Phase Transitions Models

Yaniv Almog (Louisiana State University)
Petru Mironescu (University Claude Bernard Lyon 1)

April 30 – May 5, 2017

1 Overview

The term phase transition (or phase change) is most commonly used to describe transitions between different states of matter (solid/liquid/gas, superconducting/normal, ferromagnetic/paramagnetic, isotropic/nematic, etc.). Second-order phase transition models have been in the focus of mathematical research for a number of decades. As opposed to first-order models, where the transition occurs along a sharp interface (e.g. the surface of a droplet), second-order ones, developed under the impulsion of Lev Landau, phenomenologically include a smoothing (gradient like) term leading to diffuse interfaces and transition phenomena. Mathematically, one is lead to consider in the models a small parameter (typically, $\epsilon > 0$) interpreted as the characteristic length of the interface, and to replace the discrete order parameter u (with e.g. $u = 0$ or $u = 1$ in the case of a two-phase fluid) by a continuous one. This order parameter could be either a scalar, as in the discrete case, or a complex u (with $|u|^2$ interpreted as a density) or a probabilistic function of the orientation of molecules (the Q-tensor below).

Mathematical issues within these models are related to the study of the well-posedness of the boundary conditions, the behavior of minimizers or critical points of the appropriate energy functional, approximate description of transition layers, description of metastable states, asymptotics as $\epsilon \to 0$, justification of first-order transition models as limits of the second-order one. More specialized directions concern the sound justification of physical observation as expulsion of magnetic flux (Meissner effect), existence of critical fields, existence of lattices of vortices in type II superconductors (Abrikosov lattices), etc.

A very partial list of second-order phase transition models include

1. The van der Waals-Cahn-Hilliard theory of phase transitions in a fluid. In this theory, the total energy of the fluid filling the container $\Omega \subset \mathbb{R}^n$ is assumed to be given by

$\epsilon^2|\nabla\rho|^2 + W(\rho)$, where ϵ is a small parameter and $W : \mathbb{R} \to [0,\infty)$ is a two-well potential, vanishing at a and b. A typical example is $W(\rho) = \rho^2(1-\rho)^2$, with $a = 0$ and $b = 1$. When $\epsilon = 0$, minimizers take only the values a and b. In the limit $\epsilon \to 0$, minimizers or critical points of bounded energy of the rescaled energy

$$F_\epsilon(\rho) = \int_\Omega \left(\frac{1}{\epsilon}|\nabla\rho|^2 + \epsilon W(\rho) \right) ,$$

are expected to get closer and closer to a and b. In the typical example above, the limit should be the characteristic function of a subset $A \subset \Omega$. The shape of A depends on the constraint on ρ: mass constraint $\displaystyle\int_\Omega \rho = m$, contact energy with the walls of the container, for example of the form $\epsilon\sigma(\rho)$, etc. In each case, minimizers approximate a two-phase configuration satisfying a variational principle related to the equilibrium configuration of liquid drops.

Variants of the above functional include vector-valued unknowns $\rho : \Omega \to \mathbb{R}^d$ and adapted potentials $W : \mathbb{R}^d \to [0,\infty)$.

2. The Ginzburg-Landau model. This model and its variant are relevant for the theory of superconductivity and Bose-Einstein condensates.

   Its simplest version is given by the energy functional

$$E_\epsilon(u) = \int_\Omega \left(\frac{1}{2}|\nabla u|^2 + \frac{1}{4\epsilon^2}(1-|u|^2)^2 \right) , \tag{1}$$

   where $u \in H^1(\Omega,\mathbb{C})$, $\Omega \subset \mathbb{R}^n$, and $\epsilon > 0$ is a (small) parameter. The physically relevant quantity here is $|u|^2$, which plays the role of a density. The unknown function u can be subject to various boundary conditions (Dirichlet, semi-stiff, etc.).

   There are numerous generalizations and modifications for this functional. One can, for instance, discuss the above model on manifolds, to consider $u \in H^1(\Omega,\mathbb{R}^n)$, etc. One can also consider time-dependent gradient flow (with either heat, Schrdinger or wave operator for the time derivatives).

   This simplified energy is obtained by neglecting the effect of magnetic field in the Ginzburg-Landau model of superconductivity. In two dimensions, the full energy functional takes the form

$$G_\epsilon(u) = \int_\Omega \left(|\nabla_A u|^2 + |\nabla A - h_{ex}|^2 + \frac{1}{2\epsilon^2}(1-|u|^2)^2 \right) . \tag{2}$$

   In the above $A \in H^1(\Omega,\mathbb{R}^2)$ denotes the magnetic vector potential (∇A is the magnetic field), h_{ex} is the applied magnetic field and $u \in H^1(\Omega,\mathbb{C})$ denotes the superconductivity order parameter. The minimization of G_ϵ can be carried out without any prescribed boundary conditions, but one can also prescribe boundary conditions other than the natural ones, on some subset of the boundary.

   Another variant is obtained by adding a traping potential, leading to the Bose-Einstein model for condensates. The effect of electric current can also be added to the Ginzburg-Landau model of superconductivity, in which case the problem is not variational anymore (it cannot be formulated in terms of an energy functional that needs to be minimized).

Other variants include spin models for ferromagnetic materials. Mathematically, this involves two unknown wave functions u_1, u_2, weakly coupled through the potential terms.

3. Oseen-Frank model of nematic and smectic liquid crystals. Liquid crystals are an intermediate state between liquids and solid crystals. Their main mathematical feature is the orientation of the molecules. In the simplest model, one associates to each molecule in the container $\Omega \subset \mathbb{R}^2$ or $\mathbb{R}^3$ an orientation $n = n(x) \in \mathbb{RP}^2$, and the energy to minimize is $\displaystyle\int_\Omega |\nabla n|^2$ (equal elastic constants). One may further simplify by replacing the physically realistic target $\mathbb{RP}^2$ by $\mathbb{S}^2$.

   A first sophistication of this model consists of introducing a more general dependence of the energy on n. The general form of the Oseen-Frank energy density for a nematic liquid crystal in the absence of external electromagnetic fields is given by

$$\begin{aligned}\mathcal{F}_N(n, \nabla n) = K_1|\nabla \cdot n|^2 + K_2|n \cdot (\nabla n) + \tau|^2 + \\ + K_3|n(\nabla n)|^2 + (K_2 + K_4)(\mathrm{tr}(\nabla n)^2 - |\nabla \cdot n|^2)\,. \end{aligned} \tag{3}$$

   In the above, K_i $(i = 1, 2, 3, 4)$ are dimensionless elastic coefficients which depend on the material, and τ is a real number representing the chiral pitch in some liquid crystals.

   Smectic crystals are liquid crystals disposed in twisted or tilted layers. A typical Oseen-Frank model for such crystals is

$$J(\psi, n) = \int_\Omega \left(|(i\nabla + qn)\psi|^2 + \mu \left(-|\psi|^2 + \frac{1}{2}|\psi|^4 \right) + \mathcal{F}_N(n, \nabla n) \right)\,. \tag{4}$$

   The number q is the characteristic smectic layer number: $2\pi/q$ is the characteristic layer thickness. The constant μ must be positive. The additional complex order parameter ψ has the following interpretation: $|\psi|$ characterizes the strength of the density modulation, while the (suitable normalized) phase of ψ measures the smectic layer displacement relative to that of perfect 1D crystalline order of layer periodicity $2\pi/q$.

   The minimization of (2) is usually carried over all $(\psi, n) \in H^1(\Omega, \mathbb{C}) H^1(\Omega, \mathbb{S}^2)$.

4. The Landau-de Gennes phase transition models. Oseen-Frank models cannot explain lines of disclination observed in 3D liquid crystals. The Landau-de Gennes phenomenological model describes liquid crystals not via the director n, but uses instead a 33 symmetric matrix $Q(x)$, interpreted as the (suitably normalized) covariance matrix of the probability distribution of $n(x) \in \mathbb{RP}^2$.

   In this case, the total energy takes the form

$$E_\epsilon(Q) = \int_\Omega \left(f_e(\nabla Q) + f_{LdG}(Q) \right)\,,$$

where the elastic energy is given by

$$f_e(\nabla Q) := \frac{L_1}{2}|\nabla Q|^2 + \frac{L_2}{2} Q_{ij,j} Q_{ik,k} + \frac{L_3}{2} Q_{ik,j} Q_{ij,k}$$
$$= \sum_{j=1}^{3} \left\{ \frac{L_1}{2}|\nabla Q_j|^2 + \frac{L_2}{2}\left(\mathrm{div} Q_j\right)^2 + \frac{L_3}{2}\nabla Q_j \cdot \nabla Q_j^T \right\}, \quad \text{(5a)}$$

while the bulk Landau-de Gennes energy density is

$$f_{LdG}(Q) := a \,\mathrm{tr}\left(Q^2\right) + \frac{2b}{3}\mathrm{tr}\left(Q^3\right) + \frac{c}{2}\left(\mathrm{tr}\left(Q^2\right)\right)^2 . \quad \text{(5b)}$$

Temperature and material depending constants a, b,c determine the critical points of the bulk energy, whose nature governs the (meta)stability of the isotropic and nematic phases and the behavior of the liquid crystal. In type II liquid crystals, the molecules will tend to be aligned most of the time, leading to a Q-tensor of the approximate form $Q(x) = n(x) \otimes n(x) - (1/3)I_3$. In small regions (diffuse points or lines) Q will differ much from this form, one of the options (but not the only one) consisting of being close to $Q = 0$ (as in isotropic liquids).

5. Micromagnetics. In certain asymptotic regimes, the magnetization of a material contained in a thin film in $\mathbb{R}^3$ is described (at the mesoscopic level) by a 3D vector field $m : \Omega \subset \mathbb{R}^2$ taking values into $\mathbb{S}^2$. In dimensional reductions procedures, one is then led to the study of the asymptotic behavior of functionals of the form

$$E_\epsilon(m) = \epsilon \int_\Omega |\nabla m|^2 + f(\epsilon) \int_\Omega \left||\nabla|^{-1/2} \left(\nabla \cdot m\right)\right|^2 ,$$

where $f(\epsilon) \to 0$ as $\epsilon \to 0$; the given f accounts of the characteristics of the asymptotic regime.

6. The Bloch-Torrey model of diffusion-weighted magnetic resonance imaging (DW-MRI). For a magnetization M and an external magnetic field B the time-dependent equations

$$\frac{dM}{dt} = MB + h^2 \Delta M ,$$

where h is a parameter. In two dimensions the steady-state problem reduces to a Schrdinger equation with purely imaginary potential.

2 Recent Developments

The problems that have been addressed in the workshop were spanned over a wide area of interest. Some of the problems that were considered are listed below.

1. Linear stability of trivial solutions. In particular, some attention was devoted to the spectral theory of non selfadjoint operators, which appear, for instance, when one considers the effect of electric current into the Ginzburg-Landau model, or when considering the Bloch-Torrey model.

2. Tunneling effects for either the Robin-Laplacian (or p-Laplacian) or the linearized Ginzbug-Landau model.
3. Weakly nonlinear analysis of either the Ginzburg-Landau model or for the smectic A liquid crystals model. These problems are characterized by boundary layer solution, decaying exponentially fast away from the boundary.
4. Analysis of singularities for the Ginzburg-Landau model. The issues considered include the analysis of local minimizers in the sense of De Giorgi in dimension 3, the interaction between local (singularities) and global analysis (genus) in the asymptotic analysis of minimizers.
5. Existence and linear stability of radially symmetric solutions of the Landau-de Gennes model.
6. New models of liquid crystals and their analysis. In this direction, topics include models for the free energy accounting of the shape the molecules and the role of the penalization terms in the free energy in preventing the escape of the Q-tensor from the physically realistic region. A related topic is the one of discrete models to nematic configuration, and the justification of the derivation of the continuous model as limit of the discrete one.
7. The transitions from isotropic to uniaxial, from uniaxial to biaxial nematic solutions for the Landau-de Gennes model, and the transition from smectic A to smectic C states for the Chen-Lubensky model. In particular, the results presented include a rigorous justification of the existence of Saturn rings and/or biaxial transitions around spherical droplets in nematic liquids.
8. Some general issues of analysis related to phase transition models. In particular, description of an appropriate functional space for the analysis of semi-stiff boundary problems, homotopy classes of Sobolev maps with prescribed singularities, lifting problems for Sobolev maps, justification of 3D to 2D dimensional reductions via asymptotic analysis of variational inequalities in large cylinders, and the rigorous analysis of variational problems under prescribed mass and energy constraints. In a different direction, applications of the ideas developed in relation with phase transition theories to the relaxation of total length minimization Plateau type problems were discussed. Attention was also focused on the use of Allen-Cahn type regularizations in the modeling of the motility of eukaryotic cells on substrates.

3 Presentation Highlights

3.1 Non selfadjoint operators

Bernard Helffer considered the complex Airy operator $-d^2/dx^2 + ix$ defined on the domain

$$D = \{(u_+, u_-) \in H^2(\mathbb{R}_+)H^2(\mathbb{R}_-) \,|\, u'_+(0) = u'_-(0) = \kappa[u_+(0) - u_-(0)]\}\,.$$

The transmission boundary condition satisfied at $x = 0$ is in frequent use when studying the above-mentioned Bloch-Torrey equations. Among other things, he presented a proof of completeness of the eigenspace, and of the simplicity of the eigenvalues. Some additional results were presented for the Robin realization of the same operator acting on $\mathbb{R}_+$ (i.e., $u'(0) = \kappa u(0)$) (cf. [29, 28]).

Yaniv Almog considered the Schrdinger operator with a purely imaginary potential $\mathcal{A}_h = -h^2\Delta + iV$ in the semiclassical limit $h \to 0$. Assuming a smooth domain and a smooth potential with no critical points ($\nabla V \neq 0$ in $\bar{\Omega}$) he obtained the left margin of the spectrum of $\mathcal{A}_h$. A lower bound of $\inf \Re\sigma(\mathcal{A}_h)$ have previously been obtained in [6, 30] for the Dirichlet realization of $\mathcal{A}_h$, an upper bound, under some significant assumptions on V, has been obtained in [8] for the Dirichlet realization. Here both upper bounds and lower bounds have been obtained in much greater generality for a variety of boundary conditions, including the above-mentioned transmission boundary condition.

Petr Siegl presented a study of the eigenfunctions of operators of the type

$$-d^2/dx^2 + |x|^\beta + iV(x) \quad ; \quad |V| \lesssim |x|^\gamma \text{ as } |x| \to \infty$$

acting on the real line, where $\beta \geq 2$ and $\gamma \geq 0$. It has been established that the system of eigenfunctions is complete. Nevertheless, very often it does not form a basis. The main result for this specific operator is that whenever $\gamma < \beta/2 - 1$ the eigenfunctions form a Riesz basis. Some negative results for the case $\gamma > \beta/2 - 1$ have been demonstrated as well (cf. [39, 43]).

3.2 Surface superconductivity

Soeren Fournais considered the 3D Ginzburg-Landau energy functional (2) in the limit $\epsilon \to 0$. It is well known that when the applied magnetic field satisfies $\epsilon^{-2} < h_{ex} < \epsilon^{-1}/\Theta_0$ ($\Theta_0 \approx 0.59$ is known as de Gennes value) the minimizer decays exponentially fast away from the boundary. The energy density function on the surface (the local energy of the minimizer per unit surface area) has been studied. A proof was presented to the fact that this energy density is monotone non-decreasing with the angle between the applied magnetic field and the local tangent plane.

Ayman Kachmar presented a study of the smectic A energy (3)–(4) in the limit where the large elastic constants force the director field to be in the chiral nematics state, i.e.,

$$n^* = (\cos(\tau x_3), \sin(\tau x_3), 0)\,,$$

where the x_3 axis direction is arbitrary. In previous works [5, 31] a reduced functional where $n = n^*$ (and hence $\mathcal{F}_N = 0$) was considered. Kachmar demonstrated that the results obtained for the reduced function can be reproduced for the full functional (3)–(4), in the limit of large elastic constants (cf. [41]).

Michele Correggi began by reviewing some of the results he has obtained with Rougerie on the behavior of the minimizer of (2) near the boundary, in the surface superconductivity regime. It has been conjectured by Pan [45] that for any critical point of (2) the solution becomes uniformly distributed along the boundary as $\epsilon \to 0$. Coreggi and Rougerie proved this conjecture for the global minimizer (cf. [24]). He then discussed the effects of curvature and corners on the energy [22, 25].

3.3 Tunneling and Weyl asymptotics

Nicolas Raymond considered the Robin Laplacian $\mathcal{L}_h = -h^2\Delta$ defined on

$$D = \{u \in H^2(\Omega) \,|\, h^{1/2}\frac{\partial u}{\partial \nu}\Big|_{\partial\Omega} = u\}$$

in the semiclassical limit $h \to 0$. The leading behavior (as well as higher order terms) of the negative eigenvalues has been obtained. Assuming two points of maximal curvature on $\partial\Omega$ for a 2D symmetric domain, it is demonstrated that the gap between the first two eigenvalues can be approximated by the gap between the first pair of eigenvalues of a simple boundary operator. The presentation also contained some insights of the L^p spectral theory of magnetic Laplacians. In particular, a localization result, similar in nature to existing L^2 results, has been obtained (cf. [40, 26]).

Hynek Kovařk considered the p-Laplace operator with Robin boundary conditions on Euclidean domains with sufficiently regular boundary. In particular, the asymptotic behavior of the first eigenvalue, given by

$$\Lambda(\Omega, p, \alpha) := \inf_{\substack{u \in W^{1,p}(\Omega) \\ u \not\equiv 0}} \frac{\displaystyle\int_\Omega |\nabla u|^p \mathrm{d}x - \alpha \int_{\partial\Omega} |u|^p \mathrm{d}\sigma}{\displaystyle\int_\Omega |u|^p \mathrm{d}x},$$

when the strength, α, of the (negative) boundary term grows to infinity, depends on the geometry of the domain. Localization of the corresponding minimizers, near the point of maximal mean curvature, has been obtained as well [38].

Virginie Bonnaillie-Nol devoted her presentation to the semiclassical analysis of the Neumann realization of the magnetic Laplacian $(-ih\nabla + A)^2$ (where $\nabla A = \hat{\imath}_3$) on a smooth planar domain. As in the presentation of Raymond a symmetric domain is considered, with precisely two points on the boundary where the maximal curvature is attained (an ellipse for example). By obtaining WKB expansions of the eigenfunctions a formal derivation of the gap between the first two eigenvalues is achieved (cf. [15]).

3.4 Liquid crystals

Peter Pallfy-Muhoray reported a study where the effects of particle shape on the behavior of soft condensed matter systems were considered. A simple orientational density functional form of the Helmholtz free energy including both long-range attractive and short-range repulsive interactions is provided. It is applied to an example, taking into account nematic order due to both temperature–dependent attractive (Maier-Saupe) and concentration dependent repulsive (Onsager) interactions. The shape dependence of the attractive interactions originates in the polarizability, while the shape dependence of the repulsive interactions arises through the excluded volume. The varying phase behavior due to the relative contributions of these two effects has also been considered (cf. [46]).

Xiaoyu Zheng continued the presentation of Pallfy-Muhoray, and provided more details as to how the Onsager model can be modified to account for hard core repulsion, including the effect of shape-dependent excluded volume. A detailed derivation of the new model from the Helmholtz free energy was presented. Unlike the Onsager model where the pressure remains finite for arbitrarily high densities, the new model predicts divergence of the pressure at a critical density.

Dmitry Golovaty presented a Gamma-convergence result of the Landau-de Gennes (LdG) model (5) for a nematic liquid crystalline film in the limit of vanishing thickness. The film is assumed to be attached to a fixed surface, where an anchoring energy of the form

$$f_s(Q,\nu) = \alpha\left[(Q\nu\cdot\nu)-\beta\right]^2 + \gamma\left|(I_3-\nu\otimes\nu)\,Q\nu\right|^2 \ ,$$

is assumed, where ν is a unit normal vector, and $\alpha,\gamma>0$, $\beta\in\mathbb{R}$ are given parameters. In the limit of vanishing thickness, Γ-convergence to a limiting surface energy is proved. Then, the limiting problem was discussed in several parameter regimes (cf. [27]).

Dan Phillips considered a surface stabilized ferroelectric liquid crystal cell which, after being cooled from the smectic-A to the smectic-C phase forms V-shaped (chevron like) defects. The defects create an energy barrier that prevent (for the Γ-limit) switching between equilibrium patterns. To obtain such a transition, a gradient flow for a Chen-Lubensky energy is examined. The flow allows the order parameter to vanish, and consequently it is possible to overcome the energy barrier (cf. [44]).

Patricia Bauman presented a study of minimizers, on a bounded domain, of the Landau-de Gennes functional (5) where instead of (5a) use is made of the Maier-Saupe energy

$$f_{ms}(Q) = \begin{cases} -K|Q|^2 + \inf\limits_{\rho\in A_Q}\int_{\mathbb{S}^2}\rho(\mathbf{p})\ln(\rho(\mathbf{p}))d\mathbf{p}\,, & \text{if } Q\in\mathcal{M} \\ \infty\,, & \text{otherwise} \end{cases},$$

where

$$\begin{aligned} A_Q := \{\rho\in L^1(\mathbb{S}^2;\mathbb{R}) : \rho\geq 0, s\int_{\mathbb{S}^2}\rho(\mathbf{p})d\mathbf{p} = 1, \\ Q = \int_{\mathbb{S}^2}\left(\mathbf{p}\otimes\mathbf{p}-\frac{1}{3}I_3\right)\rho(\mathbf{p})d\mathbf{p}\}\,, \end{aligned} \tag{6}$$

and

$$\mathcal{M} = \{Q\in\mathbb{R}^{33}\,|\,Q^t = Q\,;\ \mathrm{Tr}Q = 0\,;\ \sigma(Q)\in(-1/3,2/3)\,\}\,.$$

Note that $\mathcal{M}$ is the set of physically acceptable states, in view of the relation betwen Q and ρ given in (6). Using the fact that the energy density is singular outside the physically realistic range, it is proved that minimizers are regular and, in several model problems, take on values strictly within the physical range (cf. [9]).

Lia Bronsard provided an instructive illustration of the advantage of the Landau-de Gennes model over the more rigid Oseen-Frank or Ericksen theories. She considered a spherical colloidal particle immersed in a liquid crystal, satisfying homeotropic weak anchoring at the surface of the colloid (with strength parameter W) and approaching a uniform uniaxial state at infinity. The analysis is performed in the case of the Landau-de Gennes model with equal elastic constants, i.e., in (5) one takes $L_1 = L_2 = L_3 := L$.

For small balls (i.e., $r \ll L^{1/2}$) and relatively strong anchoring, she proved the existence of a limiting quadrupolar configuration, with a "Saturn ring" defect, corresponding to an exchange of eigenvalues of the Q-tensor. Relatively strong anchoring means that r is of the order of L/W; the limiting shape depends on the limiting ratio $\frac{rL}{W}$. An interesting feature of this result is the explicit form of the quadrupolar configurations. The Saturn ring defect appears as a discontinuity in the principal eigenvector of $Q(x)$, the Q-tensor passing through a uniaxial state as eigenvalue branches cross via an "eigenvalue exchange" mechanism. In the large particle limit, she was able to analyze the strong anchoring (Dirichlet) condition under the extra assumption that the minimizer is axially symmetric. In this setting, she obtained that the limiting map when $r \gg L^{1/2}$ is the unique uniaxial axially symmetric minimizer of the Oseen-Frank energy which is compatible with the behavior at infinity of the liquid crystal (cf. [4]). Some of the striking features of this analysis: the Oseen-Frank model does not allow line defects as in the Saturn ring, and the numerical simulations based on the Ericksen model do not provide the correct radius of the ring.

Arghir Zărnescu gave a general overview of the research project of the group he forms with Radu Ignat, Luc Nguyen and Valeriy Slastikov, and of some of their main achievements. His presentation served as an introduction to the one of Luc Nguyen. In particular, he put in perspective the Landau-de Gennes and the Ginzburg-Landau models, the former one being a higher dimensional, more complex version than the latter. It turns out that new interesting features appear, connected to new phenomena which are specific to this type of models. A typical example is the uniqueness and the stability of radial solutions. While it is well understood for decades for the Ginzburg-Landau model, its resolution for the Landau-de Gennes model required new ideas and techniques which are of independent interest, in particular new separation of variables and uniqueness techniques. His presentation was based on [33, 34, 35, 36].

Luc Nguyen detailed one of the new features presented in the previous lecture. In Ginzburg-Landau theory, it is known that the hedgehog $f(r)e^{i\theta}$ is energy minimizing. In the Landau-de Gennes setting, the hedgehog $f(r)\frac{x}{|x|}$ is minimizing in certain regimes, but not in all of them. Another way to present this is that even if the energy functional and the boundary data are invariant under the orthogonal group, the minimizer need not have this property. A striking result presented is that even for two dimensional liquid crystals, uniqueness is a non-trivial matter. More specifically, if the boundary datum on $\partial\mathbb{D}$ has no topological obstruction, the minimizers are "unique and rotationally symmetric" (cf. [36]). As an application, he derived the existence of multiple non-minimizing rotationally symmetric critical points.

Giacomo Canevari presented recent progress related to nematic shells. These are rigid colloidal particles with a typical dimension in the micrometer scale coated with a thin film of nematic liquid crystal whose molecular orientation is subjected to a tangential anchoring. The recent interest in their study is related to the possibility of using them as building blocks of meso-atoms with a controllable valence. Mathematically, they are described as compact boundaryless two dimensional surfaces M embedded into $\mathbb{R}^3$, together with a unit-norm tangent vector field $n : M \to TM$. Such a smooth n need not exist, and even in H^1 n does not exist in a surface of non zero Euler characteristic, by the weak form of the Poincar-Hopf's theorem (see also Robert Jerrard's presentation). He presented a discrete-to-continuous approach of nematic shells. It consists of discretizing the surface using triangulations, and to define the tangent vectors only on the vertices of the triangulation, avoiding in this way all topological obstructions. A discrete energy is defined, mimicking the standard Dirichlet energy. The main result presented is the Γ-convergence of the discrete energy as $\epsilon \to 0$. The second order expansion involves, at the minimal energy level, the Euler characteristic of the surface and a renormalized energy in the spirit of [13] (cf. [19]). A striking fact about the renormalized energy is that it keeps trace of the discrete structures used to discretize the surface M around each singularity.

Jinhae Park discussed the nature of minimizers for isotropic-nematic 1D interface problem in case of equal elastic constants in (5), i.e., $L_1 = L_2 = L_3 := L$. In this setting, it is interesting to allow non positive values of the parameter L. The matter of discussion is the stability and/or minimality of 1D interfaces, i.e., of entire critical points of (5) depending only on x_3 and satisfying appropriate anchoring conditions at $x_3 = \infty$. This issue is investigated under the assumption $b^2 = 27ac$, meaning that the bulk energy of the normal and the nematic phase are equal. When $L = 0$, it is proved that the minimizer must be a kink similar to the one for the Modica-Mortola functional. Assuming $Q(-\infty) = 0$, the anchoring condition at ∞ is proved to play a crucial role when $L \neq 0$: homeotropic, planar and tilt anchoring lead to different analysis. For example in the case of homeotropic anchoring it is proved that the uniaxial equilibrium is stable when $L \leq 0$, but unstable when $L > 0$ (cf. [47]).

3.5 Other aspects of the Ginzburg-Landau theories

Nicolas Rougerie considered a mean-field approximation of multi-particle Hamiltonian, appropriate for "almost bosonic" 2D anyons. The order parameter associated with these anyons minimizes the energy functional

$$\mathcal{E}_\beta^{\rm af}[u] := \int_{\mathbb{R}^2} \left\{ \left| \left(-i\nabla + \beta \mathbf{A}[|u|^2]\right) u \right|^2 + V(\mathbf{r})|u|^2 \right\} \, d\mathbf{r}, \tag{7}$$

where V is a trapping potential and

$$\mathbf{A}[\lambda] := \nabla_\perp \log |\mathbf{r}| * \lambda \, .$$

After providing some physical background, the energy and the density (u) asymptotics in the limit $\beta \to \infty$ were presented [23].

Kirill Samokhin presented the challenges of the study of non centrosymmetric superconductors. One of their noticeable features is the possibility of unusual nonuniform superconducting states even without any external field. In such situations, the strong spin-orbit coupling of electrons with the crystal lattice makes it necessary to describe superconductivity in terms of one or more nondegenerate bands characterized by helicity. He also explained how the origin of non uniform superconducting states can be traced in the first-order gradient terms in the Ginzburg-Landau free energy (cf [48]). He gave some insight concerning the topological classification of the superconducting states using the integer-valued Maurer-Cartan invariants and the Bogoliubov-Wilson loops, with focus, for a two-dimensional setting, on the corresponding wave function topology.

tienne Sandier presented a first progress towards the description of local minimizers of the simplified Ginzburg-Landau functional (1) in 3D. An entire solution of (1) is locally minimizing in the sense of De Giorgi if $E_\epsilon(u+\phi, B_R) \geq E_\epsilon(u, B_R)$ for every $R > 0$ and $\phi \in C_c^\infty(B_R; \mathbb{C})$. Such solutions are classified in 2D (they are either constant, or, up to an isometry, the unique radial solution of degree 1 at infinity, u_{rad}). Their classification in dimension ≥ 3 is widely open. He presented the following result: an entire solution whose average energy is sufficiently small, in the sense that

$$\liminf_{R\to\infty} \frac{E(u, B_R)}{R \ln R} < 2\pi,$$

must be constant [49]. Here, 2π is precisely the density of the 2D solution u_{rad} considered as a function of three variables. This may open the way for classifying the local minimizers in 3D as constants or, up to isometries, the 2D solution u_{rad}.

Robert Jerrard focused on the analysis of the functional

$$G_\epsilon(u) = \int_S \left(\frac{1}{2}|Du|_g^2 + \frac{1}{4\epsilon^2} F(|u|_g^2) \right),$$

with $u : S \to TS$ a tangent vector field, and S a (two dimensional) surface. He explained a Γ-convergence result at the second order of G_ϵ as $\epsilon \to 0$. In particular, he showed that energy minimizers u_ϵ converge outside a finite number of singularities to a canonical vector field u^* of unit length, whose number of singularities is $|2-2\mathbf{g}|$, g being the genus of the (compact) surface S (cf. [32]). In addition, he obtained a second order expansion of the energy $G_\epsilon(u_\epsilon)$ involving a renormalized energy in the spirit of the one devised by Bethuel, Brezis and Hlein for the Dirichlet problem in the plane (cf. [13]). The remarkable aspect of this analysis is that the role of the Dirichlet condition is played by the topology of S, more specifically by its Euler characteristic.

Radu Ignat presented a uniqueness (up to symmetries) asymptotic result for minimizers of the Ginzburg-Landau E_ϵ functional for $\mathbb{R}^3$ (and not complex) valued unknown functions u_ϵ. His starting point is the following well-known symmetry result for $\mathbb{S}^2$-valued harmonic maps: the Dirichlet energy $\int_{\mathbb{D}} |\nabla n|^2$, with $\mathbb{D}$ the unit disc and $n : \mathbb{D} \to \mathbb{S}^2$ subject to the boundary condition $n(e^{i\theta}) = (e^{ki\theta}, 0)$ has exactly two solutions, one such that $n_3 > 0$, the other one such that $n_3 < 0$. These solutions are of the form $(f(r)e^{ki\theta}, g(r))$, with $r := |x|$. One expects this uniqueness (up to the sign) and special form of the solutions to propagate to minimizers of E_ϵ on $\mathbb{D}$, at least for small ϵ. This is indeed the case. He presented elements of the proof, with emphasis on the crucial steps and ideas in [37].

3.6 Miscelaneous topics

Leonid Berlyand presented a study of two types of models describing the motility of eukaryotic cells on substrates. The first one, a phase-field model, consists of the Allen-Cahn equation for the scalar phase field function coupled with a vectorial parabolic equation for the orientation of the acting filament network. In the sharp interface limit the equation of the motion of the cell boundary has been derived. The existence of two distinct regimes of the physical parameters is then established and the existence of traveling waves in one of them is proved. The second model type is a non-linear free boundary problem for a Keller-Segel type system of PDEs in 2D with area preservation and curvature entering the boundary conditions. A family of radially symmetric standing wave solutions (corresponding to a resting cell) are obtained. Then, with the aid of topological tools, traveling wave solutions (describing steady motion) with non-circular shape are shown to bifurcate from the standing wave. The bifurcation analysis explains, how varying a single (physical) parameter allows the cell to switch from rest to motion (cf. [12, 10]).

Gershon Wolansky considered a non-local Liouville equation

$$\Delta\psi = \frac{e^{-\lambda\psi}}{\|e^{-\lambda\psi}\|_1} \text{ in } \Omega \subset \mathbb{R}^n\,, \quad \psi|_{\partial\Omega} = 0\,,$$

where $\lambda > 0$. The physical motivation behind this equation is a variational problem for entropy maximization under prescribed mass and energy. He presented an unconditional existence and uniqueness proof in case of electrostatic (repulsive) self-interaction, and conditional existence and uniqueness in dimension two in the case of gravitational (attractive) self-interaction.

Stan Alama considered a a nonlocal isoperimetric functional with a confinement term, derived as the sharp interface limit of a variational model for self-assembly of diblock copolymers under confinement by nanoparticle inclusion. This functional appears as the sharp interface limit of a model of diblock copolymer/nanoparticle blend where a large number static nanoparticles serve as a confinement term, penalizing the energy outside of a fixed region. In a periodic setting, this energy takes the form

$$\mathcal{E}_{\gamma,\sigma,\mu}(u) := \int_{\mathbb{T}^3} |Du| + \gamma \|u - m\|^2_{H^{-1}(\mathbb{T}^3)} + \sigma \int_{\mathbb{T}^3} (u-1)^2.$$

Here, μ is a measure with density on $\mathbb{T}^3$ and the BV unknown density function u is subject to the mass constraint $\int_{\mathbb{T}^3} = m$.

The following asymptotic regime naturally appears in connection with the sharp interface limit of the Ohta-Kawasaki functional, modeling the self-assembly of diblock copolymers: $m \to 0$, $\gamma, \sigma \to \infty$.

In this regime and after a suitable rescaling, a two terms expansion for the energy without confinement term was presented, involving a small parameter η (representing, roughly speaking, the radius of the small particles). The first term captures the location of droplets in the limit $\eta \to 0$ (through a sum of Dirac masses); the second one, a Coulomb type interaction between droplets. Much more delicate is the analysis of the case with confinement. This is obtained in presence of confinement densities of μ which are spatially variable and attain a nondegenerate maximum. Under such an assumption, it is possible to obtain a two-terms asymptotic expansion exhibiting a separation of length scales due to competition between the nonlocal repulsive and confining attractive effects in the energy. Two different asymptotic behaviours may occur, according to the total volume of the droplets: either the minority phase splits into several droplets at an intermediate scale, or the minimizers form a single droplet converging to the maximum of the confinement density (cf [1]).

Michel Chipot presented new aspects of the justification of dimensional reduction for infinitely large cylinders, theory he developed over the last decade [20, 21]. More specifically, he established the existence of minimal solutions (local minimizers in the sense of De Giorgi) to some variational elliptic inequalities. These solutions are obtained by appropriate truncations of the unbounded domain. A typical situation is the one of an infinite (straight) cylinder, but the techniques allow considering more general cylinder like domains, in particular bounded by appropriate graphs. Uniqueness of the minimal solutions is obtained via adapted comparison principles.

Peter Sternberg introduced a non-standard isoperimetric problem in the plane associated with a metric having a degenerate conformal factor at two points. More specifically, he considers the minimization problem

$$\inf E(\gamma) \text{ with } \gamma : [0,1] \to \mathbb{R}^2,\ E(\gamma) := \int_0^1 F(\gamma)|\gamma'|.$$

The competitors must satisfy $\gamma(0) = \mathbf{p}_-$, $\gamma(1) = \mathbf{p}_+$ and the "enclosed area" condition $\displaystyle\int_\gamma \omega = const.$, with $\omega := -p_2 dp_1$.

The conformal factor $F : \mathbb{R}^2 \to [0, \infty)$ vanishes exactly at $\mathbf{p}$.

Existence of minimizers is related to the existence of traveling wave solutions to a Hamiltonian system associated with the energy functional

$$H(u) := \int \left(\frac{1}{2}|\nabla u|^2 + W(u)\right), \text{ with } W(u) := F^2(u).$$

Minimizer for the one-well problem exist for quadratic potentials F^2, and need not exist for more degenerate ones. He explained how to obtain existence for the two-wells problem assuming separate existence for the one-well ones at $\mathbf{p}$ (cf. [3]). This result has implications on the existence of traveling waves. It is also possible to derive a limitation for the maximal propagation speed for these traveling waves through an explicit upper bound depending on the conformal factor F.

Giandomenico Orlandi discussed a relaxation of the Steiner tree problem, consisting of finding a minimal (for various metrics) connected graph containing given points. He proposed a variational approximation of this problem, as well as of the Gilbert-Steiner irrigation problem for the Euclidean distance in the plane. The relaxation involves Modica-Mortola or Ginzburg-Landau type functionals. More generally, he considered the Plateau problem in 2D with coefficients into a normed group. He presented elements of the proof of the fact that these approximations do indeed Γ converge to the original problems (cf. [14]), and thus offer an alternative approach for handling such questions known to be NP hard.

Itai Shafrir presented a natural notion of class within Sobolev spaces of sphere-valued maps, with focus on the spaces $W^{1,1}(\Omega; \mathbb{S}^1)$ and $W^{1,2}(\Omega; \mathbb{S}^2)$. More specifically, two maps are in the same class if they have "the same singularities" (the same distributional Jacobian). The latter functional setting is relevant for liquid crystals. He introduced the metric and Hausdorff distance between two classes, and gave their precise values (cf. [18, 17, 16]). The former distance can be interpreted as the minimal energy required to move the singularities from one place to the other, and its exact value involves the Wasserstein distance between the Jacobians of maps.

Petru Mironescu presented a functional analytic setting adapted to the study of the semi-stiff problems. A typical relevant space in this case is $W^{1/p,p}(\mathbb{S}^1; \mathbb{S}^1)$, with $1 < p < \infty$. Such a space is critical for lifting and weak convergence matters: bubbling phenomena appear, and there is no phase control or preservation of the degree in the weak limit. He described the behavior of weakly convergent sequences, demonstrating that non compactness can appear only via the conformal group of the unit disc (profile decomposition cf. [42]) and gave applications of the profile decomposition to the existence of critical points for semi-stiff problems [11].

4 Future Perspectives

The meeting revealed the emergence of new techniques and intermediate problems that in the near future should facilitate the ground for approaching several problems that seemed out of reach before:

1. Study of stability, uniqueness and other qualitative properties of radial solutions of vector-valued radially symmetric functionals.
2. Classification of locally minimizing entire solutions of the Ginzburg-Landau functional in dimension ≥ 3.
3. Complete analysis of Landau-de Gennes models with penalization terms confining the Q-tensor within a physically realistic region.
4. Sharp analysis of the biaxial escape phenomenon in nematics.
5. Rigorous asymptotic analysis of many order parameters Ginzburg-Landau type functionals – beyond the p-waves models.
6. Linear stability analysis of hydrodynamic flow in a tube of arbitrary cross section.
7. Rigorous analysis of tunneling effects for the Neumann magnetic Laplacian and other operators.
8. Determination of the preferred orientation of the helical axis in nearly cholesteric smectic A liquid crystals.
9. Analyzing the behaviour of the superconductivity order the boundary layer in a three-dimensional setting, in the surface superconductivity parameter regime.

References

[1] S. Alama, L. Bronsard, R. Choksi and I. Topaloglu, *Droplet phase in a nonlocal isoperimetric problem under confinement*, arXiv preprint arXiv:1609.03589 (2016).

[2] S. Alama, L. Bronsard, R. Choksi and I. Topaloglu, *Ground-states for the liquid drop and TFDW models with long-range attraction*, arXiv preprint arXiv:1707.06674 (2017).

[3] S. Alama, L. Bronsard, A. Contreras, J. Dadok and P. Sternberg, *A Degenerate Isoperimetric Problem and Traveling Waves to a Bi-stable Hamiltonian System*, arXiv preprint arXiv:1504.00423 (2015).

[4] S. Alama, L. Bronsard and X. Lamy, *Minimizers of the Landau-de Gennes energy around a spherical colloid particle*, arXiv preprint arXiv:1504.00421 (2015).

[5] Y. ALMOG, *Thin boundary layers of chiral smectics*, Calculus of Variations and Partial Differential Equations, 33 (2008), pp. 299–328.

[6] Y. ALMOG, *The stability of the normal state of superconductors in the presence of electric currents.* SIAM J. Math. Anal. 40 (2) (2008), pp. 824–850.

[7] Y. ALMOG, D. GREBENKOV AND B. HELFFER, *On a Schrödinger operator with a purely imaginary potential in the semiclassical limit*, arXiv preprint arXiv:1703.07733 (2017).

[8] Y. ALMOG AND R. HENRY, *Spectral analysis of a complex Schrdinger operator in the semiclassical limit.* SIAM J. Math. Anal. 44 (2016), pp. 2962–2993.

[9] P. BAUMAN AND D. PHILLIPS, *Regularity and the behavior of eigenvalues for minimizers of a constrained Q*, Calculus of Variations and Partial Differential Equations, 55 (2016), pp. 1–22.

[10] L. BERLYAND, J. FUHRMANN AND V. RYBALKO, *Bifurcation of traveling waves in a Keller-Segel type free boundary model of cell motility*, arXiv preprint arXiv:1705.10352 (2017).

[11] L. BERLYAND, P. MIRONESCU, V. RYBALKO AND É. SANDIER, *Minimax critical points in Ginzburg-Landau problems with semi-stiff boundary conditions: existence and bubbling*, Comm. Partial Differential Equations 39(5) (2014), pp. 946–1005.

[12] L. BERLYAND, M. POTOMKIN AND V. RYBALKO, *Phase-field model of cell motility: Traveling waves and sharp interface limit*, C. R. Math. Acad. Sci. Paris 354 (2016), pp. 986–992.

[13] F. BETHUEL, H. BREZIS AND F. HÉLEIN, Ginzburg-Landau vortices, Progress in Nonlinear Differential Equations and their Applications, 13, Birkhäuser Boston Inc., Boston, MA, 1994.

[14] M. BONAFINI, G. ORLANDI AND É. OUDET, *Variational approximation of functionals defined on 1-dimensional connected sets: the planar case*, arXiv preprint arXiv:1610.03839 (2016).

[15] V. BONNAILLIE-NOËL, F. HÉRAU AND N. RAYMOND, *Curvature induced magnetic bound states: towards the tunneling effect for the ellipse* (2016).

[16] H. BREZIS, P. MIRONESCU AND I. SHAFRIR, *Distances between classes in $W^{1,1}(\Omega;\mathbb{S}^1)$*, arXiv preprint arXiv:1606.01526 (2016).

[17] H. BREZIS, P. MIRONESCU AND I. SHAFRIR, *Distances between homotopy classes of $W^{s,p}(\mathbb{S}^N;\mathbb{S}^N)$*, ESAIM Control Optim. Calc. Var. 22(4) (2016), pp. 1204–1235.

[18] H. BREZIS, P. MIRONESCU AND I. SHAFRIR, *Distances between classes of sphere-valued Sobolev maps*, C. R. Math. Acad. Sci. Paris 354(7) (2016), pp.677–684.

[19] G. CANEVARI AND A. SEGATTI, *Defects in Nematic Shells: a Γ-convergence discrete-to-continuum approach*, arXiv preprint arXiv:1612.07720 (2017).

[20] M. CHIPOT, ℓ goes to plus infinity, Birkhuser Advanced Texts: Basler Lerhbcher, Birkhuser Verlag, Basel, viii+181 pp, 2002.

[21] M. CHIPOT, Asymptotic issues for some partial differential equations, Imperial College Press, London, ix+252 pp, 2016.

[22] M. CORREGGI AND E. L. GIACOMELLI, *Surface superconductivity in presence of corners*, Rev. Math. Phys., 29 (2017), 1750005.

[23] M. CORREGGI, D. LUNDHOLM AND N. ROUGERIE, *Local density approximation for the almost-bosonic anyon gas*, arXiv preprint arXiv:1611.00942 (2016).

[24] M. CORREGGI AND N. ROUGERIE, *On the Ginzburg-Landau functional in the surface superconductivity regime*, Commun. Math. Phys., 332 (2014), pp. 1297–1343.

[25] M. CORREGGI AND N. ROUGERIE, *Effects of boundary curvature on surface superconductivity*, Lett. Math. Phys., 106 (2016), 445.

[26] S. FOURNAIS, L. L. TREUST, N. RAYMOND AND J. VAN SCHAFTINGEN, *Semiclassical Sobolev constants for the electro-magnetic Robin Laplacian*, arXiv preprint arXiv:1603.02810 (2016).

[27] D. GOLOVATY, A. MONTERO AND P. STERNBERG, *Dimension reduction for the Landau-de Gennes model on curved nematic thin films*, arXiv preprint arXiv:1611.03011 (2016).

[28] D. S. GREBENKOV AND B. HELFFER, *On spectral properties of the Bloch-Torrey operator in two dimensions.* Submitted. Preprint: http://arxiv.org/abs/1608.01925.

[29] D. S. GREBENKOV, B. HELFFER AND R. HENRY, *The complex Airy operator with a semi-permeable barrier.* To appear in SIAM J. Math. Anal (2017). Preprint: http://arxiv.org/abs/1603.06992.

[30] R. HENRY, *On the semi-classical analysis of Schrdinger operators with purely imaginary electric potentials in a bounded domain*, arXiv preprint arXiv:1405.6183 (2014).

[31] B. HELFFER AND X.-B. PAN, *Reduced Landau–de Gennes functional and surface smectic state of liquid crystals*, Journal of Functional Analysis, 255 (2008), pp. 3008–3069.

[32] R. IGNAT AND R. JERRARD, *Interaction energy between vortices of vector fields on Riemannian surfaces*, arXiv preprint arXiv:1701.06546 (2017).

[33] R. IGNAT, L. NGUYEN, V. SLASTIKOV AND A. ZĂRNESCU, *Uniqueness results for an ODE related to a generalized Ginzburg-Landau model for liquid crystals*, arXiv preprint arXiv:1404.1724 (2014).

[34] R. Ignat, L. Nguyen, V. Slastikov and A. Zărnescu, *Stability of the melting hedgehog in the Landau-de Gennes theory of nematic liquid crystals*, arXiv preprint arXiv:1404.1729 (2014).

[35] R. Ignat, L. Nguyen, V. Slastikov and A. Zărnescu, *Instability of point defects in a two-dimensional nematic liquid crystal model*, arXiv preprint arXiv:1503.03670 (2015).

[36] R. Ignat, L. Nguyen, V. Slastikov and A. Zărnescu, *Stability of point defects of degree $\frac{1}{2}$ in a two-dimensional nematic liquid crystal model*, arXiv preprint arXiv:1601.02812 (2016).

[37] R. Ignat, L. Nguyen, V. Slastikov and A. Zărnescu, *On the uniqueness of minimisers of Ginzburg-Landau functionals*, arXiv preprint arXiv:1708.05040 (2017).

[38] H. Kovařík and K. Pankrashkin, *On the p-Laplacian with Robin boundary conditions and boundary trace theorems*, Calculus of Variations and Partial Differential Equations, 56 (2017), p. 49.

[39] D. Krejcirik and P. Siegl, *Pseudomodes for Schroedinger operators with complex potentials*, arXiv preprint arXiv:1705.01894 (2017).

[40] A. Kachmar, P. Keraval and N. Raymond, *Weyl formulae for the Robin Laplacian in the semiclassical limit*, Confluentes Math. (2016).

[41] A. Kachmar, X.-B. Pan et al., *Existence of surface smectic states of liquid crystals*, arXiv preprint arXiv:1602.06241 (2016).

[42] P. Mironescu, *Profile decomposition and phase control for circle-valued maps in one dimension*, C. R. Math. Acad. Sci. Paris 353(12) (2015), pp. 1087–1092.

[43] B. Mityagin and P. Siegl, *Local form-subordination condition and Riesz basisness of root systems*, arXiv preprint arXiv:1608.00224 (2016).

[44] L. Mrad and D. Phillips, *Dynamic analysis of chevron structures in liquid crystal cells*, Molecular Crystals and Liquid Crystals, 647 (2017), pp. 66–91.

[45] X. B. Pan, *Surface superconductivity in applied magnetic fields above H_{C_2}*, Comm. Math. Phys., 228 (2002), pp. 327–370.

[46] P. Pallfy-Muhoray, M. Y. Pevnyi, E. G. Virga and X. Zheng, *The Effects of Particle Shape in Orientationally Ordered Soft Materials*, IAS/Park City Mathematics Series (to appear).

[47] J. Park, W. Wang, P. Zhang, Z. Zhang, *On minimizers for the isotropic-nematic interface problem*, Calculus of Variations and Partial Differential Equations 56(2) (2017), pp. 1–15.

[48] K. SAMOKHIN, *Symmetry and topology of two-dimensional noncentrosymmetric superconductors*, arXiv preprint arXiv:1511.07493 (2015).

[49] É. SANDIER AND I. SHAFRIR, *Small energy Ginzburg-Landau minimizers in* $\mathbb{R}^3$, arXiv preprint arXiv:1612.00821 (2017).