Dimension-independent singular potential calculation

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1 Introduction

The order parameter for a nematic liquid crystal system is the Q-tensor, which, in d-dimensions, is given by:

$$Q = \int_{S^{d-1}} \rho(\mathbf{p}) \left(\mathbf{p} \otimes \mathbf{p} - \tfrac{1}{d} I \right) d^d \mathbf{p} \tag{1}$$

where here ρ is a probability distribution function of molecular orientations of the nematic molecules. Because the nematic molecules are agnostic to which direction along a particular axis they point, we must have that $\rho(\mathbf{p}) = \rho(-\mathbf{p})$. Here S^{d-1} is the $d-1$-dimensional sphere. Note that, by this definition, Q is traceless and symmetric.

The particular Q-tensor value that a particular equilibrium configuration takes on is dependent on the system's free energy:

$$F[Q] = E[Q] - TS[Q] \tag{2}$$

We seek to write down an expression for this free energy which is numerically calculable from the Q-tensor. To do this, we find some appropriate mean-field expression for the energy E and calculate S by maximizing it subject to constraint (1) for ρ.

2 Singular potential

Consider the standard definition for S:

$$S = -N k_B \int_{S^{d-1}} \rho(\mathbf{p}) \log(4\pi \rho(\mathbf{p})) d^d \mathbf{p} \tag{3}$$

To maximize (3) subject to (1), we cast it as a Lagrange multiplier problem. To this end, we write down a Lagrangian:

$$\begin{aligned} \mathcal{L}[\rho] &= S + \Lambda : \left(\int_{S^{d-1}} \rho(\mathbf{p}) \left(\mathbf{p} \otimes \mathbf{p} - \tfrac{1}{d} I \right) d^d \mathbf{p} - Q \right) \\ &= \int_{S^{d-1}} \rho(\mathbf{p}) \left[-N k_B \log(4\pi \rho(\mathbf{p})) + \Lambda : \left(\mathbf{p} \otimes \mathbf{p} - \tfrac{1}{d} I \right) \right] d^d \mathbf{p} - \Lambda : Q \end{aligned} \tag{4}$$

Here Λ is also traceless and symmetric. Taking the variation yields:

$$\mathcal{L}[\rho] = \int_{S^{d-1}} \left[-N k_B \log(4\pi \rho(\mathbf{p})) + \Lambda : \left(\mathbf{p} \otimes \mathbf{p} - \tfrac{1}{d} I \right) - N k_B \right] \delta\rho \, d^d \mathbf{p} \tag{5}$$

Since this is for an arbitrary variation $\delta\rho$ we get that:

$$\begin{aligned} &- N k_B \log(4\pi \rho(\mathbf{p})) + \Lambda : \left(\mathbf{p} \otimes \mathbf{p} - \tfrac{1}{d} I \right) - N k_B = 0 \\ &\implies \rho(\mathbf{p}) = \frac{1}{4\pi e} \exp\left(\frac{1}{N k_B} \Lambda : (\mathbf{p} \otimes \mathbf{p}) \right) \exp\left(-\frac{1}{N k_B d} \Lambda : I \right) \end{aligned} \tag{6}$$