

On Some Spectral Problems and Asymptotic Limits Occuring in the Analysis of Liquid Crystals

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ABSTRACT

On the basis of de Gennes' theory of analogy between liquid crystals and superconductivity, the second author introduced the critical wave number Q_{c3} of liquid crystals, which is an analog of the upper critical field H_{c3} for superconductors, and he predicted the existence of a surface smectic state, which was supposed to be an analog of the surface superconducting state. In this article we study this problem and our study relies on the Landau-de Gennes functional of liquid crystals in connection with a simpler functional called the reduced Ginzburg-Landau functional which appears to be relevant when some of the elastic constants are large. We discuss the behavior of the minimizers of these functionals. We describe briefly some results obtained by Bauman-Carme Calderer-Liu-Phillips, and present more recent results on the reduced Ginzburg-Landau functional obtained by the authors. This paper is partially extracted of lectures given by the first author in Recife and Serrambi in August 2008.

RESUMEN

Sobre la base de teoría de Gennes, la analogía entre cristales líquidos y superconductividad, el segundo autor introdujo el número de onda crítico Q_{c3} de cristales líquidos, el cual es un análogo del campo crítico superior H_{c3} para superconductores, él predijo la existencia de una superficie “smectic state”, la cual fué supuesta ser un análogo de la superficie de estado de superconductividad. En este artículo estudiamos este problema y nuestro estudio se basa en el funcional de Landau-de Gennes de cristales líquidos en conexión con un simple funcional llamado el funcional de Ginzburg-Landau reducido que resulta ser relevante cuando algunas de las constantes elásticas son grandes. Nosotros discutimos el comportamiento de los minimizadores de esos funcionales. Describimos brevemente algunos resultados obtenidos por Bauman-Carme Calderer-Liu-Phillips, y presentamos resultados más recientes sobre el funcional de Ginzburg-Landau reducido obtenidos por los autores. Este artículo es parcialmente extraído de las conferencias dadas por el primer autor en Recife y Serrambi en Agosto 2008.

Key words and phrases: *Liquid crystals, surface smectic state, Landau-de Gennes functional, reduced Ginzburg-Landau functional, critical wave number, critical elastic coefficients.*

Math. Subj. Class.: *82D30, 82D55, 35J55, 35Q55.*

1 Introduction

In [P1], based on the de Gennes analogy between liquid crystals and superconductivity [dG1, dGP], one of the authors (X. Pan) introduced the critical wave number Q_{c3} (which is an analog of the upper critical field H_{c3} for superconductors) and predicted the existence of a surface smectic state, which was supposed to be an analog of the surface superconducting state. The phase transition between the nematic state and smectic state of liquid crystals as the wave number varies around Q_{c3} was studied in [P1]. Bauman, Calderer, Liu and Phillips [BCLP] studied the phase transition of liquid crystals for a different set of parameters¹. In this article (which is partially extracted of lectures given by one of the authors (B. Helffer) in Recife and Serrambi in August 2008), we study this problem which relies on the Landau-de Gennes functional (modeling the properties of liquid crystals) in connection with a simpler functional called the reduced Ginzburg-Landau functional which appears to be relevant when some of the elastic constants are large. We discuss the behavior of the minimizers. We describe mainly some results obtained by Bauman-Carme Calderer-Liu-Phillips [BCLP], Pan [P1, P4, P5] and more recent results on the reduced Ginzburg-Landau functional obtained in [HP2, HP3]. We also add a few new results.

All these results 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 with $\kappa \rightarrow \infty$, where $\Theta_0 \in (0, 1)$ is the lowest eigenvalue of the Schrödinger operator with a unit magnetic field in the half plane.

¹In particular [P1] considers the case where $K_2 + K_4 = 0$ and in [BCLP] it is assumed that $c_0 \leq K_2 + K_4 \leq c_1$ where c_0 and c_1 are fixed positive constants.

This is also a natural extension of what was done by Fournais and Helffer in superconductivity in continuation of previous results of Lu-Pan, Bernoff-Sternberg, Helffer-Morame and many others (See [FH4] and references therein).

We will only present some of the results, emphasize on some points, recall some basic material and refer to the original papers or works in progress for more details and proofs.

2 Some Questions in the Theory of Liquid Crystals and First Answers

2.1 The model

The model in liquid crystals can be described² by the functional

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

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*,
- $\nabla_{q\mathbf{n}}$ is the magnetic gradient: $\nabla_{q\mathbf{n}} = \nabla - iq\mathbf{n}$,
- τ is a real number measuring the chiral pitch,
- $\mathbf{K} = (K_1, K_2, K_3)$ with $K_1 > 0$, $K_2 > 0$ and $K_3 > 0$ is the triple of the *elastic coefficients* or *Frank coefficients*,
- $\kappa > 0$ depends on the material and on temperature and is called the *Ginzburg-Landau parameter* of the liquid crystal.

This functional is called the Landau-de Gennes functional. We are interested in minimizing the functional over the pairs $(\psi, \mathbf{n}) \in H^1(\Omega, \mathbb{C}) \times V(\Omega, \mathbb{S}^2)$, where $H^1(\Omega, \mathbb{C})$ is the standard Sobolev space for complex-valued functions, $V(\Omega, \mathbb{S}^2)$ consists of vector fields \mathbf{n} such that $\operatorname{div} \mathbf{n} \in L^2(\Omega)$, $\operatorname{curl} \mathbf{n} \in L^2(\Omega, \mathbb{R}^3)$ and $|\mathbf{n}(x)|^2 = 1$ almost everywhere. We refer to [C], [BCLP] and [P1, P4, P6]

²This is an already simplified model where boundary terms (see [BCLP, P1]) have been eliminated. With the notations of these authors, we are considering as in [HP2] the case $K_2 + K_4 = 0$.

for a more complete discussion of the mathematical issues and a discussion of the contents of the references to the physics literature [dG1, dG2, dGP]. We only mention here that the physical interpretation is that \mathbf{n} is the molecular director field and that, if we write

$$\psi(x) = \rho(x)e^{i\phi(x)},$$

where $\rho(x) \geq 0$ and $\phi(x)$ is a real function, we recover the molecular mass density by

$$\delta(x) = \rho_0(x) + \rho(x) \cos \phi(x),$$

where $\rho_0(x)$ is some given reference density.

Observing that we have the lower bound

$$\mathcal{E}^{\mathbf{K}}[\psi, \mathbf{n}] \geq -\frac{\kappa^2}{2}|\Omega|, \quad (2.1)$$

it is not too difficult to show that this functional admits minimizers. But the main questions are then:

- What is the minimum of the energy ?
- What is the nature of the minimizers ?

Of course the answer depends heavily on the various parameters and we will only be able to give answers in some asymptotic regimes.

As in the theory of superconductivity, a special role will be played by some critical points of the functional, the pairs $(0, \mathbf{n})$, where \mathbf{n} is a minimizer of the so called Oseen-Frank functional:

$$\mathbf{n} \mapsto \mathcal{E}_{OF}^{\mathbf{K}}[\mathbf{n}] := \int_{\Omega} \{K_1 |\operatorname{div} \mathbf{n}|^2 + K_2 |\mathbf{n} \cdot \operatorname{curl} \mathbf{n} + \tau|^2 + K_3 |\mathbf{n} \times \operatorname{curl} \mathbf{n}|^2\} dx.$$

These special solutions are called “nematic phases” and one is naturally asking if they are minimizers or local minimizers of the functional $\mathcal{E}^{\mathbf{K}}$.

In any case, the minimizers of $\mathcal{E}^{\mathbf{K}}$ satisfy some Euler-Lagrange equation. We do not write the complete system but note that the variation with respect to the order parameter leads to

$$-\nabla_{q\mathbf{n}}^2 \psi - \kappa^2 \psi + \kappa^2 |\psi|^2 \psi = 0 \quad \text{in } \Omega, \quad (2.2)$$

together with the boundary condition

$$\nu \cdot \nabla_{q\mathbf{n}} \psi = 0 \quad \text{on } \partial\Omega, \quad (2.3)$$

where ν denotes the normal to the boundary.

Using the maximum principle for $u = |\psi|^2$ which can be seen as a solution of

$$\begin{cases} -\Delta u + \kappa^2 u(1-u) \geq 0 & \text{in } \Omega, \\ \frac{\partial u}{\partial \nu} = 0 & \text{on } \partial\Omega, \end{cases}$$

one can show that

$$\|\psi\|_{L^\infty(\Omega)} \leq 1. \quad (2.4)$$

2.2 A universal upper bound

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

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

It has been shown in [BCLP] that $\mathcal{C}(\tau)$ consists of the vector fields \mathbb{N}_τ^Q such that, for some $Q \in \operatorname{SO}(3)$,

$$\mathbb{N}_\tau^Q(x) \equiv Q \mathbb{N}_\tau(Q^t x), \quad x \in \Omega, \tag{2.5}$$

where

$$\mathbb{N}_\tau(y_1, y_2, y_3) = (\cos(\tau y_3), \sin(\tau y_3), 0), \quad y \in \mathbb{R}^3. \tag{2.6}$$

This is also equivalent, as $|\mathbf{n}|^2 = 1$, to

$$\operatorname{div} \mathbf{n} = 0, \quad \mathbf{n} \cdot \operatorname{curl} \mathbf{n} + \tau = 0, \quad \mathbf{n} \times \operatorname{curl} \mathbf{n} = \mathbf{0}. \tag{2.7}$$

So the last three terms in the functional $\mathcal{E}^{\mathbf{K}}$ vanish if and only if $\mathbf{n} \in \mathcal{C}(\tau)$.

As a consequence, if we denote by

$$C(K_1, K_2, K_3, \kappa, q, \tau) = \inf_{(\psi, \mathbf{n}) \in H^1(\Omega, \mathbb{C}) \times V(\Omega, \mathbb{S}^2)} \mathcal{E}^{\mathbf{K}}[\psi, \mathbf{n}], \tag{2.8}$$

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

$$C(K_1, K_2, K_3, \kappa, q, \tau) \leq c(\kappa, q, \tau), \tag{2.9}$$

where

$$c(\kappa, q, \tau) = \inf_{\mathbf{n} \in \mathcal{C}(\tau)} \inf_{\psi \in H^1(\Omega, \mathbb{C})} \mathcal{G}_{q\mathbf{n}}[\psi], \tag{2.10}$$

and $\mathcal{G}_{q\mathbf{n}}[\psi]$ is the so called reduced Ginzburg-Landau functional which will be defined in the next subsection.

2.3 Reduced Ginzburg-Landau functional

Given a vector field \mathbf{A} , the reduced Ginzburg-Landau functional $\mathcal{G}_{\mathbf{A}}$ with magnetic potential \mathbf{A} is defined on $H^1(\Omega, \mathbb{C})$ by

$$\psi \mapsto \mathcal{G}_{\mathbf{A}}[\psi] = \int_{\Omega} \{ |\nabla_{\mathbf{A}} \psi|^2 - \kappa^2 |\psi|^2 + \frac{\kappa^2}{2} |\psi|^4 \} dx. \tag{2.11}$$

The standard Ginzburg-Landau functional with external vector field $\sigma \mathcal{H}^e$ (where $\mathcal{H}^e = \operatorname{curl} \mathbf{F}$ is a divergence free vector field on $\overline{\Omega}$) (see [FH4] and references therein) takes the form

$$\mathcal{E}_{GL}[\psi, \mathbf{A}] = \mathcal{G}_{\kappa\sigma\mathbf{A}}[\psi] + \kappa^2 \sigma^2 \int_{\mathbb{R}^3} |\operatorname{curl} \mathbf{A} - \mathcal{H}^e|^2 dx \tag{2.12}$$

where

- Ω is a bounded and simply connected domain,
- $(\psi, \mathbf{A}) \in H^1(\Omega, \mathbb{C}) \times \dot{H}_{\text{div}, \mathbf{F}}^1(\mathbb{R}^3, \mathbb{R}^3)$,
- $\dot{H}_{\text{div}, \mathbf{F}}^1(\mathbb{R}^3, \mathbb{R}^3) = \{ \mathbf{A} \mid \text{div } \mathbf{A} = 0, \mathbf{A} - \mathbf{F} \in \dot{H}^1(\mathbb{R}^3, \mathbb{R}^3) \}$,
- $\dot{H}^1(\mathbb{R}^3)$ denotes the homogeneous Sobolev space, i.e. the closure of $C_0^\infty(\mathbb{R}^3)$ under the norm $u \mapsto \|\nabla u\|_{L^2(\mathbb{R}^3)}$, and $\dot{H}^1(\mathbb{R}^3, \mathbb{R}^3)$ denotes the corresponding space of vector fields.

So the Oseen-Frank energy in liquid crystals theory replaces the magnetic energy measuring the square of the L^2 norm of $\text{curl } \mathbf{A} - \mathcal{H}^e$ in \mathbb{R}^3 in Ginzburg-Landau theory.

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

$$c(\kappa, q, \tau) = \inf_{\mathbf{n} \in \mathcal{C}(\tau), \psi \in H^1(\Omega, \mathbb{C})} \mathcal{G}[\psi, q\mathbf{n}] \leq 0, \quad (2.13)$$

and if $\mathbf{n} \in \mathcal{C}(\tau)$, then the following equality holds

$$\mathcal{E}^{\mathbf{K}}[\psi, \mathbf{n}] = \mathcal{G}[\psi, q\mathbf{n}]. \quad (2.14)$$

3 A Limiting Case: The Case of Large Frank Constants

We have seen that in full generality (2.9) holds. Conversely, it can be shown (see [BCLP, P1, HP2]) that when the elastic parameters tend to $+\infty$, the converse is asymptotically true.

Proposition 3.1.

$$\lim_{K_1, K_2, K_3 \rightarrow +\infty} C(K_1, K_2, K_3, \kappa, q, \tau) = c(\kappa, q, \tau). \quad (3.1)$$

So $c(\kappa, q, \tau)$ is a good approximation for the minimal value of $\mathcal{E}^{\mathbf{K}}$ for large K_j 's.

Of course, a basic initial remark for the proof is that if (ψ, \mathbf{n}) is a minimizer $\mathcal{E}^{\mathbf{K}}$ then we always have

$$\mathcal{E}_{OF}^{\mathbf{K}}[\mathbf{n}] \leq \frac{\kappa^2 |\Omega|}{2}. \quad (3.2)$$

Remark 3.2.

In [BCLP], the authors used instead the bound

$$\mathcal{E}_{OF}^{\mathbf{K}}[\mathbf{n}] \leq C(\Omega)q^2\tau^2, \quad (3.3)$$

which is obtained from the universal upperbound

$$C(K_1, K_2, K_3, \kappa, q, \tau) \leq C(\Omega)q^2\tau^2 - \frac{\kappa^2 |\Omega|}{2}. \quad (3.4)$$

This upper bound is obtained (see Lemma 1 in [BCLP]) by computing the energy of the pair $(\psi, \mathbf{n}) = (e^{iqx \cdot \mathbb{N}_\tau(x)}, \mathbb{N}_\tau(x))$, with \mathbb{N}_τ defined in (2.6).

This gives the two following controls

$$\|\operatorname{div} \mathbf{n}\|_{L^2(\Omega)}^2 \leq \frac{\kappa^2 |\Omega|}{2K_1}, \quad (3.5)$$

and

$$\|\operatorname{curl} \mathbf{n} - \tau \mathbf{n}\|_{L^2(\Omega)}^2 \leq \frac{\kappa^2 |\Omega|}{2 \min\{K_2, K_3\}}. \quad (3.6)$$

We also have

$$\|\nabla_{\mathbf{q}\mathbf{n}} \psi\|_{L^2(\Omega)}^2 \leq \frac{\kappa^2 |\Omega|}{2}. \quad (3.7)$$

Remark 3.3.

1. *This limiting case where all the elastic coefficients tend to $+\infty$ appears naturally in the transition from smectic-C to nematic phase (see [dG2]).*
2. *As observed by D. Phillips in a conference in Ryukoku University in Japan, it would be also interesting to have the result with fixed $K_1 > 0$, in the limit when K_2 and K_3 tend to $+\infty$. A modification of the proof in [HP2] leads indeed (see Lemma 3.4) to this result. For parameters in different regime (in particular $c_0 < K_2 + K_4 < c_1$), the same conclusion was obtained in [BCLP].*
3. *An interesting open problem is to control the rate of convergence in (3.1) (see [Ray3]).*

Proof of Proposition 3.1

To illustrate the last point of the remark and to complete the proof of the proposition, we need the following result ³

Lemma 3.4.

Let $\tau_0 > 0$ and $C_0 > 0$. Then for any $\epsilon > 0$, there exists $\alpha > 0$ such that if $\mathbf{n} \in V(\Omega, \mathbb{S}^2)$, $\tau \in (0, \tau_0]$, and

$$\begin{aligned} \|\operatorname{curl} \mathbf{n} + \tau \mathbf{n}\|_{L^2(\Omega)} &\leq \alpha, \\ \|\operatorname{div} \mathbf{n}\|_{L^2(\Omega)} &\leq C_0 \tau, \end{aligned}$$

then there exists $Q \in SO(3)$ such that

$$\|\mathbf{n} - \mathbb{N}_\tau^Q\|_{L^4(\Omega)} \leq \epsilon. \quad (3.8)$$

Proof. We give the proof in the case of a fixed $\tau > 0$.

If it were not true, we will find $\epsilon_0 > 0$ and a bounded sequence $\mathbf{n}_j \in V(\Omega, \mathbb{S}^2)$ such that $\|\operatorname{div} \mathbf{n}_j\|_{L^2(\Omega)}$ is bounded,

$$\lim_{j \rightarrow +\infty} \|\operatorname{curl} \mathbf{n}_j + \tau \mathbf{n}_j\|_{L^2(\Omega)} = 0,$$

³The same conclusion was proved in [BCLP] (Lemma 4) in the case where $K_2 + K_4 \geq c_0 > 0$ and hence $\|\nabla \mathbf{n}\|_{L^2(\Omega)}^2$ can be controlled by the energy.

and

$$\inf_{Q \in SO(3)} \|\mathbf{n}_j - \mathbb{N}_\tau^Q\|_{L^4(\Omega)} \geq \epsilon_0.$$

From the assumptions, it is clear that the sequence is bounded in $V(\Omega, \mathbb{S}^2)$, and hence bounded in $H_{loc}^1(\Omega, \mathbb{R}^3)$ (see [P4], Lemma 2.3), hence we can extract a subsequence, still denoted by \mathbf{n}_j , and find \mathbf{n}_∞ such that \mathbf{n}_j tends weakly to \mathbf{n}_∞ in $H_{loc}^1(\Omega, \mathbb{R}^3)$. One can also show that $|\mathbf{n}_\infty|^2 = 1$ a.e. in Ω and that $\text{curl } \mathbf{n}_\infty + \tau \mathbf{n}_\infty = 0$. So \mathbf{n}_∞ belongs to $\mathcal{C}(\tau)$ and there exists $Q \in SO(3)$ such that $\mathbf{n}_\infty = \mathbb{N}_\tau^Q$. Now by compactness of the injection of $H_{loc}^1(\Omega, \mathbb{R}^3)$ in $L_{loc}^4(\Omega, \mathbb{R}^3)$, we get that \mathbf{n}_j tends to \mathbf{n}_∞ in $L_{loc}^4(\Omega, \mathbb{R}^3)$. Let D be a compact subset of Ω such that $|\Omega \setminus D| < \epsilon_0/48$. For large j we have

$$\int_D |\mathbf{n}_j - \mathbf{n}_\infty|^4 dx < \frac{\epsilon_0^4}{3}.$$

Then

$$\int_\Omega |\mathbf{n}_j - \mathbf{n}_\infty|^4 dx \leq \int_D |\mathbf{n}_j - \mathbf{n}_\infty|^4 dx + 16|\Omega \setminus D| < \frac{2\epsilon_0^4}{3},$$

which leads to a contradiction. ■

The control of the rate of convergence in Proposition 3.1 should pass through a good knowledge of $\alpha(\epsilon)$.

The second step in the proof of Proposition 3.1 consists in observing that, if (ψ, \mathbf{n}) is a minimizer, we can, for any $Q \in SO(3)$, get the lower bound

$$\begin{aligned} \mathcal{G}[\psi, q\mathbf{n}] &= \|\nabla_{q\mathbf{n}} \psi\|_{L^2(\Omega)}^2 - \kappa^2 \|\psi\|_{L^2(\Omega)}^2 + \frac{\kappa^2}{2} \|\psi\|_{L^4(\Omega)}^4 \\ &\geq (1 - \eta) \|\nabla_{q\mathbb{N}_\tau^Q} \psi\|_{L^2(\Omega)}^2 - \kappa^2 \|\psi\|_{L^2(\Omega)}^2 + \frac{\kappa^2}{2} \|\psi\|_{L^4(\Omega)}^4 \\ &\quad - \frac{q^2}{\eta} |\Omega|^{1/2} \|\mathbf{n} - \mathbb{N}_\tau^Q\|_{L^4(\Omega)}^2. \end{aligned} \tag{3.9}$$

Here we have used Cauchy-Schwarz inequality and (2.4). This we can rewrite, using (3.7), in the form

$$\mathcal{G}[\psi, q\mathbf{n}] \geq \mathcal{G}[\psi, q\mathbb{N}_\tau^Q] - \frac{\eta}{2} \kappa^2 |\Omega| - \frac{q^2}{\eta} |\Omega|^{1/2} \|\mathbf{n} - \mathbb{N}_\tau^Q\|_{L^4(\Omega)}^2. \tag{3.10}$$

This gives

$$\mathcal{G}[\psi, q\mathbf{n}] \geq c(\kappa, q, \tau) - \frac{\eta}{2} \kappa^2 |\Omega| - \frac{q^2}{\eta} |\Omega|^{1/2} \|\mathbf{n} - \mathbb{N}_\tau^Q\|_{L^4(\Omega)}^2. \tag{3.11}$$

Putting together the estimates, we obtain

$$\mathcal{E}_{OF}^{\mathbf{K}}(\mathbf{n}) \leq \frac{\eta}{2} \kappa^2 |\Omega| + \frac{q^2}{\eta} |\Omega|^{1/2} \|\mathbf{n} - \mathbb{N}_\tau^Q\|_{L^4(\Omega)}^2, \tag{3.12}$$

and

$$\begin{aligned} c(\kappa, q, \tau) &\geq C(K_1, K_2, K_3, \kappa, q, \tau) \\ &\geq c(\kappa, q, \tau) - \frac{\eta}{2}\kappa^2|\Omega| - \frac{q^2}{\eta}|\Omega|^{1/2}\|\mathbf{n} - \mathbb{N}_\tau^Q\|_{L^4(\Omega)}^2. \end{aligned} \tag{3.13}$$

These estimates are valid for any $\eta > 0$ and any $Q \in SO(3)$. The remainder on the right hand side can be chosen arbitrarily small by choosing first η small. Then we can use (3.5) and (3.6) to have $\|\operatorname{curl} \mathbf{n} + \tau \mathbf{n}\|_{L^2(\Omega)}$ and $\|\operatorname{div} \mathbf{n}\|_{L^2(\Omega)}$ small and using Lemma 3.4 (and a good choice of Q) to have $\|\mathbf{n} - \mathbb{N}_\tau^Q\|_{L^4(\Omega)}$ small.

4 Analysis of the Reduced Ginzburg-Landau Functional

We now analyze the non-triviality of the minimizers realizing $c(\kappa, q, \tau)$. As for the Ginzburg-Landau functional in superconductivity, this question is closely related to the analysis of the lowest eigenvalue $\lambda_1^N(\mathbf{q}\mathbf{n})$ of the Neumann realization of the magnetic Schrödinger operator $-\nabla_{\mathbf{q}\mathbf{n}}^2$ in Ω that we met already when describing the Euler-Lagrange equation associated to the functional. Namely $\lambda_1^N = \lambda_1^N(\mathbf{q}\mathbf{n})$ is the lowest eigenvalue of the following problem

$$\begin{cases} -\nabla_{\mathbf{q}\mathbf{n}}^2 \phi = \lambda_1^N \phi & \text{in } \Omega, \\ \nu \cdot \nabla_{\mathbf{q}\mathbf{n}} \phi = 0 & \text{on } \partial\Omega, \end{cases} \tag{4.1}$$

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

But the new point is that we will minimize $\lambda_1^N(\mathbf{q}\mathbf{n})$ over $\mathbf{n} \in \mathcal{C}(\tau)$. So we shall actually meet the quantity:

$$\mu_*(q, \tau) = \inf_{\mathbf{n} \in \mathcal{C}(\tau)} \lambda_1^N(\mathbf{q}\mathbf{n}). \tag{4.2}$$

We preliminarily observe the

Lemma 4.1.

If $(\psi, \mathbf{q}\mathbf{n})$ is a nontrivial minimizer of \mathcal{G} , then $\mathcal{G}[\psi, \mathbf{q}\mathbf{n}] < 0$.

The proof is simple. ψ is a solution of the (Euler-Lagrange) equation (2.2) with Neumann condition (2.3). Multiplying (2.2) by $\overline{\psi}$ and integrating over Ω , we have, after an integration by parts and taking account of the boundary condition (2.3),

$$\int_{\Omega} \{|\nabla_{\mathbf{q}\mathbf{n}} \psi|^2 - \kappa^2(1 - |\psi|^2)|\psi|^2\} dx = 0, \tag{4.3}$$

and hence

$$c(\kappa, q, \tau) = \mathcal{G}_{\mathbf{q}\mathbf{n}}[\psi] = -\frac{\kappa^2}{2} \int_{\Omega} |\psi|^4 dx < 0. \tag{4.4}$$

This gives:

$$\frac{1}{2}(\mu_*(q, \tau) - \kappa^2)\|\psi\|_{L^2(\Omega)}^2 \leq \frac{1}{2}(\lambda_1^N(\mathbf{q}\mathbf{n}) - \kappa^2)\|\psi\|_{L^2(\Omega)}^2 = c(\kappa, q, \tau). \tag{4.5}$$

Hence, when $c(\kappa, q, \tau) < 0$, we should have $\mu_*(q, \tau) < \kappa^2$. Pushing forward, one has the main comparison statement (analogous to a statement in Fournais-Helffer [FH3] for surface superconductivity) in [HP2]:

Proposition 4.2.

$$-\frac{\kappa^2|\Omega|}{2}[1 - \kappa^{-2}\mu_*(q, \tau)]^2 \leq c(\kappa, q, \tau) \quad (4.6)$$

and

$$c(\kappa, q, \tau) \leq -\frac{\kappa^2}{2}[1 - \kappa^{-2}\mu_*(q, \tau)]_+^2 \sup_{\mathbf{n} \in \mathcal{C}(\tau)} \sup_{\phi \in Sp(q\mathbf{n})} \frac{(\int_{\Omega} |\phi|^2 dx)^2}{\int_{\Omega} |\phi|^4 dx}, \quad (4.7)$$

where $Sp(q\mathbf{n})$ is the eigenspace associated to $\lambda_1^N(q\mathbf{n})$, and $[\cdot]_+$ denotes the positive part of the enclosed quantity.

For the upper bound, we can minimize $\mathcal{G}[\psi, q\mathbf{n}]$ over the pairs (ψ, \mathbf{n}) with $\psi = t\psi_{q\mathbf{n}}$, where $\psi_{q\mathbf{n}}$ is an eigenfunction of $-\nabla_{q\mathbf{n}}^2$, $t \in \mathbb{C}$, and $\mathbf{n} \in \mathcal{C}(\tau)$.

For the lower bound, we have just to use the Hölder inequality and (4.4) and (4.5).

This completes the (sketch of the) proof that $c(\kappa, q, \tau)$ is strictly negative if and only if $\mu_*(\kappa, \tau) < \kappa^2$.

5 Main Questions

As a consequence of Proposition 4.2, we obtain that the transition from a nematic phase to a smectic phase is strongly related to the analysis of the solution of

$$1 - \kappa^{-2}\mu_*(q, \tau) = 0. \quad (5.1)$$

This is a pure spectral problem concerning a family indexed by $\mathbf{n} \in \mathcal{C}(\tau)$ of Schrödinger operators with magnetic field $-\nabla_{q\mathbf{n}}^2$.

Remark 5.1.

In the analysis of (5.1), the monotonicity of $q \mapsto \mu_(q, \tau)$ is an interesting open question (see Fournais-Helffer [FH3] for the phase transition from normal state to surface superconducting state of type II superconductors).*

This will permit indeed to find a unique solution of (5.1) permitting a natural definition of the critical value $Q_{c3}(\kappa, \tau)$.

We hope to answer this question in [HP3] in the case of a strictly convex domain.

We have proved in [HP2] that if τ stays in a bounded interval, then $Q_{c3}(\kappa, \tau)$ and $\mu_*(q, \tau)$ can be controlled in two regimes

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

where

$$\sigma = q\tau,$$

which, as it appears already in [BCLP], is in some sense the leading parameter in the theory. We mention that if we examine the magnetic Schrodinger operator $-\nabla_{q\mathbf{n}}^2$, the parameter σ corresponds indeed to the intensity of the magnetic field corresponding to the magnetic potential $q\mathbf{n}$, with $\mathbf{n} \in \mathcal{C}(\tau)$. This will be detailed in Sections 7 and 8.

6 A Simpler Question

A simpler question, which was first introduced in [P1], and partially solved in [P5] with the help of [P3, HM4], but can be completed under the additional assumption below by a careful control (see [HP2, HP3]) of the uniformity in the proof of [HM4], can be stated as follows:

Question 6.1.

Given a strictly convex open set $\Omega \subset \mathbb{R}^3$, find the direction \mathbf{h} of the constant magnetic field giving asymptotically as $\sigma \rightarrow +\infty$ the lowest energy for the Neumann realization in Ω of the Schrödinger operator with magnetic field $\sigma\mathbf{h}$.

Let us present shortly the answer to this question. We assume that

Assumption 6.2.

At each point of $\partial\Omega$ the curvature tensor has two strictly positive eigenvalues $\kappa_1(x)$ and $\kappa_2(x)$, so that

$$0 < \kappa_1(x) \leq \kappa_2(x).$$

Under this assumption, the set $\Gamma_{\mathbf{h}}$ of boundary points where \mathbf{h} is tangent to $\partial\Omega$, i.e.

$$\Gamma_{\mathbf{h}} := \{x \in \partial\Omega \mid \mathbf{h} \cdot \nu(x) = 0\}, \tag{6.1}$$

is a regular submanifold of $\partial\Omega$:

$$d^T(\mathbf{h} \cdot \nu)(x) \neq 0, \forall x \in \Gamma_{\mathbf{h}}, \tag{6.2}$$

where d^T denotes the tangential gradient along $\Gamma_{\mathbf{h}}$. The basic example where this assumption is satisfied is the ellipsoid.

For any given \mathbf{h} , let $F_{\mathbf{h}}$ be the magnetic potential such that

$$\text{curl } \mathbf{F}_{\mathbf{h}} = \mathbf{h} \quad \text{and} \quad \text{div } \mathbf{F}_{\mathbf{h}} = 0 \quad \text{in } \Omega, \quad \mathbf{F}_{\mathbf{h}} \cdot \nu(x) = 0 \quad \text{on } \partial\Omega.$$

We have the following two-term asymptotics of $\lambda_1^N(\sigma\mathbf{F}_{\mathbf{h}})$ of the Neumann Laplacian $-\nabla_{\sigma\mathbf{F}_{\mathbf{h}}}^2$, (due to Helffer-Morame-Pan [HM4, P3]).

Theorem 6.3.

If Ω and \mathbf{h} are as above, then, as $\sigma \rightarrow +\infty$,

$$\lambda_1^N(\sigma \mathbf{F}_{\mathbf{h}}) = \Theta_0 \sigma + \widehat{\gamma}_{\mathbf{h}} \sigma^{2/3} + \mathcal{O}(\sigma^{2/3-\eta}), \quad (6.3)$$

for some $\eta > 0$.

Moreover η is independent of \mathbf{h} and the control of the remainder is uniform with respect to \mathbf{h} .

Here $\Theta_0 \in (0, 1)$, $\delta_0 \in (0, 1)$ and $\widehat{\nu}_0 > 0$ are spectral quantities (see in the Appendix), and $\widehat{\gamma}_{\mathbf{h}}$ is defined by

$$\widehat{\gamma}_{\mathbf{h}} := \inf_{x \in \Gamma_{\mathbf{h}}} \widetilde{\gamma}_{\mathbf{h}}(x), \quad (6.4)$$

where

$$\widetilde{\gamma}_{\mathbf{h}}(x) := 2^{-2/3} \widehat{\nu}_0 \delta_0^{1/3} |k_n(x)|^{2/3} \left(1 - (1 - \delta_0) |T_{\mathbf{h}}(x) \cdot \mathbf{h}|^2\right)^{1/3}. \quad (6.5)$$

Here $T_{\mathbf{h}}(x)$ is the oriented, unit tangent vector to $\Gamma_{\mathbf{h}}$ at the point x and

$$k_n(x) = |d^T(\mathbf{h} \cdot \nu)(x)|.$$

Note that the constant Θ_0 has been denoted by β_0 in [LuP1, LuP2, LuP3] and in [P1, P3, P4] etc.

Here is now the answer to the question 6.1. We have just to determine $\inf_{\mathbf{h} \in \mathbb{S}^2} \widehat{\gamma}_{\mathbf{h}}$ or equivalently

$$\inf_{\mathbf{h} \in \mathbb{S}^2} \inf_{x \in \Gamma_{\mathbf{h}}} |k_n(x)|^{2/3} \left(1 - (1 - \delta_0) |T_{\mathbf{h}}(x) \cdot \mathbf{h}|^2\right)^{1/3}.$$

So everything is reduced to the analysis of the map

$$\Gamma_{\mathbf{h}} \ni x \mapsto k_n(x)^2 \left(1 - (1 - \delta_0) |T_{\mathbf{h}}(x) \cdot \mathbf{h}|^2\right).$$

As observed in the appendix of [HM3], where the comparison is done between the results of [P3] and [HM4], this last expression can be written in the form

$$\begin{aligned} \Gamma_{\mathbf{h}} \ni x \mapsto & \kappa_1(x)^2 \cos^2 \phi(x) + \kappa_2(x)^2 \sin^2 \phi(x) \\ & - (1 - \delta_0) (\kappa_1(x) - \kappa_2(x))^2 \sin^2 \phi(x) \cos^2 \phi(x), \end{aligned}$$

where, for $x \in \partial\Omega$, $\phi(x)$ is defined by writing

$$\mathbf{h} = \cos \phi(x) \mathbf{u}_1(x) + \sin \phi(x) \mathbf{u}_2(x),$$

with $(\mathbf{u}_1(x), \mathbf{u}_2(x))$ being the orthonormal basis of the curvature tensor at x , associated to the eigenvalues $\kappa_1(x)$ and $\kappa_2(x)$.

We easily observe that, is $0 < \kappa_1 \leq \kappa_2$ the function

$$[0, 1] \ni t \mapsto \kappa_1^2 t + \kappa_2^2 (1 - t) - (1 - \delta_0) (\kappa_1 - \kappa_2)^2 t (1 - t),$$

admits a minimum at $t = 1$. Hence, when minimizing over \mathbf{h} and $x \in \Gamma_{\mathbf{h}}$, it is rather easy to show that the infimum is obtained by first choosing a point x_0 of $\partial\Omega$ where $\kappa_1(x)$ is minimum and then taking $\mathbf{h} = \mathbf{u}_1(x_0)$. This leads to the following proposition which was conjectured and partially proved by X. Pan [P5] and then completed in [HP2].

Proposition 6.4.

Under Assumption 6.2, we have

$$\inf_{\mathbf{h} \in \mathbb{S}^2} \widehat{\gamma}_{\mathbf{h}} = \inf_{x \in \partial\Omega} (\kappa_1(x))^{2/3}, \tag{6.6}$$

hence

$$\inf_{\mathbf{h} \in \mathbb{S}^2} \lambda_1^N(\sigma \mathbf{F}_{\mathbf{h}}) = \Theta_0 \sigma + \inf_{x \in \partial\Omega} (\kappa_1(x))^{2/3} \sigma^{2/3} + \mathcal{O}(\sigma^{2/3-\eta}). \tag{6.7}$$

This answers Question 6.1.

7 Semi-Classical Case: $q\tau$ Large

When looking at the general problem, various questions 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 to this case. A first analysis [HM4, P3, HP2] (semi-classical in spirit) gives:

Theorem 7.1.

As $\sigma = q\tau \rightarrow +\infty$,

$$\mu_*(q, \tau) = \Theta_0 q\tau + \mathcal{O}((q\tau)^{2/3}), \tag{7.1}$$

where the remainder is controlled uniformly for ⁴ $\tau \in (0, \tau_0]$.

This is a consequence of

$$\lambda_1^N(q\mathbf{n}) = \Theta_0 q\tau + \mathcal{O}((q\tau)^{2/3}), \tag{7.2}$$

with $\mathcal{O}((q\tau)^{2/3})$ uniform with respect to $\mathbf{n} \in \mathcal{C}(\tau)$ and $\tau \in (0, \tau_0]$.

The reader could be astonished to have this uniformity. The first thing is to observe that, when Ω has no holes, it is not the magnetic potential $\mathbf{A} = q\mathbf{n}$ which is important in the analysis of the Neumann groundstate energy of $-\nabla_{\mathbf{A}}^2$ but the magnetic field which is $-q\tau \mathbf{n}$. We observe that the magnetic field is of constant strength $q\tau$ and that its variation is controlled if $\tau \in (0, \tau_0]$. The analysis of [HM4] which was devoted to the constant magnetic field case can go through (see [HP2]).

This leads (assuming the monotonicity of μ_* with respect to q), to obtain for the solution $Q_{c3}(\kappa, \tau)$ of (5.1) the expansion

$$\tau Q_{c3}(\kappa, \tau) = \frac{\kappa^2}{\Theta_0} + \mathcal{O}(\kappa^{4/3}). \tag{7.3}$$

We refer to [HP2] and to the last section for a discussion of this critical wave number.

We hope to give in [HP3] a two-term asymptotic of $\mu_*(q, \tau)$ and consequently of $Q_{c3}(\kappa, \tau)$ for large κ (with $\tau \in (0, \tau_0]$).

⁴This condition can be relaxed [Ray2] at the price of a worse remainder.

8 Perturbative Case: $q\tau$ Small

A second analysis (perturbative in spirit) gives (see [HP2])

Theorem 8.1.

As $\sigma = q\tau \rightarrow 0$,

$$\mu_*(q, \tau) = \Theta(\tau)(q\tau)^2 + \mathcal{O}((q\tau)^4), \quad (8.1)$$

where the remainder is controlled uniformly for $\tau \in (0, \tau_0]$, and $\tau \mapsto \Theta(\tau)$ is a continuous function on $[0, \tau_0]$ such that

$$\Theta(0) = \inf_{\mathbf{h} \in \mathbb{S}^2} \frac{1}{|\Omega|} \int_{\Omega} |\mathbf{F}_{\mathbf{h}}|^2 dx. \quad (8.2)$$

One can also give an asymptotic of $c(\kappa, q, \tau)$, see [HP2].

Theorem 8.2.

Let Ω be a bounded smooth domain in \mathbb{R}^3 and $\tau_0 > 0$. Then, there exist positive constants $C_1(\tau_0)$, $C_2(\tau_0)$ and $\sigma_1(\tau_0)$, such that, for any q, τ, κ satisfying

$$\tau \in (0, \tau_0], \quad \sigma = q\tau \in (0, \sigma_1], \quad \kappa \geq C_1(\tau_0)\sigma, \quad (8.3)$$

we have

$$\left| c(q, \tau, \kappa) + \frac{\kappa^2}{2} |\Omega| - \sigma^2 |\Omega| \Theta(\tau) \right| \leq C_2(\tau_0)(1 + \kappa^{-2})\sigma^4. \quad (8.4)$$

As a corollary and using (2.1), we immediately obtain under the same assumptions

$$\left| \inf_{(\psi, \mathbf{n}) \in H^1(\Omega, \mathbb{C}) \times V(\Omega, \mathbb{S}^2)} \mathcal{E}^{\mathbf{K}}[\psi, \mathbf{n}] + \frac{\kappa^2}{2} |\Omega| \right| \leq C(\tau_0)(q\tau)^2(1 + \kappa^{-2}). \quad (8.5)$$

This estimate is independent of the elastic parameters.

Remark 8.3.

It would be good to have a second term in this last expansion.

9 Coming Back to the Main Functional

We finish this survey by presenting the following results regarding the non-triviality of minimizers. Similar but less accurate results have been obtained in [BCLP]. For the corresponding results for superconductors see Giorgi and Phillips [GioP] and Lu and Pan [LuP1, LuP2, LuP3].

It is a consequence of (8.4) and of (2.9) that

Proposition 9.1.

Let Ω be a bounded smooth domain in \mathbb{R}^3 , $\tau_0 > 0$ and $\kappa_0 > 0$. Then, for any q, τ, κ satisfying

$$\tau \in (0, \tau_0], \quad \sigma = q\tau \in (0, \sigma_1], \quad \kappa \geq C_1(\tau_0)\sigma, \quad \kappa \geq \kappa_0, \quad (9.1)$$

the minimizers of $\mathcal{E}^{\mathbf{K}}$ are non trivial.

We note that the constants involved in the previous statement are independent of the elastic coefficients. The next proposition will show that, if σ/κ and the elastic constants are sufficiently large, the minimizers are the nematic phases.

Proposition 9.2.

For any τ_0 and any σ_0 , there exists a constant $C > 0$ such that, if

$$\tau \in (0, \tau_0], \quad q\tau \geq \sigma_0, \quad q\tau \geq C(1 + q^2)(1 + \kappa^2),$$

then the functional $\mathcal{E}^{\mathbf{K}}$ has no minimizer with $\psi \neq 0$.

Proof. Let (ψ, \mathbf{n}) be a minimizer, with ψ not trivial. So

$$\mathcal{E}^{\mathbf{K}}[\psi, \mathbf{n}] < 0.$$

We should keep in mind what we have obtained in (2.2). In particular, we deduce, like for getting (4.3), that

$$\|\nabla_{q\mathbf{n}}\psi\|_{L^2(\Omega)}^2 \leq \kappa^2\|\psi\|_{L^2(\Omega)}^2. \tag{9.2}$$

As in the proof of Proposition 3.1, we can compare with some element in $\mathcal{C}(\tau)$. For any $Q \in SO(3)$, we have

$$\|\nabla_{q\mathbb{N}_\tau^Q}\psi\|_{L^2(\Omega)}^2 \leq 2\|\nabla_{q\mathbf{n}}\psi\|_{L^2(\Omega)}^2 + 2q^2\|\mathbf{n} - \mathbb{N}_\tau^Q\|_{L^4(\Omega)}^2\|\psi\|_{L^4(\Omega)}^2. \tag{9.3}$$

Then, one can use (9.2) and the so called diamagnetic inequality⁵ and this, together with Sobolev's injection of $H^1(\Omega, \mathbb{C})$ in $L^4(\Omega, \mathbb{C})$, leads to

$$\begin{aligned} \|\psi\|_{L^4(\Omega)}^2 &= \|\psi\|_{L^4(\Omega)}^2 \\ &\leq C(\Omega)(\|\nabla|\psi|\|_{L^2(\Omega)}^2 + \|\psi\|_{L^2(\Omega)}^2) \\ &\leq C(\Omega)(\|\nabla_{q\mathbf{n}}\psi\|_{L^2(\Omega)}^2 + \|\psi\|_{L^2(\Omega)}^2). \end{aligned} \tag{9.4}$$

Hence we obtain, using the characterization of the groundstate energy,

$$\lambda_1^N(q\mathbb{N}_\tau^Q) \leq 2(\kappa^2 + C(\Omega)(1 + \kappa^2)q^2\|\mathbf{n} - \mathbb{N}_\tau^Q\|_{L^4(\Omega)}^2). \tag{9.5}$$

We now choose some Q and observe that, for any $\sigma_0 > 0$, there exists \widehat{C} , such that, if $q\tau$ is larger than σ_0 , we have from the proof of Theorem 7.1 (uniformly with respect to $\tau \in (0, \tau_0]$)

$$\frac{q\tau}{\widehat{C}} \leq \lambda_1^N(q\mathbb{N}_\tau^Q). \tag{9.6}$$

This implies

$$\frac{q\tau}{\widehat{C}} \leq 2(1 + q^2\|\mathbf{n} - \mathbb{N}_\tau^Q\|_{L^4(\Omega)}^2)(1 + \kappa^2). \tag{9.7}$$

The observation –and this is again independent of the elastic coefficients– is that

$$\frac{q\tau}{\widehat{C}} \leq 2(1 + 4|\Omega|^{1/2}q^2)(1 + \kappa^2). \tag{9.8}$$

⁵We recall that diamagnetic inequality says that, for any $u \in H_{loc}^1$ and any magnetic potential \mathbf{A} in L_{loc}^2 we have $|\nabla|u|| \leq |\nabla_{\mathbf{A}}u|$, almost everywhere.

The proof is finished by taking $C = 4 \max\{1, 4|\Omega|^{1/2}\hat{C}\}$. ■

Hence, this is only if we want to have a more precise information about the transition between nematic phase and smectic phase that we will have to use that some of the elastic constants are large. Let us give a statement, in this direction.

Proposition 9.3.

For any $\tau_0 > 0$, any $k_1^0 > 0$, any $\epsilon > 0$, there exists κ_0 and, for any q , $C(\epsilon, \tau_0, q)$ such that if ⁶

- $\kappa \geq \kappa_0$,
- $\tau \in (0, \tau_0]$,
- $K_1 \geq k_1^0 \kappa^2 / \tau$,
- $\min_{j=2,3} K_j \geq C(\epsilon, \tau_0, q) \kappa^2$,
- $q\tau \geq (1 + \epsilon) \kappa^2 / \Theta_0$,

then the functional has no minimizers with $\psi \neq 0$.

Proof. We have to improve the argument starting from (9.3) which we replace for any $\eta > 0$ by

$$\|\nabla_{q\mathbb{N}_\tau^Q} \psi\|_{L^2(\Omega)}^2 \leq (1 + \eta) \|\nabla_{q\mathbf{n}} \psi\|_{L^2(\Omega)}^2 + \left(1 + \frac{1}{\eta}\right) q^2 \|\mathbf{n} - \mathbb{N}_\tau^Q\|_{L^4(\Omega)}^2 \|\psi\|_{L^4(\Omega)}^2. \quad (9.9)$$

This leads to replace (9.5) by

$$\lambda_1^N(q\mathbb{N}_\tau^Q) \leq (1 + \eta) \kappa^2 + C(\Omega, \eta) (1 + \kappa^2) q^2 \|\mathbf{n} - \mathbb{N}_\tau^Q\|_{L^4(\Omega)}^2, \quad (9.10)$$

with two free parameters η and Q .

We first choose $\eta = \epsilon/2$. We can now use Lemma 3.4 together with (3.5) and (3.6) in order to get

$$C(\Omega, \eta) q^2 \|\mathbf{n} - \mathbb{N}_\tau^Q\|_{L^4(\Omega)}^2 \leq \frac{\epsilon}{2}.$$

This leads to our choice of Q . This time we have to use the uniform asymptotic established in (7.2). ■

Remark 9.4.

The results of this section have to be compared with similar, but less accurate, results of [BCLP].

⁶We can in the second item alternatively assume $K_1 \geq k_1^0 q^2 \tau$.

Application to the critical wave numbers

Proposition 9.3 admits a converse using what we know about $c(\kappa, q, \tau)$. This converse result is independent of the Frank constants. More precisely, we can introduce (following [P1]):

For $\kappa > 0, \tau > 0$, we define

$$\begin{aligned} \underline{Q}_{c3}(\kappa, \tau) &= \inf\{q > 0 : \psi = 0 \text{ is the minimizer of } \mathcal{G}_{qn} \text{ for all } \mathbf{n} \in \mathcal{C}(\tau)\}, \\ \overline{Q}_{c3}(\kappa, \tau) &= \inf\{q > 0 : \psi = 0 \text{ is the unique minimizer of } \mathcal{G}_{q'\mathbf{n}} \\ &\quad \text{for all } q' > q, \mathbf{n} \in \mathcal{C}(\tau)\}. \end{aligned} \tag{9.11}$$

and

$$\begin{aligned} \overline{Q}_{c3}^{\mathbf{K}}(\kappa, \tau) &= \inf\{q > 0 : \text{the } (0, \mathbf{n}) \text{ } (\mathbf{n} \in \mathcal{C}(\tau)) \text{ are minimizer of } \mathcal{E}^{\mathbf{K}} \}, \\ \underline{Q}_{c3}^{\mathbf{K}}(\kappa, \tau) &= \inf\{q > 0 : \text{the } (0, \mathbf{n}) \text{ } (\mathbf{n} \in \mathcal{C}(\tau)) \text{ are the unique} \\ &\quad \text{minimizers of } \mathcal{E}^{\mathbf{K}} \text{ for all } q' > q\}. \end{aligned} \tag{9.12}$$

Here we have explicated in the notation the dependence on $\mathbf{K} = (K_1, K_2, K_3)$.

It results of course of the universal estimate (2.9) that

$$\overline{Q}_{c3}^K(\kappa, \tau) \leq \overline{Q}_{c3}(\kappa, \tau) \quad \text{and} \quad \underline{Q}_{c3}^K(\kappa, \tau) \leq \underline{Q}_{c3}(\kappa, \tau), \tag{9.13}$$

for any elastic constants.

Proposition 9.3 implies that for large κ and sufficient large elastic constants the critical wave numbers satisfy

$$\tau \lim_{K_j \rightarrow +\infty} \overline{Q}_{c3}^{\mathbf{K}}(\kappa, \tau) \sim \frac{\kappa^2}{\Theta_0} \quad \text{and} \quad \tau \lim_{K_j \rightarrow +\infty} \underline{Q}_{c3}^{\mathbf{K}}(\kappa, \tau) \sim \frac{\kappa^2}{\Theta_0}. \tag{9.14}$$

A The De Gennes Family

The family of operators $H(\xi)$

$$H(\xi) = D_t^2 + (t - \xi)^2 \tag{A.1}$$

on the half-line with Neumann boundary condition at 0 appears initially in the analysis of the problem in the half plane $\mathbb{R}_+^2 := \{x_1 > 0\}$ of the Neumann realization of the magnetic Schrodinger operator with constant magnetic field $D_{x_1}^2 + (D_{x_2} - x_1)^2$. Here we write $D_t = \frac{1}{i} \frac{\partial}{\partial t}$. The lowest eigenvalue of the operator $H(\xi)$,

$$\xi \mapsto \mu(\xi)$$

admits a unique minimum at $\xi_0 > 0$. For analyzing the variation of $\mu(\xi)$, it is useful to combine the following two formulas

- The Feynman-Hellmann formula:

$$\mu'(\xi) = -2 \int_0^{+\infty} (t - \xi) u_\xi(t)^2 dt,$$

where u_ξ is the normalized groundstate of $H(\xi)$.

- The Bolley-Dauge-Helffer formula [DaH]:

$$\mu'(\xi) = u_\xi(0)^2(\xi^2 - \mu(\xi)) .$$

This permits to show that $\mu(\xi)$ has a unique minimum, which is attained at $\xi_0 > 0$. Moreover

$$\lim_{\xi \rightarrow +\infty} \mu(\xi) = 1 , \quad \lim_{\xi \rightarrow -\infty} \mu(\xi) = +\infty .$$

Graph of $\mu(\xi)$ and comparison with Dirichlet realization

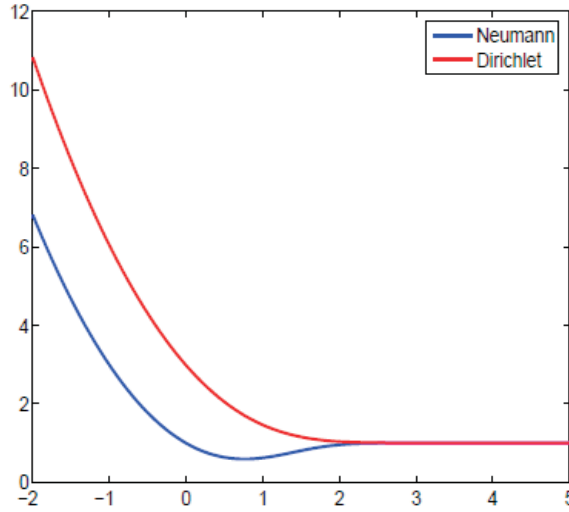


Figure 1: De Gennes model, computed by V. Bonnaillie-Noël

Two constants have played a role in the main text. The first one is Θ_0 :

$$0 < \Theta_0 = \mu(\xi_0) = \inf_{\xi \in \mathbb{R}} \mu(\xi) < 1 . \quad (\text{A.2})$$

We have

$$\xi_0^2 = \Theta_0 \sim 0.59 . \quad (\text{A.3})$$

The second one is:

$$\delta_0 = \frac{1}{2} \mu''(\xi_0) . \quad (\text{A.4})$$

B Montgomery's Model

We have also met the following family (depending on ρ) of quadratic oscillators:

$$D_t^2 + (t^2 - \rho)^2 . \quad (\text{B.1})$$

Denoting by $\nu(\rho)$ the lowest eigenvalue of this operator, Pan and Kwek [PK] (see also [Hel]) have shown that there exists a unique minimum of $\nu(\rho)$ leading to a new universal constant

$$\hat{\nu}_0 = \inf_{\rho \in \mathbb{R}} \nu(\rho) . \quad (\text{B.2})$$

One has (Feynman-Hellmann Formula)

$$\rho_{min} = 2 \int t^2 u_{\rho_{min}}^2 dt ,$$

where u_ρ denotes the normalized groundstate.

Numerical computations confirm that the minimum is attained for a positive value of ρ :

$$\rho_{min} \sim 0.35 ,$$

and that this minimum is

$$\Theta_{min} \sim 0.5698 .$$

Numerical computations also suggest that the minimum is non degenerate. This result is proved in [Hel].

Acknowledgements

The first author would like to thank F. Cardoso and A. Sá Barreto for their kind invitation at this conference and the opportunity to give a mini-course the week before, and he also thank his collaborators (particularly V. Bonnaillie-Noël, S. Fournais), his student N. Raymond (whose Master thesis inspires partially this survey) and also P. Bauman and D. Phillips for useful discussions.

The second author was partly supported by the National Natural Science Foundation of China grant no. 10471125, 10871071, the Science Foundation of the Ministry of Education of China grant no. 20060269012, and the National Basic Research Program of China grant no. 2006CB805902.

Received: November, 2008. Revised: February, 2009.

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