Scaling behavior of kinetic orientational distributions for dilute nematic polymers in weak shear

M. Gregory Forest\textsuperscript{a}, Ruhai Zhou\textsuperscript{a}, Qi Wang\textsuperscript{b}

\textsuperscript{a} Department of Mathematics, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA
\textsuperscript{b} Department of Mathematical Sciences, Florida State University, Tallahassee, FL 32306, USA

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Abstract


1. Introduction

A classical benchmark of continuum, mesoscopic, and molecular theory for nematic polymers is the ability to predict conditions under which monodomain flow-alignment occurs (cf. [24,25]), the resultant most probable direction of alignment (the “major director”), the relative focusing or spreading of the orientational distribution (the order parameters), and to parametrize these properties in terms of model parameters. As one passes down from coarser to finer scale models, the ability to do explicit analysis is compromised. Leslie–Ericksen (L–E) continuum theory [1,2] gives explicit in-plane alignment condition and Leslie angle formula, which depend only on Miesowicz viscosities, independent of shear rate, without information on the spread of the orientational distribution. These results apply only to strongly nematic, small-molecular-weight liquids (liquid crystals), so that continuum theory gives no information for dilute concentrations of nematic polymers; indeed, there is no concentration parameter in the theory.

Quiescent nematic polymers have multiple stable phases (isotropic in the dilute regime, nematic at high concentrations, with bistability in an overlap regime). When shear flow is imposed, steady alignment sometimes occurs, and it is a challenge of mesoscopic or kinetic theory to predict a most probable alignment angle in terms of model parameters, and to ascertain whether the distribution is steady or oscillatory. This analog of the Leslie alignment angle is known to vary with shear rate and concentration, and there is ample theoretical evidence for strong dependence on molecular aspect ratio at nematic concentrations [7,10,18,19]. Mesoscopic models describe shear-aligned steady states, but explicit formulas are only available in the weak shear limit [12–19]. In this limit, the authors derived the Leslie angle dependence upon molecular aspect ratio and concentration, whereas shear rate dependence requires higher order asymptotic analysis [19] or direct numerical simulation [18,19]. Furthermore, the Leslie angle of stable states varies abruptly for dilute versus concentrated nematics, as expected since the flow-aligned solution branches arise from two distinct quiescent states (the isotropic and the nematic).

In kinetic theory, exact expressions for the orientational probability distribution function in shear flow are not yet available, although several useful and illustrating approximations have been derived [3,4,6,7,9–11,21,23]. The utility of explicit formulas lies in their prediction of how molecular alignment features scale with properties of the nematic polymer and flow. The difficulty in gaining explicit formulas is not surprising, with very little analytical progress since the seminal paper of Onsager [20] and the above references. New insights, Constantin et al. [26], appear to be emerging. Marrucci and Maffettone [22] finessed the problem by restricting to two dimensions and made remarkable progress, especially in the explanation of negative normal stress differences. Numerical simulations [27–29] show that shear-perturbed nematic equilibria have significant high-order spherical harmonic amplitudes, and there is no natural known classical distribution that resolves the numerical results. Furthermore, all
nematic equilibria are orientationally degenerate [8,20,29,30], so their perturbed properties are inherently complex; the breakup and persistence of the orthogonal group of nematic equilibria has only succumbed to partial analysis in mesoscopic models [19].

By comparison, the isotropic branch is trivial (constant) for kinetic theory as well as mesoscopic theory, so one might expect to be able to carry out a weak-shear asymptotic analysis for this shear-deformed isotropic branch. Such an analysis is relevant experimentally only in the dilute regime below the “clearing transition”, where quiescent nematic polymers are isotropic (except for a short interval of bi-stability). Imposed shear flows in the isotropic concentration range are known to induce weak birefringence (cf. [22]), with peaks in the orientational distribution focused in the shear plane, at the Leslie alignment angle, as predicted from essentially all mesoscopic models [18,19]. See et al. [23] developed a singular perturbation analysis in the weak flow limit, centered at the isotropic transition, in order to show that flow perturbations shift the instability of the isotropic state to lower concentrations.

Our goal in this paper is to establish analytical scaling properties of the perturbed isotropic branch directly from kinetic theory in the weak shear limit, and to give explicit formulas for the alignment angle, degrees of alignment, and normal and shear stresses, parametrized in terms of molecular parameters and normalized shear rate. Our analysis is complementary to See et al. [23], in that it applies everywhere except in a neighborhood of the isotropic transition. To complete the flow-perturbed analysis of isotropic equilibria for all concentrations, we show how to connect the regular expansion away from the isotropic transition to the singular expansion employed in [23]. We show, for example, that the isotropic instability corresponds to a fifth-order degeneracy in the marginal stability condition for the linearized Smoluchowski equation. This degeneracy (with a multiplicity five linearized eigenvalue) occurs for all concentrations, and we show the eigenfunctions are precisely the second-moment tensor basis. From this analytical structure, we show how the quiescent, highly degenerate, isotropic bifurcation point splits, separated by a gap with no persistent isotropic states, into a pair of saddle-nodes, or turning points. The See et al. [23] bifurcation curve is the “left” turning point, marking the onset of instability of the shear-perturbed isotropic branch at lower concentrations than the quiescent values. The right turning point marks the continuation of unstable isotropic equilibria in shear.

We employ the Doi kinetic theory, extended to include a finite aspect ratio of spheroidal molecules [5]; we then develop a weak-shear asymptotic expansion of the probability distribution function (f) by an extension of the seminal methods of Kuzuu and Doi [3,4] and See et al. [23]. At leading order, the quiescent equilibrium distribution functions consist of: the isotropic state (f = 1/(4π)) for all concentrations N (dimensionless), which is stable only for 0 < N < N_c = 5; and, a pair of nematic equilibria above a critical concentration N_1 ≈ 4.49. For the quiescent nematic equilibria [20], weak shear asymptotic corrections are thus far inaccessible to our analysis. We are nonetheless motivated by the approximations predicted by Semenov [21], Stepanov [31], Archer and Larson [7] and Kroger and Sellers [10] for the shear-aligned nematic steady state, which provide an expression for the Leslie tumbling parameter, λ,

$$\lambda = a \frac{5P_2 + 16P_4 + 14}{35P_2},$$

where $a = (r^2 - 1)/(r^2 + 1)$, r is the molecular aspect ratio, and $P_2, P_4$ are equilibrium values of the second and fourth moments of the PDF f, given in terms of Legendre polynomials. The Leslie alignment angle $\phi$ for flow-aligning nematics is then given by

$$\cos(2\phi) = \lambda^{-1}.$$
which takes the same form in mesoscopic tensor analysis [12–19]. (As we shall confirm below, the kinetic theory analog of the Leslie tumbling parameter for the isotropic branch in weak shear is a “flow-aligning parameter”, since dilute concentrations of nematic polymers do not tumble at weak to moderate shear rates.) According to (1), flow-alignment occurs only when \( |\lambda| \geq 1 \). The moments \( P_{2,4} \) are concentration-dependent, and can be computed numerically as functions of \( N \); therefore if \( |a| = 1 \), the Leslie angle and unsteady transition can be tabulated versus \( N \). The molecular geometry parameter \( a \) lies between \( a = -1 \) for infinitely thin discs, \( a = 0 \) for spherical molecules, and \( a = +1 \) for infinitely thin rods; \( |a| \) decreases monotonically from 1 to 0 from extreme aspect ratios to the spherical molecule limit. From (1), as noted by Archer and Larson, the effect of reducing the aspect ratio, e.g. from \( a = 1 \) to \( a = 0.8 (r = 3) \), can be quite significant. If the infinite aspect ratio nematic liquid is tumbling, lowering aspect ratio will only enhance tumbling, i.e., shorten the period. However, a flow-aligned infinite aspect ratio liquid is transformed by lowering aspect ratio to either reduce the Leslie angle downward (toward the flow axis) or cause a tumbling transition. This effect due to aspect ratio has been explored in [18] for a variety of mesoscopic closure approximations to the Doi theory, and in [19] from an analytical tensor method which yields precise curves \( N(a) \) along which the steady-unsteady transition occurs. These phenomena are specific to the nematic state in weak shear, and rigorous analysis only exists from mesoscopic tensor models in the weak shear limit, together with the elegant kinetic PDF treatments of Semenov [21] and Marrucci and Maffettone [22].

By focusing on the weak-shear continuation of the isotropic state, at low and high concentrations, we will derive explicit kinetic theory formulas of the form (1). Indeed, we will construct the stationary PDF, then its moments, and all average orientation properties become explicit. We thereby affirm the validity of such exact kinetic theory expressions.

Our regular asymptotic analysis is shown to become disordered where the isotropic state destabilizes, precisely the focus of the See et al. [23] analysis. Indeed, their formulas are sufficient to give the alignment properties of states on the bifurcation branch, although they did not choose to extract this information in their paper. To close the book on the deformation of isotropic equilibria in weak flows for all concentrations, we show how to deduce the See et al. [23] expansion in powers of \( Pe^{1/2} \), where \( Pe \) is the normalized shear rate. This scaling is equivalent to showing the quiescent bifurcation point of the isotropic instability splits into two turning points (two saddle-node bifurcations), separated by a gap in concentrations of \( O(Pe^{1/2}) \) around \( N = 5 \). Inside the gap the quiescent isotropic stationary distributions do not persist in weak shear. The right turning point and construction of the PDF for \( N > 5 + O(Pe^{1/2}) \) are given, corresponding to unstable, nearly isotropic persistent states, not believed to be physically realizable. We note, as a curiosity, that nearly isotropic monodomains of concentrated nematic polymers are transiently observed in numerical simulations of structure formation in shear cells [32,33], associated with local defects that mediate neighboring incompatible orientational patterns, as anticipated by Marrucci and Greco [30].

2. Kinetic theory for LCPs of spheroidal molecules

Let \( f(m, t) \) be the orientational probability distribution function for molecules with axis of symmetry \( m \) on the unit sphere \( S^2 \) in a linear flow field

\[
\mathbf{v} = (\Omega + D) \cdot \mathbf{x},
\]

where \( \Omega \) and \( D \) are the angular and linear deformation rates, respectively. The PDF equation for LCPs is given by

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = \mathcal{L} f,
\]

with \( \mathcal{L} \) the linearized tensor operator.

To close the book on the deformation of isotropic equilibria in weak flows for all concentrations, we show how to deduce the See et al. [23] expansion in powers of \( Pe^{1/2} \), where \( Pe \) is the normalized shear rate. This scaling is equivalent to showing the quiescent bifurcation point of the isotropic instability splits into two turning points (two saddle-node bifurcations), separated by a gap in concentrations of \( O(Pe^{1/2}) \) around \( N = 5 \). Inside the gap the quiescent isotropic stationary distributions do not persist in weak shear. The right turning point and construction of the PDF for \( N > 5 + O(Pe^{1/2}) \) are given, corresponding to unstable, nearly isotropic persistent states, not believed to be physically realizable. We note, as a curiosity, that nearly isotropic monodomains of concentrated nematic polymers are transiently observed in numerical simulations of structure formation in shear cells [32,33], associated with local defects that mediate neighboring incompatible orientational patterns, as anticipated by Marrucci and Greco [30].
where $\Omega$ and $D$ are vorticity and rate-of-strain tensors, respectively. The Smoluchowski (kinetic) equation for $f(m, t)$ is given by [5]

$$\frac{Df}{Dt} = R \cdot [D_r(m)(R f + \frac{1}{kT} f/RV)] - R \cdot [m \times m f],$$

$$m = \Omega \cdot m + a[D \cdot m - D : m m],$$

(4)

where $D_r(m)$ is the rotary diffusivity which we hold constant, $D_r(m) = D^0_r$, to make connection with [28,34]; $k$ is the Boltzmann constant; $T$ is the absolute temperature; $R = m \times (\partial/\partial m)$ is the rotational gradient operator; and $(D/Dt)(\cdot)$ denotes the material derivative $(\partial/\partial t)(\cdot) + v \cdot \nabla (\cdot)$. In (4), the second moment of $m$,

$$M = \langle mm \rangle = \int_{|m| \leq 1} mm f(m, t) \, dm,$$

(5)

enters through the mean-field Maier–Saupe excluded-volume potential $V$,

$$V = -\frac{3}{2}NkTmm : M.$$

(6)

The mesoscopic orientation tensor $Q$ is the traceless form of $M$, whose eigenvalues and eigenvectors provide the mesoscopic order parameters and directors:

$$Q = M - \frac{1}{3}I.$$

(7)

At issue here is the Smoluchowski kinetic equation for an imposed simple shear flow, given in Cartesian coordinates $(x, y, z)$ by

$$v = \dot{\gamma}(y, 0, 0),$$

(8)

where $\dot{\gamma}$ is the shear rate, assumed constant. The corresponding rate-of-strain $D$ and vorticity tensors $\Omega$ are:

$$D = \frac{1}{2} \dot{\gamma} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \Omega = \frac{1}{2} \dot{\gamma} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

(9)

We non-dimensionalize the velocity equation (3), (8) and kinetic equation (4) with respect to the relaxation timescale $\tau_0 = (D^0_r)^{-1}$, which introduces the fundamental flow parameter, the Peclet number,

$$Pe = \dot{\gamma}/D^0_r.$$

3. Important expansions

We employ spherical harmonic expansions [27,28] with the basis $Y^m_l(\theta, \phi)$, defined by

$$Y^m_l(\theta, \phi) = P^m_l(\cos \theta)e^{im\phi},$$

(10)

where $P^m_l(\cos \theta)$ are normalized Legendre polynomials. We now develop expansion formulas for the various terms in the Smoluchowski equation (4), which we will then combine to derive the weak shear construction of $f$. 
From (8), \( x \) is the flow direction, \( y \) is the direction of the velocity gradient, and \( z \) is the vorticity direction.

Because of the even parity of the distribution function \( f \), that is, \( f(-m) = f(m) \), only those spherical harmonics \( Y_l^m \) with even \( l \) are considered.

### 3.1. Maier–Saupe potential

For any integrable function \( g = g(m) \) on the unit sphere \( ||m|| = 1 \), define \( T_g \) as

\[
T_g = \langle mm \rangle_g
\]

with

\[
\langle mm \rangle_g = \int_{||m|| = 1} mm g(m) \, dm.
\]

Since \( mm \) is in the span of the first six spherical harmonics, by orthogonality

\[
\langle mm \rangle_{Y_l^m} = 0, \quad \text{for } l > 2.
\]

Therefore, after some calculation, one can write \( T_g \) as an expansion with only six terms:

\[
T_g = \frac{4\pi}{3} \langle Y_0^0 \rangle g Y_0^0 + \frac{8\pi}{15} \sum_{m=-2}^{2} (-1)^m \langle Y_{-m}^m \rangle g Y_m^m.
\]

From this expansion, by the orthogonality property of the harmonics,

\[
\begin{align*}
&T_{Y_0^0} = \frac{4\pi}{3} Y_0^0, \\
&T_{Y_m^m} = \frac{8\pi}{15} Y_m^m, \quad m = -2, -1, 0, 1, 2, \\
&T_{Y_l^m} = 0, \quad \text{otherwise.}
\end{align*}
\]

We note that \( T_g \) is a linear function of \( g \).

The Maier–Saupe potential for the distribution function \( f \) is then given by

\[
V_{MS} = -\frac{3}{2} kTN \langle mm \rangle = -\frac{3}{2} kTN \left( \frac{4\pi}{3} \langle Y_0^0 \rangle Y_0^0 + \frac{8\pi}{15} \sum_{m=-2}^{2} (-1)^m \langle Y_{-m}^m \rangle Y_m^m \right).
\]

### 3.2. Shear flow

The last term in (4) is the shear flow contribution, which can be written as

\[
\mathcal{R} \cdot (m \times f) = \frac{1}{2} \text{Pe} \left( -1 + a \cos 2\phi \frac{\partial f}{\partial \phi} + \frac{1}{2} a \sin 2\theta \sin 2\phi \frac{\partial f}{\partial \theta} \right) - \frac{3}{2} a \text{Pe} \left( \sin^3 \theta \sin 2\phi \right) f
\]

where the linear function \( G(f) \) can be expressed as

\[
G(f) = a \sqrt{\frac{8\pi}{15}} \left( \frac{1}{2} Y_1^1 - Y_2^{-1} \right) R_1 f + \frac{1}{2} (Y_1^1 + Y_2^{-1}) R_2 f + \frac{1}{2} (Y_2^1 + Y_2^{-1}) R_3 f
\]

\[
- \frac{3}{2} \sqrt{\frac{8\pi}{15}} \ln(Y_2^1 - Y_2^{-1}) f.
\]
\[ R_x, R_y \text{ and } R_z \] are three components of the operator \( R \) in Cartesian coordinates. Applied to the spherical harmonics, we have

\[ iG(Y^m_l) = mY^m_l + a \left( \sum_{p=-2}^{2} a_{l,m,p} Y^{m-2}_{l+p} - \sum_{p=-2}^{2} a_{l,-m,p} Y^{m+2}_{l+p} \right), \]

where the coefficients are determined by

\[
\begin{align*}
\alpha_{l,m,-2} &= \frac{(l - 2) \sqrt{(-3 + l + m)(-2 + l + m)(-1 + l + m)(l + m)}}{2 \sqrt{(-3 + 2l)(1 + 2l)(1 + 2l)}} \\
\alpha_{l,m,0} &= -\frac{3 \sqrt{(1 + l - m)(2 + l - m)(-1 + l + m)(l + m)}}{2(-1 + 2l)(3 + 2l)} \\
\alpha_{l,m,2} &= \frac{(3 + l) \sqrt{(1 + l - m)(2 + l - m)(3 + l - m)(4 + l - m)}}{2 \sqrt{(1 + 2l)(5 + 2l)(3 + 2l)}} \\
\alpha_{l,n,p} &= 0, \quad \text{if } p \neq -2, 0, 2.
\end{align*}
\]

3.3. The Smoluchowski equation for steady states

Steady states of (4) satisfy

\[ R \cdot R f - \frac{3}{2} N R \cdot (f R T f) - \frac{1}{2} PeG(f) = 0. \] (19)

Recall the fundamental spectral property of the rotational diffusion operator \( R \cdot R \),

\[ R \cdot Y^m_l = -l(l + 1)Y^m_l. \] (20)

4. Approximate steady solutions in weak shear

We expand the orientational distribution function \( f \) in the Peclet number \( Pe \):

\[ f = \frac{1}{\sqrt{4\pi}} (f_0 + Pe f_1 + Pe^2 f_2 + Pe^3 f_3 + \cdots), \] (21)

and the goal is to determine \( f_0, f_1, f_2, \ldots \) associated with the isotropic quiescent state. If we insert this expansion into (19), we have

\[ R \cdot R f - \frac{3}{2} N R \cdot (f R T f) - \frac{1}{2} PeG(f) \]

\[ = \frac{1}{\sqrt{4\pi}} \left\{ \sum_{k=0}^{3N} \left( \frac{3N}{4\pi} \right) \sum_{k_1=0}^{3N} \sum_{k_2=0}^{3N} \sum_{k_3=0}^{3N} \right\}. \] (22)
4.1. Leading order terms and linearized stability

The terms independent of $Pe$ give the quiescent Smoluchowski equation for $f_0$,

$$
\mathbf{R} \cdot \mathbf{R} f_0 - \frac{3N}{4\sqrt{\pi}} \mathbf{R} \cdot (f_0 \mathbf{R} T f_0) = 0.
$$

(23)

With the normalization

$$
\int |\mathbf{m}| \, df = 1,
$$

(24)

the isotropic state is

$$
f_0 = Y_0^0 = \frac{1}{\sqrt{4\pi}}
$$

(25)

which solves (23) for all concentrations $N$. Two nematic branches (for $N > 4.49$) are computed numerically in [27–29], which Onsager [20] characterized analytically. Several valiant attempts (cf. [3,4,7,10,21]) have been made to characterize the flow-induced stable branch(es) of nematic solutions analytically. Absent thus far of an explicit basis for the linearized Smoluchowski equation about the quiescent nematic branch, we restrict hereafter to the isotropic branch.

The linearized Smoluchowski equation about this isotropic solution takes the form

$$
\frac{df}{dt} = \mathbf{R} \cdot \mathbf{R} f - \frac{3N}{4\sqrt{\pi}} (\mathbf{R} \cdot (f_0 \mathbf{R} T f) + \mathbf{R} \cdot (f \mathbf{R} T f_0)) = \mathbf{R} \cdot \mathbf{R} f - \frac{3N}{8\pi} \mathbf{R} \cdot \mathbf{R} T f.
$$

(26)

By formulas (14) and (20), we deduce a basis of independent eigenfunctions of this linearized system. For example,

$$
Y_{k}^{2}, \quad k = -2, -1, 0, 1, 2
$$

(27)

are five eigenfunctions corresponding to the multiplicity five eigenvalue $\lambda_1 = -6(1 - (N/5))$;

$$
Y_{k}^{4}, \quad k = -4, -3, \ldots, 3, 4
$$

(28)

are nine eigenfunctions corresponding to the multiplicity nine eigenvalue $\lambda_2 = -20$;

$$
Y_{k}^{6}, \quad k = -6, -5, \ldots, 5, 6
$$

(29)

are 13 eigenfunctions corresponding to multiplicity thirteen eigenvalue $\lambda_3 = -42$; and in general, we have the eigenfunctions of

$$
Y_{k}^{2l}, \quad k = -2l, \ldots, 2l
$$

(30)

corresponding to the eigenvalues $\lambda_2 = -2l(2l + 1), l = 2, 3, \ldots, \infty$. This “block diagonal structure” of the linearized Doi equation is the key to analysis of the isotropic transition in weak flows (cf. See et al. [23] and our discussion below). From this observation, one immediately deduces isotropic solutions are: asymptotically stable if $N < 5$, and unstable for $N > 5$. The isotropic transition at $N = 5$ is associated with a multiplicity five neutral eigenvalue ($\lambda_1 = 0$). This observation explains why the isotropic instability transition in weak shear is likely to produce a singular expansion for the bifurcation curve, $N - 5 = O(Pe^{1/2})$, for some exponent $\alpha$ to be determined. Indeed, See et al. [23] posited $\alpha = 1/2$ and demonstrated self-consistency of an expansion for $f$ in the asymptotic parameter $Pe^{1/2}$. We return to this issue below.
4.2. First order solvability analysis

The terms of order \( Pe \) determine a non-homogeneous equation for \( f_1 \):

\[
\mathbf{R} \cdot \mathbf{R} f_1 - \frac{3N}{4\sqrt{\pi}} (\mathbf{R} \cdot (f_0 RT_f) + \mathbf{R} \cdot (f_1 RT_f)) - \frac{1}{2} G(f_0) = 0. \tag{31}
\]

Since

\[ T_f = T_0 = \frac{4\pi}{3}, \tag{32} \]

which is constant so that \( RT_f = 0 \), and

\[
G(f_0) = \sqrt{\frac{6}{\pi}} a (Y_0^2 - Y_0^{-2}), \tag{33}
\]

(31) reduces to

\[
\mathbf{R} \cdot \mathbf{R} f_1 - \frac{3N}{8\pi} \mathbf{R} \cdot RT_f - \sqrt{\frac{3}{10}} a (Y_1^2 - Y_1^{-2}) = 0. \tag{34}
\]

The normalization condition (24) together with (25) imply

\[
\int_{|m|=1} f_1 \, dm = 0. \tag{35}
\]

Therefore, the first order correction to the isotropic state is explicitly and uniquely solvable:

\[
f_1 = \frac{i}{2} \sqrt{\frac{5}{6N-3}} (Y_1^2 - Y_1^{-2}). \tag{36}
\]

which is real since \( Y_1^{-2} \) is the complex conjugate of \( Y_1^2 \).

4.3. Second-order solvability

The second-order terms give

\[
\mathbf{R} \cdot \mathbf{R} f_2 - \frac{3N}{4\sqrt{\pi}} [\mathbf{R} \cdot (f_0 RT_f) + \mathbf{R} \cdot (f_1 RT_f)] - \frac{1}{2} G(f_1) = 0, \tag{37}
\]

or equivalently,

\[
\mathbf{R} \cdot \mathbf{R} f_2 - \frac{3N}{8\pi} \mathbf{R} \cdot RT_f = \frac{3N}{4\sqrt{\pi}} \mathbf{R} \cdot (f_1 RT_f) + \frac{1}{2} G(f_1). \tag{38}
\]

Denote

\[
a_1 = \frac{1}{2} \sqrt{\frac{5}{6N-3}}, \tag{39}
\]

then we have

\[
f_1 = i a_1 (Y_1^2 - Y_1^{-2}). \tag{40}
\]
Now we expand the right hand side of (38) in spherical harmonics. The following formulas are needed:

\[
(R f_1) \cdot (R T f_1) = -\frac{1}{2} \pi \sigma_1 R(Y_2^0 - Y_2^{-2}) \cdot R(Y_2^0 - Y_2^{-2})
\]

\[
= \frac{\alpha}{3N} \sqrt{\pi} \sigma_1 (21Y_0^0 - 3\sqrt{3}Y_0^2 - 2Y_0^4 + \sqrt{70}(Y_4^4 + Y_4^{-4}))
\]

\[
f_1(R \cdot RT f_1) = -\frac{1}{2} \pi \sigma_1 (Y_2^0 - Y_2^{-2}) R \cdot R(Y_2^0 - Y_2^{-2})^2
\]

\[
= \frac{\alpha}{3N} \sqrt{\pi} \sigma_1 (-14Y_0^0 + 4\sqrt{3}Y_0^2 - 2Y_0^4 + \sqrt{70}(Y_4^4 + Y_4^{-4})),
\]

which give

\[
R \cdot (f_1 RT f_1) = (R f_1) \cdot (R T f_1) + f_1(R \cdot RT f_1)
\]

\[
= \frac{\alpha}{3N} \sqrt{\pi} \sigma_1 (6\sqrt{3}Y_0^2 - 102Y_0^4 + 5\sqrt{70}(Y_4^4 + Y_4^{-4})).
\]

We also expand \(G(f_1)\)

\[
G(f_1) = i\alpha \left( G(Y_2^0) - G(Y_2^{-2}) \right)
\]

\[
= \alpha \left[ 2(Y_2^0 + Y_2^{-2}) - \frac{2}{\sqrt{\pi}} \left( \sqrt{Y_0^2} - \frac{10}{3} Y_0^4 + \frac{70}{3} (Y_4^4 + Y_4^{-4}) \right) \right].
\]

Therefore, the solution to (38) has the form

\[
f_z = f_z^{(1)}(Y_2^0, Y_2^{1}, Y_2^{-1}, Y_2^{-2}) + f_z^{(2)}(Y_4^0, Y_4^{1}, Y_4^{-1}).
\]

where \(f_z^{(1)}\) is a linear function of \(Y_2^0, Y_2^{1}, Y_2^{-1}, Y_2^{-2}\), \(f_z^{(2)}\) is a linear function about \(Y_4^0, Y_4^{1}, Y_4^{-1}\). By formula (14), (38) reduces to

\[
-6 \left( 1 - \frac{N}{3} \right) f_z^{(1)} - 20 f_z^{(2)} = \frac{3N}{4\sqrt{\pi}} R \cdot (f_1 RT f_1) + \frac{1}{2} G(f_1).
\]

Then from (44) and (45), we finally arrive at the explicit formulas to construct the second-order term \(f_z\) in the expansion (21) of \(f\):

\[
f_z^{(1)} = \frac{1}{2} \left( \frac{5}{6} \right)^{1/2} \frac{a}{6(N - 5)^2} \left( \frac{5\sqrt{3}}{7} - \frac{a}{N - 5} \right) \left( Y_0^2 + Y_0^4 + Y_0^6 + Y_0^8 \right)
\]

\[
f_z^{(2)} = \frac{\sqrt{3}}{168\sqrt{6}} \frac{a^2}{(N - 5)^3} \left( \sqrt{Y_0^2} - 5\sqrt{27}(Y_4^4 + Y_4^{-4}) \right).
\]

We note that any projection onto the second moment of \(f\), that is, any closure approximation, will induce errors in the term \(f_z^{(2)}\).

4.4. The isotropic-nematic transition (See et al. [23])

Note from (36) the above regular perturbation expansion is valid except near the instability transition \(N = 5\). To make contact with the fundamental analysis of this bifurcation by See et al. [23], we present
two results that link our regular asymptotic expansion with their scaling behavior. First, we recall their method. They seek a singular asymptotic expansion in a neighborhood of \( N = 5 \), for \( 0 < Pe \ll 1 \), by postulating \( O(Pe^{1/2}) \) as the correct scaling:

\[
N = 5 + cPe^{1/2} + O(Pe),
\]

\[
f = \frac{1}{\sqrt{4\pi}} (f_0 + Pe^{1/2} f_1 + Pe^{2} f_2 + \cdots).\]

This scaling assumption, that \((N - 5)^2 = O(Pe)\), characterizes turning points. Indeed, the breakup of the fifth-order degeneracy, Eq. (27), that characterizes the isotropic instability at \( N = 5 \), is often a pair of turning points, but degree 5 leaves open the possibility for two disconnected continuous branches to form \([36,37]\), or even for “cusp”-like behavior.

At leading order the isotropic state, independent of \( N \), is \( f_0 = Y_0^0 = 1/\sqrt{4\pi} \). At order \( O(Pe^{1/2}) \),

\[
\mathcal{R} \cdot \mathcal{R} f_1 - \frac{15}{8\pi} \mathcal{R} \cdot \mathcal{R} T f_1 = 0.
\]

By (14) and (20), any function \( f_1 \) in the sub-space spanned by the first five spherical harmonics, \( S^{(5)} = \text{span}(Y_k^l, k = -2, -1, 0, 1, 2) \), identically satisfies (52). Furthermore, if \( f_1 \) satisfies (52), it must lie in \( S^{(5)} \). This fact is equivalent to the earlier observation that the multiplicity-five neutral eigenvalue, \( \lambda_1 = 0 \), has \( S^{(5)} \) as its eigenbasis. To construct \( f_1 \), we must continue to the next order, \( O(Pe) \), and the equation for \( f_2 \) is:

\[
\mathcal{R} \cdot \mathcal{R} f_2 - \frac{15}{8\pi} \mathcal{R} \cdot \mathcal{R} T f_2 - \frac{\mathcal{R} \cdot \mathcal{R} f_1}{5} \mathcal{R} \cdot \mathcal{R} T f_1 - 2\sqrt{\pi} \mathcal{R} \cdot (f_1 \mathcal{R} f_1) - \frac{1}{2} G(f_0) = 0.
\]

As noted above, the first two terms vanish on \( S^{(5)} \), but then solvability requires the remaining terms must also vanish on \( S^{(5)} \):

\[
\frac{1}{\sqrt{2}} \mathcal{R} \cdot \mathcal{R} f_1 + 2\sqrt{\pi} \mathcal{R} \cdot (f_1 \mathcal{R} f_1) + \frac{1}{2} G(f_0)|_{y=0} = 0.
\]

This gives us a system of equations for the averages of the five second spherical harmonics with respect to \( f_1 \); \( (Y_2^2)_{ij}, (Y_1^2)_{ij}, (Y_2^0)_{ij}, (Y_2^1)_{ij}, (Y_2^2)_{ij} \). (We note these averages are equivalent to the second-moment tensor, Eqs. (65)-(70).)

For simplicity, let \( x = (Y_2^2)_{ij}, y = \mathfrak{R}((Y_2^1)_{ij}), z = \mathfrak{R}((Y_1^2)_{ij}), u = \mathfrak{R}((Y_2^2)_{ij}), v = \mathfrak{R}((Y_2^0)_{ij}) \) (where \( \mathfrak{R} \) and \( \mathfrak{I} \) represent the real and imaginary parts, respectively). Then we derive from (54) the following 5 equations:

\[
14cy - 5\sqrt{3}\sqrt{6}(y^2 - u^2) + 4xy = 0, \quad 6(7c - 10\sqrt{3})z + (30\sqrt{3}uv - 35\sqrt{\frac{3}{10}}) = 0,
\]

\[
7cu + 5\sqrt{3}(xu + \sqrt{6}xy + vu) = 0, \quad 7cv + 5\sqrt{3}(xv + \sqrt{6}(cu - uv)) = 0,
\]

\[
7cx + 5\sqrt{3}(x^2 - 2y^2 - 2z^2 + u^2 + v^2) = 0.
\]

Analysis of these equations shows one must have \( u = v = y = 0 \), and \( x, z \) and \( c \) satisfy:

\[
6(7c - 10\sqrt{3})z - 35\sqrt{\frac{3}{10}}u = 0,
\]

\[
14cy - 5\sqrt{3}\sqrt{6}(y^2 - u^2) + 4xy = 0.
\]
\[ 7cx + 5\sqrt{3}(x^2 - 2z^2) = 0. \]  

(57)

To close this system, we follow See et al. [23] and append the marginal stability condition (the Jacobian of (56), (57) is singular), which gives

\[ 500(c^2 + 2z^2) - 49a^2 = 0. \]  

(58)

These three equations ((56)-(58)) are explicitly solvable for \( c, x \) and \( z \). One solution yields the bifurcation curve along which the perturbed isotropic state becomes unstable:

\[ N = 5 - \frac{5(2^{1/3})\sqrt{7a}}{(3^{1/3})\sqrt{21 - 7\sqrt{3}}}Pe^{1/2} \approx 5 - 1.869\sqrt{|a|}Pe^{1/2}, \]  

(59)

as well as the perturbed solution at order \( O(Pe^{1/2}) \):

\[ \langle Y^2 \rangle_{f_1} = \frac{7(\sqrt{3} - 1)\sqrt{7a}}{2(2^{1/3})(3^{1/3})\sqrt{5}(21 - 7\sqrt{3})}Pe^{1/2} \approx -0.21\sqrt{|a|}Pe^{1/2}, \quad \langle Y^1 \rangle_{f_1} = \Re(\langle Y^2 \rangle_{f_1}) = 0, \]

(60)

\[ 3i(\langle Y^2 \rangle_{f_1}) = -\text{sgn}(a)\frac{7\sqrt{7a}}{2(2^{1/3})(3^{1/3})\sqrt{5}(21 - 7\sqrt{3})}Pe^{1/2} \approx -0.38\text{sgn}(a)\sqrt{|a|}Pe^{1/2}. \]

We thereby recover the result in [23] for \( a = 1 \), equation (59), together with the extension of the scaling behavior to finite aspect ratio rods (0 \( < a \leq 1 \)) or platelets (\( -1 \leq a < 0 \)). This explicit construction is translated below into a precise form of the second-moment orientation tensor.

To check these asymptotic predictions, we solve the Smoluchowski equation numerically using continuation software AUTO [38] to determine the bifurcation curve (59). For \( Pe = 1, 2, 5 \times 10^{-4} \), the transition occurs numerically at

\[ \frac{N - 5}{Pe^{1/2}} = 1.870, 1.867, 1.860, \]  

(61)

respectively, which brackets the theoretical result (59).

We further observe there is another solution to ((56)-(58)), to the right of \( N = 5 \), marking the continuation of the unstable isotropic branch in weak shear:

\[ N = 5 + \frac{5(2^{1/3})\sqrt{7a}}{(3^{1/3})\sqrt{21 - 7\sqrt{3}}}Pe^{1/2} \approx 5 + 1.869\sqrt{|a|}Pe^{1/2}. \]  

(62)

These two bifurcations reveal a gap around \( N = 5 \), of width \( O(Pe^{1/2}) \), in which the isotropic equilibria fail to persist in weak shear, as confirmed by our numerical simulations [29].

Our second calculation aims to deduce the \( O(Pe^{1/2}) \) scaling law at the isotropic transition. We assume \( N = 5 + m + \text{HOT} \), where \( m \) obeys a scaling law \( m = c \cdot Pe^\alpha, \alpha > 0 \), with \( c \) to be determined by solvability and marginal stability conditions, and HOT indicates high order terms. We also assume

\[ f = \frac{1}{\sqrt{|a|}}(f_0 + f_1 + \text{HOT}), \]  

(63)

where \( f_1 = O(Pe^0) \) lies in \( S^{(1)} \) (as in [23]), and \( \alpha, \beta \) are to be determined. Then we project the Smoluchowski equation onto the space \( S^{(1)} \) by neglecting all higher order terms. Details are left to the strong
at heart. We arrive at the same linear system (55), with $a$ replaced by $a\text{Pe}$, $c$ replaced by $m$, and we are able to deduce that $m \approx \pm 1.869|a|\text{Pe}^{1/2}$ and $\alpha = \beta = 1/2$. Together with the See et al. [23] results, we have now established the quiescent isotropic instability bifurcation splits apart into two opposite facing turning points, separated by a gap of $O(\text{Pe}^{1/2})$.

5. Alignment properties from the PDF construction

The explicit construction of the PDF through first- and second-order shear-induced corrections,

$$f \approx \frac{1}{\sqrt{4\pi}}(f_0 + \text{Pe}f_1 + \text{Pe}^2f_2),$$

(64)
is now used to infer physical properties of the shear-perturbed isotropic branch. We first note that the construction of $f$ contains only $\mathcal{Y}^m_l$ with $m$ even. From [35], if $f$ has zero projections onto $\mathcal{Y}^m_l$ for all $m$ odd, then $f$ is an in-plane solution of the shear-driven Smoluchowski equation. This notion extends to kinetic theory the traditional definition of in-plane Leslie–Ericksen director and mesoscopic orientation tensors, discussed shortly. The terminology “in-plane” means in the shear deformation plane of the flow and flow gradient. We note at this point that through $O(\text{Pe}^2)$, we have established the weak-shear deformation of the isotropic branch persists as a unique steady distribution, aligned in the flow deformation plane. We now extract more detailed information about the alignment properties of the shear-perturbed isotropic branch.

The traditional measure of orientation is to project $f$ onto the second-moment tensor $\mathcal{Q}$ [35]:

$$Q_{xx} = \frac{2}{3} \sqrt{\frac{8\pi}{15}} \mathcal{R}(a_{2,2}) \langle \mathcal{Y}^0_0 \rangle_f,$$

(65)

$$Q_{yy} = \frac{2}{3} \sqrt{\frac{8\pi}{15}} \mathcal{R}(a_{2,2}) \langle \mathcal{Y}^0_0 \rangle_f,$$

(66)

$$Q_{xy} = -\frac{8\pi}{15} \mathcal{I}(a_{2,2}) \langle \mathcal{Y}^0_0 \rangle_f,$$

(67)

$$Q_{xz} = -\frac{8\pi}{15} \mathcal{I}(a_{2,1}) \langle \mathcal{Y}^0_1 \rangle_f,$$

(68)

$$Q_{yz} = \frac{8\pi}{15} \mathcal{I}(a_{2,1}) \langle \mathcal{Y}^0_1 \rangle_f,$$

(69)

where we recall

$$a^0_l = (-1)^m \langle \mathcal{Y}^{-m}_l \rangle_f,$$

(70)

and $\mathcal{R}(\cdot)$ and $\mathcal{I}(\cdot)$ represent the real and the imaginary part, respectively. From the exact expansions through $O(\text{Pe}^2)$ we deduce (with $\alpha_1$ given in (39))

$$\langle \mathcal{Y}^0_0 \rangle_f = \frac{1}{\sqrt{4\pi}} \frac{25\sqrt{\text{Re} \alpha_1}}{42(\text{N} - 5)} \text{Pe}^2,$$

(71)
\[ \langle Y_1^2 \rangle_f = 0 \]  
\[ \langle Y_2^{-1} \rangle_f = \frac{1}{\sqrt{4\pi}} \cdot a Pe \left( \frac{5}{6(N-5)} Pe + i \right). \]  

which now gives the explicit second-moment tensor projection of \( f \) for \( N \) away from 5:

\[ Q = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \]

\[ -Pe^2 \frac{5a}{36(5-N)^2} \left[ -\frac{5a}{7(N-5)} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right]. \]  

This explicit construction is remarkably similar to the Doi closure model for \( Q \) \cite{19}. We can now explicitly provide the eigenvalues and eigenvectors of \( Q \) to determine the mesoscopic alignment properties of the explicit kinetic PDF:

- The eigenvalues of \( Q \) through \( O(\text{Pe}) \) are distinct, in descending order,
  \[ \lambda_1 = \frac{Pe}{6} \left| \frac{a}{5-N} \right|, \quad \lambda_2 = 0, \quad \lambda_3 = -\frac{Pe}{6} \left| \frac{a}{5-N} \right|. \]  

We deduce \( Q \) is biaxial. The degree of biaxiality, \( 0 \leq b \leq 1 \), \cite{16} is defined by

\[ b = \sqrt{1 - \frac{6\text{Tr}(Q^2)}{\text{Tr}(Q^3)}}, \]  

which is depicted in Fig. 1(left) versus \( N \) using the \( O(\text{Pe}^2) \) eigenvalue formulas for \( \text{Pe} = 0.1 \). This is one measure of the relative focusing of the distribution function with respect to the three director axes, with \( b = 1 \) corresponding to maximum biaxiality. Note the distribution remains defocused until \( N \) approaches the nematic transition.

\[ \text{Fig. 1. Left: biaxiality parameter } b \text{ for } \text{Pe} = 0.1, a = 1. \text{ Right: scaling behavior of the Leslie angle versus concentration (N) for } \text{Pe} = 0.1 \text{ and } a = 1. \text{ The solid line indicates stable solutions, the dashed line corresponds to unstable solutions.} \]
The shear-induced flow birefringence is measured by the differences in eigenvalues of $\mathbf{Q}$, which from the $O(\text{Pe})$ formulas for $\lambda_i$ are:

$$
\lambda_1 - \lambda_2 = \left| \frac{a}{5 - N} \right| \frac{\text{Pe}}{6},
\lambda_3 - \lambda_2 = -\left| \frac{a}{5 - N} \right| \frac{\text{Pe}}{6}.
$$

These are depicted in Fig. 4 versus $N$ for $\text{Pe} = 0.1$ using the $O(\text{Pe}^2)$ formulas.

The above construction breaks down in an $O(\text{Pe}^3)$ neighborhood of the critical concentration $N = 5$ where the isotropic state becomes unstable. Our singular analysis shows a gap forms, $(5 - 1.869\text{Pe}^{1/2}, 5 + 1.869\text{Pe}^{1/2})$, where the quiescent isotropic state does not persist. This result confirms mesoscopic second-
Fig. 2. Left: the distribution function \( f(\theta, \phi) \) approximated by second-order expansion. Right: the contour plot of the distribution function \( f(\theta, \phi) \). The parameters chosen are: \( a = 1 \) (infinitely thin rods), \( N = 2 \), \( Pe = 0.1 \). The peak of the distribution is at \( \theta = \pi/2 \) (i.e., in-plane major director) with Leslie alignment angle \( \phi \approx \pi/4 \).

Moment tensor analysis [19] and numerical simulations of both kinetic theory [28,29] and mesoscopic tensor models [13,18]. Based on the singular asymptotics in Section 4.2, we now construct the explicit second-moment tensor projection of \( f \) along the isotropic-nematic transition curve:

\[
Q = \mathbf{0} + Pe^{1/2} \begin{pmatrix}
7(\sqrt{3} - 1)\sqrt{|a|} & 1 & 0 & 0 \\
30(2^{1/3})(3^{1/3})\sqrt{21 - 7\sqrt{3}} & 0 & 1 & 0 \\
0 & 0 & -2 & 0 \\
\end{pmatrix}
+ \text{sgn}(a) \begin{pmatrix}
7\sqrt{|a|} & 0 & 1 & 0 \\
5(2^{1/3})(3^{1/3})\sqrt{21 - 7\sqrt{3}} & 1 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{pmatrix}.
\]

(81)

Fig. 3. Scaling behavior of the Leslie alignment angle versus normalized shear rate \( (Pe) \) and concentration \( (N) \).
Fig. 4. Order parameters for $Pe = 0.1$ and $a = 1$. The solid curve ($0 \leq N \leq 4.8$) is the stable flow-aligning branch, while the dashed curve is the unstable flow-aligning branch. The isotropic state ($d_1 = d_2 = d_3 = 1/3$) lies at the center ($N = 0$) and then biaxial states emerge as $N$ increases toward 4.8.

The eigenvalues of this tensor are

$$
\lambda_1 = 0.17\sqrt{|a|Pe}, \quad \lambda_2 = -0.06\sqrt{|a|Pe}, \quad \lambda_3 = -0.11\sqrt{|a|Pe}.
$$

(82)

Therefore, $Q$ is biaxial. The shear-induced flow birefringence is given by

$$
\lambda_1 - \lambda_3 = 0.28\sqrt{|a|Pe}, \quad \lambda_2 - \lambda_3 = 0.05\sqrt{|a|Pe}.
$$

(83)

Comparison of (74) and (81) reveals a "jump" in the scaling behavior and in the $Q$ tensor components as one passes through the bifurcation curve.

6. Rheological properties

The extra stress in dimensional form is given by [5]

$$
\tau = (2\eta + 3kTc^0(a))D + 3\eta kT[IQ - N(Q + \frac{1}{4}I)Q + NQ : (mmmm)] + 3kT[c^1(a)BM + MD] + c^2(a)D : (mmmm)],
$$

where

$$
\begin{align*}
\zeta_1 &= \zeta^{00}, & \zeta_1 &= \zeta^{00}\left(\frac{1}{I_3} - \frac{1}{I_1}\right), & \zeta_2 &= \zeta^{00}\left[\frac{J_1}{I_1J_3} + \frac{1}{I_1} - \frac{2}{I_3}\right], & r &= \frac{1 + a}{1 - a}, \\
I_1 &= 2r \int_0^\infty \frac{dx}{\sqrt{(r^2 + x)(1 + x)^3}}, & I_3 &= r(r + 1) \int_0^\infty \frac{dx}{\sqrt{(r^2 + x)(1 + x)^3(r^2 + x)}} \\
I_4 &= r(r + 1) \int_0^\infty \frac{dx}{\sqrt{(r^2 + x)(1 + x)^3(r^2 + x)}}.
\end{align*}
$$

(84)

(85)
where \( \nu \) is the number density of LCP molecules per unit volume, and \( \varepsilon^{(0)} \) is a free parameter depending on \( a \) that must be experimentally fitted. In the calculations below, because we do not know the exact dependence of \( \zeta_0 \) on \( a \), we choose constant \( \zeta_0 = 0.01 \). For rod-like polymers \( r = 10 \) (\( a \approx 0.98 \)), from (85), the values of these parameters are computed: \( \zeta_1 \approx 0.0004, \quad \zeta_2 \approx 0.15, \quad \zeta_3 \approx 0.01 \). For discotic polymers \( r = 1 \) (\( a \approx -0.98 \)), \( \zeta_1 \approx -0.044, \quad \zeta_2 \approx 0.053, \quad \zeta_3 \approx 0.05 \). We neglect the isotropic viscosity, i.e., \( \eta = 0 \), and non-dimensionalize by a characteristic entropic stress \( \tau_0 = 3kT \).

The second-moment tensor \( Q \) has been explicitly constructed in (74). To compute the stress tensor \( \tau \), we also need to construct the fourth-moment tensor \( \langle \sigma \rangle \). They are explicitly given in the Appendix A.

The steady shear stress \( \sigma \) and the first and second normal stress differences \( N_1, N_2 \) in dimensionless form are defined by

\[
\begin{align*}
N_1 &= \tau_{xx} - \tau_{yy}, \\
N_2 &= \tau_{yy} - \tau_{zz}, \\
\sigma &= \tau_{xy}/Pe.
\end{align*}
\]

Through \( O(Pe^2) \), explicit expansions for these rheological properties follow from our analysis:

\[
\begin{align*}
N_1 &= \frac{1}{18(5 - N)} a^2 Pe^2 + O(Pe^4), \\
N_2 &= \frac{3a^3 - 7a + 42(\zeta_1 + 12\zeta_2) a Pe^2 + O(Pe^4)}, \\
\sigma &= \frac{1}{30}(a^2 + 10\zeta_1 + 2\zeta_2 + 15\zeta_3) + \frac{1}{Re} + O(Pe^2).
\end{align*}
\]

Presuming the isotropic viscosity is negligible \( (1/Re = 0) \), these features are plotted in Fig. 5 for a rod-like aspect ratio \( r = 10 \) and Fig. 6 for a plate-like aspect ratio \( r = 1/10 \). The essential results are:

- Both \( N_1 \) and \( N_2 \) are of order \( O(Pe^2) \) for \( N \) sufficiently dilute, and therefore, nearly zero in weak shear.
- \( N_1 > 0 \) and \( N_2 < 0 \) at stable dilute concentrations, \( 0 < N < 5 - \delta \), with \( \delta = O(Pe^{1/2}) \).
- As \( N \) approaches 5, \( N_1 \) and \( N_2 \) grow in magnitude, but the asymptotic expansions break down in this limit. These properties of \( N_1 \) and \( N_2 \) confirm mesoscopic predictions [19].
- The scaled apparent viscosity \( \sigma \) is independent of concentration \( N \) at \( O(Pe) \), then exhibits “concentration thinning” for both rods and discotics, as the concentration increases towards the nematic transition.

![Fig. 5. Scaled normal stress differences \( N_1, N_2 \), and apparent viscosity \( \eta \) for rod-like polymers \( r = 10 \) at \( Pe = 0.1 \).](image-url)
We are unaware of experimental data to benchmark these predictions. However, they are consistent with numerical simulations of the full kinetic equation for infinite aspect ratio rods [29]. We note the normal stress differences $N_1$ and $N_2$ qualitatively confirm the mesoscopic predictions in [19]. The shear stress $\sigma$ confirms mesoscopic behavior except near the instability transition, where the “thinning” or “thickening” of $\sigma$ is sensitive to closure approximations [19].

7. Conclusion

The goals outlined in the abstract and introduction have been met. An explicit construction and stability analysis of the PDF of Doi kinetic theory in the dilute concentration and weak flow regime have been provided. The formulas are confirmed by direct numerical simulations, and then used to infer experimental data for the primary alignment of the PDF, the relative focusing of the distribution, and stress measurements. Most importantly, these constructions provide rigorous scaling behavior of flow-aligned steady orientational distributions in weak shear with respect to molecular and flow parameters. Our results are complementary to the analysis of See et al. [23], who determined the scaling behavior of the isotropic instability transition in weak flow. Together, our analyses covers the weak flow perturbation properties of the isotropic state for all concentrations.

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Appendix A

Suppose $f(m)$ has the spherical harmonic expansion

$$f(m) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} a_{lm} Y_{lm}^m(\theta, \phi).$$

(A.1)
Denote by \( \mathcal{M} \) the fourth-moment tensor \((mmmm)\). Components of \( \mathcal{M} \) can be computed as (nine of them are independent):

\[
\begin{align*}
\mathcal{M}_{1111} &= \frac{1}{105} \sqrt{\pi} \left( 42a_{00} - 12\sqrt{5}a_{20} + 12\sqrt{30}a_{12} + 6a_{40} - 4\sqrt{10}a_{14} + 2\sqrt{70}a_{14} \right) \\
\mathcal{M}_{1112} &= \frac{2}{\sqrt{2}} \sqrt{\frac{\pi}{5}} \left( -3\sqrt{2}(a_{12}) + 3(a_{42}) - \sqrt{7}(a_{44}) \right) \\
\mathcal{M}_{1113} &= -\frac{2}{\sqrt{21}} \sqrt{\frac{\pi}{5}} \left( 3\sqrt{5}a_{21} - 3a_{41} + \sqrt{10}a_{43} \right) \\
\mathcal{M}_{1122} &= \frac{1}{105} \sqrt{\pi} \left( 14a_{00} + 2a_{40} - 2\sqrt{3}a_{22} - 2\sqrt{15}a_{24} \right) \\
\mathcal{M}_{1123} &= \frac{2}{\sqrt{21}} \sqrt{\frac{\pi}{5}} \left( \sqrt{3}(a_{21}) - 3(a_{41}) + \sqrt{7}a_{43} \right) \\
\mathcal{M}_{1133} &= \frac{1}{105} \sqrt{\pi} \left( -3\sqrt{2}(a_{12}) + 3(a_{22}) - \sqrt{7}(a_{44}) \right) \\
\mathcal{M}_{1222} &= \frac{1}{105} \sqrt{\pi} \left( 42a_{00} - 12\sqrt{5}a_{20} - 12\sqrt{30}a_{12} + 6a_{40} + 4\sqrt{10}a_{14} + 2\sqrt{70}a_{14} \right) \\
\mathcal{M}_{1223} &= \frac{2}{\sqrt{21}} \sqrt{\frac{\pi}{5}} \left( \sqrt{5}a_{21} + \sqrt{3}(a_{41}) + \sqrt{10}a_{43} \right) \\
\mathcal{M}_{1233} &= \frac{2}{\sqrt{21}} \sqrt{\frac{\pi}{5}} \left( 3\sqrt{5}a_{21} + 3a_{41} + \sqrt{7}a_{43} \right) \\
\mathcal{M}_{1333} &= \frac{2}{\sqrt{21}} \sqrt{\frac{\pi}{5}} \left( 3\sqrt{5}a_{21} + 3a_{41} + \sqrt{7}a_{43} \right) \\
\mathcal{M}_{2222} &= \frac{1}{105} \sqrt{\pi} \left( 14a_{00} + 2\sqrt{3}a_{20} - 8a_{40} + 2\sqrt{30}a_{12} + 4\sqrt{10}a_{14} + 2\sqrt{70}a_{14} \right) \\
\mathcal{M}_{2223} &= \frac{2}{\sqrt{21}} \sqrt{\frac{\pi}{5}} \left( 3\sqrt{5}a_{21} + 3a_{41} + \sqrt{7}a_{43} \right) \\
\mathcal{M}_{2233} &= \frac{2}{\sqrt{21}} \sqrt{\frac{\pi}{5}} \left( 3\sqrt{5}a_{21} + 3a_{41} + \sqrt{7}a_{43} \right) \\
\mathcal{M}_{2333} &= \frac{2}{\sqrt{21}} \sqrt{\frac{\pi}{5}} \left( 3\sqrt{5}a_{21} + 3a_{41} + \sqrt{7}a_{43} \right) \\
\mathcal{M}_{3333} &= \frac{2}{\sqrt{21}} \sqrt{\frac{\pi}{5}} \left( 3\sqrt{5}a_{21} + 3a_{41} + \sqrt{7}a_{43} \right) \\
\mathcal{M}_{4444} &= \frac{1}{105} \sqrt{\pi} \left( 42a_{00} + 16a_{40} + 24\sqrt{5}a_{20} \right).
\end{align*}
\]
References

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