

Mathematical models and analysis of liquid crystals and gels

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In this series of lectures, we address mathematical models of materials systems that, in recent decades, have inspired many developments in partial differential equations. From physical point of view, such problems arise in soft condensed matter and are also linked to relevant applications in optics and mechanics. Liquid crystal phases found in organic and synthetic compounds are intermediate between solids and liquids. Gels consist of solids that can hold solvent. Both types of properties are often encountered as coexisting in physical and biological systems. Mathematically, such problems span many topics from calculus of variations, homogenization, nonlinear elasticity, to diffusive and hyperbolic dynamics.

1 Liquid crystals and phase transitions: M.Carme Calderer

In this first lecture, I will address problems of minimizing the total energy of a nematic liquid crystal subject to prescribed boundary conditions and constraints. Nematic liquid crystals have orientational ordering and tend to align along preferred directions, either determined by (anchoring) Dirichlet boundary conditions or by applied electric and magnetic fields. Positional ordering, in addition to the orientational one, develops upon lowering the temperature, causing a symmetry breaking in the system. In smectic phases, centers of mass of molecules tend to arrange themselves into one-dimensional arrays. Mathematically, the problem bears some analogies with that of phase transitions between

metal and superconductor in type II superconductivity. Additional symmetry breaking may cause the emergence of ferroelectricity in smectic liquid crystals. This introduces nonlocal phenomena due to the interaction of the molecular polarization field with its own induced electric field. Minimization of the energy is then subject to electrostatic constraints. We will discuss problems of bending of filaments and membranes.

2 Nonlinear elasticity of elastomers and gels: M.Carne Calderer

This talk examines recent applications of calculus of variations and nonlinear elasticity to study equilibrium phenomena in liquid crystal elastomers and gels. In the former, we explore the significantly different properties of the energy that result from the interaction of the anisotropy of liquid crystals with the nonlinear elastic properties of polymers. In particular, we analyze the physical and mathematical significance of the "soft elastomer modes". Indeed, the basic signature of liquid crystal elastomers is their capability of experiencing large deformations when the director aligns itself along principal directions of stretch. Static problems for gels are characterized by the presence of nonlinear constraints related to balance of mass. The Euler-Lagrange equations for the associated energies give systems that couple the equilibrium equations of elasticity with the Cahn-Hilliard ones for the solvent volume fraction. We also examine how the combination of the chemistry and network elasticity of gels opens up to exciting new applications in the field of pharmacology, biomedical devices and modeling of biological tissue.

3 Evolution problems in liquid crystals and gels: M.Carne Calderer

In the case of gels, we will address mathematical properties of the time dependent models. The governing systems consist of balance of mass and linear momentum for the polymer and solvent components. A realistic model of gels should account for elastic deformation, solvent transport, solvent diffusion and viscoelasticity. We will consider mathematical analogies of stationary regimes of gels with porous media systems and Darcy's law. We will address issues of well-posedness of initial-boundary value problems in some cases. In problems related to gels, a source of difficulty is the coexistence in the model of the Lagrangian formulation of solids with the Eulerian one of fluids. In three dimensional problems, this requires restricting the analysis to regimes with small elastic stretches but with arbitrarily large angles of local rotation.

4 Homogenization of nematic composites, Parts I and II: Dmitry Golovaty

I will review some recent results in homogenization for nematic liquid crystalline suspensions.

First, I will consider a nonlinear problem for a Ginzburg-Landau functional with a (positive or negative) surface energy term corresponding to soft anchoring of the nematic on surfaces of the inclusions. Assuming that inclusions are separated by distances of the same order as their size, I will outline the procedure for finding a limiting functional as the size of inclusions approaches zero. The approach is based on a generalization of the variational method of mesocharacteristics.

Second, I will consider a similar problem for ferronematics—dilute suspensions of ferromagnetic particles in a nematic—where the energy is supplemented by terms describing interaction between the suspension and the magnetic field. For a pure nematic, the energy density of interaction between the magnetic field and the nematic director is given by a quadratic term that is minimized when the director is parallel to the field. For a ferronematic, the additional, indirect coupling between the nematic and the field is introduced into the energy via anchoring of nematic molecules on the surfaces of the particles. Assuming that the particles are identical prolate spheroids with fixed positions but variable orientations, I will show that the influence of particles on the suspension can be accounted for by an effective nonlinear potential. For needle-like particles of large eccentricity, the model reduces to a known expression of Brochard and de Gennes.

5 Free boundary problem related to gel swelling: Ming Chen

We consider the time evolution of a gel formed when, an almost dry polymer initially confined to the rectangular strip $-1 < x < 1$, at time $t = 0$ is brought into contact with its own solvent, located in $x < -1$ and $x > 1$. The polymer interface grows towards the solvent, which in turn, diffuses into the polymer region. We perform a change of variables that transform the problem into one of fixed boundary. The governing system is of weakly dissipative hyperbolic type. We study well-posedness of such a system for the case that the total extensional stress is an increasing function of the strain. Whereas this condition is satisfied for entangled linear polymeric materials used in biomedical devices, we find that it may fail in polysaccharide gels occurring in living systems. We argue that this may indicate the onset of de-swelling. These mechanisms are relevant to motility phenomena in some bacteria.