Report on Research in Groups

Mathematical Problems in Liquid Crystals

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Topics

Despite their phenomenal success at a technological level, liquid crystals remain a mysterious material, difficult to model and understand conceptually. The challenge of describing even the simplest and most ubiquitous of liquid crystaline systems – the nematic liquid crystals – using a model that is both comprehensive and simple enough to manipulate efficiently has led to the existence of several major competing theories.

A benchmark test of any liquid crystal model is its predictive capacity with regard to certain patterns, called defects. Predicting the appearance and behaviour of these defects is obviously of utter importance in the manufacturing of liquid crystal displays.

So far, there has been yet no clear understanding as to what the defects are from mathematical point of view. In the Oseen-Frank theory defects are interpreted as discontinuities of the vector fields describing the optical director and they are classified in terms of topological invariants of vector fields. In Ericksen's theory defects are points of isotropic melting, i.e. points where the order parameter vanishes [4]. The defects, in the work of De Gennes [6] are regarded as discontinuities of eigenvectors. However, at the moment, there exists only a very limited understanding of how to characterize these discontinuities analytically [11], [13].

These challenging issues brought us together in order to investigate several key open problems in one of the most comprehensive theories, but least understood mathematically, the Landau-De Gennes Q-tensor theory. From the mathematical point of view the structure of Q-tensor equations has similarities with the Ginzburg-Landau system [2], particularly its $3D$ version, and can be regarded as an approximate harmonic map system [13]. Therefore one can try to study the singularities and defects using methods developed in Ginzburg-Landau theory. However, some of the most challenging aspects of the Q-tensor equations are related to the additional degrees of freedom present in Q-tensor theory and therefore the problem is more complicated and requires new analytical tools to tackle it.

Goals

We focused on understanding the so-called melting hedgehog –the expected universal structure around melting points – and we studied its basic qualitative features, related to its profile and energetic stability. The main challenge has been to develop suitable tools for handling the high dimensionality of the problem. More precisely we studied and obtained various results on:

- fine qualitative properties of the scalar profile of the melting hedgehog;
- existence and uniqueness for singular ODEs that generalise the ones used for describing the melting hedgehog;
- local stability of the melting hedgehog depending on the parameters of the nonlinear potential;

We also studied and made some progress on related problems[1] :

- understanding the universality of melting hedgehog as a prototype for melting points, at least in the case of local minimizers;
- understanding the profile of general isotropic melting points;
- criteria for determining symmetry-breaking solutions, in particular axially symmetric solutions, corresponding to hedgehog boundary conditions;
- existence of large perturbations, that reduce the energy of the melting hedgehog solution.

[1] These will constitute subject of future research by the same group during 2014, in particular, in April at The Mathematisches Forschungsinstitut Oberwolfach.

Organization

The first month of our work, in 2011, focused on studying the stability of the melting hedgehog defect. Our initial starting point was the work [14] that considers what can be regarded as a toy-problem for our higher dimensional case. We understood that there are two main aspects to study separately:

- the ODE governing the underlying scalar profile;
- the techniques necessary for dealing with the high-dimensionality of the possible perturbations that could lower the energy.

We realized that substantially different higher dimensional analogues of the available techniques are necessary. We developed most of these techniques, reducing the study of the stability problem to understanding the interactions between three scalar functions.

In the last two months of the programme, in 2012, after a one-week meeting in Bristol, we focused first on the problem of understanding the above mentioned interactions between three scalar functions, which proved to be a challenging task requiring the refinement of previously developed tools. Also some natural independent questions, related to the ODE problem, were raised and answered partially.

In the final month of our meeting in 2012 (as well as the last week of our meeting in 2011) we focused on several related challenging problems mentioned in previous section.

In addition to these activities we benefited from the interactions with participants of the trimester program "Mathematical challenges of materials science and condensed matter physics". Some of the participants had interactions with local PDE experts working on related subjects, namely Radu Ignat had interactions with Mathias Kurzke and Arghir Zarnescu had discussions with Soeren Bartels and Alex Raisch.

Our research group will continue the study of the problems mentioned before and expand on the ideas obtained during this meeting, in future meetings such as in April 2014 at The Mathematisches Forschungsinstitut Oberwolfach.

Main Results

The results of our work have been divided into two papers to be submitted soon, namely [9] studying the ODE problem, and [10], studying the tensorial stability problem. These have been announced in [8].

We mention now the main results contained in [9] and [10]. To this end we consider the following Landau-de Gennes energy functional:

$$\mathscr{F}(Q) = \int_{\mathbb{R}^3} \left[\frac{1}{2}|\nabla Q|^2 + f_B(Q)\right] dx, \quad Q \in H^1(\mathbb{R}^3, \mathscr{S}_0),$$

where

$$\mathscr{S}_0 \stackrel{\text{def}}{=} \{Q \in \mathbb{R}^{3\times 3},\, Q = Q^t,\, \text{tr}(Q) = 0\}$$

denotes the set of Q-tensors (i.e., traceless symmetric matrices in $\mathbb{R}^{3\times 3}$, see [1] for their physical interpretation). The bulk energy density f_B accounts for the bulk effects and has the following form

$$f_B(Q) = -\frac{a^2}{2}|Q|^2 - \frac{b^2}{3}\text{tr}(Q^3) + \frac{c^2}{4}|Q|^4, \tag{0.1}$$

where $a^2, c^2 > 0$ and $b^2 \geq 0$ are constants and $|Q|^2 \stackrel{\text{def}}{=} \text{tr}(Q^2)$. A critical point of the functional $\mathscr{F}$ satisfies the Euler-Lagrange equation

$$\Delta Q = -a^2\, Q - b^2[Q^2 - \frac{1}{3}|Q|^2\, Id] + c^2\, |Q|^2\, Q, \tag{0.2}$$

where the term $\frac{1}{3}b^2\,|Q|^2\, Id$ is a Lagrange multiplier that accounts for the tracelessness constraint. It is well known that solutions of (0.2) are smooth (see for instance [13]).

Remark 1 We should point out now that although the equation (0.2) *seems to depend on three parameters a^2, b^2 and c^2, there is only one independent parameter in the problem which can be chosen to be a^2 for fixed b^2 and c^2 (after a suitable rescaling $Q \mapsto \lambda Q(x/\mu)$ for two parameters $\lambda, \mu > 0$).*

We were interested in studying the *radially-symmetric* solution of (0.2). For that, a measurable $\mathscr{S}_0$-valued map $Q : \mathbb{R}^3 \to \mathscr{S}_0$ is called radially-symmetric if

$$Q(Rx) = R\, Q(x)\, R^t \text{ for any rotation } R \in SO(3) \text{ and a.e. } x \in \mathbb{R}^3.$$

In fact, such a map $Q(x)$ has only one degree of freedom: there exists a measurable radial scalar function $u : (0, +\infty) \to \mathbb{R}$ such that $Q(x) = u(|x|)\,\overline{\mathrm{H}}(x)$ for a.e. $x \in \mathbb{R}^3$, where $\overline{\mathrm{H}}$ is the so called *hedgehog*:

$$\overline{\mathrm{H}}(x) = \frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3} Id$$

and the radial scalar profile u of Q is given by $u(|x|) = \frac{3}{2}\mathrm{tr}(Q(x)\overline{\mathrm{H}}(x))$ for a.e. $x \in \mathbb{R}^3$.

We focused on the stability and properties of the profile of the following radially symmetric solution of (0.2), called *melting hedgehog* :

$$H(x) = u(|x|)\overline{\mathrm{H}}(x) \tag{0.3}$$

where the radial scalar profile u is the unique *positive* solution of the following semilinear ODE:

$$u''(r) + \frac{2}{r}\,u'(r) - \frac{6}{r^2}\,u(r) = F(u(r)) \quad \text{for} \quad r > 0 \tag{0.4}$$

subject to boundary conditions $u(0) = 0$ and $\lim_{r\to\infty} u(r) = s_+$ where

$$F(u) = -a^2\,u - \frac{b^2}{3}\,u^2 + \frac{2c^2}{3}\,u^3 \tag{0.5}$$

and $s_+ \stackrel{\text{def}}{=} \frac{b^2+\sqrt{b^4+24a^2c^2}}{4c^2}$ is the positive zero of F.

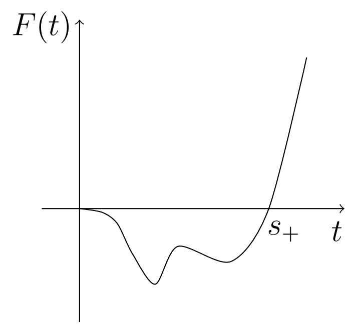
Our main result concerned the local stability of the melting hedgehog (see [10]). We highlight that H is a critical point of (0.2), but has infinite energy $\mathscr{F}$, i.e., $\mathscr{F}(H) = \infty$. Therefore, the stability issue was carried out by analyzing the following second variation of the modified functional $\mathscr{F}$ at the point H in the direction $V \in C_c^\infty(\mathbb{R}^3; \mathscr{S}_0)$, denoted by $\mathscr{Q}(V)$:

$$\begin{aligned}\mathscr{Q}(V) &= \frac{1}{2}\frac{d^2}{dt^2}\int_{\mathbb{R}^3}\Big[\frac{1}{2}|\nabla(H + t\,V)|^2 + f_B(H + t\,V) - \frac{1}{2}|\nabla H|^2 - f_B(H)\Big]\,dx \\ &= \int_{\mathbb{R}^3}\Big[\frac{1}{2}|\nabla V|^2 + \big(-\frac{a^2}{2} + \frac{c^2u^2}{3}\big)|V|^2 - b^2\,u\,\mathrm{tr}(\bar{H}\,V^2) + c^2\,u^2\,\mathrm{tr}^2(\bar{H}\,V)\Big]\,dx.\end{aligned} \tag{0.6}$$

Theorem 0.1 *There exists $a_0^2 > 0$ such that for all $a^2 < a_0^2$ the melting hedgehog H defined at* (0.3) *is a locally stable critical point of* (0.2)*, i.e., $\mathcal{Q}(V) \geq 0$ for all $V \in C_c^\infty(\mathbb{R}^3; \mathscr{S}_0)$. Moreover $\mathcal{Q}(V) = 0$ if and only if $V \in \mathrm{span}\{\partial_{x_i} H\}_{i=1}^3$, i.e., the kernel of the second variation is generated by translations of $H(x)$.*

There exists $a_1^2 > 0$ so that for any $a^2 > a_1^2$ there exists $V_* \in C_c^\infty(\mathbb{R}^3; \mathscr{S}_0)$ such that $\mathcal{Q}(V_*) < 0$. Any such V_* cannot be purely uniaxial (i.e., $V_*(x)$ has three different eigenvalues for some point $x \in \mathbb{R}^3$).

In order to study the stability we had to understand the underlying scalar profile. We have in fact studied a more general ODE. We obtained an existence and uniqueness result of solution for a special type of semilinear ODE that generalizes (0.4). Let $F : \mathbb{R} \to \mathbb{R}$ be a C^1 function satisfying the following conditions:



$$\begin{cases} F(0) = F(s_+) = 0, \ F'(s_+) > 0, \\ F(t) < 0 \ \text{ if } \ t \in (0, s_+), \\ F(t) > 0 \ \text{ if } \ t > s_+, \end{cases} \tag{0.7}$$

for some $s_+ > 0$.

Figure 1: A schematic graph of F on $\mathbb{R}_+$.

We focused on the following semilinear ODE:

$$u''(r) + \frac{p}{r} u'(r) - \frac{q}{r^2} u(r) = F(u(r)) \quad \text{on } (0, R) \tag{0.8}$$

where we assume

$$p, q \in \mathbb{R} \text{ and } q > 0.$$

We present the result for the case of finite domains (i.e., $(0, R)$ with $R \in (0, +\infty)$) and the infinite domain $(0, +\infty)$ (i.e. $R = +\infty$) under the limit conditions

$$u(0) = 0, \quad u(R) = s_+, \tag{0.9}$$

with the standard convention $u(\infty) = \lim_{r\to\infty} u(r) = s_+$ if $R = +\infty$.

Theorem 0.2 *Under the assumption* (0.7)*, there exists a unique non-negative solution u of* (0.8) *with boundary conditions* (0.9)*. Moreover, this solution is strictly increasing.*

Under some additional conditions on the nonlinearity we are able to prove the uniqueness of solutions in the general class of nodal (sign changing) solutions. Further fine properties of the solution, necessary for proving Theorem 0.1, are also established. See [9].

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