Mean-field model for polar nematics

F. Bisi[a], A.M. Sonnet[b], E.G. Virga[a]

a Dipartimento di Matematica and CNISM, Università di Pavia, via Ferrata, 1, 27100 Pavia, Italy
b Department of Mathematics, University of Strathclyde, Livingstone Tower, 26 Richmond Street, Glasgow G1 1XH, UK

The existence of uniaxial liquid crystals with polar molecules, having all the dipoles aligned in a parallel pattern, is classically ruled out(1).
Typically, there are two different avenues to a mean-field theory for liquid crystals: the first is based on short-range, repulsive, steric forces, whilst the second is based on long-range, globally attractive, dispersion forces. Purely polar steric interactions have been shown to have the potential of inducing unexpected orientationally ordered states(2).
In general, in real molecules anisotropies both in shape and in polarizability coexist; it has been shown that dispersion forces interaction can be combined with hard-core repulsion in a formal theory, based on a steric fourth-rank tensor(3). Starting from this, we build an interaction Hamiltonian incorporating the average electric dipolar energy exchanged between molecules with the same excluded region. Under the assumption of a spheroidal shape for the molecules, we propose a mean-field model with three scalar order parameters that allow us to identify both uniaxial and biaxial polar phases. By means of a numerical bifurcation analysis, we discuss the dependence of the stability of diferent phases upon two interaction parameters, one for the degree of intrinsic biaxiality in the shape tensor and one for the relative orientation of the electric dipole within each molecule.

References

(1) de Gennes, P.G.; Prost, J. The Physics of Liquid Crystals, 2nd ed.; Clarendon Press: Oxford (UK), 1993; p. 12.
(2) Bisi, F.; Rosso, R.; Virga, E.G.; Durand, G.E. *Phys. Rev. E* **2008**, *78*, 011705.
(3) Sonnet, A.M.; Virga, E.G. *Phys. Rev. E* **2008**, *77*, 031704.