Maier-Saupe free energy in weak form

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1   Introduction

Here we will find the time evolution equation according to the Maier-Saupe free energy, and then put it into weak form so that it can be solved by a finite element method.

2   Maier-Saupe free energy and equations of motion

We begin by defining the tensor order parameter of the nematic system in terms of the probability distribution of the molecular orientation:

$$Q_{ij}(\mathbf{x}) = \int_{S^2} \left(\xi_i \xi_j - \tfrac{1}{3}\delta_{ij} \right) p(\xi; \mathbf{x}) d\xi \tag{1}$$

where $p(\xi; \mathbf{x})$ is the probability distribution of molecular orientation in local equilibrium at some temperature T and position $\mathbf{x}$. Note that this quantity is traceless and symmetric. Then the mean field free energy is given by:

$$F\left[Q_{ij}\right] = H\left[Q_{ij}\right] - T\Delta S \tag{2}$$

where H is the energy of the configuration, and ΔS is the entropy relative to the uniform distribution. We choose H to be:

$$H\left[Q_{ij}\right] = \int_{\Omega} \left\{ -\alpha Q_{ij}Q_{ji} + f_e\left(Q_{ij}, \partial_k Q_{ij}\right) \right\} d\mathbf{x} \tag{3}$$

with α some interaction parameter and f_e the elastic free energy density. The entropy is given by:

$$\Delta S = -nk_B \int_{\Omega} \left(\int_{S^2} p(\xi; \mathbf{x}) \log\left[4\pi p(\xi; \mathbf{x})\right] d\xi \right) d\mathbf{x} \tag{4}$$

where n is the number density of molecules. Now, in general for a given Q_{ij} there is no unique $p(\xi; \mathbf{x})$ given by (1). Hence, there is no unique ΔS. To find the appropriate ΔS corresponding to some fixed Q_{ij}, we seek to maximize the entropy density for a fixed Q_{ij} via the method of Lagrange multipliers. This goes as follows:

$$\begin{aligned}
\mathcal{L}[p] &= \Delta s[p] - \Lambda_{ij}Q_{ij}[p] \\
&= \int_{S^2} p(\xi)\left(\log\left[4\pi p(\xi)\right] - \Lambda_{ij}\left(\xi_i\xi_j - \tfrac{1}{3}\delta_{ij} \right) \right) d\xi
\end{aligned} \tag{5}$$

Here we've taken the spatial dependence to be implicit, since each of these are local quantities, and we're minimizing them *locally*. So, define a variation in p given by:

$$p'(\xi) = p(\xi) + \varepsilon\eta(\xi) \tag{6}$$

Then we have that:

$$
\begin{aligned}
\frac{\delta \mathcal{L}}{\delta p} &= \frac{d\mathcal{L}[p']}{d\varepsilon}\bigg|_{\varepsilon=0} \\
&= \frac{d\mathcal{L}[p']}{dp'}\frac{dp'}{d\varepsilon}\bigg|_{\varepsilon=0} \\
&= \int_{S^2}\left(\log\left[4\pi p(\xi)\right] - \Lambda_{ij}\left(\xi_i\xi_j - \tfrac{1}{3}\delta_{ij}\right) + 1\right)\eta(\xi)d\xi
\end{aligned}
\tag{7}
$$

Since this is for an arbitrary variation η, we must have that

$$
\log\left[4\pi p(\xi)\right] - \Lambda_{ij}\left(\xi_i\xi_j - \tfrac{1}{3}\delta_{ij}\right) + 1 = 0
\tag{8}
$$

Solving for $p(\xi)$ yields:

$$
p(\xi) = \frac{1}{4\pi}\exp\left[-\left(\tfrac{1}{3}\Lambda_{ij}\delta_{ij} + 1\right)\right]\exp\left[\Lambda_{ij}\xi_i\xi_j\right]
\tag{9}
$$

However, $p(\xi)$ is a probability distribution, so we need to normalize it over the domain. When we do this, the constant factors out front cancel and we're just left with:

$$
p(\xi) = \frac{\exp\left[\Lambda_{ij}\xi_i\xi_j\right]}{Z\left[\Lambda\right]}
\tag{10}
$$

$$
Z\left[\Lambda\right] = \int_{S^2}\exp[\Lambda_{ij}\xi_i\xi_j]d\xi
\tag{11}
$$

Now p is uniquely defined in terms of the Lagrange multipliers Λ_{ij}. Plugging this back into the constraint equation (1) we get:

$$
\begin{aligned}
Q_{ij} &= \frac{1}{Z[\Lambda]}\left(\int_{S^2}\left(\xi_i\xi_j\exp[\Lambda_{kl}\xi_k\xi_l] - \tfrac{1}{3}\delta_{ij}\exp[\Lambda_{kl}\xi_k\xi_l]\right)d\xi\right) \\
&= \frac{1}{Z[\Lambda]}\left(\frac{\partial Z[\Lambda]}{\partial \Lambda_{ij}} - \tfrac{1}{3}\delta_{ij}Z[\Lambda]\right) \\
&= \frac{\partial \log Z}{\partial \Lambda_{ij}} - \tfrac{1}{3}\delta_{ij}
\end{aligned}
\tag{12}
$$