Q-tensor dimension

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1 Definition of the Q-tensor

In general, the Q-tensor is defined as:

$$Q = \langle \mathbf{m} \otimes \mathbf{m} \rangle - \tfrac{1}{d} I \tag{1}$$

where $\mathbf{m}$ is a unit vector representing the direction of the nematic molecules, d is the dimension, and I is the $d \times d$ itentiy matrix. This way, the Q-tensor is a traceless, symmetric $d \times d$ tensor. For a fully 3D configuration, this becomes:

$$Q = \int_{S^2} \rho(\mathbf{p}) \left(\mathbf{p} \otimes \mathbf{p} - \tfrac{1}{3} I \right) d^3\mathbf{p} \tag{2}$$

where $\rho(\mathbf{p})$ is such that $\rho(\mathbf{p}) = \rho(-\mathbf{p})$ given the nematic symmetry, and S^2 is the 2D sphere. Since Q is traceless and symmetric, we may write it in components as:

$$Q = \begin{bmatrix} Q_1 & Q_2 & Q_3 \\ Q_2 & Q_4 & Q_5 \\ Q_3 & Q_5 & -(Q_1 + Q_4) \end{bmatrix} \tag{3}$$

For the quasi-2D case (which corresponds to a thin film), we force Q to be uniform in the $\hat{\mathbf{z}}$ direction, and also force the initial director to be in the x-y plane. For a uniaxial system, $Q = S\left(\hat{\mathbf{n}} \otimes \hat{\mathbf{n}} - \tfrac{1}{3} I \right)$ so that the Q-tensor everywhere takes the following form:

$$Q = \begin{bmatrix} Q_1 & Q_2 & 0 \\ Q_2 & Q_4 & 0 \\ 0 & 0 & -(Q_1 + Q_4) \end{bmatrix} \tag{4}$$

In this case, it is described by 3 degrees of freedom. By virtue of the fact that Λ and Q are simultaneously diagonalized, none of the terms which arise in the equation of motion for isotropic elasticity will cause the x-z or y-z components to become nonzero. I have not verified for the anisotropic terms, but the numerical plots indicate that $Q_3 = Q_5 = 0$ for systems which are initialized in that way, and also for which gradients in the $\hat{\mathbf{z}}$ direction are zero.

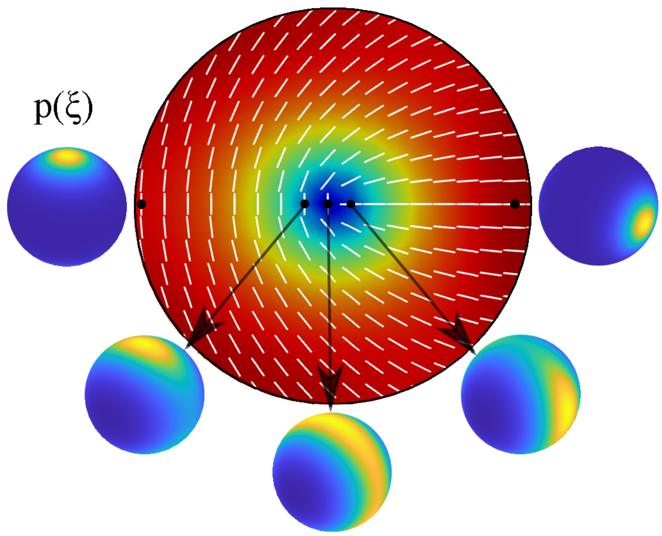
The way that this manifests for the probability distribution function is such that:

$$\int_{S^2} \rho(x, y, z) \, xz \, dS = \int_{S^2} \rho(x, y, z) \, yz \, dS = 0 \tag{5}$$

One simple way to ensure this (and perhaps the only way, given freedom in the x- and y-directions) is to enforce:

$$\rho(x, y, z) = \rho(x, y, -z) \tag{6}$$

Indeed, looking at Cody's plot of a defect with corresponding probability distribution function colormaps, we see that each configuration is symmetric about the x-y plane:



For a fully 2D Q-tensor, the definition in terms of a probability distribution function is:

$$Q = \int_{S^1} \rho(\mathbf{p}) \left(\mathbf{p} \otimes \mathbf{p} - \tfrac{1}{2} I \right) d^2\mathbf{p} \tag{7}$$

where S^1 is just the circle. In this case, it may be written in terms of components as:

$$Q = \begin{bmatrix} Q_1 & Q_2 \\ Q_2 & -Q_1 \end{bmatrix} \tag{8}$$

One way to compare this to the quasi-2D case is to understand it as a special case wherein $Q_4 = -Q_1$:

$$Q = \begin{bmatrix} Q_1 & Q_2 & 0 \\ Q_2 & -Q_1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{9}$$

This places a further constraint on the corresponding 3D probability distribution function:

$$\int_{S^2} \rho(\mathbf{p})\, z^2 \, d^3\mathbf{p} = \tfrac{1}{3} \tag{10}$$

It is unclear to me whether there is a way to write a 3D probability distribution function constrained to be a product of some function of z and some 2D PDF $\rho(x, y)$. As a cursory attempt to investigate the effect of this constraint on the PDF, we calculate the singular potential for Q-tensor values of the following form and plot the corresponding PDFs:

$$Q = \begin{bmatrix} S & 0 & 0 \\ 0 & -S & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{11}$$

Note that eq. (11) and eq. (9) are separated by a rotation in the x-y plane, so it is sufficient to only plot (11).

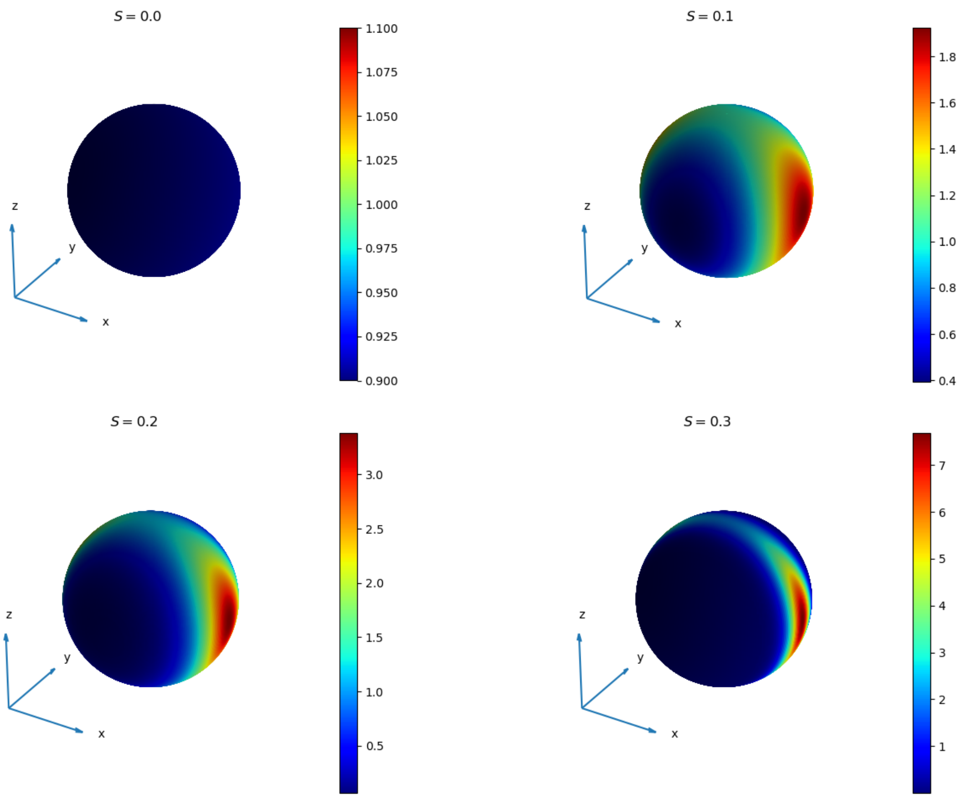


Figure 1: Probability distribution function for Q-tensor values of the form (9)

The only characteristic that stands out to me about these plots is that the PDF value in the direction of the z-axis is always intermediate between that of the x- and y-axes. This is to be expected because the z-axis eigenvalue will, by definition, be midway between the other two.

I suppose the only other question to consider is whether the PDF corresponding to the fully 2D case (that is, the one that maximizes the entropy given a fixed 2D Q-tensor) has any relationship to the full 3D PDF.