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Global orientation dynamics for liquid crystalline polymers

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Abstract

We study global orientation dynamics of the Doi–Smoluchowski equation with the Maier–Saupe potential on the sphere, which arises in the modeling of rigid rod-like molecules of polymers. Using the orientation tensor we first reconfirm the structure and number of equilibrium solutions established in [H.L. Liu, H. Zhang, P.W. Zhang, Axial symmetry and classification of stationary solutions of Doi–Onsager equation on the sphere with Maier–Saupe potential, Comm. Math. Sci. 3 (2) (2005) 201–218]. We then examine global orientation dynamics in terms of eigenvalues of the orientation tensor via the Doi closure approximation. It is shown that for small intensity $0 < \alpha < 4$, all states will evolve into the isotropic phase; for large intensity $\alpha > 4.5$, all states will evolve into the nematic prolate phase; and for the intermediate intensity $4 < \alpha < 4.5$, an initial state will evolve into either the isotropic phase or the stable phase of two nematic prolate phases, depending on whether such an initial configuration crosses a critical threshold. Moreover, the uniaxial symmetry structure is shown to be preserved in time.

Keywords: Doi–Smoluchowski equation; Rigid rod-like polymers; Phase transition; Orientation dynamics; Asymptotic stability

1. Introduction

Rod-like polymer solutions exist in an isotropic phase at low concentrations, but will undergo a phase transition to a nematic phase if the molecule concentration exceeds a certain critical value. The phase transition problem of this type was first described by Onsager [20] via a variational approach, assuming that steady states correspond to minimizers of a free energy. Doi [5] made the first attempt at developing a molecular theory for liquid crystalline polymers via the kinetic equation. Doi's model is based on Onsager's expression for the free energy of a solution containing rod-like polymeric molecules, and provides a dynamic description of the isotropic–nematic phase transition that occurs as the polymer intensity changes. The kinetic model also serves as a framework within which the effect of external fields on the isotropic–nematic phase transition can be studied. In this paper we shall examine global orientation dynamics in rigid rod-like polymers in the absence of external fields.

The mathematical model we adopt is the Doi–Smoluchowski equation on the sphere

$$\frac{\partial f}{\partial t} = D_r \mathcal{R} \cdot (\mathcal{R} f + f \mathcal{R} U), \quad m \in \mathbb{S}^2, \tag{1}$$

where $f(t, m)$ denotes the orientational probability distribution function (PDF) for rod-like, rigid molecules with axis of symmetry m on the unit sphere $\mathbb{S}^2$. D_r is the averaged rotational diffusivity, which will be set to 1. $\mathcal{R} := m \times \frac{\partial}{\partial m}$ is the gradient operator. U is the mean-field interaction potential, which here considered is the Maier–Saupe [19] one:

$$U(m) = \alpha \int_{|m'|=1} |m \times m'|^2 f(m') \mathrm{d}m'. \tag{2}$$

It is well known that the presence of flow fields affects the phase transition as modeled by the Doi kinetic equation [5], based on which various phase transition diagrams to equilibrium states in rigid rod-like polymers have been observed in both experiments and numerical simulations, see e.g. [7,10–13,17,18].

Recently the Doi–Smoluchowski model (1) has attracted a great deal of attention in the mathematics community [2–4,8,

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15]. In particular, the equilibrium solutions are governed by the Doi–Onsager equation

$$\mathcal{R} \cdot (\mathcal{R} f + f \mathcal{R} U) = 0, \tag{3}$$

subject to the usual normalization

$$\int_{|m|=1} f(m) \mathrm{d}m = 1. \tag{4}$$

Concerning the structure of equilibrium solutions of (1), Constantin et al. [2] reduced the Doi–Onsager model (3) into nonlinear equations with two parameters and classified these solutions in the high intensity limit. They also proved that the isotropic state is the only possible solution at low enough intensity. Recently in [16] Liu et al. were able to reduce the Doi–Onsager equation (3) into a nonlinear equation with only one parameter and gave an explicit representation of all equilibrium solutions. Hence a definite answer to the Onsager conjecture [20] with the Maier–Saupe potential (2) was achieved: (i) all equilibrium solutions are necessarily uniaxially symmetric. (ii) The number of equilibrium states and their qualitative behavior for the Doi–Onsager equation hinge on whether the intensity α crosses two critical values: $\alpha^* \approx 6.731393$ and 7.5. A different proof of the uniaxial symmetry was done independently and at about the same time by Fatkullin and Slastikov [9]; See also [21] for a further effort in this direction. We note that the situation is much better understood in the two-dimensional case when the orientation variable lives on the circle, see [3,15,4,8,16] for recent investigations.

In this paper we focus our attention on the Doi–Smoluchowski equation (1) on the sphere. We first utilize the orientation tensor to reconfirm results obtained in [16] as mentioned above. We then examine global dynamics of the orientation tensor, and prove time-asymptotic stability of some equilibrium solutions. Equilibrium solutions correspond to either isotropic or nematic phases. More precisely, the uniform distribution $f = 1/4\pi$ corresponds to the isotropic phase; The case when f is concentrated at some particular director corresponds to the nematic phase, which includes the prolate and oblate states.

Following the Doi closure assumption we obtain a closed dynamic equation for the orientation tensor. The main tool to study the orientation dynamics is to derive the spectral equations from the closed orientation model. Due to the unit orientation trace, the spectral dynamics is governed by a 2×2 polynomial (of degree three) system. All phase behaviors are analyzed using some elementary phase plane analysis. For a dynamical system, a set in phase space is called a *global invariant* if the solution remains in this set for all time.

Our main results regarding the orientation dynamics are summarized as follows:

- *Global invariant*. All uniaxial states are global invariants of the orientation model.
- *Time-asymptotic stability.* The number of equilibrium states for the orientation model of the Doi–Smoluchowski equation hinges on whether the intensity α crosses two critical values: $\alpha = 4$ and 4.5. Moreover,
  - (i) if $0 < \alpha < 4$, only isotropic phase exists and is stable;
  - (ii) if $4 < \alpha < 4.5$, there are three equilibrium phases (one isotropic and two nematic prolate phases), among which both the isotropic phase and one nematic prolate phase are stable.
  - (iii) If $\alpha > 4.5$, there are three equilibrium phases (isotropic, nematic oblate and nematic prolate). Only the nematic prolate phase is stable.
- *Global orientation dynamics.* For small intensity $0 < \alpha < 4$, all states will evolve into the isotropic phase; for large intensity $\alpha > 4.5$, all states will evolve into the nematic prolate phase; for $4 < \alpha < 4.5$, any given initial state will evolve into either the isotropic phase or the stable phase of two nematic prolate phases, depending on whether such an initial state crosses a critical threshold.

We note that due to the use of closure approximation the critical intensities here are slightly different from those identified in [16]. Nevertheless the qualitative behavior and number of equilibrium states are the same. The global orientation dynamics described above is expected to be carried over to the full Doi–Smoluchowski equation (1).

This paper is organized as follows: in Section 2, we use the orientation tensor to reconfirm the uniaxial symmetry of equilibrium solutions and their sharp classification, obtained in [16]. The use of the orientation tensor makes phase transition picture more transparent. Section 3 is devoted to the closure approximation and derivation of the spectral dynamics of the orientation model. Finally in Section 4, time-asymptotic stability of equilibria and global phase behavior are obtained via the elementary phase plane analysis.

2. Uniaxial symmetry and number of equilibrium solutions

2.1. Uniaxial symmetry

Let $f(m)$ be a general local distribution of molecular orientations, the traceless order tensor Q is defined as

$$Q := \int_{|m|=1} \left(m \otimes m - \frac{1}{3} I \right) f(m) \mathrm{d}m.$$

The local physical properties are linked to the degree of symmetry of Q. The nematic is *biaxial* where the three eigenvalues of the order tensor are all different; it is uniaxial if two eigenvalues coincide; finally, it becomes isotropic if all three eigenvalues coincide.

Applying the usual eigendecomposition upon Q we obtain

$$Q = \lambda_1 e_1 \otimes e_1 + \lambda_2 e_2 \otimes e_2 + \lambda_3 e_3 \otimes e_3,$$

where λ_i is the i-th eigenvalue of Q, e_i is the corresponding right eigenvector. From now on we take $\{e_1, e_2, e_3\}$ as a local orthonormal basis.

Since $\mathrm{Tr}(Q) = \sum_j^3 \lambda_j = 0$, we introduce two independent parameters to express three eigenvalues

$$\alpha\lambda_1 = -a - \frac{b}{3}, \qquad \alpha\lambda_2 = a - \frac{b}{3},$$

$$\alpha\lambda_3 = \frac{2b}{3}, \quad \forall \alpha > 0. \tag{5}$$

Then we have

$$\alpha Q = a(e_2 \otimes e_2 - e_1 \otimes e_1) + b\left(e_3 \otimes e_3 - \frac{1}{3}I\right), \tag{6}$$

I is the unit tensor, a and b are given by

$$2a = \alpha Q : (e_2 \otimes e_2 - e_1 \otimes e_1),$$
$$\frac{2}{3}b = \alpha Q : (e_3 \otimes e_3), \tag{7}$$

where the operator : is the tensor inner product defined by $A : B = \mathrm{Tr}(A^\top B)$. From (7) it follows an α-free relation

$$3aQ : e_3 \otimes e_3 + bQ : (e_1 \otimes e_1 - e_2 \otimes e_2) = 0. \tag{8}$$

We consider the Doi–Onsager equation (3) with (4), the equilibrium distribution state is known to be determined by the Boltzmann relation

$$f = \frac{\mathrm{e}^{-U}}{\int_{|m|=1} \mathrm{e}^{-U}\mathrm{d}m} = \frac{\mathrm{e}^{-V}}{\int_{|m|=1} \mathrm{e}^{-V}\mathrm{d}m},$$

where, in virtue of the Maier–Saupe potential defined in (2), $U = V + \frac{2}{3}\alpha$ with

$$V = -m \otimes m : (\alpha Q) = a(m_1^2 - m_2^2) + b\left(\frac{1}{3} - m_3^2\right). \tag{9}$$

These together when inserted into (8) yield

$$F(a, b) = 0,$$

where

$$F(a, b) = \int_{|m|=1} [b(m_1^2 - m_2^2) + a(3m_3^2 - 1)]\mathrm{e}^{-V}\mathrm{d}m.$$

Clearly for any given $b \in \mathbb{R}$, one has

$$F(0, b) = F(\pm b, b) = 0.$$

It was shown in [16] that these are only zeros on the a–b plane, corresponding to three scenarios $\lambda_j = \lambda_k$, $j \neq k$. The uniaxial symmetry is thus confirmed. Considering the rotational symmetry we can give all possible equilibrium solutions in term of an order parameter η and a director $n \in \mathbb{S}^2$. In summary we state the following

Theorem 2.1 (*[16]*). *All equilibrium solutions to the Doi–Onsager equation (3) with the Maier–Saupe potential (2) are necessarily invariant with respect to rotations around a director $n \in \mathbb{S}^2$, i.e., it is uniaxially symmetric. Moreover, the distribution function may be expressed as*

$$f(m) = k\mathrm{e}^{\eta(m\cdot n)^2}, \quad k = \left[4\pi \int_0^1 \mathrm{e}^{bz^2}\mathrm{d}z\right]^{-1},$$

where $\eta \in \mathbb{R}$ is an order parameter.

Note that the director n is unspecified as a consequence of the rotational invariance of the equilibrium states.

2.2. Characterization of equilibrium solutions

We now study the structure and number of all equilibrium solutions, which are either isotropic or uniaxial. Without loss of generality, we consider the case where the axis of uniaxial symmetry is e_3, i.e. $a = 0$. Thus (9) gives

$$V = b\left(\frac{1}{3} - m_3^2\right).$$

Thereby the Boltzmann distribution takes the form

$$f = k\mathrm{e}^{bm_3^2}, \quad k = \left[4\pi \int_0^1 \mathrm{e}^{bz^2}\mathrm{d}z\right]^{-1}.$$

Note that b has to satisfy (7)

$$b = \frac{3\alpha}{2}Q : (e_3 \otimes e_3) = \frac{\alpha}{2}\left(3\int_{|m|=1} m_3^2 f(m)\mathrm{d}m - 1\right).$$

A simple calculation using spherical coordinates leads to

$$\alpha = \frac{2b}{12k\pi \int_0^1 z^2\mathrm{e}^{bz^2}\mathrm{d}z - 1} = G(b),$$

where

$$G(b) := \frac{\int_0^1 \mathrm{e}^{bz^2}\mathrm{d}z}{\int_0^1 z^2(1 - z^2)\mathrm{e}^{bz^2}\mathrm{d}z}.$$

Here $\alpha = G(b)$ indicates the relation between α and b, besides the isotropic case $b = 0$ for any $\alpha > 0$.

It is elementary to verify that the function $G(b)$ has the following property:

(1) $4 \le G(b) < \infty$, $G(0) = 7.5$ and $G'(0) = -5/7 < 0$;
(2) $G(\pm\infty) = \infty$.

The latter is evidenced by the following two asymptotic limits:

$$\lim_{b\to\infty} \frac{G(b)}{b} = 1, \qquad \lim_{b\to-\infty} \frac{G(b)}{|b|} = 2.$$

Further we can show that G has only one global minimum $\alpha^* \in (4, 7.5)$ at $b^* > 0$, whose numerical evaluation given in [16] is

$$\alpha^* = \min_b G(b) \approx 6.731393.$$

Uniqueness of the minimizer is implied by the fact that $G'' > 0$ whenever $G'(b) = 0$.

In order to justify this fact we set $\langle g\rangle := \int_0^1 g(z)\mathrm{e}^{bz^2}\mathrm{d}z$ and express G as

$$G = \langle 1\rangle / \langle z^2(1 - z^2)\rangle. \tag{10}$$

Differentiation in terms of b gives

$$G'(b)\langle z^2(1 - z^2)\rangle + G\langle z^4(1 - z^2)\rangle = \langle z^2\rangle.$$

For b where $G'(b) = 0$ we have

$$\langle z^2\rangle\langle z^2(1 - z^2)\rangle = \langle 1\rangle\langle z^4(1 - z^2)\rangle, \tag{11}$$

and further $G''(b)$ satisfies

$$G''(b)\langle z^2(1-z^2)\rangle + G\langle z^6(1-z^2)\rangle = \langle z^4\rangle.$$

This when combined with (10) and (11) yields

$$\begin{aligned} G''(b)\langle z^2(1-z^2)\rangle^2 &= \langle z^4\rangle\langle z^2(1-z^2)\rangle - \langle 1\rangle\langle z^6(1-z^2)\rangle \\ &= \langle z^4 - z^2\rangle\langle z^2(1-z^2)\rangle \\ &\quad - \langle 1\rangle\langle z^6(1-z^2) - z^4(1-z^2)\rangle \\ &= -\langle z^2(1-z^2)\rangle^2 + \langle 1\rangle\langle z^4(1-z^2)^2\rangle \end{aligned}$$

which, by the Hölder inequality, is clearly positive.

These properties of G enable us to arrive at the following

Theorem 2.2 (*[16]*). *The number of equilibrium solutions of the Doi–Onsager equation (3) on the sphere hinges on whether the intensity α crosses two critical values: $\alpha^* \approx 6.731393$ and 7.5, where*

$$\alpha^* = \min_{\eta} \frac{\int_0^1 e^{\eta z^2} dz}{\int_0^1 (z^2 - z^4) e^{\eta z^2} dz}. \tag{12}$$

All solutions are given explicitly by

$$f = k e^{\eta (m\cdot n)^2},$$

where $n \in \mathbb{S}^2$ is a parameter, $\eta = \eta(\alpha) \neq 0$ and $k = [4\pi \int_0^1 e^{\eta z^2} dz]^{-1}$ are determined by α through

$$\alpha = \frac{\int_0^1 e^{\eta z^2} dz}{\int_0^1 (z^2 - z^4) e^{\eta z^2} dz}. \tag{13}$$

More precisely,

(i) *If $0 < \alpha < \alpha^*$, there exists one solution $f_0 = 1/4\pi$.*

(ii) *If $\alpha = \alpha^*$, there exist two distinct solutions $f_0 = 1/4\pi$ and $f_1 = k_1 e^{\eta_1 (m\cdot n)^2}$, $\eta_1 > 0$.*

(iii) *If $\alpha^* < \alpha < 7.5$, there exist three distinct solutions $f_0 = 1/4\pi$ and $f_i = k_i e^{\eta_i (m\cdot m)^2}$, $\eta_i > 0$ $(i = 1, 2)$.*

(iv) *If $\alpha = 7.5$, there exist two distinct solutions $f_0 = 1/4\pi$ and $f_1 = k_1 e^{\eta_1 (m\cdot n)^2}$, $\eta_1 > 0$.*

(v) *If $\alpha > 7.5$, there exist three distinct solutions $f_0 = 1/4\pi$ and $f_i = k_i e^{\eta_i (m\cdot n)^2}$ $(i = 1, 2)$, $\eta_1 > 0$, $\eta_2 < 0$.*

3. Dynamics of orientation tensor

Having reviewed some remarkable properties of equilibrium states, we proceed to study dynamics of solutions to the Doi–Smoluchowski equation

$$\frac{\partial f}{\partial t} = \mathcal{R}\cdot(\mathcal{R} f + f \mathcal{R} U), \quad m \in \mathbb{S}^2, \tag{14}$$

with the Maier–Saupe potential (2). Eq. (14) is nonlinear and nonlocal for f, and its mathematical analysis is not trivial. In this context the phenomenological theory in nematics proves to be useful. De Gennes [6] showed that the dynamics of nematics is essentially described by the Landau theory of phase transition and proposed a phenomenological nonlinear equation for the orientation tensor Q:

$$\frac{\partial}{\partial t} Q = -L \frac{\partial A}{\partial Q},$$

where L is a phenomenological kinetic coefficient and A is the free energy, which, near transition point, can be expanded into the following form

$$A = K_2 \mathrm{Tr}(Q^2) + K_3 \mathrm{Tr}(Q^3) + K_4 \mathrm{Tr}(Q^4) + K_4'(\mathrm{Tr}(Q^2))^2,$$

where $K_2, \ldots, K_4'$ are constants. Doi and Edwards [5] derived a closed equation of this type from approximating the kinetic equation, which we will follow.

3.1. A closure system for orientation tensor

An evolution equation for the orientation order tensor is obtained from the Eq. (14) by taking the second moment over m to yield

$$\frac{d}{dt}\langle mm\rangle = -6\left\langle mm - \frac{1}{3} I\right\rangle - \langle \mathcal{R}\cdot U m + m\mathcal{R}\cdot U\rangle,$$

which for the Maier–Saupe potential leads to

$$\dot{Q} = -6Q + 2\alpha(Q\cdot\langle mm\rangle + \langle mm\rangle\cdot Q) - 4\alpha Q : \langle mmmm\rangle. \tag{15}$$

This equation governs the evolution of the structure in polymer solutions in the absence of flow and external forces.

Since the kinetic equation is difficult to solve, as usual we choose to use the moment equation to solve for the structure tensor Q. However, (15) involves the fourth rank tensor $\langle mmmm\rangle$, which must also be obtained. A closure problem arises because the evolution equation for $\langle mmmm\rangle$ involved the sixth rank tensor $\langle mmmmmm\rangle$. This requires closure approximation to express high-order moments in terms of lower ones. Following Doi [5], we employ the quadratic closure approximation

$$Q : \langle mmmm\rangle = Q : \langle mm\rangle\langle mm\rangle.$$

These approximations maintain the trace of the governing equations and are exact in the limit of perfect orientation order.

The resulting equation becomes

$$\dot{Q} = F(Q) \tag{16}$$

where

$$F(Q) := \left(\frac{4\alpha}{3} - 6\right) Q + 4\alpha Q^2 - 4\alpha \mathrm{Tr}(Q^2)\left(Q + \frac{1}{3} I\right).$$

Doi's equation for Q can be recovered by simply adding a factor D_r, an averaged rotational diffusion coefficient, and effects from the flow. As noted in [5], D_r may depend on Q because of the tube dilation.

3.2. Spectral dynamics of the structure tensor

It is usually difficult to quantify directly all entries in the structure tensor Q. As observed in the equilibrium case, eigenvalues of the orientation tensor play a special role in governing the entries of Q, in particular the orientation order of our interest. We now study the dynamics for the eigenvalues $\lambda(Q)$, which is real due to the symmetry of Q. We mention in passing that the spectral dynamics of velocity gradients has played very important roles in the study of a class of Eulerian flows [14]. The following lemma plays a key role.

Lemma 3.1. *Consider the closed dynamical system of Q, (16). Let $\lambda := \lambda(Q)$ be an eigenvalue of Q. Then the dynamics of λ is governed by the following*

$$\dot{\lambda} = \left(\frac{4\alpha}{3} - 6\right)\lambda + 4\alpha\lambda^2 - 4\alpha\sum_{j=1}^{3}\lambda_j^2\left(\lambda + \frac{1}{3}\right). \tag{17}$$

Proof. Let the left (right) eigenvectors of Q associated with λ be $l(r)$, normalized so that $lr = 1$. Then one has

$$Qr = \lambda r, \qquad lQ = \lambda l.$$

Differentiation of the first relation with respect to t yields

$$\dot{Q}r + Q\dot{r} = \dot{\lambda}r + \lambda\dot{r}.$$

Multiplying l on the left of the above equation and using $lQ = \lambda l$ we obtain

$$l\dot{Q}r = \dot{\lambda}.$$

It is clear that

$$lQ^2r = \lambda^2, \qquad \mathrm{Tr}(Q^2) = \sum_{j=1}^{3}\lambda_j^2.$$

A combination of above facts gives the Eq. (17) as asserted. □

By the spectral dynamics described above, we have a closed 3×3 dynamical system

$$\dot{\lambda}_i = \left(\frac{4\alpha}{3} - 6\right)\lambda_i + 4\alpha\lambda_i^2 - 4\alpha\sum_{j=1}^{3}\lambda_j^2\left(\lambda_i + \frac{1}{3}\right),$$
$$i = 1, 2, 3.$$

Taking the difference of any two equations indexed by i and k we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}(\lambda_i - \lambda_k) = (\lambda_i - \lambda_k)\left[\left(\frac{4\alpha}{3} - 6\right) + 4\alpha(\lambda_i + \lambda_k) - 4\alpha\sum_{j=1}^{3}\lambda_j^2\right], \quad i \neq k.$$

This implies that $\lambda_i = \lambda_k$ for $i \neq k$, corresponding to uniaxial equilibria, are global invariants. We can thus claim the following

Theorem 3.2. *The uniaxial symmetry of the orientation distribution function is preserved in time with the orientation model (16).*

The next natural question is whether an arbitrary distribution will become uniaxial as time evolves.

It follows from (5) that

$$\frac{2a}{\alpha} = \lambda_2 - \lambda_1, \qquad \lambda_3 - \lambda_2 = \frac{c}{\alpha}, \quad c := b - a.$$

In addition to the invariants $\lambda_1 = \lambda_2$ ($a = 0$) and $\lambda_2 = \lambda_3$ ($a = b$), the third invariant $\lambda_1 = \lambda_3$ corresponds to the line $b = -a$, that is $c = -2a$ in the a–c plane. The reduced system for (a, c) is

$$\dot{a} = aP(a, c), \quad P(a, c) := \left[\left(\frac{4\alpha}{3} - 6\right) - \frac{8}{3}(a + c) - \frac{8}{3\alpha}(4a^2 + 2ac + c^2)\right], \tag{18}$$

$$\dot{c} = cN(a, c), \quad N(a, c) := \left[\left(\frac{4\alpha}{3} - 6\right) + \frac{4}{3}(4a + c) - \frac{8}{3\alpha}(4a^2 + 2ac + c^2)\right]. \tag{19}$$

This is a polynomial dynamical system on a 2D plane. We shall investigate both the linear stability of equilibria and the global dynamics of general solutions via performing some phase portrait analysis.

4. Stability of equilibrium microstructure and global dynamics

4.1. Linear stability of equilibrium phases

Considering the order of eigenvalues and three invariants of the system (18)–(19), we restrict attention to an order $\lambda_1 < \lambda_2 < \lambda_3$, that is the first quadrant in the a–c plane. The other five regions can be discussed similarly.

First we observe that inside this region

$$N - P = 4(2a + c) > 0,$$

thus all possible equilibrium points necessarily lie on the boundary $\{(a, c), a = 0 \text{ or } c = 0\}$ corresponding to $\lambda_1 = \lambda_2 < \lambda_3$ or $\lambda_1 < \lambda_2 = \lambda_3$, respectively. We now check number of equilibria and their dynamic stability in terms of the intensity α.

On the c-axis, $a = 0$, the c-coordinate of equilibria must satisfy

$$cN(0, c) = c\left[\left(\frac{4\alpha}{3} - 6\right) + \frac{4}{3}c - \frac{8}{3\alpha}c^2\right] = 0,$$

that is $c = 0$ or $c = \frac{\alpha}{4}(1 \pm 3\sqrt{1 - 4/\alpha})$ for $\alpha \geq 4$; and on the a-axis, $c = 0$, the a-coordinate of equilibria must satisfy

$$aP(a, 0) = a\left[\left(\frac{4\alpha}{3} - 6\right) - \frac{8}{3}a - \frac{32}{3\alpha}a^2\right] = 0,$$

that is $a = 0$ or $a = \frac{\alpha}{8}(-1 \pm 3\sqrt{1 - 4/\alpha})$ for $\alpha \geq 4$.

Therefore there are three cases to be distinguished in terms of α:

(1) $0 < \alpha < 4$, $(0, 0)$ is the only equilibrium point of (18)–(19);

(2) $4 < \alpha < 4.5$, there are three zeros $(0, 0)$, $(0, c_1^*)$ and $(0, c_2^*)$ with

$$c_1^* = \frac{\alpha}{4}(1 + 3\sqrt{1 - 4/\alpha}) > c_2^* = \frac{\alpha}{4}(1 - 3\sqrt{1 - 4/\alpha}) > 0.$$

Note in this case other two equilibrium points $(a_1^*, 0)$ and $(a_2^*, 0)$ on c-axis lie on negative axis $a < 0$:

$$0 > a_1^* = \frac{\alpha}{8}(-1 + 3\sqrt{1 - 4/\alpha}) > a_2^* \\ = \frac{\alpha}{8}(-1 - 3\sqrt{1 - 4/\alpha}),$$

which are outside of the first quadrant of the a–c plane.
(3) $4.5 < \alpha$, there are three zeros $(0, 0)$, $(0, c_1^*)$ and $(a_1^*, 0)$ with $c_1^* > 0$ and $a_1^* > 0$.

In order to check the stability of (a^*, c^*), we look for solutions of the form $a(t) = a^* + \epsilon\bar{a}$ and $c(t) = c^* + \epsilon\bar{c}$, for small ϵ, the local dynamics of (a, c) is expected to be governed by the linearized system

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\bar{a}\\ \bar{c}\end{pmatrix} = A(a^*, c^*)\begin{pmatrix}\bar{a}\\ \bar{c}\end{pmatrix},$$

where $A(0, 0) = \left(\frac{4\alpha}{3} - 6\right) I$, for $(0, c^*)$

$$A(0, c^*) := \begin{pmatrix} -4c^* & 0 \\ \dfrac{16}{3\alpha}c^*(\alpha - c^*) & \dfrac{4c^*}{3\alpha}(\alpha - 4c^*)\end{pmatrix},$$

and for $(a^*, 0)$

$$A(a^*, 0) := \begin{pmatrix} -\dfrac{8a^*}{3\alpha}(\alpha + 8a^*) & -\dfrac{8}{3\alpha}a^*(\alpha + 2a^*) \\ 0 & 8a^*\end{pmatrix},$$

where relations satisfied by c^*, a^* have been used. The two eigenvalues of $A(0, 0)$ are $\frac{4\alpha}{3} - 6$, thus $(0, 0)$ is a stable nodal point for $\alpha < 4.5$ and becomes unstable for $\alpha > 4.5$.

Two eigenvalues for $A(0, c^*)$ are

$$\rho_1(c^*) = -4c^*, \qquad \rho_2(c^*) = \frac{4}{3\alpha}c^*(\alpha - 4c^*).$$

Thus for $4 < \alpha < 4.5$, $\rho_1(c_1^*) < 0$ and $\rho_2(c_1^*) < 0$, the equilibrium point $(0, c_1^*)$ is a stable node. Further $(0, c_2^*)$ is an unstable saddle since $\rho_1(c_2^*) < 0 < \rho_2(c_2^*)$.

For the case $\alpha > 4.5$, $(0, c_1^*)$ with $c_1^* > 0$ is a stable node and $(a_1^*, 0)$ with $a_1^* > 0$ is an unstable saddle since two eigenvalues for $A(a^*, 0)$:

$$\rho_1(a^*) = -\frac{8}{3\alpha}a^*(\alpha + 8a^*), \qquad \rho_2(a^*) = 8a^*,$$

have different sign for $a^* = a_1^*$. We thus have distinguished all cases.

We now examine the phase behavior. Note that for the equilibrium $(0, c^*)$ one has

$$\lambda_1 = \lambda_2 = -\frac{c^*}{3\alpha}, \qquad \lambda_3 = \frac{2c^*}{3\alpha}.$$

Here the two nematic phases given by the two solutions $c_1^* > c_2^* > 0$ make up a transcritical bifurcation from the isotropic state $c^* = 0$. Nematic phases that have prolate symmetry with $c^* > 0$ are referred to as "Nematic P". For equilibrium points $(a^*, 0)$ one has

$$\lambda_1 = \frac{-4a^*}{3\alpha}, \qquad \lambda_2 = \lambda_3 = \frac{2a^*}{3\alpha},$$

which for $a^* > 0$ gives the nematic oblate state, referred to as "Nematic O".

Thus the time-asymptotic stability of equilibria can be summarized in the following

Theorem 4.1. *The number of equilibrium states for the closed orientation model (16) of the Doi–Smoluchowski equation on the sphere hinges on whether the intensity* α *crosses two critical values:* $\alpha = 4$ *and* 4.5.
Moreover,

(i) *if* $0 < \alpha < 4$, *only isotropic phase exists and is stable;*

(ii) *if* $4 < \alpha < 4.5$, *there are three equilibrium phases, among which both the isotropic phase and one nematic P phase are stable, another nematic P phase is unstable.*

(iii) *if* $\alpha > 4.5$, *there are three equilibrium phases. Only the nematic P phase is stable, both isotropic and nematic O phases are unstable.*

Remark 4.2. (1) Due to the approximation nature of the closure system the critical intensities here are different from those stated in Section 2. Nevertheless the qualitative behavior and number of equilibrium states are the same. The dynamic stability is expected to be carried over to the full Doi–Smoluchowski equation.
(2) From the phase plane analysis, there exist up to seven equilibrium states, but for each spectral order, only three states are relevant. It is important to remember that these three equilibrium states are just three of the infinite number of possibilities, because the director $\{e_1, e_2, e_3\}$ can be oriented arbitrarily.
(3) Due to the uniaxial symmetry of the equilibrium states one may express the uniaxial orientational tensor by

$$Q = \eta\left(n \otimes n - \frac{1}{3}I\right),$$

with a scalar parameter η given by

$$\eta = \frac{3}{2}\langle (m \cdot n)^2\rangle - \frac{1}{2}.$$

Substitution into $F(Q) = 0$ gives

$$g(\eta) = \eta\left(\left(\frac{4\alpha}{3} - 6\right) + \frac{4\alpha}{3}\eta - \frac{8\alpha}{3}\eta^2\right) = 0,$$

which gives three distinct structural parameters

$$\eta_1 = 0, \qquad \eta_{2,3} = \frac{1}{4} \pm \frac{3}{4}\left[1 - \frac{4}{\alpha}\right]^{1/2}.$$

This can also lead to two critical intensities $\alpha = 4, 4.5$, as observed previously, see e.g. [1,5]. However the above simple decompositions can give a misleading dynamic picture. Since the dynamics is dictated by an one-dimensional equation, $\dot{\eta} = g(\eta)$, in which the destabilizing effects of fluctuations have been completely ignored. Therefore a faithful picture can not be observed.

4.2. Nonlinear stability and global dynamics

We shall explore a qualitative approach to examine the global orientation dynamics. One of the main ingredient to an understanding of the global dynamics of a given dynamical system is to identify the boundary of two regions with different phase behavior.

First for the case $0 < \alpha < 4$, there is only one stable equilibrium point $(0, 0)$ in finite plane. In the first quadrant of the vector field, $\dot{a} < 0$ and $\dot{c} < 0$, showing that all vector fields flow towards the origin. The system is dissipative and the $(0, 0)$ is globally stable.

When α crosses 4, bifurcation occurs and a new structural pattern forms for $4 < \alpha < 4.5$. There are three critical points: $(0, 0)$ stable node, $(0, c_1^*)$ stable node and $(0, c_2^*)$ saddle. For the saddle $(0, c_2^*)$ we have

$$(A(0, c_2^*) - \rho I)\xi = 0,$$

one has $\xi = (1, -1)^\top$ corresponding to $\rho_1 = -4c_2$ and $\xi_2 = (0, 1)^\top$ for $\rho_2 > 0$. Thus the unstable separatrix leaves $(0, c_2^*)$ along $a = 0$ and the stable one enters $(0, c_2^*)$ along $c = c_2^* - a$.

We now look at the level curve of vector fields of the system. From $P(a, c) = 0$ it follows

$$a^2 + \frac{1}{3}\left(a + c + \frac{\alpha}{2}\right)^2 = \frac{\alpha}{4}(\alpha - 3),$$

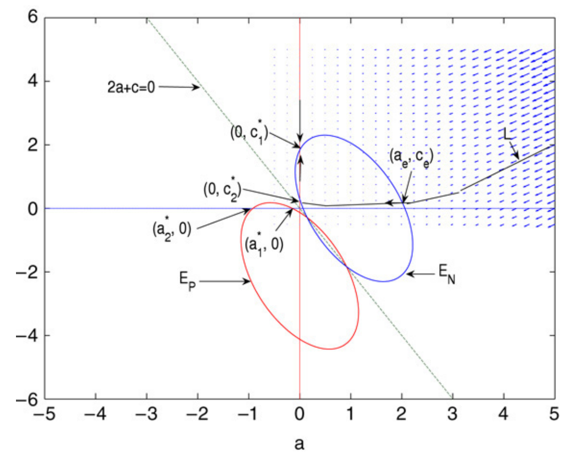
which is an ellipse, denoted by E_P, for $\alpha > 3$; and the set $N = 0$ can be written as

$$\left(a - \frac{\alpha}{4}\right)^2 + \frac{1}{3}\left(a + c - \frac{\alpha}{4}\right)^2 = \frac{\alpha}{4}(\alpha - 3),$$

also an ellipse E_N for $\alpha > 3$. Both ellipses intersect at two points on the line $2a + c = 0$ in the fourth quadrant for $3 < \alpha < 4.5$. Also the E_N intersects with $a = 0$ at two points $(0, c_1^*)$ and $(0, c_2^*)$. The stable separatrix approaches the saddle from inside the ellipse E_N, where $N > 0$ and $P < 0$, from the vector field (aP, cN) it follows that this trajectory must enter into the inside of E_N from its right, at say (a_e, c_e). Outside of E_N, both P and N are negative, no limit cycle exists. Thus the right branch of the stable manifold, L, will pass (a_e, c_e) and extend to the far field in negative time, and is uniquely defined by

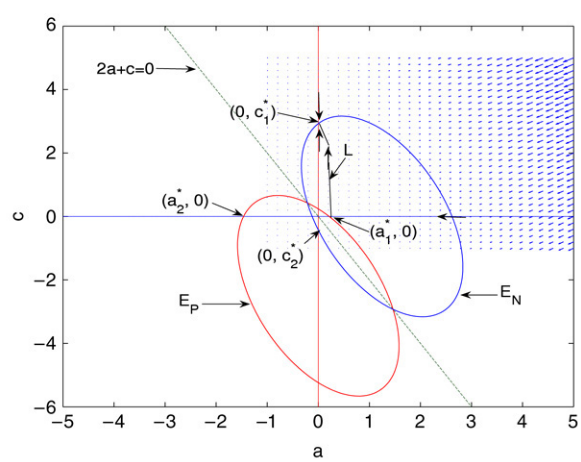
$$\frac{\mathrm{d}c}{\mathrm{d}a} = \frac{cN(a, c)}{aP(a, c)}, \qquad a(c_e) = a_e.$$

Thus the whole region $\{(a, c)|a \geq 0, c \geq 0\}$ is divided by L into two subregions. Any initial state from the upper region will be attracted to $(0, c_1^*)$ and those trajectories below the curve will be attracted to another stable node $(0, 0)$. Only initial states on L will approach the saddle $(0, c_2^*)$. Note that more information about 'behavior at infinity' can be obtained via the Poincaré compactification, though we do not present details here.



This figure shows what was described above.

We now turn to the global dynamics for the case $\alpha > 4.5$. In this case both E_N and E_P are still ellipses, but have overlap in the first quadrant. A phase field analysis shows that the one unstable separatrix of the saddle $(a_1^*, 0)$ will extend up and approach the stable node $(0, c_1^*)$. In this case the whole region is also divided by this separatrix into two regions, but trajectories in either region will be attracted to $(0, c_1^*)$; except for the states on $c = 0$ which will lead to the saddle $(a_1^*, 0)$ along $\{a \geq 0, c = 0\}$. In this case $(0, c_1^*)$ is a global stable equilibrium, see the following figure.



In summary we conclude the following

Theorem 4.3. *Consider the closed orientation model (16) of the Doi–Smoluchowski equation on the sphere. Given initial states lie in any region of a spectral order, then*

(i) *if $0 < \alpha < 4$, all initial states will evolve into the isotropic state;*

(ii) *if $4 < \alpha < 4.5$, there exists a critical threshold for the initial configuration. An initial state will evolve into either the isotropic phase or the stable phase of two nematic prolate phases, depending on whether such an initial state crosses the critical threshold.*

(iii) *If $\alpha > 4.5$, all initial states will evolve into the nematic prolate phase.*

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