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# A new proof on axisymmetric equilibria of a three-dimensional Smoluchowski equation

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**Abstract**
We consider equilibrium solutions of the Smoluchowski equation for rodlike nematic polymers with a Maier–Saupe excluded volume potential. The purpose of this paper is to present a new and simplified proof of classical well-known results: (1) all equilibria are axisymmetric and (2) modulo rotational symmetry, the number and type of axisymmetric equilibria are characterized with respect to the strength of the excluded volume potential. These results confirm the phase diagram of equilibria obtained previously by numerical simulations (Faraoni *et al* 1999 *J. Rheol.* **43** 829–43, Forest *et al* 2004 *Rheol. Acta* **43** 17–37, Larson and Ottinger 1991 *Macromolecules* **24** 6270–82).

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## 1. Introduction

The isotropic–nematic (I–N) first-order phase transition in hard rod gases and liquids is a classical topic, which was first explained theoretically by Onsager in terms of an excluded volume potential [20]. Later Maier and Saupe re-examined the I–N transition with a simpler potential that now bears their names [19]. The Maier–Saupe potential is a quartic approximation of the Onsager potential, which affords sufficient degrees of freedom to capture the hysteresis loop in an order parameter representation of isotropic and anisotropic equilibria. Indeed, this idea is the kernel of Onsager's insight.

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Doi and Edwards [7] employed a second-moment closure approximation of the Smoluchowski equation for the probability density function (PDF) to further illustrate the robustness of the I–N transition with coarse-grained models and an excluded-volume potential. Since then, numerous numerical studies and semi-analytical studies have provided detailed bifurcation diagrams for equilibrium solutions of the Smoluchowski equation as well as its various closure approximations [1, 6, 15, 16, 21].

These references yield overwhelming evidence that all anisotropic equilibria of the Smoluchowski equation are axisymmetric. In [10], the authors prove this result for all second-moment closure models with a quartic, rotationally invariant, excluded-volume potential. The rotational invariance of all equilibria is the key ingredient exploited by Onsager to prove the I–N transition is a first-order. This O(3) symmetry of equilibria is made explicit for the Smoluchowski equation in [14]. The parametrization of orientational degeneracy of nematic equilibria is a prerequisite to rigorous analysis of selection criteria when full rotational symmetry is broken by applied fields [11–13, 15]. The proof that all kinetic model equilibria are axisymmetric remained open until quite recently, when Constantin, Kevrekidis and Titi, and other groups [3–5, 9, 18], began to revisit Onsager's seminal papers and provide modern rigorous proofs about stationary solutions.

Two groups have recently proved that all anisotropic equilibrium solutions of the Smoluchowski equation, or equivalently the Euler–Lagrange equation of the free energy for rodlike nematic polymers with the Maier–Saupe excluded volume potential, must be axisymmetric [8, 17]. Both proofs use elaborate estimates on a scalar integral equation involving the eigenvalues (or equivalently order parameters) of the second moment of the PDF. In this paper, we present a different and more transparent proof for the same result independent of the work of [8, 17]. Our proof uses elementary calculus. We also give a new proof on the existence and the number of nematic phases modulo orientational symmetry of the PDF. Our method in proving the number of nematic phases is particularly interesting and may be extended to solve many other problems. It predicts global properties of a function by studying its local behaviour at a hypothetical point with certain properties.

## 2. All anisotropic equilibria of the Smoluchowski equation are axisymmetric

The governing equation for stiff rod nematic polymers interacting by excluded-volume effects, absent of external fields and flow, is the Smoluchowski equation [7]:

$$\frac{\partial \rho}{\partial t} = D\frac{\partial}{\partial \boldsymbol{u}}\cdot\left(\frac{1}{k_{\mathrm{B}}T}\frac{\partial V}{\partial \boldsymbol{u}}\rho + \frac{\partial \rho}{\partial \boldsymbol{u}}\right), \tag{1}$$

where $\boldsymbol{u}$ is the unit vector representing the orientation of the rodlike nematic polymer, $\partial/\partial\boldsymbol{u}$ the orientational gradient operator [2], $\rho(\boldsymbol{u}, t)$ the PDF for the rodlike nematic polymers with orientation $\boldsymbol{u}$ at time $t$, $D$ the rotational diffusion constant, $k_{\mathrm{B}}$ the Boltzmann constant and $T$ the absolute temperature. In (1), $V(\boldsymbol{u}, [\rho])$ is the mean field excluded volume potential, which depends on the PDF $\rho(\boldsymbol{u}, t)$. Thus, equation (1) is nonlinear in the moments of $\rho$.

We adopt the Maier–Saupe potential:

$$V(\boldsymbol{u}, [\rho]) = -bk_{\mathrm{B}}T(\boldsymbol{u}\otimes\boldsymbol{u}) : \langle\boldsymbol{u}\otimes\boldsymbol{u}\rangle, \tag{2}$$

where $b = 3N/2$ and $N$ is the dimensionless concentration. $b$ can be viewed as the strength of the excluded volume potential. Here $\langle\boldsymbol{u}\otimes\boldsymbol{u}\rangle$ denotes the second moment of the PDF or the mean of the random variable $\boldsymbol{u}\otimes\boldsymbol{u}$ on the unit sphere weighted by the probability density $\rho(\boldsymbol{u}, t)$:

$$\langle\boldsymbol{u}\otimes\boldsymbol{u}\rangle = \int_S(\boldsymbol{u}\otimes\boldsymbol{u})\rho(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}. \tag{3}$$

In equilibrium, the solution of the Smoluchowski equation is given by the Boltzmann distribution:

$$\rho(\boldsymbol{u}) = \frac{\exp(-V(\boldsymbol{u},[\rho]))}{\int_S \exp(-V(\boldsymbol{u},[\rho]))\,\mathrm{d}\boldsymbol{u}}. \tag{4}$$

It is clear that the equilibrium is completely determined by the second moment tensor $\langle \boldsymbol{u}\otimes\boldsymbol{u}\rangle$ should it be known. However, $\langle \boldsymbol{u}\otimes\boldsymbol{u}\rangle$ depends on the PDF. Moreover, as we will show, not all choices of $\langle \boldsymbol{u}\otimes\boldsymbol{u}\rangle$ are allowed. Because $\langle \boldsymbol{u}\otimes\boldsymbol{u}\rangle$ is symmetric and trace one, it can be diagonalized by rotating the Cartesian coordinate system onto its principal axes. Without loss of generality, we assume that the Cartesian system is chosen such that $\langle \boldsymbol{u}\otimes\boldsymbol{u}\rangle$ is diagonal. We denote $\boldsymbol{u} = (u_1, u_2, u_3)$ in the coordinate system. By assumption,

$$\langle \boldsymbol{u}\otimes\boldsymbol{u}\rangle = \begin{pmatrix} \frac{1}{3}+r_1 & 0 & 0 \\ 0 & \frac{1}{3}+r_2 & 0 \\ 0 & 0 & \frac{1}{3}+r_3 \end{pmatrix}, \tag{5}$$

where $(r_1, r_2, r_3)$ are given by

$$r_1 = \langle u_1^2\rangle - \tfrac{1}{3}, \qquad r_2 = \langle u_2^2\rangle - \tfrac{1}{3}, \qquad r_3 = \langle u_3^2\rangle - \tfrac{1}{3}, \tag{6}$$

and satisfy

$$\begin{aligned} &0 \leqslant \tfrac{1}{3}+r_1 < 1, \qquad 0 \leqslant \tfrac{1}{3}+r_2 < 1, \qquad 0 \leqslant \tfrac{1}{3}+r_3 < 1, \\ &r_1+r_2+r_3 = \langle u_1^2+u_2^2+u_3^2\rangle - 1 = 0. \end{aligned} \tag{7}$$

The $r_k$, as eigenvalues of the second moment of $\rho$, are therefore implicitly defined by the PDF. For simplicity, we absorb $k_{\mathrm{B}}T$ into $b$. The Maier–Saupe potential can be recast in these coordinates,

$$V(\boldsymbol{u}) = -b(r_1u_1^2 + r_2u_2^2 + r_3u_3^2 + \tfrac{1}{3}).$$

The equilibrium PDF is expressed as follows:

$$\rho(\boldsymbol{u}) = \frac{\exp[b(r_1u_1^2 + r_2u_2^2 + r_3u_3^2)]}{\int_S \exp[b(r_1u_1^2 + r_2u_2^2 + r_3u_3^2)]\,\mathrm{d}\boldsymbol{u}}. \tag{8}$$

In the analysis below, we treat $b$ as a variable (it is either the normalized volume fraction of rods or the reciprocal of temperature) and view the PDF and all averages (expectations) as functions of $b$. Specifically, we define functions as follows:

$$R_1(b) = \langle u_1^2\rangle - \tfrac{1}{3}, \qquad R_2(b) = \langle u_2^2\rangle - \tfrac{1}{3}, \qquad R_3(b) = \langle u_3^2\rangle - \tfrac{1}{3},$$

where the average is taken with respect to the PDF given in (8). If $(r_1, r_2, r_3)$ corresponds to an equilibrium for $b = b_0$, then functions $R_1(b)$, $R_2(b)$ and $R_3(b)$ must satisfy

$$\begin{aligned} &R_1(0) = 0, \qquad R_2(0) = 0, \qquad R_3(0) = 0, \\ &R_1(b_0) = r_1, \qquad R_2(b_0) = r_2, \qquad R_3(b_0) = r_3. \end{aligned} \tag{9}$$

It is important to note that $R_k(b)$ is a function of $b$ while $r_k$ is a fixed value.

To simplify the presentation, we introduce some shorthand notation:

$$h_1 = u_1^2 - \langle u_1^2\rangle, \qquad h_2 = u_2^2 - \langle u_2^2\rangle, \qquad h_3 = u_3^2 - \langle u_3^2\rangle. \tag{10}$$

We note that $h_1, h_2, h_3$ are random variables and functions of $b$. They satisfy the following constraints:

$$h_1 + h_2 + h_3 = 0 \qquad \text{and} \qquad \langle h_1\rangle = \langle h_2\rangle = \langle h_3\rangle = 0. \tag{11}$$

Any solution of (1) with three distinct eigenvalues of the second moment is called biaxial. PDFs with two distinct eigenvalues of the second moment are called uniaxial (axisymmetric). The isotropic state corresponds to $r_1 = r_2 = r_3 = 0$.

**Theorem 1.** *All anisotropic equilibria of the Smoluchowski equation with the Maier–Saupe excluded volume potential are axisymmetric. The isotropic state is a non-degenerate equilibrium for all non-zero strengths of the potential.*

To prove this theorem, we need a lemma.

**Lemma 1.** *Suppose $r_1 > r_2$. Then for $b > 0$, we have*

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

*where $h_1$, $h_2$, $h_3$ are defined in (10).*

**Remark 1.** $\langle h_3h_1\rangle = \langle (u_3^2 - \langle u_3^2\rangle)(u_1^2 - \langle u_1^2\rangle)\rangle$ is the correlation of $u_3^2$ and $u_1^2$.

**Remark 2.** This lemma does not impose any condition on $r_3$.

**Remark 3.** We can permute $(r_1, r_2, r_3)$ and apply this lemma to any pair of $(r_1, r_2, r_3)$.

For example, if $r_2 > r_3$, then we have

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

**Proof of lemma 1.** To prove this lemma, we first point out the fact that the function

$$g(r) = \frac{\int_0^{2\pi} \cos 2\theta \exp(r\cos 2\theta)\,\mathrm{d}\theta}{\int_0^{2\pi} \exp(r\cos 2\theta)\,\mathrm{d}\theta} \tag{12}$$

is an increasing function of $r$, which was proved in [4]. We rewrite $\langle h_3(h_1 - h_2)\rangle$ as

$$\begin{aligned}\langle h_3(h_1 - h_2)\rangle &= \langle (u_3^2 - \langle u_3^2\rangle)(u_1^2 - u_2^2 + \langle u_2^2\rangle - \langle u_1^2\rangle)\rangle \\ &= \langle (u_3^2 - \langle u_3^2\rangle)(u_1^2 - u_2^2)\rangle.\end{aligned}$$

We select the axis associated with $u_3$ as the $z$-axis and establish a spherical coordinate system $(\phi, \theta)$ where $\phi$ is the polar angle and $\theta$ is the azimuthal angle. We express everything in terms of $(\phi, \theta)$:

$$u_1^2 - u_2^2 = \sin^2\phi\cos^2\theta - \sin^2\phi\sin^2\theta = \sin^2\phi\cos 2\theta,$$

$$u_3^2 = \cos^2\phi.$$

The Maier–Saupe potential is

$$\begin{aligned}V(\phi,\theta) &= -b(r_1\sin^2\phi\cos^2\theta + r_2\sin^2\phi\sin^2\theta + r_3\cos^2\phi) \\ &= -b(a_1\sin^2\phi + a_2\sin^2\phi\cos 2\theta + r_3\cos^2\phi),\end{aligned}$$

where

$$a_1 = \frac{r_1 + r_2}{2}, \qquad a_2 = \frac{r_1 - r_2}{2} > 0.$$

The probability density is

$$\rho(\phi,\theta) = \frac{\exp[b(a_1\sin^2\phi + a_2\sin^2\phi\cos 2\theta + r_3\cos^2\phi)]}{\int_0^{\pi}\int_0^{2\pi}\exp[b(a_1\sin^2\phi + a_2\sin^2\phi\cos 2\theta + r_3\cos^2\phi)]\,\mathrm{d}\theta\sin\phi\,\mathrm{d}\phi}.$$

Notice that the probability density satisfies

$$\int_0^{2\pi}\cos 2\theta\rho(\phi,\theta)\,\mathrm{d}\theta = g(ba_2\sin^2\phi)\int_0^{2\pi}\rho(\phi,\theta)\,\mathrm{d}\theta,$$

where function $g(r)$ defined in (12) is an increasing function of $r$. Because $b > 0$ and $a_2 > 0$, $g(ba_2 \sin^2\phi)$ is an increasing function of $\sin^2\phi$.

Let $\cos^2\phi_0 = \langle u_3^2\rangle = \langle\cos^2\phi\rangle$. Writing the average in terms of $(\phi, \theta)$, we obtain

$$
\begin{aligned}
\langle (u_3^2 - \langle u_3^2\rangle)(u_1^2 - u_2^2)\rangle
&= \int_0^{\pi} (\cos^2\phi - \cos^2\phi_0)\sin^2\phi \left(\int_0^{2\pi} \cos 2\theta\, \rho(\phi,\theta)\,\mathrm{d}\theta\right)\sin\phi\,\mathrm{d}\phi\\
&= \int_0^{\pi} (\cos^2\phi - \cos^2\phi_0)\sin^2\phi\, g(ba_2\sin^2\phi) \left(\int_0^{2\pi} \rho(\phi,\theta)\,\mathrm{d}\theta\right)\sin\phi\,\mathrm{d}\phi\\
&= \langle (\cos^2\phi - \cos^2\phi_0)\sin^2\phi\, g(ba_2\sin^2\phi)\rangle\\
&= \langle (\cos^2\phi - \cos^2\phi_0)\{\sin^2\phi\, g(ba_2\sin^2\phi) - \sin^2\phi_0\, g(ba_2\sin^2\phi_0)\}\rangle < 0.
\end{aligned}
$$

Here we used that $g(ba_2\sin^2\phi)$ is an increasing function of $\sin^2\phi$ and $\cos^2\phi = 1 - \sin^2\phi$ is a decreasing function of $\sin^2\phi$. □

**Proof of theorem 1.** The PDF (8) depends on $b$. Its derivative with respect to $b$ is given by

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}b}\rho(\boldsymbol{u}) &= [(r_1u_1^2 + r_2u_2^2 + r_3u_3^2) - \langle r_1u_1^2 + r_2u_2^2 + r_3u_3^2\rangle]\cdot\rho(\boldsymbol{u})\\
&= (r_1h_1 + r_2h_2 + r_3h_3)\cdot\rho(\boldsymbol{u}).
\end{aligned}
$$

The derivative of $R_k(b)$ with respect to $b$ is given by

$$
R_k'(b) = \langle u_k^2(r_1h_1 + r_2h_2 + r_3h_3)\rangle = \langle h_k(r_1h_1 + r_2h_2 + r_3h_3)\rangle,
$$

taking into account the fact $\langle h_1\rangle = \langle h_2\rangle = \langle h_3\rangle = 0$.

We prove the theorem by contradiction. Suppose there is a set of distinct $(r_1, r_2, r_3)$ satisfying equation (6) with probability density (8) for $b = b_0 > 0$. Without loss of generality, we assume $r_1 > r_2 > r_3$. Because $r_1 + r_2 + r_3 = 0$, we have $r_1 > 0$ and $r_3 < 0$.

We consider the function

$$
F(b) = r_2R_1(b) - r_1R_2(b).
$$

Equation (9) implies that $F(0) = F(b_0) = 0$. To establish the contradiction, we are going to prove that

$$
F'(b) > 0 \qquad \text{for } b > 0.
$$

Taking the derivative of $F(b)$ with respect to $b$, we have

$$
\begin{aligned}
F'(b) &= r_2R_1'(b) - r_1R_2'(b)\\
&= r_2\langle h_1(r_1h_1 + r_2h_2 + r_3h_3)\rangle - r_1\langle h_2(r_1h_1 + r_2h_2 + r_3h_3)\rangle.
\end{aligned}
$$

Using $h_1 = -(h_2 + h_3)$ and $h_2 = -(h_1 + h_3)$, we obtain

$$
\begin{aligned}
F'(b) &= r_2\langle h_1[(r_2 - r_1)h_2 + (r_3 - r_1)h_3]\rangle - r_1\langle h_2[(r_1 - r_2)h_1 + (r_3 - r_2)h_3]\rangle\\
&= r_2(r_2 - r_1)\langle h_1h_2\rangle + r_2(r_3 - r_1)\langle h_1h_3\rangle - r_1(r_1 - r_2)\langle h_1h_2\rangle - r_1(r_3 - r_2)\langle h_2h_3\rangle.
\end{aligned}
$$

Splitting the term of $\langle h_1h_3\rangle$ into two using the identity $(r_3 - r_1) = (r_3 - r_2) + (r_2 - r_1)$, combining two terms of $\langle h_1h_2\rangle$ and using $r_1 + r_2 = -r_3$, we arrive at

$$
\begin{aligned}
F'(b) &= r_2(r_3 - r_2)\langle h_1h_3\rangle + r_2(r_2 - r_1)\langle h_1h_3\rangle - r_3(r_2 - r_1)\langle h_1h_2\rangle - r_1(r_3 - r_2)\langle h_2h_3\rangle\\
&= (r_3 - r_2)[r_2\langle h_1h_3\rangle - r_1\langle h_2h_3\rangle] + (r_2 - r_1)[r_2\langle h_1h_3\rangle - r_3\langle h_1h_2\rangle].
\end{aligned}
$$

Applying the identity

$$
\alpha_1\beta_1 - \alpha_2\beta_2 = \tfrac{1}{2}[(\alpha_1 - \alpha_2)(\beta_1 + \beta_2) + (\alpha_1 + \alpha_2)(\beta_1 - \beta_2)]
$$

and using $r_1 + r_2 = -r_3$ and $r_2 + r_3 = -r_1$, we finally obtain

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

In the above, all coefficients are positive, and lemma 1 dictates that all correlation terms are positive as well. Therefore, we conclude that

$$F'(b) > 0 \qquad \text{for } b > 0,$$

which clearly contradicts (9). Therefore, there cannot exist three distinct $r_k$ satisfying equation (6) with PDF (8). That is, the equilibrium solutions of the Smoluchowski equation are parametrized by three $r_k$ of which at least two must be equal.

## 3. Number of equilibria

Given that all equilibria are axisymmetric, we now investigate their multiplicity (modulo rotational invariance). We select the axis of symmetry as the $z$-axis. We next establish a corresponding spherical coordinate system. Let $\phi$ be the polar angle measured from the $z$-axis, $0 \leqslant \phi \leqslant \pi$. Let $\theta$ be the azimuthal angle, the angle on the $xy$-plane measured counterclockwise from the $x$-axis, $0 \leqslant \theta \leqslant 2\pi$. We express $\boldsymbol{u}$ in terms of $(\phi, \theta)$:

$$\boldsymbol{u} = (u_1, u_2, u_3) = (\sin(\phi)\cos(\theta), \sin(\phi)\sin(\theta), \cos(\phi)). \tag{13}$$

Because of axisymmetry, (5) becomes

$$\langle \boldsymbol{u} \otimes \boldsymbol{u} \rangle = \begin{pmatrix} \frac{1}{2}\langle \sin^2(\phi)\rangle & 0 & 0 \\ 0 & \frac{1}{2}\langle \sin^2(\phi)\rangle & 0 \\ 0 & 0 & \langle \cos^2(\phi)\rangle \end{pmatrix}, \tag{14}$$

and the Maier–Saupe potential simplifies accordingly:

$$\begin{aligned} (\boldsymbol{u} \otimes \boldsymbol{u}) : \langle \boldsymbol{u} \otimes \boldsymbol{u} \rangle &= \tfrac{1}{2}\sin^2(\phi)\langle \sin^2(\phi)\rangle + \cos^2(\phi)\langle \cos^2(\phi)\rangle \\ &= \tfrac{1}{2}(3\langle \cos^2(\phi)\rangle - 1)\cos^2(\phi) - \tfrac{1}{2}(\langle \cos^2(\phi)\rangle - \tfrac{1}{3}) + \tfrac{1}{3}. \end{aligned} \tag{15}$$

Notice that the last two terms on the right side of (15) are constants, independent of $\phi$. Thus, the Maier–Saupe potential (up to a constant) is

$$V(\phi) = -b\tfrac{1}{2}(3\langle \cos^2(\phi)\rangle - 1)\cos^2(\phi). \tag{16}$$

Here we introduce a new variable following Constantin and Vukadinovic [5]:

$$r \stackrel{\text{def}}{=} b\tfrac{1}{2}(3\langle \cos^2(\phi)\rangle - 1), \tag{17}$$

where we note that $\frac{1}{2}(3\langle \cos^2(\phi)\rangle - 1)$ is the *Flory order parameter*.

We rewrite the potential as

$$V(\phi) = -r\cos^2(\phi), \tag{18}$$

so that the Boltzmann distribution (4) in spherical coordinates has the form:

$$\rho(\phi) = \frac{\exp(r\cos^2(\phi))}{2\pi\int_0^{\pi}\exp(r\cos^2(\phi))\sin(\phi)\,\mathrm{d}\phi}. \tag{19}$$

We emphasize that $r$ has to satisfy equation (17) with PDF given by (19):

$$r = b\frac{1}{2}\left(\frac{3\int_0^\pi \cos^2(\phi)\exp(r\cos^2(\phi))\sin(\phi)\,\mathrm{d}\phi}{\int_0^\pi \exp(r\cos^2(\phi))\sin(\phi)\,\mathrm{d}\phi} - 1\right). \tag{20}$$

Using $w = \cos(\phi)$, (20) becomes

$$r = b\frac{1}{2}\frac{\int_0^1 (3w^2 - 1)\exp(rw^2)\,\mathrm{d}w}{\int_0^1 \exp(rw^2)\,\mathrm{d}w}.$$

Integrating by parts and collecting terms to the left, we obtain

$$r(1 - bf(r)) = 0, \tag{21}$$

where $f(r)$ is given by

$$f(r) \stackrel{\text{def}}{=} \frac{\int_0^1 w^2(1-w^2)\exp(rw^2)\,\mathrm{d}w}{\int_0^1 \exp(rw^2)\,\mathrm{d}w}. \tag{22}$$

The equilibrium equation (21) is a nonlinear integral equation for the scaled Flory order parameter $r$. For each solution of equation (21), the corresponding equilibrium solution of equation (1) is given by (19). Therefore, the number of equilibrium solutions equals the number of solutions of (21). We first note that $r = 0$ solves (21) for all values of $b$. When $r = 0$, from (18) it follows that $r_1 = r_2 = r_3 = 0$ and

$$\langle \boldsymbol{u} \otimes \boldsymbol{u} \rangle = \tfrac{1}{3} I,$$

which translates back to the PDF as the isotropic solution $\rho = 1/4\pi$.

For $b = 0$, $r = 0$ is the only solution of (21). For $b > 0$, non-zero solutions of (21) must satisfy

$$\frac{1}{b} = f(r). \tag{23}$$

**Theorem 2.** *$f(r)$ defined in (22) has the following properties.*

*(1)* $f(0) = \frac{2}{15}$.
*(2)* $0 < f(r) < \frac{1}{4}$.
*(3)* $\lim_{r\to-\infty} f(r) = 0$ and $\lim_{r\to+\infty} f(r) = 0$.
*(4) There exists $r^* > 0$, such that $f'(r^*) = 0$, $f'(r) > 0$ for $r < r^*$ and $f'(r) < 0$ for $r > r^*$.*

**Proof of theorem 2.** To prove this theorem, we first point out a fact of calculus of one variable.

Suppose $f(r)$ satisfies the property that $f'(r_0) = 0$ implies $f''(r_0) < 0$. If $f(r)$ attains a maximum at $r^*$, then we have

$$f'(r) > 0 \quad \text{for } r < r^* \qquad \text{and} \qquad f'(r) < 0 \quad \text{for } r > r^*.$$

As we will see, this simple fact of calculus plays a very important role in the proof of property (4) below. It enables us to predict the global behaviour of a function by studying its local behaviour at a hypothetical point with certain properties. Now we prove the four properties listed one by one.

(1) $f(0) = \int_0^1 w^2(1-w^2)\,\mathrm{d}w = \frac{1}{3} - \frac{1}{5} = \frac{2}{15}$.
(2) $0 < w^2(1-w^2) < \frac{1}{4}$ for $w \in (0,1)\backslash\left\{\frac{1}{\sqrt{2}}\right\}$ lead to

$$0 < f(r) = \frac{\int_0^1 w^2(1-w^2)\exp(rw^2)\,\mathrm{d}w}{\int_0^1 \exp(rw^2)\,\mathrm{d}w} < \frac{1}{4}.$$

(3) To prove $\lim_{r\to-\infty} f(r) = 0$, we consider for any $r < 0$ and $1 > \varepsilon > 0$,

$$\int_0^\varepsilon \exp(rw^2)\,\mathrm{d}w = \int_0^\varepsilon \exp[r(\varepsilon - s)^2]\,\mathrm{d}s = \int_0^\varepsilon \exp[r\varepsilon^2 - 2r\varepsilon s + rs^2]\,\mathrm{d}s$$

$$\geqslant \exp(r\varepsilon^2)\cdot\int_0^\varepsilon \exp(-rs^2)\,\mathrm{d}s \geqslant \int_\varepsilon^1 \exp(rw^2)\,\mathrm{d}w \cdot \int_0^\varepsilon \exp(-rs^2)\,\mathrm{d}s.$$

Here we have used $-2r\varepsilon s + rs^2 \geqslant -2rs^2 + rs^2 = -rs^2$.
Since $\lim_{r\to-\infty}\int_0^\varepsilon \exp(-rs^2)\,\mathrm{d}s = \infty$, we obtain the result below.
For any $\varepsilon > 0$, there exists an $M$ such that $r < -M$ implies

$$\int_0^\varepsilon \exp(rw^2)\,\mathrm{d}w \geqslant \frac{1}{\varepsilon}\cdot\int_\varepsilon^1 \exp(rw^2)\,\mathrm{d}w.$$

It follows that

$$0 < f(r) \leqslant \frac{\varepsilon^2\int_0^\varepsilon \exp(rw^2)\,\mathrm{d}w + (1/4)\int_\varepsilon^1 \exp(rw^2)\,\mathrm{d}w}{\int_0^\varepsilon \exp(rw^2)\,\mathrm{d}w} < \varepsilon^2 + \frac{\varepsilon}{4}.$$

Thus, we have $\lim_{r\to-\infty} f(r) = 0$.
$\lim_{r\to+\infty} f(r) = 0$ is proved in a similar way.

(4) Because $\lim_{r\to\pm\infty} f(r) = 0$ and $f(r) > 0$, $f(r)$ attains a maximum at $r^*$. Using the simple fact of calculus we pointed out above, we see that, to prove property (4), we only need to prove that $f'(r_0) = 0$ implies $f''(r_0) < 0$.

For the simplicity of presentation, we consider random variable $W$ with probability density

$$\rho(\omega) = \frac{\exp(rw^2)}{\int_0^1 \exp(rw^2)\,\mathrm{d}w}.$$

Then we have $f(r) = \langle W^2(1-W^2)\rangle$. The derivative of $\rho(w)$ with respect to $r$ is

$$\frac{\mathrm{d}}{\mathrm{d}r}\rho(w) = (w^2 - \langle W^2\rangle)\cdot\rho(w).$$

Taking derivatives of $f(r) = \langle W^2(1-W^2)\rangle$, we have

$$\begin{aligned}
f'(r) &= \langle W^2(1-W^2)(W^2 - \langle W^2\rangle)\rangle \\
&= \langle W^2(1-W^2)W^2\rangle - \langle W^2(1-W^2)\rangle\cdot\langle W^2\rangle \\
&= \langle\{W^2(1-W^2) - \langle W^2(1-W^2)\rangle\}W^2\rangle \\
&= \langle\{\langle W^2(1-W^2)\rangle - W^2(1-W^2)\}(1-W^2)\rangle, \\
f''(r) &= \langle\{\langle W^2(1-W^2)\rangle - W^2(1-W^2)\}(1-W^2)(W^2 - \langle W^2\rangle)\rangle \\
&\quad + \left(\frac{\mathrm{d}}{\mathrm{d}r}\langle W^2(1-W^2)\rangle\right)\cdot\langle(1-W^2)\rangle \\
&= \langle\{\langle W^2(1-W^2)\rangle - W^2(1-W^2)\}W^2(1-W^2)\rangle \\
&\quad - \langle\{\langle W^2(1-W^2)\rangle - W^2(1-W^2)\}(1-W^2)\rangle\cdot\langle W^2\rangle + f'(r)\cdot(1-\langle W^2\rangle) \\
&= \langle W^2(1-W^2)\rangle^2 - \langle\{W^2(1-W^2)\}^2\rangle + f'(r)\cdot(1-2\langle W^2\rangle).
\end{aligned}$$

Here we have used

$$\frac{\mathrm{d}}{\mathrm{d}r}\langle W^2(1-W^2)\rangle = f'(r)$$

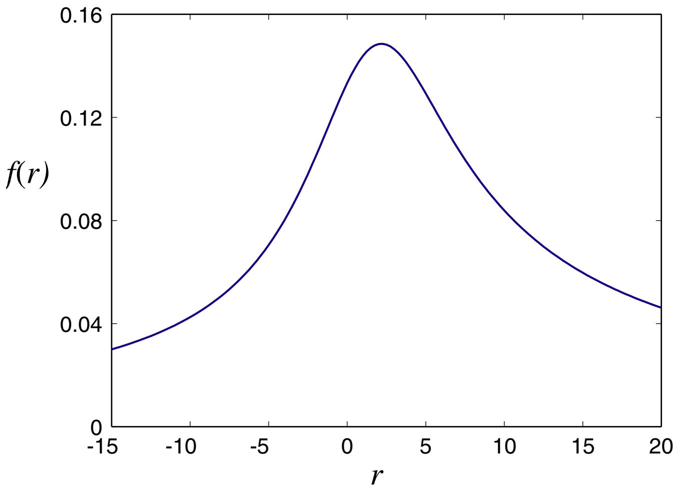


**Figure 1.** Graph of function $f(r)$ defined in (22).

and

$$\langle \{\langle W^2(1-W^2)\rangle - W^2(1-W^2)\}(1-W^2)\rangle = f'(r).$$

Suppose $f'(r_0) = 0$. Then we have

$$f''(r_0) = \langle W^2(1-W^2)\rangle^2 - \langle \{W^2(1-W^2)\}^2\rangle = -\mathrm{var}\{W^2(1-W^2)\} < 0.$$

Then it follows that $f'(r) > 0$ for $r < r^*$ and $f'(r) < 0$ for $r > r^*$.

Finally we have

$$f'(0) = \left(\int_0^1 w^4(1-w^2)\,\mathrm{d}w\right) - \left(\int_0^1 w^2(1-w^2)\,\mathrm{d}w\right)\cdot\left(\int_0^1 w^2\,\mathrm{d}w\right) = \frac{4}{315} > 0,$$

which implies $r^* > 0$.

$r^*$ and $f(r^*)$ can be estimated numerically using a nonlinear equation solver (such as the bisection method) and a numerical integration method (such as Simpson's method). Our numerical results show

$$r^* \approx 2.178\,287\,9748, \qquad f(r^*) \approx 0.148\,555\,599\,922\,54.$$

A plot of $f(r)$ is shown in figure 1. □

**Corollary.** *Let* $b^* = 1/f(r^*) \approx 6.731\,486\,3965$.

*(1) For* $b < b^*$, *(21) has one solution,* $r = 0$.
*(2) For* $b = b^*$, *(21) has two solutions,* $r = 0$ *and* $r = r^*$.
*(3) For* $b^* < b < \frac{15}{2}$, *(21) has three solutions* $r = 0$, $r = r_1$ *and* $r = r_2$ *where* $0 < r_1 < r^*$ *and* $r_2 > r^*$.
*(4) For* $b = \frac{15}{2}$, *(21) has two solutions* $r = 0$ *and* $r = r_2$ *where* $r_2 > r^*$.
*(5) For* $b > \frac{15}{2}$, *(21) has three solutions* $r = 0$, $r = r_1$ *and* $r = r_2$ *where* $r_1 < 0$ *and* $r_2 > r^*$.

**Remark.** Our numerical value of $b^*$ is slightly different from the numerical value of 6.731 393 reported in [17].

## 4. The 2D case

Our approach also works for the 2D Smoluchowski equation. In the proof given by Constantin and Vukadinovic [5] for the 2D problem, the key step is to prove that the function

$$f(r) = \frac{\int_0^{2\pi} \cos^2\phi \exp(r\cos\phi)\,\mathrm{d}\phi}{\int_0^{2\pi} \exp(r\cos\phi)\,\mathrm{d}\phi}$$

is an increasing function of $r$. Constantin and Vukadinovic [5] proved that $f(r)$ is strictly increasing by viewing it as the solution of a differential equation. Here we use the simple fact of calculus pointed out in the proof of theorem 2 above. Again, the main idea of our approach is to predict the global behaviour of a function by studying its local behaviour.

We first prove that $f(r)$ satisfies the property that $f'(r_0) = 0$ implies $f''(r_0) > 0$.

We consider random variable $\Phi$ with probability density

$$\rho(\phi) = \frac{\exp(r\cos\phi)}{\int_0^{2\pi} \exp(r\cos\phi)\,\mathrm{d}\phi}.$$

Then we have $f(r) = \langle\cos^2\Phi\rangle$. The derivative of $\rho(\phi)$ with respect to $r$ is

$$\frac{\mathrm{d}}{\mathrm{d}r}\rho(\phi) = (\cos\phi - \langle\cos\Phi\rangle)\cdot\rho(\phi).$$

Taking derivatives of $f(r) = \langle\cos^2\Phi\rangle$, we have

$$\begin{aligned} f'(r) &= \langle\cos^2\Phi(\cos\Phi - \langle\cos\Phi\rangle)\rangle \\ &= \langle(\cos^2\Phi - \langle\cos^2\Phi\rangle)\cos\Phi\rangle, \\ f''(r) &= \langle(\cos^2\Phi - \langle\cos^2\Phi\rangle)\cos\Phi(\cos\Phi - \langle\cos\Phi\rangle)\rangle - \left(\frac{\mathrm{d}}{\mathrm{d}r}\langle\cos^2\Phi\rangle\right)\cdot\langle\cos\Phi\rangle \\ &= \langle(\cos^2\Phi - \langle\cos^2\Phi\rangle)\cos^2\Phi\rangle \\ &\quad - \langle(\cos^2\Phi - \langle\cos^2\Phi\rangle)\cos\Phi\rangle\cdot\langle\cos\Phi\rangle - f'(r)\cdot\langle\cos\Phi\rangle \\ &= \langle\cos^4\Phi\rangle - \langle\cos^2\Phi\rangle^2 - 2f'(r)\cdot\langle\cos\Phi\rangle. \end{aligned}$$

Here we have used

$$\frac{\mathrm{d}}{\mathrm{d}r}\langle\cos^2\Phi\rangle = f'(r)$$

and

$$\langle(\cos^2\Phi - \langle\cos^2\Phi\rangle)\cos\Phi\rangle = f'(r).$$

Suppose $f'(r_0) = 0$. Then we have

$$f''(r_0) = \langle\cos^4\Phi\rangle - \langle\cos^2\Phi\rangle^2 = \mathrm{var}\,\{\cos^2\Phi\} > 0.$$

Now we show that $f'(r) > 0$ for $r > 0$.

Because $f'(0) = 0$ we obtain $f''(0) > 0$ , which means that $f'(r) > 0$ for $r \in (0, \varepsilon)$.

Let $r_0 = \sup\{q|q > 0 \text{ and } f'(r) > 0 \text{ in } (0, q)\}$. If $r_0 = \infty$, then it is true that $f'(r) > 0$ for $r > 0$. If $r_0 < \infty$, then we have $f'(r_0) = 0$ and consequently $f''(r_0) > 0$. That means $f'(r) < 0$ for $r \in (r_0 - \varepsilon, r_0)$, which contradicts the definition of $r_0$.

## 5. Conclusion

We have presented three new proofs for the type and number of the equilibrium solutions of the Smoluchowski equation with Maier–Saupe excluded volume potential in 2D and 3D, respectively. Although the conclusions are not new, the approach is new and systematic and has potential applicability to other questions such as selection criteria for stationary solutions of a Smoluchowski equation in the presence of axisymmetric external flow and/or external fields coupled to an excluded-volume potential.

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## References

[1] Bhave A V, Menon R K, Armstrong R C and Brown R A 1993 A constitutive equation for liquid crystalline polymer solutions *J. Rheol.* **37** 413–41
[2] Bird B, Armstrong R C and Hassager O 1987 *Dynamics of Polymeric Liquids* vol 1 (New York: Wiley)
[3] Constantin P, Kevrekidis I and Titi E S 2004 Asymptotic states of a Smoluchowski equation *Arch. Ration. Mech. Anal.* **174** 365–84
[4] Constantin P, Kevrekidis I and Titi E S 2004 Remarks on a Smoluchowski equation *Discrete Contin. Dynam. Syst.* **11** 101–12
[5] Constantin P and Vukadinovic J 2005 Note on the number of steady states for a two-dimensional Smoluchowski equation *Nonlinearity* **18** 441–3
[6] Doi H M and Larson R G 1990 The effect of steady flow fields on the isotropic–nematic phase transition of rigid rod-like polymers *J. Chem. Phys.* **92** 792–800
[7] Doi M and Edwards S F 1986 *The Theory of Polymer Dynamics* (Oxford: Oxford University Press)
[8] Fatkullin I and Slastikov V 2005 Critical points of the Onsager functional on a sphere *Preprint*
[9] Fatkullin I and Slastikov V 2005 A note on the Onsager model of nematic phase transitions *Commun. Math. Sci.* **3** 21–6
[10] Forest M G, Wang Q and Zhou H 2000 Exact banded patterns from a Doi-Marrucci-Greco model of nematic liquid crystal polymers *Phys. Rev.* E **61** 6655–62
[11] Forest M G, Wang Q and Zhou H 2000 Homogeneous pattern selection and director instabilities of nematic liquid crystal polymers induced by elongational flows *Phys. Fluids* **12** 490–8
[12] Forest M G, Wang Q and Zhou H 2001 On the flow-phase diagram for discotic liquid crystals in uniaxial extension and compression *Liq. Cryst.* **28** 717–20
[13] Forest M G, Wang Q and Zhou R 2004 The weak shear kinetic phase diagram for nematic polymers *Rheol. Acta* **43** 17–37
[14] Forest M G, Zhou R and Wang Q 2002 Symmetries of the Doi kinetic theory for nematic polymers of arbitrary aspect ratio: at rest and in linear flows *Phys. Rev.* E **66** 031712
[15] Forest M G, Zhou R and Wang Q 2003 Full-tensor alignment criteria for sheared nematic polymers *J. Rheol.* **47** 105–27
[16] Larson R and Ottinger H 1991 Effect of molecular elasticity on out-of-plane orientations in shearing flows of liquid-crystalline polymers *Macromolecules* **24** 6270–82
[17] Liu H, Zhang H and Zhang P 2005 Axial symmetry and classification of stationary solutions of Doi-Onsager equation on the sphere with Maier–Saupe potential *Commun. Math. Sci.* **3** 201–18
[18] Luo C, Zhang H and Zhang P 2005 The structure of equilibrium solutions of the one-dimensional Doi equation *Nonlinearity* **18** 379–89
[19] Maier W and Saupe A 1959 A simple molecular statistical theory of the nematic crystalline-liquid phase. I *Z. Naturf.* a **14** 882–9
[20] Onsager L 1949 The effects of shape on the interaction of colloidal particles *Ann. N. Y. Acad. Sci.* **51** 627–59
[21] Wang Q 1997 Comparative studies on closure approximations in flows of liquid crystal polymers. I. Elongational flows *J. Non-Newtonian Fluid Mech.* **72** 141–62