On homogenization of liquid crystals

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Liquid crystals

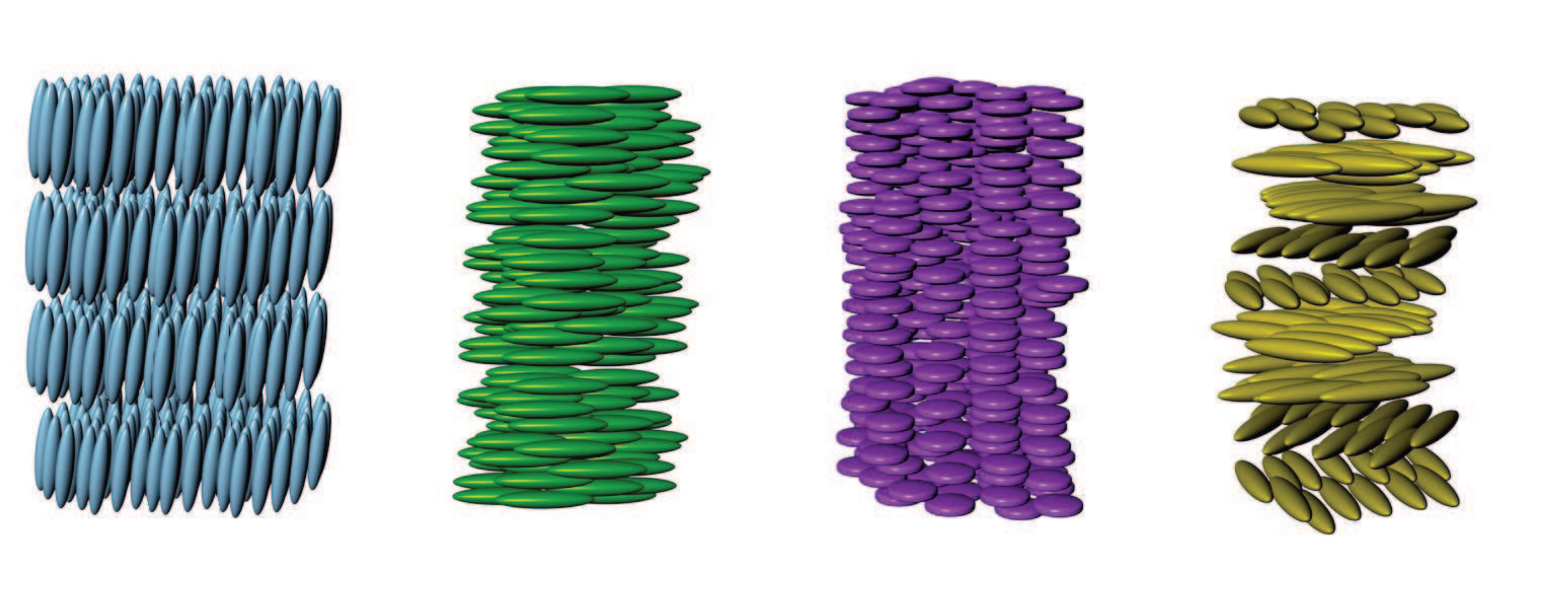

Figure 1: The structure of smectic (left), nematic calamitic and discotic (center) and cholesteric (right) liquid crystals.

Dynamics of nematic liquid crystals

The Ericksen-Leslie system describing the dynamics of nematic liquid crystals, has the form

$$\begin{cases} \dot{\mathbf{u}} - \mu\Delta\mathbf{u} = -\nabla p - \frac{\partial}{\partial x_j}\left(\frac{\partial\mathcal{F}}{\partial\mathbf{n}_{x_j}}\cdot\nabla\mathbf{n}\right) + \mathbf{F} + f, \quad \text{div}\,\mathbf{u} = 0, \\ J\ddot{\mathbf{n}} - 2q\mathbf{n} + \mathbf{h} = g + \mathbf{G}, \quad \|\mathbf{n}\| = 1, \end{cases} \tag{1}$$

where summation on repeated indices is understood and $\mathbf{n}_{x_j} := \frac{\partial}{\partial x_j}\mathbf{n}$. Here, $\mathbf{u}$ is the *spatial velocity vector field (the Eulerian)*, $\mathbf{n}$ is the *director field*, $\mu > 0$ is the *viscosity coefficient*, $J > 0$ is the *moment of inertia of the molecule*, $\mathbf{F}(x,t)$ and $\mathbf{G}(x,t)$ are given *external forces*, and $\dot{} := \frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla$ is the *material derivative*. The terms f and g correspond to the dissipative part of the stress tensor and intrinsic body force, respectively, and they depend on $\mathbf{u}$, $\mathbf{n}$. The *Oseen-Zöcher-Frank free energy* $\mathcal{F}(\mathbf{n},\nabla\mathbf{n})$ is defined by

$$\mathcal{F} := K\mathbf{n}\cdot\text{curl}\,\mathbf{n} + \frac{1}{2}\left(K_1(\text{div}\,\mathbf{n})^2 + K_2(\mathbf{n}\cdot\text{curl}\,\mathbf{n})^2 + K_3\|\mathbf{n}\times\text{curl}\,\mathbf{n}\|^2\right).$$

The *molecular field* $\mathbf{h}$ is defined by

$$\mathbf{h} := \frac{\partial\mathcal{F}}{\partial\mathbf{n}} - \frac{\partial}{\partial x_j}\left(\frac{\partial\mathcal{F}}{\partial\mathbf{n}_{x_j}}\right).$$

Dynamics of nematic liquid crystals

The *pressure* p and the Lagrange multiplier $2q$ are determined, respectively, by $\operatorname{div}\mathbf{u} = 0$ and $\|\mathbf{n}\| = 1$. Since the liquid crystal is nematic, we necessarily have $K = 0$. We assume that

$$K_1 > 0, \quad K_2 = K_3 > 0, \tag{2}$$

which includes the important case of the one constant approximation. In this case, the i^{th} component of the molecular field has the expression

$$h_i = (K_2 - K_1)\mathbf{n}_{k x_k x_i} - K_2 \mathbf{n}_{i x_k x_k} + q' \mathbf{n}_i,$$

where q' is a scalar function depending on $\mathbf{n}$ and its derivatives. We are interested in the non-dissipative case, i.e., $f = g = 0$.
Define linear differential operator $\mathcal{L}$ by

$$\mathcal{L}\mathbf{v} := (K_2 - K_1)\nabla(\operatorname{div}\mathbf{v}) - K_2 \Delta \mathbf{v}. \tag{3}$$

Dynamics of nematic liquid crystals

Given the Ericksen-Leslie system (1), define the new vector field

$$\boldsymbol{\nu} := \mathbf{n} \times \dot{\mathbf{n}}.$$

With all these hypotheses and notations, system (1) becomes

$$\dot{\mathbf{u}} - \mu\Delta\mathbf{u} = -\nabla p + (\mathcal{L}\mathbf{n} \cdot \nabla\mathbf{n}) + \mathbf{F}, \quad \operatorname{div}\mathbf{u} = 0, \tag{4}$$

$$J\dot{\boldsymbol{\nu}} = \mathcal{L}\mathbf{n} \times \mathbf{n} + \mathbf{n} \times \mathbf{G}, \tag{5}$$

$$\dot{\mathbf{n}} = \boldsymbol{\nu} \times \mathbf{n}, \tag{6}$$

with unknowns $\mathbf{u}$, $\boldsymbol{\nu}$, $\mathbf{n}$. Thus, the Ericksen-Leslie system (1) implies the new first order system (4)–(6).

Dynamics of nematic liquid crystals

Conversely, if the initial conditions of the first order system (4)–(6) satisfy the identities

$$\|\mathbf{n}(x,0)\| = 1, \qquad \mathbf{n}(x,0) \perp \boldsymbol{\nu}(x,0),$$

at time $t = 0$, then for any $t > 0$ we have

$$\|\mathbf{n}\| \equiv 1, \qquad \boldsymbol{\nu} = \mathbf{n} \times \dot{\mathbf{n}}, \qquad 2q = \mathbf{n} \cdot \mathbf{h} - J\|\boldsymbol{\nu}\|^2,$$

and (4)–(6) turns into (1). Thus, under these hypotheses on the initial conditions, the first order system (4), (5), (6) is equivalent to the original Ericksen-Leslie system (1)

We focus on the system (4)–(6) (with $J \neq 0$, which differs from the case studied in the preceding papers) and prove existence and uniqueness of solutions for 3-dimensional periodic media as well as for the problem in a bounded domain.

Periodic media. Notation and definitions

Let $Q_T := (0, T) \times \mathbb{T}$, where $\mathbb{T} = \mathbb{R}^3/\mathbb{Z}^3$ is the 3-dimensional torus. We shall study the system (4)–(6) in Q_T with initial conditions

$$\mathbf{u}(0, x) = \mathbf{u}_0, \quad \boldsymbol{\nu}(0, x) = \boldsymbol{\nu}_0, \quad \mathbf{n}(0, x) = \mathbf{n}_0. \tag{7}$$

Here $\mathbf{u}$, $\boldsymbol{\nu}$, $\mathbf{n}$ are unknown vector fields, p is an unknown scalar function, and J, K_i, μ are fixed strictly positive numbers.

Periodic media. Notation and definitions

- $L_2(\mathbb{T}) := \left\{\mathbf{v} : \mathbb{T} \to \mathbb{R}^3 \mid \|\mathbf{v}\|_2^2 := \int_{\mathbb{T}} \|\mathbf{v}\|^2 d\mathbf{x} < \infty\right\}$;
- $W_2^m(\mathbb{T})$ is the Sobolev space of functions on $\mathbb{T}$ having m distributional derivatives in $L_2(\mathbb{T})$;
- for any $\mathbf{v} \in W_2^m(\mathbb{T})$, $m \in \mathbb{N}$, define

$$\|D^m\mathbf{v}\|_2^2 := \sum_{i_1+i_2+i_3=m} \left\| \frac{\partial^m \mathbf{v}}{\partial x_1^{i_1} \partial x_2^{i_2} \partial x_3^{i_3}} \right\|_2^2 ;$$

- $Sol(\mathbb{T}) := \{\mathbf{v} : \mathbb{T} \to \mathbb{R}^3 \mid \mathbf{v} \in C^\infty(\mathbb{T}),\ \operatorname{div} \mathbf{v} = 0\}$;
- $Sol(Q_T) := \{\mathbf{v} \in C^\infty(Q_T) \mid \mathbf{v}(t,\cdot) \in Sol(\mathbb{T}),\ \forall t \in (0,T)\}$;
- $Sol_2(\mathbb{T})$ is the closure of $Sol(\mathbb{T})$ in the norm $L_2(\mathbb{T})$;
- $Sol_2^m(\mathbb{T})$ is the closure of $Sol(\mathbb{T})$ in the norm $W_2^m(\mathbb{T})$.

Periodic media. Notation and definitions

Definition 1. *A quadruple* $(\mathbf{u}, \boldsymbol{\nu}, \mathbf{n}, \nabla p)$ *is a* strong solution *of problem* (4)–(7) *in the domain* Q_T *if*

- (i) $\mathbf{u}$ *is a time-dependent vector field in* $L_2((0,T); Sol_2^3(\mathbb{T}))$, $\mathbf{u}_t \in L_2(Q_T)$*;*
- (ii) $\boldsymbol{\nu}$ *is a vector field in* $L_\infty((0,T); W_2^2(\mathbb{T}))$, $\boldsymbol{\nu}_t \in L_\infty((0,T); L_2(\mathbb{T}))$*;*
- (iii) $\mathbf{n}$ *is a vector field in* $L_\infty((0,T); W_2^3(\mathbb{T}))$, $\mathbf{n}_t \in L_\infty((0,T); W_2^1(\mathbb{T}))$*;*
- (iv) $\nabla p \in L_2(Q_T)$*;*
- (v) $\mathbf{u}$, $\mathbf{n}$, $\boldsymbol{\nu}$ *satisfy the initial conditions* (7), *i.e.,* $(\mathbf{u}, \mathbf{n}, \boldsymbol{\nu}) \rightharpoonup (\mathbf{u}_0, \mathbf{n}_0, \boldsymbol{\nu}_0)$ *weakly in* $L_2(\mathbb{T})$ *as* $t \to 0$*;*
- (vi) *equations* (4)–(6) *hold almost everywhere.*

Periodic media. Main results

Theorem 1. *Suppose* $\mathbf{u}_0 \in Sol_2^2(\mathbb{T}),\ \boldsymbol{\nu}_0 \in W_2^2(\mathbb{T}),\ \mathbf{n}_0 \in W_2^3(\mathbb{T})$*, and* $\mathbf{F} \in L_2((0,T);W_2^1(\mathbb{T}))$*,* $\mathbf{G} \in L_1((0,T);W_2^2(\mathbb{T}))$*.*
Then there exists some $0 < T_0 < T$ *such that the solution* (*as in Definition* 1) *of problem* (4)–(6) *exists in* Q_{T_0}*.*

Theorem 2. *Under the hypotheses of Theorem 1, let* $(\mathbf{u}_1, \boldsymbol{\nu}_1, \mathbf{n}_1, p_1)$ *and* $(\mathbf{u}_2, \boldsymbol{\nu}_2, \mathbf{n}_2, p_2)$ *be solutions of the problem* (4)–(7) *in the domain* Q_T*. Then, for some* $0 < T_0 \le T$

$$(\mathbf{u}_2, \boldsymbol{\nu}_2, \mathbf{n}_2, \nabla p_2) = (\mathbf{u}_1, \boldsymbol{\nu}_1, \mathbf{n}_1, \nabla p_1)$$

almost everywhere in Q_{T_0}*.*

Bounded domain. Notation and definitions

Let Ω be a bounded domain in $\mathbb{R}^3$ and consider nematic liquid crystal flow in the cylinder $\Omega \times \mathbb{R}$.

We study equations (4)–(6) in the domain $(0, T) \times \Omega$ with initial conditions (7) and additional boundary conditions

$$\mathbf{u}\big|_{\partial\Omega} = 0, \quad \mathbf{n} - \boldsymbol{n_1}\big|_{\partial\Omega} = 0, \quad \boldsymbol{\nu}|_{\partial\Omega} = 0 \quad \text{for any} \quad t > 0, \tag{8}$$

where $\boldsymbol{n}_1$ is a given vector field on Ω.

Condition $\mathbf{u}\big|_{\partial\Omega} = 0$ means that the domain has impenetrable boundary and that the fluid moves without slipping; $\mathbf{n} - \boldsymbol{n_1}\big|_{\partial\Omega} = 0$ describes the director position at the boundary. The third condition comes from the original Ericksen-Leslie system and means that $\dot{\mathbf{n}} = 0$ at the boundary.

Bounded domain. Notation and definitions

We let $Q_T := (0, T) \times \Omega$ and introduce the function spaces

$$\overset{\circ}{Sol}(\Omega) := \{\mathbf{v} : \Omega \to \mathbb{R}^3 \mid \mathbf{v} \text{ has compact support, } \operatorname{div} \mathbf{v} = 0\},$$

$$\overset{\circ}{Sol}(Q_T) := \{\mathbf{v} \in C^\infty(Q_T) \mid \mathbf{v}(t, \cdot) \in \overset{\circ}{Sol}(\Omega), \forall t\},$$

$$\overset{\circ}{Sol}{}_2^m(\Omega) \text{ is the closure of } \overset{\circ}{Sol}(\Omega) \text{ in the norm } W_2^m(\Omega).$$

Bounded domain. Notation and definitions

Definition 2. *The quadruple* $(\mathbf{u}, \boldsymbol{\nu}, \mathbf{n}, \nabla p)$ *is a* strong solution *of problem* (4)–(7), (8) *in the domain* Q_T *if*

- $\mathbf{u}$ *is a vector field in* $L_2((0,T); \overset{\circ}{Sol}{}_2^1(\Omega)) \cap L_2((0,T); W_2^3(\Omega))$, $\mathbf{u}_t \in L_2(Q_T)$;
- $\boldsymbol{\nu}$ *is a vector field in* $L_\infty((0,T); \overset{\circ}{W}{}_2^1(\Omega)) \cap L_\infty((0,T); W_2^2(\Omega))$, $\boldsymbol{\nu}_t \in L_\infty((0,T); L_2(\Omega))$;
- $\mathbf{n} - \boldsymbol{n}_1$ *is a vector field in* $L_\infty((0,T); \overset{\circ}{W}{}_2^1(\Omega)) \cap L_\infty((0,T); W_2^3(\Omega))$, *where* $\boldsymbol{n}_1$ *is a given constant vector field, and* $\mathbf{n}_t \in L_\infty((0,T); W_2^1(\Omega))$;
- $\nabla p \in L_2(Q_T)$;
- $\mathbf{u}$, $\mathbf{n}$, $\boldsymbol{\nu}$ *satisfy initial conditions* (7), *i.e.,* $(\mathbf{u}, \mathbf{n}, \boldsymbol{\nu}) \rightharpoonup (\mathbf{u}_0, \mathbf{n}_0, \boldsymbol{\nu}_0)$ *weakly in* $L_2(\Omega)$ *as* $t \to 0$;
- *equations* (4)–(6) *hold almost everywhere.*

Bounded domain. Main results

Theorem 3. *Assume that* Ω *is a Lipschitz domain and for almost all* $\mathbf{x} \in \partial\Omega$ *the boundary is the graph of a* C^2*-function in some neighborhood of* $\mathbf{x}$*. Let* $\boldsymbol{n}_1 = const$*,* $\mathbf{n}_0 \in \overset{\circ}{W}{}_2^3(\Omega)$*,* $\boldsymbol{\nu}_0 \in W_2^2(\Omega)$*,* $\mathbf{u_0} \in \overset{\circ}{S}ol_2^1(\Omega) \cap W_2^2(\Omega)$*,* $\Delta\mathbf{u}_0\big|_{\partial\Omega} = 0$*, and assume that for some* $d > 0$ *we have*

$$\mathbf{n}_0(x) = const, \quad \boldsymbol{\nu}_0(x) = 0 \quad \textit{if} \quad dist(x, \partial\Omega) < d.$$

Then problem (4)–(7), (8) *has a unique solution in* Q_T *for some* $T > 0$*.*

Theorem 4. *Suppose* Ω*,* $\mathbf{n}_0$*,* $\boldsymbol{\nu}_0$*,* $\mathbf{u_0}$*,* $\boldsymbol{n}_1$ *satisfy the conditions of Theorem* 3*. Assume also that* $\mathbf{F} \in L_2((0,T); W_2^1(\Omega))$*,* $\mathbf{G} \in L_1((0,T); W_2^2(\Omega))$*,* $\mathbf{G}$ *equal to zero in a neighborhood of* $\partial\Omega$*. Then the solution of* (4)–(7), (8) *exists and is unique for some* $T > 0$*.*

Mixture of liquid crystals

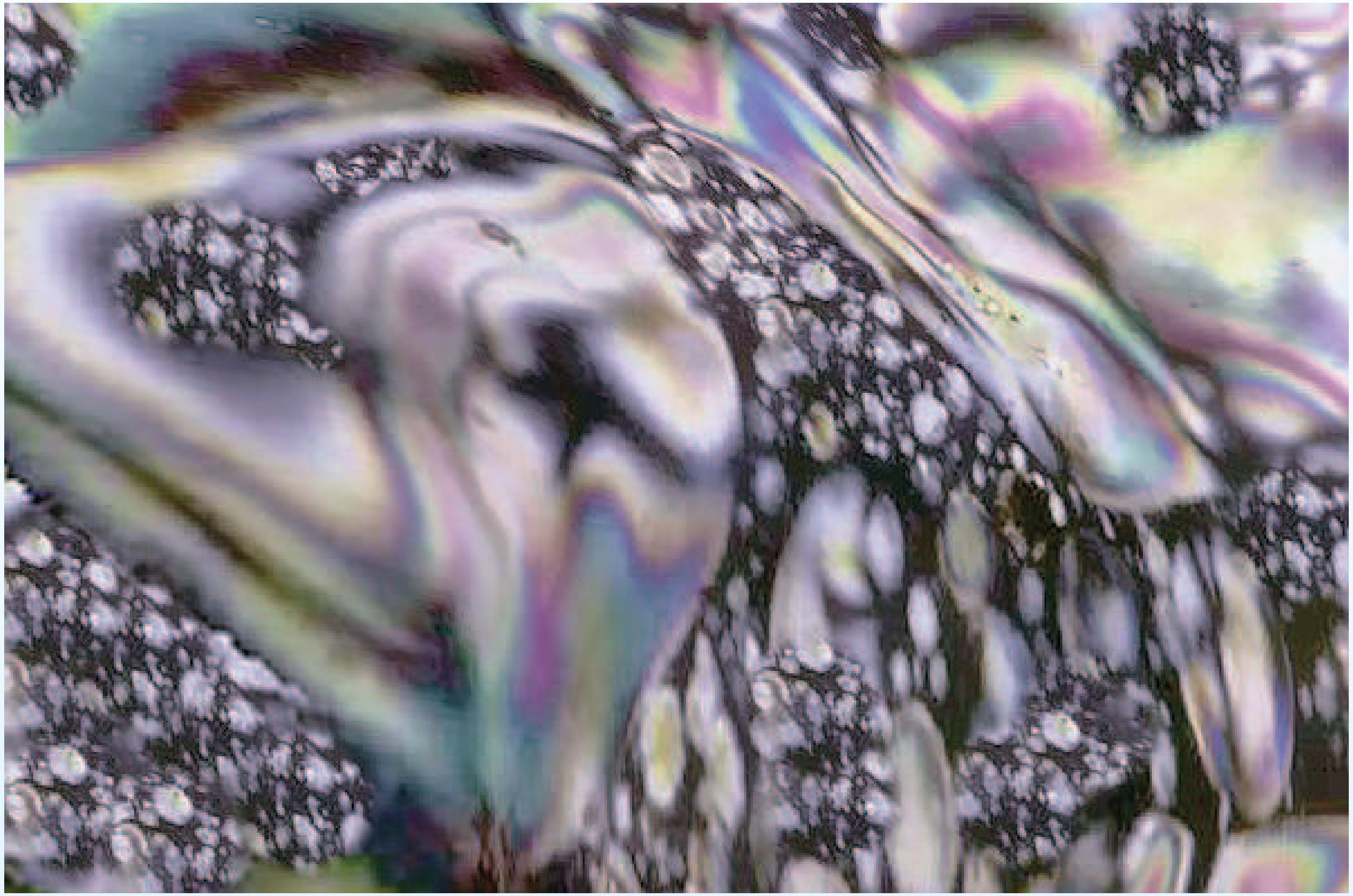

Figure 2: Liquid crystal with inhomogeneous microstructure.

Dynamics of nematic liquid crystals

Keeping the density in the equations and simplifying the system according to Lin and Liu, we have

$$\dot{\rho} = 0, \tag{9}$$

$$\rho\, \dot{u}_i = \sigma_{ji_{x_j}}, \quad \mathrm{div}\,\mathbf{u} = 0. \tag{10}$$

$$g_i + \pi_{ji_{x_j}} = 0 \tag{11}$$

with boundary and initial conditions

$$\mathbf{u}(x,t) = 0, \quad \mathbf{n}(x,t) = \mathfrak{n}_0(x) \quad \text{as } x \in \partial\Omega, \tag{12}$$

$$\mathbf{u}(x,0) = \mathfrak{u}_0(x), \quad \mathbf{n}(x,0) = \mathfrak{n}_0(x), \quad \rho(x,0) = \mathfrak{p}_0(x), \tag{13}$$

where

Dynamics of nematic liquid crystals

$$\sigma_{ij} = -p\delta_{ij} - \rho\frac{\partial\mathcal{F}}{\partial\mathbf{n}_{k x_j}} + \widehat{\sigma}_{ji}, \qquad \pi_{ij} = \beta_j\mathbf{n}_i + \frac{\partial\mathcal{F}}{\partial\mathbf{n}_{i x_j}},$$

$$g_i = \gamma\mathbf{n}_i - \beta_j\mathbf{n}_{i x_j} - \rho\frac{\partial\mathcal{F}}{\partial\mathbf{n}_i} + \widehat{g}_i, \qquad \widehat{g}_i = \lambda_1 N_i + \lambda_2\mathbf{n}_j A_{ji}, \tag{14}$$

$$\widehat{\sigma}_{ji} = \mu_1\mathbf{n}_k\mathbf{n}_l A_{kl}\mathbf{n}_i\mathbf{n}_j + \mu_2\mathbf{n}_j N_i + \mu_3\mathbf{n}_i N_j + \mu_4 A_{ij} + \mu_5\mathbf{n}_j\mathbf{n}_k A_{ki} + \mu_6\mathbf{n}_i\mathbf{n}_k A_{kj}, \tag{15}$$

here

$$\lambda_1 = \mu_2 - \mu_3, \quad \lambda_2 = \mu_5 - \mu_6 = -\mu_2 - \mu_3,$$

$$N_i = \dot{\mathbf{n}}_i + \omega_{ki}\mathbf{n}_k,$$

$$N_{ij} = \dot{\mathbf{n}}_{i x_j} + \omega_{ki}\mathbf{n}_{k x_j}$$

$$2A_{ij} = \mathbf{u}_{i x_j} + \mathbf{u}_{j x_i}, \quad 2\omega_{ij} = \mathbf{u}_{i x_j} - \mathbf{u}_{j x_i}.$$

For this system we prove the existence and the uniqueness theorems for week solutions following Lions.

Dynamics of nematic liquid crystals

Here and throughout

$$\lambda_1 < 0, \quad \mu_1 > 0, \quad \mu_4 > 0, \quad \mu_5 + \mu_6 > 0, \quad (-\lambda_1)^{\frac{1}{2}} (\mu_5 + \mu_6)^{\frac{1}{2}} > \lambda_2. \qquad (16)$$

Definition 3. *The triple* $(\rho, \mathbf{u}, \mathbf{n})$ *is called a weak solution to problem* (9)—(11), (12), (13)*, where*

- *the vector* $\mathbf{u} \in L_2((0,T); Sol_2^1(\Omega)) \cap L_\infty((0,T); Sol_2(\Omega))$,
- *the vector* $\mathbf{n} \in L_2((0,T); W_2^2(\Omega)) \cap L_\infty((0,T); W_2^1(\Omega))$,
- *the vector* $\omega \in L_2(Q_T)$,
- $\rho \in L_\infty(Q_T)$,

if

1) functions $(\rho, \mathbf{u}, \mathbf{n})$ *satisfy initial and boundary conditions* (12), (13)*,*

2) relation (11) *holds almost everywhere,*

3) relation (9) *holds as a relation for functionals on* $L_2((0,T), W_2^1(\Omega))$*,*

4) equation (10) *reads as the integral identity*

$$\int\limits_{Q_T} (\rho \mathbf{u}_{i\,t} \phi_i + \rho \mathbf{u}_j \mathbf{u}_i \phi_{i\,x_j})\, dxdt + \int\limits_{\Omega} \mathfrak{p}_0 \mathfrak{u}_{0i} \phi_i \, dx\Big|_{t=0}^{t=T} = \int\limits_{Q_T} \sigma_{ij} \phi_{i\,x_j}\, dxdt, \qquad (17)$$

for any $\overrightarrow{\phi} \in Sol(Q_T)$*.*

Dynamics of nematic liquid crystals

- If $\lambda_2 = 0$, the system satisfies the maximum principle, i.e., if $|\mathbf{n}_0| \leq 1$ on the boundary, then $|\mathbf{n}| \leq 1$ in the domain and all the integrals in identity (17) are finite.

Dynamics of nematic liquid crystals

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- In general case $\mathbf{n} \in L_2((0,T); W_2^2(\Omega)) \cap L_\infty((0,T); W_2^1(\Omega))$ leads to $\mathbf{n} \in L_8(Q_T)$, that guarantee the existence of the integrals.

Dynamics of nematic liquid crystals

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Dynamics of nematic liquid crystals

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- The initial conditions hold true since ρ_t, $\mathbf{u}_t$, $\mathbf{n}_t$ are elements of the space $L_2((0,T); H^{-1}(\Omega))$.
- The boundary conditions are fulfilled in the sense of the traces.

Liquid crystals with inhomogeneous microstructure

Consider the case of rapidly oscillating $\mathfrak{p}_\varepsilon(x)$ and define the solutions $(\rho^\varepsilon, \mathbf{u}^\varepsilon, \mathbf{n}^\varepsilon)$ for each $\mathfrak{p}_\varepsilon(x)$, which satisfies

$$\mathbf{u}^\varepsilon(x,0) = \mathfrak{u}_0(x), \quad \mathbf{n}^\varepsilon(x,0) = \mathfrak{n}_0(x), \quad \rho^\varepsilon(x,0) = \mathfrak{p}_\varepsilon(x). \tag{18}$$

We study the asymptotic behavior of solutions as $\varepsilon \to 0$.

1. family $\mathfrak{p}_\varepsilon$ is uniformly bounded and $\mathfrak{p}_\varepsilon > K_0$ for $\varepsilon > 0$;
2. there exists the limit function $\mathfrak{p}_0 \in L_\infty(\Omega)$, such that

$$\mathfrak{p}_\varepsilon \overset{*}{\rightharpoonup} \mathfrak{p}_0 \quad *\text{-weakly in } L_\infty(\Omega).$$

We construct the homogenized problem and prove the respective convergence of solutions.

Liquid crystals with inhomogeneous microstructure

Remark 1. *The simplest example is*

$$\mathfrak{p}_\varepsilon(x) = \mathfrak{p}\left(\frac{x}{\varepsilon}\right),$$

where $\mathfrak{p}$ *is 1-periodic Lipschitz function. In this case*

$$\mathfrak{p}_0 = \int_{[0,1]^3} \mathfrak{p}(\xi) d\xi.$$

For random case we have the mathematical expectation (or due to the regularity and the Birkhoff theorem the spacial mean).

Theorem 5. *Assume that*

$$\mathfrak{u}_0 \in Sol_2(\Omega), \quad \mathfrak{n}_0 \in W_2^1(\Omega), \quad \mathfrak{n}_0\big|_{\partial\Omega} \in H^{\frac{3}{2}}(\partial\Omega),$$

the family $\mathfrak{p}_\varepsilon$ *satisfies* 1—3*, and the constants* μ_i *are such that* (16) *holds. Moreover let limit problem have a unique solution.*

Then the family of weak solutions $(\rho^\varepsilon, \mathbf{u}^\varepsilon, \mathbf{n}^\varepsilon)$ *to problem* (9)—(11), (18) *converge to solutions* $(\rho^0, \mathbf{u}^0, \mathbf{n}^0)$ *to problem* (9)—(13) *in the following sense:*

$$\begin{aligned}
&\mathbf{u}^\varepsilon \rightharpoonup \mathbf{u^0} && \text{weakly in } L_2((0,T); W_2^1(\Omega)),\\
&\mathbf{n}^\varepsilon \rightharpoonup \mathbf{n^0} && \text{weakly in } L_2((0,T); W_2^2(\Omega)),\\
&\rho^\varepsilon \overset{*}{\rightharpoonup} \rho^0 && \text{*-weakly in } L_\infty(Q_T),\\
&\mathbf{u}^\varepsilon \to \mathbf{u^0} && \text{strongly in } L_3(Q_T),\\
&\mathbf{n}^\varepsilon \to \mathbf{n^0} && \text{strongly in } L_{8-\delta}(Q_T), \delta > 0.
\end{aligned} \tag{19}$$

Dynamic of smectics

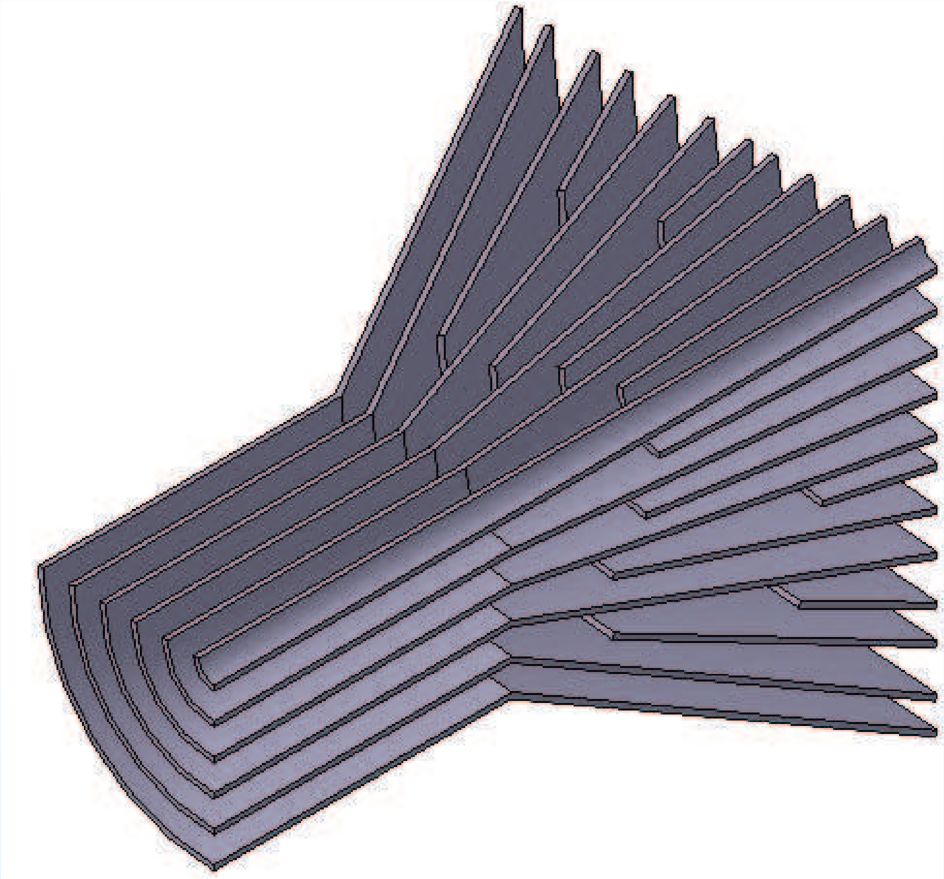

Figure 3: Smectic bifurcation.

Thank you for your attention!