Commun. Math. Sci.
Vol. 6, No. 4, pp. 949–974

A UNIFIED VIEW ON THE ROTATIONAL SYMMETRY OF EQUILIBRIA OF NEMATIC POLYMERS, DIPOLAR NEMATIC POLYMERS AND POLYMERS IN HIGHER DIMENSIONAL SPACE*

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Abstract. We study equilibrium states of the Smoluchowski equation for rigid, rod-like polymer ensembles. We start with several cases in the three dimensional space: a) nematic polymers where the only intermolecular interaction is the excluded volume effect, modeled using the Maier-Saupe potential, b) dipolar nematic polymers where the intermolecular interaction consists of the dipole-dipole potential and the Maier-Saupe potential, c) dipolar nematic polymers in the presence of a stretching elongational flow, and d) nematic polymers in higher dimensional space. For each of the cases a), b) and c), it has been established separately with various mathematical manipulations that all stable equilibrium states have rotational symmetry. In this study, we present a unified view of the rotational symmetry of cases a), b) and c). Specifically, in cases a), b) and c), the rotational symmetry is determined by a key inequality. The inequality, once established for case a), is extended elegantly to cases b) and c). Furthermore, this inequality is used in case d) to establish the rotational symmetry of equilibrium states of nematic polymers in higher dimensional space. In three dimensional space, rotational symmetry simply means axisymmetry. In higher dimensional space, rotational symmetry is more complex in structure. For example, in four dimensional space, rotational symmetry may be around a one dimensional sub-space (i.e., axisymmetry) or it may be around a two dimensional sub-space. Nevertheless, the rotational symmetry significantly simplifies the classification of equilibrium states. We calculate and present phase diagrams of nematic polymers in higher dimensional spaces.

Key words. Rotational symmetry, Smoluchowski equation, Maier-Saupe interaction potential, nematic polymers, dipolar nematic polymers, polymers in higher dimensional space.

AMS subject classifications. 35K55, 70K42.

1. Introduction and mathematical equations

The isotropic-nematic phase transition in rigid rod-like polymers is a classical topic. Onsager first examined the isotropic-nematic phase transition theoretically using the excluded volume potential [1]. Later Maier and Saupe studied the isotropic-nematic phase transition using a simpler potential that is now called the Maier-Saupe interaction potential [2]. The ensemble of rigid rod-like polymers is modeled using the meso-scale approach and the approach of mean filed potential [3]. In a meso-scale that is much larger than the micro-scale of individual polymer rods but is much smaller than the macro-scale, the ensemble of rigid rod-like polymers is characterized by its orientation distribution (a probability density). The evolution of the orientation distribution is affected by the Brownian diffusion, by the mean filed potential representing mutual interactions among polymer rods within the meso-scale range, and by external potentials. If the meso-scale orientation distribution is inhomogeneous across the macro-scale, the orientation distribution is also affected by the neighboring orientation distributions. In this paper, we study only the homogeneous case.

Let $\rho(\mathbf{m},t)$ denote the probability density of the polymer orientation at time t. Here the independent variable $\mathbf{m}$ is a vector on the unit sphere. Later, we will also

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*Received: May 20, 2008; accepted (in revised version): October 11, 2008. Communicated by Pingwen Zhang.
This work was partially supported by the US National Science Foundation.

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use $\mathbf{m}$ to denote the random variable of polymer orientation. The time evolution of the probability density $\rho(\mathbf{m},t)$ is governed by the Smoluchowski equation [3]

$$\frac{\partial\rho}{\partial t}=D_R\frac{\partial}{\partial\mathbf{m}}\cdot\left(\frac{1}{k_BT}\frac{\partial U}{\partial\mathbf{m}}\rho+\frac{\partial\rho}{\partial\mathbf{m}}\right). \tag{1.1}$$

In the above, D_R is the rotational diffusion coefficient of polymer rods, k_B is the Boltzmann constant, T is the absolute temperature, and $\frac{\partial}{\partial\mathbf{m}}$ is the orientational gradient operator [4]. At equilibrium, the solution of the Smoluchowski equation is given by the Boltzmann distribution

$$\rho(\mathbf{m})=\frac{1}{Z}\exp\left(\frac{-U(\mathbf{m})}{k_BT}\right),\quad Z=\int_S\exp(-U(\mathbf{m}))\,d\mathbf{m}, \tag{1.2}$$

where S denotes the unit sphere. It is clear from equation (1.2) that an equilibrium solution is completely determined once the potential $U(\mathbf{m})$ is known. However, equation (1.2) does not give us an explicit expression for the equilibrium solution because the potential $U(\mathbf{m})$ is unknown and depends on the probability density $\rho(\mathbf{m})$. So, a more explicit notation for the potential should be $U(\mathbf{m};\{\rho\})$, and equation (1.2) is a nonlinear equation for the equilibrium probability density $\rho(\mathbf{m})$.

The potential $U(\mathbf{m})$ contains all mutual interaction potentials and all external potentials. The mutual interactions among polymer rods include both the excluded volume effect and the dipole-dipole interaction if polymer rods are dipolar. In this study, we will first consider three cases in three dimensional space: a) nematic polymers, b) dipolar nematic polymers, and c) dipolar nematic polymers in the presence of a stretching elongational flow. Later, we will consider case d): nematic polymers in higher dimensional space, which is more complex in its mathematical structure and has more branches in its phase diagram.

Case a: nematic polymers.

For nematic polymers, Onsager modeled the excluded volume effect as [1]

$$\frac{U(\mathbf{m})_{Onsager}}{k_BT}=b\langle|\sin\theta(\mathbf{m},\mathbf{m}')|\rangle, \tag{1.3}$$

where b denotes the interaction potential strength, which is proportional to the normalized polymer concentration and inversely proportional to the absolute temperature. Here $\mathbf{m}'$ denotes the random variable of polymer orientation and $\theta(\mathbf{m},\mathbf{m}')$ is the angle between the unit vector $\mathbf{m}$ and the unit vector $\mathbf{m}'$,

$$\sin\theta(\mathbf{m},\mathbf{m}')=\mathbf{m}\times\mathbf{m}'. \tag{1.4}$$

In the Onsager potential (1.3), $\langle\cdot\rangle$ denotes the average. Specifically,

$$\langle|\sin\theta(\mathbf{m},\mathbf{m}')|\rangle=\int_S|\sin\theta(\mathbf{m},\mathbf{m}')|\rho(\mathbf{m}')d\mathbf{m}'. \tag{1.5}$$

The absolute sign $|\cdot|$ in Onsager potential (1.3) presents significant difficulties for mathematical analysis. Maier and Saupe introduced an approximation for the Onsager excluded volume potential by replacing $|\sin\theta|$ with $\sin^2\theta$:

$$\frac{U(\mathbf{m})_{MS}}{k_BT}=b\left\langle\sin^2\theta(\mathbf{m},\mathbf{m}')\right\rangle. \tag{1.6}$$

Using $\sin^2\theta = 1-\cos^2\theta$ and $\cos\theta(\mathbf{m},\mathbf{m}') = \mathbf{m}\cdot\mathbf{m}'$, and using the relation $(\mathbf{m}\cdot\mathbf{m}')^2 = (\mathbf{m}\otimes\mathbf{m}):(\mathbf{m}'\otimes\mathbf{m}')$, the Maier-Saupe potential is written as

$$\begin{aligned}\frac{U(\mathbf{m})_{MS}}{k_BT} &= b - b\left\langle\cos^2\theta(\mathbf{m},\mathbf{m}')\right\rangle \\ &= b - b\left\langle(\mathbf{m}\cdot\mathbf{m}')^2\right\rangle \\ &= b - b(\mathbf{m}\otimes\mathbf{m}):\langle\mathbf{m}'\otimes\mathbf{m}'\rangle,\end{aligned} \tag{1.7}$$

where $\mathbf{m} = (m_1, m_2, m_3)^T$ and $\mathbf{m}' = (m_1', m_2', m_3')^T$ are column vectors. The tensor product $\mathbf{m}\otimes\mathbf{m}$ is defined as

$$\mathbf{m}\otimes\mathbf{m} \equiv \mathbf{m}\mathbf{m}^T = \begin{pmatrix} m_1m_1 & m_1m_2 & m_1m_3 \\ m_2m_1 & m_2m_2 & m_2m_3 \\ m_3m_1 & m_3m_2 & m_3m_3 \end{pmatrix}. \tag{1.8}$$

The tensor contraction $A:B$ is defined as

$$A:B \equiv \operatorname{trace}(AB). \tag{1.9}$$

In (1.7), dropping the constant term, and for simplicity, using $\mathbf{m}$ to denote the random variable of polymer orientation, we write the Maier-Saupe potential as

$$\frac{U(\mathbf{m})_{MS}}{k_BT} = -b(\mathbf{m}\otimes\mathbf{m}):\langle\mathbf{m}\otimes\mathbf{m}\rangle. \tag{1.10}$$

It should be pointed out that in (1.10), the $\mathbf{m}$ inside $\langle\mathbf{m}\otimes\mathbf{m}\rangle$ is the random variable of polymer orientation while the $\mathbf{m}$ outside $\langle\mathbf{m}\otimes\mathbf{m}\rangle$ is the independent variable.

Notice, in particular, that in the Maier-Saupe potential (1.7), the effect of the orientation probability density is completely specified by the second moment $\langle\mathbf{m}\otimes\mathbf{m}\rangle$. In other words, once we know the second moment, the Maier-Saupe potential is completely determined. In comparison, the Onsager potential depends on the whole orientation probability density function. Thus, when the intermolecular interaction is modeled using the Maier-Saupe potential, an equilibrium state is completely specified by the second moment. This convenient mathematical fact motivated many authors to follow the evolution of only the second moment by introducing various closure approximations [3, 5, 6, 7, 8, 9]. The ODE systems for the second moment based on closure approximation are significantly simpler than the full Smoluchowski equations. Recently, Constantin, Kevrekidis and Titi, and other groups, began to study polymer problems based on the full Smoluchowski equations [10, 11, 12, 13, 14]. In this study, we analyze equilibrium solutions of the full Smoluchowski equations without a closure approximation.

Since the second moment $\langle\mathbf{m}\otimes\mathbf{m}\rangle$ is a symmetric matrix, it can be diagonalized by an orthogonal transformation. Let us select the coordinate system such that the second moment $\langle\mathbf{m}\otimes\mathbf{m}\rangle$ is already diagonal:

$$\langle\mathbf{m}\otimes\mathbf{m}\rangle = \begin{pmatrix} \langle m_1^2\rangle & 0 & 0 \\ 0 & \langle m_2^2\rangle & 0 \\ 0 & 0 & \langle m_3^2\rangle \end{pmatrix}. \tag{1.11}$$

In this coordinate system, the Maier-Saupe potential has a simple form

$$\frac{U(\mathbf{m})_{MS}}{k_BT} = -b\left(\langle m_1^2\rangle m_1^2 + \langle m_2^2\rangle m_2^2 + \langle m_3^2\rangle m_3^2\right). \tag{1.12}$$

Case b: dipolar nematic polymers.

For dipolar nematic polymers, the mutual interaction potential includes both the Maier-Saupe interaction and the dipole-dipole interaction. The dipole-dipole interaction potential has the form [15, 16]

$$\frac{U(\mathbf{m})_{MS}}{k_B T} = -\alpha \mathbf{m} \cdot \langle \mathbf{m} \rangle \tag{1.13}$$

where $\alpha > 0$ is the strength of the dipole-dipole interaction, which is affected by the dipole strength of each polymer rod, the polymer concentration, and the absolute temperature. The total potential for dipolar nematic polymers has the form

$$\frac{U(\mathbf{m})_{Total}}{k_B T} = -b(\mathbf{m} \otimes \mathbf{m}) : \langle \mathbf{m} \otimes \mathbf{m} \rangle - \alpha \mathbf{m} \cdot \langle \mathbf{m} \rangle . \tag{1.14}$$

Case c: dipolar nematic polymers in the presence of a stretching elongational flow.

The potential induced by the stretching elongational flow has the form [16]

$$\frac{U(\mathbf{m})_{Flow}}{k_B T} = -\frac{\alpha_0}{2}(\mathbf{m} \otimes \mathbf{m}) : (\mathbf{E} \otimes \mathbf{E}) \tag{1.15}$$

where $\mathbf{E}$ is the direction of the stretching elongation flow, and $\alpha_0 > 0$ is proportional to the rate of the stretching elongation and inversely proportional to the absolute temperature. The total potential for dipolar nematic polymers in the presence of a stretching elongational flow has the form

$$\frac{U(\mathbf{m})_{Total}}{k_B T} = -b(\mathbf{m} \otimes \mathbf{m}) : \langle \mathbf{m} \otimes \mathbf{m} \rangle - \alpha \mathbf{m} \cdot \langle \mathbf{m} \rangle - \frac{\alpha_0}{2}(\mathbf{m} \otimes \mathbf{m}) : (\mathbf{E} \otimes \mathbf{E}) . \tag{1.16}$$

Case d: nematic polymers in higher dimensional space.

The study of nematic polymer rods in higher dimensional spaces with the Maier-Saupe potential interaction is a challenging mathematical problem. This interesting mathematical problem is formulated by applying the form of the Maier-Saupe potential in three dimensional case directly to the n-dimensional case. Currently, there is no concrete physical interpretation for this mathematical problem. However, the orientation of a polymer element can have more than two degrees of freedom. For example, the orientation of a boomerang-shaped polymer element has three degrees of freedom (the same as the number of dimensions of the unit sphere in four dimensional space), albeit the molecular interaction between boomerang-shaped polymers is more complicated than the Maier-Saupe potential. It is our hope that by studying nematic polymer rods in higher dimensional spaces with the Maier-Saupe potential interaction, we will gain insight into the behavior of more complicated polymers (such as boomerang-shaped polymers) in three dimensional space.

For nematic polymers in n-dimensional space, the Maier-Saupe potential is

$$\frac{U_{MS}(\mathbf{m})}{k_B T} = -b \sum_{i=1}^{n} \langle m_i^2 \rangle m_i^2 . \tag{1.17}$$

In this paper, we discuss the rotational symmetry of these cases. We start by discussing what we mean by rotational symmetry.

In k-dimensional space, the rotational symmetry of a function $\rho(m_1,\dots,m_k)$ is intuitively defined as that the function $\rho(m_1,\dots,m_k)$ is invariant under an arbitrary rotation around the origin, which means the function ρ depends only on $m_1^2+\cdots+m_k^2$:

$$\rho(m_1,\dots,m_k)=f(m_1^2+\cdots+m_k^2).$$

In the special case of $k=1$ (functions of one variable), the rotational symmetry means $\rho(m_1)=f(|m_1|)$, that is, ρ is an even function of m_1: $\rho(m_1)=\rho(-m_1)$.

When the k-dimensional space in consideration is a sub-space of the n-dimensional space for independent variables $(m_1,\dots,m_n)$, function ρ generally depends both on $(m_1,\dots,m_k)$ and on $(m_{k+1},\dots,m_n)$. In this case, the rotational symmetry in the k-dimensional sub-space $\{(m_1,\dots,m_k)\}$ is intuitively extended as that the dependence of function ρ on $(m_1,\dots,m_k)$ is only through $m_1^2+\cdots+m_k^2$. In other words, the rotational symmetry in the k-dimensional sub-space $\{(m_1,\dots,m_k)\}$ means

$$\rho(m_1,\dots,m_k,m_{k+1},\dots,m_n)=f(m_1^2+\cdots+m_k^2,m_{k+1},\dots,m_n).$$

In this manuscript, we consider functions on the unit sphere in n-dimensional space, which satisfies $m_1^2+\cdots+m_k^2=1-(m_{k+1}^2+\cdots+m_n^2)$. Using this fact, the rotational symmetry in the k-dimensional sub-space $\{(m_1,\dots,m_k)\}$ is conveniently defined as

$$\rho(m_1,\dots,m_k,m_{k+1},\dots,m_n)=f(m_{k+1},\dots,m_n).$$

Note that a function $\rho(m_1,m_2,m_3)$ defined on the unit sphere in three dimensional space satisfies $\rho(m_1,m_2,m_3)=f(m_2,m_3)$ if and only if ρ is even in m_1: $\rho(m_1,m_2,m_3)=\rho(-m_1,m_2,m_3)$. That is, the rotational symmetry in a one-dimensional subspace means the function is even in that variable. For the case of nematic polymers without dipole-dipole interaction, the probability density ρ is always even in every independent variable. In the presence of dipole-dipole interaction, however, that is no longer true.

DEFINITION 1.1 (Rotational symmetry). *Consider a function $\rho(\mathbf{m})$ on the unit sphere in n-dimensional space. That is, the independent variable $\mathbf{m}=(m_1,m_2,\dots,m_n)^T$ is constrained by $\sum_{j=1}^n m_j^2=1$. If we can divide the n dimensions into two groups and re-number them as $\mathbf{m}^{(\mathbf{A})}=(m_1,\dots,m_k)$ and $\mathbf{m}^{(\mathbf{B})}=(m_{k+1},\dots,m_n)$ such that*

$$\rho(\mathbf{m})=f(\mathbf{m}^{(\mathbf{B})}), \tag{1.18}$$

then we say the function $\rho(\mathbf{m})$ has rotational symmetry around the sub-space $\{(m_{k+1},\dots,m_n)\}$, or equivalently we say the function $\rho(\mathbf{m})$ has rotational symmetry in the subspace $\{(m_1,\dots,m_k)\}$.

For nematic polymers in three dimensional space, an equilibrium state has the form

$$\rho(\mathbf{m})=\frac{1}{Z}\exp\left(b\left(\langle m_1^2\rangle m_1^2+\langle m_2^2\rangle m_2^2+\langle m_3^2\rangle m_3^2\right)\right) \tag{1.19}$$

which is even in every independent variable. It follows that probability density (1.19) always has rotational symmetry around $\{(m_i,m_j)\},i\neq j$, the two dimensional sub-space spanned by any two of the three principal axes of the second moment. Obviously, this rotational symmetry is not very interesting. The rotational symmetry we prefer to have for nematic polymers in three dimensional space is the one around a principal axis, which is also called axisymmetry. For example, if $\langle m_1^2\rangle = \langle m_2^2\rangle$, then probability density $\rho(\mathbf{m})$ given in (1.19) can be written as a function of m_3 only, and thus, has axisymmetry around m_3-axis. In higher dimensional space, the rotational symmetry is indeed broader and more complex in structure than the axisymmetry. An equilibrium state of nematic polymers in the n-dimensional space has the form

$$\rho(\mathbf{m}) = \frac{1}{Z}\exp\left(b\sum_{i=1}^{n}\langle m_i^2\rangle m_i^2\right). \tag{1.20}$$

For $n=4$, if $\langle m_1^2\rangle = \langle m_2^2\rangle$, then $\rho(\mathbf{m})$ has rotational symmetry around the subspace $\{(m_3, m_4)\}$; if $\langle m_1^2\rangle = \langle m_2^2\rangle = \langle m_3^2\rangle$, then $\rho(\mathbf{m})$ has rotational symmetry around the subspace $\{m_4\}$, which is the axisymmetry around m_4-axis.

The rest of the paper is organized as follows. In section 2, we introduce a key inequality, and discuss the relation between the inequality and the axisymmetry of equilibria of nematic polymers. In section 3, we show that once the inequality is established for the case of nematic polymers, it can be elegantly extended to the case of dipolar nematic polymers and the case of dipolar nematic polymers in the presence of a stretching elongational flow. Furthermore, we show that in both of these two cases, the inequality implies the axisymmetry of equilibria. In section 4, we investigate equilibrium states of nematic polymers in higher dimensional spaces. We first extend the inequality obtained in three dimensional space to n-dimensional space. Then we use the inequality to show that for nematic polymers in n-dimensional space, the second moment (a $n\times n$ matrix) has at most two distinct eigenvalues. It follows that all equilibrium states must have rotational symmetry, which significantly reduces the complexity of classifying equilibrium states. We will calculate and present the phase diagram of nematic polymers in four-, five- and six- dimensional spaces.

In the sections below, to facilitate the discussion on the unified view of rotational symmetry, it is necessary to revisit many known results. Instead of just citing them in references, we state them as propositions for two good reasons. First, these propositions are included here for the completeness of our discussion and for the convenience of readers. Second, these propositions state the known results in terms of new formulations (for example, the key inequality) and in terms of new parameters (for example, η_1 and η_2), which are specifically designed and required in our discussion here.

2. Nematic polymers in the three dimensional space

For nematic polymers, the equilibrium probability density, as given in (1.19), is completely specified by $(\langle m_1^2\rangle, \langle m_3^2\rangle, \langle m_3^2\rangle)$. To facilitate the discussion below, we introduce the shorthand notations:

$$s_1 \equiv \langle m_1^2\rangle, \quad s_2 \equiv \langle m_2^2\rangle, \quad s_3 \equiv \langle m_3^2\rangle. \tag{2.1}$$

Our goal is to show that s_1, s_2, and s_3 have at most two distinct values. That is, two out of s_1, s_2, and s_3 must be the same. The nonlinear system for (s_1, s_2, s_3) is

$$\int_S m_j^2\rho(\mathbf{m})d\mathbf{m} = s_j, \quad j = 1,2,3 \tag{2.2}$$

where the probability density is given by

$$\rho(\mathbf{m}) = \frac{1}{Z}\exp\left(b\left(s_1 m_1^2 + s_2 m_2^2 + s_3 m_3^2\right)\right). \tag{2.3}$$

Nonlinear system (2.2) can be concisely written as

$$\langle m_j^2 \rangle = s_j, \quad j = 1,2,3, \tag{2.4}$$

where the average is taken with respect to the probability density given in (2.3). Without loss of generality, we assume that (s_1, s_2, s_3) satisfies $s_1 \le s_2 \le s_3$, which can always be satisfied by re-labeling the three dimensions. With the ordering of $s_1 \le s_2 \le s_3$, the solution of nonlinear system (2.4) has several possibilities, which are listed below.

1. $s_1 = s_2$, which means that the equilibrium state is axisymmetric around the m_3-axis.
2. $s_2 = s_3$, which means that the equilibrium state is axisymmetric around the m_1-axis.
3. $s_1 < s_2 < s_3$, which means that the equilibrium state is not axisymmetric.

Our approach is to show that two out of s_1, s_2, and s_3 must be the same by excluding the case of $s_1 < s_2 < s_3$. It is clear that with the ordering of $s_1 \le s_2 \le s_3$, an equilibrium state is not axisymmetric if and only if $s_1 < s_2 < s_3$. We summarize this in a proposition below.

Proposition 2.1. *For nematic polymers, the existence of a non-axisymmetric equilibrium state is equivalent to the existence of a solution of system (2.4) with* $s_1 < s_2 < s_3$.

Consider a solution (s_1, s_2, s_3) of system (2.4). It follows directly from system (2.4) that

$$\begin{aligned} \langle m_3^2 - m_2^2 \rangle &= s_3 - s_2, \\ \langle m_3^2 - m_1^2 \rangle &= s_3 - s_1. \end{aligned} \tag{2.5}$$

Combining these two equations yields

$$\langle F(s_1, s_2, s_3, b, \mathbf{m}) \rangle = 0 \tag{2.6}$$

where the function $F(s_1, s_2, s_3, b, \mathbf{m})$ is defined as

$$F(s_1, s_2, s_3, b, \mathbf{m}) \equiv b(s_3 - s_1)(m_3^2 - m_2^2) - b(s_3 - s_2)(m_3^2 - m_1^2). \tag{2.7}$$

Thus, we obtain the proposition below about a necessary condition for non-axisymmetry.

Proposition 2.2. *For nematic polymers, the existence of a non-axisymmetric equilibrium state implies that there exists a set of* $s_1 < s_2 < s_3$ *and* $b > 0$ *such that*

$$\langle F(s_1, s_2, s_3, b, \mathbf{m}) \rangle = 0. \tag{2.8}$$

From Proposition 2.2, we arrive at a sufficient condition for the axisymmetry.

Proposition 2.3. *For nematic polymers, if we have*

$$\langle F(s_1, s_2, s_3, b, \mathbf{m}) \rangle \ne 0 \ \textit{ for all } s_1 < s_2 < s_3 \textit{ and } b > 0, \tag{2.9}$$

then all equilibrium states are axisymmetric for all values of $b > 0$.

The axisymmetry of all equilibrium states of nematic polymers in three dimensional space has been established in [15, 17, 18]. The goal of the current study is to have a unified view of rotational symmetry in many different cases. It is clear that inequality (2.9) is the key in determining the axisymmetry of nematic polymers. As we will see later, this inequality is also the key in determining i) the axisymmetry of dipolar nematic polymers, ii) the axisymmetry of dipolar nematic polymers in the presence of a stretching elongational flow, and iii) the rotational symmetry of nematic polymers in higher dimensional space. Below we will prove a stronger and a more convenient version of inequality (2.9).

We first rewrite inequality (2.9) into a simpler form by introducing new parameters.

$$\eta_1 \equiv b(s_3 - s_1), \quad \eta_2 \equiv b(s_3 - s_2). \tag{2.10}$$

With the introduction of (η_1, η_2), we use the relation $m_1^2 + m_2^2 + m_3^2 = 1$ to write the equilibrium probability density as

$$\begin{aligned} \rho(\mathbf{m}) &= \frac{1}{Z} \exp\left(b\left(s_1 m_1^2 + s_2 m_2^2 + s_3 m_3^2\right)\right), \\ &= \frac{1}{Z} \exp\left(b\left(s_1 m_1^2 + s_2 m_2^2 + s_3 m_3^2\right) - b s_3 (m_1^2 + m_2^2 + m_3^2)\right), \\ &= \frac{1}{Z} \exp\left(-b(s_3 - s_1) m_1^2 - b(s_3 - s_2) m_2^2\right), \\ &= \frac{1}{Z} \exp\left(-\eta_1 m_1^2 - \eta_2 m_2^2\right). \end{aligned} \tag{2.11}$$

Here we use the notation Z generically as the normalizing constant in different situations. For example, in equation (2.11), the Z on line 2 is different from the Z on line 1. In terms of (η_1, η_2), the function $F(s_1, s_2, s_3, b, \mathbf{m})$ becomes

$$F(\eta_1, \eta_2, \mathbf{m}) \equiv \eta_1 (m_3^2 - m_2^2) - \eta_2 (m_3^2 - m_1^2). \tag{2.12}$$

Note that with the introduction of (η_1, η_2), both the function $F(\eta_1, \eta_2, \mathbf{m})$ and the probability density $\rho(\mathbf{m})$ are independent of b. As a result, inequality (2.9) can be written into a form that involves only two parameters η_1 and η_2. From definition (2.10), we see that $s_1 < s_2 < s_3$ is equivalent to $0 < \eta_2 < \eta_1$. It follows that inequality (2.9) is equivalent to the inequality

$$\langle F(\eta_1, \eta_2, \mathbf{m}) \rangle \neq 0 \quad \text{for all } 0 < \eta_2 < \eta_1. \tag{2.13}$$

Thus, to show the axisymmetry for nematic polymers, we only need to prove inequality (2.13). The theorem below establishes a stronger version of inequality (2.13).

Theorem 2.4. *The inequality*

$$\langle F(\eta_1, \eta_2, \mathbf{m}) \rangle > 0 \quad \textit{for all } 0 < \eta_2 < \eta_1, \tag{2.14}$$

holds, where the average is with respect to the probability density given in (2.11).

The proof of Theorem 2.4 employs similar tools used in the proof of axisymmetry in [18]. We present the proof here for two reasons. First, this inequality is the key for determining rotational symmetry in many different cases. We are going to extend this inequality to other cases *based on its validity in the case of nematic polymers*. Thus, for the benefit of discussing the rotational symmetry of other cases, it is important to present a complete proof of this inequality here for the case of nematic polymers. The second reason is that the proof requires a few lemmas that will be used later when we extend this inequality to other cases. We introduce the lemmas needed before we present the proof of Theorem 2.4.

LEMMA 2.5. *Suppose u is a continuous random variable. Consider two derived random variables $f(u)$ and $g(u)$. If both $f(u)$ and $g(u)$ are continuous and strictly increasing functions of u, then we have*

$$\Big\langle \Big(f(u)-\langle f(u)\rangle\Big)\, g(u)\Big\rangle > 0, \tag{2.15}$$

or equivalently $\langle f(u)g(u)\rangle > \langle f(u)\rangle\cdot\langle g(u)\rangle$.

Proof. Since $f(u)$ is a continuous and strictly increasing function of u, there exists u_0 such that $f(u_0)=\langle f(u)\rangle$. It follows that

$$\begin{aligned}\Big\langle \Big(f(u)-\langle f(u)\rangle\Big)\, g(u)\Big\rangle &= \Big\langle \Big(f(u)-f(u_0)\Big)\, g(u)\Big\rangle\\ &= \Big\langle \Big(f(u)-f(u_0)\Big)\Big(g(u)-g(u_0)\Big)\Big\rangle > 0.\end{aligned} \tag{2.16}$$

□

LEMMA 2.6. *Consider the random variable $\mathbf{m}=(m_1,m_2,m_3)$ with the probability density given in (2.11). If $0<\eta_2<\eta_1$, then we have*

1. $\Big\langle m_1^2-m_3^2 \,\Big|\, |m_2|=u\Big\rangle$ *is a strictly increasing function of u.*
2. $\Big\langle m_2^2-m_3^2 \,\Big|\, |m_1|=u\Big\rangle$ *is a strictly increasing function of u.*
3. $\Big\langle m_1^2-m_2^2 \,\Big|\, |m_3|=u\Big\rangle$ *is a strictly increasing function of u.*

Proof. Here we present the proof for Item 1. items 2 and 3 are proved in a similar way. We adopt the spherical coordinate system with the m_2-axis as its pole. In this spherical coordinate system, we have

$$m_1=\sin\phi\sin\theta,\quad m_2=\cos\phi,\quad m_3=\sin\phi\cos\theta. \tag{2.17}$$

Using $m_1^2+m_2^2+m_3^2=1$, we write the probability density given in (2.11) as

$$\begin{aligned}\rho(\mathbf{m}) &= \frac{1}{Z}\exp\left(-\eta_1 m_1^2-\eta_2 m_2^2\right),\\ &= \frac{1}{Z}\exp\left((\eta_2-\eta_1)m_1^2+\eta_2 m_3^2\right),\\ &= \frac{1}{Z}\exp\left(\frac{\eta_1}{2}(m_3^2-m_1^2)+\frac{2\eta_2-\eta_1}{2}(m_3^2+m_1^2)\right),\\ &= \frac{1}{Z}\exp\left(\frac{\eta_1}{2}\sin^2\phi\cos 2\theta+\frac{2\eta_2-\eta_1}{2}\sin^2\phi\right).\end{aligned} \tag{2.18}$$

The conditional average has the form:

$$\begin{aligned}\Big\langle m_1^2-m_3^2 \,\Big|\, |m_2|=u\Big\rangle &= \frac{-(1-u^2)\int_0^{2\pi}\cos 2\theta \exp\left(\frac{\eta_1}{2}(1-u^2)\cos 2\theta\right)d\theta}{\int_0^{2\pi}\exp\left(\frac{\eta_1}{2}(1-u^2)\cos 2\theta\right)d\theta}\\ &= -(1-u^2)\,\sigma\Big(\frac{\eta_1}{2}(1-u^2)\Big),\end{aligned} \tag{2.19}$$

where function $\sigma(r)$ is defined as

$$\sigma(r) \equiv \frac{\int_0^{2\pi} \cos 2\theta \exp(r\cos 2\theta)\, d\theta}{\int_0^{2\pi} \exp(r\cos 2\theta)\, d\theta}. \tag{2.20}$$

In [12], it was shown that $\sigma(0)=0$ and $\sigma(r)$ is a strictly increasing function of r. It follows that the conditional average $\left\langle m_1^2 - m_3^2 \,\middle|\, |m_2| = u \right\rangle$ is a strictly increasing function of u for $|u| \le 1$ (the range of $|m_2|$). ◻

For simplicity of presentation, we introduce shorthand notations for $m_j^2 - \langle m_j^2 \rangle$. Let

$$h_1 \equiv m_1^2 - \langle m_1^2 \rangle, \quad h_2 \equiv m_2^2 - \langle m_2^2 \rangle, \quad h_3 \equiv m_3^2 - \langle m_3^2 \rangle. \tag{2.21}$$

From the definition, it is clear that $h_1 + h_2 + h_3 = 0$ is always true.

Lemma 2.7. *If $0 < \eta_2 < \eta_1$, then we have*

$$\langle h_2(h_1 - h_3) \rangle > 0, \quad \langle h_1(h_2 - h_3) \rangle > 0, \quad \langle h_3(h_1 - h_2) \rangle > 0. \tag{2.22}$$

Proof. Here we present the proof of $\langle h_2(h_1 - h_3) \rangle > 0$. The other two inequalities are proved in a similar way. We start by expressing $\langle h_2(h_1 - h_3) \rangle$ in terms of a conditional average.

$$\begin{aligned} \langle h_2(h_1 - h_3) \rangle &= \left\langle \left(m_2^2 - \langle m_2^2 \rangle\right)\left(m_1^2 - m_3^2 - \langle m_1^2 - m_3^2 \rangle\right) \right\rangle \\ &= \left\langle \left(m_2^2 - \langle m_2^2 \rangle\right)\left(m_1^2 - m_3^2\right) \right\rangle \\ &= \left\langle \left(m_2^2 - \langle m_2^2 \rangle\right) \left\langle m_1^2 - m_3^2 \,\middle|\, |m_2| \right\rangle \right\rangle. \end{aligned} \tag{2.23}$$

Lemma 2.6 tells us that $\left\langle m_1^2 - m_3^2 \,\middle|\, |m_2| \right\rangle$ is a strictly increasing function of $|m_2|$. Since $m_2^2 - \langle m_2^2 \rangle$ is also a strictly increasing function of $|m_2|$, after applying Lemma 2.5 to the right hand side of (2.23) we arrive at

$$\langle h_2(h_1 - h_3) \rangle > \left\langle m_2^2 - \langle m_2^2 \rangle \right\rangle \cdot \left\langle \left\langle m_1^2 - m_3^2 \,\middle|\, |m_2| \right\rangle \right\rangle = 0. \tag{2.24}$$

◻

Now we are ready to prove the inequality (Theorem 2.4).

Proof of Theorem 2.4. For a given set of $0 < q_2 < q_1$, we need to show $\langle F(q_1, q_2, \mathbf{m}) \rangle > 0$. Let us introduce the function

$$w(r) \equiv \frac{\langle F(rq_1, rq_2, \mathbf{m}) \rangle}{r} = q_1 \left\langle m_3^2 - m_2^2 \right\rangle, -q_2 \left\langle m_3^2 - m_1^2 \right\rangle, \tag{2.25}$$

where the average is taken with respect the probability density given in (2.11) with $\eta_1 = rq_1$ and $\eta_2 = rq_2$

$$\rho(\mathbf{m}) = \frac{\exp\left(-r\left(q_1 m_1^2 + q_2 m_2^2\right)\right)}{\int_S \exp\left(-r\left(q_1 m_1^2 + q_2 m_2^2\right)\right) d\mathbf{m}}. \tag{2.26}$$

When $r = 0$, the probability density is the uniform distribution and $\langle m_j^2 \rangle = 1/3$. It follows that $w(0) = 0$. Thus, to prove $\langle F(q_1, q_2, \mathbf{m}) \rangle = w(1) > 0$, we only need to show

$w'(r) > 0$ for $r > 0$. The derivative of the probability density (2.26) with respect to r has the form

$$\begin{aligned}\frac{d\rho(\mathbf{m})}{dr} &= -\left(q_1 m_1^2 + q_2 m_2^2\right)\rho(\mathbf{m}) + \left(\int_S \left(q_1 m_1^2 + q_2 m_2^2\right)\rho(\mathbf{m})d\mathbf{m}\right)\rho(\mathbf{m}),\\ &= -\left(q_1 m_1^2 + q_2 m_2^2 - \left\langle q_1 m_1^2 + q_2 m_2^2\right\rangle\right)\rho(\mathbf{m}),\\ &= -\left(q_1 h_1 + q_2 h_2\right)\rho(\mathbf{m}),\end{aligned} \tag{2.27}$$

where h_j is defined in (2.21). Differentiating $w(r)$ and using $\langle h_j\rangle = 0$, we obtain

$$\begin{aligned}w'(r) &= -q_1\left\langle\left(m_3^2 - m_2^2\right)\left(q_1 h_1 + q_2 h_2\right)\right\rangle + q_2\left\langle\left(m_3^2 - m_1^2\right)\left(q_1 h_1 + q_2 h_2\right)\right\rangle,\\ &= -q_1\left\langle\left(h_3 - h_2\right)\left(q_1 h_1 + q_2 h_2\right)\right\rangle + q_2\left\langle\left(h_3 - h_1\right)\left(q_1 h_1 + q_2 h_2\right)\right\rangle.\end{aligned} \tag{2.28}$$

With the help of $h_1 + h_2 + h_3 = 0$, we write $(q_1 h_1 + q_2 h_2)$ into two expressions

$$\begin{aligned}(q_1 h_1 + q_2 h_2) &= (q_1 - q_2)h_1 - q_2 h_3,\\ (q_1 h_1 + q_2 h_2) &= -(q_1 - q_2)h_2 - q_1 h_3.\end{aligned} \tag{2.29}$$

Substituting the two expressions into the two terms on the right hand side of (2.28), respectively, we obtain

$$\begin{aligned}w'(r) = &-q_1\left\langle (h_3 - h_2)\Big((q_1 - q_2)h_1 - q_2 h_3\Big)\right\rangle,\\ &+q_2\left\langle (h_3 - h_1)\Big(-(q_1 - q_2)h_2 - q_1 h_3\Big)\right\rangle,\\ = &\, q_1(q_1 - q_2)\langle h_1(h_2 - h_3)\rangle + q_1 q_2\langle h_3(h_3 - h_2)\rangle,\\ &+q_2(q_1 - q_2)\langle h_2(h_1 - h_3)\rangle - q_1 q_2\langle h_3(h_3 - h_1)\rangle,\\ = &\, q_1(q_1 - q_2)\langle h_1(h_2 - h_3)\rangle + q_2(q_1 - q_2)\langle h_2(h_1 - h_3)\rangle,\\ &+q_1 q_2\langle h_3(h_1 - h_2)\rangle.\end{aligned} \tag{2.30}$$

For $r > 0$, we have $0 < rq_2 < rq_1$, which implies that probability density (2.26) satisfies the condition of Lemma 2.7 with $\eta_1 = rq_1$ and $\eta_2 = rq_2$. Applying Lemma 2.7, we obtain that all averages on the right hand side of (2.30) are strictly positive. All coefficients on the right hand side of (2.30) are also strictly positive following from $0 < q_2 < q_1$. Therefore, we conclude that $w'(r) > 0$ for $r > 0$, which leads immediately to $\langle F(q_1, q_2, \mathbf{m})\rangle = w(1) > 0$. □

Combining the results of Proposition 2.3 and Theorem 2.4, we conclude that all equilibrium states of nematic polymers are axisymmetric for all values of $b > 0$. The inequality described in Theorem 2.4 is the key in determining the axisymmetry in the case of nematic polymers. As we will see later, this inequality (with different probability densities) also determines i) axisymmetry in the case of a dipolar nematic polymer, ii) axisymmetry in the case of a dipolar nematic polymer driven by a stretching elongational flow, and iii) rotational symmetry in the case of nematic polymers in higher dimensional space.

3. Dipolar nematic polymers

3.1. Dipolar nematic polymers in the absence of flow.

In the discussion below, we need to distinguish different averages taken with respect to different probabilities. For clarity of the presentation, we shall continue to use $\langle\cdot\rangle$ to denote the average with respect to the probability density $\rho(\mathbf{m})$ given in (2.11) for nematic polymers and we shall use $\langle\cdot\rangle_b$ to denote the average with respect to the probability density $\rho_b(\mathbf{m})$ given below for dipolar nematic polymers.

For dipolar nematic polymers, the total potential includes both the Maier-Saupe interaction and the dipole-dipole interaction [16]:

$$\frac{U(\mathbf{m})}{k_B T} = -\alpha \mathbf{m}\cdot\langle\mathbf{m}\rangle_b - b(\mathbf{m}\otimes\mathbf{m}):\langle\mathbf{m}\otimes\mathbf{m}\rangle_b. \tag{3.1}$$

The second moment $\langle\mathbf{m}\otimes\mathbf{m}\rangle_b$ is symmetric, so it can be diagonalized by an orthogonal transformation. In [16] and [19], it was shown that the the first moment $\langle\mathbf{m}\rangle$ must be parallel to one of the three principal axes of the second moment (here we adopt the convention that zero vector is parallel to any vector). We adopt the coordinate system in which the second moment $\langle\mathbf{m}\otimes\mathbf{m}\rangle_b$ is diagonal and the m_3-axis coincides with the first moment. In this coordinate system, the total potential has the form

$$\frac{U(\mathbf{m})}{k_B T} = -\alpha\langle m_3\rangle_b m_3 - b\left(\langle m_1^2\rangle_b m_1^2 + \langle m_2^2\rangle_b m_2^2 + \langle m_3^2\rangle_b m_3^2\right). \tag{3.2}$$

An equilibrium state is completely specified by $\left(\langle m_3\rangle_b, \langle m_1^2\rangle_b, \langle m_2^2\rangle_b, \langle m_3^2\rangle_b\right)$. For mathematical convenience, we introduce shorthand notations.

$$r_3 \equiv \langle m_3\rangle_b, \quad s_1 \equiv \langle m_1^2\rangle_b, \quad s_2 \equiv \langle m_2^2\rangle_b, \quad s_3 \equiv \langle m_3^2\rangle_b. \tag{3.3}$$

Our goal is to show $s_1 = s_2$. The nonlinear system for (r_3, s_1, s_2, s_3) is

$$\begin{aligned} &\langle m_3\rangle_b = r_3, \\ &\langle m_j^2\rangle_b = s_j, \quad j = 1,2,3, \end{aligned} \tag{3.4}$$

where the probability density is given by

$$\rho_b(\mathbf{m}) = \frac{1}{Z_b}\exp\left(\alpha r_3 m_3 + b\left(s_1 m_1^2 + s_2 m_2^2 + s_3 m_3^2\right)\right). \tag{3.5}$$

In [19], it was established that a necessary condition for an equilibrium state being stable is that i) the first moment must be parallel to the longest principal axis of the second moment and ii) if the first moment is non-zero, then the longest principal axis of the second moment must be strictly longer than the other two. This result implies that for $r_3 \neq 0$, a stable equilibrium solution of system (3.4) can be made to satisfy the constraint $s_1 \le s_2 < s_3$ by possibly relabeling the m_1-axis and the m_2-axis. When $r_3 \neq 0$, the m_3-axis is the only possible candidate for the axis of symmetry, and an equilibrium solution is axisymmetric if and only if $s_1 = s_2$. Our approach is to show $s_1 = s_2$ by excluding the case of $s_1 < s_2 < s_3$. When $r_3 \neq 0$, a stable equilibrium state is not axisymmetric if and only if $s_1 < s_2 < s_3$. We summarize this in the proposition below for dipolar nematic polymers. Notice that the conclusion here is the same as the conclusion for nematic polymers in Proposition 2.1.

PROPOSITION 3.1. *For dipolar nematic polymers, the existence of a stable non-axisymmetric equilibrium state is equivalent to the existence of a solution of system (3.4) with* $s_1 < s_2 < s_3$.

Here we need to point out that for dipolar nematic polymers, an equilibrium state with $r_3 \neq 0$ and $s_2 = s_3$ is not axisymmetric. But this case is excluded using the stability requirement, based on the result established in [19]. Note that (s_1, s_2, s_3)

satisfies equations of the same average form (but with different probability densities) in both the case of nematic polymers and the case of dipolar nematic polymers. As a result, the reasoning after Proposition 2.1 leading to Proposition 2.2 and 2.3 is also valid for dipolar nematic polymers. It is stated below as Proposition 3.2 and 3.3.

Proposition 3.2. *For dipolar nematic polymers, the existence of a stable non-axisymmetric equilibrium state implies that there exists a set of* $s_1 < s_2 < s_3$, r_3, $\alpha > 0$ *and* $b > 0$ *such that*

$$\langle F(s_1, s_2, s_3, b, \mathbf{m}) \rangle_b = 0, \tag{3.6}$$

where $\langle \cdot \rangle_b$ *denotes the average with respect to probability density (3.5), and the function*
$F(s_1, s_2, s_3, b, \mathbf{m})$ *is defined in (2.7).*

Proposition 3.3. *For dipolar nematic polymers, if we have*

$$\langle F(s_1, s_2, s_3, b, \mathbf{m}) \rangle_b \neq 0 \;\; \textit{for all } s_1 < s_2 < s_3, r_3, \alpha > 0 \textit{ and } b > 0, \tag{3.7}$$

then all stable equilibrium states are axisymmetric for all values of $\alpha > 0$ *and* $b > 0$.

Similar to what we did in the previous section, inequality (3.7) is simplified by introducing new parameters

$$\lambda \equiv \alpha r_3, \;\; \eta_1 \equiv b(s_3 - s_1), \;\; \eta_2 \equiv b(s_3 - s_2). \tag{3.8}$$

In terms of $(\eta_1, \eta_2, \lambda)$, the probability density (3.5) becomes

$$\begin{aligned} \rho_b(\mathbf{m}) &= \frac{1}{Z_b} \exp\left(\alpha r_3 m_3 + b\left(s_1 m_1^2 + s_2 m_2^2 + s_3 m_3^2\right)\right) \\ &= \frac{1}{Z_b} \exp\left(\lambda m_3 - \eta_1 m_1^2 - \eta_2 m_2^2\right) \end{aligned} \tag{3.9}$$

and the function $F(s_1, s_2, s_3, b, \mathbf{m})$ becomes the function $F(\eta_1, \eta_2, \mathbf{m})$ given in (2.12). Thus, inequality (3.7) is equivalent to the inequality below, which involves only $(\eta_1, \eta_2, \lambda)$.

$$\langle F(\eta_1, \eta_2, \mathbf{m}) \rangle_b \neq 0 \;\; \text{for all } 0 < \eta_2 < \eta_1 \text{ and } \lambda. \tag{3.10}$$

Therefore, to show axisymmetry for dipolar nematic polymers, we only need to prove inequality (3.10). The theorem below establishes a stronger version of inequality (3.10).

Theorem 3.4. *The inequality*

$$\langle F(\eta_1, \eta_2, \mathbf{m}) \rangle_b > 0 \;\;\; \textit{for all } 0 < \eta_2 < \eta_1 \textit{ and } \lambda \tag{3.11}$$

holds, where $\langle \cdot \rangle_b$ *denotes the average with respect to probability density (3.9).*

The proof of Theorem 3.4 requires a lemma that relates the average $\langle \cdot \rangle_b$ *to the average* $\langle \cdot \rangle$.

Lemma 3.5. *If* $f(m_1, m_2, m_3)$ *is an even function of* m_3*, then we have*

$$\langle f(m_1, m_2, m_3) \rangle_b = C_b \langle f(m_1, m_2, m_3) \cosh(\lambda m_3) \rangle, \tag{3.12}$$

where $\langle\cdot\rangle$ *denotes the average with respect to the probability density* $\rho(\mathbf{m})$ *given in (2.11) for nematic polymers, and* $\langle\cdot\rangle_b$ *denotes the average with respect to the probability density* $\rho_b(\mathbf{m})$ *given in (3.9) for dipolar nematic polymers. In the above, the coefficient* $C_b = Z/Z_b > 0$ *where* Z *is the normalizing constant in (2.11) and* Z_b *is the normalizing constant in (3.9).*

Proof. The integral expression of $\langle f(m_1,m_2,m_3)\rangle_b$ is

$$\langle f(m_1,m_2,m_3)\rangle_b = \frac{1}{Z_b}\int_S f(m_1,m_2,m_3)\exp\left(\lambda m_3 - \eta_1 m_1^2 - \eta_2 m_2^2\right) d\mathbf{m}. \tag{3.13}$$

In the integral, using change of variable $(m_3)_{new} = -(m_3)_{old}$ yields

$$\langle f(m_1,m_2,m_3)\rangle_b = \frac{1}{Z_b}\int_S f(m_1,m_2,-m_3)\exp\left(-\lambda m_3 - \eta_1 m_1^2 - \eta_2 m_2^2\right) d\mathbf{m}. \tag{3.14}$$

Combining (3.13) and (3.14), and using that $f(m_1,m_2,m_3)$ is even in m_3, we have

$$\begin{aligned}\langle f(m_1,m_2,m_3)\rangle_b &= \frac{1}{Z_b}\int_S f(m_1,m_2,m_3)\cosh(\lambda m_3)\exp\left(-\eta_1 m_1^2 - \eta_2 m_2^2\right) d\mathbf{m}\\ &= \frac{Z}{Z_b}\langle f(m_1,m_2,m_3)\cosh(\lambda m_3)\rangle. \end{aligned}\tag{3.15}$$

□

Proof of Theorem 3.4. When $\lambda = 0$, the probability density $\rho_b(\mathbf{m})$ reduces to the probability density $\rho(\mathbf{m})$, and consequently, $\langle F(\eta_1,\eta_2,\mathbf{m})\rangle_b$ reduces to $\langle F(\eta_1,\eta_2,\mathbf{m})\rangle$, which has been dealt with in Theorem 2.4. Here we focus on the case where $\lambda \neq 0$. Applying Lemma 3.5 to $F(\eta_1,\eta_2,\mathbf{m})$, noting that $F(\eta_1,\eta_2,\mathbf{m})$ is even in m_3, and then expressing the result in terms of a conditional average, we obtain

$$\begin{aligned}\langle F(\eta_1,\eta_2,\mathbf{m})\rangle_b &= C_b\langle F(\eta_1,\eta_2,\mathbf{m})\cosh(\lambda m_3)\rangle\\ &= C_b\left\langle\left\langle F(\eta_1,\eta_2,\mathbf{m})\,\middle|\,|m_3|\right\rangle\cosh(\lambda m_3)\right\rangle. \end{aligned}\tag{3.16}$$

Using the expression of $F(\eta_1,\eta_2,\mathbf{m})$ given in (2.12) and using $m_1^2+m_2^2+m_3^2=1$, we write the conditional average in (3.16) as

$$\begin{aligned}\left\langle F(\eta_1,\eta_2,\mathbf{m})\,\middle|\,|m_3|\right\rangle &= \left\langle(\eta_1(m_3^2-m_2^2)-\eta_2(m_3^2-m_1^2))\,\middle|\,|m_3|\right\rangle\\ &= \frac{\eta_1-\eta_2}{2}(3m_3^2-1)+\frac{\eta_1+\eta_2}{2}\left\langle m_1^2-m_2^2\,\middle|\,|m_3|\right\rangle. \end{aligned}\tag{3.17}$$

Lemma 2.6 tells us that $\left\langle m_1^2-m_2^2\,\middle|\,|m_3|\right\rangle$ is a strictly increasing function of $|m_3|$. Substituting this result into (3.17) yields that for $0<\eta_2<\eta_1$, the conditional average $\left\langle F(\eta_1,\eta_2,\mathbf{m})\,\middle|\,|m_3|\right\rangle$ is also a strictly increasing function of $|m_3|$. Note that for $\lambda\neq 0$, $\cosh(\lambda m_3)$ is always a strictly increasing function of $|m_3|$. Thus, the right hand side of (3.16) satisfies the condition of Lemma 2.5. Applying Lemma 2.5 and using the result of Theorem 2.4, we arrive at

$$\begin{aligned}\langle F(\eta_1,\eta_2,\mathbf{m})\rangle_b &> C_b\left\langle\left\langle F(\eta_1,\eta_2,\mathbf{m})\,\middle|\,|m_3|\right\rangle\right\rangle\cdot\langle\cosh(\lambda m_3)\rangle\\ &= C_b\langle F(\eta_1,\eta_2,\mathbf{m})\rangle\cdot\langle\cosh(\lambda m_3)\rangle > 0,\\ &\qquad\qquad \text{for all } 0<\eta_2<\eta_1 \text{ and } \lambda. \end{aligned}\tag{3.18}$$

□

Combining the results of Proposition 3.3 and Theorem 3.4, we conclude that all stable equilibrium states of dipolar nematic polymers are axisymmetric for all values of $\alpha > 0$ and $b > 0$.

3.2. Dipolar nematic polymers in the presence of a stretching elongational flow. For clarity of the presentation, we shall use $\langle\cdot\rangle_c$ to denote the average with respect to the probability density $\rho_c(\mathbf{m})$ described below for dipolar nematic polymers in the presence of a stretching elongational flow. This new notation is necessary because in the analysis below we need to distinguish these different averages.

For dipolar nematic polymers in the presence of a stretching elongational flow, the total potential also includes the potential induced by the stretching elongational flow [16, 20]:

$$\frac{U(\mathbf{m})}{k_B T} = -b(\mathbf{m}\otimes\mathbf{m}):\langle(\mathbf{m}\otimes\mathbf{m})\rangle_c - \alpha\mathbf{m}\cdot\langle\mathbf{m}\rangle_c - \frac{\alpha_0}{2}(\mathbf{m}\otimes\mathbf{m}):(\mathbf{E}\otimes\mathbf{E}), \tag{3.19}$$

where $\mathbf{E}$ is the direction of the stretching elongation. For a stretching elongational flow, we have $\alpha_0 > 0$. In [16] and [20], it was shown that the direction of the stretching elongational flow $\mathbf{E}$ and the the first moment $\langle\mathbf{m}\rangle$ must be parallel to each other and must be parallel to one of the three principal axes of the second moment. We adopt the coordinate system in which the second moment $\langle\mathbf{m}\otimes\mathbf{m}\rangle_c$ is diagonal and the m_3-axis coincides with $\mathbf{E}$. In this coordinate system, the total potential has the form

$$\frac{U(\mathbf{m})}{k_B T} = -\alpha\langle m_3\rangle_c m_3 - b\left(\langle m_1^2\rangle_c m_1^2 + \langle m_2^2\rangle_c m_2^2 + \langle m_3^2\rangle_c m_3^2\right) - \frac{\alpha_0}{2}m_3^2. \tag{3.20}$$

The situation here is similar to that in the previous subsection. An equilibrium state is completely specified by $\left(\langle m_3\rangle_c, \langle m_1^2\rangle_c, \langle m_2^2\rangle_c, \langle m_3^2\rangle_c\right)$. We introduce the following shorthand notations (r_3, s_1, s_2, s_3)

$$r_3 \equiv \langle m_3\rangle_c, \quad s_1 \equiv \langle m_1^2\rangle_c, \quad s_2 \equiv \langle m_2^2\rangle_c, \quad s_3 \equiv \langle m_3^2\rangle_c. \tag{3.21}$$

Our goal is to show that $s_1 = s_2$. The nonlinear system for (r_3, s_1, s_2, s_3) has the form

$$\begin{aligned} &\langle m_3\rangle_c = r_3, \\ &\langle m_j^2\rangle_c = s_j, \quad j = 1,2,3. \end{aligned} \tag{3.22}$$

All these things are the same as the corresponding ones in the previous subsection except that the probability density has a slightly different expression

$$\rho_c(\mathbf{m}) = \frac{1}{Z_b}\exp\left(\alpha r_3 m_3 + b\left(s_1 m_1^2 + s_2 m_2^2 + s_3 m_3^2\right) + \frac{\alpha_0}{2}m_3^2\right). \tag{3.23}$$

In [20], it was established that a necessary condition for an equilibrium state being stable is that i) the direction of the stretching elongation and the first moment must be parallel to the longest principal axis of the second moment, and ii) the longest principal axis of the second moment must be strictly longer than the other two. This result implies that a stable equilibrium solution of system (3.22) can be made to satisfy the constraint $s_1 \le s_2 < s_3$ by possibly relabeling the m_1-axis and the m_2-axis. In the presence of a stretching elongation in the m_3-direction, the m_3-axis is the only possible candidate for the axis of symmetry, and an equilibrium solution is axisymmetric if and only if $s_1 = s_2$. Our approach is to show $s_1 = s_2$ by excluding the case where $s_1 < s_2 < s_3$. In the presence of a stretching elongation, a stable equilibrium state is not axisymmetric if and only if $s_1 < s_2 < s_3$. We summarize this in the proposition below for dipolar nematic polymers driven by a stretching elongational flow. Notice that the conclusion here is the same as the conclusion in Proposition 2.1 for nematic polymers and the same as the conclusion in Proposition 3.1 for dipolar nematic polymers without flow.

Proposition 3.6. *For dipolar nematic polymers in the presence of a stretching elongational flow, the existence of a stable non-axisymmetric equilibrium state is equivalent to the existence of a solution of system (3.22) with* $s_1 < s_2 < s_3$.

Here we need to point out that in the presence of a stretching elongational flow in the m_3-direction, an equilibrium state with $s_2 = s_3$ is not axisymmetric. But this case is excluded using the stability requirement, based on the result established in [20]. Note that (s_1, s_2, s_3) satisfies equations of the same average form (but with different probability densities) in both the case of nematic polymers and the case of dipolar nematic polymers driven by a stretching elongational flow. As a result, the reasoning after Proposition 2.1 and leading to Proposition 2.2 and 2.3 is also valid for dipolar nematic polymers driven by a stretching elongational flow. It is stated below as Proposition 3.7 and 3.8.

Proposition 3.7. *For dipolar nematic polymers driven by a stretching elongational flow, the existence of a stable non-axisymmetric equilibrium state implies that there exists a set of* $s_1 < s_2 < s_3$, r_3, $\alpha > 0$, $\alpha_0 > 0$ *and* $b > 0$ *such that*

$$\langle F(s_1, s_2, s_3, b, \mathbf{m}) \rangle_c = 0, \tag{3.24}$$

where $\langle \cdot \rangle_c$ *denotes the average with respect to probability density (3.23), and the function* $F(s_1, s_2, s_3, b, \mathbf{m})$ *is defined in (2.7).*

Proposition 3.8. *For dipolar nematic polymers driven by a stretching elongational flow, if we have*

$$\langle F(s_1, s_2, s_3, b, \mathbf{m}) \rangle_c \neq 0 \ \textit{ for all } s_1 < s_2 < s_3, r_3, \alpha > 0, \alpha_0 > 0, \textit{ and } b > 0, \tag{3.25}$$

then all stable equilibrium states are axisymmetric for all values of $\alpha > 0$, $\alpha_0 > 0$, *and* $b > 0$.

After we introduce new parameters $(\lambda, \eta_1, \eta_2)$ given in (3.8), the probability density (3.23) becomes

$$\begin{aligned} \rho_c(\mathbf{m}) &= \frac{1}{Z_c} \exp\left(\alpha r_3 m_3 + b\left(s_1 m_1^2 + s_2 m_2^2 + s_3 m_3^2\right) + \frac{\alpha_0}{2} m_3^2 \right) \\ &= \frac{1}{Z_c} \exp\left(\lambda m_3 - \eta_1 m_1^2 - \eta_2 m_2^2 + \frac{\alpha_0}{2} m_3^2 \right) \end{aligned} \tag{3.26}$$

and function $F(s_1, s_2, s_3, b, \mathbf{m})$ becomes the function $F(\eta_1, \eta_2, \mathbf{m})$ defined in (2.12). Thus, inequality (3.25) is equivalent to the inequality below, which involves only $(\eta_1, \eta_2, \lambda)$ and α_0.

$$\langle F(\eta_1, \eta_2, \mathbf{m}) \rangle_c \neq 0 \ \text{ for all } 0 < \eta_2 < \eta_1, \ \lambda, \text{ and } \alpha_0 > 0. \tag{3.27}$$

Therefore, to show axisymmetry for dipolar nematic polymers driven by a stretching elongational flow, we only need to prove inequality (3.27). The theorem below establishes a stronger version of inequality (3.27).

THEOREM 3.9. *The inequality*

$$\langle F(\eta_1,\eta_2,\mathbf{m})\rangle_c > 0 \quad \textit{for all } 0<\eta_2<\eta_1,\ \lambda,\ \textit{and } \alpha_0>0 \tag{3.28}$$

holds, where $\langle\cdot\rangle_c$ *denotes the average with respect to probability density (3.26).*

The proof of Theorem 3.9 requires a lemma that relates the average $\langle\cdot\rangle_c$ *to the average* $\langle\cdot\rangle_b$.

LEMMA 3.10.

$$\langle f(m_1,m_2,m_3)\rangle_c = C_c\left\langle f(m_1,m_2,m_3)\exp\left(\frac{\alpha_0}{2}m_3^2\right)\right\rangle_b \tag{3.29}$$

holds, where $\langle\cdot\rangle_c$ *denotes the average with respect to the probability density* $\rho_c(\mathbf{m})$ *given in (3.26) and* $\langle\cdot\rangle_b$ *denotes the average with respect to the probability density* $\rho_b(\mathbf{m})$ *given in (3.9). In the above, the coefficient* $C_c = Z_b/Z_c > 0$ *where* Z_b *is the normalizing constant in (3.9) and* Z_c *is the normalizing constant in (3.26).*

Proof. It is straightforward to verify. □

Proof of Theorem 3.9. First applying Lemma 3.10 to $F(\eta_1,\eta_2,\mathbf{m})$, then applying Lemma 3.5 to $F(\eta_1,\eta_2,\mathbf{m})\exp\left(\frac{\alpha_0}{2}m_3^2\right)$, noting that $F(\eta_1,\eta_2,\mathbf{m})$ is an even function of m_3, and expressing the result in terms of conditional average, we obtain

$$\begin{aligned}\langle F(\eta_1,\eta_2,\mathbf{m})\rangle_c &= C_c\left\langle F(\eta_1,\eta_2,\mathbf{m})\exp\left(\frac{\alpha_0}{2}m_3^2\right)\right\rangle_b\\ &= C_cC_b\left\langle F(\eta_1,\eta_2,\mathbf{m})\cosh(\lambda m_3)\exp\left(\frac{\alpha_0}{2}m_3^2\right)\right\rangle\\ &= C_cC_b\left\langle\left\langle F(\eta_1,\eta_2,\mathbf{m})\,\Big|\,|m_3|\right\rangle\cosh(\lambda m_3)\exp\left(\frac{\alpha_0}{2}m_3^2\right)\right\rangle.\end{aligned} \tag{3.30}$$

In the proof of Theorem 3.4, we showed that $\left\langle F(\eta_1,\eta_2,\mathbf{m})\,\Big|\,|m_3|\right\rangle$ is a strictly increasing function of $|m_3|$ (see result (3.17) and the reasoning below it). Note that for a stretching elongational flow ($\alpha_0>0$), $\cosh(\lambda m_3)\exp\left(\frac{\alpha_0}{2}m_3^2\right)$ is a strictly increasing function of $|m_3|$, and the value of λ does not change the monotonicity. Thus, the right hand side of (3.30) satisfies the condition of Lemma 2.5. Applying Lemma 2.5 and using the result of Theorem 2.4, we arrive at

$$\begin{aligned}\langle F(\eta_1,\eta_2,\mathbf{m})\rangle_c &> C_cC_b\left\langle\left\langle F(\eta_1,\eta_2,\mathbf{m})\,\Big|\,|m_3|\right\rangle\right\rangle\cdot\left\langle\cosh(\lambda m_3)\exp\left(\frac{\alpha_0}{2}m_3^2\right)\right\rangle\\ &= C_CC_b\langle F(\eta_1,\eta_2,\mathbf{m})\rangle\cdot\left\langle\cosh(\lambda m_3)\exp\left(\frac{\alpha_0}{2}m_3^2\right)\right\rangle > 0,\\ &\qquad\text{for all } 0<\eta_2<\eta_1,\ \lambda,\ \text{and } \alpha_0>0.\end{aligned} \tag{3.31}$$

□

Combining the results of Proposition 3.8 and Theorem 3.4, we conclude that all stable equilibrium states of dipolar nematic polymers in the presence of a stretching elongational flow are axisymmetric for all values of $\alpha>0$, $\alpha_0>0$ and $b>0$. The axis of symmetry is the direction of the stretching elongational flow.

4. Nematic polymers in higher dimensional space

4.1. Rotational symmetry. For clarity of presentation, we shall use $\langle\cdot\rangle_d$ to denote the average with respect to the probability density $\rho_d(\mathbf{m})$ described below for nematic polymers in n-dimensional space ($n\geq 3$).

For nematic polymers in n-dimensional space, the Maier-Saupe interaction potential, as given in (1.17), is completely specified by the eigenvalues of the second moment $(\langle m_1^2\rangle_d,\langle m_2^2\rangle_d,\ldots\langle m_n^2\rangle_d)$. As a result, the equilibrium probability density, which is related to the Maier-Saupe interaction potential through the Boltzmann distribution, is also completely specified by $(\langle m_1^2\rangle_d,\langle m_2^2\rangle_d,\ldots\langle m_n^2\rangle_d)$. For simplicity of presentation, we introduce the following the shorthand notations for the eigenvalues of the second moment:

$$s_j\equiv\langle m_j^2\rangle_d,\quad j=1,2,\ldots,n. \tag{4.1}$$

Our goal is to show that $s_1,s_2,\ldots,s_n$ have at most two distinct values. The nonlinear system for $(s_1,s_2,\ldots,s_n)$ can be concisely written as

$$\langle m_j^2\rangle_d=s_j,\quad j=1,2,\ldots,n, \tag{4.2}$$

where the average is with respect to the probability density

$$\rho_d(\mathbf{m})=\frac{1}{Z_d}\exp\left(b\sum_{j=1}^{n}s_jm_j^2\right). \tag{4.3}$$

To show that $s_1,s_2,\ldots,s_n$ have at most two distinct values, we only need to show that any three choices out of $s_1,s_2,\ldots,s_n$ have at most two distinct values. Without loss of generality, we consider s_1, s_2, and s_3 (for any three out of $s_1,s_2,\ldots,s_n$, we can rename them s_1, s_2 and s_3 by relabeling axes of the coordinate system). We only need to show that two out of s_1, s_2, and s_3 must be the same. Again, without loss of generality, we assume that s_1, s_2, and s_3 are ordered as $s_1\leq s_2\leq s_3$. This brings us to a situation similar to the one in section 1. With the ordering of $s_1\leq s_2\leq s_3$, there are three possibilities: $s_1=s_2$, $s_2=s_3$, or $s_1<s_2<s_3$ where $s_1=s_2$ and $s_2=s_3$ are not mutually exclusive. Our approach is to show that two out of s_1, s_2, and s_3 must be the same by excluding the case of $s_1<s_2<s_3$. It is clear that with a proper relabeling of axes and with the ordering of $s_1\leq s_2\leq s_3$, the second moment of an equilibrium state has more than two distinct eigenvalues if and only if $s_1<s_2<s_3$. We summarize this in the proposition below.

PROPOSITION 4.1. *For nematic polymers in n-dimensional space ($n\geq 3$), the existence of an equilibrium state whose second moment has more than two distinct eigenvalues is equivalent to the existence of a solution of system (4.2) with $s_1<s_2<s_3$.*

Note that (s_1,s_2,s_3) satisfies equations of the same average form (but with different probability densities) in both the case of nematic polymers in three dimensional space and the case of nematic polymers in n dimensional space. It follows that the reasoning after Proposition 2.1 and leading to Proposition 2.2 and 2.3 is also valid for the n dimensional case. It is stated below as Proposition 4.2 and 4.3.

PROPOSITION 4.2. *For nematic polymers in n-dimensional space ($n\geq 3$), the existence of an equilibrium state whose second moment has more than two distinct eigenvalues implies that there exists a set of $\{s_j,\,1\leq j\leq n\}$ with $s_1<s_2<s_3$ and $b>0$ such* *that*

$$\langle F(s_1,s_2,s_3,b,\mathbf{m})\rangle_d = 0, \tag{4.4}$$

where $\langle\cdot\rangle_d$ *denotes the average with respect to probability density (4.3), and the function*
$F(s_1,s_2,s_3,b,\mathbf{m})$ *is defined in (2.7).*

Proposition 4.3. *For nematic polymers in n-dimensional space* ($n \geq 3$)*, if we have*

$$\langle F(s_1,s_2,s_3,b,\mathbf{m})\rangle_d \neq 0 \ \textit{ for all } \{s_j,\, 1\leq j\leq n\} \textit{ with } s_1<s_2<s_3 \textit{ and } b>0, \tag{4.5}$$

then for all values of $b>0$ *and for all equilibrium states the second moment has at most two distinct eigenvalues.*

Similar to what we did in section 2, we simplify inequality (4.5) by introducing a set of new parameters $\{\eta_j,\, 1\leq j\leq n\}$

$$\eta_j \equiv b(s_3 - s_j). \tag{4.6}$$

From the definition (4.6), it is clear that $s_1<s_2<s_3$ is equivalent to $0<\eta_2<\eta_1$. It is also clear that $\eta_3=0$. So the new set of parameters has only $n-1$ members instead of n members. We use the relation $\sum_{j=1}^{n} m_j^2 = 1$ to write probability density (4.3) in terms of $\{\eta_j,\, 1\leq j\leq n\}$ as

$$\begin{aligned}\rho_d(\mathbf{m}) &= \frac{1}{Z_d}\exp\left(b\sum_{j=1}^{n} s_j m_j^2 - b s_3 \sum_{j=1}^{n} m_j^2\right)\\ &= \frac{1}{Z_d}\exp\left(-\eta_1 m_1^2 - \eta_2 m_2^2 - \sum_{j=4}^{n}\eta_j m_j^2\right).\end{aligned} \tag{4.7}$$

With the introduction of $\{\eta_j,\, 1\leq j\leq n\}$, the function $F(s_1,s_2,s_3,b,\mathbf{m})$ becomes the function $F(\eta_1,\eta_2,\mathbf{m})$ defined in (2.12). It follows that inequality (4.5) is equivalent to the inequality

$$\langle F(\eta_1,\eta_2,\mathbf{m})\rangle_d \neq 0 \ \text{ for all } \{\eta_j,\, 1\leq j\leq n\} \text{ with } 0<\eta_2<\eta_1 \text{ and } \eta_3=0. \tag{4.8}$$

Therefore, to show that for all values of $b>0$ and for all equilibrium states, the second moment has at most two distinct eigenvalues, we only need to prove inequality (4.8). The theorem below establishes a stronger version of inequality (4.8).

Theorem 4.4. *The inequality*

$$\langle F(\eta_1,\eta_2,\mathbf{m})\rangle_d > 0 \ \textit{ for all } \{\eta_j,\, 1\leq j\leq n\} \textit{ with } 0<\eta_2<\eta_1 \textit{ and } \eta_3=0, \tag{4.9}$$

holds, where the average is with respect to the probability density given in (4.7).

Proof. For mathematical convenience, we decompose vector $\mathbf{m}=(m_1,m_2,\ldots,m_n)$ into two vectors: $\mathbf{m}=(\mathbf{u},\mathbf{v})$ where vectors $\mathbf{u}$ and $\mathbf{v}$ are defined as

$$\begin{aligned}&\mathbf{u} \equiv (m_1,m_2,m_3),\\ &\mathbf{v} \equiv (m_4,\ldots,m_n).\end{aligned} \tag{4.10}$$

Notice that function $F(\eta_1,\eta_2,\mathbf{m})$ has no dependence on $\mathbf{v}$. For this reason, we shall write it as $F(\eta_1,\eta_2,\mathbf{u})$ to show explicitly that it is a function of $\mathbf{u}$ only. Expressing $\langle F(\eta_1,\eta_2,\mathbf{u})\rangle_d$ in terms of a conditional average, we have

$$\langle F(\eta_1,\eta_2,\mathbf{u})\rangle_d = \left\langle \left\langle F(\eta_1,\eta_2,\mathbf{u}) \,\middle|\, \mathbf{v} \right\rangle_d \right\rangle_d. \tag{4.11}$$

On the unit sphere $\|\mathbf{m}\|_2^2 = 1$ in n-dimensional space, so we have $\|\mathbf{u}\|_2^2 + \|\mathbf{v}\|_2^2 = 1$. Let us introduce the shorthand notation $r \equiv \sqrt{1-\|\mathbf{v}\|_2^2}$. We use probability density (4.7) to express the conditional average in (4.11) in integral form.

$$\left\langle F(\eta_1,\eta_2,\mathbf{u}) \,\middle|\, \mathbf{v} \right\rangle_d = \frac{\int_{\|\mathbf{u}\|_2=r} F(\eta_1,\eta_2,\mathbf{u}) \exp\left(-\eta_1 m_1^2 - \eta_2 m_2^2\right) d\mathbf{u}}{\int_{\|\mathbf{u}\|_2=r} \exp(-\eta_1 m_1^2 - \eta_2 m_2^2)\, d\mathbf{u}}. \tag{4.12}$$

In the integrals, using the change of variable $\mathbf{u}_{old} = r\,\mathbf{u}_{new}$ and using the fact that function $F(\eta_1,\eta_2,r\mathbf{u}) = F(\eta_1 r^2,\eta_2 r^2,\mathbf{u})$, we obtain

$$\begin{aligned} &\left\langle F(\eta_1,\eta_2,\mathbf{u}) \,\middle|\, \mathbf{v} \right\rangle_d \\ &= \frac{\int_{\|\mathbf{u}\|_2=1} F(\eta_1,\eta_2,r\mathbf{u}) \exp\left(-\eta_1 r^2 m_1^2 - \eta_2 r^2 m_2^2\right) d\mathbf{u}}{\int_{\|\mathbf{u}\|_2=1} \exp(-\eta_1 r^2 m_1^2 - \eta_2 r^2 m_2^2)\, d\mathbf{u}} \\ &= \int_{\|\mathbf{u}\|_2=1} F(\eta_1 r^2,\eta_2 r^2,\mathbf{u}) \frac{\exp\left(-\eta_1 r^2 m_1^2 - \eta_2 r^2 m_2^2\right)}{\int_{\|\mathbf{u}\|_2=1} \exp(-\eta_1 r^2 m_1^2 - \eta_2 r^2 m_2^2)\, d\mathbf{u}} d\mathbf{u} \\ &= \langle F(\eta_1 r^2,\eta_2 r^2,\mathbf{u})\rangle. \end{aligned} \tag{4.13}$$

$\langle F(\eta_1 r^2,\eta_2 r^2,\mathbf{u})\rangle$ on the right hand side of (4.13) is the same as $\langle F(\eta_1,\eta_2,\mathbf{m})\rangle$ in Theorem 2.4, except that η_1 is replaced by $\eta_1 r^2$ and η_2 is replaced by $\eta_2 r^2$. For $r \neq 0$, we have $0 < \eta_1 r^2 < \eta_2 r^2$, following from $0 < \eta_1 < \eta_2$. Thus, using the result of Theorem 2.4, we arrive at

$$\left\langle F(\eta_1,\eta_2,\mathbf{u}) \,\middle|\, \mathbf{v} \right\rangle_d = \langle F(\eta_1 r^2,\eta_2 r^2,\mathbf{u})\rangle > 0 \quad \text{for } \|\mathbf{v}\|_2 < 1. \tag{4.14}$$

Substituting this result into (4.11) leads immediately to the desired conclusion. ∎

Combining the results of Proposition 4.3 and Theorem 4.4, we conclude that for nematic polymers in n-dimensional space, the second moment of equilibrium state has at most two distinct eigenvalues.

4.2. Phase diagrams of nematic polymers. Proposition 4.3 and Theorem 4.4 above tell us that the second moment has at most two distinct eigenvalues. When the the second moment has only one distinct eigenvalue, we have $s_j = 1/n$, and the corresponding probability density, as given in (4.3), is isotropic $\rho_d(\mathbf{m}) = const$. It is straightforward to verify that the isotropic state is always a solution of nonlinear system (4.2) for any value of $b > 0$. Below we focus on the more interesting situation where the the second moment has two distinct eigenvalues.

For nematic polymers in the n-dimensional space, The n eigenvalues of the second moment can take only two distinct values, denoted respectively by σ_1 and σ_2. Let n_1 denote the number of occurrences of value σ_1 among the n eigenvalues. Consequently, $n_2 = n - n_1$ is the number of occurrences of the value σ_2. Here we do not require that

σ_1 and σ_2 are ordered in any way. Instead, we assume that $0 < n_1 \le n_2 = n - n_1$, which is equivalent to

$$0 < n_1 \le n/2. \tag{4.15}$$

Note that $n_1 > 0$ because we exclude the isotropic case where all eigenvalues have the same value. Also, without loss of generality we assume that the n eigenvalues are renamed or relabeled such that

$$\begin{aligned} &s_j = \sigma_1, \;\; 1 \le j \le n_1 \\ &s_j = \sigma_2, \;\; n_1 + 1 \le j \le n. \end{aligned} \tag{4.16}$$

The n eigenvalues are constrained by $\sum_{j=1}^{n} s_j = 1$. Substituting (4.16) into the constraint, we obtain that σ_1, σ_2, and n_1 satisfy

$$n_1\sigma_1 + (n - n_1)\sigma_2 = 1, \tag{4.17}$$

from which σ_2 can be expressed in terms of n_1 and σ_1 as $\sigma_2 = (1 - n_1\sigma_1)/(n - n_1)$. Thus, an equilibrium state is completely specified by the values of n_1 and σ_1.

$$\begin{aligned} \rho_d(\mathbf{m}) &= \frac{1}{Z_d} \exp\left(b \left(\sigma_1 \sum_{j=1}^{n_1} m_j^2 + \frac{1 - n_1\sigma_1}{n - n_1} \sum_{j=n_1+1}^{n} m_j^2 \right) \right) \\ &= \frac{1}{Z_d} \exp\left(b \frac{n\sigma_1 - 1}{n - n_1} \sum_{j=1}^{n_1} m_j^2 \right) &(4.18) \\ &\equiv \frac{1}{Z_d} \exp\left(r \sum_{j=1}^{n_1} m_j^2 \right), \quad \text{where } r \equiv b \frac{n\sigma_1 - 1}{n - n_1}. &(4.19) \end{aligned}$$

The quantity $(n\sigma_1 - 1)/(n - n_1)$ may be viewed as the generalized order parameter. For the isotropic equilibrium state, we have $\sigma_1 = 1/n$ and the order parameter is $(n\sigma_1 - 1)/(n - n_1) = 0$. For $n_1 = 1$, the largest allowable value for σ_1 is $\sigma_1 = 1$, in which case, all polymer rods are aligned along the m_1-direction and the corresponding order parameter is $(n\sigma_1 - 1)/(n - n_1) = 1$. For $n_1 > 1$, the largest allowable value for σ_1 is $\sigma_1 = 1/n_1$ when the n-dimensional polymer orientation is restricted to the unit sphere $\sum_{j=1}^{n_1} m_j^2 = 1$ in n_1-dimensional space. In this case, the order parameter is $(n\sigma_1 - 1)/(n - n_1) = 1/n_1$. The nonlinear equation for σ_1 is concisely written as

$$\frac{1}{n_1} \left\langle \sum_{j=1}^{n_1} m_j^2 \right\rangle_d = \sigma_1, \tag{4.20}$$

where the average is with respect to the probability density, with σ_1 and b as the parameters, given in (4.18). We would like to obtain σ_1 as a function of b, because b is the physical parameter that can be tuned in experiments (b is proportional to the normalized polymer concentration and is inversely proportional to the absolute temperature). Mathematically, however, it is more convenient to treat $r \equiv b(n\sigma_1 - 1)/(n - n_1)$ as the independent variable and calculate $1/b$ as a function of r. With r and b as parameters, we re-write equation (4.20) as

$$\frac{1}{(n - n_1)n_1} \left\langle n \sum_{j=1}^{n_1} m_j^2 - n_1 \right\rangle_d = \frac{r}{b}, \tag{4.21}$$

where the average is with respect to the probability density given in (4.19). Note that the left hand side of (4.21) depends on r only. It does not depend on parameter b. Thus, $1/b$ as a function of r is expressed as

$$\begin{aligned}\frac{1}{b(r)} &= \frac{1}{(n-n_1)n_1}\cdot\frac{\left\langle n\sum_{j=1}^{n_1} m_j^2 - n_1\right\rangle_d}{r}\\ &= \frac{1}{(n-n_1)n_1}\cdot\frac{\int_S\left(n\sum_{j=1}^{n_1} m_j^2 - n_1\right)\exp\left(r\sum_{j=1}^{n_1} m_j^2\right)d\mathbf{m}}{r\int_S\exp\left(r\sum_{j=1}^{n_1} m_j^2\right)d\mathbf{m}}\\ &= \frac{\int_0^{\pi/2}\left(n\cos^2\phi - n_1\right)\exp\left(r\cos^2\phi\right)\cos^{(n_1-1)}\phi\sin^{(n-n_1-1)}\phi d\phi}{(n-n_1)n_1 r\int_0^{\pi/2}\exp(r\cos^2\phi)\cos^{(n_1-1)}\phi\sin^{(n-n_1-1)}\phi d\phi}. \end{aligned}\tag{4.22}$$

Applying integration by parts to the numerator and using $\left(n\cos^2\phi - n_1\right)\cos^{n_1-1}\phi\sin^{n-n_1-1}\phi d\phi = d\left(\cos^{n_1}\phi\sin^{n-n_1}\phi\right)$, we obtain

$$\begin{aligned}\frac{1}{b(r)} &= \frac{1}{(n-n_1)n_1}\cdot\frac{\int_0^{\pi/2}\exp\left(r\cos^2\phi\right)d\left(\cos^{n_1}\phi\sin^{n-n_1}\phi\right)}{r\int_0^{\pi/2}\exp(r\cos^2\phi)\cos^{(n_1-1)}\phi\sin^{(n-n_1-1)}\phi d\phi}\\ &= \frac{2}{(n-n_1)n_1}\cdot\frac{\int_0^{\pi/2}\cos^2\phi\sin^2\phi\exp\left(r\cos^2\phi\right)\cos^{(n_1-1)}\phi\sin^{(n-n_1-1)}\phi d\phi}{\int_0^{\pi/2}\exp(r\cos^2\phi)\cos^{(n_1-1)}\phi\sin^{(n-n_1-1)}\phi d\phi}\\ &= \frac{2}{(n-n_1)n_1}\cdot\left\langle\cos^2\phi\sin^2\phi\right\rangle \equiv \frac{2}{(n-n_1)n_1}\cdot f(r),\end{aligned}\tag{4.23}$$

where the average is with respect to the probability density

$$\rho(\phi) = \frac{\exp\left(r\cos^2\phi\right)\cos^{(n_1-1)}\phi\sin^{(n-n_1-1)}\phi}{\int_0^{\pi/2}\exp(r\cos^2\phi)\cos^{(n_1-1)}\phi\sin^{(n-n_1-1)}\phi d\phi}.\tag{4.24}$$

It is straightforward to verify that $f(r)\equiv\left\langle\cos^2\phi\sin^2\phi\right\rangle$ is always positive. Furthermore, $f(r)$ satisfies

$$\lim_{r\to-\infty} f(r) = 0 \quad\text{and}\quad \lim_{r\to+\infty} f(r) = 0.\tag{4.25}$$

Here we show the derivation of $\lim_{r\to+\infty} f(r) = 0$. As $r\to+\infty$, in both the numerator and the denominator of $f(r)$ the dominant contribution comes from a neighborhood near $\phi = 0$. Expanding everything in terms of ϕ and applying the Laplace method, we obtain

$$\begin{aligned}f(r) &= \frac{\int_0^{\pi/2}\exp\left(r-\frac{r}{2}\phi^2\right)\phi^{(n-n_1+1)}d\phi + \cdots}{\int_0^{\pi/2}\exp\left(r-\frac{r}{2}\phi^2\right)\phi^{(n-n_1-1)}d\phi + \cdots}\\ &= \frac{\exp(r)\cdot O\left(r^{-(n-n_1+2)/2}\right)}{\exp(r)\cdot O\left(r^{-(n-n_1)/2}\right)} = O\left(r^{-1}\right)\to 0 \quad\text{as } r\to+\infty.\end{aligned}$$

$\lim_{r\to-\infty} f(r) = 0$ can be derived in a similar way. Next we show that $f(r)$ has the property that

$$f'(r_0) = 0 \text{ implies } f''(r_0) < 0.\tag{4.26}$$

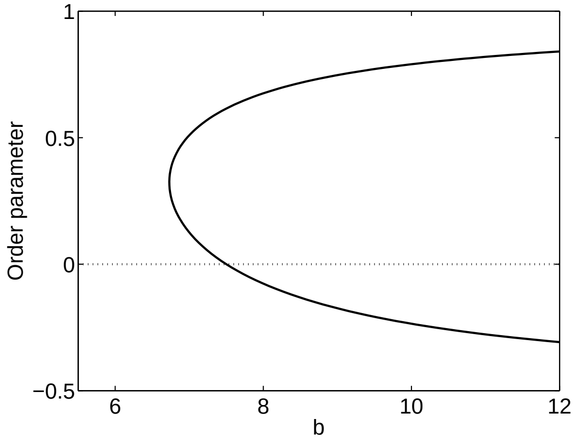

FIG. 4.1. *Phase diagram of nematic polymers in three dimensional space. The solid line shows the nematic branch that is axisymmetric with respect to the m_1-axis, and the dotted line shows the isotropic branch.*

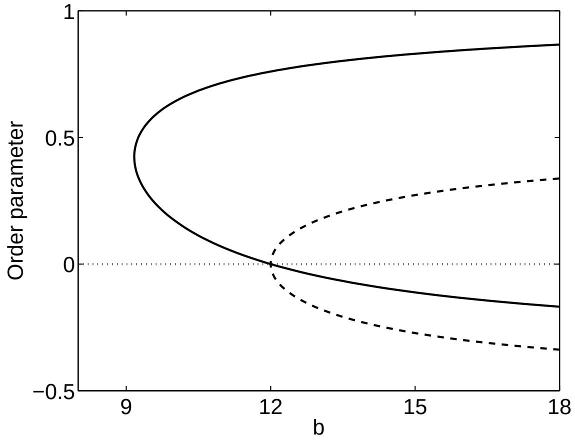

FIG. 4.2. *Phase diagram of nematic polymers in four dimensional space. The solid line shows the nematic branch for $n_1=1$, which is axisymmetric with respect to the m_1-axis, the dashed line shows the nematic branch for $n_1=2$, which has rotational symmetry around the two dimensional subspace $\{(m_1,m_2)\}$, and the dotted line shows the isotropic branch.*

Differentiating probability density (4.24) with respect to r yields

$$\frac{d\rho(\phi)}{dr}=\left(\cos^2\phi-\langle\cos^2\phi\rangle\right)\rho(\phi). \tag{4.27}$$

Using result (4.27) to calculate the derivatives of $f(r)\equiv\left\langle\cos^2\phi\sin^2\phi\right\rangle$, we arrive at

$$f'(r)=\left\langle\cos^2\phi\sin^2\phi\left(\cos^2\phi-\langle\cos^2\phi\rangle\right)\right\rangle, \tag{4.28}$$

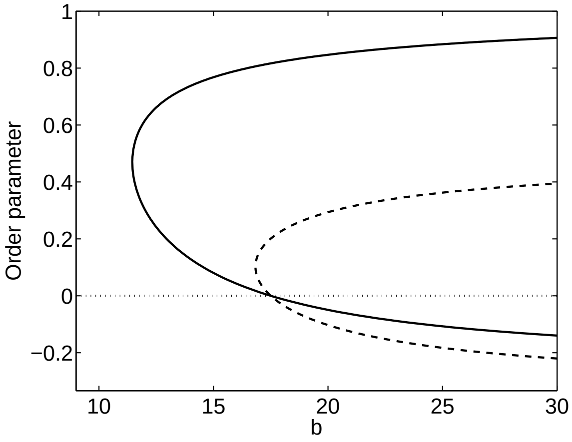

FIG. 4.3. *Phase diagram of nematic polymers in five dimensional space. The solid line shows the nematic branch for* $n_1=1$*, which is axisymmetric with respect to the* m_1*-axis, the dashed line shows the nematic branch for* $n_1=2$*, which has rotational symmetry around the two dimensional subspace* $\{(m_1,m_2)\}$*, and the dotted line shows the isotropic branch.*

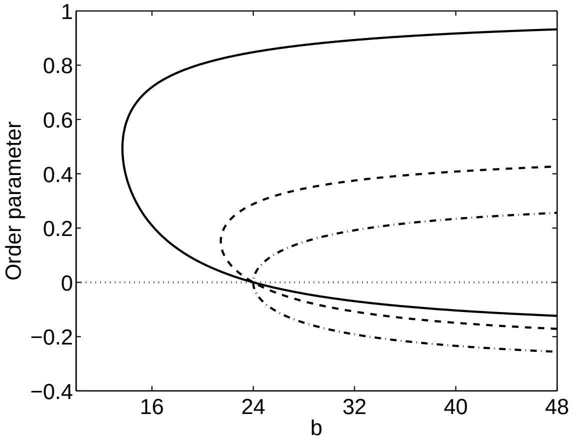

FIG. 4.4. *Phase diagram of nematic polymers in six dimensional space. The solid line shows the nematic branch for* $n_1=1$*, which is axisymmetric with respect to the* m_1*-axis, the dashed line shows the nematic branch for* $n_1=2$*, which has rotational symmetry around the two dimensional subspace* $\{(m_1,m_2)\}$*, the dashdot line shows the nematic branch for* $n_1=3$*, which has rotational symmetry around the three dimensional subspace* $\{(m_1,m_2,m_3)\}$*, and the dotted line shows the isotropic branch.*

$$\begin{aligned}
f''(r) = &\left\langle \cos^2\phi\sin^2\phi\left(\cos^2\phi - \langle\cos^2\phi\rangle\right)^2\right\rangle \\
&- \left\langle\cos^2\phi\sin^2\phi\right\rangle\cdot\left\langle\cos^2\phi\left(\cos^2\phi - \langle\cos^2\phi\rangle\right)\right\rangle \\
= &-\left\langle\cos^2\phi\sin^2\phi\left(\cos^2\phi\sin^2\phi - \langle\cos^2\phi\sin^2\phi\rangle\right)\right\rangle \\
&+\left\langle\cos^2\phi\sin^2\phi\left(\cos^2\phi - \langle\cos^2\phi\rangle\right)\right\rangle\cdot\left(1-2\left\langle\cos^2\phi\right\rangle\right) \\
= &-\mathrm{var}\left(\cos^2\phi\sin^2\phi\right) + f'(r)\left(1-2\left\langle\cos^2\phi\right\rangle\right). \qquad (4.29)
\end{aligned}$$

If $f'(r_0)=0$, then we have that $f''(r_0)=-\mathrm{var}\left(\cos^2\phi\sin^2\phi\right)<0$. Thus, we conclude that $f(r)$ satisfies property (4.26). Property (4.25) gives the existence of a maximum. Let r^* be the location where that maximum is attained. We have $f'(r^*)=0$. It follows from property (4.26) that

$$f'(r)>0 \;\text{ for }\; r<r^* \quad\text{and}\quad f'(r)<0 \;\text{ for }\; r>r^*. \tag{4.30}$$

Here we show the proof for the first half of (4.30). Combining $f'(r^*)=0$ with property (4.26) leads to $f''(r^*)<0$, which implies $f'(r)>0$ for $r\in(r^*-\epsilon,r^*)$. Now consider $q_0=\inf\{q|f'(r)>0 \text{ for } r\in(q,r^*)\}$. If q_0 is finite, then the definition of q_0 implies $f'(q_0)=0$ and $f''(q_0)\geq 0$. Applying property (4.26) to $f'(q_0)=0$ yields $f''(q_0)<0$, which contradicts that $f''(q_0)\geq 0$. Therefore, a finite q_0 is impossible and we must have $q_0=-\infty$, which leads to $f'(r)>0$ for $r<r^*$. The second half of (4.30) is proved in a similar way.

Once the correspondence between r and b is obtained, the order parameter is calculated as $(n\sigma_1-1)/(n-n_1)=r/b$. When $n=3$, the condition $0<n_1\leq n/2$ implies that $n_1=1$. The phase diagram of r/b vs b for $n=3$ is shown in Figure 4.1. When $n=4$, the condition $0<n_1\leq n/2$ allows $n_1=1$ and $n_1=2$. The phase diagram of r/b vs b for $n=4$ is shown in Figure 4.2. There are two curves in Figure 4.2: one for $n_1=1$ and the other for $n_1=2$. When $n=5$, there are two values of n_1 that satisfy the condition $0<n_1\leq n/2$: $n_1=1$ and $n_1=2$. The phase diagram of r/b vs b for $n=5$ is shown in Figure 4.3. There are two curves in Figure 4.3: one for $n_1=1$ and the other for $n_1=2$. When $n=6$, the condition $0<n_1\leq n/2$ yields three choices for n_1: $n_1=1$, $n_1=2$ and $n_1=3$. The phase diagram of r/b vs b for $n=6$ is shown in Figure 4.4. There are three curves in Figure 4.4: one for $n_1=1$, second one for $n_1=2$ and the third one for $n_1=3$.

The stability of these equilibrium branches will be investigated in a future work.

Acknowledgement. This work was partially supported by the US National Science Foundation.

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