Mathematical studies of liquid crystals

M. Carme Calderer
School of Mathematics
University of Minnesota
Minneapolis, MN 55455

July 6, 2004

Abstract

These presentations deal with mathematical problems of the liquid crystal theory.

We label as liquid crystals those materials capable of showing different degrees of molecular ordering, both, orientational and positional, according to temperature and concentration. Such materials may flow like fluids and experience deformations as elastic solids. One issue of interest is the interaction with applied electric fields within the scope of applications to devices, such as switches and artificial muscles.

We present a survey of static and flow theories of liquid crystals, emphasizing mathematical studies of existence and properties of solutions of the governing equations. The coupling between molecular ordering and elastic deformation arises in connection with elastomer polymer networks. Finally, the inclusion of fluid flow in elastic networks motivates us to introduce the problem of gel swelling.

Whereas some of the results presented here are classic, we also emphasize new and open problems.

1 Modeling Survey and Phenomenology

Liquid crystals are phases intermediate between solid and liquid. Wheres some liquid crystals consist of rigid and elongated molecules, liquid crystal phases are also exhibited by more complicated molecules (e.g., with bent-shapes) and also by some polymeric networks. We use the chemical structure of the molecule and the corresponding type of interaction to motivate the continuum theory models of the phases. We give a survey of the phenomenology for the different phases, from the nematic (with orientational order of molecules, tending to follow preferred directions of alignment), through the smectic phases (with positional order of centers of mass, arranged in layers). We address the interaction of the molecules with electric fields, describing dielectric as well as ferroelectric behaviors and their roles in applications such as to switching devices. For bent-shape molecules, we discuss the effects of the spontaneous polarization, and its role in the observed instabilities, e.g., *telephone cord shapes*. For elastic networks, we discuss the coupling between elastic deformation and electric polarization, and how the principal directions of stretch relate to the polarization field.

- Liquid crystal molecules
- Liquid crystal phases
- Mean field theory of the nematic phase
- Uniaxial and biaxial symmetries
- The Oseen-Frank theory of nematics
- Chiral liquid crystals
- Smectic A* ([5])and Smectic C* phases and positional ordering
- Ferroelectricity ([28], [26], [8])
- Theories of de Gennes, Lubensky, Chen and Renn ([16],[13], [37])
- Electric energy
- Self-field interaction energy
- Polymeric networks and elastomers ([17], [40], [27], [35], [20])

2 Variational theory of nematics and the Fredericks transition

We consider the problem of minimizing the total energy of a liquid crystal occupying a domain $\Omega \in \mathcal{R}^3$, and with prescribed boundary conditions. The admissible set consist of fields, $\mathbf{n} \in H^1(\Omega, \mathcal{S}^2)$, and the energy density is quadratic with respect to $\nabla\mathbf{n}$ and invariant with respect to the transformation $\mathbf{n} \rightarrow -\mathbf{n}$. We consider the case that electric fields are applied in the material. We present the theory developed in [24].

The Fredericks transition, which forms the theoretical basis of the application to switching devices, consists on the exchange of stability between two distinct minimizers as the value of the applied external field reaches a critical value. We address the stability analysis associated with such a phenomenon ([14], [39].

3 Composite liquid crystals and polymer systems

We consider composite systems of liquid crystal and polymer network. These are prototype models for switching devices where the inclusion of a polymer matrix plays the role of *remembering* one state of alignment. We assume that the polymer inclusions are periodically distributed in the liquid crystal domain and provide a contact energy favoring a special molecular alignment at the polymer-liquid crystal interface. We analyze a relaxed problem where the constraint $|\mathbf{n}| = 1$ is replace by a new term in the bulk energy, penalizing deviations of the length $\mathbf{n}$ from the value 1. With the application of the two-scale convergence method, we obtain an effective liquid crystal material. The Fredericks transition is analyzed in a two-dimensional geometry, corresponding to the case that the polymeric inclusions are cylinder-like.

- Composite liquid crystals and polymeric systems ([15], [12])
- Weak surface anchoring
- Relaxed energy functional ([6], [7])
- A priori estimates
- Two-scale convergence ([3], [4], [25])
- Limiting problems and effective energies
- Cylindrical geometry
- Electric energy
- Stability and critical fields: Fredericks transition ([36])

4 Flow problems

Once the static theory of a physical system is well understood, the issue often arises of deriving flow equations for such a system. We present Leslie's derivation of the governing equations of liquid crystal flow, the Leslie-Ericksen equations, as a method capable of addressing many complex material systems. Such a method is indeed an application of the approach to obtaining conservation laws by postulating a law of balance of energy together with invariance requirements. We present a survey of the existence theory of such flow, and discuss flow regimes with defects. The latter follows a generalization by Ericksen of the governing equations including the uniaxial order parameter that vanishes at defect locations.

- Balance of energy and invariance under rigid body rotations and translations [29]
- The second law of thermodynamics ([22], [23])
- Dissipation inequality (Ericksen) ([21]
- The Leslie-Ericksen system [29]
- Existence theory ([30], [31])
- Liquid crystals with variable degree of orientation ([23], [10])
- Defect surfaces and chevron pattern in flow ([34], [11], [9])

5 Liquid crystals and gels

We proceed with the flow problems of the previous section by presenting the flow theory of smectic A as developed by Weinan E. We mention an application to the study of formation of smectic filaments from the isotropic phase. We derive the dissipation inequality and discuss the problem of existence of solutions to the governing equations following the analysis of Liu.

The final part of this presentation deals with models of gels from the point of view of two-component mixtures: Elastic solid and Newtonian fluid. We discuss the role of electric ions in the swelling phenomena, and conclude with the formulation of a Riemann problem proposed as model to analyze and simulate the motion of the swelling front.

- Flow theory of smectic A [18]
- Filaments in the isotropic-smectic A transition [19]
- Existence results for the flow equations [32]
- Models of gels as mixtures of elastic networks and liquids [33]
- Modeling the ion effects of the system [1]
- Free energy: elastic, mixing and electrostatic contributions [1]
- The phenomena of gel swelling ([2], [38])
- Formulation of dynamic swelling in terms of Riemann problems [33]

References

[1] P. Addad, *Physical Properties of Polymeric Gels*, Chichester, 1996.

[2] J. M. A.E. English, S. Mafe and et.al., *Equilibrium swelling properties of polyampholytic hydrogels*, J.Chem. Phys., 104 (1996), pp. 8713–8720.

[3] G. Allaire, *Homogenization and two-scale convergence*, SIAM J. Math. Anal., 23 (1992), pp. 1482–1518.

[4] ———, *Two-scale convergence and homogenization of periodic structures.* Lecture Notes, School on Homogenization, ICTP, Trieste, 1993.

[5] P. Bauman, M. C. Calderer, C. Liu, and D. Phillips, *The phase transition between chiral nematic and smectic a liquid crystals*, Arch. Rat. Mech. Anal., (2002), pp. 161–186.

[6] F. Bethuel, H. Brézis, and J.-M. Coron, *Relaxed energies for harmonic maps*, in Variational methods (Paris, 1988), Birkhäuser Boston, Boston, MA, 1990, pp. 37–52.

[7] F. Bethuel, H. Brézis, and F. Hélein, *Ginzburg-Landau vortices*, Birkhäuser Boston Inc., 1994.

[8] M. Calderer, *Superconductivity analogies, ferroelectricity and flow defects in liquid crystals*, in Recent Progress in Computational and Applied PDEs, Kluwer Academic/Plenum Publishers, 2002, pp. 10–25.

[9] M. C. Calderer and C. Liu, *Liquid crystal flow: dynamic and static configurations*, SIAM J. Appl. Math., 60 (2000), pp. 1925–1949.

[10] ———, *Poiseuille flow of nematic liquid crystals*, Int. J. Engr. Sci. Mech., 39 (2000), pp. 1007–1022.

[11] M. C. Calderer and B. Mukherjee, *Chevron patterns in liquid crystal flows*, Physica D, 98 (1996), pp. 201–224.

[12] M. C. Calderer and Q. Shen, *Static configurations of nematic liquid crystals and polymer composites*, Math.Meth.Appl.Sci., in press, (2002).

[13] J. Chen and T. Lubensky, *Landau-ginzburg mean-field theory for the nematic to smectic c and nematic to smectic a liquid crystal transistions*, Phys. Rev. A, 14 (1976), pp. 1202–1297.

[14] N. A. Clark and S. T. Lagerwall, *Submicrosecond bistable electro-optic switching in liquid crystals*, Applied Physics Letters, 36 (1980), pp. 899–901.

[15] G. P. Crawford and S. Zumer, *Liquid crystals in complex geometries*, Taylor & Francis, 1996.

[16] P. G. de Gennes and J. Prost, *The physics of liquid crystals*, Oxford University Press, 1993.

[17] A. DeSimone and G. Dolzmann, *Material instabilities in nematic elastomers*, Physica D, 136 (2000), pp. 175–191.

[18] W. E, *Nonlinear continuum theory of smectic a liquid crystals*, Arch. Rat. Mech. Anal., 137 (1997), pp. 159–175.

[19] W. E and P. Palffy-Muhoray, *Dynamics of filaments during the isotropic to smectic a phase transition*, J. Non. Sci., 9 (1999), pp. 417–437.

[20] M. W. E. M. Terentjev and T. C. Lubensky, *Fluctuations and long–range order in smectic elastomers*, Europhys. Lett., 30 (1995), pp. 343–348.

[21] J. Ericksen, *Conservation laws for liquid crystals*, Trans. Soc. Rheol., 5 (1961), pp. 22—34.

[22] J. Ericksen, *Continuum theory of nematic liquid crystals*, Res. Mechanica, 21 (1987), pp. 381–392.

[23] J. Ericksen, *Liquid crystals with variable degree of orientation*, Arch Rath. Mech. Anal., 113 (1991), pp. 97–120.

[24] R. Hardt, D. Kinderlehrer, and F. H. Lin, *Existence and partial regularity of static liquid crystal configurations*, Comm. Math. Phys., 105 (1987), pp. 547–570.

[25] U. Hornung, *Homogenization and Porous Media*, Springer, New York, 1997.

[26] M. C. J. Park, *Variational problems for ferroelectric liquid crystals*, Submitted, (2004).

[27] I. Kundler and H. Finkelmann, *Director reorientation via stripe–domains in nematic elastomers: influence of cross–link density, anisotropy of the network and smectic clusters*, Macromol. Chem. Phys., 199 (1998), pp. 677–686.

[28] S. Lagerwall, *Ferroelectric and Antiferroelectric Liquid Crystals*, Wiley-VCH, 1999.

[29] F. M. Leslie, *Theory of flow phenomena in liquid crystals*, Advances in Liquid Crystals, 4 (1979), pp. 1–81.

[30] F.-H. Lin and C. Liu, *Nonparabolic dissipative systems modeling the flow of liquid crystals*, Comm. Pure Appl. Math., 48 (1995), pp. 501–537.

[31] ——, *Existence of solutions for the ericksen-leslie system*, Arch.Rat. Mech. Anal, 154 (2000), pp. 135–156.

[32] C. Liu, *Dynamic theory for incompressible smectic-a liquid crystals: Existence and regularity*, Discrete and Continuous Dynamical Systems, 6 (2000), pp. 591–608.

[33] M.C.Calderer and H.W.Weinberger, *Dynamical studies of gel swelling*, Preprint, (2004).

[34] B. Mukherjee, S. Mazumder, and M. C. Calderer, *Poiseuille flow of liquid crystals: highly oscillatory regimes*, J. non-Newtonian Fluid Mech., accepted, 99 (2001), pp. 37–55.

[35] E. Nishikawa and H. Finkelmann, *Smectic-a liquid single crystal elastomers–strain induced break-down of smectic layers*, Macromol. Chem. Phys., 200 (1999), pp. 312–322.

[36] D. P. P. Bauman and Q. Shen, *On singular limits in polymer stabilized liquid crystals*, Royal Soc. of Edinburgh, Ser A., to appear, (2002).

[37] S. Renn and T. Lubensky, *An abrikosov twist-grain-boundary phase in smectic liquid crystals*, Phys. Rev. A, 38 (1988), pp. 2133–2147.

[38] T. Tanaka and D. Filmore, *Kinetics of selling of gels*, J. Chem. Phys., 70 (1979), pp. 1214–1218.

[39] E. G. Virga, *Variational theories for liquid crystals*, Chapman & Hall, 1994.

[40] M. Warner and E. M. Terentjev, *Nematic elastomers–a new state of matter*, Prog. Polym. Sci., 21 (1996), pp. 853–891.