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Characterization of stable kinetic equilibria of rigid, dipolar rod ensembles for coupled dipole–dipole and Maier–Saupe potentials

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Abstract

We study equilibria of the Smoluchowski equation for rigid, dipolar rod ensembles where the intermolecular potential couples the dipole–dipole interaction and the Maier–Saupe interaction. We thereby extend previous analytical results for the decoupled case of the dipolar potential only (Fatkullin and Slastikov 2005 *Nonlinearity* **18** 2565–80; Ji *et al Phys. Fluids* at press; Wang *et al* 2005 *Commun. Math. Sci.* **3** 605–20) or the Maier–Saupe potential only (Constantin *et al* 2004 *Arch. Ration. Mech. Anal.* **174** 365–84; Constantin *et al* 2004 *Discrete Contin. Dyn. Syst.* **11** 101–12; Constantin and Vukadinovic 2005 *Nonlinearity* **18** 441–3; Constantin 2005 *Commun. Math. Sci.* **3** 531–44; Fatkullin and Slastikov 2005 *Commun. Math. Sci.* **3** 21–6; Liu *et al* 2005 *Commun. Math. Sci.* **3** 201–18; Luo *et al* 2005 *Nonlinearity* **18** 379–89; Zhou *et al* 2005 *Nonlinearity* **18** 2815–25; Zhou and Wang *Commun. Math. Sci.* at press), and prove certain numerical observations for equilibria of coupled potentials (Ji *et al Phys. Fluids* at press). We first derive stability conditions, on the magnitude of the polarity vector (the first moment of the orientational probability distribution function) and on the direction of the polarity. We then prove that all stable equilibria of rigid, dipolar rod dispersions are either isotropic or prolate uniaxial. In particular, all stable anisotropic equilibrium distributions admit the following remarkable symmetry: the peak axis of orientation is aligned with both the polarity vector (first moment) and the distinguished director of the uniaxial second moment tensor. The stability is essential in establishing the axisymmetry. To demonstrate that the

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stability is indeed required, we show that there exist unstable non-axisymmetric equilibria.

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1. Introduction

The Smoluchowski equation describing the behaviour of rigid rod ensembles in a viscous solvent, often called rigid nematic polymers or rod-like dispersions, has recently received significant attention from analytical perspectives [4–7, 9–13, 15, 16, 18, 19]. The Smoluchowski equation provides more accurate descriptions based on physical principles than the mesoscopic orientation tensor equation with approximation closure rules. It is mathematically much more challenging. Led by Constantin *et al* [4–7], the mathematical groups started to study the Smoluchowki equation directly. Whereas most treatments have investigated equilibria with only the Maier–Saupe interaction, a couple of papers deal with rigid rod ensembles subject to only the dipole–dipole interaction without the Maier–Saupe interaction [11, 18]. Based on the formalism of Doi and Hess, a new kinetic theory for imposed kinematics of magnetic rod suspensions was recently proposed, and numerical solutions were calculated in simple flows [1, 2].

Prior to the coupling of an external hydrodynamic or magnetic field, it is prudent to first understand the space of quiescent equilibria of the Smoluchowski equation. When the individual rods are dipolar, and they are sufficiently crowded (semi-dilute) as to be affected by the Maier–Saupe interaction, this means that one must combine the analyses referenced above and address the coupling of the dipole–dipole interaction and the Maier–Saupe interaction. From this rigorous basis, one can then entertain imposed external fields. It is noteworthy that rigorous proofs for the Smoluchowski equation and its equilibrium distributions have only been provided in the last couple of years, for both limits of decoupled potentials, even though the essential results were known by formal arguments since Onsager's seminal paper [17], and modern numerical simulations have detailed the probability distributions for quite general interaction potentials.

This paper addresses equilibria of the Smoluchowski equation for fully coupled potentials. We are guided by recent numerical investigations [14], for which we prove the primary physical results regarding the properties of stable equilibria. In particular, it was shown in [14] that the polarity vector (first moment of the orientational probability distribution function (PDF)) of all anisotropic equilibria must be a principal axis of the second moment tensor of PDF. Several types of equilibria, all obeying this symmetry, are found using numerical continuation software, including isotropic, prolate and oblate uniaxial and biaxial states. For equilibria obeying this symmetry, the PDF reduces, in a coordinate system specified by the orthogonal frame of the second moment tensor, to a Boltzmann distribution parametrized by three order parameters and material parameters. This is the key analytical foundation for all previous rigorous analyses, which then proceed from the detailed properties of the Boltzmann parametrization; our analysis likewise begins from this representation of the PDF of the Smoluchowski equation for the coupled potential. From a physical perspective of observable PDFs for dipolar rigid rod ensembles in a viscous solvent, the primary result established in this paper is a proof of the numerical observation in [14]: all stable equilibria for coupled dipolar and Maier–Saupe potentials are either isotropic or prolate uniaxial. Thus, all oblate uniaxial and biaxial equilibria, which indeed exist, are necessarily unstable. We remark that this result significantly reduces any numerical computation of stable equilibria, since one may posit an appropriate Boltzmann distribution with symmetry reduced degrees of freedom! In order to prove the main result in the paper, a series of lemmas is developed. Each lemma addresses some aspects of the probability density function, which are essential in the proof of the main theorem.

2. Equilibria of rigid, dipolar rod ensembles or 'extended nematics'

We denote the inherent dipole of rigid rods by a unit vector $\boldsymbol{m}$, and let $\rho(\boldsymbol{m})$ denote the probability density function of the dipolar direction for the 'extended nematic' defined as ensembles of rigid rods with inherent dipoles. The evolution of the probability density function for the rod ensemble is governed by the Smoluchowski equation [8]:

$$\frac{\partial \rho}{\partial t} = D\frac{\partial}{\partial \boldsymbol{m}} \cdot \left(\frac{1}{k_B T} \frac{\partial U}{\partial \boldsymbol{m}} \rho + \frac{\partial \rho}{\partial \boldsymbol{m}} \right), \tag{1}$$

where $\partial/\partial \boldsymbol{m}$ is the orientational gradient operator [3], D the rotational diffusivity, k_B the Boltzmann constant and T the absolute temperature. For extended nematics, the total mean-field interaction potential $U(\boldsymbol{m})$ consists of two parts: the dipole–dipole interaction and the Maier–Saupe interaction,

$$U(\boldsymbol{m}) = -\alpha\langle \boldsymbol{m}\rangle \cdot \boldsymbol{m} - b\langle \boldsymbol{m} \otimes \boldsymbol{m}\rangle : \boldsymbol{m} \otimes \boldsymbol{m}, \tag{2}$$

where α denotes the strength of the dipole–dipole interaction and b represents the strength of the Maier–Saupe interaction. It should be pointed out that the mean-field interaction potential $U(\boldsymbol{m})$ is the part of the interaction potential *per molecule* that is proportional to the polymer concentration, which is the second virial coefficient of the chemical potential. In (2), for simplicity, we have normalized the potential by $k_B T$. In this paper, we consider the case of $\alpha > 0$, which means energetically a dipole tends to align with surrounding dipoles.

Equilibrium solutions of the Smoluchowski equation are given by the Boltzmann distribution [8]

$$\rho_{\text{eq}}(\boldsymbol{m}) = \frac{1}{Z}\exp[-U(\boldsymbol{m})], \qquad Z = \int_S \exp[-U(\boldsymbol{m})]\mathrm{d}\boldsymbol{m}, \tag{3}$$

where Z is the total partition function and $S = \{\boldsymbol{m} | \|\boldsymbol{m}\| = 1\}$ is the unit sphere. Notice that the Smoluchowski equation (1) is nonlinear: the mean-field interaction potential depends on $\langle \boldsymbol{m}\rangle$ and $\langle \boldsymbol{m} \otimes \boldsymbol{m}\rangle$ which, in turn, depends on the probability density. As a result, the Boltzmann distribution provides an implicit expression for equilibria. The nonlinear integral equation for $\langle \boldsymbol{m}\rangle$ is

$$\langle \boldsymbol{m}\rangle = \int_S \boldsymbol{m}\rho_{\text{eq}}(\boldsymbol{m})\mathrm{d}\boldsymbol{m}, \tag{4}$$

while the nonlinear integral equation for $\langle \boldsymbol{m} \otimes \boldsymbol{m}\rangle$ is

$$\langle \boldsymbol{m} \otimes \boldsymbol{m}\rangle = \int_S \boldsymbol{m} \otimes \boldsymbol{m}\rho_{\text{eq}}(\boldsymbol{m})\mathrm{d}\boldsymbol{m}. \tag{5}$$

Since $\langle \boldsymbol{m} \otimes \boldsymbol{m}\rangle$ is symmetric, it can be diagonalized by an orthogonal transformation. We choose a Cartesian coordinate system such that $\langle \boldsymbol{m} \otimes \boldsymbol{m}\rangle$ is diagonal. Furthermore, we select the positive direction of the z-axis such that if $\langle \boldsymbol{m}\rangle$ is not zero, then $\langle \boldsymbol{m}\rangle$ has a positive component along the z-axis. This choice of coordinates removes orientational degeneracy of all equilibria. Any orthogonal transformation of coordinates yields another equilibrium, so that isotropic equilibria are unchanged whereas any anisotropic equilibrium corresponds to an orthogonal group, S^2, of equilibria.

For the convenience of discussion below, we introduce notations for the components of $\langle \boldsymbol{m} \rangle$ and $\langle \boldsymbol{m} \otimes \boldsymbol{m} \rangle$ in the selected Cartesian coordinate system:

$$
\begin{aligned}
&\boldsymbol{m} = (m_1, m_2, m_3),\\
&q_i \equiv \langle m_i \rangle, \quad q_3 > 0 \qquad \text{if } (q_1, q_2, q_3) \neq 0,\\
&s_i \equiv \langle m_i^2 \rangle,\\
&U(\boldsymbol{m}) = -\alpha(q_1 m_1 + q_2 m_2 + q_3 m_3) - b(s_1 m_1^2 + s_2 m_2^2 + s_3 m_3^2).
\end{aligned} \tag{6}
$$

In this Cartesian coordinate system, an equilibrium is completely specified by $\{q_i, s_i, i = 1, 2, 3\}$. The nonlinear equations for $\{q_i, s_i\}$ are

$$q_i = \int_S m_i \rho_{\text{eq}}(\boldsymbol{m}) \mathrm{d}\boldsymbol{m}, \tag{7}$$

$$\delta_{ij} s_i = \int_S m_i m_j \rho_{\text{eq}}(\boldsymbol{m}) \mathrm{d}\boldsymbol{m}. \tag{8}$$

In the following, we present all theorems with respect to the coordinates above unless stated otherwise.

First, we recall the theorem proved in [14].

Theorem 1. *If an equilibrium solution satisfies $q_3 > 0$, then both q_1 and q_2 must vanish.*

This theorem states that the polarity vector, if non-zero, must be in the direction of one of the principal axes of the second order moment tensor. Next, we give an alternative proof of the theorem, which sets the stage for subsequent characterization of our principal focus: the symmetric subgroup of stable equilibria.

Proof of theorem 1. We prove $q_1 = 0$ by contradiction. Suppose there is a solution satisfying $q_3 > 0$ and $q_1 \neq 0$. We are going to show that $q_3 > 0$ and $q_1 \neq 0$ leads to $\frac{1}{q_1}\langle m_1 m_3 \rangle > 0$, which contradicts the selection of the Cartesian coordinate system:

$$
\begin{aligned}
\frac{1}{q_1}\langle m_1 m_3 \rangle &= \frac{1}{q_1 Z} \int_S m_1 m_3 \exp[-U(m_1, m_2, m_3)] \mathrm{d}\boldsymbol{m}\\
&= \frac{1}{q_1 Z} \int_{m_3 > 0} m_1 m_3 \{\exp[-U(m_1, m_2, m_3)] - \exp[-U(m_1, m_2, -m_3)]\} \mathrm{d}\boldsymbol{m}.
\end{aligned} \tag{9}
$$

In the above equation, the second factor of the integrand is

$$
\begin{aligned}
\gamma_1(m_1, m_2, m_3) &\equiv \exp[-U(m_1, m_2, m_3)] - \exp[-U(m_1, m_2, -m_3)]\\
&= 2\sinh(\alpha q_3 m_3) \exp(\alpha q_1 m_1) \exp[\alpha q_2 m_2 - U_{\text{MS}}(\boldsymbol{m})],
\end{aligned} \tag{10}
$$

where $U_{\text{MS}}(\boldsymbol{m}) = -b(s_1 m_1^2 + s_2 m_2^2 + s_3 m_3^2)$ is the Maier–Saupe potential, which is an even function of m_1, m_2 and m_3. Substituting into (9), we get

$$
\begin{aligned}
\frac{1}{q_1}\langle m_1 m_3 \rangle &= \frac{1}{q_1 Z} \int_{m3 > 0} m_1 m_3 \gamma_1(m_1, m_2, m_3) \mathrm{d}\boldsymbol{m}\\
&= \frac{1}{q_1 Z} \int_{m_1 > 0, m_3 > 0} m_1 m_3 \{\gamma_1(m_1, m_2, m_3) - \gamma_1(-m_1, m_2, m_3)\} \mathrm{d}\boldsymbol{m}\\
&= \frac{4}{Z} \int_{m_1 > 0, m_3 > 0} m_1 m_3 \sinh(\alpha q_3 m_3) \frac{\sinh(\alpha q_1 m_1)}{q_1} \times \exp[\alpha q_2 m_2 - U_{\text{MS}}(\boldsymbol{m})] \mathrm{d}\boldsymbol{m}.
\end{aligned} \tag{11}
$$

The integrand in (11) satisfies

$$m_1 m_3 \sinh(\alpha q_3 m_3) \frac{\sinh(\alpha q_1 m_1)}{q_1} \exp[\alpha q_2 m_2 - U_{\mathrm{MS}}(\boldsymbol{m})] > 0$$
$$\text{for } m_1 > 0,\ m_3 > 0,\ q_3 > 0 \text{ and } q_1 \neq 0. \tag{12}$$

It leads to $\frac{1}{q_1}\langle m_1 m_3 \rangle > 0$, which contradicts the selection of the Cartesian coordinate system. Therefore, we must have $q_1 = 0$; $q_2 = 0$ can be proved in a similar way.

To facilitate the analysis below, we introduce a lemma.

Lemma 1. *Let $\boldsymbol{u} = (u_1, u_2, \ldots, u_n)$ denote a point in the n-dimensional space. Consider a region A, which can be the whole n-dimensional space or an n-dimensional sub-region of the n-dimensional space or a lower-dimensional sub-region of the n-dimensional space (such as the unit sphere in the three-dimensional space). Consider a family of v-dependent probability density functions over the region A:*

$$\rho(\boldsymbol{u}, v) = \frac{1}{Z} \exp[v f_1(\boldsymbol{u}) + f_2(\boldsymbol{u})],$$
$$Z = \int_A \exp[v f_1(\boldsymbol{u}) + f_2(\boldsymbol{u})] \mathrm{d}\boldsymbol{u}. \tag{13}$$

Let $\langle\cdot\rangle$ denote the mean and var$\{\cdot\}$ denote the variance, taken with respect to the probability density $\rho(\boldsymbol{u}, v)$. Let us treat v as an independent variable and consider two functions:

$$g_1(v) \equiv \langle f_1(\boldsymbol{u})\rangle, \tag{14}$$
$$g_2(v) \equiv \langle f_1^2(\boldsymbol{u})\rangle. \tag{15}$$

We have the following

- If var$\{f_1(\boldsymbol{u})\} > 0$ for all v, then $g_1(v)$ is strictly increasing for all v.
- If var$\{f_1^2(\boldsymbol{u})\} > 0$ for all v and $g_2'(0) = 0$, then $g_2(v)$ is strictly increasing for all $v > 0$ and $g_2(v)$ is strictly decreasing for all $v < 0$.

Remark 1. The two conditions 'var$\{f_1(\boldsymbol{u})\} > 0$ for all v' and 'var$\{f_1^2(\boldsymbol{u})\} > 0$ for all v' are usually easy to verify. The only condition left to verify is $g_2'(0) = 0$.

Proof of lemma 1. Differentiating $\rho(\boldsymbol{u}, v)$ with respect to v gives

$$\frac{\mathrm{d}}{\mathrm{d}v}\rho(\boldsymbol{u}, v) = [f_1(\boldsymbol{u}) - \langle f_1(\boldsymbol{u})\rangle]\rho(\boldsymbol{u}, v). \tag{16}$$

From the derivative of the probability density, it follows immediately that

$$g_1'(v) = \langle f_1(\boldsymbol{u})[f_1(\boldsymbol{u}) - \langle f_1(\boldsymbol{u})\rangle]\rangle = \mathrm{var}\{f_1(\boldsymbol{u})\}. \tag{17}$$

Thus, var$\{f_1(\boldsymbol{u})\} > 0$ for all v implies that $g_1(v)$ is strictly increasing for all v.

To prove the property of $g_2(v)$, we point out a useful fact from calculus.

- Suppose function $f(v)$ satisfies $f'(v_0) = 0$ and further obeys the property that wherever $f'(v^*)$ is zero $f''(v^*)$ must be positive. Then we have $f'(v) > 0$ for all $v > v_0$ and $f'(v) < 0$ for all $v < v_0$.

It is important to point out that this simple fact of calculus allows us to study the global behaviour of a function from its local properties; this observation is key to our earlier analysis of equilibria of Maier–Saupe potentials [17]. Differentiating $g_2(v)$ yields

$$g_2'(v) = \langle f_1^2(\boldsymbol{u})[f_1(\boldsymbol{u}) - \langle f_1(\boldsymbol{u})\rangle]\rangle, \tag{18}$$

$$\begin{aligned} g_2''(v) &= \frac{\mathrm{d}}{\mathrm{d}v}\langle f_1^3(\boldsymbol{u})\rangle - \left(\frac{\mathrm{d}}{\mathrm{d}v}\langle f_1^2(\boldsymbol{u})\rangle\right)\cdot\langle f_1(\boldsymbol{u})\rangle - \langle f_1^2(\boldsymbol{u})\rangle\cdot\frac{\mathrm{d}}{\mathrm{d}v}\langle f_1(\boldsymbol{u})\rangle \\ &= \langle f_1^3(\boldsymbol{u})[f_1(\boldsymbol{u}) - \langle f_1(\boldsymbol{u})\rangle]\rangle - \langle f_1^2(\boldsymbol{u})[f_1(\boldsymbol{u}) - \langle f_1(\boldsymbol{u})\rangle]\rangle\cdot\langle f_1(\boldsymbol{u})\rangle \\ &\quad - \langle f_1^2(\boldsymbol{u})\rangle\cdot\langle f_1(\boldsymbol{u})[f_1(\boldsymbol{u}) - \langle f_1(\boldsymbol{u})\rangle]\rangle \\ &= \langle f_1^2(\boldsymbol{u})[f_1^2(\boldsymbol{u}) - \langle f_1^2(\boldsymbol{u})\rangle]\rangle - 2\langle f_1^2(\boldsymbol{u})[f_1(\boldsymbol{u}) - \langle f_1(\boldsymbol{u})\rangle]\rangle\langle f_1(\boldsymbol{u})\rangle \\ &= \mathrm{var}\{f_1^2(\boldsymbol{u})\} - 2g_2'(v)\langle f_1(\boldsymbol{u})\rangle. \end{aligned} \tag{19}$$

It is clear that function $g_2(v)$ satisfies the property that $g_2'(v^*) = 0$ implies $g_2''(v^*) > 0$. The condition of the lemma specifies that $g_2'(0) = 0$. From the simple fact of calculus we pointed out above that it follows that $g_2'(v) > 0$ for all $v > 0$ and $g_2'(v) < 0$ for all $v < 0$.

Theorem 2. *If an equilibrium solution satisfies $q_3 > 0$, then α and s_3 must satisfy $\alpha s_3 > 1$.*

Proof of theorem 2. We prove by contradiction. Suppose $\alpha s_3 \leqslant 1$. From theorem 1, we see that $q_3 > 0$ implies $q_1 = q_2 = 0$. The parameter q_3 has a fixed value in the equilibrium solution $\rho_{\mathrm{eq}}(\boldsymbol{m})$. Here we rename it v and treat it as an independent variable. We consider the probability density

$$\rho(\boldsymbol{m}, v) = \frac{1}{Z}\exp[\alpha v m_3 + b(s_1 m_1^2 + s_2 m_2^2 + s_3 m_3^2)],$$

$$Z = \int_S \exp[\alpha v m_3 + b(s_1 m_1^2 + s_2 m_2^2 + s_3 m_3^2)]\mathrm{d}\boldsymbol{m}.$$

Note that $\rho(\boldsymbol{m}, v)|_{v=q_3} = \rho_{\mathrm{eq}}(\boldsymbol{m})$. Consider the function

$$F(v) \equiv v - \langle m_3\rangle, \tag{20}$$

where the average $\langle\cdot\rangle$ is taken with respect to the probability density $\rho(\boldsymbol{m}, v)$ and is a function of v. $F(v)$ satisfies $F(0) = 0$ and $F(q_3) = 0$. We are going to show that $\alpha s_3 \leqslant 1$ implies that $F'(v) > 0$ for $v \in (0, q_3)$, which contradicts $F(0) = F(q_3) = 0$.
Differentiating with respect to v yields

$$\begin{aligned} &\frac{\partial}{\partial v}\rho(\boldsymbol{m}, v) = \alpha(m_3 - \langle m_3\rangle)\rho(\boldsymbol{m}, v), \\ &\frac{\mathrm{d}}{\mathrm{d}v}\langle m_3\rangle = \alpha\langle m_3\,(m_3 - \langle m_3\rangle)\rangle = \alpha\left(\langle m_3^2\rangle - \langle m_3\rangle^2\right), \\ &F'(v) = 1 - \alpha\langle m_3^2\rangle + \alpha\langle m_3\rangle^2. \end{aligned} \tag{21}$$

To show $F'(v) > 0$ for $v \in (0, q_3)$, we only need to show $\alpha\langle m_3^2\rangle < 1$ for $v \in (0, q_3)$. Because of the assumption $\alpha s_3 \leqslant 1$, we have $\alpha\langle m_3^2\rangle_{v=q_3} \leqslant 1$. Thus, to show $\alpha\langle m_3^2\rangle < 1$ for $v \in (0, q_3)$, we only need to show $\langle m_3^2\rangle$ is strictly increasing for $v > 0$.

Let us apply lemma 1 with A = the unit sphere, $f_1(\boldsymbol{m}) = \alpha m_3$ and $f_2(\boldsymbol{m}) = b(s_1 m_1^2 + s_2 m_2^2 + s_3 m_3^2)$. When $v = 0$, the probability density $\rho(\boldsymbol{m}, 0)$ is an even function of m_3. So the condition of part 2 of lemma 1 is satisfied:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}v}\langle f_1^2(\boldsymbol{m})\rangle|_{v=0} &= \langle f_1^2(\boldsymbol{m})[f_1(\boldsymbol{m}) - \langle f_1(\boldsymbol{m})\rangle]\rangle|_{v=0} \\ &= \alpha^3\langle m_3^3\rangle|_{v=0} - \alpha^3\langle m_3^2\rangle|_{v=0}\langle m_3\rangle|_{v=0} = 0. \end{aligned} \tag{22}$$

It follows from lemma 1 that $\langle m_3^2\rangle = \frac{1}{\alpha^2}\langle f_1^2(\boldsymbol{m})\rangle$ is strictly increasing for $v > 0$. This leads immediately to $F'(v) > 0$ for $v \in (0, q_3)$, which contradicts $F(0) = F(q_3) = 0$. Therefore, $\alpha s_3 > 1$.

3. Free energy and stability

Consider an arbitrary probability density $\rho(\boldsymbol{m})$, not necessarily an equilibrium probability density. The free energy of the probability density $\rho(\boldsymbol{m})$ is given by [11]

$$\begin{aligned} G[\rho] &= \int_S \rho(\boldsymbol{m}) \ln \rho(\boldsymbol{m}) \mathrm{d}\boldsymbol{m} - \frac{\alpha}{2}\int_S\int_S \boldsymbol{m}'\cdot\boldsymbol{m}\ \rho(\boldsymbol{m}')\rho(\boldsymbol{m})\mathrm{d}\boldsymbol{m}'\,\mathrm{d}\boldsymbol{m} \\ &\quad -\frac{b}{2}\int_S\int_S \boldsymbol{m}'\otimes\boldsymbol{m}' : \boldsymbol{m}\otimes\boldsymbol{m}\ \rho(\boldsymbol{m}')\rho(\boldsymbol{m})\mathrm{d}\boldsymbol{m}'\,\mathrm{d}\boldsymbol{m} \\ &= \int_S \rho(\boldsymbol{m}) \ln \rho(\boldsymbol{m}) \mathrm{d}\boldsymbol{m} - \frac{\alpha}{2}\langle\boldsymbol{m}\rangle\cdot\langle\boldsymbol{m}\rangle - \frac{b}{2}\langle\boldsymbol{m}\otimes\boldsymbol{m}\rangle : \langle\boldsymbol{m}\otimes\boldsymbol{m}\rangle \\ &\equiv G_{\mathrm{ent}}[\rho] + G_1[\rho] + G_2[\rho], \end{aligned} \tag{23}$$

where $G_{\mathrm{ent}}[\rho]$ is the entropic part of the free energy and $G_1[\rho]$ and $G_2[\rho]$ are the free energy parts corresponding to the two mutual interactions: dipole–dipole interaction and the Maier–Saupe interaction, respectively.

In the above $\langle\cdot\rangle$ denotes the mean taken with respect to the probability density $\rho(\boldsymbol{m})$. For the clarity of analysis below, we introduce different notations for means taken with respect to different probability densities.

- Let $\langle\cdot\rangle_{\mathrm{eq}}$ denote the mean taken with respect to the equilibrium probability density.
- Let $\langle\cdot\rangle$ denote the mean taken with respect to a general probability density (for example, a perturbed probability density near the equilibrium probability density).

Now we prove two theorems that relate the second moment, the dipole–dipole interaction strength (α) and the stability of equilibria.

Theorem 3. *If an equilibrium solution satisfies $q_i = 0$ and $\alpha s_i > 1$ for $i = 1$ or $i = 2$ or $i = 3$, then it is unstable.*

Proof of theorem 3. With the choice of coordinates, only q_3 may be non-zero. Without loss of generality, we prove the theorem for $i = 2$. To prove instability, we only need to show that the free energy $G[\rho]$ does not attain a local minimum at $\rho_{\mathrm{eq}}(\boldsymbol{m})$. More precisely, we show that if $\alpha s_2 > 1$, then there exists a perturbed probability density $\tilde{\rho}(\boldsymbol{m})$ arbitrarily close to the equilibrium probability density $\rho_{\mathrm{eq}}(\boldsymbol{m})$ such that

$$G[\tilde{\rho}(\boldsymbol{m})] < G[\rho_{\mathrm{eq}}(\boldsymbol{m})]. \tag{24}$$

We consider the perturbed probability density

$$\tilde{\rho}(\boldsymbol{m}) = (1 + \varepsilon m_2)\rho_{\mathrm{eq}}(\boldsymbol{m}). \tag{25}$$

Since $\langle m_2\rangle_{\mathrm{eq}} = q_2 = 0$, we have $\int_S \tilde{\rho}(\boldsymbol{m})\mathrm{d}\boldsymbol{m} = 1$, which indicates $\tilde{\rho}(\boldsymbol{m})$ is a probability density function. We calculate the three parts of the free energy with the perturbed probability density $\tilde{\rho}(\boldsymbol{m})$.

Using the Taylor expansion

$$(a + \Delta x)\ln(a + \Delta x) = a \ln a + [\ln a + 1]\Delta x + \frac{1}{2a}(\Delta x)^2 + \cdots, \tag{26}$$

we have

$$G_{\mathrm{ent}}[\tilde{\rho}] = \int_S \rho(\boldsymbol{m}) \ln \rho(\boldsymbol{m}) \mathrm{d}\boldsymbol{m}$$

$$= \int_S \rho_{\mathrm{eq}}(\boldsymbol{m}) \ln \rho_{\mathrm{eq}}(\boldsymbol{m}) \mathrm{d}\boldsymbol{m} + \varepsilon \int_S m_2 \rho_{\mathrm{eq}}(\boldsymbol{m})[\ln \rho_{\mathrm{eq}}(\boldsymbol{m}) + 1] \mathrm{d}\boldsymbol{m}$$

$$+ \varepsilon^2 \int_S m_2^2 \rho_{\mathrm{eq}}^2(\boldsymbol{m}) \frac{1}{2\rho_{\mathrm{eq}}(\boldsymbol{m})} \mathrm{d}\boldsymbol{m} + \cdots,$$

$$= G_{\mathrm{ent}}[\rho_{\mathrm{eq}}] + \varepsilon^2 \frac{1}{2} \langle m_2^2 \rangle_{\mathrm{eq}} + \cdots. \tag{27}$$

Because $q_1 = 0$ and $q_2 = 0$, the equilibrium probability density $\rho_{\mathrm{eq}}(\boldsymbol{m})$ is an even function of m_1 and m_2. The first moment of the perturbed probability density and $G_1[\tilde{\rho}]$ are

$$\langle \boldsymbol{m} \rangle = \langle \boldsymbol{m} \rangle_{\mathrm{eq}} + \varepsilon \langle \boldsymbol{m} m_2 \rangle_{\mathrm{eq}} = (0, 0, q_3) + \varepsilon\, (0, \langle m_2^2 \rangle_{\mathrm{eq}}, 0), \tag{28}$$

$$G_1[\tilde{\rho}] = -\frac{\alpha}{2} \langle \boldsymbol{m} \rangle \cdot \langle \boldsymbol{m} \rangle$$

$$= G_1[\rho_{\mathrm{eq}}] - \varepsilon^2 \frac{\alpha}{2} \langle m_2^2 \rangle_{\mathrm{eq}}^2. \tag{29}$$

The second moment of the perturbed probability density is

$$\langle \boldsymbol{m} \otimes \boldsymbol{m} \rangle = \langle \boldsymbol{m} \otimes \boldsymbol{m} \rangle_{\mathrm{eq}} + \varepsilon \langle \boldsymbol{m}\boldsymbol{m} m_2 \rangle_{\mathrm{eq}}$$

$$= \begin{pmatrix} s_1 & 0 & 0 \\ 0 & s_2 & 0 \\ 0 & 0 & s_3 \end{pmatrix} + \varepsilon \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \langle m_3 m_2^2 \rangle_{\mathrm{eq}} \\ 0 & \langle m_3 m_2^2 \rangle_{\mathrm{eq}} & 0 \end{pmatrix}. \tag{30}$$

Substituting the above into $G_2[\tilde{\rho}]$ yields

$$G_2[\tilde{\rho}] = \frac{b}{2} \langle \boldsymbol{m} \otimes \boldsymbol{m} \rangle : \langle \boldsymbol{m} \otimes \boldsymbol{m} \rangle$$

$$= G_2[\rho_{\mathrm{eq}}] - \varepsilon^2 b \langle m_3 m_2^2 \rangle_{\mathrm{eq}}^2. \tag{31}$$

Combining (27), (29) and (31) we obtain

$$G[\tilde{\rho}] - G[\rho_{\mathrm{eq}}] = \varepsilon^2 \frac{1}{2} \langle m_2^2 \rangle_{\mathrm{eq}} - \varepsilon^2 \frac{\alpha}{2} \langle m_2^2 \rangle_{\mathrm{eq}}^2 - \varepsilon^2 b \langle m_3 m_2^2 \rangle_{\mathrm{eq}}^2 + \cdots$$

$$\leqslant -\varepsilon^2 \frac{1}{2} s_2(\alpha s_2 - 1) + \cdots. \tag{32}$$

If $\alpha s_2 > 1$, then for ε sufficiently small we have $G[\tilde{\rho}] < G[\rho_{\mathrm{eq}}]$, which implies the equilibrium solution ρ_{eq} is unstable.

Theorem 4. *If an equilibrium solution satisfies $q_3 > 0$ and $s_3 \leqslant s_2$, then it is unstable.*

Proof of theorem 4. Theorem 1 shows that $q_3 > 0$ implies $q_1 = q_2 = 0$. It follows from theorem 2 that $q_3 > 0$ implies $\alpha s_3 > 1$. Combining these results with the condition $s_2 \geqslant s_3$, we obtain $q_2 = 0$ and $\alpha s_2 \geqslant \alpha s_3 > 1$. Theorem 3 implies that the equilibrium solution is unstable.

4. All stable solutions are axisymmetric

In this section, we show that all *stable* equilibrium solutions must be prolate uniaxial (axisymmetric). Note that the stability requirement is essential in establishing the axisymmetry. The existence of unstable non-axisymmetric equilibrium solutions is presented in the appendix.

We first recall the result proved for pure (non-dipolar) nematic rod ensembles where $\langle \boldsymbol{m} \rangle = 0$ [11, 19].

Theorem 5. *For pure nematics, the stable equilibria satisfy either* $s_1 = s_2 = s_3$ *(isotropic phase) or* $s_3 > s_1 = s_2$ *(prolate phase) in the selected coordinate system.*

Below for the case of extended nematic equilibria in which $\langle \boldsymbol{m} \rangle$ may be non-zero, we are going to show that if $\langle \boldsymbol{m} \rangle \neq 0$ (i.e. $q_1 = q_2 = 0$ and $q_3 > 0$ by the selection of the coordinate system and by the result of theorem 1), then a stable equilibrium solution must be uniaxial. Furthermore, the axis of symmetry must be the major director (i.e. the eigenvector of the second moment corresponding to the largest eigenvalue). That is, $\langle m_1^2 \rangle = \langle m_2^2 \rangle < \langle m_3^2 \rangle$.

Before we go into the details of proving the axisymmetry, let us describe the general approach we are going to use in the proof. A key step in the proof for the case of pure (non-dipolar) nematics is that we renamed b as v and treated v as an independent variable [19]. For pure nematics, we parametrized the probability function by introducing

$$r_i \equiv s_i - \langle m_i^2 \rangle_{v=0} \tag{33}$$

and proved that $h_i \equiv m_i^2 - \langle m_i^2 \rangle$ has the property

$$\langle h_3(h_1 - h_2) \rangle < 0 \qquad \text{if } r_1 > r_2. \tag{34}$$

Then the function

$$F(v) \equiv r_2(\langle m_1^2 \rangle - \langle m_1^2 \rangle_{v=0}) - r_1(\langle m_2^2 \rangle - \langle m_2^2 \rangle_{v=0})$$

satisfies $F(0) = F(b) = 0$, which will lead to a contradiction if the axisymmetry is violated. For the extended nematics, the definition of r_i is non-trivial. Note that for a definition of r_i to work in the proof, it has to preserve property (34). For the extended nematics, definition (33) does not preserve property (34). Lemmas 2–5 presented below are the intermediate steps leading to a successful definition of r_i for the extended nematics. Then finally in theorem 6, the results of these lemmas are used to prove the axisymmetry.

Lemma 2. *Consider a family of* r*-dependent probability density functions of* θ

$$\rho(\theta, r) = \frac{1}{Z} \exp[a_1 r^2 \cos 2\theta + a_4 r \cos\theta],$$

$$Z = \int_0^{2\pi} \exp[a_1 r^2 \cos 2\theta + a_4 r \cos\theta] \mathrm{d}\theta. \tag{35}$$

Let

$$g(r, a_1, a_4) \equiv \langle \cos 2\theta \rangle, \tag{36}$$

where the average is taken with respect to the probability density (35). If $a_1 > 0$, then $g(r, a_1, a_4)$ is a strictly increasing function of r for $r > 0$.

Note two aspects of this lemma. First, there is no condition imposed on a_4. Second, a special case of lemma 2 with $a_4 = 0$ was proved in [5] and was used in [19] to prove that all equilibria of pure (non-dipolar) nematic polymers are axisymmetric.

Proof of lemma 2. To prove lemma 2, let us replace r^2 by v_1, replace r by v_2 and treat v_1 and v_2 as two independent variables. a_1 and a_4 are treated as parameters. The probability density becomes

$$\rho(\theta, v_1, v_2) = \frac{1}{Z}\exp[a_1 v_1 \cos 2\theta + a_4 v_2 \cos\theta],$$

$$Z = \int_0^{2\pi} \exp[a_1 v_1 \cos 2\theta + a_4 v_2 \cos\theta]\mathrm{d}\theta. \quad (37)$$

Consider the function

$$g_3(v_1, v_2) \equiv \langle \cos 2\theta \rangle. \quad (38)$$

We first fix v_2 and treat v_1 as a variable. Let us apply lemma 1 with $A = [0, 2\pi]$, $f_1(\theta) = a_1 \cos 2\theta$ and $f_2(\theta) = a_4 v_2 \cos\theta$. Clearly, $\mathrm{var}(f_1) > 0$. It follows that $\langle f_1(\theta)\rangle = a_1\langle \cos 2\theta\rangle = a_1 g_3(v_1, v_2)$ is strictly increasing for all v_1, which means $g_3(v_1, v_2)$ is a strictly increasing function of v_1 for all v_1.

If $a_4 = 0$, then $g_3(v_1, v_2)$ does not depend on v_2. Suppose $a_4 \neq 0$. We fix v_1 and treat v_2 as a variable. Let us apply lemma 1 with $A = [0, 2\pi]$, $f_1(\theta) = a_4 \cos\theta$ and $f_2(\theta) = a_1 v_1 \cos 2\theta$. When $v_2 = 0$, expressing $\cos 2\theta = 2\cos^2\theta - 1$, we see that the probability density at $v_2 = 0$ is an even function of $\cos\theta$ which implies $\langle \cos^k\theta\rangle|_{v_2=0} = 0$ for any odd integer k. So the condition of part 2 of lemma 1 is satisfied: $\mathrm{var}(f_1^2) > 0$ and

$$\frac{\mathrm{d}}{\mathrm{d}v_2}\langle f_1^2(\theta)\rangle|_{v_2=0} = \langle f_1^2(\theta)[f_1(\theta) - \langle f_1(\theta)\rangle]\rangle|_{v_2=0}$$

$$= a_4^3\langle \cos^3\theta\rangle|_{v_2=0} - a_4^3\langle \cos^2\theta\rangle|_{v_2=0}\langle \cos\theta\rangle|_{v_2=0} = 0. \quad (39)$$

It follows that $\langle f_1^2(\theta)\rangle = a_4^2\langle \cos^2\theta\rangle = a_4^2\frac{g_3(v_1,v_2)+1}{2}$ is strictly increasing for all $v_2 > 0$, which means $g_3(v_1, v_2)$ is a strictly increasing function of v_2 for all $v_2 > 0$ if $a_4 \neq 0$. If $a_4 = 0$, $g_3(v_1, v_2)$ does not depend on v_2.

By definition, function g_3 is related to g by

$$g(r, a_1, a_4) = g_3(r^2, r). \quad (40)$$

Since $g_3(v_1, v_2)$ is a strictly increasing function of v_1 for all v_1 and is either independent of v_2 (if $a_4 = 0$) or a strictly increasing function of v_2 for $v_2 > 0$ (if $a_4 \neq 0$), we conclude that $g(r, a_1, a_4)$ is a strictly increasing function of r for $r > 0$.

Lemma 3. *Consider a family of v-dependent probability density functions of $\boldsymbol{m}$:*

$$\rho(\boldsymbol{m}, v) = \frac{1}{Z}\exp[c_4 m_3 + c_1 m_3^2 + v(c_2 m_2^2 + c_3 m_3^2)],$$

$$Z = \int_S \exp[c_4 m_3 + c_1 m_3^2 + v(c_2 m_2^2 + c_3 m_3^2)]\mathrm{d}\boldsymbol{m}. \quad (41)$$

Let $\langle\cdot\rangle$ denote the average taken with respect to $\rho(\boldsymbol{m}, v)$. Let $h_j \equiv m_j^2 - \langle m_j^2\rangle$. h_j has the properties

$$h_1 + h_2 + h_3 = 0,$$

$$\langle h_1\rangle = \langle h_2\rangle = \langle h_3\rangle = 0. \quad (42)$$

Suppose (c_1, c_2, c_3, c_4) satisfy the condition $c_1 + vc_3 > vc_2 > 0$ for all $v > 0$. For $v > 0$, we have

$$\langle h_1(h_3 - h_2)\rangle < 0,$$

$$\langle h_2(h_3 - h_1)\rangle < 0,$$

$$\langle h_3(h_2 - h_1)\rangle < 0. \quad (43)$$

Remark. $\langle h_1(h_3 - h_2)\rangle$ is the correlation of h_1 and $(h_3 - h_2)$.

Proof of lemma 3. Below we present the proof of $\langle h_1(h_3 - h_2)\rangle < 0$. $\langle h_2(h_3 - h_1)\rangle < 0$ and $\langle h_3(h_2 - h_1)\rangle < 0$ can be proved in a similar way.

Expressing in terms of m_1, m_2, m_3, we have

$$\langle h_1(h_3 - h_2)\rangle = \langle (m_1^2 - \langle m_1^2\rangle)(m_3^2 - m_2^2)\rangle. \tag{44}$$

We select the x-axis (the axis associated with m_1) as the direction of the pole of a spherical coordinate system (ϕ, θ). In the spherical coordinate system (ϕ, θ), we have

$$\begin{aligned}
&m_1 = \cos\phi, \qquad m_2 = \sin\phi\sin\theta, \qquad m_3 = \sin\phi\cos\theta,\\
&m_1^2 = \cos^2\phi,\\
&m_3^2 - m_2^2 = \sin^2\phi\cos 2\theta,\\
&c_4 m_3 + (c_1 + vc_3)m_3^2 + vc_2 m_2^2 = c_4\sin\phi\cos\theta + a_1\sin^2\phi\cos 2\theta + a_2\sin^2\phi,
\end{aligned} \tag{45}$$

where the coefficients a_1 and a_2 are

$$\begin{aligned}
a_1 &= \frac{c_1 + v(c_3 - c_2)}{2} > 0,\\
a_2 &= \frac{c_1 + v(c_3 + c_2)}{2}.
\end{aligned} \tag{46}$$

The probability density function (41) becomes

$$\begin{aligned}
\rho(\phi, \theta) &= \frac{1}{Z}\exp[a_1\sin^2\phi\cos 2\theta + c_4\sin\phi\cos\theta]\exp[a_2\sin^2\phi],\\
Z &= \int_0^{\pi}\int_0^{2\pi}\exp[a_1\sin^2\phi\cos 2\theta + c_4\sin\phi\cos\theta]\mathrm{d}\theta\,\exp[a_2\sin^2\phi]\sin\phi\,\mathrm{d}\phi.
\end{aligned} \tag{47}$$

We compare $\exp[a_1\sin^2\phi\cos 2\theta + c_4\sin\phi\cos\theta]$ with the probability density in lemma 2 and identify $(c_4, \sin\phi)$ with (a_4, r) in lemma 2. It follows that $\rho(\phi, \theta)/\int_0^{2\pi}\rho(\phi, \theta)\mathrm{d}\theta$ is a probability density function of θ and has the same form as the one in lemma 2. Applying lemma 2 gives

$$\int_0^{2\pi}\cos 2\theta\rho(\phi, \theta)\mathrm{d}\theta = g(\sin\phi, a_1, c_4)\int_0^{2\pi}\rho(\phi, \theta)\mathrm{d}\theta, \tag{48}$$

where $g(r, a_1, a_4)$ is defined in (36), and for $a_1 > 0$, $g(r, a_1, a_4)$ is a strictly increasing function of r for $r > 0$.

Let $\cos^2\phi_0 = \langle\cos^2\phi\rangle$. Writing $\langle h_1(h_3 - h_2)\rangle$ in spherical coordinates, we have

$$\begin{aligned}
\langle h_1(h_3 - h_2)\rangle &= \langle (m_1^2 - \langle m_1^2\rangle)(m_3^2 - m_2^2)\rangle\\
&= \int_0^{\pi}(\cos^2\phi - \cos^2\phi_0)\sin^2\phi\left(\int_0^{2\pi}\cos 2\theta\rho(\phi, \theta)\mathrm{d}\theta\right)\sin\phi\,\mathrm{d}\phi\\
&= \int_0^{\pi}(\cos^2\phi - \cos^2\phi_0)\sin^2\phi g(\sin\phi, a_1, c_4)\left(\int_0^{2\pi}\rho(\phi, \theta)\mathrm{d}\theta\right)\sin\phi\,\mathrm{d}\phi\\
&= \langle (\cos^2\phi - \cos^2\phi_0)\sin^2\phi g(\sin\phi, a_1, c_4)\rangle\\
&= \langle (\cos^2\phi - \cos^2\phi_0)[\sin^2\phi g(\sin\phi, a_1, c_4) - \sin^2\phi_0 g(\sin\phi_0, a_1, c_4)]\rangle < 0.
\end{aligned}$$

In the above we have used the fact that $\sin^2\phi g(\sin\phi, a_1, c_4)$ is a strictly increasing function of $\sin\phi$ and that $\cos^2\phi = 1 - \sin^2\phi$ is a strictly decreasing function of $\sin\phi$.

Lemma 4. *Consider a family of v-dependent probability density functions of* $\boldsymbol{m}$*:*

$$\rho(\boldsymbol{m}, v) = \frac{1}{Z}\exp[c_4 m_3 + c_1 m_3^2 + v(c_2 m_2^2 + c_3 m_3^2)],$$

$$Z = \int_S \exp[c_4 m_3 + c_1 m_3^2 + v(c_2 m_2^2 + c_3 m_3^2)]\mathrm{d}\boldsymbol{m}.$$

Let $\langle\cdot\rangle$ denote the average taken with respect to $\rho(\boldsymbol{m}, v)$. Suppose (c_1, c_2, c_3, c_4) satisfy the condition $c_1 + vc_3 > vc_2 > 0$ for all $v > 0$ and $c_4 \neq 0$. Then we have

1. $\langle m_3^2\rangle_{v=0}$ is a strictly increasing function of c_1 for all c_1;
2. $\langle m_3^2\rangle_{v=0} > \frac{1}{3} > \langle m_1^2\rangle_{v=0} = \langle m_2^2\rangle_{v=0}$;
3. for $v > 0$, $\langle m_3^2\rangle - \langle m_3^2\rangle_{v=0} > \langle m_2^2\rangle - \langle m_2^2\rangle_{v=0}$.

Remark. Note that condition $c_1 + vc_3 > vc_2 > 0$ for all $v > 0$ implies that $c_1 \geqslant 0$, $c_3 \geqslant c_2 > 0$.

Proof of lemma 4.
Proof of item 1. To prove that $\langle m_3^2\rangle_{v=0}$ is a strictly increasing function of c_1 for all c_1, we treat c_1 as the independent variable and fix $v = 0$ and other parameters. Applying lemma 1 with A = unit sphere, $f_1(\boldsymbol{m}) = m_3^2$, and $f_2(\boldsymbol{m}) = c_4 m_3$, we arrive at that $\langle m_3^2\rangle_{v=0}$ is a strictly increasing function of c_1 for all c_1.

Proof of item 2. For $c_1 \geqslant 0$, using item 1, we have

$$\langle m_3^2\rangle_{v=c_4=0} \geqslant \langle m_3^2\rangle_{v=c_1=c_4=0}. \tag{49}$$

Next we treat c_4 as the independent variable and fix $v = 0$ and other parameters. We apply lemma 1 with A = unit sphere, $f_1(\boldsymbol{m}) = m_3$ and $f_2(\boldsymbol{m}) = c_1 m_3^2$. It is straightforward to verify that the condition of lemma 1 is satisfied. Thus, we obtain that $\langle m_3^2\rangle_{v=0}$ is a strictly increasing function of c_4 for all $c_4 > 0$ and a strictly decreasing function of c_4 for all $c_4 < 0$. That is, $\langle m_3^2\rangle_{v=0}$ attains the global minimum at $c_4 = 0$. Thus, for $c_4 \neq 0$, we have

$$\langle m_3^2\rangle_{v=0} > \langle m_3^2\rangle_{v=c_4=0}. \tag{50}$$

When $c_1 = c_4 = v = 0$, the probability density gives a uniform distribution, which leads to

$$\langle m_3^2\rangle_{v=c_1=c_4=0} = \langle m_2^2\rangle_{v=c_1=c_4=0} = \langle m_1^2\rangle_{v=c_1=c_4=0} = \tfrac{1}{3}. \tag{51}$$

Combining (49), (50) and (51), we obtain

$$\langle m_3^2\rangle_{v=0} > \langle m_3^2\rangle_{v=c_4=0} \geqslant \langle m_3^2\rangle_{v=c_1=c_4=0} = \tfrac{1}{3}. \tag{52}$$

Using the fact $m_1^2+m_2^2+m_3^2 = 1$ and the fact that at $v = 0$ the probability density is independent of m_1 and m_2, we have

$$\langle m_1^2\rangle_{v=0} = \langle m_2^2\rangle_{v=0} = \tfrac{1}{2}(1 - \langle m_3^2\rangle_{v=0}) < \tfrac{1}{3}. \tag{53}$$

Proof of item 3. To prove item 3, we only need to show that for $v > 0$

$$\langle m_3^2\rangle - \langle m_2^2\rangle > \langle m_3^2\rangle_{v=0} - \langle m_2^2\rangle_{v=0}. \tag{54}$$

That is, $\langle m_3^2\rangle - \langle m_2^2\rangle$ is a strictly increasing function of v. Recall that h_j is defined as $h_j = m_j^2 - \langle m_j^2\rangle$ and satisfies $\langle h_j\rangle = 0$. Taking the derivative with respect to v, we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}v}\rho(\boldsymbol{m}, v) &= [c_3(m_3^2 - \langle m_3^2\rangle) + c_2(m_2^2 - \langle m_2^2\rangle)]\rho(\boldsymbol{m}, v)\\ &= [c_3h_3 + c_2h_2]\rho(\boldsymbol{m}, v),\\ \frac{\mathrm{d}}{\mathrm{d}v}\langle m_3^2 - m_2^2\rangle &= \langle (m_3^2 - m_2^2)(c_3h_3 + c_2h_2)\rangle\\ &= \langle (h_3 - h_2)(c_3h_3 + c_2h_2)\rangle\\ &= \left\langle (h_3 - h_2)\left(\frac{c_3 + c_2}{2}(h_3 + h_2) + \frac{c_3 - c_2}{2}(h_3 - h_2)\right)\right\rangle.\end{aligned}$$

Using $h_3 + h_2 = -h_1$ and using the result of lemma 3, we get

$$\frac{\mathrm{d}}{\mathrm{d}v}\langle m_3^2 - m_2^2\rangle = -\frac{c_3 + c_2}{2}\langle h_1(h_3 - h_2)\rangle + \frac{c_3 - c_2}{2}\langle (h_3 - h_2)^2\rangle > 0. \tag{55}$$

Here we have used $(c_3 + c_2)/2 > 0$, $(c_3 - c_2)/2 \geqslant 0$, $\langle h_1(h_3 - h_2)\rangle < 0$ and $\langle (h_3 - h_2)^2\rangle > 0$.

Lemma 5. *Consider the equilibrium probability density:*

$$\begin{aligned}\rho_{\mathrm{eq}}(\boldsymbol{m}) &= \frac{1}{Z}\exp[\alpha q_3 m_3 + b((s_2 - s_1)m_2^2 + (s_3 - s_1)m_3^2)],\\ Z &= \int_S \exp[\alpha q_3 m_3 + b((s_2 - s_1)m_2^2 + (s_3 - s_1)m_3^2)]\mathrm{d}\boldsymbol{m}.\end{aligned} \tag{56}$$

We first define functions $c_1(\sigma)$, $c_2(\sigma)$, $c_3(\sigma)$ and $c_4(\sigma)$ as follows:

$$\begin{aligned}c_1(\sigma) &\equiv b\frac{3\sigma - 1}{2},\\ c_2(\sigma) &\equiv s_2 - s_1,\\ c_3(\sigma) &\equiv s_3 - s_1 - \frac{3\sigma - 1}{2},\\ c_4(\sigma) &\equiv \alpha q_3,\end{aligned} \tag{57}$$

where q_3 and s_i $(i = 1, 2, 3)$ are the first and second moments of the equilibrium solution, respectively. We construct a family of (σ, v)-dependent probability density functions of the form (41):

$$\begin{aligned}\rho(\boldsymbol{m}, \sigma, v) &= \frac{1}{Z}\exp[c_4(\sigma)m_3 + c_1(\sigma)m_3^2 + v(c_2(\sigma)m_2^2 + c_3(\sigma)m_3^2)],\\ Z &= \int_S \exp[c_4(\sigma)m_3 + c_1(\sigma)m_3^2 + v(c_2(\sigma)m_2^2 + c_3(\sigma)m_3^2)]\mathrm{d}\boldsymbol{m}.\end{aligned} \tag{58}$$

It is straightforward to verify that

$$\rho(\boldsymbol{m}, \sigma, v)|_{v=b} = \rho_{\mathrm{eq}}(\boldsymbol{m}). \tag{59}$$

Let $\langle\cdot\rangle_\sigma$ be the mean taken with respect to probability density $\rho(\boldsymbol{m}, \sigma, v)$. We define a mapping $\eta = H(\sigma)$ as

$$\eta = H(\sigma) \equiv \langle m_3^2\rangle_\sigma|_{v=0}. \tag{60}$$

Using the value of η, we set parameters $c_1(\eta)$, $c_2(\eta)$, $c_3(\eta)$ and $c_4(\eta)$ and construct probability density $\rho(\boldsymbol{m}, \eta, v)$ by replacing $c_j(\sigma)$ in (58) with $c_j(\eta)$.

Suppose $q_3 > 0$. If σ satisfies the conditions

1. $\sigma \geqslant \frac{1}{3}$ and $H(\sigma) > \sigma$ (i.e. $\eta > \sigma$),
2. $c_1(\sigma) + vc_3(\sigma) > vc_2(\sigma) > 0$ for all $v > 0$,

then $\eta = H(\sigma)$ has the properties

1. $\eta > \frac{1}{3}$ and $H(\eta) > \eta$,
2. $c_1(\eta) + vc_3(\eta) > vc_2(\eta) > 0$ for all $v > 0$.

Remark. Mapping $\eta = H(\sigma)$ preserves the property $c_1 + vc_3 > vc_2 > 0$ for all $v > 0$. As long as this condition is satisfied, lemmas 3 and 4 can be applied. As we will see, lemmas 3 and 4 will play an essential role in the proof of the main result that all stable equilibrium solutions are either isotropic or prolate uniaxial.

Proof of lemma 5.
Proof of item 1. From item 1 of the condition: $\sigma \geqslant \frac{1}{3}$ and $\eta = H(\sigma) > \sigma$, we have $\eta > \frac{1}{3}$ and

$$c_1(\eta) = b\frac{3\eta - 1}{2} > b\frac{3\sigma - 1}{2} = c_1(\sigma) \geqslant 0. \tag{61}$$

Note that $c_4(\sigma) = \alpha q_3$ is independent of σ and that $\langle m_3^2 \rangle_{v=0}$ is independent of c_2 and c_3. In other words, $\langle m_3^2 \rangle_{v=0}$ depends on σ only through its dependence on c_1. Result 1 of lemma 4 shows that $\langle m_3^2 \rangle_{v=0}$ is a strictly increasing function of c_1. Thus, $c_1(\eta) > c_1(\sigma)$ gives us

$$H(\eta) = \langle m_3^2 \rangle_\eta |_{v=0} > \langle m_3^2 \rangle_\sigma |_{v=0} = H(\sigma) = \eta. \tag{62}$$

Proof of item 2. Now we prove $c_1(\eta) + vc_3(\eta) > vc_2(\eta) > 0$ for $v > 0$. Notice that $c_2(\sigma) = s_2 - s_1$ is independent of σ. So $vc_2(\eta) > 0$ for $v > 0$ follows directly from $vc_2(\sigma) > 0$ for $v > 0$. We have already obtained $c_1(\eta) > 0$. Hence, we only need to prove $c_3(\eta) - c_2(\eta) > 0$.

Item 2 of the condition, $c_1(\sigma) + vc_3(\sigma) > vc_2(\sigma) > 0$ for all $v > 0$, allows us to apply lemma 4 with probability density $\rho(\boldsymbol{m}, \sigma, v)$. Using result 3 of lemma 4 at $v = b$, we have

$$\langle m_3^2 \rangle_\sigma |_{v=0} = \eta,$$

$$\langle m_1^2 \rangle_\sigma |_{v=0} = \langle m_2^2 \rangle_\sigma |_{v=0} = \frac{1-\eta}{2},$$

$$s_3 - \langle m_3^2 \rangle_\sigma |_{v=0} - (s_2 - \langle m_2^2 \rangle_\sigma |_{v=0}) = s_3 - s_2 - \frac{3\eta - 1}{2} > 0,$$

which immediately leads to

$$c_3(\eta) - c_2(\eta) = s_3 - s_2 - \frac{3\eta - 1}{2} > 0. \tag{63}$$

Theorem 6. *If a stable equilibrium solution satisfies $q_3 > 0$, then $s_3 > s_1 = s_2$. Thus, all stable anisotropic equilibria obey prolate, uniaxial symmetry.*

Proof of theorem 6. We prove the conclusion in several steps.

Theorem 4 indicates that if an equilibrium solution with $q_3 > 0$ is stable, then we have $s_3 > s_1$ and $s_3 > s_2$. We need to show $s_1 = s_2$. We prove it by contradiction. Suppose $s_2 > s_1$.

Step 1. Let $\sigma_0 = \frac{1}{3}$. With the assumption $s_2 > s_1$, it is straightforward to verify that $c_1(\sigma_0) + vc_3(\sigma_0) > vc_2(\sigma_0) > 0$ for $v > 0$. This allows us to apply lemma 4. Result 2 of lemma 4 implies that $H(\sigma_0) = \langle m_3^2\rangle_{\sigma_0}|_{v=0} > \frac{1}{3} = \sigma_0$. Thus, the two conditions of lemma 5 are satisfied for $\sigma_0 = \frac{1}{3}$. Starting from $\sigma_0 = \frac{1}{3}$, we construct a sequence $\{\sigma_n\}$:

$$\sigma_k = H(\sigma_{k-1}). \tag{64}$$

Lemma 5 guarantees that for each new σ_k the two conditions of lemma 5 are satisfied and that $\sigma_k > \sigma_{k-1}$. Since σ_k is the average of m_3^2, we have $\sigma_k \leqslant 1$. So the sequence $\{\sigma_k\}$ is strictly increasing and bounded. Hence the sequence $\{\sigma_k\}$ has a well-defined limit as $k \to \infty$. Let $\sigma = \lim_{k\to\infty} \sigma_k$. Lemma 5 implies that $\sigma > \frac{1}{3}$. Let us introduce

$$r_3 \equiv s_3 - \sigma,$$
$$r_2 \equiv s_2 - \frac{1-\sigma}{2},$$
$$r_1 \equiv s_1 - \frac{1-\sigma}{2}.$$

We have

$$c_1(\sigma) = b\frac{3\sigma - 1}{2} > 0,$$
$$c_2(\sigma) = s_2 - s_1 = r_2 - r_1 > 0,$$
$$c_3(\sigma) = s_3 - s_1 - \frac{3\sigma - 1}{2} = r_3 - r_1.$$

Since the mapping $\sigma_k = H(\sigma_{k-1})$ preserves the property $c_1 + vc_3 > vc_2 > 0$ for $v > 0$, in the limit of $k \to \infty$, we have $c_3(\sigma) \geqslant c_2(\sigma)$. We already know that $c_1(\sigma) > 0$ and $c_2(\sigma) > 0$. Combining these results, we have

$$r_1 + r_2 + r_3 = 0,$$
$$r_3 \geqslant r_2 > r_1,$$
$$r_3 > 0, \qquad r_1 < 0,$$

and $c_1(\sigma), c_2(\sigma), c_3(\sigma)$ satisfy

$$c_1(\sigma) + vc_3(\sigma) > vc_2(\sigma) > 0, \qquad \text{for } v > 0.$$

Thus, lemmas 3 and 4 can be applied to the limit probability density, which has the form

$$\rho(\boldsymbol{m}, \sigma, v) = \frac{1}{Z}\exp[\alpha q_3 m_3 + b\frac{3\sigma - 1}{2}m_3^2 + v((r_2 - r_1)m_2^2 + (r_3 - r_1)m_3^2)],$$
$$Z = \int_S \exp[\alpha q_3 m_3 + b\frac{3\sigma - 1}{2}m_3^2 + v((r_2 - r_1)m_2^2 + (r_3 - r_1)m_3^2)]\mathrm{d}\boldsymbol{m}. \tag{65}$$

The limit probability density $\rho(\boldsymbol{m}, \sigma, v)$ satisfies

$$\langle m_3^2\rangle|_{v=0} = \sigma,$$
$$\langle m_1^2\rangle|_{v=0} = \langle m_2^2\rangle|_{v=0} = \frac{1 - \langle m_3^2\rangle|_{v=0}}{2} = \frac{1-\sigma}{2},$$
$$\langle m_2^2\rangle|_{v=b} - \langle m_2^2\rangle|_{v=0} = s_2 - \frac{1-\sigma}{2} = r_2,$$
$$\langle m_1^2\rangle|_{v=b} - \langle m_1^2\rangle|_{v=0} = s_1 - \frac{1-\sigma}{2} = r_1.$$

Here for simplicity we write $\langle\cdot\rangle_\sigma$ simply as $\langle\cdot\rangle$.

Step 2. Consider the function

$$F(v) \equiv r_2(\langle m_1^2\rangle - \langle m_1^2\rangle_{v=0}) - r_1(\langle m_2^2\rangle - \langle m_2^2\rangle_{v=0}). \tag{66}$$

$F(v)$ satisfies $F(0) = F(b) = 0$. Using the supposition $s_2 > s_1$, we are going to show that $F'(v) < 0$ for $v > 0$, which contradicts $F(0) = F(b) = 0$. Let $h_j \equiv m_j^2 - \langle m_j^2\rangle$. (h_1, h_2, h_3) satisfies

$$\begin{aligned} &h_1 + h_2 + h_3 = 0,\\ &\langle h_1\rangle = \langle h_2\rangle = \langle h_3\rangle = 0. \end{aligned} \tag{67}$$

Using the result of lemma 3, we have

$$\langle h_1(h_3 - h_2)\rangle < 0,$$

$$\langle h_2(h_3 - h_1)\rangle < 0,$$

$$\langle h_3(h_2 - h_1)\rangle < 0,$$

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}v}\rho(\boldsymbol{m}, \sigma, v) &= [(r_3 - r_1)(m_3^2 - \langle m_3^2\rangle) + (r_2 - r_1)(m_2^2 - \langle m_2^2\rangle)]\rho(\boldsymbol{m}, v)\\ &= (r_3h_3 + r_2h_2 + r_1h_1)\rho(\boldsymbol{m}, v)\\ &= [(r_3 - r_2)h_3 + (r_1 - r_2)h_1]\rho(\boldsymbol{m}, v), \end{aligned} \tag{68}$$

$$\begin{aligned} F'(v) &= r_2\langle m_1^2[(r_3 - r_2)h_3 + (r_1 - r_2)h_1]\rangle - r_1\langle m_2^2[(r_3 - r_2)h_3 + (r_1 - r_2)h_1]\rangle\\ &= \langle (r_2h_1 - r_1h_2)[(r_3 - r_2)h_3 + (r_1 - r_2)h_1]\rangle. \end{aligned} \tag{69}$$

Using $r_1 + r_2 = -r_3$, we have

$$r_2h_1 - r_1h_2 = \tfrac{1}{2}[r_3(h_2 - h_1) + (r_2 - r_1)(h_1 + h_2)]. \tag{70}$$

On the other hand, using $r_2 + r_3 = -r_1$ and adding $r_1(h_1 + h_2 + h_3) = 0$ to it, we have

$$\begin{aligned} r_2h_1 - r_1h_2 &= \tfrac{1}{2}[(r_2 - r_3)h_1 + (r_2 + r_3)h_1 - 2r_1h_2]\\ &= \tfrac{1}{2}[(r_2 - r_3)h_1 - r_1h_1 - 2r_1h_2 + r_1(h_1 + h_2 + h_3)]\\ &= \tfrac{1}{2}[(r_3 - r_2)(h_2 + h_3) + r_1(h_3 - h_2)]. \end{aligned}$$

Substituting these two expressions for $r_2h_1 - r_1h_2$ into $F'(v)$, we obtain

$$\begin{aligned} F'(v) &= \tfrac{1}{2}\langle [r_3(h_2 - h_1) + (r_2 - r_1)(h_1 + h_2)](r_3 - r_2)h_3\rangle\\ &\quad + \tfrac{1}{2}\langle [(r_3 - r_2)(h_2 + h_3) + r_1(h_3 - h_2)](r_1 - r_2)h_1\rangle\\ &= \tfrac{1}{2}r_3(r_3 - r_2)\langle h_3(h_2 - h_1)\rangle + \tfrac{1}{2}(r_2 - r_1)(r_3 - r_2)\langle h_3(h_2 + h_1)\rangle\\ &\quad - \tfrac{1}{2}(r_2 - r_1)(r_3 - r_2)\langle h_1(h_2 + h_3)\rangle + \tfrac{1}{2}(-r_1)(r_2 - r_1)\langle h_1(h_3 - h_2)\rangle\\ &= \tfrac{1}{2}r_3(r_3 - r_2)\langle h_3(h_2 - h_1)\rangle + \tfrac{1}{2}(r_2 - r_1)(r_3 - r_2)\langle h_2(h_3 - h_1)\rangle\\ &\quad + \tfrac{1}{2}(-r_1)(r_2 - r_1)\langle h_1(h_3 - h_2)\rangle. \end{aligned} \tag{71}$$

In the above expression, all coefficients are non-negative and all correlations are negative. The coefficient of the third term $(-r_1)(r_2 - r_1)$ is strictly positive. So the sum must be strictly negative. That is, $F'(v) < 0$ for $v > 0$, which contradicts $F(0) = F(b) = 0$. Therefore, we conclude $s_1 = s_2$.

For an axisymmetric equilibrium with the z-axis as the axis of symmetry, we have

$$s_1 = s_2 = \frac{1 - s_3}{2}.$$

So a stable equilibrium state of the extended nematic polymers is completely specified by the values of q_3 and s_3. The nonlinear integral equation for q_3 and s_3 is

$$q_3 = \int_S m_3 \rho_{\mathrm{eq}}(\boldsymbol{m}) \mathrm{d}\boldsymbol{m},$$

$$s_3 = \int_S m_3^2 \rho_{\mathrm{eq}}(\boldsymbol{m}) \mathrm{d}\boldsymbol{m}, \tag{72}$$

where the equilibrium probability density is given by

$$\rho_{\mathrm{eq}}(\boldsymbol{m}) = \frac{1}{Z} \exp\left[\alpha q_3 m_3 + b \frac{3s_3 - 1}{2} m_3^2\right],$$

$$Z = \int_S \exp\left[\alpha q_3 m_3 + b \frac{3s_3 - 1}{2} m_3^2\right] \mathrm{d}\boldsymbol{m}. \tag{73}$$

Numerical solutions of equation (72) have been carried out in [14]. The solution structure, affected by two parameters α and b, appears to be significantly more complicated than that of pure (non-dipolar) nematics. The theoretical study of the solution structure of equation (72) will be the subject of a future work.

5. Conclusions

The stable equilibria of rigid, dipolar rod ensembles (so-called extended nematics) are shown to be either isotropic or prolate uniaxial. Furthermore, the distinguished axis of symmetry of stable anisotropic equilibria is identical to the first moment of the PDF (the polarity vector) and the major director of the second moment of the PDF (eigenvector associated with the largest principal value). The property of axisymmetry greatly simplifies any procedure for obtaining physically observable equilibria, whether it is numerical or some form of asymptotic approximation scheme involving closure models. We anticipate the analytical approach developed in this paper can be extended to Smoluchowski equations with more complex potentials or with external fields.

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Appendix. Existence of unstable non-axisymmetric equilibrium solutions

In this appendix, we show that the *extended* nematic polymers do admit non-axisymmetric equilibrium states if the stability requirement is removed. Specifically, we only need to show the existence of a non-axisymmetric equilibrium state for one set of (b, α).

Theorem 1 shows that if $q_3 \neq 0$ then we must have $q_1 = q_2 = 0$. Using this result, we simplify the nonlinear equations (7) and (8) to

$$q_3 = \int_S m_3 \rho_{\rm eq}(\boldsymbol{m}) {\rm d}\boldsymbol{m}, \tag{74}$$

$$s_i = \int_S m_i^2 \rho_{\rm eq}(\boldsymbol{m}) {\rm d}\boldsymbol{m}, \quad i = 1, 2, 3 \tag{75}$$

where the equilibrium probability density is given by

$$\rho_{\rm eq}(\boldsymbol{m}) = \frac{1}{Z} \exp[\alpha q_3 m_3 + b(s_1 m_1^2 + s_2 m_2^2 + s_3 m_3^2)],$$

$$Z = \int_S \exp[\alpha q_3 m_3 + b(s_1 m_1^2 + s_2 m_2^2 + s_3 m_3^2)] {\rm d}\boldsymbol{m}. \tag{76}$$

Note that the equilibrium probability density $\rho_{\rm eq}(\boldsymbol{m})$ depends on α and q_3 only through its dependence on the combination $\lambda \equiv \alpha q_3$. Once the value of $\lambda \equiv \alpha q_3$ is given, $\rho_{\rm eq}(\boldsymbol{m})$ no longer depends on the individual value of α or q_3. The key in constructing non-axisymmetric equilibrium solutions is to treat $\lambda \equiv \alpha q_3$ as a parameter and to satisfy equation (74) by adjusting the value of α. Mathematically, with the introduction of $\lambda \equiv \alpha q_3$ as the new parameter and with α as the new unknown, equation (74) becomes

$$\frac{\lambda}{\alpha} = \int_S m_3 \rho_{\rm eq}(\boldsymbol{m}) {\rm d}\boldsymbol{m}. \tag{77}$$

Using the constraint $s_1 + s_2 + s_3 = 1$, we see that only the first two component equations in (75) are needed; the third component equation follows automatically from the first two. We keep s_1 and s_2 as the unknowns and write $s_3 = 1 - s_1 - s_2$. Below is our new formulation:

- we treat s_1, s_2 and α as unknowns;
- we treat b and λ as parameters;
- we have three equations: (77) plus the first two components of (75).

The equilibrium probability density has the form

$$\rho_{\rm eq}(\boldsymbol{m}; s_1, s_2; b, \lambda) = \frac{1}{Z} \exp[\lambda m_3 + b(s_1 m_1^2 + s_2 m_2^2 + (1 - s_1 - s_2) m_3^2)],$$

$$Z = \int_S \exp[\lambda m_3 + b(s_1 m_1^2 + s_2 m_2^2 + (1 - s_1 - s_2) m_3^2)] {\rm d}\boldsymbol{m}. \tag{78}$$

If $\lambda = 0$, then both sides of (77) are identically zero and equation (77) is automatically satisfied. If $\lambda \neq 0$, the equilibrium probability density can be written as

$$\rho_{\rm eq}(\boldsymbol{m}) = \exp(\lambda m_3) \times (\text{an even function of } \boldsymbol{m}).$$

Hence, the right side of (77) is non-zero and is of the same sign as λ. It follows that equation (77) can always be satisfied by selecting a suitable positive value for α. Therefore, in our new formulation with $\lambda \equiv \alpha q_3$ as a parameter and α as an unknown, we gain the freedom of being able to solve for α separately from equation (77) after (s_1, s_2) has been determined. The equation for (s_1, s_2) is

$$s_1 = \int_S m_1^2 \rho_{\rm eq}(\boldsymbol{m}) {\rm d}\boldsymbol{m}, \qquad s_2 = \int_S m_2^2 \rho_{\rm eq}(\boldsymbol{m}) {\rm d}\boldsymbol{m}. \tag{79}$$

Note that in the new formulation, α does not appear in the equation for (s_1, s_2) (79). This feature of the new formulation is very useful for our purpose of demonstrating the existence of non-axisymmetric equilibrium solutions. Before we go into details, let us outline the steps we will take in constructing a non-axisymmetric equilibrium solution.

- We first solve equation (79) for $\lambda = 0$. Specifically, we take $b = 8$ and pick the prolate solution $(s_1^{(0)}, s_2^{(0)})$ whose major director is parallel to the y-axis.
- For general λ, we write equation (79) as a variational problem by introducing energy function $G_1(s_1, s_2, \lambda)$. We prove that $(s_1^{(0)}, s_2^{(0)})$ (the solution we pick for $\lambda = 0$) is an isolated global minimizer of $G_1(s_1, s_2, 0)$.
- Since $(s_1^{(0)}, s_2^{(0)})$ is an isolated global minimizer of $G_1(s_1, s_2, 0)$, we can find a small rectangle centred around $(s_1^{(0)}, s_2^{(0)})$ such that the minimum of $G_1(s_1, s_2, 0)$ on the boundary of rectangle is strictly larger than $G_1(s_1^{(0)}, s_2^{(0)}, 0)$.
- We show that $\partial G_1(s_1, s_2, \lambda)/\partial\lambda$ is uniformly bounded by 1 for all values of (s_1, s_2, λ). So we can find a small positive λ_1 such that the minimum of $G_1(s_1, s_2, \lambda_1)$ on the boundary of rectangle is strictly larger than $G_1(s_1^{(0)}, s_2^{(0)}, \lambda_1)$, which implies that as a function of (s_1, s_2), $G_1(s_1, s_2, \lambda_1)$ attains a minimum inside the rectangle. Therefore, for $\lambda = \lambda_1$ equation (79) has a solution near $(s_1^{(0)}, s_2^{(0)})$ (the solution we pick for $\lambda = 0$).
- Finally, we show that the solution we constructed in this way for $\lambda = \lambda_1$ is indeed non-axisymmetric.

We start with the case of $\lambda = 0$. In this case, equation (79) with equilibrium probability density given in (78) reduces to the case of pure (non-dipolar) nematic polymers. From the theoretical results of pure nematic polymers [11, 15, 19], we know that for $b > 7.5$ there is only one family of rotation-equivalent prolate equilibrium states. In the analysis below we fix $b = 8$. We select the prolate equilibrium state whose major director is parallel to the y-axis. Thus, for $\lambda = 0$, a solution of equation (79) is given by

$$s_1^{(0)} = \frac{1}{3} - \frac{1}{3}s^{(0)} < \frac{1}{3}, \qquad s_2^{(0)} = \frac{1}{3} + \frac{2}{3}s^{(0)} > \frac{1}{3}, \tag{80}$$

where $s^{(0)} \equiv \frac{3}{2}(\langle m_2^2\rangle - \frac{1}{3}) > 0$ is the order parameter of the prolate solution. Here we use the notations $(s_1^{(0)}, s_2^{(0)})$ to show explicitly that the solution corresponds to the case of $\lambda = 0$. In order to construct a non-axisymmetric solution, we introduce two energy functions for probability density of the form (78), which is completely specified by $(s_1, s_2;\ \lambda)$. Recall that b has been fixed at $b = 8$. We first rewrite equation (79) as a variational problem by introducing the energy function

$$G_1(s_1, s_2; \lambda) \equiv \frac{b}{2}(s_1^2 + s_2^2 + (1 - s_1 - s_2)^2) - \ln Z, \tag{81}$$

where the partition function Z is given in (78). Here s_1 and s_2 are treated as independent variables while b and λ are treated as parameters. It is straightforward to verify that a critical point of energy function G_1 is equivalent to a solution of equation (79). Furthermore, we have the theorem below.

Theorem A1. *$(s_1^{(0)}, s_2^{(0)})$ is an isolated global minimizer of $G_1(s_1, s_2;\ 0)$.*

Proof of theorem A1. In the proof, λ is fixed at $\lambda = 0$. We consider the free energy of pure nematic (non-dipolar) polymers for probability density of the form (78):

$$G_2(s_1, s_2) \equiv \int_S \rho(\boldsymbol{m}) \ln \rho(\boldsymbol{m}) \mathrm{d}\boldsymbol{m} - \frac{b}{2}\langle \boldsymbol{m} \otimes \boldsymbol{m}\rangle : \langle \boldsymbol{m} \otimes \boldsymbol{m}\rangle. \tag{82}$$

In [11], it was concluded that for $b > 7.5$ only the family of prolate equilibrium states is stable with respect to the Maier–Saupe interaction and is the global minimizer of the free energy of the pure nematic (non-dipolar) polymers. The isotropic solution and the family of oblate solutions are unstable for $b > 7.5$. In other words, the probability density (78) with

$(s_1^{(0)}, s_2^{(0)})$ is a global minimizer of the right-hand side of (82). Consequently, $(s_1^{(0)}, s_2^{(0)})$ is a global minimizer of $G_2(s_1, s_2)$. It should be pointed out that in the discussion of stability we must always specify what are the interactions. For example, a stable state with respect to only the Maier–Saupe interaction may be unstable with respect to the Maier–Saupe interaction plus the dipole–dipole interaction. Using form (78), we can write $G_2(s_1, s_2)$ as

$$\begin{aligned} G_2(s_1, s_2) &= b(s_1\langle m_1^2\rangle + s_2\langle m_2^2\rangle + (1 - s_1 - s_2)\langle m_3^2\rangle) - \ln Z - \frac{b}{2}(\langle m_1^2\rangle^2 + \langle m_2^2\rangle^2 + \langle m_3^2\rangle^2) \\ &= -\frac{b}{2}[(\langle m_1^2\rangle - s_1)^2 + (\langle m_2^2\rangle - s_2)^2 + (\langle m_3^2\rangle - (1 - s_1 - s_2))^2] + G_1(s_1, s_2; 0) \end{aligned} \tag{83}$$

which implies

$$\begin{aligned} &G_1(s_1, s_2; 0) \geqslant G_2(s_1, s_2), \\ &G_1(s_1, s_2; 0) = G_2(s_1, s_2) \qquad \text{if } (s_1, s_2) \text{ is a solution of (79).} \end{aligned} \tag{84}$$

Since $(s_1^{(0)}, s_2^{(0)})$ is a solution of (79) and a global minimizer of $G_2(s_1, s_2)$, it follows that $(s_1^{(0)}, s_2^{(0)})$ is a global minimizer of $G_1(s_1, s_2; 0)$. As we pointed out earlier, all global minimizers of $G_1(s_1, s_2; 0)$ are solutions of equation (79). Property (84) also tells us that for $b > 7.5$ neither the isotropic state nor the oblate equilibrium state is a global minimizer of $G_1(s_1, s_2; 0)$ because neither of them is a global minimizer of $G_2(s_1, s_2)$. Suppose $(\tilde{s_1}, \tilde{s_2})$ corresponds to the isotropic state or an oblate equilibrium state. Since $(\tilde{s_1}, \tilde{s_2})$ is a solution of (79), we have $G_1(\tilde{s_1}, \tilde{s_2}, 0) = G_2(\tilde{s_1}, \tilde{s_2})$. For $b > 7.5$, a prolate equilibrium state is a global minimizer of the free energy while neither the isotropic state nor an oblate equilibrium state is. Thus, we must have $G_2(\tilde{s_1}, \tilde{s_2}) > G_2(s_1^{(0)}, s_2^{(0)})$. It follows that $G_1(\tilde{s_1}, \tilde{s_2}, 0) > G_1(s_1^{(0)}, s_2^{(0)}, 0)$. That is, $(\tilde{s_1}, \tilde{s_2})$ is not a global minimizer of $G_1(s_1, s_2; 0)$. Therefore, a global minimizer of $G_1(s_1, s_2; 0)$ must come from the family of rotation-equivalent prolate equilibrium states. In the framework of probability density (78), the principal axes of the second moment are restricted to be parallel to the axes of the coordinate system. With this restriction, the family of rotation-equivalent prolate equilibrium states consists of only three solutions: $(s_1^{(0)}, s_2^{(0)})$, $(s_2^{(0)}, s_1^{(0)})$ and $(s_1^{(0)}, s_1^{(0)})$. Therefore, $(s_1^{(0)}, s_2^{(0)})$ is an isolated global minimizer of $G_1(s_1, s_2; 0)$. This completes the proof of theorem A1.

Let $R(d)$ denote the rectangle $[s_1^{(0)} - d, s_1^{(0)} + d] \times [s_2^{(0)} - d, s_2^{(0)} + d]$ and let $\partial R(d)$ denote the boundary of the rectangle. Theorem A1 tells us that there exists $d_0 > 0$ such that

$$G_1(s_1, s_2; 0) > G_1(s_1^{(0)}, s_2^{(0)}; 0) \qquad \text{for } (s_1, s_2) \in R(d_0)\backslash(s_1^{(0)}, s_2^{(0)}). \tag{85}$$

Let $\delta \equiv \min(d_0, s^{(0)}/6)$ where $s^{(0)} > 0$ is the order parameter of the prolate solution. Let

$$D(\lambda) \equiv \min_{(s_1,s_2)\in\partial R(\delta)} G_1(s_1, s_2; \lambda) - G_1(s_1^{(0)}, s_2^{(0)}; \lambda). \tag{86}$$

Property (85) implies that $D(0) > 0$. Differentiating (81) with respect to λ yields

$$\left|\frac{\partial}{\partial\lambda} G_1(s_1, s_2; \lambda)\right| = |\langle m_3\rangle| \leqslant 1.$$

We select $\lambda_1 = D(0)/4 > 0$. Since $\frac{\partial}{\partial\lambda} G_1(s_1, s_2; \lambda)$ is uniformly bounded by 1, we have $D(\lambda_1) \geqslant D(0)/2 > 0$, which implies that function $G_1(s_1, s_2; \lambda_1)$ must attain a minimum inside the rectangle $R(\delta)$. Recall that all critical points of $G_1(s_1, s_2; \lambda)$ are solutions of equation (79). Thus, for $\lambda_1 = D(0)/4 > 0$, equation (79) has a solution $(s_1^{(1)}, s_2^{(1)}) \in R(\delta)$.

Once we know $(s_1^{(1)}, s_2^{(1)})$, equation (77) is satisfied by selecting $\alpha_1 = \lambda_1/\langle m_3\rangle > 0$. In this way, we constructed an equilibrium solution. From the selection of δ given above, we obtain

$$\begin{aligned}
&\tfrac{1}{3} - \tfrac{1}{2}s^{(0)} < s_1^{(1)} < \tfrac{1}{3} - \tfrac{1}{6}s^{(0)} \\
&\tfrac{1}{3} + \tfrac{1}{2}s^{(0)} < s_2^{(1)} < \tfrac{1}{3} + \tfrac{5}{6}s^{(0)} \\
&\tfrac{1}{3} - \tfrac{2}{3}s^{(0)} < s_3^{(1)} = 1 - s_1^{(1)} - s_2^{(1)} < \tfrac{1}{3}
\end{aligned} \tag{87}$$

where $s^{(0)} > 0$ is the order parameter of the prolate equilibrium solution. Equation (87) shows that $s_2^{(1)}$ is still the only eigenvalue (of the second moment) that is above $1/3$. Both $s_1^{(1)}$ and $s_3^{(1)}$ are below $1/3$. If the equilibrium solution were to be axisymmetric, then the only possible choice for the axis of symmetry would be the y-axis. As we pointed out earlier in the discussion of equation (77), for $\lambda > 0$ we have $\langle m_3\rangle > 0$ which implies that the first moment (polarity vector) is parallel to the z-axis. Therefore, it is clear that the equilibrium solution we constructed above is non-axisymmetric.

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