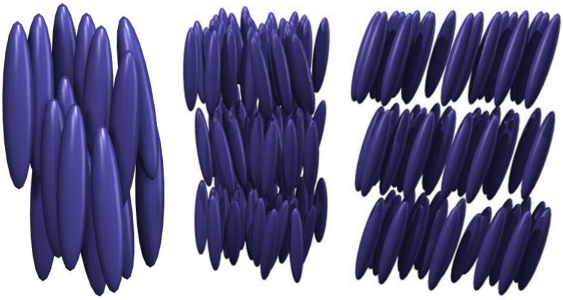


Figure : Nematic(left), Smectic A(middle), Smectic C(right)

Chiral Liquid Crystal

Figure : Chiral Phase

Chiral Liquid Crystal

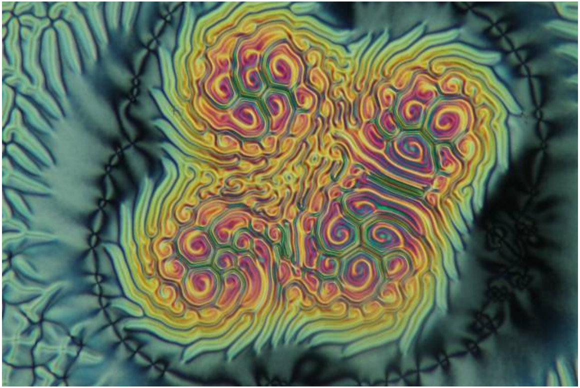


Figure : from tywkiwdbi.blogspot.com

Chiral Smectic C Phase

- Smectic C + Chiral molecules
- $\mathbf{P} = P_0 \mathbf{n} \times \nabla\omega$: P_0 is a fixed constant depending on the material

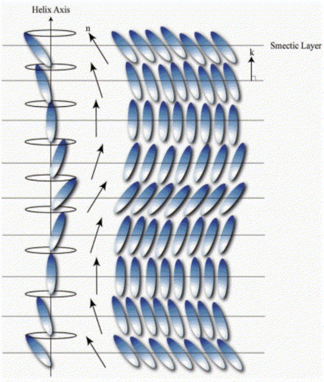


Figure : from www.sciencedirect.com

Tristable Switching

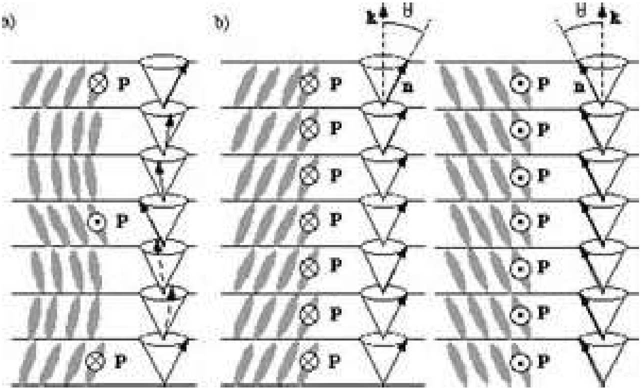
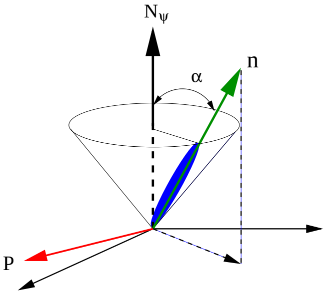


Figure : from www.gekandfly.com

Chiral Smectic C Phase

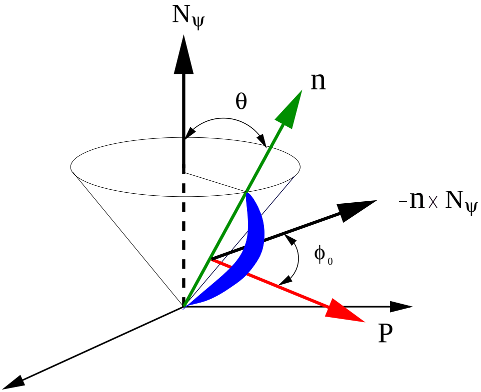
Variables: **n**, **P**, $\psi = \rho e^{i\omega}$ (level sets of ω are corresponding to smectic layers)

$$\mathbf{N}_\psi = -\frac{i}{2}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) = \rho^2\nabla\omega.$$



Bent Core Molecules

$$\mathbf{N}_\psi = -\frac{i}{2}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) = \rho^2\nabla\omega.$$



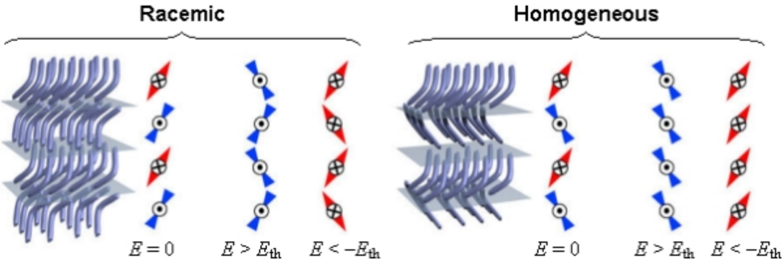


Figure : from barrett-group.mcgill.ca

How to describe liquid crystals?

Suppose that molecules occupy a C^2-domain Ω in $\mathbf{R}^3$,

- nematic liquid crystals : $\mathbf{n}$, a map from Ω to $\mathbb{S}^2$
- smectic liquid crystals: $\mathbf{n}$, $\psi = \rho e^{i\omega}$ (level sets of ω are corresponding to smectic layers)
- chiral smectic and bent core molecules: $\mathbf{n}, \psi, \mathbf{P}$(polarization field)

Nematic Liquid Crystals

Minimize the Oseen-Frank Energy of nematic liquid crystals

$$\mathcal{W} = \int_\Omega F_{OF}$$

$$F_{OF} = K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n} + \tau)^2 + K_3|\mathbf{n} \times \nabla \times \mathbf{n} + \mathbf{b}|^2$$

$$+(K_2 + K_4)(\mathrm{tr}(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2)$$

$$\mathbf{n} : \Omega \to \mathbb{S}^2$$

where $0 < K_2 + K_4 \leq \min\{K_1, K_3\}, K_4 \leq 0, \tau \in \mathbf{R}$, and $\mathbf{b} \in L^2(\Omega)$.

Smectic Liquid Crystals

Investigate minimum energy configurations of

$$\mathcal{E}_{Sm} = \int_{\Omega} \{F_{OF} + F_{Sm} + F_P + F_E\}$$

subject to

$$-\nabla \cdot ((I + \varepsilon_a \mathbf{n} \otimes \mathbf{n})\mathbf{E}) = \nabla \cdot \mathbf{P} \text{ in } \Omega,$$

$$-\nabla \cdot \varepsilon_0 E = 0 \text{ in } \mathbf{R}^3 - \Omega,$$

$$\nabla \times \mathbf{E} = 0 \text{ in } \mathbf{R}^3,$$

$$[(I + \varepsilon_a \mathbf{n} \otimes \mathbf{n})\mathbf{E} - \varepsilon_0 \mathbf{E}] \cdot \nu = (\mathbf{P} \cdot \nu) \text{ on } \partial\Omega,$$

where ν is outward normal vector to the boundary.

$$F_{Sm} = a_\perp |D_\perp \cdot D_\perp \psi|^2 - c_\perp |D_\perp \psi|^2 + a_\| |D_\| \cdot D_\| \psi|^2 + c_\| |D_\| \psi|^2 + r|\psi|^2 + \frac{g}{2}|\psi|^4$$

$$F_P = B(\nabla \mathbf{P})^2 + \frac{1}{\eta^2}(|\mathbf{P}|^2 - P_0^2)^2$$

or $\quad \frac{1}{\eta^2}|\mathbf{P}|^2[(|\mathbf{P}|^2 - P_0^2)^2 - \alpha]^2$

$$F_E = -\frac{1}{2}[(I + \varepsilon_a \mathbf{n} \otimes \mathbf{n})\mathbf{E}] \cdot \mathbf{E} - \mathbf{E} \cdot \mathbf{P}$$

$$\tilde{F}_p = B|\nabla \mathbf{P}|^2 + \frac{1}{\eta^2}(|\mathbf{P}|^2 - P_0^2)^2 + \frac{1}{2}K_c \left| (\mathbf{n} \times \mathbb{N}_\psi \cdot \mathbf{P})^2 (\mathbf{n} \cdot \mathbb{N}_\psi)^2 - \chi_0^2 |\mathbf{P}|^4 |\mathbb{N}_\psi|^4 \right|^s$$

where

$D = \nabla - iq\mathbf{n}, \quad D_\| = (\mathbf{n} \cdot \nabla - iq)\mathbf{n}, \quad D_\perp = D - D_\|, \psi = \rho e^{i\omega}, r = a(T - T^*), a > 0, g > 0, a_\perp > 0, a_\| > 0, B > 0.$

Nematic Energy $\mathcal{W}$

$$H^1(\Omega, \mathbf{R}^3) = \{\mathbf{u} : \Omega \to \mathbf{R}^3 : \mathbf{u} \in L^2, \nabla \mathbf{u} \in L^2\}$$

$$H^1(\Omega, \mathbb{S}^2) = \{\mathbf{n} \in H^1(\Omega, \mathbf{R}^3) : |\mathbf{n}| = 1 \text{ a.e. in } \Omega\}$$

$$\mathcal{A}(\mathbf{n}_0) = \{\mathbf{n} \in H^1(\Omega, \mathbb{S}^2) : \mathbf{n} = \mathbf{n}_0 \text{ on } \partial\Omega\}$$

THEOREM 1(Hardt-Kinderlehrer-Lin, 1985): For any Lipschitz function $\mathbf{n}_0 : \partial\Omega \to \mathbb{S}^2$, there exists an $\mathbf{n} \in \mathcal{A}(\mathbf{n}_0)$ such that

$$\mathcal{W}(\mathbf{n}) = \inf_{\mathbf{u} \in \mathcal{A}(\mathbf{n}_0)} \mathcal{W}(\mathbf{u}).$$

THEOREM 2(Hardt-Kinderlehrer-Lin, 1985): If $\mathbf{n} \in \mathcal{A}(\mathbf{n}_0)$ is a minimizer of $\mathcal{W}$, $\mathbf{n}$ is Hölder continuous (smooth) on $\Omega \setminus Z$ for some closed subset Z of Ω which has one dimensional Hausdorff measure zero. In fact,

$$Z = \left\{ a \in \Omega : \limsup_{r \downarrow 0} r^{-1} \int_{\mathbb{B}_r(a)} |\nabla \mathbf{n}|^2 \, d\mathbf{x} > 0 \right\}.$$

Note: $A \subset \mathbf{R}^n, 0 \leq s < \infty, 0 < \delta \leq \infty$,

$$\mathcal{H}^s_\delta(A) = \inf \left\{ \sum_{j=1}^{\infty} \alpha(s) \left(\frac{\text{diam } C_j}{2} \right)^s : A \subset \cup_{j=1}^{\infty} C_j, \text{diam } C_j \leq \delta \right\}$$

where

$$\alpha(s) = \frac{\pi^{\frac{s}{2}}}{\Gamma\left(\frac{s}{2}+1\right)}, \Gamma(s) = \int_0^\infty e^{-x} x^{s-1} \, dx (0 < s < \infty)$$

$$\mathcal{H}^s(A) = \lim_{\delta \to 0} \mathcal{H}^s_\delta(A) = \sup_{\delta > 0} \mathcal{H}^s_\delta(A)$$

is called s-dimensional Hausdorff measure on $\mathbf{R}^n$

In the case, $K_1 = K_2 = K_3 = K, K_4 = 0$,
THEOREM 3(Schoen and Uhlenbeck, 1983): If $\mathbf{n}$ is a minimizer, then $\mathbf{n}$ is Hölder continuous (smooth) on $\Omega \setminus Z$ where Z is a set of finite points.
If $\mathbf{n}$ is a minimizer of $\int_\Omega K|\nabla \mathbf{n}|^2$, then $\mathbf{n}$ satisfies

$$\Delta \mathbf{n} + |\nabla \mathbf{n}|^2 \mathbf{n} = 0, \quad |\mathbf{n}| = 1, \quad \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

whose solutions are called harmonic maps.

Remark

- $\frac{x}{|x|}$ is only the stable minimizer if $K_1 \leq K_2$ on $B(0,1)$ with $\mathbf{n}(x) = x$ on $\mathbb{S}^2$(B. Ou, 1992)
- $\frac{x}{|x|}$ is unstable if $8(K_2 - K_1) + K_3 < 0$(Helein, 1987)
- $\frac{x}{|x|}$ is not an energy minimizer if $K_1 >> K_2 = K_3$(S.-Y. Lin, 1988, Cohen and Taylor,1990, Kinderlerher and Ou, 1992)

Other Related Works and Open Question

Schoen and Uhlenbeck(J. of Diff. Geometry, 1982, 1983), Almgren and Lieb(Annals of math, 1988), Hardt and Kinderlehrer (H. Poincare, 1987), Hardt (Bull. of AMS, 1997), Hardt, Kinderlehrer, and Lin (Comm. Math. Phys., 1986,1988, 1990), Hardt and Lin(1986, 1993), Kinderlehrer and Ou (1992, 1993), Lin (1989, 1991), Lin and Poon(1993), Brezis and Coron, and Lieb(1986), Cohen et al (1989, 1990), L. Simon(1996),...

Open Problem: Is the singular set Z finite in THEOREM 2? Some numerical simulations showed that it seems to be finite, but there is no theoretical result. Monotonicity inequality is the main issue.

Smectic Liquid Crystals

Consider

$$\mathcal{E}_{Sm} = \int_{\Omega} \{F_{OF} + F_{Sm} + F_P + F_E\}$$

subject to

$$-\nabla \cdot ((I + \varepsilon_a \mathbf{n} \otimes \mathbf{n})\mathbf{E}) = \nabla \cdot \mathbf{P} \text{ in } \Omega,$$

$$-\nabla \cdot \mathbf{E} = 0 \text{ in } \mathbf{R}^3 - \Omega,$$

$$\nabla \times \mathbf{E} = 0 \text{ in } \mathbf{R}^3,$$

$$[(I + \varepsilon_a \mathbf{n} \otimes \mathbf{n})\mathbf{E} - \varepsilon_0 \mathbf{E}] \cdot \nu = (\mathbf{P} \cdot \nu) \text{ on } \partial\Omega,$$

where ν is outward normal vector to the boundary.

$$F_{Sm} = a_\perp |D_\perp \cdot D_\perp \psi|^2 - c_\perp |D_\perp \psi|^2 + a_\| |D_\| \cdot D_\| \psi|^2 + c_\| |D_\| \psi|^2 + r|\psi|^2 + \frac{g}{2}|\psi|^4$$ (Chen-Lubensky,1976)

$$F_P = B(\nabla \mathbf{P})^2 + \frac{1}{\eta^2}(|\mathbf{P}|^2 - P_0^2)^2$$

$$F_E = -\frac{1}{2}[(I + \varepsilon_a \mathbf{n} \otimes \mathbf{n})\mathbf{E}] \cdot \mathbf{E} - \mathbf{E} \cdot \mathbf{P}$$

where

$D = \nabla - iq\mathbf{n}, \quad D_\| = (\mathbf{n} \cdot \nabla - iq)\mathbf{n}, \quad D_\perp = D - D_\|, \psi = \rho e^{i\omega}, r = a(T - T^*), a > 0, g > 0, a_\perp > 0, a_\| > 0, B > 0.$

Smectic Energy $\mathcal{E}_{Sm}$

Prior works regarding to the smectic energy:

- Phase Transition between chiral nematic and chiral smectic A (P. Bauman, M. Calderer, C. Liu and D. Phillips, Arch. Ration. Mech. Anal. 2002)
- Asymptotic limit for Smectic A (B.Heffler and X.B. Pan, J. Funct. Anal. 2008)
- Study with small Ginzburg-Landau parameter(X.B. Pan, SIAM, 2006)
- Existence results and asymptotic study for $|\psi| = 1$ (with M. Calderer, SIAM, 2006)
- Existence and other results with $\psi\big|_{\partial\Omega} = 0$ (S. Joo and D. Phillips, Comm. Math. Phys, 2007)
- Asymptotic Study with a special geometry (with Chen, and Shen, DCDS-A, 2010)

Smectic Energy $\mathcal{E}_{Sm}$

- Bent Core Fibers (P. Bauman and D. Phillips, DCDS, 2012)
- Partial Regulairy for Smectic A (D.Liu, Nonlinear Anal. 2013)
- Study undulation (G. Cervera and S. Joo, Arch. Ration. Mech. Anal., 2012)
- Dynamics of smectic C $\psi\big|_{\partial\Omega} = 0$ (M. C. Calderer and S. Joo, SIAM J. App. Math, 2008)
- There are many other works with different types of smectic energies in the literature which I am not able to list all of them(M. Cepic,B. Zeks,N. Vaupotic, M. Copic, S. Kralj, R. Kamien,...)

Uniformly Smectic States

$$\mathcal{B} = \left\{(\psi, \mathbf{n}) \in H^1(\Omega; \mathbb{C}) \times H^1(\Omega; \mathbb{S}^2) : D_\perp\psi, D_\parallel\psi \in H(div; \Omega)\right\}$$

$$H(div; \Omega) = \left\{\mathbf{v} \in L^2(\Omega; \mathbb{C}^3) : div\mathbf{v} \in L^2(\Omega)\right\}$$

$$\mathcal{F} = \int_\Omega F_{OF} + F_{Sm}$$

$$\mathcal{B}_0 = \left\{(\psi, \mathbf{n}) \in \mathcal{B} : |\psi| = \rho_0 \text{ a.e. in } \Omega\right\}$$

$$\mathcal{F} = \int_\Omega F_{OF} + F_{Sm}$$

THEOREM 4 [with P. Bauman and D. Phillips, submitted]If $\mathcal{K}$ is a non-empty, weakly closed subset of $\mathcal{B}_0$, then there exists $(\tilde{\psi}, \tilde{\mathbf{n}}) \in \mathcal{K}$ such that

$$\mathcal{F}(\tilde{\psi}, \tilde{\mathbf{n}}) = \inf_{(\psi, \mathbf{n}) \in \mathcal{K}} \mathcal{F}(\psi, \mathbf{n}).$$

Strong Anchoring Boundary Conditions

$$\mathcal{B}_1 = \left\{(\psi, \mathbf{n}) \in \mathcal{B} : \psi - \psi_0 \in H_0^1(\Omega)\right\}$$

THEOREM 5 [with P. Bauman and D. Phillips, submitted] If $\mathcal{K}$ is a non-empty, weakly closed subset of $\mathcal{B}_1$, then there exists $(\tilde{\psi}, \tilde{\mathbf{n}}) \in \mathcal{K}$ such that

$$\mathcal{F}(\tilde{\psi}, \tilde{\mathbf{n}}) = \inf_{(\psi, \mathbf{n}) \in \mathcal{K}} \mathcal{F}(\psi, \mathbf{n}).$$

Weak Anchoring Conditions

$$\mathcal{B}_2 = \left\{(\psi, \mathbf{n}) \in \mathcal{B} : \nabla_\perp \psi \cdot \nu := (\nabla\psi - (\mathbf{n} \cdot \nabla\psi)\mathbf{n}) \cdot \nu \in L^2(\partial\Omega)\right\}$$

THEOREM 6 [with P. Bauman and D. Phillips, submitted] Let $\mathcal{K}$ be a non-empty, weakly closed subset of $\mathcal{B}_2$. Then there exists $(\tilde{\psi}, \tilde{\mathbf{n}}) \in \mathcal{K}$ such that

$$\tilde{\mathcal{F}}(\tilde{\psi}, \tilde{\mathbf{n}}) = \inf_{(\psi,\mathbf{n})\in\mathcal{K}} \tilde{\mathcal{F}}(\psi, \mathbf{n}),$$

$$\tilde{\mathcal{F}}(\psi, \mathbf{n}) = \mathcal{F}(\psi, \mathbf{n}) + \alpha_1 \int_{\partial\Omega} |\psi - g_1|^2 + \alpha_2 \int_{\partial\Omega} |\nabla_\perp \psi \cdot \nu - g_2|^2,$$

with $\alpha_1 \geq 0, \alpha_2 > 0$, and $g_1, g_2 \in L^2(\partial\Omega)$.

Bookshelf Geometry

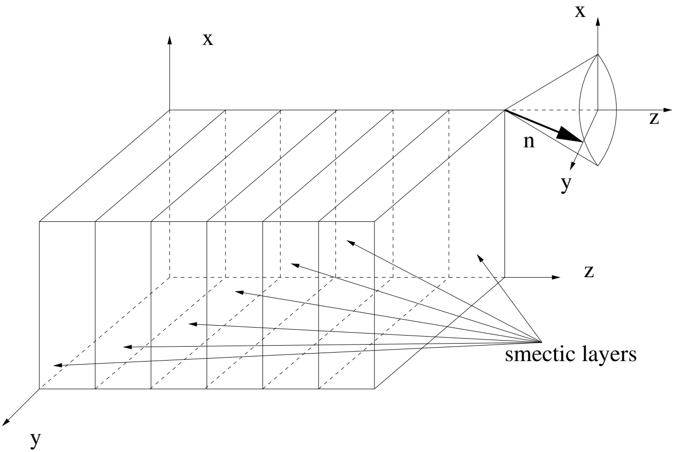


Figure : Bookshelf Geometry

Partial Regularity

Assuming a special geometry(a bookshelf geometry) with saturation ($|\mathbf{P}| = P_0$), we have

$$\mathcal{E}(\mathbf{n}, \mathbf{p}, \varphi) = \int_\Omega \{F_N + F_P + F_\varphi\}\, d\mathbf{x} + \frac{1}{2}\varepsilon_0 \int_{\mathbf{R}^3\setminus\Omega} |\nabla\varphi|^2\, d\mathbf{x}$$

$$\begin{cases} -\nabla\cdot((\varepsilon_\perp \mathbf{I} + \varepsilon_a \mathbf{n}\otimes\mathbf{n})\nabla\varphi) = \nabla\cdot\mathbf{p} \text{ in } \Omega, \\ -\Delta\varphi = 0 \text{ in } \mathbf{R}^3 - \Omega, \\ -[(\varepsilon_\perp \mathbf{I} + \varepsilon_a \mathbf{n}\otimes\mathbf{n})\nabla\varphi - \varepsilon_0\nabla\varphi]\cdot\nu = \mathbf{p}\cdot\nu \text{ on } \partial\Omega, \end{cases}$$

where $a > 0$, $a^2 + c^2 = 1$, $|\mathbf{n}| = |\mathbf{p}| = 1$,

$$F_N = K_1(\nabla\cdot\mathbf{n})^2 + K_2(\mathbf{n}\cdot\nabla\times\mathbf{n}+\tau)^2 + K_3|\mathbf{n}\times(\nabla\times\mathbf{n})-\mathbf{p}|^2$$

$$+(K_2+K_4)(tr(\nabla\mathbf{n})^2-(\nabla\cdot\mathbf{n})^2)+\frac{1}{\epsilon^2}\Big((n_3-a)^2+(n_1^2+n_2^2-c^2)^2\Big),$$

$$F_P = B|\nabla\mathbf{p}|^2 + \alpha\left[(\mathbf{n}\times\mathbf{e}_3\cdot\mathbf{p})^2(\mathbf{n}\cdot\mathbf{e}_3)^2-\chi_0^2\right]^2,$$

$$F_\varphi = \frac{1}{2}(\varepsilon_\perp|\nabla\varphi|^2+\varepsilon_a(\mathbf{n}\cdot\nabla\varphi)^2),$$

with $\alpha > 0, \epsilon > 0$, and a potential function φ for electric field $\mathbf{E}$, i.e. $\mathbf{E} = \nabla\varphi$.

THEOREM 7[with K. Kang, to appear in DCDS-A, 2013] If $(\mathbf{n}, \mathbf{p})$ is a minimizing pair and $\frac{1}{r_0}\int_{\mathbb{B}_{r_0}(a)} \left(|\nabla \mathbf{n}|^2 + |\nabla \mathbf{p}|^2\right) dx < \epsilon^2$ on $\mathbb{B}_{r_0}(a)$ for some $r_0 > 0$, then

$$\frac{1}{r}\int_{\mathbb{B}_r(a)} \left(|\nabla \mathbf{n}|^2 + |\nabla \mathbf{p}|^2\right) dx \le Cr^{\beta}$$

for any $\mathbb{B}_r(a) \subset \mathbb{B}_{r_0}(a) \subset \Omega$. Moreover, $\mathbf{n}$ and $\mathbf{p}$ are Hölder continuous on $\Omega \setminus Z$ where Z is a closed subset of Ω of one dimensional Hausdorff measure zero. Moreover, if $K_1 = K_2 = K_3 = K > 0$, then Z is a finite subset of Ω.

LEMMA 8 (Hybrid inequality) Let Ω be a domain of smooth boundary and $a \in \Omega$. Suppose that $(\mathbf{n}, \mathbf{p}, \varphi)$ be a minimizing triple in Ω. Then for any $\mathbb{B}_\rho(a) \subset \Omega$ and for any $0 < \lambda < 1$ there exists $C_0 > 0$ such that the following inequality is satisfied:

$$\left(\frac{\rho}{2}\right)^{-1} \int_{\mathbb{B}_{\frac{\rho}{2}}(a)} (|\nabla \mathbf{n}|^2 + |\nabla \mathbf{p}|^2)\, dx$$

$$\leq \lambda \rho^{-1} \int_{\mathbb{B}_\rho(a)} (|\nabla \mathbf{n}|^2 + |\nabla \mathbf{p}|^2)\, dx$$

$$+C_0\left(\rho^\beta + \lambda^{-1}\rho^{-3} \int_{\mathbb{B}_\rho(a)} (|\mathbf{n} - \mu_1|^2 + |\mathbf{p} - \mu_2|^2)\, dx\right),$$

where $\mu_1, \mu_2 \in \mathbf{R}^3$ are arbitrary constant vectors and $0 < \beta \leq \frac{1}{2}$.

LEMMA 9 (Energy decay estimate) Let $(\mathbf{n}, \mathbf{p}, \varphi) \in W^{1,2}(\Omega; \mathbb{S}^2) \times W^{1,2}(\Omega; \mathbb{S}^2) \times W^{1,2}(\mathbf{R}^3)$ be a minimizer in Ω. There exist ϵ_0, r_0, η and $\theta < 1$ such that if $\frac{1}{r_0}\mathbb{E}_{r_0}(\mathbf{n}, \mathbf{p}) < \epsilon_0^2$, then for any r with $0 < r < r_0$

$$\frac{1}{\theta r}\mathbb{E}_{\theta r}(\mathbf{n}, \mathbf{p}) \leq \theta \max \left\{ \eta r^{\beta}, \frac{1}{r}\mathbb{E}_r(\mathbf{n}, \mathbf{p}) \right\}.$$

where

$$\mathbb{E}_r(\mathbf{n}, \mathbf{p}) := \int_{\mathbb{B}_r(a)} (|\nabla \mathbf{n}|^2 + |\nabla \mathbf{p}|^2)$$

LEMMA 10 Let $a \in \Omega$. Suppose that $(\mathbf{n}, \mathbf{p}, \varphi) \in \mathcal{A}$ is a minimizer for $\mathcal{E}$. Assume further that there exist $\epsilon > 0$ and $r_0 > 0$ with $\mathbb{B}_{r_0}(a) \subset \Omega$ such that

$$\frac{1}{r_0}\mathbb{E}_{r_0}(\mathbf{n}, \mathbf{p}) = \frac{1}{r_0}\int_{\mathbb{B}_{r_0}(a)} \left(|\nabla \mathbf{n}|^2 + |\nabla \mathbf{p}|^2\right)\, dx < \epsilon^2.$$

Then there exists $\beta \in (0, 1)$ such that for any r with $r < r_0$,

$$\frac{1}{r}\mathbb{E}_{r}(\mathbf{n}, \mathbf{p}) = \frac{1}{r}\int_{\mathbb{B}_{r}(a)} \left(|\nabla \mathbf{n}|^2 + |\nabla \mathbf{p}|^2\right)\, dx \le Cr^{\beta}.$$

Moreover, **n** and **p** are Hölder continuous at a.

The set of singularities is

$$Z = \left\{ a \in \Omega : \limsup_{r \to 0} r^{-1} \int_{\mathbb{B}_r(a)} \left(|\nabla \mathbf{n}|^2 + |\nabla \mathbf{p}|^2 \right) \, dx > 0 \right\}$$

In case that $K_1 = K_2 = K_3 = K > 0$, Z is at most discrete set due to the following monotonicity type inequality

$$\frac{1}{s} \int_{\mathbb{B}_s} \left(K|\nabla \mathbf{n}|^2 + B|\nabla \mathbf{p}|^2 \right) - \frac{1}{r} \int_{\mathbb{B}_r} \left(K|\nabla \mathbf{n}|^2 + B|\nabla \mathbf{p}|^2 \right) \geq -C(s^\beta - r^\beta)$$

for some $C > 0$ and $0 < r < s < \mathrm{dist}(a, \partial\Omega)$

One-dimensional Problem: Polarization with an applied electric field

After scalings, we obtain

$$\int_0^1 \left\{ \frac{\varepsilon^2}{2}(u'(x))^2 + f(u) - Eu \right\} dx$$

where E is applied electric field and

$$f(u) = \frac{1}{6}u^2[(u^2-1)^2 - \alpha].$$

The corresponding Euler-Lagrange equations is

$$-\varepsilon^2 u''(x) + f'(u) = E \text{ in } [0,1]$$

with $u'(0) = u'(1) = 0$.

Solvability condition:

$$E = \int_0^1 f'(u(x))$$

Note that for any real $\lambda \in \mathbf{R}$, $u = \lambda$ is a solution.
We then choose solutions satisfying $\int_0^1 u = \lambda$ for each $\lambda \in \mathbf{R}$. If u is such a solution, then u satisfies

$$-\varepsilon^2 u''(x) + f'(u) = \int_0^1 f'(u)\, dx \text{ in } [0,1]$$

$$u'(0) = u'(1) = 0, \ \int_0^1 u\, dx = \lambda$$

One-dimensional Problem

New energy:

$$\mathbb{E}(u) = \int_0^1 \left\{ \frac{\varepsilon^2}{2}(u'(z))^2 + f(u) \right\} dz, u'(0) = u'(1) = 0, \int_0^1 u = \lambda$$

$$f(u) = \frac{1}{6}u^2 \left[(u^2 - 1)^2 - \alpha \right]$$

For a fixed number λ, E plays a role of Lagrange multiplier for the constraint $\int_0^1 u = \lambda$.

We rewrite the Euler-Lagrange equation as by

$$\varepsilon^2 w - K(w, \lambda) = 0,$$

$$\frac{d^2}{dx^2} K(w, \lambda) = f'(w + \lambda) - \int_0^1 f'(w(s) + \lambda) ds.$$

Let

$$\mathcal{X} = \left\{ w \in C^2[0,1] : w'(0) = w'(1) = 0, \int_0^1 w \, dx = 0 \right\},$$

$$\mathcal{Z} = \left\{ z \in C^0[0,1] : \int_0^1 z \, dx = 0 \right\},$$

Choose $\mathcal{Y} = \mathcal{Z}$ and define $F : \mathcal{Y} \times \mathbf{R} \to \mathcal{Y}$ by

$$F(w, \lambda) = w - \varepsilon^{-2} K(w, \lambda).$$

Define $G : \mathcal{X} \times \mathbf{R} \to \mathcal{Z}$ by

$$G(w, \lambda) = -\varepsilon^2 w'' + f'(w + \lambda) - \int_0^1 f'(w(s) + \lambda)\, ds.$$

Then $G(0, \lambda) = 0$ for any $\lambda \in \mathbf{R}$ and

$$D_w G(0, \lambda) = -\varepsilon^2 w'' + f''(\lambda) w$$

LEMMA 11 For a sufficiently small $\varepsilon > 0$, there exist $\lambda_i (i = 1, 2, ..., 2K)$ such that $G(\cdot, \lambda_i) : \mathcal{X} \to \mathcal{Z}$ is a nonlinear Fredholm operator with Fredholm index 0 where $0 < \lambda_1 < \lambda_2 < \cdots < \lambda_K$, $\lambda_i < 0 (i = K + 1, \cdots, 2K)$

By Lyapunov-Schmidt Reduction and Crandall-Rabinowitz Theorem,

LEMMA 11 For each λ_i in LEMMA 10, there exists a nontrivial C^1- curve $\mathcal{C}$ which passes through $(0, \lambda_i)$,

$$\mathcal{C} : \{(w(s), \lambda(s)) : s \in (-\delta, \delta), (w(0), \lambda_i) = (0, \lambda_i)\},$$

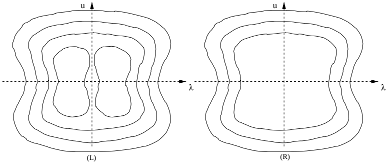
such that

$$G(w(s), \lambda(s)) = 0 \text{ for all } s \in (-\delta, \delta)$$

and all solutions of $G(x, \lambda) = 0$ in a neighborhood of $(0, \lambda_i)$ are either on the trivial line or on the nontrivial curve $\mathcal{C}$. The intersection $(0, \lambda_i)$ is called a bifurcation point.

Since F is also nonlinear Fredholm operator(in fact, $K(w, \lambda)$ is compact operator), we can define Leray-Schauder degree. By the homotopy invariance of the degree, we finally obtain

THEOREM 12 [JCMS, 2010]Let $\mathcal{M}_k (1 \leq k \leq K)$ be a maximal connected subset of the closure of the nontrivial solution branch bifurcating from $(0, \lambda_k)$. Then $\mathcal{M}_k$ is bounded and thus a closed curve.


u
λ
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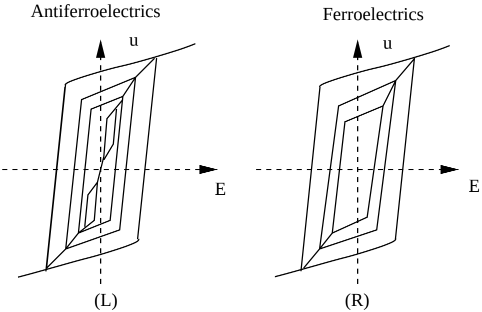
Antiferroelectrics
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Ferroelectrics
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General Theory of Liquid Crystals

- Landau-de Gennes energy:

$$\mathcal{E}_{LD} = \int_{\Omega} (F_{el} + f_{bulk})$$

$$\mathcal{F}_{el} = \frac{1}{2}\left(L_1 Q_{ij,k} Q_{ij,k} + L_2 Q_{ij,j} Q_{kj,k} + L_3 Q_{ij,k} Q_{ik,j}\right)$$

$$f_{bulk} = \frac{A}{2}\mathrm{tr}\, Q^2 - \frac{B}{3}\mathrm{tr}\, Q^3 + \frac{C}{4}\left(\mathrm{tr}\, Q^2\right)^2, \; Q_{ij,k} = \frac{\partial Q_{ij}}{\partial x_k}$$

Defects:singular points

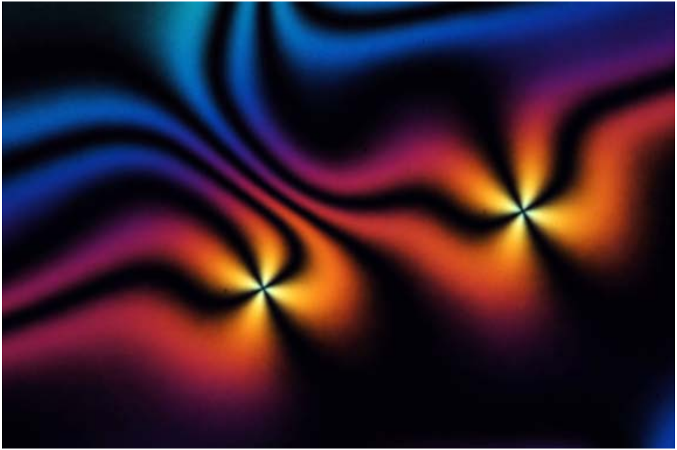

Figure : Singularities of Degree 1 for the Oseen-Frank Energy

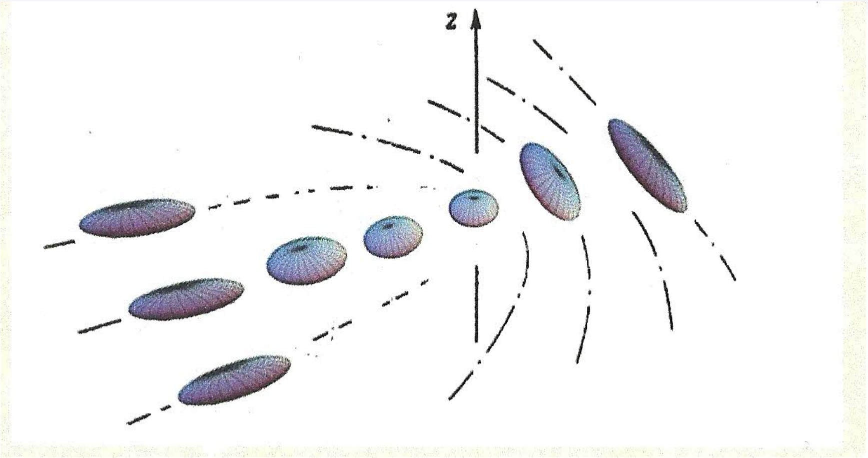

Figure : Singularity of $\frac{1}{2}$ degree(picture is taken from Pelcovits-IMA workshop 2005

- Study singularities of $\frac{1}{2}$-degrees [with Bauman and Phillips, Archive Ration. Mech. Analysis, 2012]

Thank you for your attention and have a wonderful day!