[pex44] Maier-Saupe theory II: free energy, entropy, order parameter

This is the continuation of [pex43], where we have solved the variational problem and determined the one-parameter orientation function, $f(\theta, b) = A(b) \exp\left(b \cos^2\theta\right)$ with an explicit expression for the amplitude $A(b)$.
(a) Use Mathematica to calculate analytic expressions for the order parameter,

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

and the entropy,

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

(b) Use ParametricPlot of Mathematica to plot entropy $\Delta S/k_B$ versus order parameter $\mathcal{N}$. Interpret the shape of the curve thus obtained.
(c) From these ingredients and the enthalpy,

$$\Delta H = -\frac{1}{2} u [\mathcal{N}(b)]^2,$$

we express the scaled free energy, $\Delta\hat{F} \doteq \Delta F/k_{\rm B}T$, as a function of the parameter b and the scaled coupling constant $\hat{u} \doteq u/k_{\rm B}T$:

$$\Delta\hat{F}(b, \hat{u}) = -\frac{1}{2}\hat{u}[\mathcal{N}(b)]^2 - \Delta\hat{S}(b),$$

where $\Delta\hat{S} = \Delta S/k_{\rm B}$ is a dimensionless entropy. Plot $\Delta\hat{F}(b, \hat{u})$ versus $\mathcal{N}(b)$ for $\hat{u} = 3, 4, \ldots, 7$. Note that the thermal energy, k_BT, is used as energy scale for both the coupling strength and the free energy itself. For each value of $\hat{u}$, the order parameter $\mathcal{N}$ settles at the value for which the free energy, $\Delta\hat{F}$, has a minimum.

[adapted from Jones 2002]

Solution: