Dense liquid crystals and duality methods for finding equilibria

J. M. Taylor (University of Oxford) in collaboration with X. Zheng and P. Palffy-Muhoray (KSU)

- Our work is concerned with the derivation and analysis of a new model for describing dense, homogeneous liquid crystal systems.
- We minimise the free energy

$$\mathcal{F}_\eta(f) = \int_{\mathbb{S}^2} f(p) \ln f(p) - f(p) \ln \left(\int_{\mathbb{S}^2} (p \cdot q)^2 f(q) \, dq - \eta \right) \, dp$$

over all probability distributions $f \in \mathcal{P}(\mathbb{S}^2)$ describing the distribution of orientations.

- Intuitively, the model aims to capture the idea that at higher concentrations there is very little configuration space available to molecules, and that the pressure should diverge at a finite saturation limit.

$$\mathcal{F}_\eta(f) = \int_{\mathbb{S}^2} f(p) \ln f(p) - f(p) \ln \left(\int_{\mathbb{S}^2} (p \cdot q)^2 f(q) \, dq - \eta \right) \, dp$$

- In general, variations cannot find solutions. $\mathcal{P}(\mathbb{S}^2)$ has empty (relative) interior in L^1 and all non-trivial minimisers are on the boundary of the domain in L^∞.
- The energy is not convex, but is convex "enough" to apply duality methods to overcome this smoothness issues.
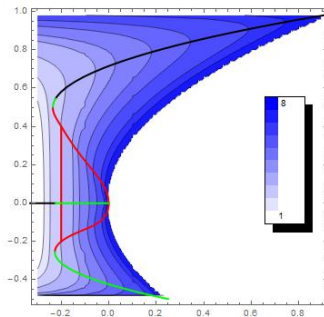
- The analysis allows a feasible numerical scheme, and new phase behaviour is found for solutions.
- A Van-der Waals type equation of state can be obtained, demonstrating diverging pressure as the system reaches saturation.