Rotational Diffusion and Viscosity of Liquid Crystals

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Today:

- Summary of the continuum Leslie-Ericksen approach to nematic viscosity: symmetry and basic physical features
- Building the Microscopic theory of continuum linear response: general principles and available options
- Part 1 – Mean-field Microscopic Stress Tensor, from first principles, examine rod-like and disk-like limiting cases
- Part 2 – Kinetic theory of rotational diffusion:
  a) from stochastic Langevin to kinetic Fokker-Planck formulation
  b) eliminating fast variables (velocities) – Smoluchovski equation
  c) equilibrium case – spectrum of rotational relaxation modes
- Part 3 – Solving non-equilibrium kinetic equation:
  a) the “Doi trick”
  b) antisymmetric stress tensor
- Final steps: Leslie coefficients – limits of rod- & disk-like nematic; smectic; experiment
- The missing link: translational part of viscosity...
Leslie-Ericksen continuum

Balance of local forces (stress) and local torques (nematic):

\[
\frac{\delta (L)}{\delta (u)} - \frac{\delta (T\dot{S})}{\delta (\dot{u})} = 0
\]

\[
\frac{\delta (L)}{\delta (n)} - \frac{\delta (T\dot{S})}{\delta (\dot{n})} = 0
\]

Lagrangian

\[
L = \int dx \left( \frac{1}{2} \rho \dot{u}^2 - F[n, \nabla n, u, E] \right)
\]

Entropy production

\[
T\dot{S} = \int dx (R[n, \dot{u}])
\]

Potential energy:
- Frank elasticity
- Order-parameter expansion
- Smectic (n-layer coupling)
- Gels (n-elastic matrix coupling)

Dissipation function: friction arising from relative motion of fluid and internal variable \(n\)
(Q: symmetry criteria?.. A: assign a dissipation to each principal deformation mode)

Linear nematic viscosity (Leslie-Ericksen): strain rates + \(n\)-rotation rates

\[
R = A_1 (n \cdot \dot{\varepsilon} \cdot n)^2 + 2A_4 [n \times \dot{\varepsilon} \times n]^2 + 4A_5 ([n \times \varepsilon] \cdot n)^2
\]

\[
+ \frac{1}{2} \gamma_1 \left( \frac{d}{dt} [n \times (\Omega - \omega)] \right)^2 + \gamma_2 (n \cdot \varepsilon \cdot \frac{d}{dt} [n \times (\Omega - \omega)])
\]

Here:
\[
\dot{\varepsilon} = \frac{1}{2} (\nabla \dot{u} + \nabla \dot{u}^T) \equiv D
\]
\[
\Omega = \frac{1}{2} \text{curl} \ \dot{u} \Leftrightarrow W
\]
Relative to \(\omega = [n \times \delta n]\)
Symmetry: 3 flow geometries

Viscous flow:

\[ R = A_1 (n \cdot \varepsilon \cdot n)^2 + 2A_4 [n \times \varepsilon \times n]^2 + 4A_5 ([n \times \varepsilon] \cdot n)^2 + \frac{1}{2} \gamma_1 (\frac{d}{dt} [n \times (\Omega - \omega)])^2 + \gamma_2 (n \cdot \varepsilon \cdot \frac{d}{dt} [n \times (\Omega - \omega)]) \]

Elastic deformation:

\[ F = C_1 (n \cdot \varepsilon \cdot n)^2 + 2C_4 [n \times \varepsilon \times n]^2 + 4C_5 ([n \times \varepsilon] \cdot n)^2 + \frac{1}{2} D_1 [n \times (\Omega - \omega)]^2 + D_2 (n \cdot \varepsilon \cdot [n \times (\Omega - \omega)]) \]

\[ A_1 = \frac{1}{2} (\alpha_1 + \alpha_4 + \alpha_5 + \alpha_6) \]

\[ A_4 = \frac{1}{4} \alpha_4 \]

\[ A_5 = \frac{1}{8} (2\alpha_4 + \alpha_5 + \alpha_6) \]
Anisotropic continuum with linear friction

Viscous flow:

\[ R = A_1 (n \cdot D \cdot n)^2 + 2A_4 [n \times D \times n]^2 + 4A_5 ([n \times D] \cdot n)^2 + \frac{1}{2} \gamma_1 (\frac{d}{dt} [n \times (\Omega - \omega)])^2 + \gamma_2 (n \cdot D \cdot \frac{d}{dt} [n \times (\Omega - \omega)]) \]

Frank elasticity:

\[ F = \frac{1}{2} K (\nabla n)^2 \]

Penalises local torques... balanced by boundaries or by viscous torques (antisymmetric visc. stress)

Balance of forces:

\[ \rho \dot{u} + \rho (u \cdot \nabla)u = \nabla \cdot [\sigma_{\text{visc}} + \sigma_{\text{elast}}] \]

Balance of torques:

\[ I \frac{d}{dt} [n \times \dot{n}] = K \nabla^2 n - \gamma_1 \frac{d}{dt} [n \times (O - \omega)] + \gamma_2 (n \cdot D) \]

Assuming \( \gamma_1 \sim \gamma_2 \), non-dimensional number:

\[ E_{\text{Fr}} = \frac{\gamma (\nabla v)}{K (\nabla^2 n)} \sim \frac{\gamma L v}{K} \gg 1 \]

Improvements

- \( Q_{ij} \) theory (Sonnet & Virga)
- Flow with \( n \)-gradients
- Compressible medium (acoustics)
- Non-Newtonian (beyond \( G^* = C + i \omega A \))
Microscopic Theory of Viscosity

**General scheme:**
1) Determine the **Microscopic Stress tensor**, $\sigma^M$, from local molecular dynamics
2) Identify the kinetic (Fokker-Planck) equation for ensemble in flow
3) Solve is to find the (non-equilibrium) molecular distribution function
4) The answer:
   Macroscopic (continuum) stress tensor $\sigma = \int s^M(\Theta) P(\Theta, \nabla \nu) d\Theta \Rightarrow [\alpha] \nabla \nu$

**Bits of history:**
- 1975-1982 Diogo-Martins
- 1978 Tsebers
- 1982 Marucci
- 1980-1983 Kuzuu-Doi
- 1989-1991 Osipov-Terentjev
- 1990-1995 S.T. Wu (expt)
Microscopic Stress tensor

"Number" density
\[ \rho(x) = \sum_\alpha \delta(x - \mathbf{r}_\alpha) \]

Momentum (rigid body rotation)
\[ \mathbf{p}(x) = \sum_\alpha \sum_{\beta} m_\beta (\mathbf{v}_\alpha + ?_\alpha \times \mathbf{r}_{\alpha\beta}) \delta(x - \mathbf{r}_\alpha - \mathbf{r}_{\alpha\beta}) \]

\[ \frac{d\mathbf{p}(x)}{dt} = -\nabla \cdot \mathbf{S}^M \]

…evaluating the \( t \)-derivative
\[ \dot{\mathbf{p}}(x) = \sum_\alpha \sum_{\beta} m_\beta [\dot{\mathbf{v}}_\alpha + ?_\alpha \times \dot{\mathbf{r}}_{\alpha\beta} + ?_\alpha \times \mathbf{r}_{\alpha\beta}] \delta(x - \mathbf{r}_\alpha - \mathbf{r}_{\alpha\beta}) - m_\beta [\mathbf{v}_\alpha + ?_\alpha \times \mathbf{r}_{\alpha\beta}] (\dot{\mathbf{r}}_{\alpha} + \dot{\mathbf{r}}_{\alpha\beta}) \cdot \nabla \delta(x - \mathbf{r}_\alpha - \mathbf{r}_{\alpha\beta}) \]

…formally expanding in powers of \( \mathbf{r}_{\alpha\beta} \)
\[ \delta(x - \mathbf{r}_\alpha - \mathbf{r}_{\alpha\beta}) = \delta(x - \mathbf{r}_\alpha - \mathbf{r}_{\alpha\beta}) \cdot \nabla_x \delta(x - \mathbf{r}_\alpha) + O(\mathbf{r}_{\alpha\beta}, \nabla^2) \]

…we obtain the translational and the orientational parts of \( \mathbf{S}^M \):
\[ \mathbf{S}^M = \sum_\alpha m [\mathbf{v}_\alpha \mathbf{v}_\alpha] \delta(x - \mathbf{r}_\alpha) - \frac{1}{2} \sum_{\alpha \neq \alpha'} [\mathbf{r}_{\alpha\alpha'} F_{\alpha\alpha'}] \delta(x - \mathbf{r}_\alpha) \]
\[ + \sum_\alpha [\mathbf{I} \omega^2 - \mathbf{?} (\mathbf{I} \times \mathbf{?}) - \mathbf{?} \times \mathbf{I} \times \mathbf{?} - \mathbf{I} \times (\mathbf{I}^{-1} \cdot \mathbf{G}) - \mathbf{\times} (\mathbf{I}^{-1} \cdot \mathbf{G}) \mathbf{\frac{1}{2} Tr} (\mathbf{I})] \delta(x - \mathbf{r}_\alpha) \]
Uniaxial particles; Uniaxial mean-field

\[ I_{ik} = I_\perp \delta_{ik} + (I_\parallel - I_\perp) a_i a_k \]

Also: the torque

\[ G_i(r_\alpha) = -\varepsilon_{ijk} a_j \frac{\partial}{\partial a_k} \sum_{\alpha \neq \alpha} U(r_\alpha - r_\alpha, a_\alpha, a_\alpha) \]

Finally (only orientational part):

\[ s^M = \sum_\alpha \left[ \frac{p^2 - 1}{p^2 + 1} I_\perp (? \times a \otimes ? \times a + ? a (? \cdot a) - \omega^2 a a) \right] \Rightarrow \sum_\alpha 3k_B T \frac{p^2 - 1}{p^2 + 1} (aa - \frac{1}{3} d) \delta (x - r_\alpha) \]

Averaging over (fast) angular velocity distribution gives the “kinetic” part of \( \sigma^M \) (which is the momentum flux due to motion of molecules, in contrast to the “potential” part of \( \sigma^M \) representing the flux due to intermolecular forces.

In a dilute gas, e.g. a solution of rod-polymers, the kinetic part, \( \sigma^M = \Sigma 3k_B T (aa - 1/3) \), is the main contribution; but in a dense molecular liquid - the potential part is dominant.

Ellipsoid: \( p = a/b \)

\[ I_\perp = \frac{1}{3} m(a^2 + b^2); \quad I_\parallel = \frac{2}{3} mb^2 \]

Cylinder: \( p = a/b \)

\[ I_\perp = \frac{1}{12} m(a^2 + 3b^2); \quad I_\parallel = \frac{1}{2} mb^2 \]
Non-equilibrium distribution function

Mean-field kinetic theory

Full Fokker-Planck description with sources (velocity gradients) is reduced due to two-step relaxation feature: the distribution of velocities relays much faster to the Maxwell-like form with the mean

\[ O = \frac{1}{2} \frac{p^2 - 1}{p^2 + 1} (a \times D \cdot a) + \frac{1}{2} \text{curl} \nu - \frac{1}{2} (a \cdot \text{curl} \nu) a \]

Separation of time scales is assured:

\[ \alpha = \frac{\tau_\omega}{\tau_a} = \frac{k_B T I_\perp}{\gamma^2} \ll 1 \quad D_{\text{rot}} = \frac{k_B T}{\gamma} \]

The reduced Smoluchowski equation (for pdf only dependent on coordinates) relaxes much slower to the steady state; dissipation and effective friction forces during this relaxation is the main source of viscous response in dense liquids.

\[ \partial_t P + \alpha \partial_a (OP) = \alpha^2 \partial_a \left( \partial_a P - \frac{G}{k_B T} P \right) \]

\[ + \alpha^2 \partial_a [(\Omega \cdot \partial_a) \partial_a P] + \alpha^2 \frac{I_{\parallel}}{I_{\perp}} \partial_a [(a \cdot \text{curl} \nu) (O \times a) P] \]

Equilibrium is, of course:

\[ P = e^{-\frac{U(a \cdot n)}{k_B T}} \]
From stochastic (Langevin) to kinetic (F-P)

Full angular velocity of uniaxial object: \( \dot{\omega} = \gamma \omega + \xi \quad \rightarrow \quad L = I_\parallel \dot{\omega} + I_\perp \dot{\omega} \)

Equation of (rotational) motion:
\[
\dot{L} = I_\parallel \dot{\omega} + I_\perp \ddot{\omega} = -\gamma (\omega + O) + G + \xi
\]

\[
\partial_t P(\omega, t) = \frac{\partial}{\partial \omega} (\dot{\omega} P) - \frac{\partial}{\partial \omega} (G) - \frac{\partial}{\partial \omega} (\dot{\omega} P) +
+ \frac{\partial^2}{\partial \omega \partial \omega} \left[ \frac{1}{I_\parallel} (\delta - aa) \cdot \langle \omega \omega \rangle (\delta - aa) P \right] + \frac{\partial^2}{\partial \omega^2} \left[ \frac{1}{I_\perp} a \cdot \langle \omega \omega \rangle \cdot a P \right]
\]

\[
\langle \omega \omega \rangle = 2\gamma_\perp k_B T \delta + 2(\gamma_\parallel - \gamma_\perp) k_B T \langle \omega \rangle
\]

Arrive at full F-P equation for rotational motion:
\[
\partial_t P + \partial_\omega G = \left( \frac{1}{I_\perp} \frac{\partial}{\partial \omega} \left[ (O - \omega) P + \frac{1}{2} k_B T \frac{\partial}{\partial \omega} (\delta - aa) P + \frac{1}{\gamma_\perp} (\omega \times a) P \right] + \frac{\gamma_\parallel}{I_\parallel} \left( \frac{\partial}{\partial \omega} \left[ \frac{1}{2} k_B T \frac{\partial}{\partial \omega} P \right] \right) \right)
\]
Eliminating fast variables

Integrating out ? and ?

1) Ignore the relaxation of ? (too fast):

Put in

\[ P = e^{-\frac{I_{||}}{2k_BT}(\frac{1}{2}a \cdot \text{curl})^2} \tilde{P}(a, ?, t) \]

and integrate over ?

\[
\begin{aligned}
\partial_t P + \partial_a (? P) + \frac{\partial}{\partial ?} ([\delta - aa] \frac{G}{I_\perp} P) &= \\
&= \gamma_\perp \frac{\partial}{\partial ?} \left[ (? - O)P + \frac{1}{2} \frac{k_BT}{I_\perp} \frac{\partial}{\partial ?} (\delta - aa)P + \frac{I_\parallel}{2\gamma_\perp} (a \cdot \text{curl})(? \times a)P \right]
\end{aligned}
\]

2) Ignore the relaxation of ? (faster than the coordinate a):

Naively:

\[ P = e^{-\frac{I_\perp}{2k_BT}(? - O)^2} \tilde{P}(a, t) \]

and integrate over ?

\[ \partial_t P = \partial_a (OP) \] (!)

Diffusive corrections to the coordinate-only kinetic equation arise from the last bits of non-relaxed Maxwell distribution:

\[ P = e^{-\frac{I_\perp}{2k_BT}(? - O)^2} \left[ \tilde{P}(a, t) + \left( \frac{\tau_o}{\tau_a} \right) Y(a, [? - O]) \right] \]

Substitute to F-P, only retain leading terms in \( \alpha \ll 1 \) and expand in powers of small deviation (\( \omega - \Omega \)), matching the terms of the same order gives \( Y(a, [\omega - \Omega]) \).

THEN integrate over ? …..
Solving the F-P equation

\[ \partial_t P + \alpha \partial_a (OP) = \alpha^2 \partial_a (\partial_a P - \frac{1}{k_B T} [\partial_a U_{MF}] P) \]
\[ + \alpha^2 \sqrt{\frac{I \parallel}{I \perp}} \partial_a [(a \cdot \text{curl} v)(O \times a) P] + \alpha^2 \partial_a [(O \cdot \partial_a) O P] \]

\[ \Gamma = -\partial_a U_{MF}(a \cdot n) \]

Spectrum of rotational relaxation modes: eigenfunction expansion in equilibrium fluid

\[ \partial_t P = -\Lambda(a) P(a,t) \quad \rightarrow \quad P = w_0(a) + \sum_{n=1}^{\infty} c_n e^{\frac{-t}{\tau_n}} w_n(a) \]

Look for solutions in the form \( w_n(a) = f_n(\theta) w_0(a) \)

\[ \frac{1}{\sin \theta} e^{\frac{-U(\theta)}{k_B T}} \partial \left( e^{\frac{-U(\theta)}{k_B T}} \sin \theta \frac{\partial f_n}{\partial \theta} \right) = -\frac{1}{\alpha^2 \tau_n} f_n \]

 Gives self-consistent integral equation for \( w_n \)

\[ w_n(\theta) = e^{\frac{-U(\theta)}{k_B T}} \left[ C - \frac{1}{\alpha^2 \tau_n} \int_0^\theta \frac{1}{\sin x} e^{\frac{U(x)}{k_B T}} dx \int_0^x w_n(z) \sin z \, dz \right] \]

\[ U_{MF}(a \cdot n) = JS \sin^2 \theta \]
Equilibrium relaxation time(s)

Could only solve by expansion to leading order in the smallest non-zero eigenvalue \([1/\tau_1]\) (i.e. the longest relaxation time \(\tau_1\)):

\[
w_n(\theta) = w_0 + \left[ \frac{1}{\alpha_2 \tau_1} \right] w_1 + \left[ \frac{1}{\alpha_2 \tau_1} \right]^2 w_2 + ...
\]

\[
w_n(\theta) = e^{-\frac{U(\theta)}{k_B T}} \left[ 1 - \frac{1}{\alpha^2 \tau_1} \int_0^\theta \frac{1}{\sin x} e^{\frac{U(x)}{k_B T}} dx \int_0^x e^{-\frac{U(z)}{k_B T}} \sin z \, dz \right]
\]

Condition of periodicity states: \(w(\theta = \pi) = w(0) = \text{const} \) (of order 1 for normalized \(w\) ) gives:

\[
\frac{1}{\alpha^2 \tau_1} \int_0^\pi \frac{1}{\sin x} e^{\frac{U(x)}{k_B T}} dx \int_0^x e^{-\frac{U(z)}{k_B T}} \sin z \, dz \approx 1
\]

The longest relaxation time [of diffusion over the orientational barrier \(U(\theta)\) ]:

\[
U_{MF} = JS \sin^2 \theta
\]

\[
S \to 0 \quad \tau_1 \approx \frac{\gamma}{k_B T} \left( 1 + \frac{JS}{k_B T} + ... \right)
\]

\[
S \to 1 \quad \tau_1 \approx \frac{\gamma}{k_B T} \left( \frac{k_B T}{JS} \right)^{3/2} e^{\frac{JS}{k_B T}}
\]

Felderhof, and many others... (1989-now)
Solving the non-equilibrium F-P eq.

In order to calculate the ensemble average of microscopic stress tensor $\sigma^M$ in a system with flow gradients, we need to find the correction to equilibrium pdf $P(a,\omega,t)$

$$\Rightarrow \sum_\alpha 3k_BT\left\langle (aa - \frac{1}{3}d) \delta(x - r_\alpha) \right\rangle_{eq.} = \text{const \{pressure\}}$$

$$\Rightarrow \sum_\alpha \left\langle a \partial_a U(a \cdot n) \delta(x - r_\alpha) \right\rangle_{eq.} = 0 \{\text{symmetry}\}$$

$$\partial_t P + \alpha \partial_a (OP) = \alpha^2 \partial_a (\partial_a P - \frac{1}{k_BT}[\partial_a U_{MF}]P)$$

It turns out that there is no need to average the symmetric part of $\sigma^M$ (there is a “trick” allowing its direct evaluation). To average the antisymmetric part, describing the torques, we may only consider the $t$-dependent rotation of $n$ (without any $\Omega \sim \nabla v$).

**Symmetric part of $\langle \sigma^M \rangle$:**

$$<S^M>_{\text{sym}} = \rho \frac{p^2 - 1}{p^2 + 1} \left( 3k_BT(aa - \frac{1}{3}d) + \frac{1}{2} \left( a \frac{\partial U}{\partial a} + \frac{\partial U}{\partial a} a - 2aaa \cdot \frac{\partial U}{\partial a} \right) \right) \bar{P}(a,t)$$

**L.H.S.**

$$\Rightarrow \frac{\partial}{\partial t} \langle aa - \frac{1}{3}d \rangle + \frac{p^2 - 1}{p^2 + 1} \left[ 2D : \langle aaa \rangle - D \cdot \langle aa \rangle - \langle aa \rangle \cdot D \right] - \frac{1}{2} [W \cdot \langle aa \rangle - \langle aa \rangle \cdot W]$$

$$\Rightarrow <\sigma^M>_{\text{sym}} = -\frac{\rho k_BT}{\alpha^2} \frac{p^2 - 1}{p^2 + 1} \left[ \frac{\partial}{\partial t} Q - G(\nabla v;\langle aa \rangle;\langle aaaa \rangle) \right]$$
Solving the non-equilibrium F-P eq.

\[ \partial_t P + \alpha \partial_a (OP) = \alpha^2 \partial_a (\partial_a P - \frac{1}{k_B T} [\partial_a U_{MF}] P) \]

\[ 0 = \alpha^2 \partial_a (\partial_a P_{eq} - \frac{1}{k_B T} [\partial_a U_{MF}] P_{eq}) \]

To average the antisymmetric part of \( \sigma^M \), describing the torques, we may only consider the \( t \)-dependent rotation of \( n \) (without any \( \Omega \sim \nabla v \)).

\[ \partial^2_a Y - \frac{1}{k_B T} [\partial_a U] \partial_a Y = \frac{3JS}{\alpha^2 k_B T} (a \cdot n)(a \cdot \dot{n})[1+Y] \]

Using the fact that \((n \cdot \dot{a})\) is negligibly small.

Thus find

\[ Y \approx -\frac{\gamma}{k_B T} \frac{(JS / k_B T)}{2 + (JS / k_B T)} (a \cdot n)(a \cdot \dot{n}) \]

And the average

\[ \langle \sigma^M \rangle_{\text{antisym}} = \frac{1}{2} \rho \int (a \partial_a U - \partial_a U \cdot a) e^{-U/k_B T} Y da \]

\[ \approx \frac{1}{70} \rho \gamma \frac{(JS / k_B T)^2}{2 + (JS / k_B T)} (7 + 5S - 12S_4) [\hat{n}\hat{n} - \hat{m}\hat{m}] \]
Leslie coefficients, and consequences

\[ \alpha_1 = -\rho \gamma \left( \frac{p^2 - 1}{p^2 + 1} \right)^2 S_4 \]
\[ \alpha_2 = -\frac{1}{2} \rho \gamma \left( \frac{p^2 - 1}{p^2 + 1} \right) S + g_1 \]
\[ \alpha_3 = -\frac{1}{2} \rho \gamma \left( \frac{p^2 - 1}{p^2 + 1} \right) S - g_1 \]
\[ \alpha_4 = -\frac{1}{35} \rho \gamma \left( \frac{p^2 - 1}{p^2 + 1} \right)^2 \left( 7 - 5S - 2S_4 \right) \]
\[ \alpha_5 = \frac{1}{2} \rho \gamma \left( \frac{p^2 - 1}{p^2 + 1} \right) \left[ S + \frac{1}{7} \left( \frac{p^2 - 1}{p^2 + 1} \right) (3S + 4S_4) \right] \]
\[ \alpha_6 = \frac{1}{2} \rho \gamma \left( \frac{p^2 - 1}{p^2 + 1} \right) \left[ -S + \frac{1}{7} \left( \frac{p^2 - 1}{p^2 + 1} \right) (3S + 4S_4) \right] \]

Torque balance not always possible: director rotation vs. tumbling

\[ \tan \theta = \sqrt{\frac{\alpha_3}{\alpha_2}} = \sqrt{\frac{(\ldots p \ldots) - g_1}{(\ldots p \ldots) + g_1}} \]

Rods (\( p \gg 1 \)) give \( \tan \theta \sim 1; \quad \theta \sim 45^\circ \)

Disks (\( p \ll 1 \)) suggest \( \tan \theta \gg 1; \quad \theta \sim 90^\circ \)
Conclusions

- First-principle derivation of the microscopic stress tensor
- Derivation of full F-P equation allows any level of accuracy, as long as the corresponding HD problem is resolved
- Separation of time scales gives the relevant (Smoluchowski) equation, with the hierarchy of sources in powers of $\alpha = (\tau_w / \tau_a) << 1$
- Leslie coefficients expressed either as an expansion in powers of $\{S\}$, or as Arrhenius-style activation exponentials $\{\exp -D/kT\}$

- What about inhomogeneous particle density $\rho(x) = \Sigma \delta(r_\alpha - x)$ (i.e. in mixtures)?
- How to solve for the full spectrum of relaxation modes (including $\theta-\phi$ coupling)?
- Non-axisymmetric particles (the derivation depends on general $I_{ik}$)?
- Non-axisymmetric mean-field $U(a \cdot n)$ (e.g. biaxial phases, or smectics)?
- Could one re-formulate the whole theory in terms of Q-tensor?
- Moving away from the mean-field approximation (pair correlation functions)?

The translational part of viscous coefficients, giving a part of $\alpha_4$ (and all of the residual isotropic viscosity!..) is a totally different story...
Thank you