Spectral theory for magnetic Schrödinger operators and applications to liquid crystals (after Bauman-Calderer-Liu-Phillips, Pan, Helffer-Pan)

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In [P2], based on the de Gennes analogy between liquid crystals and superconductivity [dG2], X. Pan introduced the critical wave number Q_{c_3} (which is an analog of the upper critical field H_{c_3} for superconductors) and predicted the existence of a surface smectic state, which was supposed to be an analog of the surface superconducting state. In this talk we study an approximate form of the Landau-de Gennes model of liquid crystals, and examine the behavior of minimizers. Our results (obtained with X. Pan) suggest that a liquid crystal with large Ginzburg-Landau parameter κ will be in the surface smectic state if the number $q\tau$ lies asymptotically between κ^2 and κ^2/Θ_0, where Θ_0 is the lowest eigenvalue of the Schrödinger operator with a unit magnetic field in the half space, which satisfies $0 < \Theta_0 < 1$.

The energy for the model in Liquid Crystals can be written[1] as

$$\mathcal{E}[\psi,\mathbf{n}] = \int_\Omega \Big\{ |\nabla_{q\mathbf{n}}\psi|^2 - \kappa^2|\psi|^2 + \frac{\kappa^2}{2}|\psi|^4 + K_1\,|\operatorname{div}\mathbf{n}|^2 + K_2\,|\mathbf{n}\cdot \operatorname{curl}\mathbf{n} + \tau|^2 + K_3\,|\mathbf{n}\times \operatorname{curl}\mathbf{n}|^2 \Big\}\, dx\,,$$

where :

- $\Omega \subset \mathbb{R}^3$ is the region occupied by the liquid crystal,
- ψ is a complex-valued function called the *order parameter*,
- $\mathbf{n}$ is a real vector field of unit length called *director field*,
- q is a real number called *wave number*,
- τ is a real number measuring the chiral pitch,
- $K_1 > 0$, $K_2 > 0$ and $K_3 > 0$ are called the *elastic coefficients*,
- $\kappa > 0$ depends on the material and on temperature.

[1] This is an already simplified model where boundary terms have been eliminated.

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Of course the answer depends heavily on the various parameters !! As in the theory of superconductivity, a special role will be played by the following critical points of the functional, i.e. the pairs

$$(0, \mathbf{n}) \ ,$$

where **n** should minimize the second part :

$$\int_\Omega \left\{ K_1 \,|\, \mathrm{div}\ \mathbf{n}|^2 + K_2 \,|\mathbf{n} \cdot \ \mathrm{curl}\ \mathbf{n} + \tau|^2 + K_3 \,|\mathbf{n} \times \ \mathrm{curl}\ \mathbf{n}|^2 \right\} dx \ .$$

These special solutions are called "nematic phases" and one is naturally asking if they are minimizers of the functional.

For $\tau > 0$, let us consider $\mathcal{C}(\tau)$ the set of the $\mathbb{S}^2$-valued vectors satisfying :

$$\text{curl } \mathbf{n} = -\tau \mathbf{n} \,, \quad \text{div } \mathbf{n} = 0 \,.$$

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It can be shown that $\mathcal{C}(\tau)$ consists of the vector fields $\mathbb{N}_\tau^Q$ such that, for some $Q \in SO(3)$,

$$\mathbb{N}_\tau^Q(x) \equiv Q\mathbb{N}_\tau(Q^t x) \,, \quad \forall x \in \Omega, \tag{1}$$

where

$$\mathbb{N}_\tau(y_1, y_2, y_3) = (\cos(\tau y_3), \sin(\tau y_3), 0) \,, \ \forall y \in \mathbb{R}^3 \,. \tag{2}$$

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Note that is also equivalent, when $|\mathbf{n}|^2 = 1$ to

$$\text{div }\mathbf{n} = 0, \quad \mathbf{n}\cdot\ \text{curl }\mathbf{n} + \tau = 0, \quad \mathbf{n}\times\ \text{curl }\mathbf{n} = 0\,. \tag{3}$$

So the last three terms in the functional vanish iff $\mathbf{n} \in \mathcal{C}(\tau)$.

As a consequence, if we denote by

$$C(K_1, K_2, K_3, \kappa, q, \tau) = \inf_{(\psi, \mathbf{n}) \in \mathbb{V}(\Omega)} \mathcal{E}[\psi, \mathbf{n}]\,,$$

the infimum of the energy over the natural maximal form domain of the functional, then

$$C(K_1, K_2, K_3, \kappa, q, \tau) \leq c(\kappa, q, \tau)\ , \tag{4}$$

where

$$c(\kappa, q, \tau) = \inf_{\mathbf{n} \in \mathcal{C}(\tau)} \inf_{\psi} \mathcal{G}_{q\mathbf{n}}(\psi) \tag{5}$$

and $\mathcal{G}_{q\mathbf{n}}(\psi)$ is the so called the reduced Ginzburg-Landau functional.

Given a vector field $\mathbf{A}$, this functional is defined on $H^1(\Omega, \mathbb{C})$ by

$$\psi \mapsto \mathcal{G}_{\mathbf{A}}[\psi] = \int_\Omega \{|\nabla_{\mathbf{A}}\psi|^2 - \kappa^2|\psi|^2 + \frac{\kappa^2}{2}|\psi|^4\}\, dx\,. \tag{6}$$

For convenience, we also write $\mathcal{G}_{\mathbf{A}}[\psi]$ as $\mathcal{G}[\psi, \mathbf{A}]$.
So we have

$$c(\kappa, q, \tau) = \inf_{\mathbf{n}\in\mathcal{C}(\tau), \psi\in H^1(\Omega,\mathbb{C})} \mathcal{G}[\psi, q\mathbf{n}]\,. \tag{7}$$

and

$$\mathcal{E}(\psi, \mathbf{n}) = \mathcal{G}[\psi, q\mathbf{n}]\,, \tag{8}$$

if

$$\mathbf{n} \in \mathcal{C}(\tau)\,.$$

We have seen that in full generality that

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Conversely, it can be shown [BCLP, P2, HP2], that when the elastic parameters tend to $+\infty$, the converse is asymptotically true.

Proposition 1

$$\lim_{K_1, K_2, K_3 \to +\infty} C(K_1, K_2, K_3, \kappa, q, \tau) = c(\kappa, q, \tau)\ . \tag{10}$$

So $c(\kappa, q, \tau)$ is a good approximation for the minimal value of $\mathcal{E}$ for large K_j's.
Note that an interesting open problem is to control the rate of convergence in (10).

We now examine the non-triviality of the minimizers realizing $c(\kappa, q, \tau)$.

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As for the Ginzburg-Landau functional in superconductivity, this question is closely related to the analysis of the lowest eigenvalue $\mu(q\mathbf{n})$ of the Neumann realization of the magnetic Schrödinger operator

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As for the Ginzburg-Landau functional in superconductivity, this question is closely related to the analysis of the lowest eigenvalue $\mu(q\mathbf{n})$ of the Neumann realization of the magnetic Schrödinger operator

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in Ω, with

$$\nabla_{q\mathbf{n}} = \nabla - iq\mathbf{n}\ ,$$

namely $\mu = \mu(q\mathbf{n})$ is the lowest eigenvalue of the following problem

$$\begin{cases} -\nabla^2_{q\mathbf{n}}\phi = \mu\phi & \text{in } \Omega, \\ \nu \cdot \nabla_{q\mathbf{n}}\phi = 0 & \text{on } \partial\Omega, \end{cases} \qquad (11)$$

where ν is the unit outer normal of $\partial\Omega$.

But the new point is that we will minimize over $\mathbf{n} \in \mathcal{C}(\tau)$. So we shall actually meet

$$\mu_*(q,\tau) = \inf_{\mathbf{n}\in\mathcal{C}(\tau)} \mu(q\mathbf{n}). \tag{12}$$

Our main comparison statement (which is the analog of a statement in Fournais-Helffer [FH3] for surface superconductivity) is :

Proposition 2

$$-\frac{\kappa^2}{2}\,[1-\kappa^{-2}\mu_*(q,\tau)]_+^2 \inf_{\mathbf{n}\in\mathcal{C}(\tau)} \inf_{\{\mathcal{G}_{q\mathbf{n}}[\psi]=c(\kappa,q,\tau)\}} \frac{(\int_\Omega |\psi|^2\,dx)^2}{\int_\Omega |\psi|^4\,dx} \leq c(\kappa,q,\tau)\,. \tag{13}$$

and

$$c(\kappa,q,\tau) \leq -\frac{\kappa^2}{2}[1-\kappa^{-2}\mu_*(q,\tau)]_+^2 \sup_{\mathbf{n}\in\mathcal{C}(\tau)} \sup_{\phi\in\mathcal{S}p(q\mathbf{n})} \frac{(\int_\Omega |\phi|^2\,dx)^2}{\int_\Omega |\phi|^4\,dx}\,, \tag{14}$$

where $\mathcal{S}p(q\mathbf{n})$ is the eigenspace associated to $\mu(q\mathbf{n})$.

The first inequality implies, using Hölder,

$$-\frac{\kappa^2|\Omega|}{2}[1-\kappa^{-2}\mu_*(q,\tau)]^2 \leq c(\kappa,q,\tau) \tag{15}$$

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This shows also that $c(\kappa,q,\tau)$ is strictly negative if and only $\mu_*(\kappa,\tau) < \kappa^2$.

As a consequence of Proposition 2, we obtain that the transition from nematic phases to non-nematic phases (the so called smectic phases) is strongly related to the analysis of the solution of

$$1 - \kappa^{-2}\mu_*(q,\tau) = 0 \,. \tag{16}$$

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In the analysis of (16), the monotonicity of $q \mapsto \mu_*(q,\tau)$ is an interesting question (see Fournais-Helffer [FH3] in Surface Superconductivity).

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This will permit indeed to find a unique solution of (16) permitting a natural definition of the critical value $Q_{C3}(\kappa,\tau)$.

One can also be interested in giving lower bounds for $\sup_{\phi\in\mathcal{S}p(q\mathbf{n})} \frac{(\int_\Omega |\phi|^2\,dx)^2}{\int_\Omega |\phi|^4\,dx}$, which becomes more simply

$$\frac{(\int_\Omega |\phi|^2\,dx)^2}{\int_\Omega |\phi|^4\,dx}$$

for the eigenfunction ϕ if $\mu(q\mathbf{n})$ is of multiplicity 1.
We have proved with Pan that if τ stays in a bounded interval, then this quantity and $\mu_*(q,\tau)$ can be controlled in two regimes

- $\sigma \to 0$,
- $\sigma \to +\infty$

where

$$\sigma = q\tau$$

which is in some sense the leading parameter in the theory.

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A simpler question which is partially solved in Pan [P2] (with the help of [HM3]) and corresponds to the case $\tau = 0$ is the following :

Given a strictly convex open set, find the direction **h** of the constant magnetic field giving asymptotically as $\sigma \to +\infty$ the lowest energy for the Neumann realization in Ω of the Schrödinger operator with magnetic field σ **h**.

When looking to the general problem, various problems occur. The magnetic field $-q\tau\mathbf{n}$ (corresponding when $\mathbf{n} \in \mathcal{C}(\tau)$ to the magnetic potential $q\mathbf{n}$) is no more constant, so one should extend the analysis of Helffer-Morame [HM3] to this case.

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A first analysis (semi-classical in spirit) gives, as $\sigma = q\tau \to +\infty$,

$$\mu_*(q,\tau) = \Theta_0(q\tau) + \mathcal{O}((q\tau)^{\frac{2}{3}}) \tag{17}$$

where the remainder is controlled uniformly for[2] $\tau \in]0, \tau_0]$.

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This leads (assuming the uniqueness of Q_{C3}), to

$$\tau\, Q_{C3}(\kappa,\tau) = \frac{\kappa^2}{\Theta_0} + \mathcal{O}(\kappa^{\frac{4}{3}})\,. \qquad (18)$$

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A second analysis (perturbative in spirit) gives as $\sigma = q\tau \rightarrow O$,

$$\mu_*(q,\tau) = \Theta(\tau)(q\tau)^2 + \mathcal{O}((q\tau)^4) \tag{19}$$

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$$\Theta(0) = \inf_{\mathbf{h}\in\mathbb{S}^2} \frac{1}{|\Omega|}\int_\Omega |\mathbf{A_h}|^2\, dx \,, \tag{20}$$

where $\mathbf{A_h}$ is the unique solution in Ω of

$$\text{div } \mathbf{A_h} = 0 \,, \quad \text{curl } \mathbf{A_h} = \mathbf{h} \,, \text{ and } \mathbf{A_h}\cdot\nu = 0 \text{ on } \partial\Omega \,. \tag{21}$$

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One can also give an asymptotic of $c(\kappa, q, \tau)$.

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