

## BOUNDARY CONDITIONS FOR THE MICROSCOPIC FENE MODELS\*

CHUN LIU<sup>†</sup> AND HAILIANG LIU<sup>‡</sup>

**Abstract.** We consider the microscopic equation of finite extensible nonlinear elasticity (FENE) models for polymeric fluids under a steady flow field. It is shown that for the underlying Fokker–Planck type of equations, any preassigned distribution on the boundary will become redundant once the nondimensional number  $Li := \frac{Hb}{k_B T} \geq 2$ , where  $H$  is the elasticity constant,  $\sqrt{b}$  is the maximum dumbbell extension,  $T$  is the temperature, and  $k_B$  is the usual Boltzmann constant. Moreover, if the probability density function is regular enough for its trace to be defined on the sphere  $|m| = \sqrt{b}$ , then the trace is necessarily zero when  $Li > 2$ . These results are consistent with our numerical simulations as well as some recent well-posedness results by preassuming a zero boundary distribution.

**Key words.** microscopic finite extensible nonlinear elasticity models, boundary condition, polymer fluids, Fokker–Planck equation, Fichera function

**AMS subject classifications.** 34F05, 35K65, 35K20, 65C30

**DOI.** 10.1137/060667700

**1. Introduction.** The two-scale macro-micro models have been proven successful in describing the dynamics of many polymeric fluids. The systems usually consist of a macroscopic momentum equation (the force balance equation) and a microscopic evolution of the probability distribution functions (PDFs) through Fokker–Planck equations [4, 5]. The coupling of the micro-macro interaction is through the transport of the PDF in the microscopic equations and the induced elastic stress in the macroscopic equations. It is through this interaction, the competition between the kinetic energy and the (multiscale) elastic energies, that all different hydrodynamical and rheological properties of these materials arise [5, 14]. Let  $y$  be the macroscopic Eulerian (observer’s) coordinate and  $m$  the microscopic molecule configurational variable. The distinguished representation of the variables represents the nature of the scale separation of these models. Let  $u = u(y, t)$  be the macroscopic velocity field of the flow and  $y(X, t)$  be the induced flow map (trajectory) with macroscopic material coordinate  $X$ .  $f = f(t, m, y)$ ,  $(m, y) \in \mathbb{R}^{2d}$  is the PDF of the molecule separation. The dependence of the macroscopic coordinate of  $f$  is attributed to the macroscopic anisotropy of the materials. Moreover, the models assume that the microscopic deformation is the same as the macroscopic deformation through the macroscopic covariant (or anticovariant) deformation of  $m$ . In the case of  $m = F\tilde{m}$ , with  $F = \frac{\partial y}{\partial X}$  the (macroscopic) deformation tensor induced by the flow map  $y(X, t)$ , and  $\tilde{m}$  the undeformed configuration, we have the following microscopic evolution equation [17]:

$$(1.1) \quad \partial_t f + u \cdot \nabla_y f + \nabla_m \cdot (\kappa m f) = \frac{2}{\gamma} [(\nabla_m \cdot (\nabla_m U f) + k_B T \Delta_m f)],$$

\*Received by the editors August 18, 2006; accepted for publication (in revised form) January 10, 2008; published electronically April 11, 2008.

<http://www.siam.org/journals/siap/68-5/66770.html>

<sup>†</sup>Department of Mathematics, Pennsylvania State University, 218 McAllister Building, University Park, PA 16802 (liu@math.psu.edu). This author’s research was partially supported by NSF grants DMS-0405850 and DMS-0509094.

<sup>‡</sup>Mathematics Department, Iowa State University, Carver Hall 434, Ames, IA 50011 (hliu@iastate.edu). This author’s research was partially supported by NSF grant DMS-0505975 and the Ames Laboratory (DOE facility).

where  $\kappa = \nabla_y u$  is the strain rate tensor;  $U$  denotes the spring potential;  $\gamma$  is the friction coefficient;  $T$  is the absolute temperature; and  $k_B$  is the Boltzmann constant. Equation (1.1) models both the convection and stretching of the polymers by the macroscopic flow and the microscopic convection diffusion evolution. The latter mechanism can be interpreted with its corresponding SDE [11, 16]:

$$dm = \left( -\frac{2}{\gamma} \nabla_m U \right) dt + \sqrt{\frac{4k_B T}{\gamma}} dW_t,$$

where  $W_t$  is a standard Brownian motion, which in turn gives the Fokker–Planck dynamic to the PDF. Much of the material properties can be attributed to different microscopic energies. The simplest spring potential is given by the Hookean law  $U(m) = H|m|^2/2$ , where  $H$  is the elasticity constant. This potential has the distinguished feature that the system is closed under second moment closure, which yields the usual Oldroyd models [3, 5, 17]. A more commonly used model is with the following finite extensible nonlinear elasticity (FENE) potential:

$$U(m) = -\frac{Hb}{2} \log \left( 1 - \frac{|m|^2}{b} \right),$$

which takes into account a finite-extensibility constraint by assigning infinite energy when the molecule length approaches  $\sqrt{b}$ , the maximum dumbbell extension [3]. In this case, the convective spring force becomes

$$(1.2) \quad \nabla_m U = \frac{Hm}{1 - |m|^2/b},$$

which also becomes infinity on the boundary of  $B_{\sqrt{b}}$ . Intuitively, this should mean that the Fokker–Planck equation (1.1) is defined only on the open ball  $\Omega = \{m \in \mathbb{R}^d : |m|^2 < b\}$ , where  $d = 2, 3$ , disregarding the boundary condition preimposed on the solution of (1.1). On the other hand, the diffusion due to the thermofluctuation does have infinite propagation speed. Also, the Brownian motion is unbounded in the  $L^\infty$  norm. The main complexity with the FENE potential lies mainly with the singularity of the equation at the boundary. In this paper, we will discuss boundary conditions for the Fokker–Planck equation alone, with the fluid velocity being steady and homogeneous. The velocity gradient will be treated as a constant matrix. Observe that since (1.1) experiences singularity on the sphere  $|m| = \sqrt{b}$ , the data may not necessarily be well defined. The main issues of our interest in this work are the following:

- Are the boundary conditions necessary or redundant?
- If the PDF solution is regular enough to have a trace on the boundary, what is its trace, regardless of whether or not the data is preimposed?

These issues for the underlying FENE models are fundamental and attracted much attention in the study of the well-posedness in certain weighted Sobolev spaces (see, e.g., [15]) as well as in the two-dimensional SDE framework [13]. However, the whole issue remained open. Our key observation in this paper is that the answer to the above questions hinges on whether the nondimensional quantity

$$(1.3) \quad Li := \frac{Hb}{k_B T}$$

crosses a critical value 2. The main goals of this paper are to show two new results: (i) for the underlying Fokker–Planck equation (1.1), any boundary condition will

become redundant once the nondimensional number  $Li \geq 2$ ; (ii) if the PDF  $f$  is regular enough for its trace to be defined on the sphere  $|m| = \sqrt{b}$ , then the trace is necessarily zero when  $Li > 2$ . Physically speaking, no boundary condition is necessary for the case with the given spring at low temperature or the case at fixed temperature with the large product of  $H$  and  $b$ . To put our work in a proper perspective we recall that well-posedness of the coupled micro-macro system or Fokker–Planck equation alone has attracted much attention recently [2, 6, 7, 12]. In particular, the local existence results of [23] in the weighted Sobolev space will also force the zero boundary condition. Up to now, most works have been with prescribed boundary conditions. On the other hand, numerical simulations seemed to indicate that the solutions are not sensible to such boundary conditions. We also refer the reader to [15] for the study of large-time behavior of the coupled micro-macro system and a rigorous formulation of the no-flux boundary condition. We now proceed to identify the key quantity  $Li$  defined in (1.3) by making the following scaling:

$$(y, u, t, m, b) \rightarrow \left( \frac{y}{L_0}, \frac{u}{U_0}, \frac{t}{T_c}, \frac{m}{l}, \frac{b}{l^2} \right),$$

where  $T_c := L_0/U_0$  is the macroscopic convective time scale and  $l := \sqrt{\frac{k_B T}{H}}$  serves as the mesoscopic length scale of the spring. We further introduce the nondimensional parameter  $De = \frac{T_r}{T_c}$ , where  $T_r = \frac{\gamma}{4H}$  characterizes the mesoscopic relaxation time scale of the spring, and  $De$  is often called the Deborah number, which is a unique parameter in non-Newtonian fluids. Putting all of the above together and still using  $(y, u, t, m, b)$  for the scaled quantities, (1.1) thus reduces to

$$(1.4) \quad \partial_t f(t, m) + \nabla_m \cdot (\kappa m f) = \frac{1}{2De} (\nabla_m \cdot (\nabla_m U f) + \Delta_m f),$$

where  $\kappa = \nabla_y u$  is the steady homogeneous velocity gradient.  $\text{Tr}(\kappa) = \nabla_y \cdot u = 0$  for the incompressible flow. Note that the corresponding square of radius for the nondimensional configuration variable  $m$  is exactly the key parameter  $Li = b/l^2 = \frac{Hb}{k_B T}$  as given in (1.3) (though still denoted by  $b$  in what follows). The potential in nondimensional form thus reads

$$(1.5) \quad \nabla_m U = \frac{m}{1 - |m|^2/b}.$$

In order to simplify the notation, we simply take  $De = 1$  and obtain

$$(1.6) \quad \partial_t f(t, m) + \nabla_m \cdot (\kappa m f) = \frac{1}{2} (\nabla_m \cdot (\nabla_m U f) + \Delta_m f).$$

For (1.6) with scaled potential (1.5) our first result is that  $b = 2$  is a critical extension parameter for deciding whether boundary conditions are necessary for a well-defined problem (in the sense that the well-posedness results are expected to be obtained in standard Sobolev spaces).

**THEOREM 1.1.** *Consider (1.6) in  $\{m \mid |m| < \sqrt{b}\}$  for  $t > 0$  subject to certain initial data. The extension parameter  $b = 2$  is a critical value in the sense that the Dirichlet boundary condition leads to a well-defined problem, provided that (i) when  $b < 2$ , the distribution  $f$  on boundary  $|m|^2 = b$  must be imposed; and (ii) when  $b \geq 2$ , any preassigned distribution on boundary  $|m|^2 = b$  will become redundant.*

It is known that the parameter range of physical interest is  $b > 2$  [3]. Therefore, in this regime for  $b$ , the original problem can be formulated as follows: find a distribution function  $f(t, m)$  such that (1.6) holds for  $t > 0$  and

$$(1.7) \quad f(0, m) = f_0(m), \quad |m| < \sqrt{b},$$

where  $f_0 \geq 0$  is a given bounded measurable function.

Here we would like to make several remarks:

(1) The statement in this theorem is justified based on the use of Fichera’s criterion [8], which is sketched in the appendix.

(2) The well-posedness for the case  $b < 2$  with imposed distribution on  $|m| = \sqrt{b}$  follows from Theorem 4.2 in the appendix, with an extra constraint on the nontrivial shear rate  $k$ . The proof of the well-posedness for the case  $b \geq 2$  is more delicate. In this work the redundancy of boundary conditions is stated in the sense of trace for weak solutions. We note that boundary conditions can also be discussed in terms of trajectories of the stochastic process; see, e.g., Stroock and Varadhan [20]. The second order linear equations with nonnegative characteristic form attracted much interest in the 1960’s and 1970’s [18, 21]. The existence results are customarily in Sobolev spaces with certain disjointness assumptions on the relevant boundary parts with the irrelevant parts and the non(negative) characteristic parts. Regularity of solutions with continuity up to the boundary can be further discussed [18]. As for the FENE models considered in this paper, we will present a description of the existence of the full system (coupled with the flow field) in a separate paper.

(3) The corresponding analogue of this statement in the SDE framework is known [13], where for the two-dimensional case the authors show that if  $b \geq 2$ , then the trajectories of the stochastic process representing the evolution of the end-to-end vector does not touch the boundary of radius  $\sqrt{b}$ , which means the polymer does not reach its maximal extensibility. Our second result determines the trace of the PDF on the sphere  $|m|^2 = b$ .

**THEOREM 1.2.** *Consider the initial value problem (1.6)–(1.7) in  $|m| < \sqrt{b}$ . Let  $f_0(m)$  be a bounded measurable function with  $\text{supp}(f_0(m)) \subset \{m, |m| \leq \sqrt{b^*}, b^* < b\}$ . Then for  $b > 2$  the solution  $f(t, m)$  of (1.6) remains bounded and satisfies*

$$|f| \leq |f_0| \left( \frac{b - |m|^2}{b - b^*} \right)^{b/2 - \alpha} e^{Kt},$$

where  $\alpha$  and  $K$  satisfy

$$0 < \alpha < \frac{b}{2} - 1, \quad K > K^* := \frac{\beta^2}{16b\alpha(b - 2 - 2\alpha)} - \rho(b - 2\alpha)$$

with  $\beta = \rho(b - \alpha)r^2 + 2\alpha(d + b - 2 - 2\alpha)$  and  $\rho = \sqrt{\text{Tr}(\kappa^\top \kappa)}$ .

In comparison we mention that the solution to the SDE associated with (1.6) is shown to exist and has trajectorial uniqueness if and only if  $b \geq 2$  [12]. We also refer the reader to [2] for an existence result with prescribed zero boundary data. Our results also show that for  $b \geq 2$  well-posedness requires no prescribed boundary value on  $|m|^2 = b$ , and for  $b > 2$  the distribution function, if regular enough to have a trace, must have zero trace:

$$(1.8) \quad f(t, m)|_{|m|=\sqrt{b}} = 0.$$

In other words, one is not allowed to prescribe boundary data on the sphere  $|m| = \sqrt{b}$  other than (unnecessary)  $f = 0$  or a natural no-flux boundary condition. The difficulty of the problem lies in the singularity of the equation occurring at the boundary. The key to our approach is to rewrite the equation into a second order equation having standard nonnegative characteristic form, for which we apply the Fichera function criterion to check when boundary conditions are unnecessary [8, 18, 21]. We further investigate the trace of the PDF on the sphere  $|m| = \sqrt{b}$  where no data is preimposed. Our approach is to convert the equation by a delicate transformation in such a way that the resulting equation supports a maximum principle. This paper is organized as follows: in section 2, we use the Fichera function criterion to prove Theorem 1.1. Section 3 is devoted to the trace analysis of the PDF on the sphere  $|m| = \sqrt{b}$ . The presentation is split into two parts, without and with homogeneous flow involved.

**2. Critical parameter  $b = 2$  and boundary conditions.** In this section we shall show that  $b = 2$  is a critical value in the sense that for  $b < 2$  a boundary condition is necessary and when  $b \geq 2$  the boundary distribution becomes redundant. Note that (1.6) has a singular lower order term on boundary  $|m| = \sqrt{b}$ ; our approach is to first transform this equation into a second equation degenerating near the boundary. We then employ the method of the Fichera function [1, 8, 18, 21] to study the corresponding relevant boundary value points on the boundary [18], as sketched in the appendix. We now introduce the following transformation:

$$(2.1) \quad f(t, m) = g(t, m) \exp(-U(m)),$$

which gives

$$(2.2) \quad \partial_t g + \nabla_m \cdot (\kappa m g) - \nabla_m U \cdot (\kappa m g) = \frac{1}{2} [\Delta_m g - \nabla_m U \cdot \nabla_m g].$$

The right-hand side of the equation becomes the dual form of the original Fokker-Planck equation [9, 19]. We note a different transformation in [6, 10, 22],  $f(t, m) = g(t, m) \exp(-U(m)/2)$ , which was used to remove the singularity at the boundary in the resulting equation. Applying further rescaling,

$$(2.3) \quad x = \sqrt{2}m, \quad r^2 = 2b, \quad v(t, x) = g(t, m),$$

we obtain

$$(2.4) \quad \partial_t v + \nabla_x \cdot (\kappa x v) + a(x) \cdot (\nabla_x v - \kappa x v) = \Delta_x v,$$

where

$$a(x) := \frac{bx}{r^2 - |x|^2}.$$

Note that  $\nabla_x \cdot (\kappa x) = \text{Tr}(\kappa) = 0$ ; the above equation reduces to

$$(2.5) \quad \partial_t v + (a(x) + \kappa x) \cdot \nabla_x v - a(x) \cdot \kappa x v = \Delta_x v.$$

Once  $v$  is determined, the PDF  $f$  can be recovered through

$$(2.6) \quad f(t, m) = v(t, \sqrt{2}m)(1 - |m|^2/b)^{b/2}.$$

Rewrite (2.5) as

$$(2.7) \quad L(v) = 0, \quad x \in \mathbb{R}^d,$$

where

$$L(v) := (r^2 - |x|^2)\Delta_x v - (r^2 - |x|^2)v_t - (bx + (r^2 - |x|^2)\kappa x) \cdot \nabla_x v + bx^\top \kappa x v$$

has a standard form:

$$L(v) := a^{kj}(\xi)D_{kj}v + b^k(\xi)D_k v + c(\xi)v = 0, \quad k, j = 0 \dots d.$$

Here the repeated indices are summed from 1 to  $d$ ,  $\xi = (t, x)$ :

$$a^{00} = 0, \quad b^0 = -(r^2 - |x|^2), \quad c(\xi) = bx^\top \kappa x$$

and

$$a^{kk}(\xi) = (r^2 - |x|^2), \quad b^k = -[bx_k + (r^2 - |x|^2)\kappa_{kj}x_j], \quad k = 1 \dots d.$$

Note that the new equation is degenerate at boundary  $|x| = r$ . This second order equation has nonnegative characteristic form in domain  $\Omega = \{(t, x), 0 < t < T^*, |x| < r\}$  for any  $T^* > 0$ , since

$$a^{kj}(\xi)y_k y_j \geq 0$$

for any real vector  $y$  and any point  $\xi \in \Omega$ . Hence there are no negative characteristic points on the boundary.

Next we check the sign of Fichera's function

$$\mathfrak{F} = (b^k - a_{\xi_j}^{kj})n_k$$

at points on  $\partial\Omega$ . At boundary  $|x| = r$ ,  $0 < t < T^*$ , one has  $n_0 = 0$ ,  $n_k = -x_k/r$ ,  $k = 1 \dots d$ ; thus

$$\begin{aligned} \mathfrak{F}(t, x) &= \sum_{k=1}^d (b^k - a_{x_k}^{kk})n_k \\ &= \sum_{k=1}^d (-bx_k + 2x_k) \cdot (-x_k/r) \\ &= (b - 2)r. \end{aligned}$$

If  $\mathfrak{F} \geq 0$ , that is,  $b \geq 2$ , all boundary points are irrelevant and no boundary condition is needed. Otherwise, in the case  $b < 2$ , all boundary points are relevant and an appropriate boundary condition has to be imposed. We now examine the boundary  $t = T^*$  and  $|x| < r$ , on which one has  $n^0 = -1$ ,  $n^k = 0$ ; thus

$$\begin{aligned} \mathfrak{F}(t, x) &= (b^k - a_{\xi_j}^{kj})n_k = b^0 n_0 \\ &= r^2 - |x|^2 > 0. \end{aligned}$$

No condition needs to be imposed at  $t = T^*$  either. Similarly at  $t = 0$ ,  $|x| < r$ , one obtains  $\mathfrak{F}(t, x) = |x|^2 - r^2 < 0$ ; thereby a condition at  $t = 0$ , the initial condition, has to be imposed. This completes the proof of Theorem 1.1.

*Remark.* For the transformed equation  $L[v] = 0$  with  $\kappa = 0$ , we have

$$\frac{1}{2}D_i b^i - \frac{1}{2}D_{ij} a^{ij} - c = d \left(1 - \frac{b}{2}\right) > 0$$

for  $b < 2$ . Hence the existence theorem (Theorem 4.2) in the appendix applies only to the case  $b < 2$ .

**3. The trace of the distribution function on the sphere  $|m| = \sqrt{b}$  for  $b > 2$ .** We now restrict ourselves to the case of  $b > 2$ . The proof in the above section shows that the presence of the fluid velocity does not affect the relevancy of the boundary points with respect to the equation. In this section, we will show, if the solution exists and assumes a trace on the boundary, that the trace of the resulting PDF has to be zero.

**3.1. No-flow case.** We will start from the case  $\kappa = 0$ . Equation (2.4) becomes

$$(3.1) \quad \partial_t v + a(x) \cdot \nabla_x v = \Delta_x v, \quad a(x) := \frac{bx}{r^2 - |x|^2},$$

with the initial condition

$$v(0, x) = v_0(x) = f_0 \left( \frac{x}{\sqrt{2}} \right) \left( 1 - \frac{|x|^2}{r^2} \right)^{-b/2}, \quad \text{supp}(v_0) \subset [-r, r];$$

we are going to show that there exists an  $\alpha$  satisfying  $0 < \alpha < b/2$  and a  $K > 0$  such that

$$|v(t, x)| \leq M e^{Kt} (r^2 - x^2)^{-\alpha} \quad \forall t > 0.$$

Combining with the original transformation (2.1) and (2.3), which yield

$$f(t, m) = v(t, x)(1 - |x|^2/r^2)^{b/2},$$

we arrive at

$$(3.2) \quad |f(t, m)| \leq C(r^2 - x^2)^{b/2-\alpha} e^{Kt}.$$

This leads to the zero trace for the PDF:

$$f(t, m)|_{|m|^2=b} = 0 \quad \forall t > 0.$$

The main difficulty of Theorem 1.2 lies in the singularity at the boundary. Equation (2.7) for  $v$  solves  $L(v) = 0$  with

$$L(v) := (r^2 - |x|^2)\Delta_x v - bx \cdot \nabla_x v - (r^2 - |x|^2)\partial_t v.$$

We now introduce the transformation

$$v(t, x) := w(t, x)(r^2 - |x|^2)^{-\alpha} e^{Kt},$$

with  $\alpha$  and  $K$  to be determined. A simple calculation gives

$$\begin{aligned} \partial_t v &= (w_t + Kw)(r^2 - |x|^2)^{-\alpha} e^{Kt}, \\ \nabla_x v &= [\nabla_x w (r^2 - |x|^2)^{-\alpha} + 2\alpha w x (r^2 - |x|^2)^{-\alpha-1}] e^{Kt}, \\ \Delta_x v &= [\Delta_x w (r^2 - |x|^2)^{-\alpha} + 4\alpha x \cdot \nabla_x w (r^2 - |x|^2)^{-\alpha-1} \\ &\quad + 4\alpha(\alpha + 1)w|x|^2(r^2 - |x|^2)^{-\alpha-2}] e^{Kt} \\ &\quad + 2\alpha d w (r^2 - |x|^2)^{-(\alpha+1)} e^{Kt}. \end{aligned}$$

Substitution of these terms into the equation  $L(v) = 0$  multiplied by  $(r^2 - |x|^2)^{\alpha+1} e^{-Kt}$  gives

$$A(w) = 0,$$

where the operator  $A(w)$  is defined as

$$A(w) := (r^2 - |x|^2)^2 \Delta_x w + (4\alpha - b)(r^2 - |x|^2)x \cdot \nabla_x w - (r^2 - |x|^2)^2 \partial_t w + c(x)w,$$

in which the coefficient

$$c(x) = -K(r^2 - |x|^2)^2 + 2\alpha[dr^2 + (2\alpha + 2 - d - b)|x|^2].$$

In order to apply a maximum principle to  $A(w) = 0$ , we need to choose  $\alpha$  and  $K$  such that  $c < 0$  in  $\Omega(T^*)$ . Setting  $|x|^2 = \theta r^2$ , we have

$$c = -Kr^4(1 - \theta)^2 + 2\alpha dr^2 + 2\alpha(2\alpha + 2 - d - b)\theta r^2 = -r^2 \{Kr^2\theta^2 - 2((2\alpha + 2 - d - b)\alpha + Kr^2)\theta + Kr^2 - 2d\alpha\}.$$

Thus as a function of  $\theta$ ,  $c$  achieves its maximum

$$c = K^{-1}\alpha \{2Kr^2(2\alpha + 2 - b) + \alpha(2\alpha + 2 - d - b)^2\}$$

at

$$\theta^* = 1 + \frac{\alpha}{Kr^2}(2 - d - b + 2\alpha).$$

The coefficient  $c$  can be made negative if its maximum value is negative, which is true provided that

$$\alpha < \frac{b}{2} - 1$$

and

$$Kr^2 > \frac{\alpha(d + b - 2 - 2\alpha)^2}{2(b - 2 - 2\alpha)} > 0.$$

With these choices we apply the maximum principle [18] to the equation  $A(w) = 0$  and find that  $w$  achieves a positive maximum only at initial time, i.e., in the region  $\{(0, x), |x| < r^2\}$ . Therefore we have

$$0 \leq w(t, x) \leq \|w(0, \cdot)\|_{L^\infty}.$$

Note that

$$w_0(x) = v_0(x)(r^2 - |x|^2)^\alpha = f_0(m)r^b(r^2 - |x|^2)^{\alpha - b/2}.$$

Assume that  $f_0(m) \neq 0$  for  $|m|^2 \leq b^* < b$ . Then

$$\|w_0\|_\infty \leq \|f_0\|_\infty r^b (r^2 - 2b^*)^{\alpha - b/2}.$$

Thus from

$$f(t, m) = v(t, x)(1 - |x|^2/r^2)^{b/2} = w(t, x)r^{-b}(r^2 - |x|^2)^{b/2 - \alpha}e^{Kt},$$

it follows that

$$|f(t, m)| \leq \|f_0\|_\infty \leq \left(\frac{r^2 - |x|^2}{r^2 - 2b^*}\right)^{b/2 - \alpha} e^{Kt}.$$

Replacing  $r^2 = 2b$  and  $|x|^2 = 2|m|^2$  we have obtained the desired estimate stated in Theorem 1.2. Therefore the trace of  $f$  on the sphere  $|m| = \sqrt{b}$  must be null.



**3.2. Coupled with flow  $\kappa \neq 0$ .** We now show the null trace when flow is involved. In this case (2.7) has the form  $L(v) = 0$  with

$$L(v) := (r^2 - |x|^2)\Delta_x v - (bx + (r^2 - |x|^2)\kappa x) \cdot \nabla_x v - (r^2 - |x|^2)\partial_t v + (bx^\top \kappa x)v.$$

We again apply the transformation

$$v(t, x) := w(t, x)(r^2 - |x|^2)^{-\alpha} e^{Kt},$$

with  $\alpha$  and  $K$  to be determined. This transformation applied to  $L(v)(r^2 - |x|^2)^{\alpha+1} e^{-Kt}$  leads to the following equation:

$$B(w) = 0,$$

with the operator  $B(w)$  being

$$B(w) = (r^2 - |x|^2)^2 \Delta_x w + (r^2 - |x|^2)[(4\alpha - b)x - (r^2 - |x|^2)\kappa x] \cdot \nabla_x w - (r^2 - |x|^2)^2 \partial_t w + c(x)w,$$

and the coefficient of the last term being

$$c(x) = -K(r^2 - |x|^2)^2 + 2\alpha[dr^2 + (2\alpha + 2 - d - b)|x|^2] + (b - 2\alpha)x^\top \kappa x(r^2 - |x|^2).$$

Using a similar argument as in the no-flow case, we proceed to determine  $\alpha$  and  $K$  so that  $c$  stays negative in  $\Omega(T)$ . Let  $\rho$  be the largest eigenvalues of the deformation tensor

$$S = (\kappa + \kappa^\top)/2;$$

one has

$$x^\top \kappa x \leq \rho|x|^2.$$

We first choose  $\alpha$  in such a way that  $\alpha < b/2 - 1$ , which implies  $h - 2\alpha > 0$ . Thus we obtain

$$\begin{aligned} c(x) &\leq \bar{c} = -K(r^2 - |x|^2)^2 + 2\alpha[dr^2 + (2\alpha + 2 - d - b)|x|^2] \\ &\quad + \rho(b - 2\alpha)|x|^2(r^2 - |x|^2) \\ &= -[K + \rho(b - 2\alpha)]|x|^4 + [2Kr^2 + \rho(h - 2\alpha)r^2 \\ &\quad + 2\alpha(2\alpha + 2 - d - b)]|x|^2 + 2\alpha dr^2 - Kr^4 \\ &\leq 2\alpha dr^2 - Kr^4 \\ &\quad + \frac{[2Kr^2 + \rho(b - 2\alpha)r^2 + 2\alpha(2\alpha + 2 - d - b)]^2}{4[K + \rho(h - 2\alpha)]} \\ &\leq 2\alpha r^2(2\alpha + 2 - b) + \frac{\beta^2}{4[K + \rho(b - 2\alpha)]}, \end{aligned}$$

where

$$\beta := \rho(b - 2\alpha)r^2 - 2\alpha(2\alpha + 2 - d - b).$$

Therefore we can choose  $K$  such that

$$K > \frac{\beta^2}{8\alpha r^2(b - 2 - 2\alpha)} - \rho(b - \alpha),$$

and the following is always true:

$$c(x) \leq \bar{c} < 0, \quad |x| \leq r^2.$$

We thus can apply the maximum principle [18] to the equation

$$B(w) = 0$$

and obtain that  $u$  achieves its positive maximum only at initial time, i.e., in the region  $\{(0, x), |x| < r^2\}$ . This will give the result that

$$0 \leq w(t, x) \leq \|w(0, \cdot)\|_{L^\infty}.$$

Converting back to  $f$  we prove the results stated in Theorem 1.2.

**4. Appendix.** In this appendix, we recall some basic facts concerning the Fichera function which we used in section 2. Consider the second order equation

$$L[u] := a^{jk} D_{jk}u + b^i D_i u + cu = f \text{ in } \Omega$$

with the condition

$$a^{ij}(x)\xi_i\xi_j \geq 0$$

for any  $\xi \in \mathbb{R}^d$  and  $x \in \Omega$ . This class of equations with noncharacteristic form includes equations of elliptic and parabolic types, first order equations, the equations of Brownian motion, and others. The first boundary value problem in its general form was set up by Fichera [8]. We assume that  $a^{ij} \in C^2(\Omega)$ ,  $b^i \in C^1(\Omega)$ , and  $c \in C^0(\Omega)$ . Let  $n$  denote the unit outward normal vector to  $\Gamma = \partial\Omega$  at  $x \in \Gamma$ . The Fichera function is defined as

$$\mathfrak{F} = (b^k - D_j a^{kj})n_k(x) : \Gamma \rightarrow \mathbb{R}.$$

Thus the boundary is classified into several parts based on the sign of Fichera function  $\mathfrak{F}$ :

$$\Gamma = \Gamma_e \cup \Gamma_h,$$

where  $\Gamma_e := \{x \in \Gamma, a^{ij}n_i n_j > 0\}$  is the noncharacteristic (positive characteristic) part, and  $\Gamma_h := \{x \in \Gamma, a^{ij}n_i n_j = 0\}$ , in which there are two subsets (irrelevant and relevant parts):

$$\Gamma_+ = \{x, \mathfrak{F}(x) \geq 0\}, \quad \Gamma_- = \{x, \mathfrak{F}(x) < 0\}.$$

The classical theory of Fichera [8] says that the Dirichlet boundary condition leads to a well-posed problem: find a function  $u$  in  $\Omega \cup \Gamma$  such that

$$(4.1) \quad L(u) = f \text{ in } \Omega, \quad u = g \text{ on } \Gamma_e \cup \Gamma_-.$$

In other words, no Dirichlet boundary data is necessarily imposed on  $\Gamma_-$ , where  $\mathfrak{F} \geq 0$ .

It was shown that the sign of the Fichera function at points on  $\Gamma_h$  does not change under smooth nondegenerate changes of independent variables in the equation. Consequently, we have the following theorem.

**THEOREM 4.1** (see [18]). *The subsets  $\Gamma_e, \Gamma_+, \Gamma_-$  of the boundary  $\Gamma$ , defined for the operator  $L$ , remain invariant under smooth nonsingular changes of independent variables in the equation.*

To define the weak solution for the underlying problem, we introduce an adjoint operator as

$$L^*[v] = -D_{ij}(a^{ij}v) - D_i(b^i v) + cv.$$

Then for  $v \in C^2(\bar{\Omega})$  and  $v = 0$  on  $\Gamma_e \cup \Gamma_-$  the weak formulation of the equation becomes

$$\int_{\Omega} uL^*[v]dx = \int_{\Omega} vL[u]dx.$$

*Weak solution in  $L^2(\Omega)$ .* A bounded measurable function  $u(x)$  will be called a weak solution of the above problem with  $u \in \{L^2(\Omega), u = 0, x \in \Gamma_e \cup \Gamma_-\}$  if

$$\int_{\Omega} uL^*[v]dx = (f, v)$$

for all  $v \in \{C^2(\bar{\Omega}), v = 0, x \in \Gamma_e \cup \Gamma_-\}$ , where  $(\cdot, \cdot)$  denotes the inner product in  $L^2$ . Weak solution in other spaces such as the  $L^p$  space or general Hilbert space can be defined; and solution smoothness can be further studied once existence of a weak solution is established. Existence results have been proven under various assumptions, e.g., the following theorem.

**THEOREM 4.2.** *Suppose the inequality*

$$\frac{1}{2}D_i b^i - \frac{1}{2}D_{ij} a^{ij} - c \geq c_0 > 0$$

*is satisfied in  $\bar{\Omega}$ , and let  $f \in L^2(\Omega)$ . Then there exists a function  $u \in L^2(\Omega)$  which is a weak solution of (4.1) in the sense stated above.*

**Acknowledgments.** We acknowledge discussion with and suggestions by Gary Lieberman. We also thank the referees for valuable suggestions and pointing out two relevant references [13, 15]. We also want to thank the IMA for the hospitality and support during our stay for the *Thematic Year on Mathematics of Materials and Macromolecules: Multiple Scales, Disorder, and Singularities*.

#### REFERENCES

- [1] M. BARDI AND S. BOTTACIN, *Characteristic and Irrelevant Boundary Points for Viscosity Solutions of Nonlinear Degenerate Elliptic Equations*, Preprint 25, Dip. di Matematica P. E. A, University di Padova, Padova, Italy, 1998.
- [2] J. W. BARRETT, C. SCHWAB, AND E. SULI, *Existence of global weak solutions for some polymeric flow models*, Math. Models Methods Appl. Sci., 15 (2005), pp. 939–983.
- [3] R. B. BIRD, C. F. CURTISS, R. C. ARMSTRONG, AND P. HASSAGER, *Dynamics of Polymeric Liquids, Volume 2: Kinetic Theory*, Wiley Interscience, New York, 1987.
- [4] R. B. BIRD, O. HASSAGER, R. C. ARMSTRONG, AND C. F. CURTISS, *Dynamics of Polymeric Fluids, 2, Kinetic Theory*, John Wiley and Sons, New York, 1977.
- [5] M. DOI AND S. F. EDWARDS, *The Theory of Polymer Dynamics*, Oxford University Press, Oxford, UK, 1986.

- [6] Q. DU, C. LIU, AND P. YU, *FENE dumbbell model and its several linear and nonlinear closure approximations*, Multiscale Model. Simul., 4 (2005), pp. 709–731.
- [7] W.-N. E, T. LI, AND P. ZHANG, *Well-posedness for the dumbbell model of polymeric fluids*, Comm. Math. Phys., 248 (2004), pp. 409–427.
- [8] G. FICHERA, *Sulle equazioni differenziali lineari ellittico-paraboliche del secondo ordine*, Atti Accad. Naz. Lincei. Mem. Cl. Sci. Fis. Mat. Nat. Sez. I (8), 5 (1956), pp. 1–30.
- [9] C. W. GARDINER, *Handbook of Stochastic Methods*, Springer, Berlin, 1997.
- [10] Y. GUO, *The Vlasov-Maxwell-Boltzmann system near Maxwellians*, Invent. Math., 153 (2003), pp. 593–630.
- [11] P. HALIN, G. LIELENS, R. KEUNINGS, AND V. LEGAT, *The Lagrangian particle method for macroscopic and micro-macro viscoelastic flow computations*, J. Non-Newtonian Fluid Mech., 79 (1998), pp. 387–403.
- [12] B. JOURDAIN, T. LILIÈVRE, AND C. LE BRIS, *Existence of solution for a micro-macro model of polymeric fluid: The FENE model*, J. Funct. Anal., 209 (2004), pp. 162–193.
- [13] B. JOURDAIN AND T. LILIÈVRE, *Mathematical analysis of a stochastic differential equation arising in the micro-macro modelling of polymeric fluids*, in Probabilistic Methods in Fluids, I. M. Davies, N. Jacob, A. Truman, O. Hassan, K. Morgan, and N. P. Weatherill, eds., World Scientific, River Edge, NJ, 2002, pp. 205–223.
- [14] R. G. LARSON, *The Structure and Rheology of Complex Fluids*, Oxford University Press, New York, 1995.
- [15] C. LE BRIS, B. JOURDAIN, T. LILIÈVRE, AND F. OTTO, *Long-time asymptotic of a multi-scale model for polymeric fluid flows*, Arch. Ration. Mech. Anal., 181 (2006), pp. 97–148.
- [16] C. LE BRIS AND P. L. LIONS, *Renormalized solutions of some transport equations with partially  $W^{1,1}$  velocities and applications*, Ann. Mat. Pura Appl. (4), 183 (2004), pp. 97–130.
- [17] F. H. LIN, C. LIU, AND P. ZHANG, *On a micro-macro model for polymeric fluids near equilibrium*, Comm. Pure Appl. Math., 60 (2006), pp. 838–866.
- [18] O. A. OLEINIK AND E. V. RADKEVIĆ, *Second Order Equations with Nonnegative Characteristic Form*, AMS, Providence, RI, and Plenum Press, New York, 1973.
- [19] F. OTTO AND C. VILLANI, *Generalization of an inequality by Talagrand and links with the logarithmic Sobolev inequality*, J. Funct. Anal., 173 (2000), pp. 361–400.
- [20] D. STROOK AND S. R. S. VARADHAN, *On degenerate elliptic-parabolic operators of second order and their associated diffusions*, Comm. Pure Appl. Math., 25 (1972), pp. 651–713.
- [21] K. TAIRA, *Diffusion Processes and Partial Differential Equations*, Academic Press, Boston, 1988.
- [22] P. YU, Q. DU, AND C. LIU, *From micro to macro dynamics via a new closure approximation to the FENE model of polymeric fluids*, Multiscale Model. Simul., 3 (2005), pp. 895–917.
- [23] H. ZHANG AND P. ZHANG, *Local existence for the FENE-dumbbell model of polymeric fluids*, Arch. Ration. Mech. Anal., 181 (2006), pp. 373–400.