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Elastic Constants of Biaxial Nematic liquid Crystals

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A microscopic theory is developed for the bulk and surface elastic constants of biaxial nematic liquid crystals. Our expressions depend on generalized orientational order parameters and on the direct pair correlation function.

Keywords: Biaxial nematic; elastic constants

INTRODUCTION

Liquid crystals exhibit a rich variety of phases. The most common among them is the uniaxial nematic [1]. The biaxial nematic (N_B) which in phenomenological approaches almost always accompanies the uniaxial one [1], was only detected in lyotropic systems [2, 3]. Important information concerning the nature of anisotropic organization in nematics can be extracted from their elastic constants. In particular, the values of the elastic constants determine most of the observed phenomena such as defect shapes, flow patterns, optical properties, *etc.* Furthermore, they play a crucial rôle in almost all applications of liquid crystalline materials. While the elastic constants of uniaxial nematics are well understood, the corresponding studies of elasticity for biaxial nematics are scarce [4–8]. To fill this gap, our

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attempt in this paper is a derivation of the elastic energy with a view to relating phenomenological elastic constants to molecular quantities. The first step towards this goal is a microscopic formulation of the elastic energy for biaxial liquid crystals. By performing these studies we also hope to provide a possible hint as to why thermotropic biaxial nematics have not been discovered so far. One of the possible hypotheses is that the biaxial nematic constants associated with the secondary directors are so small that thermal fluctuations prevent the formation of a stable N_B phase. Valuable hints concerning this issue could again be obtained from numerical estimates of the elastic constants.

We start by recalling that the orientational order in nematic liquid crystals is generally described on a mesoscopic level by a second-order, symmetric and traceless tensor field $\mathbf{Q}$. The three eigenvectors of $\mathbf{Q}$, the *directors* $\mathbf{l}$, $\mathbf{m}$ and $\mathbf{n}$, are mutually orthogonal. The eigenvalues corresponding to $\mathbf{l}$, $\mathbf{m}$ and $\mathbf{n}$ are $-(1/3)(S-T)$, $-1/3(S+T)$ and $(2/3)S$, where the quantities S and T denote the uniaxial and biaxial order parameters, respectively.

Elastic deformations in biaxial nematics generally affect both the eigenvectors and eigenvalues of $\mathbf{Q}$. However, it is often assumed that only the directors are position-dependent functions, whereas the scalar order parameters S and T remain constant. Our analysis is restricted to this particular case, also known as *hard biaxial nematic phase* [4].

Nematic liquid crystals are viscoelastic materials. Thus any inhomogeneity in the director fields will contribute to an elastic energy. In a continuum approach the elastic energy is obtained as an expansion around the undistorted ground state with respect to gradients of the directors. It was derived by Saupe [5]; Trebin [6]; Brand and Pleiner [7] and Govers and Vertogen [8]. In this paper we shall refer to the version as proposed by Trebin [6]. It reads

$$\begin{aligned}\mathcal{F}_{\text{elast}} = &\frac{1}{2}K_{l1}(\operatorname{div}\mathbf{l})^2 + \frac{1}{2}K_{l2}(\mathbf{l}\cdot\operatorname{curl}\mathbf{l})^2 + \frac{1}{2}K_{l3}(\mathbf{l}\times\operatorname{curl}\mathbf{l})^2 \\ &+ \frac{1}{2}K_{m1}(\operatorname{div}\mathbf{m})^2 + \frac{1}{2}K_{m2}(\mathbf{m}\cdot\operatorname{curl}\mathbf{m})^2 + \frac{1}{2}K_{m3}(\mathbf{m}\times\operatorname{curl}\mathbf{m})^2 \\ &+ \frac{1}{2}K_{n1}(\operatorname{div}\mathbf{n})^2 + \frac{1}{2}K_{n2}(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 + \frac{1}{2}K_{n3}(\mathbf{n}\times\operatorname{curl}\mathbf{n})^2 \\ &+ \frac{1}{2}K_{mn}(\mathbf{m}\cdot\operatorname{curl}\mathbf{n})^2 + \frac{1}{2}K_{nl}(\mathbf{n}\cdot\operatorname{curl}\mathbf{l})^2 + \frac{1}{2}K_{lm}(\mathbf{l}\cdot\operatorname{curl}\mathbf{m})^2 \\ &+ \frac{1}{2}K_{l4}\operatorname{div}[(\mathbf{l}\cdot\nabla)\mathbf{l} - \mathbf{l}\operatorname{div}\mathbf{l}] + \frac{1}{2}K_{m4}\operatorname{div}[(\mathbf{m}\cdot\nabla)\mathbf{m} - \mathbf{m}\operatorname{div}\mathbf{m}] \\ &+ \frac{1}{2}K_{n4}\operatorname{div}[(\mathbf{n}\cdot\nabla)\mathbf{n} - \mathbf{n}\operatorname{div}\mathbf{n}]. \qquad (1)\end{aligned}$$

Here K_{ij} denote the 15 linearly independent elastic constants. In (1), the twelve expressions starting from K_{l1} up to K_{lm} describe the bulk deformations of a biaxial nematic (*splay*, *twist* and *bend* distortions, respectively). The last three summands are divergence terms. Thus they contribute to elastic deformations close to surfaces.

Clearly, the continuum theory based upon (1) does not provide any information about the magnitude of the biaxial elastic constants. To this aim we need a microscopic approach. A purpose of this paper is to establish a connection between the elastic constants entering the expression (1) and molecular quantities. We generalize the density-functional approach [9–11] and express the biaxial elastic constants in terms of the the direct pair correlation function and of the one-particle distribution function of the ordered biaxial nematic phase.

MICROSCOPIC EXPRESSIONS FOR BIAXIAL ELASTIC CONSTANTS

The microscopic expression for the elastic free energy can be found by calculating the free energy difference, F, between deformed and undeformed equilibrium biaxial nematic states, characterized by one-particle distributions $\rho_d(\mathbf{1})$ and $\rho_u(\mathbf{1}) \equiv \rho(\mathbf{1})$ (SDF), respectively, where $(\mathbf{1}) \equiv (\mathbf{r}_1, \boldsymbol{\Omega}_1)$. To second order in the density difference $\delta\rho = \rho_d - \rho$ the expression for F may be written as [11]

$$\beta F = \int \rho_d(\mathbf{1}) \ln \frac{\rho_d(\mathbf{1})}{\rho(\mathbf{1})} d(\mathbf{1}) - \int \delta\rho(\mathbf{1}) d(\mathbf{1}) - \frac{1}{2!} \int\int c(\mathbf{r}_{12}, \boldsymbol{\Omega}_1, \boldsymbol{\Omega}_2, [\rho]) \delta\rho(\mathbf{1}) \delta\rho(\mathbf{2}) d(\mathbf{1}) d(\mathbf{2}) + \cdots, \quad (2)$$

where c is the direct pair correlation function (DPCF) of the undeformed, homogeneously oriented biaxial nematic, $d(\mathbf{1}) = d\mathbf{r}_1 d\boldsymbol{\Omega}_1$, β is the inverse temperature, and $\int d(\mathbf{1})\, \rho(\mathbf{1}) = N$ (N being the average number of particles in the system). Finally, $\mathbf{r}_1$, $\mathbf{r}_2$ and $\boldsymbol{\Omega}_1$, $\boldsymbol{\Omega}_2$ denote the positions and orientational tripods of a pair of biaxial molecules; $\mathbf{r}_{12}$ is the separation vector between the molecular centers.

The expression (2) is accurate up to second order in deformations and, in the limit of long-wavelength deformations, can serve as a definition of the elastic free energy for biaxial nematics. Assuming that the gradient expansion holds for the SDF [10, 11] and integrating by parts the expression

(2), we obtain the microscopic analogon of (1). It has the form

$$\beta F_{\text{elast}} = \int d\mathbf{r} A_{k\alpha\beta}(\partial_\alpha n_\beta^{(k)}) + \int d\mathbf{r} B_{k\alpha\beta\gamma}(\partial_\alpha \partial_\beta n_\gamma^{(k)}) + \int d\mathbf{r} M_{k'k''\alpha\beta\gamma'\gamma''}(\partial_\alpha n_{\gamma'}^{(k')})(\partial_\beta n_{\gamma''}^{(k'')}), \tag{3}$$

where

$$A_{k\alpha\beta} = -\frac{1}{2}\int d\mathbf{r}_{12} d\boldsymbol{\Omega}_1 d\boldsymbol{\Omega}_2 \; c(\mathbf{r}_{12}, \boldsymbol{\Omega}_1, \boldsymbol{\Omega}_2)\delta\rho(\boldsymbol{\Omega}_1) r_{12}^\alpha \Delta_{k\beta}(\boldsymbol{\Omega}_2) \tag{4}$$

$$B_{k\alpha\beta\gamma} = -\frac{1}{2}\int d\mathbf{r}_{12} d\boldsymbol{\Omega}_1 d\boldsymbol{\Omega}_2 \; c(\mathbf{r}_{12}, \boldsymbol{\Omega}_1, \boldsymbol{\Omega}_2)\delta\rho(\boldsymbol{\Omega}_1) r_{12}^\alpha r_{12}^\beta \Delta_{k\gamma}(\boldsymbol{\Omega}_2) \tag{5}$$

$$M_{k'k''\alpha\beta\gamma'\gamma''} = \frac{1}{2}\int d\mathbf{r}_{12} d\boldsymbol{\Omega}_1 d\boldsymbol{\Omega}_2 \; c(\mathbf{r}_{12}, \boldsymbol{\Omega}_1, \boldsymbol{\Omega}_2) \times r_{12}^\alpha r_{12}^\beta \Delta_{k'\gamma'}(\boldsymbol{\Omega}_1)\Delta_{k''\gamma''}(\boldsymbol{\Omega}_2). \tag{6}$$

In (3)–(6), $n_\gamma^{(k)}$ is the γ-th component of the k-th vector of the director tripod ($\mathbf{n}^{(1)} \equiv \mathbf{l}$, $\mathbf{n}^{(2)} \equiv \mathbf{m}$, $\mathbf{n}^{(3)} \equiv \mathbf{n}$) and r_{12}^β is the β-component of $\mathbf{r}_{12}$. Furthermore, we introduced the abbreviation

$$\Delta_{k\gamma}(\Omega) \equiv \frac{\partial \rho}{\partial \Omega_{jk}} \Omega_{j\gamma}, \tag{7}$$

where $\Omega_{jk} = \boldsymbol{\Omega}^{(j)} \cdot \mathbf{n}^{(k)}$ is the matrix of all directional cosines between the tripod of molecular orientations and the tripod of the directors.

Now, the 15 linearly independent biaxial deformations (1) can be extracted from (3) in the systematic way as follows. First of all we write F_{elast}, Eq. (3), in a local frame $(\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}})$ at point $\mathbf{r}$, that coincides with the three orthonormal directors $\mathbf{l}(\mathbf{r}) = [1, 0, 0]$, $\mathbf{m}(\mathbf{r}) = [0, 1, 0]$ and $\mathbf{n}(\mathbf{r}) = [0, 0, 1]$. The orthonormality requirements impose six constraints on the nine components of $\mathbf{l}(\mathbf{r})$, $\mathbf{m}(\mathbf{r})$ and $\mathbf{n}(\mathbf{r})$ and, consequently, on the first order terms $\partial_\alpha n_\beta^{(k)}$. Out of 27 partial derivatives $\partial_\alpha n_\beta^{(k)}$ one can select 9 *independent* derivatives, say $\partial_\alpha l_2 \equiv l_{2,\alpha}$, $\partial_\alpha n_1 \equiv n_{1,\alpha}$ and $\partial_\alpha n_2 \equiv n_{2,\alpha}$, which considerably reduce the number of terms in the expansion F_{elast}. In particular, they allow F_{elast} to be written as a sum of only 45 *linearly independent* bilinear deformations $(\partial_\alpha n_\beta^{(k)})(\partial_\gamma n_\delta^{(l)})$ (to contrast with 378 terms in the original expansion (3)). In order to express F_{elast} in a coordinate-free notation we

further use the relations:

$$\begin{array}{lll} \operatorname{div}\mathbf{l} = l_{2,y} - n_{1,z}, & \mathbf{l}\cdot\operatorname{curl}\mathbf{l} = -n_{1,y} - l_{2,z}, & \mathbf{l}\cdot\operatorname{curl}\mathbf{m} = -n_{2,y}, \\ \operatorname{div}\mathbf{m} = -l_{2,x} - n_{2,z}, & \mathbf{m}\cdot\operatorname{curl}\mathbf{m} = -l_{2,z} + n_{2,x}, & \mathbf{m}\cdot\operatorname{curl}\mathbf{n} = n_{1,z}, \\ \operatorname{div}\mathbf{n} = n_{1,x} + n_{2,y}, & \mathbf{n}\cdot\operatorname{curl}\mathbf{n} = n_{2,x} - n_{1,y}, & \mathbf{n}\cdot\operatorname{curl}\mathbf{l} = l_{2,x}. \end{array}$$

They allow to replace the local, partial derivatives of the directors by the invariant combinations of the combinations of the directors and of their first derivatives. Finally, by making use of the relations

$$\begin{aligned} [\mathbf{l}\times\operatorname{curl}\mathbf{l}]^2 &= (\operatorname{div}\mathbf{n})^2 + 2(\operatorname{div}\mathbf{n})(\mathbf{l}\cdot\operatorname{curl}\mathbf{m}) + (\mathbf{l}\cdot\operatorname{curl}\mathbf{m})^2 \\ &\quad + (\mathbf{n}\cdot\operatorname{curl}\mathbf{l})^2, \\ [\mathbf{m}\times\operatorname{curl}\mathbf{m}]^2 &= (\operatorname{div}\mathbf{l})^2 + 2(\operatorname{div}\mathbf{l})(\mathbf{m}\cdot\operatorname{curl}\mathbf{n}) \\ &\quad + (\mathbf{l}\cdot\operatorname{curl}\mathbf{m})^2 + (\mathbf{m}\cdot\operatorname{curl}\mathbf{n})^2, \\ [\mathbf{n}\times\operatorname{curl}\mathbf{n}]^2 &= (\operatorname{div}\mathbf{m})^2 + 2(\operatorname{div}\mathbf{m})(\mathbf{n}\cdot\operatorname{curl}\mathbf{l}) \\ &\quad + (\mathbf{m}\cdot\operatorname{curl}\mathbf{n})^2 + (\mathbf{n}\cdot\operatorname{curl}\mathbf{l})^2, \\ \operatorname{div}[(\mathbf{l}\cdot\nabla)\mathbf{l} - \mathbf{l}(\operatorname{div}\mathbf{l})] &= -\frac{1}{2}(\mathbf{l}\cdot\operatorname{curl}\mathbf{l})^2 + \frac{1}{2}(\mathbf{m}\cdot\operatorname{curl}\mathbf{m})^2 + \frac{1}{2}(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 \\ &\quad - (\mathbf{m}\cdot\operatorname{curl}\mathbf{m})(\mathbf{n}\cdot\operatorname{curl}\mathbf{n}) + 2(\operatorname{div}\mathbf{l})(\mathbf{m}\cdot\operatorname{curl}\mathbf{n}) \\ &\quad + 2(\mathbf{m}\cdot\operatorname{curl}\mathbf{n})^2, \\ \operatorname{div}[(\mathbf{m}\cdot\nabla)\mathbf{m} - \mathbf{m}(\operatorname{div}\mathbf{m})] &= \frac{1}{2}(\mathbf{l}\cdot\operatorname{curl}\mathbf{l})^2 - \frac{1}{2}(\mathbf{m}\cdot\operatorname{curl}\mathbf{m})^2 + \frac{1}{2}(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 \\ &\quad - (\mathbf{l}\cdot\operatorname{curl}\mathbf{l})(\mathbf{n}\cdot\operatorname{curl}\mathbf{n}) + 2(\operatorname{div}\mathbf{m})(\mathbf{n}\cdot\operatorname{curl}\mathbf{l}) \\ &\quad + 2(\mathbf{n}\cdot\operatorname{curl}\mathbf{l})^2, \\ \operatorname{div}[(\mathbf{n}\cdot\nabla)\mathbf{n} - \mathbf{n}(\operatorname{div}\mathbf{n})] &= \frac{1}{2}(\mathbf{l}\cdot\operatorname{curl}\mathbf{l})^2 + \frac{1}{2}(\mathbf{m}\cdot\operatorname{curl}\mathbf{m})^2 - \frac{1}{2}(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 \\ &\quad - (\mathbf{l}\cdot\operatorname{curl}\mathbf{l})(\mathbf{m}\cdot\operatorname{curl}\mathbf{m}) + 2(\operatorname{div}\mathbf{n})(\mathbf{l}\cdot\operatorname{curl}\mathbf{m}) \\ &\quad + 2(\mathbf{l}\cdot\operatorname{curl}\mathbf{m})^2, \end{aligned}$$

and after disregarding terms that contain an odd number of the directors of a given kind we arrive at the 15, D_{2h}-symmetric and linearly independent biaxial deformations corresponding to (1). The biaxial elastic constants are expressed by appropriate linear combinations of the tensor components $M_{k'k''\alpha\beta\gamma'\gamma''}$.

In order to obtain explicit expressions, however, we have to evaluate the integrals contained in (6). This is achieved by means of an invariant expansion of the SDF and DPCF in terms of *Wigner matrices*. They depend on the set of three Euler angles denoting the orientation $\mathbf{\Omega}$ of a biaxial

molecule. By exhausting the orthonormality properties of the Wigner matrices all angular integrals can be solved analytically. In the framework of a second-rank approximation for the Wigner expansions the biaxial elastic constants are given by

$$\begin{aligned} K_{l1} = K_{l3} = K_l(1,-2), \qquad & K_{l2} = K_l(1,4), \quad K_{l4} = K_l(1,1), \\ K_{m1} = K_{m3} = K_m(1,-2), \qquad & K_{m2} = K_m(1,4), \quad K_{m4} = K_m(1,1), \\ K_{n1} = K_{n3} = K_n(1,-2), \qquad & K_{n2} = K_n(1,4), \quad K_{n4} = K_n(1,1), \\ & K_{lm} = K_{mn} = K_{nl} = 0 \end{aligned} \tag{8}$$

where the two arguments in brackets in (8) are substituted for a_1 and a_2 in the following expressions:

$$\begin{aligned} K_l(a_1,a_2) = a_1\rho_0^2 \Bigg\{ & \frac{16}{15}\sqrt{5\pi}\Bigg[\left(I_{220}^{20}+I_{220}^{02}\right)\langle R_{20}^2\rangle\langle R_{22}^2\rangle + \left(I_{220}^{22}+I_{220}^{\bar{2}2}\right)\langle R_{22}^2\rangle^2 \\ & + \frac{1}{2}I_{220}^{00}\langle R_{20}^2\rangle^2\Bigg] - \frac{8}{45}\sqrt{30\pi}\Bigg[\frac{3}{2}I_{220}^{00}\langle R_{00}^2\rangle\langle R_{20}^2\rangle \\ & + \left(I_{220}^{02}+2I_{220}^{20}\right)\langle R_{00}^2\rangle\langle R_{22}^2\rangle + \left(I_{220}^{20}+2I_{220}^{02}\right)\langle R_{02}^2\rangle\langle R_{20}^2\rangle \\ & + 3\left(I_{220}^{22}+I_{220}^{\bar{2}2}\right)\langle R_{02}^2\rangle\langle R_{22}^2\rangle\Bigg]\Bigg\} + a_2\rho_0^2\Bigg\{\frac{8}{105}\sqrt{70\pi}\Bigg[\frac{1}{2}I_{222}^{00}\langle R_{20}^2\rangle^2 \\ & + \left(I_{222}^{20}+I_{222}^{02}\right)\langle R_{20}^2\rangle\langle R_{22}^2\rangle + \left(I_{222}^{22}+I_{222}^{\bar{2}2}\right)\langle R_{22}^2\rangle^2\Bigg] \\ & - \frac{8}{315}\sqrt{105\pi}\Bigg[\frac{3}{2}I_{222}^{00}\langle R_{00}^2\rangle\langle R_{20}^2\rangle + 3\left(I_{222}^{22}+I_{222}^{\bar{2}2}\right)\langle R_{02}^2\rangle\langle R_{22}^2\rangle \\ & + \left(I_{222}^{02}+2I_{222}^{20}\right)\langle R_{00}^2\rangle\langle R_{22}^2\rangle + \left(I_{222}^{20}+2I_{222}^{02}\right)\langle R_{02}^2\rangle\langle R_{20}^2\rangle\Bigg]\Bigg\} \end{aligned} \tag{9}$$

$$\begin{aligned} K_m(a_1,a_2) = a_1\rho_0^2 \Bigg\{ & \frac{8}{15}\sqrt{30\pi}\Bigg[\frac{1}{2}I_{220}^{00}\langle R_{00}^2\rangle\langle R_{20}^2\rangle + I_{220}^{20}\langle R_{00}^2\rangle\langle R_{22}^2\rangle \\ & + I_{220}^{02}\langle R_{02}^2\rangle\langle R_{20}^2\rangle + \left(I_{220}^{22}+I_{220}^{\bar{2}2}\right)\langle R_{02}^2\rangle\langle R_{22}^2\rangle\Bigg] \\ & + \frac{16}{15}\sqrt{5\pi}\Bigg[\frac{1}{2}I_{220}^{00}\langle R_{20}^2\rangle^2 + \left(I_{220}^{20}+I_{220}^{02}\right)\langle R_{20}^2\rangle\langle R_{22}^2\rangle \\ & + \left(I_{220}^{22}+I_{220}^{\bar{2}2}\right)\langle R_{22}^2\rangle^2\Bigg]\Bigg\} + a_2\rho_0^2\Bigg\{\frac{8}{105}\sqrt{105\pi} \\ & \times\Bigg[I_{222}^{20}\langle R_{00}^2\rangle\langle R_{22}^2\rangle + \frac{1}{2}I_{222}^{00}\langle R_{00}^2\rangle\langle R_{20}^2\rangle + I_{222}^{02}\langle R_{02}^2\rangle\langle R_{20}^2\rangle \end{aligned}$$

$$+\left(I_{222}^{22}+I_{\bar{2}22}^{22}\right)\langle R_{02}^2\rangle\langle R_{\bar{2}2}^2\rangle\Big]+\frac{8}{105}\sqrt{70\pi}\Big[\frac{1}{2}I_{222}^{00}\langle R_{20}^2\rangle^2$$
$$+\left(I_{222}^{20}+I_{222}^{02}\right)\langle R_{20}^2\rangle\langle R_{\bar{2}2}^2\rangle+\left(I_{\bar{2}22}^{22}+I_{\bar{2}\bar{2}2}^{22}\right)\langle R_{\bar{2}2}^2\rangle^2\Big]\Big\} \tag{10}$$

$$K_n(a_1,a_2)=a_1\rho_0^2\Big\{\frac{8}{15}\sqrt{5\pi}\Big[\frac{3}{4}I_{220}^{00}\langle R_{00}^2\rangle^2-\frac{1}{2}I_{220}^{00}\langle R_{20}^2\rangle^2$$
$$+\frac{3}{2}\left(I_{220}^{20}+I_{220}^{02}\right)\langle R_{00}^2\rangle\langle R_{02}^2\rangle$$
$$+\left(I_{220}^{22}+I_{\bar{2}20}^{22}\right)\left(\frac{3}{2}\langle R_{02}^2\rangle^2-\langle R_{\bar{2}2}^2\rangle^2\right)$$
$$-\left(I_{220}^{20}+I_{220}^{02}\right)\langle R_{20}^2\rangle\langle R_{\bar{2}2}^2\rangle\Big]$$
$$+\frac{4}{45}\sqrt{30\pi}\Big[\left(I_{220}^{02}-I_{220}^{20}\right)\langle R_{00}^2\rangle\langle R_{\bar{2}2}^2\rangle+\left(I_{220}^{20}-I_{220}^{02}\right)\langle R_{02}^2\rangle\langle R_{20}^2\rangle\Big]\Big\}$$
$$+a_2\rho_0^2\Big\{\frac{4}{105}\sqrt{70\pi}\Big[\frac{3}{4}I_{222}^{00}\langle R_{00}^2\rangle^2-\frac{1}{2}I_{222}^{00}\langle R_{20}^2\rangle^2$$
$$+\frac{3}{2}\left(I_{222}^{20}+I_{222}^{02}\right)\langle R_{00}^2\rangle\langle R_{02}^2\rangle$$
$$+\left(I_{222}^{22}+I_{\bar{2}22}^{22}\right)\left(\frac{3}{2}\langle R_{02}^2\rangle^2-\langle R_{\bar{2}2}^2\rangle^2\right)-\left(I_{222}^{20}+I_{222}^{02}\right)\langle R_{20}^2\rangle\langle R_{\bar{2}2}^2\rangle\Big]$$
$$-\frac{4}{315}\sqrt{105\pi}\Big[\left(I_{222}^{02}-I_{222}^{20}\right)\langle R_{02}^2\rangle\langle R_{20}^2\rangle+\left(I_{222}^{20}-I_{\bar{2}22}^{02}\right)\langle R_{00}^2\rangle\langle R_{\bar{2}2}^2\rangle\Big]\Big\} \tag{11}$$

In (9)–(11) $\langle R_{mn}^l\rangle$ are generated orientational order parameters [12] and $I_{l_1l_2l}^{n_1n_2}$ stands for radial integrals of the DPCF expansion coefficients.

$$I_{l_1l_2l}^{n_1n_2}=\int dr\, r^4 c_{l_1l_2l}^{n_1n_2}(r) \tag{12}$$

Though quantitative conclusions cannot be drawn from the general expressions (8)–(11), a few qualitative features are evident. First of all, due to the second rank approximation our expressions (8) reveal a *splay-bend degeneracy* of all directors, *i.e.*, $K_{l1}=K_{l3}$, $K_{m1}=K_{m3}$, $K_{n1}=K_{n3}$. Reasonably, in a purely uniaxial phase, where $\langle R_{mn}^l\rangle=\langle P^l\rangle\delta_{m0}\delta_{n0}$, the only nonzero elastic constants are those that affect the uniaxial director **n**.

Secondly, the mixed elastic constants K_{lm}, K_{mn} and K_{nl} vanish. This indicates that these quantities depend on higher than second rank order

parameters. Thus, they should be much smaller than the remaining elastic constants.

Finally, our expressions (8)–(11) are independent of any particular molecular model. They can now be used to estimate the biaxial elastic constants for model biaxial liquid crystals. This will be performed in our forthcoming publication for the lattice model studied by Biscarini *et al.* [12].

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