

## Research Article

# Extendability of Equilibria of Nematic Polymers

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Received 9 May 2008; Accepted 30 October 2008

Recommended by Nobuyuki Kenmochi

The purpose of this paper is to study the extendability of equilibrium states of rodlike nematic polymers with the Maier-Saupe intermolecular potential. We formulate equilibrium states as solutions of a nonlinear system and calculate the determinant of the Jacobian matrix of the nonlinear system. It is found that the Jacobian matrix is nonsingular everywhere except at two equilibrium states. These two special equilibrium states correspond to two points in the phase diagram. One point is the folding point where the stable prolate branch folds into the unstable prolate branch; the other point is the intersection point of the nematic branch and the isotropic branch where the unstable prolate state becomes the unstable oblate state. Our result establishes the existence and uniqueness of equilibrium states in the presence of small perturbations away from these two special equilibrium states.

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## 1. Introduction

Liquid crystal polymers (LCPs) consisting of rigid rodlike macromolecules in a viscous solvent have wide technological applications [1–4]. The most common theoretical framework for modeling nematic polymers is to represent the nematogenic molecules as rigid rods and to describe the ensemble with an orientational probability density function (pdf) [5]. Equilibrium orientational distribution is related to the interaction potential by the Boltzmann relation. Recently, rigorous mathematical analysis on the equilibrium states of nematic polymers has garnered serious attention from mathematicians led by Constantin and Titi [6–22]. For example, various proofs for the axisymmetry of equilibrium states with only the Maier-Saupe interaction were given in [8, 19] for the 2-D case and in [9, 18, 20] for the 3-D case; the equilibrium states for the case where dipole-dipole interaction is coupled to the Maier-Saupe interaction were studied in [17, 21]. Not surprisingly, many mathematical issues of polymers are still unexplored. In particular, to our knowledge, the extendability of the equilibrium states has never been attempted.

| Report Documentation Page                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |                                    |                                     |                                                           | Form Approved<br>OMB No. 0704-0188                  |                                 |
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| 1. REPORT DATE<br><b>MAY 2008</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                    | 2. REPORT TYPE                      |                                                           | 3. DATES COVERED<br><b>00-00-2008 to 00-00-2008</b> |                                 |
| 4. TITLE AND SUBTITLE<br><b>Extendability of Equilibria of Nematic Polymers</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                    |                                     |                                                           | 5a. CONTRACT NUMBER                                 |                                 |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                    |                                     |                                                           | 5b. GRANT NUMBER                                    |                                 |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                    |                                     |                                                           | 5c. PROGRAM ELEMENT NUMBER                          |                                 |
| 6. AUTHOR(S)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                    |                                     |                                                           | 5d. PROJECT NUMBER                                  |                                 |
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| 7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)<br><b>Naval Postgraduate School, Department of Applied Mathematics, Monterey, CA, 93943</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                                    |                                     |                                                           | 8. PERFORMING ORGANIZATION REPORT NUMBER            |                                 |
| 9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                    |                                     |                                                           | 10. SPONSOR/MONITOR'S ACRONYM(S)                    |                                 |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                    |                                     |                                                           | 11. SPONSOR/MONITOR'S REPORT NUMBER(S)              |                                 |
| 12. DISTRIBUTION/AVAILABILITY STATEMENT<br><b>Approved for public release; distribution unlimited</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                    |                                     |                                                           |                                                     |                                 |
| 13. SUPPLEMENTARY NOTES                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                    |                                     |                                                           |                                                     |                                 |
| 14. ABSTRACT                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                    |                                     |                                                           |                                                     |                                 |
| 15. SUBJECT TERMS                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                    |                                     |                                                           |                                                     |                                 |
| 16. SECURITY CLASSIFICATION OF:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                    |                                     | 17. LIMITATION OF ABSTRACT<br><b>Same as Report (SAR)</b> | 18. NUMBER OF PAGES<br><b>10</b>                    | 19a. NAME OF RESPONSIBLE PERSON |
| a. REPORT<br><b>unclassified</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | b. ABSTRACT<br><b>unclassified</b> | c. THIS PAGE<br><b>unclassified</b> |                                                           |                                                     |                                 |

In our previous study [21], it was revealed that for large values of the nematic strength and small perturbations, there exists at least one solution near the corresponding unperturbed pure nematic solution. In [21], we concluded the existence using complicated free energy arguments. Moreover, in [21] only existence was established whereas the uniqueness was not addressed at all. Our goal in the current study is to establish rigorously the extendability, both existence and uniqueness, of the equilibrium states of nematic polymers in the presence of small perturbations. Notice that all equilibrium states of nematic polymers are axisymmetric [9, 18, 20]. To facilitate the discussion of extendability, we introduce two new variables for the nonlinear system governing the equilibrium states: one variable is proportional to the order parameter of the pdf; the other variable is proportional to the biaxial order parameter, which measures the deviation of the pdf from being axisymmetric. One advantage of this approach is that the Jacobian matrix is diagonal at equilibrium states. We will show that the Jacobian determinant of the nonlinear system is nonzero everywhere except at two equilibrium states. These two equilibrium states correspond to two points in the phase diagram: one point is the folding point where the stable prolate branch folds into the unstable prolate branch; the other point is the intersection point of the nematic states and the isotropic states where the unstable prolate state becomes the unstable oblate state. The extendability of the equilibrium states except these two states follows immediately from the implicit function theorem.

## 2. Nonlinear system for equilibrium states, Jacobian matrix, and its determinant

We now briefly recall the mathematical description for equilibrium states of rigid rodlike nematic polymers. The orientation direction of each polymer rod is denoted by a unit vector  $\mathbf{m}$ . In this study, by “pure nematic polymers,” we mean the case where the Maier-Saupe interaction potential is the only potential. The Maier-Saupe potential is given by

$$U(\mathbf{m}) = -b\langle \mathbf{m}\mathbf{m} \rangle : \mathbf{m}\mathbf{m}, \quad (2.1)$$

where the tensor product  $\mathbf{m}\mathbf{m}$  and the tensor double contraction  $\mathbf{A} : \mathbf{B}$  are defined as

$$\mathbf{m}\mathbf{m} \equiv \begin{bmatrix} m_1m_1 & m_1m_2 & m_1m_3 \\ m_2m_1 & m_2m_2 & m_2m_3 \\ m_3m_1 & m_3m_2 & m_3m_3 \end{bmatrix}, \quad (2.2)$$

$$\mathbf{A} : \mathbf{B} \equiv \text{trace}(\mathbf{A}\mathbf{B}).$$

In (2.1),  $b = 3N/2$ ,  $N$  is the normalized polymer concentration describing the strength of intermolecular interactions, and  $\langle \mathbf{m}\mathbf{m} \rangle$  is the second moment of the orientation distribution:

$$\langle \mathbf{m}\mathbf{m} \rangle \equiv \int_{\|\mathbf{m}\|=1} \mathbf{m}\mathbf{m} \rho(\mathbf{m}) d\mathbf{m}, \quad (2.3)$$

where  $\rho(\mathbf{m})$  is the orientational probability density function (pdf) of the ensemble of polymer rods. For convenience, potential (2.1) has been normalized with respect to  $k_B T$ , where  $k_B$

is the Boltzmann constant and  $T$  the absolute temperature. For pure nematic polymers, equilibrium states are described by the Boltzmann distribution [5]:

$$\rho(\mathbf{m}) = \frac{1}{Z} \exp[-U(\mathbf{m})], \quad (2.4)$$

where  $Z = \int_S \exp[-U(\mathbf{m})] d\mathbf{m}$  is the partition function and  $S$  is the unit sphere.

We choose the coordinate system such that the second moment  $\langle \mathbf{m}\mathbf{m} \rangle$  is diagonal:

$$\langle \mathbf{m}\mathbf{m} \rangle = \begin{bmatrix} \langle m_1^2 \rangle & 0 & 0 \\ 0 & \langle m_2^2 \rangle & 0 \\ 0 & 0 & \langle m_3^2 \rangle \end{bmatrix}. \quad (2.5)$$

As a consequence, the Maier-Saupe potential can be written as

$$U(\mathbf{m}) = -b(\langle m_1^2 \rangle m_1^2 + \langle m_2^2 \rangle m_2^2 + \langle m_3^2 \rangle m_3^2). \quad (2.6)$$

The most significant conclusion for pure nematic polymers is that all equilibrium states are axisymmetric [9, 18, 20]. Since not all equilibrium states of a perturbed nematic polymer ensemble are necessarily axisymmetric, to study the extendability, we formulate the problem without using the axisymmetry so that non-axisymmetric perturbations are allowed. The axisymmetry will be useful in our analysis because the extendability is determined by the Jacobian determinant evaluated at the unperturbed equilibrium state, which is axisymmetric. The definition and derivation of the Jacobian matrix, however, require non-axisymmetric formulation. For pure nematic polymers, the total potential is completely specified by the second moment  $\langle \mathbf{m}\mathbf{m} \rangle$ . As a result of the Boltzmann relation (2.4), an equilibrium state is completely specified by the second moment  $\langle \mathbf{m}\mathbf{m} \rangle$ . Because of the constraint  $m_1^2 + m_2^2 + m_3^2 = 1$ , an equilibrium state is completely specified by

$$s_1 \equiv \langle m_1^2 \rangle, \quad s_2 \equiv \langle m_2^2 \rangle. \quad (2.7)$$

At a pure nematic equilibrium state without perturbation, we have  $s_1 = s_2$  or  $s_1 = 1 - s_1 - s_2$  (which means  $s_1 = s_3$ ) or  $s_2 = 1 - s_1 - s_2$  (which means  $s_2 = s_3$ ). At an equilibrium state, we select the coordinate system such that the equilibrium satisfies  $s_1 = s_2$ . In terms of  $(s_1, s_2)$ , the Maier-Saupe potential can be expressed as

$$\begin{aligned} U(\mathbf{m}) &= -b(s_1 m_1^2 + s_2 m_2^2 + (1 - s_1 - s_2) m_3^2) \\ &= -b \left[ \frac{1}{2} (s_2 - s_1) (m_2^2 - m_1^2) + \left( 1 - \frac{3}{2} (s_1 + s_2) \right) m_3^2 \right] + \text{const.} \end{aligned} \quad (2.8)$$

Consequently, the equilibrium pdf is given by

$$\rho(\mathbf{m}) = \frac{1}{Z} \exp \left\{ b \left[ \frac{1}{2} (s_2 - s_1) (m_2^2 - m_1^2) + \left( 1 - \frac{3}{2} (s_1 + s_2) \right) m_3^2 \right] \right\}. \quad (2.9)$$

At an equilibrium state,  $(s_1, s_2)$  satisfies the nonlinear system:

$$s_1 - \langle m_1^2 \rangle = 0, \quad s_2 - \langle m_2^2 \rangle = 0. \quad (2.10)$$

The form of the equilibrium pdf (2.9) motivates us to introduce  $(\eta_1, \eta_2)$ :

$$\eta_1 \equiv b \left[ 1 - \frac{3}{2}(s_1 + s_2) \right], \quad \eta_2 \equiv b \frac{(s_2 - s_1)}{2}. \quad (2.11)$$

Here  $\eta_1$  is proportional to the order parameter of the pdf while  $\eta_2$  is proportional to the biaxial order parameter, which measures the deviation of the pdf from being axisymmetric. As we will see, one advantage of using  $(\eta_1, \eta_2)$  is that the Jacobian matrix is diagonal at equilibrium states. In terms of  $(\eta_1, \eta_2)$ , the pdf has the expression

$$\rho(\mathbf{m}, \eta_1, \eta_2) = \frac{\exp [\eta_2(m_2^2 - m_1^2) + \eta_1 m_3^2]}{\int_S \exp [\eta_2(m_2^2 - m_1^2) + \eta_1 m_3^2] d\mathbf{m}}. \quad (2.12)$$

The second advantage of using  $(\eta_1, \eta_2)$  is that the pdf does not depend on  $b$  explicitly. Later on, this property will enable us to write  $b$  as a function of  $r$  which is the equilibrium value of  $\eta_1$ . At an equilibrium state, the nonlinear system for  $(\eta_1, \eta_2)$  is

$$\begin{aligned} F_1(\eta_1, \eta_2; b) &\equiv \frac{\eta_1}{b} - \frac{1}{2}(3\langle m_3^2 \rangle - 1) = 0, \\ F_2(\eta_1, \eta_2; b) &\equiv \frac{\eta_2}{b} - \frac{1}{2}\langle m_2^2 - m_1^2 \rangle = 0. \end{aligned} \quad (2.13)$$

In this paper, we study the extendability of equilibrium states of nematic polymers in the presence of small perturbations. We consider a perturbed version of system (2.13):

$$\begin{aligned} F_1(\eta_1, \eta_2; b) &= \epsilon_1, \\ F_2(\eta_1, \eta_2; b) &= \epsilon_2. \end{aligned} \quad (2.14)$$

Mathematically, we study the existence and uniqueness of solution of system (2.14) near a solution of system (2.13) for small  $\epsilon_1$  and  $\epsilon_2$ . According to the implicit function theorem, the existence and uniqueness are determined by the Jacobian determinant of  $(F_1(\eta_1, \eta_2), F_2(\eta_1, \eta_2))$ . To calculate the Jacobian matrix, we first calculate the derivatives of pdf (2.12):

$$\begin{aligned} \frac{\partial}{\partial \eta_1} \rho(\mathbf{m}, \eta_1, \eta_2) &= (m_3^2 - \langle m_3^2 \rangle) \rho(\mathbf{m}, \eta_1, \eta_2), \\ \frac{\partial}{\partial \eta_2} \rho(\mathbf{m}, \eta_1, \eta_2) &= (m_2^2 - m_1^2 - \langle m_2^2 - m_1^2 \rangle) \rho(\mathbf{m}, \eta_1, \eta_2). \end{aligned} \quad (2.15)$$

Recall that at a pure nematic equilibrium state without perturbation, we have selected our coordinate system such that  $\eta_2 = 0$ . Evaluating the partial derivatives of  $F_1$  and  $F_2$  at the equilibrium ( $\eta_1 = r, \eta_2 = 0$ ) yields

$$\begin{aligned}
\left. \frac{\partial}{\partial \eta_1} F_1(\eta_1, \eta_2; b) \right|_{\eta_1=r, \eta_2=0} &= \frac{1}{b} - \frac{3}{2} \langle m_3^2 (m_3^2 - \langle m_3^2 \rangle) \rangle = \frac{1}{b} - \frac{3}{2} \text{var} (m_3^2), \\
\left. \frac{\partial}{\partial \eta_2} F_1(\eta_1, \eta_2; b) \right|_{\eta_1=r, \eta_2=0} &= -\frac{3}{2} \langle m_3^2 (m_2^2 - m_1^2 - \langle m_2^2 - m_1^2 \rangle) \rangle = 0, \\
\left. \frac{\partial}{\partial \eta_1} F_2(\eta_1, \eta_2; b) \right|_{\eta_1=r, \eta_2=0} &= -\frac{1}{2} \langle (m_2^2 - m_1^2) (m_3^2 - \langle m_3^2 \rangle) \rangle = 0, \\
\left. \frac{\partial}{\partial \eta_2} F_2(\eta_1, \eta_2; b) \right|_{\eta_1=r, \eta_2=0} &= \frac{1}{b} - \frac{1}{2} \langle (m_2^2 - m_1^2) (m_2^2 - m_1^2 - \langle m_2^2 - m_1^2 \rangle) \rangle, \\
&= \frac{1}{b} - \frac{1}{2} \langle (m_2^2 - m_1^2)^2 \rangle.
\end{aligned} \tag{2.16}$$

Here we point out that the Jacobian matrix of system (2.13) evaluated at an equilibrium state is diagonal, which is caused by the axisymmetry of the equilibrium state.

It follows that the determinant of Jacobian matrix of system (2.13) at the equilibrium is

$$\det \left( \frac{\partial (F_1, F_2)}{\partial (\eta_1, \eta_2)} \right) \Big|_{\eta_1=r, \eta_2=0} = \left( \frac{1}{b} - \frac{3}{2} \text{var} (m_3^2) \right) \cdot \left( \frac{1}{b} - \frac{1}{2} \langle (m_2^2 - m_1^2)^2 \rangle \right). \tag{2.17}$$

In (2.17), all averages are evaluated using the equilibrium pdf

$$\rho(\mathbf{m}, \eta_1, \eta_2) \Big|_{\eta_1=r, \eta_2=0} = \frac{1}{Z} \exp(r m_3^2). \tag{2.18}$$

For pure nematic polymers, an equilibrium state is completely specified by  $r$ . The governing equation for  $r$  is the first equation of (2.13):  $F_1(r, 0; b) = 0$ , whereas the second equation of (2.13) is satisfied automatically when  $\eta_2 = 0$ . We introduce a new function:

$$F(\eta; b) \equiv F_1(\eta, 0; b) = \frac{\eta}{b} - \frac{1}{2} (3 \langle m_3^2 \rangle - 1). \tag{2.19}$$

The governing equation for  $r$  is  $F(r; b) = 0$ . It follows directly from the definition that function  $F(\eta; b)$  is related to the (1, 1) element of the Jacobian matrix at equilibrium as

$$\left. \frac{\partial}{\partial \eta_1} F_1(\eta_1, \eta_2; b) \right|_{\eta_1=r, \eta_2=0} = \left. \frac{\partial}{\partial \eta} F(\eta; b) \right|_{\eta=r}. \tag{2.20}$$

As we will find later, this relation is a key tool for determining the sign of the (1, 1) element of the Jacobian matrix at equilibrium. In the above, we have used variables  $\eta$  and  $r$  more or less interchangeably. Later on when necessary, we will use  $\eta$  to denote the independent variable

of functions and use  $r$  to denote the particular value of  $\eta$  that satisfies  $F(r; b) = 0$ . For that purpose, we will continue using these two variables.

### 3. Extendability of equilibria of nematic polymers

To obtain more specific properties of equilibrium states of nematic polymers, we rewrite the governing equation for  $r$  using spherical coordinates. We select the  $m_3$ -axis as the pole of the spherical coordinate system. The equilibrium pdf given in (2.18) becomes

$$\rho(\phi, \theta; r) = \frac{\exp(r \cos^2 \phi)}{2\pi \int_0^\pi \exp(r \cos^2 \phi) \sin \phi d\phi}, \quad (3.1)$$

where  $\phi$  is the polar angle and  $\theta$  the azimuthal angle. Here we need to point out that  $r$  is not the radius in the spherical coordinate system. It is a parameter of the equilibrium state. Substituting equilibrium pdf (3.1) into  $(1/2)(3\langle m_3^2 \rangle - 1)$ , using a change of variable  $u = \cos \phi$ , and integrating by parts, we have

$$\frac{1}{2}(3\langle m_3^2 \rangle - 1) = r \cdot \frac{\int_0^1 (u^2 - u^4) \exp(r u^2) du}{\int_0^1 \exp(r u^2) du}. \quad (3.2)$$

Thus,  $F(\eta; b)$  defined in (2.19) becomes  $F(\eta; b) = \eta[1/b - f(\eta)]$ , where  $f(\eta)$  is defined as

$$f(\eta) \equiv \frac{\int_0^1 u^2 (1 - u^2) \exp(\eta u^2) du}{\int_0^1 \exp(\eta u^2) du}. \quad (3.3)$$

The equation for  $r$ ,  $F(r; b) = 0$ , becomes

$$r \left[ \frac{1}{b} - f(r) \right] = 0. \quad (3.4)$$

Equation (3.4) has a trivial solution  $r = 0$  for arbitrary value of  $b$ , which corresponds to the isotropic branch of the nematic polymer phase diagram. At  $r = 0$ , the equilibrium pdf is uniform,  $\rho(\phi, \theta; 0) = 1/4\pi$ . It follows that

$$\begin{aligned} \langle m_j^2 \rangle &= \frac{1}{3}, \\ \langle m_j^4 \rangle &= \langle m_3^4 \rangle = \int_0^1 u^4 du = \frac{1}{5}, \\ \langle m_i^2 m_j^2 \rangle &= \langle m_1^2 m_3^2 \rangle = \frac{1}{2} \int_0^1 u^2 (1 - u^2) du = \frac{1}{15}, \quad i \neq j, \\ \text{var}(m_3^2) &= \langle m_3^4 \rangle - \langle m_3^2 \rangle^2 = \frac{1}{5} - \frac{1}{9} = \frac{4}{45}, \\ \langle (m_2^2 - m_1^2)^2 \rangle &= \langle m_2^4 \rangle - 2\langle m_1^2 m_2^2 \rangle + \langle m_1^4 \rangle = \frac{2}{5} - \frac{2}{15} = \frac{4}{15}. \end{aligned} \quad (3.5)$$

Substituting these results into (2.16), we obtain

$$\begin{aligned}\left.\frac{\partial}{\partial \eta_1} F_1(\eta_1, \eta_2; b)\right|_{\eta_1=0, \eta_2=0} &= \frac{1}{b} - \frac{3}{2} \text{var}(m_3^2) = \frac{1}{b} - \frac{2}{15}, \\ \left.\frac{\partial}{\partial \eta_2} F_2(\eta_1, \eta_2; b)\right|_{\eta_1=0, \eta_2=0} &= \frac{1}{b} - \frac{1}{2} \langle (m_2^2 - m_1^2)^2 \rangle = \frac{1}{b} - \frac{2}{15}.\end{aligned}\quad (3.6)$$

Therefore, when  $b \neq 15/2$ , the Jacobian matrix is nonsingular and thereby the isotropic equilibrium is extendable. At  $b = 15/2$ , the isotropic branch intersects with the nematic branch.

The remaining solutions of (3.4), if any, satisfy

$$\frac{1}{b} - f(r) = 0. \quad (3.7)$$

In [20], it has been shown that the function  $f(\eta)$  has the following properties:

- (1)  $f(0) = 2/15$ ,  $\lim_{\eta \rightarrow +\infty} f(\eta) = 0$  and  $\lim_{\eta \rightarrow -\infty} f(\eta) = 0$ ;
- (2)  $f(\eta)$  attains its maximum at  $\eta = \eta^* = 2.1782879748 > 0$ , where the maximum is  $f(\eta^*) = 0.14855559992254 > 0$ ;
- (3)  $f'(\eta) > 0$  for  $\eta < \eta^*$  and  $f'(\eta) < 0$  for  $\eta > \eta^*$ .

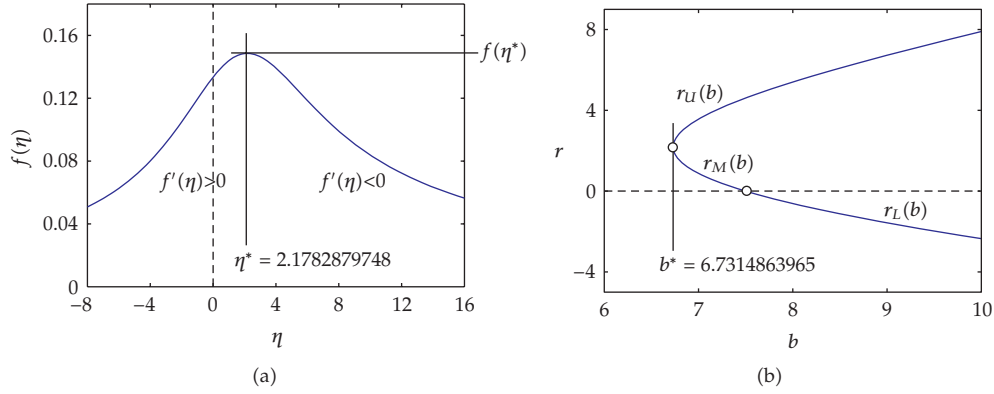
A graph of  $f(\eta)$  is shown in Figure 1(a). Thus, we draw conclusions below for (3.7) as follows.

- (i) The critical value of  $b$  is  $b^* = 1/f(\eta^*) = 6.7314863965$ .
- (ii) For  $b < b^*$ , (3.7) has no solution.
- (iii) At  $b = b^*$ , (3.7) has one solution  $r(b^*) = \eta^* > 0$ .
- (iv) For  $b^* < b < 2/15$ , (3.7) has two solutions:  $r_U(b) > \eta^* > 0$  and  $0 < r_M(b) < \eta^*$ .
- (v) At  $b = 2/15$ , (3.7) has two solutions:  $r_U(2/15) > \eta^* > 0$  and  $r(2/15) = 0$ .
- (vi) For  $b > 2/15$ , (3.7) has two solutions:  $r_U(b) > \eta^* > 0$  and  $r_L(b) < 0$ .

As mentioned before, we use subscript “U” to denote to the “Upper” part of the phase diagram where  $r > \eta^*$ , subscript “M” to denote to the “Middle” part of the phase diagram, where  $0 < r < \eta^*$ , and subscript “L” to denote to the “Lower” part of the phase diagram, where  $r < 0$ . The phase diagram for nematic polymers is shown in Figure 1(b). In the terminologies of nematic polymers, curve segment  $r_U(b)$  is the stable part of the prolate branch;  $r_M(b)$  is the unstable part of the prolate branch; and  $r_L(b)$  is the unstable oblate branch.

Recall that  $b$  is the strength of the Maier-Saupe interaction, which is proportional to the normalized polymer concentration and is inversely proportional to the temperature.  $r$ , the solution of  $F(r; b) = 0$ , has the expression  $r = b \cdot (1/2)(3\langle m_3^2 \rangle - 1)$ , where  $(1/2)(3\langle m_3^2 \rangle - 1)$  is the order parameter. Thus, from physical considerations, it is desirable to use  $b$  as the independent variable and treat  $r$  as a function of  $b$ . However,  $r(b)$  is a multivalued function of  $b$  and for  $b < b^*$  function  $r(b)$  is not even defined. Mathematically, it is much more convenient if we use  $r$  as the independent variable and treat  $b$  as a function of  $r$ .  $b(r)$  is a





**Figure 1:** (a) Graph of function  $f(\eta)$ ; (b) phase diagram of nematic polymers.

single-value function of  $r$  and is defined for all values of  $r$  in  $(-\infty, +\infty)$ . Below, we will adopt this new formulation of viewing  $b$  as a function of  $r$ . In the new formulation, function  $b(r)$  is determined from (3.7) as  $b(r) = 1/f(r)$ . In terms of this new formulation, the stable part of the prolate branch  $r_U(b)$  can be simply represented as  $b(r)$  for  $r > \eta^*$ ; the unstable part of the prolate branch  $r_M(b)$  as  $b(r)$  for  $0 < r < \eta^*$ ; and the unstable oblate branch  $r_L(b)$  as  $b(r)$  for  $r < 0$ . Now we discuss the extendability of these branches. Using relation (2.20),  $F(\eta; b) = \eta[1/b - f(\eta)]$ , and  $1/b - f(r) = 0$ , we arrive at

$$\begin{aligned}
 \left. \frac{\partial}{\partial \eta_1} F_1(\eta_1, \eta_2; b(r)) \right|_{\eta_1=r, \eta_2=0} &= \left. \frac{\partial}{\partial \eta} F(\eta; b(r)) \right|_{\eta=r} \\
 &= \left[ \frac{1}{b(r)} - f(\eta) \right] \bigg|_{\eta=r} - \eta f'(\eta) \bigg|_{\eta=r} \\
 &= -r f'(r) = \begin{cases} > 0, & \text{for } r > \eta^* \\ < 0, & \text{for } 0 < r < \eta^* \\ > 0, & \text{for } r < 0. \end{cases}
 \end{aligned} \tag{3.8}$$

To study the  $(2,2)$  element of Jacobian matrix, we first rewrite  $(1/2)\langle (m_2^2 - m_1^2)^2 \rangle$  by substituting equilibrium pdf (3.1) into  $(1/2)\langle (m_2^2 - m_1^2)^2 \rangle$  and using substitution  $u = \cos \phi$ ,

$$\frac{1}{2} \langle (m_2^2 - m_1^2)^2 \rangle = \frac{1}{4} \frac{\int_0^1 (1-u^2)^2 \exp(ru^2) du}{\int_0^1 \exp(ru^2) du}. \tag{3.9}$$

Using (2.16),  $b(1) = 1/f(r)$ , the expression of  $f(r)$  given in (3.3), and result (3.9), we have

$$\begin{aligned}
 \left. \frac{\partial}{\partial \eta_2} F_2(\eta_1, \eta_2; b(r)) \right|_{\eta_1=r, \eta_2=0} &= \frac{1}{b(r)} - \frac{1}{2} \langle (m_2^2 - m_1^2)^2 \rangle \\
 &= \frac{1}{4} \frac{\int_0^1 (1-u^2)(5u^2-1) \exp(ru^2) du}{\int_0^1 \exp(ru^2) du} \equiv g(r).
 \end{aligned} \tag{3.10}$$

It is straightforward to verify that  $g(0) = 0$ . Below, we want to show that  $g(r) > 0$  for  $r > 0$  and  $g(r) < 0$  for  $r < 0$ . To facilitate the analysis below, we write  $g(r)$  as an average

$$g(r) = \frac{1}{4} \langle (1 - u^2)(5u^2 - 1) \rangle, \quad (3.11)$$

where the average is with respect to the pdf  $\rho(u; r) = \exp(ru^2) / \int_0^1 \exp(ru^2) du$ .

**Lemma 3.1.** *Function  $g(r)$  given in (3.11) has the property that  $g(r) = 0$  implies  $g'(r) > 0$ .*

*Proof of Lemma 3.1.* We first calculate the derivative of the pdf:  $(\partial/\partial r)\rho(u; r) = (u^2 - \langle u^2 \rangle)\rho(u; r)$ , which leads to

$$\begin{aligned} g'(r) &= \frac{1}{4} \langle (1 - u^2)(5u^2 - 1)(u^2 - \langle u^2 \rangle) \rangle \\ &= \frac{1}{20} \langle (1 - u^2)(5u^2 - 1)^2 \rangle + \frac{1}{5} (1 - 5\langle u^2 \rangle) g(r). \end{aligned} \quad (3.12)$$

Thus, whenever  $g(r) = 0$ , we have  $g'(r) = (1/20) \langle (1 - u^2)(5u^2 - 1)^2 \rangle > 0$ .  $\square$

Lemma 3.1 together with  $g(0) = 0$  leads to  $g(r) > 0$  for  $r > 0$  and  $g(r) < 0$  for  $r < 0$ . Combining this result on  $g(r)$  with result (3.8) on  $-rf'(r)$ , we arrive at

$$\det \left( \frac{\partial(F_1, F_2)}{\partial(\eta_1, \eta_2)} \right) \Big|_{\eta_1=r, \eta_2=0} = (-rf'(r))g(r) = \begin{cases} > 0, & \text{for } r > \eta^*, \\ < 0, & \text{for } 0 < r < \eta^*, \\ < 0, & \text{for } r < 0. \end{cases} \quad (3.13)$$

Therefore, we conclude that all nematic equilibrium states (stable or unstable) are extendable except for the equilibrium state at  $(r = 0, b = 15/2)$  and the equilibrium state at  $(r = \eta^*, b = b^*)$ .

#### 4. Conclusions

In this work, we studied the extendability of equilibrium states of nematic polymers with the Maier-Saupe intermolecular potential. We found that the Jacobian matrix of the nonlinear system is nonsingular except at two special equilibrium states. The significance of this result is its implication on the existence and uniqueness of equilibrium states of a perturbed system, in the neighborhood of the unperturbed equilibrium states.

#### Acknowledgments

H. Wang was partially supported by the National Science Foundation. H. Zhou was supported in part by the Air Force Office of Scientific Research under Grant no. F1ATA06313G003.

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