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Variational analysis of liquid crystals

Análisis variacional de cristales líquidos

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This is an exposition of the role played by the calculus of variations in the field of liquid crystals, in particular the way it provides a sound foundation to the mathematical modelling and numerical study of their response to the confining material's geometry and to external electromagnetic stimuli.

Keywords: liquid crystal, calculus of variations, partial order, **Q**-tensor, Landau-de Gennes, topological defects.

Resumen. Se expone del rol del cálculo de variaciones en el área de los cristales líquidos, en particular el modo en que proporciona un cimiento sólido al modelamiento matemático y el estudio numérico de su respuesta a la geometría del material que lo contiene y a estimulos electromagnéticos externos.

Palabras claves: Cristales líquidos, Cálculo de variaciones, Landau-de Gennes, Transición de fase.

Mathematics Subject Classification: 35B36, 49S05, 49J10, 49J45, 49K10, 49K20, 49K30, 49N60, 82B21, 82D30.

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> *"In physics we have dealt hitherto only with periodic crystals. To a humble physicist's mind, these are very interesting and complicated objects; they constitute one of the most fascinating and complex material structures by which inanimate nature puzzles his wits. Yet, compared with the aperiodic crystal, they are rather plain and dull. The difference in structure is of the same kind as that between an ordinary wallpaper in which the same pattern is repeated again and again in regular periodicity and a masterpiece of embroidery, say a Raphael tapestry, which shows no dull repetition, but an elaborate, coherent, meaningful design traced by the great master."*
>
> *Erwin Schrödinger,* What is Life? *[24]*

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1. The science and technology of liquid crystals

1.1. How do LCDs work?

A liquid crystal display consists of a light source (be it the fluorescent lamps of the traditional displays or the modern LED backlight) and an array of red, green and blue pixels capable of blocking as well as of transmiting the light emitted by that source. The method used to either block or let the light go through a pixel, depending on the colour that the screen should have in that particular point to display a given image, consists in depositing a liquid crystal between two electrodes, located behind the colour filter of the pixel, and then ask the liquid crystal to either block or transmit the light. But how can such a request be made to a liquid crystal? By having placed it between two electrodes it is possible to generate a voltage gradient and, with it, an electric field that changes the orientation of the liquid crystal. In a single pixel, whose characteristic length is of approximately $100\mu m$ (a tenth of a milimiter, just as a hair or a needle), there are about a thousand million liquid crystal molecules. One of their many special properties is their capacity to interact with the applied electric field, making it possible to align the thousand million molecules along a single direction, preventing light from passing. In order to understand why the orientation of the LC molecules determines whether light passes through the pixel, it is necessary to understand first the effect of light polarization.

1.2. Light polarization

Light is composed of particles called photons which, apart from travelling at the speed of the light in a given direction, also vibrate in a plane perpendicular to it. In general the direction in which photons vibrate within that plane is random (i.e., light is composed of photons that vibrate in different directions within that plane and, given any fixed direction, there are as many photons vibrating close to that direction as there are vibrating close to any other). However, in some occasions part of the light is absorbed by various media and only those photons vibrating in a specific direction remain; the light is then said to be polarized in that direction. An instance of this occurs when light is reflected in a window or in water; in this case most of the photons of the reflected light vibrate parallel to the surface. The same happens, although possibly to a less extent, when light is reflected from any non-metallic surface. This is the principle behind Polarid filters, invented by Edwin Land in 1929, made out of long-chain hydrocarbons that absorb any light with an electric field parallel to them. These filters are used, for example, in sunglasses, by aligning the hydrocabons horizontally in order to absorb the light reflected by roads and other horizontal surfaces.

Going back to liquid crystals, apart from being able to align with the electric field generated by the electrodes, they also possess the ability to interact with polarized light and modify its polarization direction. If in the two electrodes the LC molecules are parallel to the surface, but pointing to different directions on the two electrodes, and if in the intermediate region the molecules twist gradually until they attain their final orientation, the liquid crystal receives light polarized in the direction of the LC molecules on one electrode and ends up giving light polarized in the direction of the LC on the other electrode. Thanks to this the pixel is able to transmit light even if crossed polarized filters are placed behind the electrodes, as long as, in each electrode, the liquid crystal aligns with the polarization axis of the polarizer. In contrast, when the electric field is turned on, the alignment of the LC molecules no longer coincides with the directions permitted by the polarizers, the light is completely absorbed by the end polarized and the pixel becomes dark.

1.3. The fourth state of matter

Even though plasma is commonly regarded as the fourth state of matter, it is not very common. “On earth, plasmas can be found in the glass envelopes of fluorescent lights and in the picture elements of some large-area television sets. Only in the heavens will plasma be commonly encountered, in the form of northern (or southern) lights, or in stars, galactic trails, and other astrophysical phenomena, but on our planet, there are *no* free-standing plasmas. Liquid crystals, on the other hand, are indeed a terrestrial fourth state of matter.” [11, Preface].

The story begins in 1888 with the Austrian botanist and chemist Friedrich Reinitzer who, in his attempts to discover the molecular formula of cholesterol (which was only discovered in the 1930’s thanks to the work of Adolf Windaus and Heinrich Wieland), was struck to find that the Cholesteryl benzoate he extracted from carrots had not one but two melting points. At the time the general idea was that all matter normally had one melting point, where it turns from solid to liquid, and a boiling point where it turns from liquid to gas. However, at 145.5°C this cholesterol substance melted from its solid state into a turbid liquid which existed until 178.5°C where the cloudiness suddenly disappeared, giving way to a clear transparent liquid. Being unable to explain this discovery, the name of Otto Lehmann, a german physicist expert in crystal optics, came to his mind. Lehmann had invented a very special microscope. On the one hand, it was a polarizing microscope: it was fitted with two polarizers in such a way that liquid and gases appeared black, whereas minerals and crystals could actually be seen; moreover, the image changed if the orientation of the crystal changed. Being, hence, extremely valuable for identifying crystals and resolving the details of the crystal structure, these microscopes were very popular in the 19th century due to the prominent role of geology and mineralogy in the mining industry. On the other hand, Lehmann had added a hot stage to the microscope and in that way he could study what happened to the samples upon heating. Lehmann was fascinated with Reinitzer samples because he saw images, containing straight worm-like objects, that looked like no other sample he had studied before and, most of all, because those objects were flowing, coalescing, separating, and exhibiting all sorts of phenomena (as opposed to the images produced from classical crystals which were perfectly still). He went even further in his excitement to the point of truly believing that he had discovered the secret of life [10].

That crystals can be studied under polarized light is due to the fact their atoms are arranged in a definite pattern, possessing special discrete translational and rotational symmetries. At the other end, that liquids and gases look black under polarizing microscopes is a consequence of the mobility their molecules gain by having higher temperature than solids, mobility that increases its disorder ending up in molecules having a random orientation even in very small regions of the material, each molecule also eventually taking all possible orientations as it evolves in time. Since Reitnitzer's turbid fliuds did not looked black under his microscope, Lehmann knew that their constitutent molecules could not be completely disordered as in a traditional liquid; they had to exhibit some form of order, as in crystalline solids. Initially he thought that the substances were composed of crystals that were flowing in a liquid, as suggested by his famous 1889 article entitled 'On Flowing Crystals'. Conclusive experiments and early theories between 1910 and 1930, in particular the work of Georges Friedel, finally confirmed that the substances were not just a mixture of solid and liquid components but an entirely new phase of matter.

1.4. Applications to medicine, biology, astrophysics, and topology

Far for being rare materials, liquid crystals are part of our daily life. Not only they are present in our flat-screen TV's, laptops, and mobiles: cholesterol, soap, cosmetics, the myelin that electrically insulates the axon of some nerve cells, viruses such as the tobacco mosaic virus, and human blood also have liquid crystal phases (though not at room temperature as the synthetic LC used in displays). Our DNA has also been found recently to have a liquid crystalline structure [3].

A captivating example of an application of LC to medicine is the recent patent of Popov et al. [22] of a non-invasive sensor capable of rapidly detecting if a patient is infected with, e.g., ebola or other given viruses. In this sensor a common liquid cyrstal is coated with an antibody against ebola, inducing a parallel alignment of the LC molecules on the top surface. If a drop of blood infected with ebola enters in contact with the LC sample, the antibody coating reacts with the virus in the blood at the coat is removed from the LC, leaving it exposed to air. This induces a perpendicular aligment on the top surface, completely changing the orientation of the molecules throughout the sample and producing well-defined optical signatures. In contrast, if the virus is not present in the drop of blood, the antibody remains and no change is perceived in the optical textures produced by the LC.

Regarding biology, it is of fundamental importance to understand what holds together the delicate and mobile structure of a cell membrane and how does it form [25], as well as the formation and the governing mechanism for the ion channels in the membranes which are responsible for many of the biological functions. Liquid crystals are commonly regarded as a first necessary step towards a proper understanding of biological membranes, not only because the membranes are liquid crystalline themselves, also because both in liquid crystals and in membranes the fundamental question is how do their molecules attain diverse degrees of order (and compared to the order exhibited by the passive LC, the problem of studying membranes and living organisms is much more complex).

Special mention ought to be made of the fertile interaction between the fields of liquid crystals and topology. One of the most attractive features of liquid crystals is the presence of very small regions inside which the average orientation of the molecules changes dramatically, as will be discussed in the following sections. These *topological defects*, which appear in various parts of an LC sample and are not independent but interact with each other, are not exclusive to LC systems but can be found also in superconductors, in superfluids, in dislocations and disclinations in metals, just to mention a few examples. However, due to their unique optical properties, in liquid crystal systems it is possible to easily visualize and study topological defects, so that, for instance, experiments with LC may lead to predictions about the cosmic strings formed on the boundaries of regions that spread at the speed of light upon the cooling and expansion of the early universe [8]. Also, open problems from knot theory can now be studied through liquid crystalline optical realizations, such as in the work of I. Smalyukh and his co-workers, e.g. [1, 2, 28, 18, 26, 27].

2. Mathematical modelling

Part of the impressive development of the LCD industry has been made possible and/or accompanied by the analytical and numerical understanding of the behaviour of liquid crystals in response to various external electromagnetic stimuli or, for example, changes in the design of the specimens where they are deposited. As already explained, the interaction with light and other electromagnetic fields characteristic of liquid crystals is due to the ability of their molecules to sustain highly ordered states. There are various ways to measure the amount of order; this exposition will focus on the 1991 Nobel Prize winner approach by Landau & de Gennes. Consider a material point $\mathbf{x}$ in the region Ω occupied by the liquid crystal. Let $\delta > 0$ be small compared to the macroscopic length-scale, but large enough to contain enough molecules for a statistical description to be valid. Let $N(\mathbf{x})$ be the number of molecules entirely contained in $B(\mathbf{x}, \delta)$ and $\mathbf{p}_i \in \mathbb{S}^2$ be the orientation of the i-th molecule at a given fixed time (here $\mathbb{S}^2$ denotes the unit sphere in $\mathbb{R}^3$). By the statistical head-to-tail symmetry of the molecules, it is physically more significant to represent the orientation by the pair $\pm\mathbf{p}_i$ of antipodal unit vectors, or with the tensor product $\mathbf{p}_i \otimes \mathbf{p}_i$, which corresponds to the projection along that direction (regarded as a linear transformation from $\mathbb{R}^3 \to \mathbb{R}^3$). Since it is prohibitive to follow every single molecule, this collection of orientations will be described macroscopically by a (Borel) probability measure $\mu_{\mathbf{x}}$ on $\mathbb{S}^2$ that is to be regarded as an approximation of $\dfrac{1}{N}\displaystyle\sum_{i=1}^{N}\frac{1}{2}(\delta_{\mathbf{p}_i} + \delta_{-\mathbf{p}_i})$. This probability measure $\mu_{\mathbf{x}}$ is still very complex to study, so only a finite-dimensional approximation of it, consisting of a finite number of its moments, will be chosen as the *order parameter*. Now, the measure $\mu_{\mathbf{x}}$ will be required to respect the head-to-tail symmetry, so that $\mu_{\mathbf{x}}(E) = \mu_{\mathbf{x}}(-E)$ for every Borel $E \subset \mathbb{S}^2$; due to this, the first moment $\int_{\mathbb{S}^2} \mathbf{p}\, \mathrm{d}\mu_{\mathbf{x}}(\mathbf{p})$ vanishes and, hence, does not contribute in the description of the LC. For the *isotropic* distribution $\frac{1}{4\pi}\, \mathrm{d}A(\mathbf{p})$ (in which all orientations occur with the same probability; here $A(E)$ is the area of E for every Borel $E \subset \mathbb{S}^2$) the second moment is $\frac{1}{4\pi}\int_{\mathbb{S}^2} \mathbf{p}\otimes\mathbf{p}\, \mathrm{d}A(\mathbf{p}) = \frac{1}{3}\mathbf{1}$ (here $\mathbf{1}$ denotes the 3×3 identity matrix). The *de Gennes* $\mathbf{Q}$*-tensor*

$$\mathbf{Q}(\mathbf{x}) := \int_{\mathbb{S}^2} \left(\mathbf{p}\otimes\mathbf{p} - \frac{1}{3}\mathbf{1}\right) \mathrm{d}\mu_{\mathbf{x}}(\mathbf{p}) \tag{1}$$

is then a measure of the deviation of the second moment of $\mu_{\mathbf{x}}$ from that of the isotropic state.

It is easy to see that the projection matrices $\mathbf{p}\otimes\mathbf{p}$ are symmetric. Since $\mathbf{Q}$ is, then, the limit of (Lebesgue) sums of symmetric matrices, it is symmetric itself. Therefore, by the spectral theorem, it admits a decomposition of the form

$$\mathbf{Q}(\mathbf{x}) = \lambda_1(\mathbf{x})\mathbf{n}_1(\mathbf{x})\otimes\mathbf{n}_1(\mathbf{x}) + \lambda_2(\mathbf{x})\mathbf{n}_2(\mathbf{x})\otimes\mathbf{n}_2(\mathbf{x}) + \lambda_3(\mathbf{x})\mathbf{n}_3(\mathbf{x})\otimes\mathbf{n}_3(\mathbf{x}),$$

where $\{\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3\}$ is an orthonormal basis of eigenvectors of $\mathbf{Q}$ with corresponding eigenvalues λ_1, λ_2, λ_3. Furthermore,

$$\operatorname{tr}\mathbf{Q} = \int_{\mathbb{S}^2} (\operatorname{tr}\mathbf{p}\otimes\mathbf{p} - 1)\, \mathrm{d}\mu_{\mathbf{x}}(\mathbf{p}) = 0,$$

hence $\lambda_1+\lambda_2+\lambda_3 = 0$. Assuming, without loss of generality, that $\lambda_1 \geq \lambda_2 \geq \lambda_3$, the above decomposition is unique if and only if the three eigenvalues are different. If this is the case, the molecules around $\mathbf{x}$ are said to be in the *biaxial* state. There is a preferred orientation $\mathbf{n}_1$ but knowing this is insufficient to describe the state of order of the molecules; it must be taken into account that among the orientations of their projections onto the plane $\mathbf{n}_1^\perp$ orthogonal to $\mathbf{n}_1$ there is also a preferred direction $\mathbf{n}_2$. If, at the other end, the three eigenvalues are equal, then $\mathbf{Q}(\mathbf{x}) = \mathbf{0}$ and the second moment of $\mu_{\mathbf{x}}$ is unable to detect any alignment of the molecules around $\mathbf{x}$. This is to say, the second moment is the same of that of a regular liquid; around that point the liquid crystal is said to have melted, or to be in its *isotropic* state. The last possibility is that two of the eigenvalues are equal and the other differs. If the equal eigenvalues are the smallest two then $\mathbf{Q} = \frac{3\lambda_1}{2}\left(\mathbf{n}_1 \otimes \mathbf{n}_1 - \frac{1}{3}\mathbf{1}\right)$ and the molecules tend to align along the direction of $\pm\mathbf{n}_1$, but their projections onto $\mathbf{n}_1^\perp$ point equally likely in every direction. If, on the other hand, it is the two largest eigenvalues that are equal, then the representation $\mathbf{Q} = s\left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{1}\right)$ continues to be valid and the projection of the orientation of the individual molecules onto $\mathbf{n}^\perp$ continues to point equally likely in every direction, but s is now negative and rather than having a preferred direction what the molecules now prefer is to align along a plane (the plane $\mathbf{n}^\perp$). They are, respectively, the *positive uniaxial* and the *negative uniaxial* states.

Equilibrium states of a liquid crystal sample are sought via the principle of minimum energy, which postulates that in any closed system the thermodynamic free energy tends to decrease and attain a minimum value. Phenomenological models usually consider the following contributions to the total free energy:

- A term corresponding to any distortion to the structure of the material (spatial variations of the molecular alignment, i.e. of the **Q**-tensor). It makes it possible to capture the elastic response of the LC.
- The so-called *thermotropic potential* which determines the state (the amount of order) preferred by the liquid crystal at different temperatures.
- The energy coming from externally applied electric and/or magnetic fields.
- Surface energy terms representing the interaction energy between the bounding surface and the LC molecules on that surface.

The simplest (and simplistic) form of the elastic energy is

$$\int_\Omega \frac{L}{2}|\nabla\mathbf{Q}(\mathbf{x})|^2\,\mathrm{d}\mathbf{x}, \tag{2}$$

where $L > 0$ is an elastic constant. Regarding the thermotropic potential, the special form proposed by de Gennes [9] in order to study the transition from the isotropic phase to the nematic phase (in which at every material point molecules start to align along a preferred direction) is

$$\psi_B(\mathbf{Q},\theta) = a(\theta)\operatorname{tr}\mathbf{Q}^2 - \frac{2b}{3}\operatorname{tr}\mathbf{Q}^3 + c\operatorname{tr}\mathbf{Q}^4, \tag{3}$$

where $a(\theta) = \alpha(\theta-\theta^*)$ for some constants $\alpha > 0$ and $\theta^* > 0$, and where $b, c > 0$ are constants independent of the temperature θ. Above the critical temperature θ^* the isotropic state $\mathbf{Q}^*$ is a global minimizer of this quartic form of the thermotropic potential. In contrast, when $\theta < \theta^*$ the minimum of the polynomial is attained only at uniaxial states $\mathbf{Q} = s\left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{1}\right)$ and only when *scalar order parameter* s takes the special value $s_+ := \frac{b+\sqrt{b^2-24ac}}{4c}$. The surface energies considered are typically of the form $-\dfrac{1}{2}\displaystyle\int_{\partial\Omega} K\left(s^{-1}\mathbf{Q}(\mathbf{x})\bar{\mathbf{n}}(\mathbf{x})\cdot\bar{\mathbf{n}}(\mathbf{x}) + \frac{1}{3}\right)\mathrm{d}S(\mathbf{x})$, a consequence being that the free energy is reduced when the molecules at the surface align parallel to the prescribed direction $\bar{\mathbf{n}}(\mathbf{x})$. The presence of the surface energy turns into a Dirichlet condition (referred to as the *strong anchoring* condition) when the anchoring constant $K \to +\infty$. Refer to [19] for numerical simulations of the minimization of this phenomenological free energy in the case of a real life LC device.

3. Rigorous analysis

3.1. Orientability and comparison between models

The Landau-de Gennes theory is able to capture non-orientable topological defects and half-integer indices (as in the case study in [19]), as well as truly biaxial states. However, most studies of liquid crystals are made either with the simpler model of Ericksen, which describes the amount of order by means of a preferred direction $\mathbf{n}(\mathbf{x})$ and a scalar order parameter $s(\mathbf{x})$ only, or with the Oseen-Frank model in which $s(\mathbf{x})$ is furthermore assumed to be constant. Regarding orientability, the main result is due to Ball & Zarnescu [5, 6]:

> *If* $\Omega \subset \mathbb{R}^3$ *is a bounded simply-connected domain of class* C^0 *and* $\mathbf{Q} \in W^{1,2}(\Omega, \mathbb{R}^{3\times 3})$ *is such that for almost every* $\mathbf{x} \in \Omega$ *there exists* $\mathbf{n}(\mathbf{x}) \in \mathbb{S}^2$ *such that*
>
> $$\mathbf{Q}(\mathbf{x}) = s\left(\mathbf{n}(\mathbf{x}) \otimes \mathbf{n}(\mathbf{x}) - \frac{1}{3}\mathbf{1}\right), \tag{4}$$
>
> *for some constant* $s > 0$, *then there exists a unit vector field* $\mathbf{n} \in W^{1,1}(\Omega, \mathbb{S}^2)$ *for which* (4) *holds.*

Thus, for simply-connected domains, the Oseen-Frank model can be regarded as the minimization of the Landau-de Gennes energy functional in the restricted class of $\mathbf{Q}$-tensor-valued maps that are uniaxial at almost every $\mathbf{x} \in \Omega$ and have a prescribed constant scalar order parameter.

For the *one-constant* approximation (2) it was proved in [17] that as $L \to 0$ minimizers of the full Landau-de Gennes functional do converge (in the strong topology of the Hilbert space $H^1(\Omega; \mathbb{R}^{3\times 3})$) to minimizers of the simplified Oseen-Frank model. Nevertheless, for other asymptotic regimes such as the low temperature limit, it has been proved [12, 16, 14, 15] that the approximation ceases to be valid near the defects' cores since there points with maximal biaxiality and points with negative uniaxiality necessarily exist. Understanding the internal structure of the defects remains an open problem.

3.2. Numerical analysis

In work by Nochetto, Walker & Zhang [20] a piecewise-linear finite element scheme is proposed for the orientable Ericksen model with a variable scalar order parameter. They are able to rigorously prove that their numerical discretization Γ-converges to the continuum variational problem. For the required energy lower bound, the convexity of the energy on each variable is exploited. For the construction of recovery sequences necessary for the energy upper bounds, they require a result of approximation of Sobolev maps by smooth maps such as the one by Pakzad & Rivière [21]. The difficulty in the density result is that the smooth maps that approximate the director $\mathbf{n} \in W^{1,2}(\Omega, \mathbb{S}^2)$ must satisfy the unit-length constraint. The result of Pakzad & Rivière can be used provided that the liquid crystal is far from melting (that the scalar order parameter $s(\mathbf{x})$ is bounded away from zero), but in Ericksen's model this fails around defects (which the model accommodates via melting). Nochetto, Walker & Zhang overcome this obstacle in the orientable case but for non-orientable fields the problem remains open.

3.3. Derivation of the de Gennes potential

The commonly used quartic thermotropic potential (3) was originally conceived as what should intuitively be a Taylor expansion, around the isotropic state, of the true thermodynamic bulk potential. A rigorous justification only appeared recently (40 years later), and is due to Ball & Majumdar [4]. First, the bulk potential $\psi_B(\mathbf{Q}, \theta)$ is identified with the minimum of the free energy per particle at temperature $\theta > 0$ given by

$$I_\theta(\rho) = U(\rho) - \theta\eta(\rho),$$

where U is an interaction term given by

$$U(\rho) = \frac{1}{2}\int_{\mathbb{S}^2}\int_{\mathbb{S}^2} K(\mathbf{p}, \mathbf{q})\rho(\mathbf{p})\rho(\mathbf{q})\,\mathrm{d}\mathbf{p}\,\mathrm{d}\mathbf{q}$$

and $\eta(\rho)$ is the entropy term given by

$$\eta(\rho) = -k_B\int_{\mathbb{S}^2} \rho(\mathbf{p})\ln\rho(\mathbf{p})\,\mathrm{d}\mathbf{p},$$

among all probability density functions $\rho = \rho(\mathbf{p}) \in L^1(\mathbb{S}^2)$ giving rise to a macroscopic probability measure μ whose second moment produces exactly the **Q**-tensor $\mathbf{Q}$. The regularity and other analytical properties of ψ_B are thoroughly studied for the mean-field Maier-Saupe theory where the interaction kernel is postulated to be of the form

$$K(\mathbf{p}, \mathbf{q}) = 2\kappa\left(\frac{1}{3} - (\mathbf{p}\cdot\mathbf{q})^2\right)$$

for some constant κ independent of temperature. This enables a rigorous Taylor expansion around $\mathbf{Q} = \mathbf{0}$ which almost coincides with (3), showing that some corrections are necessary regarding the dependance on the temperature of the coefficients of the polynomial (which, in particular, changes the predicted nematic initiation temperature).

3.4. Harmonic maps

The study of liquid crystals has proved to be a fertile meeting point between continuum mechanics and differential geometry, the most spectacular result being probably the following, due to Schoen & Uhlenbeck [23] and to Brezis, Coron & Lieb [7]:

> *Any minimizer of* $\int_\Omega |\nabla \mathbf{n}(\mathbf{x})|^2 \,\mathrm{d}\mathbf{x}$ *over all* $\mathbf{n} \in H^1(\Omega; \mathbb{S}^2)$ *with prescribed boundary values* $\mathbf{n}|_{\partial\Omega} = \bar{\mathbf{n}}$ *is smooth in* Ω *except for a finite number of point defects located at points* $\mathbf{x}_i \in \Omega$*. Moreover,*
>
> $$\mathbf{n}(\mathbf{x}) \sim \pm \mathbf{R}_i \frac{\mathbf{x} - \mathbf{x}_i}{|\mathbf{x} - \mathbf{x}_i|} \text{ as } \mathbf{x} \to \mathbf{x}_i$$
>
> *for some* $\mathbf{R}_i \in SO(3)$.

In the more physical case of an elastic energy involving different energetic costs for the twist, bend, splay, and saddle-splay of the director field, Hardt, Kinderlehrer & Lin [13] have the impressive result that minimizers over all $\mathbf{n} \in H^1(\Omega; \mathbb{S}^2)$ with prescribed boundary data are analytic outside a closed subset of Ω whose Hausdorff dimension is less than one.

References

[1] P. J. Ackerman and I. I. Smalyukh, *Diversity of knot solitons in liquid crystals manifested by linking of preimages in torons and hopfions*, Preprint.

[2] ———, *Static three-dimensional topological solitons in fluid chiral ferromagnets and colloids*, Preprint.

[3] J. Arsuaga, M.-C. Calderer, L. Hiltner, and M. Vezquez, *A liquid crystal model of viral dna encapsidation*, arXiv:1712.00629, 2017.

[4] J. M. Ball and A. Majumdar, *Nematic liquid crystals: from maier-saupe to a continuum theory*, Molecular Crystals and Liquid Crystals **525** (2010), 1–11.

[5] J. M. Ball and A. Zarnescu, *Orientable and non-orientable line fields for uniaxial nematic liquid crystals*, Molecular Crystals and Liquid Crystals **495** (2008), 573–585.

[6] ———, *Orientability and energy minimization in liquid crystal models*, Arch. Ration. Mech. Anal. **202** (2011), 493–535.

[7] H. Brezis, J. M. Coron, and E. H. Lieb, *Harmonic maps with defects*, Comm. Math. Phys. **107** (1986), 649–705.

[8] M. Cruz, N. Turok, P. Vielva, E. Martínez-González, and M. Hobson, *A Cosmic Microwave Background Feature Consistent with a Cosmic Texture*, Science **318** (2007), no. 5856, 1612–1614.

[9] P. G. de Gennes, *Short range order defects in the isotropic phase of nematics and cholesterics*, Molecular Crystals and Liquid Crystals **12** (1971), no. 3, 193–214.

[10] D. Dunmur, *Liquid crystals: structured fluids for applications*, DiStruc Innovative Training Network Public Lectures, 2016, Web, 6 June 2018, https://www.youtube.com/watch?v=y3iJIPhn5GY.

[11] D. Dunmur and T. Sluckin, *Soap, Science & Flat-Screen TVs*, Oxford University Press, 2014.

[12] E. C. Gartland and S. Mkaddem, *On the local instability of radial hedgehog configurations in nematic liquid crystals under Landau-de Gennes free-energy models*, Phys. Rev. E. **59** (1999), 563–567.

[13] R. Hardt, D. Kinderlehrer, and F.-H. Lin, *Existence and partial regularity of static liquid crystal configurations*, Comm. Math. Phys. **105** (1986), no. 4, 547–570.

[14] D. Henao and A. Majumdar, *Symmetry of Uniaxial Global Landau-de Gennes Minimizers in the Theory of Nematic Liquid Crystals*, SIAM J. Math. Anal. **44** (2012), 3217–3241.

[15] D. Henao, A. Majumdar, and A. Pisante, *Uniaxial versus biaxial character of nematic equilibria in three dimensions*, Calculus of Variations and Partial Differential Equations **56** (apr 2017), no. 2, 55.

[16] A. Majumdar, *The Landau-de Gennes theory of nematic liquid crystals: Uniaxiality versus Biaxiality*, Commun. Pure Appl. Anal. **11** (2012), 1303–1337.

[17] A. Majumdar and A. Zarnescu, *Landau-de Gennes theory of nematic liquid crystals: the Oseen-Frank limit and beyond*, Arch. Rational Mech. Anal. **196** (2010), 227–280.

[18] A. Martinez, M. Ravnik, B. Lucero, R. Žumer, S. Visvanathan, and I. I. Smalyukh, *Mutually tangled colloidal knots and induced defect loops in nematic fields*, Nat. Mater. **13** (2014), 258–263.

[19] N. J. Mottram and C. Newton, *Introduction to* **Q***-Tensor Theory*, arXiv:1409.3542, 2014.

[20] R. Nochetto, S. Walker, and W. Zhang, *A Finite Element Method for Nematic Liquid Crystals with Variable Degree of Orientation*, SIAM J. Numer. Anal. **55** (2017), no. 3, 1357–1386.

[21] M. R. Pakzad and T. Rivière, *Weak density of smooth maps for the Dirichlet energy between manifolds*, Geom. Funct. Anal. **13** (2003), no. 1, 223–257.

[22] P. Popov, L. W. Honaker, E. E. Kooijman, E. K. Mann, and A. I. Jákli, *A liquid crystal biosensor for specific detection of antigens*, Sensing and Bio-sensing Research **8** (2016), 31–35.

[23] R. Schoen and K. Uhlenbeck, *A regularity theory for harmonic maps*, J. Differential Geom. **17** (2016), no. 2, 307–335.

[24] E. Schrödinger, *What is Life?: The Physical Aspect of the Living Cell*, Cambridge University Press, 1948.

[25] J. Seddon and R. Templer, *The world of liquid crystals*, New Scientist, 18 May 1991.

[26] M. Tasinkevych, M. G. Campbell, and I. I. Smalyukh, *Splitting, linking, knotting, and solitonic escape of topological defects in nematic drops with handles*, Proc. Natl. Acad. Sci. USA **111** (2014), no. 46, 16268–16273.

[27] U. Tkalec, M. Ravnik, S. Žumer, S. Čopar, and I. Muševič, *Reconfigurable knots and links in chiral nematic colloids*, Science **333** (2011), no. 6038, 62–65.

[28] S. Čopar, U Tkalec, I. Muševič, and S. Žumer, *Knot theory realizations in nematic colloids*, Proc. Natl. Acad. Sci. USA **112** (2015), no. 6, 1675–1680.