Discontinuous order parameters in liquid crystal theories

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Continuum theories of liquid crystals describe defects in different ways. For example, in the Oseen-Frank theory the mean molecular orientation of a nematic liquid crystal is described by a director field **n**. In the case of equal elastic constants it is known that the only possible discontinuities of **n** in energy-minimizing configurations are isolated point defects[1]. While this is not known to be the case for unequal elastic constants, natural candidates for line defects have infinite energy. One possible way out of this problem is to modify the growth of the free-energy density for very large $\nabla\mathbf{n}$, so that it grows subquadratically, but this introduces a new difficulty, that, for example, an index ½ singularity is nonorientable, so that a description in terms of a vector field **n** is questionable. As regards two-dimensional defects, in which **n** jumps across a surface, the calculation of the energy of such configurations depends on how the gradient $\nabla\mathbf{n}$ of **n** is interpreted, but in the usual interpretation of this gradient (mathematically, as a weak derivative) such configurations are not allowed.

In the Landau – de Gennes theory defects are not described by singularities in the **Q**-tensor order parameter, energy minimizers being expected to be smooth, something that can be proved under appropriate hypotheses. Thus defects have to be described differently, for example in terms of singular behaviour of eigenvectors of **Q**. Thus there is no problem regarding infinite-energy line defects, and also the theory respects the overall head-to-tail symmetry of molecules, so that the problem of orientability disappears too. However the advantage of a clean mathematical interpretation of defects as singularities is lost. Singularities in which **Q** jumps across a surface are again not allowed according to the usual interpretation of $\nabla\mathbf{Q}$.

There are, however, indications that at small length-scales there can be sharp discontinuities of such order parameters across surfaces. Examples are discontinuities that arise when a liquid crystal is confined between surfaces on which conflicting boundary conditions are specified[2-4]. There is a natural mathematical framework for describing such situations energetically, in which the underlying order parameter belongs to a space of mappings of bounded variation, and there is an additional energy term involving an integral over the interface where the order parameter jumps, the integrand depending on the values of the order parameter on each side of the interface. Such models have proved useful, for example, in models of fracture mechanics[5], and they naturally predict that surface discontinuities are energetically preferred for some problems involving small length-scales.

The talk will explore the possibilities of such models and how they might lead to a possible description of observed defects as singularities.

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