

Density functional theory for nematics at high densities

Peter Palffy-Muhoray*

mpalffy@cpip.kent.edu

Interparticle interactions in condensed matter can be regarded to consist of long range attractive forces originating in London dispersion, and short range repulsive forces originating in Pauli exclusion. Although particles with short range interactions are usually modelled as impenetrable rigid solid bodies, density functional theories typically allow configurations with arbitrarily high particle densities. We consider the regions of validity of Onsager’s theory for colloidal particles, and present a simple ‘hard’ density functional formalism where configurations with densities greater than a critical value are strictly disallowed. We present the model, discuss the implications of the ‘hard’ aspect, and provide results from numerical calculations. Discontinuities of the derivatives of the orientational distribution function resulting from the hardness is of particular interest. The resulting equation of state allows comparison with experiment — but this has not yet been done.

This is joint work with Xiaoyu Zheng, Department of Mathematical Sciences, Kent State University.

*Liquid Crystal Institute, Kent State University, 1425 University Esplanade, Kent, OH 44242-0001, USA.