Electronic Supplementary Material (ESI) for Soft Matter.


# Supplementary Information: Relevance of saddle-splay elasticity in complex nematic geometries

Žiga Kos and Miha Ravnik

July 27, 2015

## 1 Saddle-splay free energy in Q-tensor formulation

The saddle-splay free energy density

$$f_{24} = -K_{24}\nabla \cdot [\mathbf{n}(\nabla \cdot \mathbf{n}) + \mathbf{n} \times \nabla \times \mathbf{n}], \tag{A.1}$$

can be rewritten in terms of nematic order parameter tensor $Q_{ij}$ as

$$f_{24}^{\text{ten}} = L_{24}\left(\frac{\partial Q_{jk}}{\partial x_i}\frac{\partial Q_{ik}}{\partial x_j} - \frac{\partial Q_{ij}}{\partial x_j}\frac{\partial Q_{ik}}{\partial x_k}\right) \tag{A.2}$$

by including additional contributions from biaxiality and inhomogeneous scalar order parameter, where where $K_{24}$ is the director saddle-splay elastic constant, $L_{24}$ is the tensor saddle-splay elastic constant, and $\mathbf{n}$ is the director.

The relation between Eq. A.1 and Eq. A.2 can be demonstrated by using the expanded form of the scalar order parameter tensor

$$Q_{ij} = \frac{S}{2}(3n_in_j - \delta_{ij}) + \frac{P}{2}\left(e_i^{(1)}e_j^{(1)} - e_i^{(2)}e_j^{(2)}\right) \tag{A.3}$$

in Eq. A.2. Besides the largest eigenvalue of $Q_{ij}$ – scalar order parameter $S$ – and the corresponding eigenvector – director $\mathbf{n}$ – Eq. A.3 also includes the biaxiality parameter $P$, the secondary director $\mathbf{e}^{(1)}$, and the third axis $\mathbf{e}^{(2)} = \mathbf{n} \times \mathbf{e}^{(1)}$. In our approach, Q-tensor is allowed to be biaxial, however $P$ is typically non-zero only close to defect cores[1,2]. Expanding Eq. A.2 with full Q-tensor gives many biaxial-dependent terms (see for example[3]), which from computational perspective are not very simple to implement and actually calculate with good precision. Therefore, to calculate the biaxial contributions to the saddle-splay free energy in the tensorial formulations, we rather construct an *uniaxial* order parameter tensor

$$Q_{ij}^{\text{uni}} = \frac{S}{2}(3n_in_j - \delta_{ij}) \tag{A.4}$$

from the scalar order parameter and the director (as obtained from the full $Q_{ij}$), and calculate the biaxial contribution to Eq. A.2 as

$$f_{24}^{\text{ten}} - f_{24}^{\text{ten, uni}} = L_{24}\left(\frac{\partial Q_{jk}}{\partial x_i}\frac{\partial Q_{ik}}{\partial x_j} - \frac{\partial Q_{ij}}{\partial x_j}\frac{\partial Q_{ik}}{\partial x_k}\right) - L_{24}\left(\frac{\partial Q_{jk}^{\text{uni}}}{\partial x_i}\frac{\partial Q_{ik}^{\text{uni}}}{\partial x_j} - \frac{\partial Q_{ij}^{\text{uni}}}{\partial x_j}\frac{\partial Q_{ik}^{\text{uni}}}{\partial x_k}\right) \tag{A.5}$$

Effectively, being able the account for the biaxiality, we explore the individual invariants from equation A.2 in terms of uniaxial Q-tensor:

$$\begin{aligned}\frac{\partial Q^{\rm uni}_{jk}}{\partial x_i}\frac{\partial Q^{\rm uni}_{ik}}{\partial x_j} &= \frac{9S^2}{4}\frac{\partial(n_j n_k)}{\partial x_i}\frac{\partial(n_i n_k)}{\partial x_j} \\ &+ \frac{3S}{2}\frac{\partial(n_j n_k)}{\partial x_i}\frac{1}{2}\frac{\partial S}{\partial x_j}(3n_i n_k - \delta_{ik}) \\ &+ \frac{1}{2}\frac{\partial S}{\partial x_i}(3n_j n_k - \delta_{jk})\frac{3S}{2}\frac{\partial(n_i n_k)}{\partial x_j} \\ &+ \frac{1}{4}\frac{\partial S}{\partial x_i}\frac{\partial S}{\partial x_j}(3n_j n_k - \delta_{jk})(3n_i n_k - \delta_{ik})\end{aligned} \tag{A.6}$$

$$\begin{aligned}&= \frac{9S^2}{4}\Big\{(\nabla\cdot\mathbf{n})^2 + [\mathbf{n}\times(\nabla\times\mathbf{n})]^2 - \nabla\cdot[\mathbf{n}\cdot(\nabla\cdot\mathbf{n}) + \mathbf{n}\times(\nabla\times\mathbf{n})]\Big\} \\ &+ \frac{1}{4}(\nabla S)^2 + \frac{3}{4}(\mathbf{n}\cdot\nabla S)^2 + 3S(\nabla S)[(\mathbf{n}\cdot\nabla)\mathbf{n}] - \frac{3S}{2}(\nabla\cdot\mathbf{n})(\mathbf{n}\cdot\nabla S),\end{aligned} \tag{A.7}$$

$$\begin{aligned}\frac{\partial Q^{\rm uni}_{ij}}{\partial x_j}\frac{\partial Q^{\rm uni}_{ik}}{\partial x_k} &= \frac{9S^2}{4}\frac{\partial(n_i n_j)}{\partial x_j}\frac{\partial(n_i n_k)}{\partial x_k} \\ &+ \frac{3S}{2}\frac{\partial(n_i n_j)}{\partial x_j}\frac{1}{2}\frac{\partial S}{\partial x_k}(3n_i n_k - \delta_{ik}) \\ &+ \frac{1}{2}\frac{\partial S}{\partial x_j}(3n_i n_j - \delta_{ij})\frac{3S}{2}\frac{\partial(n_i n_k)}{\partial x_k} \\ &+ \frac{1}{4}\frac{\partial S}{\partial x_j}\frac{\partial S}{\partial x_k}(3n_i n_j - \delta_{ij})(3n_i n_k - \delta_{ik})\end{aligned} \tag{A.8}$$

$$\begin{aligned}&= \frac{9S^2}{4}\Big\{(\nabla\cdot\mathbf{n})^2 + [\mathbf{n}\times(\nabla\times\mathbf{n})]^2 \\ &+ \frac{1}{4}(\nabla S)^2 + \frac{3}{4}(\mathbf{n}\cdot\nabla S)^2 - \frac{3S}{2}(\nabla S)[(\mathbf{n}\cdot\nabla)\mathbf{n}] + 3S(\nabla\cdot\mathbf{n})(\mathbf{n}\cdot\nabla S).\end{aligned} \tag{A.9}$$

Subtracting Eq. A.7 and Eq. A.9 gives the uniaxial form of the tensor-based saddle-splay volume free energy density

$$f_{24}^{\text{ten, uni}} = -L_{24}\frac{9S^2}{4}\nabla\cdot[\mathbf{n}(\nabla\cdot\mathbf{n}) + \mathbf{n}\times\nabla\times\mathbf{n}] \tag{A.10}$$

$$- L_{24}\frac{9S}{2}\left(\nabla\cdot\mathbf{n}\right)\left(\nabla S\cdot\mathbf{n}\right) + L_{24}\frac{9S}{2}\left(\nabla S\right)\left[\left(\mathbf{n}\cdot\nabla\right)\mathbf{n}\right]. \tag{A.11}$$

Comparing Eq. A.10 and Eq. A.1 gives the relation $L_{24} = 4K_{24}/9S^2$. For $K_{24} = K_2/2$ and $K_1 = K_3$ -as used in the paper-, $L_{24}$ is exactly equal to $L_1$. Eq. A.11 gives the contribution of the inhomogeneous scalar order parameter to $f_{24}^{\text{ten}}$. Note that a similar procedure is commonly applied to resolve the relations between director $K_i$ and tensorial $L_i$ elastic constants[4].

## References


[1] N. Schopohl and T. Sluckin, *Phys. Rev. Lett.*, 1987, **59**, 2582.

[2] M. Ravnik and S. Žumer, *Liq. Cryst.*, 2009, **36**, 1201.

[3] A. Poniewierski and T. Sluckin, *Molecular Physics*, 1985, **55**, 1113.

[4] K. Schiele and S. Trimper, *Phys. Stat. Sol.*, 1983, **118**, 267.