A new approach to continuum energy functionals for nematic liquid crystals

John Ball* and Apala Majumdar**

*Oxford Centre for Nonlinear Partial Differential Equations,
Mathematical Institute, 24-29 St Giles', Oxford, OX1 3LB, U.K
**Oxford Centre for Collaborative and Applied Mathematics,
Mathematical Institute, 24-29 St Giles', Oxford OX1 3LB, U.K.

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Abstract

Mean-field theories describe the state of a nematic liquid crystal in terms of a probability distribution function for the molecular orientations. The **Q**-tensor order parameter is then defined to be a normalized second moment of this probability distribution function, from which it follows that the ordered eigenvalues $\lambda_i(\mathbf{Q})$ of $\mathbf{Q}$ are constrained to satisfy

$$-\frac{1}{3} < \lambda_1(\mathbf{Q}) \leq \lambda_2(\mathbf{Q}) \leq \lambda_3(\mathbf{Q}) < \frac{2}{3}. \qquad (*)$$

The Landau-De Gennes theory is a general continuum theory for nematic liquid crystals in which the total free energy has the form $I_\theta(\mathbf{Q}) = \int_\Omega \psi(\mathbf{Q}, \nabla\mathbf{Q}, \theta)\, dx$ at temperature θ, and where the bulk free-energy density $\psi_B(\mathbf{Q}, \theta) = \psi(\mathbf{Q}, \mathbf{0}, \theta)$ is a quartic polynomial in the eigenvalues $\lambda_i(\mathbf{Q})$. It is well known that the Landau-De Gennes predictions are not consistent with the mean-field predictions in the low-temperature regime, and that (*) can be violated; the range of consistency can be quantified.

In this talk, we consider the Onsager mean-field bulk free-energy functional with the Maier-Saupe molecular interaction, and show how this leads to a new form for the bulk free energy density which satisfies $\psi_B(\mathbf{Q}, \theta) \to \infty$ as $\lambda_1(\mathbf{Q}) \to -\frac{1}{3}$ or $\lambda_3(\mathbf{Q}) \to \frac{2}{3}$. We study the asymptotics and qualitative properties of this form for ψ_B. In particular, our model also predicts a first-order isotropic-nematic phase transition and for the case of the one-constant approximation $\psi(\mathbf{Q}, \nabla\mathbf{Q}, \theta) = \psi_B(\mathbf{Q}, \theta) + \kappa(\theta)|\nabla\mathbf{Q}|^2,\ \kappa(\theta) > 0$, we show that the corresponding energy minimizers for I_θ satisfy (*). Our study is in part motivated by the interesting work of Fatkullin & Slastikov (*Nonlinearity* **18**(2005),2565-2580), where they study critical points of the free energy functional within Onsager's model of isotropic-nematic phase transitions.