[pex43] Maier-Saupe theory I: variational problem

The Maier-Saupe theory for the thermotropic transition between an isotropic liquid and a nematic phase as described in [pln74] arrives at the functional,

$$J[f] = \Delta S + \lambda_1 \mathcal{N} + \lambda_2 \mathcal{M},$$

with Lagrange multipliers, λ_1, λ_2, and where

$$\Delta S = -k_B \int_0^{\pi/2} d\theta \, \sin\theta \, [2\pi f(\theta)] \ln\big(2\pi f(\theta)\big),$$

$$\mathcal{N} = \pi \int_0^{\pi/2} d\theta \, \sin\theta \, (3\cos^2\theta - 1) f(\theta), \quad \mathcal{M} = 2\pi \int_0^{\pi/2} d\theta \, \sin\theta \, f(\theta) = 1,$$

represent entropy, order parameter, and normalization, respectively, all expressed as integrals involving the unknown orientation function $f(\theta)$.

(a) Find the extremum of the functional $J[f]$ by variational calculus to produce the orientation function,

$$f(\theta, b) = A(b) \exp\big(b \cos^2\theta\big),$$

and determine the amplitude $A(b)$ analytically by imposing the normalization condition $\mathcal{M} = 1$.

(b) Plot the orientation function $f(\theta, b)$ versus θ for $0 < \theta < \pi/2$ and several values of the parameter $b \geq 0$. Interpret the shape of the orientation function thus obtained in the context of nematic ordering.

[adapted from Jones 2002]

Solution: