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A MAXIMUM ENTROPY PRINCIPLE BASED CLOSURE METHOD FOR MACRO-MICRO MODELS OF POLYMERIC MATERIALS

Yunkyong Hyon

Department of Mathematics, Pennsylvania State University
University Park, PA 16802, USA

Jose A. Carrillo

ICREA and Departament de Matemàtiques, Universitat Autònoma de Barcelona
E-08193 Bellaterra, Spain

Qiang Du

Department of Mathematics, Pennsylvania State University
University Park, PA 16802, USA

Chun Liu

Department of Mathematics, Pennsylvania State University
University Park, PA 16802, USA

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Abstract. We consider the finite extensible nonlinear elasticity (FENE) dumbbell model in viscoelastic polymeric fluids. We employ the maximum entropy principle for FENE model to obtain the solution which maximizes the entropy of FENE model in stationary situations. Then we approximate the maximum entropy solution using the second order terms in microscopic configuration field to get an probability density function (PDF). The approximated PDF gives a solution to avoid the difficulties caused by the nonlinearity of FENE model. We perform the moment-closure approximation procedure with the PDF approximated from the maximum entropy solution, and compute the induced macroscopic stresses. We also show that the moment-closure system satisfies the energy dissipation law. Finally, we show some numerical simulations to verify the PDF and moment-closure system.

1. **Introduction.** The viscoelastic flow of rheological complex fluids is described as a multiscale-multiphysics model, called macro-micro model through the coupled continuum mechanics and kinetic theory for macroscopic and microscopic level, respectively. These coupled multiscale systems for the viscoelastic flow give various explanations for the corresponding complicated but important physical phenomena of polymeric fluids (multiscale-multiphysics). For instance, a typical interaction between different scales in rheological complex fluids is that the deformation of

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macroscopic flow will affect the structure of microscopic level through the kinematic transport, and the averaged nonlinear behaviors of molecules will affect the macroscopic level through the induced elastic stress. The induced macroscopic stress is described by the average of probability function (PDF) for the molecular configurations. The PDF is a solution to the Fokker-Planck equation at microscopic level.

To specify molecular behaviors in microscopic configuration field some physical models are designed. There are two well-known molecular models. One is the Hookean dumbbell model which is related to the Oldroyd-B model, and the other is the finite-extensible-nonlinear-elastic (FENE) spring dumbbell model [1, 2]. In this paper we consider the FENE dumbbell model. The FENE model has crucial role in describing complicated and more realistic physical phenomena of molecular behaviors, and is reformed to an enhanced model or system, for instance, FENE-P [10], FENE-L [13, 14, 17], FENE-S [19, 20], FENE-D [6], FENE-QE, FENE-QE-PLA [18].

From the modeling point of view, FENE-S [19, 20] is an approximation of the near equilibrium situation. Its numerical results show an excellent agreement for certain flow rates, and the inheritance of the energy law for the original coupled system. In [6], we introduced FENE-D system whose PDF has an additional variable related to the peak positions of PDF in certain large flow rate. This position variable is designed to catch the behavior of two peaks of FENE model in large flow rates and to complement the lack of the stretching effect of FENE-S. FENE-D also has an excellent agreement to the peak solution of PDF in large flow rate, especially, for extensional flow, and also inherits the energy law. The actual energy of FENE-D preserves the leading order term of the energy for the original system.

In this paper, we employ the maximum entropy principle (MEP) [3, 7, 11, 12, 15] for FENE model, and we also concentrate upon the near equilibrium situation. The MEP for FENE model leads to a maximizing problem subject to the constraints given by fixing certain moments of the PDF. As usual, Lagrange multipliers are employed for the constraints. This MEP approach for the FENE model was introduced by Han Wang et. al., in [18]. They used a piecewise linear approximation (PLA) technique to find the Lagrange multiplier and solve a nonlinear system with PLA. But in this paper, we first approximate a PDF from the maximum entropy solution and then we derive a moment-closure system with the approximated PDF. In this macroscopic moment-closure approximation, one important thing is that the moment-closure system satisfies an energy law analogous to the energy law of the original system. In the derivation of the energy law we shall use the approach in [4, 8, 9] using the whole entropy.

An outline of this paper is as follows. In section 2, we recall the FENE macro-micro model and some related results. The MEP for FENE model is presented in section 3 to obtain the maximum entropy solution and an approximated PDF. In section 4, we also derive the moment-closure system with the PDF and derive the corresponding energy law. We present various numerical experiments to verify the closure system in the configuration fields for several cases in section 6. Final remarks are given in section 7.

2. **The Macro-Micro models for viscoelastic fluids.** Let $\vec{Q}$ be the microscopic configuration field and $\Psi(Q)$ be a spring potential, which only depends on $Q = |\vec{Q}|$. $f(\vec{Q}, t)$ is the PDF of the configuration field $\vec{Q}$ and time t. The micro-force balance

law with the spring potential gives the following equation:

$$m\vec{Q}_{tt} + \frac{1}{\eta}\vec{Q}_t = -\nabla_{\vec{Q}}\Psi, \tag{1}$$

where $\vec{Q}_t$ is a damping and η is a damping coefficient. m is the mass of the molecule. If we consider the separation of scale in time, that is, the time-scale of small molecular behavior is much smaller than that in macroscopic level, then the damping term will be dominant in the relevant dynamics. In other words, we can neglect the inertial term and results in a gradient flow $\frac{1}{\eta}\vec{Q}_t = -\nabla_{\vec{Q}}\Psi$. Moreover, if we take into account the thermo-fluctuation, an infinitesimal quasi-static Brownian motion effect, σdB, where σ is a ratio coefficient [5], and the deformation of configuration field $\vec{Q}$ in the macroscopic flow field with Cauchy-Born type of kinematic assumption, we can obtain the following Fokker-Planck equation for $f(\vec{Q}, t)$.

$$f_t + \nabla \cdot (-\eta\nabla_{\vec{Q}}\Psi f) = \frac{\sigma^2}{2}\Delta_{\vec{Q}} f. \tag{2}$$

This equation (2) is only about microscopic behavior, there is no communication between microscopic and macroscopic effects. The connection between these two different levels is made via the deformation of configuration field $\vec{Q}$ in the flow field which is made with the use of Cauchy-Born type of kinematic assumption that passes information from macroscopic scale to microscopic scale. For the macro-micro models we have the following hydrodynamic system coupled with a incompressible momentum equations for macroscopic flow field $\vec{u} = \vec{u}(x, t)$ and the Fokker-Planck equation for microscopic molecular PDF, $f = f(\vec{x}, \vec{Q}, t)$, with molecular configuration field $\vec{Q}$ under the assumption of suitable initial and boundary conditions [1, 2, 16]:

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\vec{u} + \nabla P = \nabla\cdot\tau_p + \nu\Delta\vec{u}, \tag{3}$$

$$\nabla\cdot\vec{u} = 0, \tag{4}$$

$$\frac{\partial f}{\partial t} + (\vec{u}\cdot\nabla)f + \nabla_{\vec{Q}}\cdot(\nabla\vec{u}\vec{Q}f) = \frac{2}{\zeta}\nabla_{\vec{Q}}\cdot(\nabla_{\vec{Q}}\Psi f) + \frac{2kT}{\zeta}\Delta_{\vec{Q}} f \tag{5}$$

where τ_p is the induced stress from the microscopic configurations representing the polymer contribution to stress,

$$\tau_p = \lambda\int(\nabla_{\vec{Q}}\Psi\otimes\vec{Q})f(\vec{x}, \vec{Q}, t)d\vec{Q}, \tag{6}$$

P is the hydrostatic pressure, ν is the fluid viscosity, ζ is the elastic relaxation time of the spring, $\Psi(Q)$ is the potential of molecular, and λ is the polymer density constant. One can easily find the derivation of Fokker-Planck equation (5) in [19, 20].

In microscopic fields, the molecular is modeled by the FENE dumbbell whose beads are connected with FENE spring. The FENE spring potential is given by

$$\Psi(Q) = -\frac{HQ_0^2}{2}\ln\left(1 - \frac{Q^2}{Q_0^2}\right) \tag{7}$$

where Q_0 is the maximum dumbbell extension and H is the spring constant, and then the FENE spring force is given by

$$\nabla_{\vec{Q}}\Psi = \frac{H\vec{Q}}{1 - (Q/Q_0)^2}. \tag{8}$$

The main difficulty is caused by the nonlinearity of the FENE model in using the FENE spring potential. There is no exact equation for τ_p with FENE model because of this nonlinearity. To avoid these difficulties we apply a moment-closure approximation procedure with an approximated PDF obtained from the maximum entropy solution, see the next section. This approximation procedure also gives us the derivation of energy law without any approximation of FENE spring force.

Here, for the derivation of an approximation of the maximum entropy solution, we note the PDF ansatz, introduced in [19, 20], coming from the equilibrium solution of Fokker-Planck equation (5) without flow fields given by

$$f_{\tilde{b}} = \frac{1}{J_{\tilde{b}}}\left[1 - \frac{Q^2}{Q_0^2}\right]^{\tilde{b}/2}\left\{1 + \tilde{\beta}Q_1Q_2 + \tilde{\gamma}(Q_1^2 - Q_2^2)\right\} \tag{9}$$

where $J_{\tilde{b}}$ is the normalizing factor of PDF $f_{\tilde{b}}$ and $\tilde{b}$, $\tilde{\beta}$, $\tilde{\gamma}$ are unknowns . One can also find an enhanced PDF ansatz to catch the behavior of two peaks of FENE model in large flow rate [6].

In the next section we describe the derivation of the maximum entropy solution using the maximum entropy principle for FENE model and the approximation of the maximum entropy solution.

3. **The maximum entropy principle for FENE model.** In [6, 19, 20] the PDF ansatz for a macroscopic closure approximation for FENE model is based on the equilibrium solution for the Fokker-Planck equation without flow field. But in this paper we employ the MEP for a new PDF which maximizes the entropy for FENE model subjected to the moments.

First of all, let M_a be the moments on molecular configuration fields, which are defined by

$$M_a = \int w_a f \, d\vec{Q} \tag{10}$$

where w_a are moments of the distribution function denoted by: 1, Q_1, Q_2, Q_1Q_2, Q_1^2, Q_2^2, $\cdots$. The free energy with entropic term, denoted by s, for the FENE model in stationary situation is given by

$$s = -\int (kTf\ln f + \Psi f)\, d\vec{Q} \tag{11}$$

where Ψ is the FENE spring potential.

Next we consider a maximizing entropy problem under the constrains (10) with (11). A well-known method for this maximizing problem is to introduce the Lagrange multipliers. We denote the Lagrange multipliers with $kT\lambda_a$ for each moment M_a (10). Thus, the corresponding maximizing entropy problem is given as follows: maximize the function $S(f)$ which is defined by

$$S(f) = -kT\sum_a \lambda_a M_a - s = \int\left(-kT\sum_a \lambda_a w_a f + kTf\ln f + \Psi f\right) d\vec{Q}.$$

To solve this problem, we compute the derivative of S, and then the variational approach leads to $\delta S' = 0$, that is,

$$\left\{-kT\sum_a \lambda_a w_a + kT(1 + \ln f) + \Psi\right\}\delta f = 0. \tag{12}$$

From (12) we easily obtain the following PDF, denoted by f_M, which maximizes S.

$$f_M = Ce^{-\Psi/kT} e^{\sum_a \lambda_a w_a} \tag{13}$$

where $C > 0$ is a normalizing constant.

Remark 1. We observe that the PDF (13) is the equilibrium solution to the Fokker-Planck equation without flow fields when the Lagrange multipliers, λ_as are zero, and f_M preserves the positivity of PDF.

Using the FENE spring potential Ψ (7), the explicit form of PDF (13) is given by

$$f_M(\vec{Q}) = C \left[1 - \frac{Q^2}{Q_0^2}\right]^{HQ_0^2/(2kT)} e^{\sum_a \lambda_a w_a}. \tag{14}$$

The next step is to find the unknowns, λ_a's which remains a formidable task. Due to the nonlinearity of (14), it is impossible to compute λ_a's, analytically. Thus, we need approximation techniques to resolve this issue. A numerical technique based on a piecewise linear approximation (PLA) upon the symmetrization of the domain in (14) is introduced by Han Wang et al. [18]. Other numerical approximation techniques may also be developed solve the nonlinear system for λ_a's in (14). In our study, we employ an approximation of the exponential terms which utilizes the special features of PDE to avoid the difficulty in computing λ_a's. This leads nicely to a moment-closure approximation procedure which is, to a large extent, similar to an earlier ansatz expansion considered in [19].

We consider the following second order expansions of the exponential terms involving the moments in PDF (14):

$$f_M(\vec{Q}) \approx C \left[1 - \frac{Q^2}{Q_0^2}\right]^{HQ_0^2/(2kT)} (1 + \lambda_1 Q_1^2)(1 + \lambda_2 Q_2^2)(1 + \lambda_3 Q_1 Q_2). \tag{15}$$

In this approximation, we see that the first order terms disappear which coincides with the symmetry of the function and its domain. Although the approximation contains only three unknown parameters, the product has both the fourth and the sixth order moments. Thus, to get an explicit form of stress tensor in the numerical simulations, we simplify the PDF in (15) by taking into consideration the fact that the second order moments are crucial factors in the description of the energy and induced stress tensor for FENE model in [6, 19, 20] and the computation for high order moments can be connected to the second order moments.

Hence, we arrive at the following equation consisting of only the second order terms, Q^2, Q_1Q_2, $Q_1^1 - Q_2^2$:

$$f = \frac{1}{J} \left[1 - \frac{Q^2}{Q_0^2}\right]^{b/2} \left\{1 + \eta Q^2 + \beta Q_1 Q_2 + \gamma(Q_1^2 - Q_2^2)\right\} \tag{16}$$

with unknown variables, β, γ, η, which are related to λ_1, λ_2, λ_3, where J is the normalizing factor for PDF, and $b = HQ_0^2/(kT)$.

As in [19], the second order moments can be explicitly computed from the above PDF (16). Let $M_1 =< Q^2 >$, $M_2 =< Q_1^2 - Q_2^2 >$, $M_3 =< Q_1Q_2 >$ be the second order moments with the notation $<\cdot>$ denoting $\int \cdot f \, d\vec{Q}$, we have

$$M_1 = < Q^2 >= \frac{2Q_0^2}{2\eta Q_0^2 + b + 4}\left(1 + \frac{4\eta Q_0^2}{b+6}\right), \quad (17)$$

$$M_2 = < Q_1^2 - Q_2^2 >= \frac{4\gamma Q_0^4}{(2\eta Q_0^2 + b + 4)(b+6)}, \quad (18)$$

$$M_3 = < Q_1 Q_2 >= \frac{\beta Q_0^4}{(2\eta Q_0^2 + b + 4)(b+6)}, \quad (19)$$

and the scaling factor J is

$$J = \frac{2\pi Q_0^2}{b+2}\left(1 + \frac{2\eta Q_0^2}{b+4}\right). \quad (20)$$

Meanwhile, β, γ, η can also be easily computed from M_1, M_2, M_3 as follows:

$$\eta = \frac{2Q_0^2 - (b+4)M_1}{2Q_0^2 M_1 - 8Q_0^4/(b+6)}, \quad (21)$$

$$\gamma = \frac{(2\eta Q_0^2 + b + 4)(b+6)M_2}{4Q_0^4}, \quad (22)$$

$$\beta = \frac{(2\eta Q_0^2 + b + 4)(b+6)M_3}{Q_0^4}. \quad (23)$$

In another word, the PDF (16) is easily recovered by the second order moments.

Direct computation shows that all moments of the PDF (16) of order higher than two can be expressed in terms of the second order moments. This is a consequence of the fact that all moments of the PDF (16) can be expressed in terms of the variables β, γ, η, computed from the second order moments in (17)–(19).

Remark 2. We see that the PDF (16) is a consequence of the maximum entropy solution (14). The form of PDF (16) is similar to the PDF ansatz (9) obtained from the equilibrium solution of Fokker-Planck equation without the flow field and it is similar to the ansatz considered in [19]. In addition, the PDF (9) can be recovered from (16) by setting $\eta = 0$, $b = \tilde{b}$, $\beta = \tilde{\beta}$, $\gamma = \tilde{\gamma}$. In other words, the PDF (9) is among those PDFs which satisfy the constraints of the maximum entropy problem.

4. Moment-closure system for FENE model.

In this section, we derive the moment-closure system from the Fokker-Planck equation (5), and establish the corresponding energy law.

To obtain the moment-closure system we multiply Q^2, $Q_1^2 - Q_2^2$, Q_1Q_2 to the Fokker-Planck equation (5) and integrate by parts. Then we have the following equations for the second order moments:

$$\frac{\partial}{\partial t} < Q^2 > + \vec{u}\cdot\nabla < Q^2 > -2\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) < Q_1 Q_2 > \quad (24)$$
$$- \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) < Q_1^2 - Q_2^2 >= \frac{8kT}{\zeta} - \frac{2}{\zeta}\int (\nabla_{\vec{Q}}\Psi \cdot \nabla_{\vec{Q}} Q^2) f \, d\vec{Q},$$

$$\frac{\partial}{\partial t} < Q_1^2 - Q_2^2 > + \vec{u}\cdot\nabla < Q_1^2 - Q_2^2 > -2\left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}\right) < Q_1 Q_2 > \quad (25)$$
$$- \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) < Q^2 >= -\frac{2}{\zeta}\int (\nabla_{\vec{Q}}\Psi \cdot \nabla_{\vec{Q}} (Q_1^2 - Q_2^2)) f \, d\vec{Q},$$

$$\frac{\partial}{\partial t} < Q_1Q_2 > + \vec{u}\cdot\nabla < Q_1Q_2 > - \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) < Q^2 > \tag{26}$$
$$+ \frac{1}{2}\left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}\right) < Q_1^2 - Q_2^2 > = -\frac{2}{\zeta}\int (\nabla_{\vec{Q}}\Psi \cdot \nabla_{\vec{Q}}(Q_1Q_2)) f \, d\vec{Q}.$$

As mentioned before, the nonlinearity of FENE spring potential presents a difficulty in obtaining the exact equation for the induced stress, τ_p, from the Fokker-Planck equation (5). Also, in above equations (24)–(26) the integration terms including the spring force $\nabla_{\vec{Q}}\Psi$ need to be evaluated either analytically or numerically. But the approximation procedure provides an explicit form of moment equations (24)–(26) without the integration terms, and the inheritance of the original energy law without any approximation of the FENE spring force, $\nabla_{\vec{Q}}\Psi$.

First, we shall give an explicit form of the induced stress τ_p. By (6) and (7), the polymeric contribution to the stress takes on the form:

$$\tau_p = \begin{pmatrix} \tau_p^{11} & \tau_p^{12} \\ \tau_p^{21} & \tau_p^{22} \end{pmatrix} = \lambda H \int \frac{\vec{Q}\otimes\vec{Q}}{\left(1 - \frac{Q^2}{Q_0^2}\right)} f \, d\vec{Q}.$$

Then, taking the PDF in (16). the induced stress τ_p is given by

$$\tau_p = \lambda H \left(\frac{b+6}{b}\right)\left\{\begin{pmatrix} \frac{1}{2}M_2 & M_3 \\ M_3 & -\frac{1}{2}M_2 \end{pmatrix} + \frac{(b+4+4\eta Q_0^2)}{(b+6+4\eta Q_0^2)}\frac{M_1}{2} I\right\}. \tag{27}$$

In equation (27), we can separate the second term, a scalar multiple of the identity matrix, from the induced stress tensor τ_p, and absorb it into the pressure by defining

$$P' = P - \frac{\lambda H}{2}\left(\frac{(b+6)}{b}\frac{(b+4+4\eta Q_0^2)}{(b+6+4\eta Q_0^2)} M_1\right).$$

Then the new (trace free) stress τ_p becomes

$$\tau_p = \lambda H \left(\frac{b+6}{b}\right)\begin{pmatrix} \frac{1}{2}M_2 & M_3 \\ M_3 & -\frac{1}{2}M_2 \end{pmatrix}. \tag{28}$$

Here we also provide the explicit form of the integral terms in (24)–(26) as follows:

$$\int (\nabla_{\vec{Q}}\Psi \cdot Q^2) f \, d\vec{Q} = \frac{2H(b+6)}{b}\frac{(b+4+4\eta Q_0^2)}{(b+6+4\eta Q_0^2)} M_1, \tag{29}$$

$$\int (\nabla_{\vec{Q}}\Psi \cdot \nabla_{\vec{Q}}(Q_1^2 - Q_2^2) f \, d\vec{Q} = \frac{2H(b+6)}{b} M_2, \tag{30}$$

$$\int (\nabla_{\vec{Q}}\Psi \cdot \nabla_{\vec{Q}}(Q_1Q_2) f \, d\vec{Q} = \frac{2H(b+6)}{b} M_3. \tag{31}$$

Thus, we obtain the following moment-closure system for the original multiscale system (3)–(5) :

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u}\cdot\nabla)\vec{u} + \nabla P = \lambda \nabla\cdot\tau_p + \nu\triangle\vec{u}, \tag{32}$$

$$\nabla\cdot\vec{u} = 0, \tag{33}$$

$$\frac{\partial}{\partial t}M_1 + \vec{u}\cdot\nabla M_1 - 2\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)M_3 - \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right)M_2 \tag{34}$$

$$= \frac{8kT}{\zeta} - \frac{4H}{\zeta}\left[\frac{(b+6)}{b}\frac{(b+4+4\eta Q_0^2)}{(b+6+4\eta Q_0^2)}\right]M_1,$$

$$\frac{\partial}{\partial t}M_2 + \vec{u}\cdot\nabla M_2 - 2\left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}\right)M_3 - \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right)M_1 \tag{35}$$

$$= -\frac{4H}{\zeta}\left(\frac{b+6}{b}\right)M_2,$$

$$\frac{\partial}{\partial t}M_3 + \vec{u}\cdot\nabla M_3 - \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)M_1 + \frac{1}{2}\left(\frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}\right)M_2 \tag{36}$$

$$= -\frac{4H}{\zeta}\left(\frac{b+6}{b}\right)M_3.$$

5. **The energy law for the closure model.** We now derive the energy law corresponding to the above moment-closure system, which shows that the (24)–(26) preserves the overall energy law. To see this we recall that the original multiscale system (3)–(5) has the following energy estimate under the boundary condition $\vec{u} = 0$ on the boundary of macroscopic domain:

$$\begin{aligned}&\frac{d}{dt}\int\left\{\frac{1}{2}|\vec{u}|^2 + \lambda\int(kTf\ln f + \Psi f)\,d\vec{Q}\right\}dx\\ &\quad= -\int\left(\nu|\nabla\vec{u}|^2 + \frac{2\lambda}{\zeta}\int f|\nabla_{\vec{Q}}(kT\ln f + \Psi)|^2\,d\vec{Q}\right)dx.\end{aligned} \tag{37}$$

Since the equilibrium distribution, f_∞, for the Fokker-Planck equation (5) is given by

$$f_\infty = \frac{e^{-\Psi/kT}}{\int e^{-\Psi/kT}\,d\vec{Q}}, \tag{38}$$

we have

$$\begin{aligned}&\frac{d}{dt}\int\left\{\frac{1}{2}|\vec{u}|^2 + \lambda\int kTf\ln\left(\frac{f}{f_\infty}\right)d\vec{Q}\right\}dx\\ &\quad= -\int\left(\nu|\nabla\vec{u}|^2 + \frac{2\lambda}{\zeta}\int f\left|kT\nabla_{\vec{Q}}\ln\left(\frac{f}{f_\infty}\right)\right|^2 d\vec{Q}\right)dx.\end{aligned} \tag{39}$$

Assuming the Hookean dumbbell approximation for the spring potential, $\Psi(\vec{Q}) = |\vec{Q}|^2/2$, then then the PDF is Gaussian distributed and the integral terms related to the free energy in the above energy law (39) are expressed in explicit form. Those are given as follows:

$$\int f \ln\left(\frac{f}{f_\infty}\right) d\vec{Q} \quad = \quad \frac{1}{2}\left(-\ln(\det A) - d + \mathrm{tr}(A)\right), \tag{40}$$

$$\int f \left|\nabla_{\vec{Q}} \ln\left(\frac{f}{f_\infty}\right)\right|^2 d\vec{Q} \quad = \quad \mathrm{tr}((I - A^{-1})^2) \tag{41}$$

where $\mathrm{tr}(A)$ is the trace of tensor A [4, 8, 9] and I is the identity matrix. This bring a way to derive an energy law for the closure system (32)- (36).

Here we define a tensor $A =< \vec{Q} \otimes \vec{Q} >$ to obtain the energy law

$$A \quad = \quad \begin{pmatrix} < Q_1^2 > & < Q_1Q_2 > \\ < Q_1Q_2 > & < Q_2^2 > \end{pmatrix} = \begin{pmatrix} \frac{M_2}{2} & M_3 \\ M_3 & -\frac{M_2}{2} \end{pmatrix} + \frac{M_1}{2} I. \tag{42}$$

Then one can easily show that the tensor A satisfies the following equation obtained by a modification of (5) with $\vec{Q} \otimes \vec{Q}$.

$$\frac{\partial}{\partial t} A + \vec{u} \cdot \nabla A = \nabla \vec{u} A + A \nabla^T \vec{u} - \frac{4H}{\zeta}\left(\frac{b+6}{b}\right) A + \frac{2HM_1}{\zeta}\frac{(b+6)}{b} G(M_1) I + \frac{4kT}{\zeta} I. \tag{43}$$

where $G(M_1) = 1 - \dfrac{(b + 4 + 4\eta Q_0^2)}{(b + 6 + 4\eta Q_0^2)}$ (η is a function of M_1). Also, one can show that the tensor A satisfying the equation (43) is symmetric positive matrix in certain condition. The symmetric positivity of the tensor A plays a crucial role for derivation of energy law.

By taking the trace of the above equation, we get

$$\frac{\partial}{\partial t}\mathrm{tr}(A) = 2\nabla \vec{u} : A - \frac{4H}{\zeta}\left(\frac{b+6}{b}\right)\mathrm{tr}(A) + \frac{2HM_1}{\zeta}\frac{(b+6)}{b} G(M_1) d + \frac{4kT}{\zeta} d, \tag{44}$$

where d is dimension of space ($d = 2$ for the case considered in this work). Also, we can obtain the following equation from (43):

$$-\frac{\partial}{\partial t}\ln(\det A) = \frac{4H}{\zeta}\left(\frac{b+6}{b}\right) d - \frac{2HM_1}{\zeta}\frac{(b+6)}{b} G(M_1)\mathrm{tr}(A^{-1}) - \frac{4kT}{\zeta}\mathrm{tr}(A^{-1}). \tag{45}$$

Now we consider the following free energy equation:

$$S_E(t) = \frac{H}{2}\left(\frac{b+6}{b}\right)\mathrm{tr}(A) - \frac{kT}{2}\ln(\det A). \tag{46}$$

With help of the identity for the tensor A,

$$\mathrm{tr}((I - A^{-1})^2 A) = \mathrm{tr}(A) - 2d + \mathrm{tr}(A^{-1}),$$

we have the following energy equation:

$$\begin{aligned} &\frac{d}{dt}\int \left[\frac{1}{2}|\vec{u}|^2 + \lambda\left\{\left(\frac{H}{2}\left(\frac{b+6}{b}\right)\mathrm{tr}(A) - \frac{kT}{2}\ln(\det A)\right)\right\}\right] dx \\ = \quad & -\int \Bigg[\mu|\nabla \vec{u}|^2 + \lambda\Bigg\{\frac{kTHM_1}{\zeta}\left(\frac{b+6}{b}\right) G(M_1)\mathrm{tr}(A^{-1}) + \frac{2k^2T^2}{\zeta}\mathrm{tr}(A^{-1}) \\ & + \frac{2H^2}{\zeta}\left(\frac{b+6}{b}\right)^2 \left[(1-\tilde{G})\mathrm{tr}(A) + \frac{\tilde{G}}{2}\left\{\mathrm{tr}((I - A^{-1})^2 A - \mathrm{tr}(A^{-1}))\right\}\right]\Bigg\} \end{aligned} \tag{47}$$

where $\tilde{G} = G(M_1)\dfrac{M_1}{2} + \dfrac{2kT}{H}\left(\dfrac{b}{b+6}\right)$.

We consider the following inequality in [4] to obtain the positivity of the free energy part, $S_E(t)$, in the left hand side of the above energy law (47):

$$-\ln(\det(A)) - Q_0^2 \ln\left(1 - \frac{\mathrm{tr}(A)}{Q_0^2}\right) \geq d \tag{48}$$

for symmetric positive tensor A. Using the above equation we have

$$S_E(t) = \frac{H}{2}\left(\frac{b+6}{b}\right)\mathrm{tr}(A) - \frac{kT}{2}\ln(\det A) \tag{49}$$

$$\geq \frac{H}{2}\left(\frac{b+6}{b}\right)\mathrm{tr}(A) + \frac{kT}{2}Q_0^2 \ln\left(1 - \frac{\mathrm{tr}(A)}{Q_0^2}\right). \tag{50}$$

Then the positivity of S_E for the energy law is easily obtained by the positivity of the last equation (50) on $0 < M_1 < Q_0^2\left(1 - \frac{kTb}{H(b+6)}\right)$.

Also, we see that the positivity of the coefficient of $\mathrm{tr}(A)$ for the energy equation. Under the condition that $H \gg 1$, i.e., $b \gg 1$, we easily see that $\tilde{G} < 1$. The positivity of $\mathrm{tr}(A^{-1})$ and $\mathrm{tr}((I - A^{-1})^2 A)$ are almost trivial for symmetric positive definite matrix A. Thus, we have the energy law under the condition that $H \gg 1$, or $b \gg 1$.

6. **Numerical results.** In this section we simulate various numerical experiments to validate/verify the closure approximation based on the maximum entropy principle for the FENE model. In the numerical simulations, we consider a standard scaling and the homogeneity in the configuration field which is independent to the microscopic spatial variables. The resulting Fokker-Planck equation from (5) is derived as follows:

$$\frac{\partial f}{\partial t} + \nabla_{\vec{Q}} \cdot (\kappa \vec{Q} f) = \frac{1}{2}\left(\nabla_{\vec{Q}} \cdot (\nabla_{\vec{Q}} \Psi f) + \Delta_{\vec{Q}} f\right), \tag{51}$$

in the open domain $\Omega = \{\vec{Q} \in \mathbb{R}^2 \mid |\vec{Q}| < Q_0,\ Q_0 = \sqrt{50}\}$.

Since the Fokker-Planck equation has the analytic solution with only symmetric velocity gradients we compare the numerical results, which is obtained by the Runge-Kutta method, with those from the direct computation of the Chapman-Kolmogorov simulation for the Fokker-Planck equation. The numerical results of this direct computation are denoted by FENE.

The corresponding moment-closure system to the scaled Fokker-Planck equation (51) is given as follows:

$$\frac{\partial M_1}{\partial t} - 2(\kappa_{12} + \kappa_{21})M_3 - (\kappa_{11} - \kappa_{22})M_2 = 2 - \left[\frac{(b+6)}{b}\frac{(b+4+4\eta Q_0^2)}{(b+6+4\eta Q_0^2)}\right] M_1, \tag{52}$$

$$\frac{\partial M_2}{\partial t} - 2(\kappa_{12} - \kappa_{21})M_3 - (\kappa_{11} - \kappa_{22})M_1 = -\left(\frac{b+6}{b}\right) M_2, \tag{53}$$

$$\frac{\partial M_3}{\partial t} - \frac{1}{2}(\kappa_{12} + \kappa_{21})M_1 + \frac{1}{2}(\kappa_{12} - \kappa_{21})M_2 = -\left(\frac{b+6}{b}\right) M_3. \tag{54}$$

In numerical simulations, η in (52) is replaced by (21).

We provide the numerical simulations for shear flows using the PDF (16) obtained by the maximum entropy principle. We denote the moment-closure system (24)–(26) with the PDF (16) as FENE-M. In these simulations, the integration terms in moment-closure system (24)–(26) are evaluated by numerical integration.

In Figure 1 we first present the contour plots of the PDF obtained by FENE-S [19] in the first row, FENE-D [6] in the second row, FENE-M (24)–(26) in the last

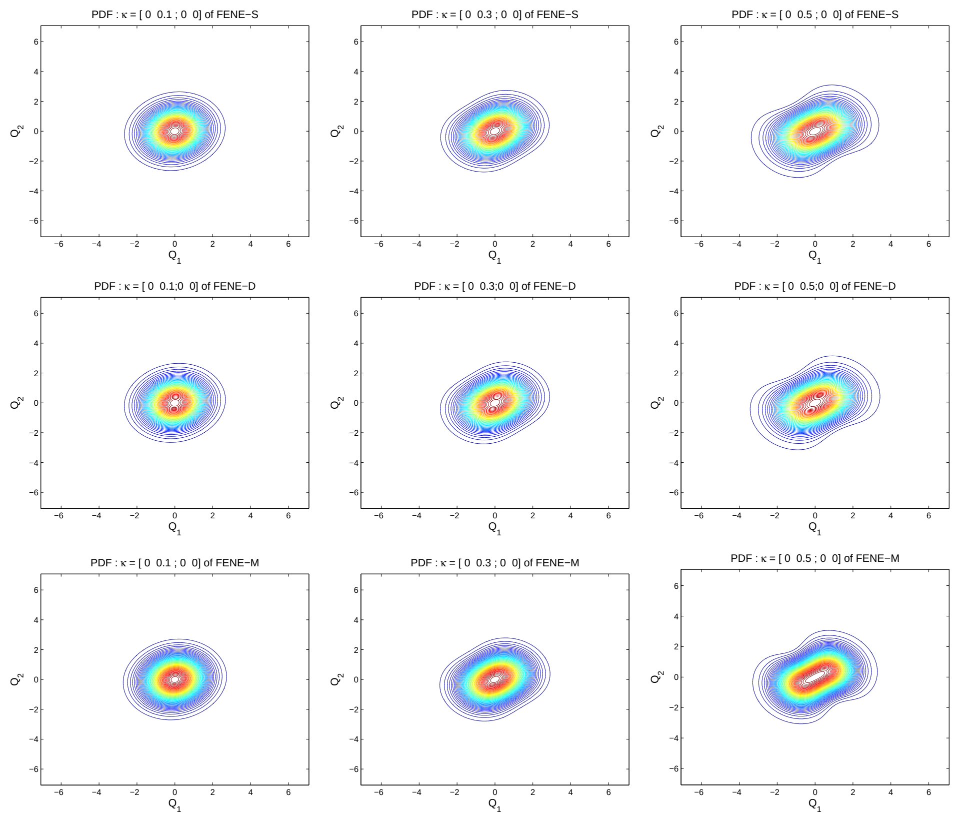

FIGURE 1. Comparison of the contour plots of the probability distribution functions solved from the FENE-S (first row), the FENE-D (second row), and the FENE-M (the last row) with $r = 0.1$, 0.3, 0.5, column-wise.

row with $\kappa_{11} = \kappa_{21} = \kappa_{22} = 0$, $\kappa_{12} = 0.1, 0.3, 0.5$ in the configuration field. FENE-S in the first row has an excellent agreement to the macroscopic stresses, normal and shear stresses for certain flow rates as it is shown in [19, 20]. We can see that FENE-D, the second row in Figure 1 shows almost identical to FENE-S for simple shear flow rates because the PDF of FENE-D is almost same as that of FENE-S for the certain simple shear flow rates [6].

Another observation in these results is the fact that FENE-M has a little bit more stretching effect around origin than that of the others. Since the stretching behavior of molecules distributes to the normal stress in macroscopic variables, we expect that the stretching effect of FENE-M around the origin makes the normal stress larger than that of FENE-S.

Next, we consider normal and shear stresses, which are the difference of the diagonal entries and the off-diagonal entry of the induced stress tensor, τ_p, respectively, in shear flows with $\kappa_{11} = \kappa_{21} = \kappa_{22} = 0$, $\kappa_{12} = r$, $0.1 \leq r \leq 1.0$. For comparison of stress results we use variation models, which are denoted by FENE-DS, FENE-D$_\alpha$, of FENE-D model in [6]. These results are presented in Figure 2. For normal stress in shear flows, the results of FENE-M model has a good agreement to FENE until $r = 0.7$. For $r > 0.7$, the normal stress results of FENE-M are overall between those of FENE and FENE-P which is on the top graph in Figure 2, and greater than FENE-S. As we see Figure 1 the stretching of FENE-M effects to its normal stress results which are larger than those of FENE-S. In the shear stress FENE-M shows also good agreement results to FENE for $0.1 \leq r \leq 1.0$. It is better than the others.

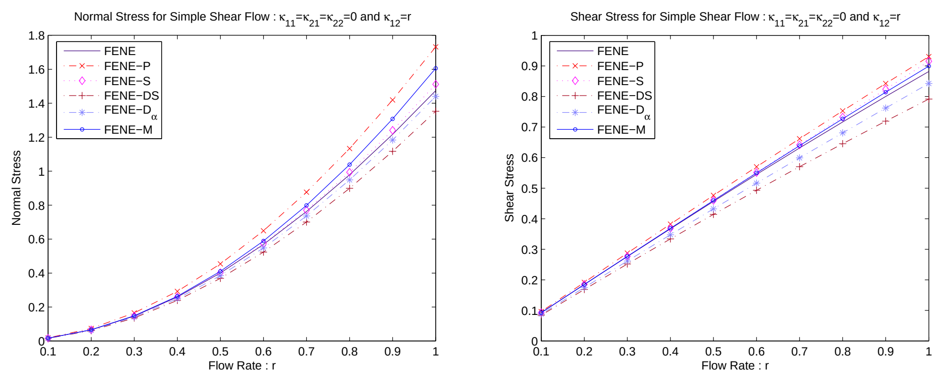

FIGURE 2. Comparison of the normal stress (first) and the shear stress (second) for the shear flow by solving Fokker-Planck and those from FENE-DS, FENE-D$_\alpha$, FENE-M models.

In Figure 3, we present the numerical results for the elastic energy computed by

$$E_{M_e} = \frac{1}{2}\left(\frac{b+6}{b}\right)\mathrm{tr}(A) - \frac{1}{2}\ln(\det A) \tag{55}$$

$$= \frac{M_1}{2}\left\{1 + \frac{6}{Q_0^2}\right\} - \frac{1}{2}\ln\left\{\left(\frac{M_1}{2}\right)^2 - \left(\frac{M_2}{2}\right)^2 - M_3^2\right\}, \tag{56}$$

containing the entropic term. It is denoted by FENE-M. Also, we present the numerical results obtained by the Chapman-Kolmogorov equation with $\int (f \ln f + \Psi f)\, d\vec{Q}$. We denote it FENE.

Since the free energy in (39), in terms of the relative energy to the equilibrium distribution function, f_∞, may include a constant difference between the free energy of original FENE (37) and that of the resulting closure FENE-M (39) due to the normalized factor. Moreover, there is no exact analytical expression for $\int (f \ln f + \Psi f)\, d\vec{Q}$ in the moment-closure approximation approach. Thus, we re-normalize the numerical results of FENE by a constant factor to match the FENE-M result at $r = 0.0$. The numerically computed elastic energy results are demonstrated in Figure 3, for varying shear rate r. From Figure 3, we can see that the growth behavior of the energy for FENE-M matches very well with that of the FENE for moderated shear rate situations. When the shear rate getting larger, say $r > 0.5$, the two energies begin to deviate and the FENE-M shows a faster growth than the FENE.

7. **Conclusion.** In this study, we employ the maximum entropy principle to obtain the maximum entropy solution (14) for the FENE model in stationary situation, and then we approximate it to the PDF (16) through (15) instead of using the maximum entropy solution (14), directly, because it is hard to solve the unknowns,

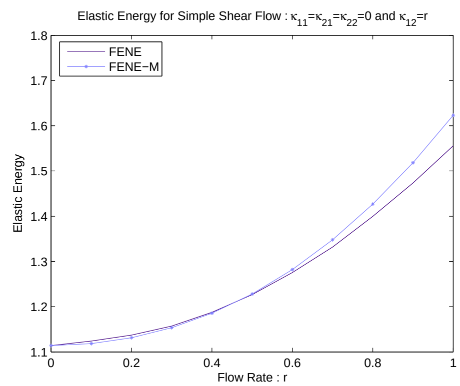

FIGURE 3. The energy results with the entropy term for FENE-M models.

λ_a's without any approximation. We also derive the moment-closure system (24)–(26) with the PDF (16), which satisfies the energy law (47) analogous to the energy law (37) of the original system (3)–(5).

Although we employ a simple approximation of the maximum entropy solution (14) for the PDF, the numerical simulations show satisfactory results in the macroscopic stresses for the shear flows. Especially, FENE-M shows a good agreement in shear stress results such as FENE-S. One of the important things in this moment closure approximation procedure is the fact that it satisfies the energy law (47). Moreover, the approximated PDF (16) makes possible to find an explicit form of the macroscopic stress tensor (27), which requires very cheap costs in the numerical computations because of the explicit form for the closure system.

At the beginning of the approximation step of the maximum entropy solution (14) we obtained the PDF (15) which is the second order approximation of (14). We reduced the PDF (15) to the PDF (16) for the connection to the second order moments because it includes the fourth order terms in microscopic field. However, we see that the PDF (15) is a good candidate for the approximation of the maximum entropy solution (14). Thus, we can apply the high order scheme which is proposed in [19] with the PDF (15) for the macroscopic moment-closure approximation procedure directly and it will be treated elsewhere.

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E-mail address: `hyon@math.psu.edu`
E-mail address: `carrillo@mat.uab.es`
E-mail address: `qdu@math.psu.edu`
E-mail address: `liu@math.psu.edu`