

KINETIC MODELS FOR POLYMERS WITH INERTIAL EFFECTS

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ABSTRACT. Novel kinetic models for both Dumbbell-like and rigid-rod like polymers are derived, based on the probability distribution function $f(t, x, n, \dot{n})$ for a polymer molecule positioned at x to be oriented along direction n while embedded in a \dot{n} environment created by inertial effects. It is shown that the probability distribution function of the extended model, when converging, will lead to well accepted kinetic models when inertial effects are ignored such as the Doi models for rod like polymers, and the Finitely Extensible Non-linear Elastic (FENE) models for Dumbbell like polymers.

1. Introduction. In this paper we derive novel kinetic models for both Dumbbell like and rigid-rod like polymers in the presence of inertial forces. The model is to describe dynamics of the probability distribution function embedded in high dimensional configuration space due to inertial effects. We then prove that the limit equation of the new model when inertial force vanishes leads to current models with no inertial effects such as the FENE model and the Doi model, respectively. This illustrates consistency of our kinetic models with existing models.

This paper is related to [39] where the derivation of a kinetic model for Dumbbell-like polymers including bead inertia is given. While [39] focuses on the derivation of the model, its extension to the Rouse model of polymers consisting of N beads attached by Hookean Dumbbells, and the transport properties of the resulting fluid, our work also develops the case of rigid-rod polymers and focuses on the relation between the inertial models and the classical inertia-free polymer models.

The wide range of applications of polymer materials has attracted new areas of academic and industrial research. The synthesis of different type of polymers has enlarged the range of applications of polymer materials to areas where mechanical properties are important. Materials made up of macro-molecules such as polymers display properties that completely differ from those made from small molecules. The

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description of polymer dynamics is often based on large assemblies of molecules, the characteristics could be modeled in terms of their statistical properties.

Most polymers are long chains or branches of repeated chemical units. The full description of each atom in the polymer by molecular dynamics is not feasible for the huge computational effort. Coarse grained models are often expected with macroscopic space and time properties of complex fluids. Typical models such as bead-spring chain for flexible polymers and the rigid rod model for liquid crystalline polymers have been established by the pioneers in polymer science.

In general, the flow modeling of polymers has to take into account the internal structure, characterized by both positional and orientational order of phases. Such incorporation is often done by adding new balance equations to those that govern structure-less Newtonian fluids. These new balances must be evaluated from the behavior of polymers. According to the relative size of the bending persistence size and the length of the polymer, two canonical types of polymers are widely studied: the Dumbbell model and the rigid-rod like model. In modeling motion of polymers, it is essential to explore an accurate method of solutions of the Langevin equation for particles undergoing Brownian movement (rotational or translational) under the influence of external fields. A large number of reviews, text books and monographs on the theory, applications and rheology of polymeric materials have appeared in the literature, see e.g. [19, 20, 21, 18, 11, 12, 1, 9, 34, 25, 38].

There are three main levels of description of polymeric fluids: atomistic modeling, kinetic modeling [12, 21], and the macroscopic approach of continuum mechanics [1]. We shall exploit the kinetic approach. Models of kinetic theory provide a coarse-grained description of molecular configurations wherein atomistic processes are ignored altogether (Doi and Edwards [12], Bird et al [1], and Ottinger[34]). Kinetic theory models for polymer solutions are most naturally exploited numerically by means of stochastic simulation or Brownian dynamics methods [34]. A kinetic theory model when equipped with an expression relating stress to molecular configurations plays an important role in developing micro-macro methods of computational rheology [36, 24]. In current kinetic theory models for polymers, the inertia of molecules is often neglected. However, neglect of inertia in some cases leads to incorrect predictions of the behavior of polymers. The forgoing considerations indicate that the inertial effects are of importance in practical applications, e.g., for short time characteristics of materials based on the relevant underlying phenomena.

It is thus the goal of this paper to model dynamics of the density distribution of polymers when the inertial force is no longer ignorable. More precisely we shall be particularly interested in modeling two canonical types of polymers: Dumbbell-like and rod-like polymers, which when inertial forces are not considered have been well understood. We first derive kinetic models including inertial effects from particle dynamics (continuum limit in the Brownian motion), we then show the limit of the augmented models when inertial forces vanish leads to the inertia-free model.

We now summarize our main results for two types of polymers.

1.1. Dumbbell-like polymers. A macromolecule is idealized as an ‘elastic dumbbell’ consisting of two ‘beads’ joined by a spring which can be modeled by an end-to-end vector n . Here n is in a bounded ball $B(0, n_0)$, which means that the extensibility of the polymers is finite. Let $f(t, x, n, p, q)$ denote the distribution function of Dumbbell-like polymers on the space variables $x \in \mathbb{R}^d$, $d = 2, 3$, the translational velocity $p \in \mathbb{R}^d$, the end-to-end vector n as well as the orientational

velocity $q \in \mathbb{R}^d$. And t is the time. The novel kinetic model to be derived is

$$\begin{aligned} \partial_t f + \nabla_x \cdot (pf) + \nabla_n \cdot (qf) + \nabla_p \cdot \left(-\frac{\zeta}{m}(p-u(x))f\right) \\ + \nabla_q \cdot \left(\left(-\frac{\zeta}{m}(q-n \cdot \nabla_x u(x)) - \frac{2F}{m}\right)f\right) = \frac{2k_B T \zeta}{m^2} \left(\frac{1}{4}\Delta_p f + \Delta_q f\right), \end{aligned} \quad (1)$$

where ζ is the frictional coefficient for the beads with mass m , k_B is the usual Boltzmann constant, T is the absolute temperature, and F is the spring force between beads. The force usually derives from a potential, and has different forms for different models. For the well known FENE potential

$$F = \frac{Hn}{1 - n^2/n_0^2},$$

where H is a spring constant [1].

The above model under the scaling

$$m = \epsilon^2, \quad \sqrt{mp} \rightarrow p, \quad \sqrt{mq} \rightarrow q,$$

leads to

$$\begin{aligned} \epsilon^2 \partial_t f + \epsilon \nabla_x \cdot (pf) + \epsilon \nabla_n \cdot (qf) \\ + \epsilon \nabla_p \cdot (\zeta u(x)f) + \epsilon \nabla_q \cdot [(\zeta n \cdot \nabla_x u - 2F)f] = Q(f), \end{aligned} \quad (2)$$

where

$$Q(f) := \zeta \nabla_p \cdot (pf + \frac{1}{2}k_B T \nabla_p f) + \zeta \nabla_q \cdot (qf + 2k_B T \nabla_q f).$$

Our result for Dumbbell like polymers could thus read as follows:

Theorem 1.1. *The limit $\epsilon \rightarrow 0$ of f is given by $f^0 = \rho M$ where $\rho = \rho(t, x, n) \geq 0$ and M are given by*

$$\rho(t, x, n) = \int f^0(t, x, n, p, q) dp dq, \quad M = \exp\left(-\frac{4p^2 + q^2}{4k_B T}\right).$$

Furthermore, $\rho(t, x, n)$ satisfies the following kinetic equation

$$\partial_t \rho + \nabla_x \cdot (u(x)\rho) + \nabla_n \cdot \left((n \cdot \nabla_x u - \frac{2F}{\zeta})\rho\right) = \frac{k_B T}{2\zeta} \Delta_x \rho + \frac{2k_B T}{\zeta} \Delta_n \rho. \quad (3)$$

1.2. Rod-like polymers. Polymers are idealized as rods of fixed length. The orientation space is $n \in \mathbb{S}^{d-1}$. Let $f(t, x, n, p, \omega)$ denote the distribution function of rod-like polymers on the space variables $x \in \mathbb{R}^d$, the translational velocity $p \in \mathbb{R}^d$, the orientational vector n as well as the angular velocity ω . Here ω is on the tangent bundle $T_n \mathbb{S}^{d-1}$. And t is the time. Our rescaled kinetic model can be formulated as

$$\begin{aligned} \epsilon \partial_t f + \nabla_x \cdot (pf) + \mathcal{R} \cdot (\omega f) + \zeta_t \nabla_p \cdot (u(x)f) \\ + \nabla_\omega \cdot ((\zeta_r n \times \nabla_x u \cdot n - \mathcal{R} \cdot U)f) = \frac{1}{\epsilon} Q(f), \end{aligned} \quad (4)$$

where

$$Q(f) = \zeta_t \nabla_p \cdot (pf + k_B T \nabla_p f) + \zeta_r \nabla_\omega \cdot (f\omega + k_B T \nabla_\omega f).$$

Here ϵ denotes the inertial parameter similar to (2), u is the fluid velocity, and U is certain interaction potential of rods. $\mathcal{R} = n \times \nabla_n$ is the rotational gradient operator, and k_B, T denote the Boltzmann constant and absolute temperature, respectively. ζ_t, ζ_r are frictional coefficients in x and n directions.

Our result for rod-like polymers then reads as follows:

Theorem 1.2. *The formal limit $\epsilon \rightarrow 0$ of f is given by $f^0 = \rho M$ where $\rho = \rho(t, x, n) \geq 0$ and M are given by*

$$\rho(t, x, n) = \int f^0(t, x, n, p, q) dp dn \omega, \quad M = \exp\left(-\frac{p^2 + \omega^2}{2k_B T}\right).$$

Furthermore, $\rho(t, x, n)$ satisfies the kinetic equation

$$\partial_t \rho + \nabla_x \cdot (u(x)\rho) + \mathcal{R} \cdot (n \times \nabla_x u \cdot \rho) = D_t \Delta_x \rho + D_r \mathcal{R} \cdot \left[\mathcal{R} \rho + \frac{\rho}{k_B T} \mathcal{R} U \right] \quad (5)$$

where

$$D_t = \frac{k_B T}{\zeta_t}, \quad D_r = \frac{k_B T}{\zeta_r}.$$

Our derivation of these kinetic models is based on establishing motion laws of polymer molecules, followed by a conversion into the kinetic description. The formal limit when inertia vanishes is justified by taking the classical approach for hydrodynamic limits. To this end a rescaling is adopted, so that the collision operator is set on fast scale, and the dissipation of the collision operator drives the states to the unique equilibrium states M . Derivation of models for Dumbbell-like polymers and the formal limit justification are given in §3, and those for rod-like polymers are given in §4. Some concluding remarks are presented in §5.

Finally, we wish to close this section by pointing to a vast body of recent work on mathematical treatment of kinetic theory models for polymers, their constitutive models as well as their coupling with fluid models (so called micro-macro models), see e.g. [37, 10, 15, 5, 4, 14, 23, 2, 7, 8, 17, 13, 32, 16, 22, 40, 3, 31, 27, 29, 6, 26, 30, 28, 33, 35, 42, 41] and references therein. These should provide guidance in establishing the various levels of mathematical theory of kinetic models developed in this work.

2. Kinetic models for Dumbbell polymers.

2.1. Equations of motion with non-trivial inertia. We consider a polymer consisting of two-beads connected by one-spring. Each bead as a coarse grained particle represents several chemical units and experiences four kinds of forces in the dilute case where there is no interaction for inter- and intra-dumbbells.

Assume the two beads are positioned at x_1 and x_2 , the Langevin equation of the beads are just balance of different forces expressed as

$$\begin{aligned} m_1 \ddot{x}_1 &= -\zeta_1 (\dot{x}_1 - u(x_1)) + F_1 + \sigma_1 \dot{W}_1, \\ m_2 \ddot{x}_2 &= -\zeta_2 (\dot{x}_2 - u(x_2)) + F_2 + \sigma_2 \dot{W}_2. \end{aligned}$$

Here W_i are independent standard Brownian motions, ζ_i are frictional coefficients for the i -th bead with mass m_i , $\sigma_i = \sqrt{2k_B T \zeta_i}$ by fluctuation-dissipation theorem, where k_B is the Boltzmann constant, and T is the temperature. The spring forces $F_1 = -F_2 = F$ by Newton's Third Law depends only on the end-to-end vector n .

A natural configuration for this underlying polymer includes both position of the polymer with these two beads connected to one spring

$$x = \frac{x_1 + x_2}{2},$$

and the end-to-end vector denoted by $n = x_2 - x_1$. We assume that $m_1 = m_2 = m$ and $\zeta_1 = \zeta_2 = \zeta$. Then the difference and average of the above two equations gives

a coupled system

$$m\dot{x} = -\zeta(\dot{x} - u(x)) + \sqrt{k_B T \zeta} \dot{W}_1, \quad (6)$$

$$m\dot{n} = -\zeta(\dot{n} - n \cdot \nabla_x u) - 2F + \sqrt{4k_B T \zeta} \dot{W}_2. \quad (7)$$

The approximation utilizes the equation $u(x) \sim (u(x_1) + u(x_2))/2$, $u(x_2) - u(x_1) \sim \nabla_x u \cdot n$, and the two new Brownian motions $(W_2 \pm W_1)/\sqrt{2}$ (still denoted by W_i).¹

If the inertia were ignored for this two beads spring system, we would have the following stochastic equations (SDE),

$$\dot{x} = u(x) + \sqrt{\frac{k_B T}{\zeta}} \dot{W}_1, \quad (8)$$

$$\dot{n} = n \cdot \nabla_x u - \frac{2F}{\zeta} + \sqrt{\frac{4k_B T}{\zeta}} \dot{W}_2. \quad (9)$$

The differential operator or the infinitesimal generator corresponding to the process $(x(t), n(t))$ is given by

$$L \equiv \langle u(x), \nabla_x \rangle + \langle n \cdot \nabla_x u - \frac{2F}{\zeta}, \nabla_n \rangle + \frac{2k_B T}{\zeta} \left(\frac{1}{4} \Delta_x + \Delta_n \right), \quad (10)$$

where

$$\nabla_x = \left(\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_d} \right), \quad \nabla_n = \left(\frac{\partial}{\partial n_1}, \dots, \frac{\partial}{\partial n_d} \right),$$

with $\langle \cdot, \cdot \rangle$ denoting the Euclidean inner product in \mathbb{R}^d . The configuration of Dumbbell like polymers can be illustrated in Figure 1:

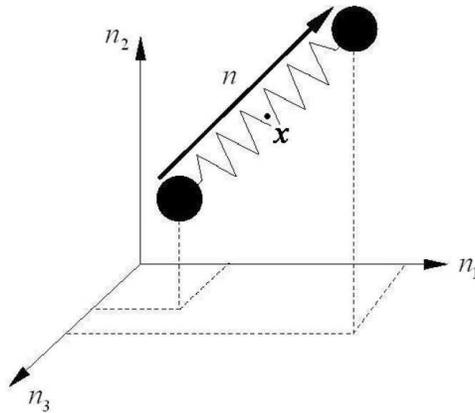


FIGURE 1. A Dumbbell like polymer

¹Here we use the fact that for any $\alpha \in [0, 1]$, $\alpha W_1(t) \pm \sqrt{1 - \alpha^2} W_2(t)$ remains a Brownian motion.

When inertial force is significant, one has to take the inertial effects into consideration. We now rewrite the system (6)-(7) into a first-order system

$$\begin{aligned}\dot{x} &= p, \\ \dot{n} &= q, \\ \dot{p} &= -\frac{\zeta}{m}(p - u(x)) + \frac{\sqrt{k_B T \zeta}}{m} \dot{W}_1, \\ \dot{q} &= -\frac{\zeta}{m}(q - n \cdot \nabla_x u(x)) - \frac{2F}{m} + \frac{\sqrt{4k_B T \zeta}}{m} \dot{W}_2.\end{aligned}$$

This system can be considered as a degenerate stochastic differential equation with a singular diffusion matrix of $4d \times 4d$. The differential operator corresponding to the process $(x(t), n(t), p(t), q(t))$ is also uniquely defined. In fact for the above dissipative stochastic differential equation with well-defined initial data, a unique solution $(x, n, p, q)(t)$ up to an explosion time is ensured if $u(x)$ and F are smooth functions of the configuration variables.

2.2. Kinetic description. We now formulate the kinetic description of the above motion laws. For a given instant t , the random variables $X = (x, n, p, q)$ can be characterized by a probability density function (PDF) $f(t, x, n; p, q)$ defined by

$$f(t, x, n; p, q,)dX = P[\{X \leq \tilde{X} \leq X + dX\}].$$

In words, the right-hand side is the probability that the random variable \tilde{X} falls between the sample space values X and $X + dX$ for different realizations of the polymer motion. Thus the above statistical ODE system can be converted into a PDE of the form

$$\begin{aligned}\partial_t f + \nabla_x \cdot (pf) + \nabla_n \cdot (qf) + \nabla_p \cdot \left(-\frac{\zeta}{m}(p - u(x))f \right) + \\ + \nabla_q \cdot \left(\left(-\frac{\zeta}{m}(q - n \cdot \nabla_x u(x)) - \frac{2F}{m} \right) f \right) = \frac{2k_B T \zeta}{m^2} \left(\frac{1}{4} \Delta_p f + \Delta_q f \right).\end{aligned}\quad (11)$$

It is known that in the case with no inertial forces the kinetic equation is also of the Fokker-Planck type. The model follows from the motion law (8)-(9) as follows:

$$\partial_t \rho + \nabla_x \cdot (u(x)\rho) + \nabla_n \cdot \left(\left(n \cdot \nabla_x u - \frac{2F}{\zeta} \right) \rho \right) = \frac{k_B T}{2\zeta} \Delta_x \rho + \frac{2k_B T}{\zeta} \Delta_n \rho, \quad (12)$$

where $\rho(t, x, n)$ denotes the corresponding probability density function.

Remark 1. The polymer scale is much smaller than the fluid scale, the diffusion in space is often ignorable. Here we make no such distinction.

It is natural to ask whether the effective dynamics in (11) is dominated by (12) when inertia vanishes. As a first step we shall identify an effective equation satisfied by the limit of f when $m \downarrow 0$, if the limit exists. In the remainder, we will always suppose that f is as smooth as needed.

2.3. Scaling. We make the following scaling

$$m = \epsilon^2, \quad \sqrt{m}p \rightarrow p, \quad \sqrt{m}q \rightarrow q,$$

to obtain

$$\begin{aligned}\epsilon^2 \partial_t f + \epsilon \nabla_x \cdot (pf) + \epsilon \nabla_n \cdot (qf) + \epsilon \nabla_p \cdot (\zeta u(x)f) + \\ + \epsilon \nabla_q \cdot [(\zeta n \cdot \nabla_x u - 2F)f] = Q(f),\end{aligned}\quad (13)$$

where

$$Q(f) := \zeta \nabla_p \cdot (pf + \frac{1}{2}k_B T \nabla_p f) + \zeta \nabla_q \cdot (qf + 2k_B T \nabla_q f).$$

The remaining task in this section is to justify the following

Theorem 2.1. *The limit $\epsilon \downarrow 0$ of the f^ϵ is given by $f^0 = \rho(t, x, n)M(p, q)$, where*

$$M = \exp\left(-\frac{4p^2 + q^2}{4k_B T}\right) \tag{14}$$

satisfying $Q(M) = 0$ and $\rho(t, x, n)$ solves the kinetic equation (12).

As usual the limit equation that is associated with (13) does not depend on details of the operator Q . Rather, it depends on Q possessing certain properties related to conservation, dissipation, and equilibria that are stated below. Note the operator Q acts on the augmented variables (p, q) only and leaves other variables (t, x, n) as parameters. Thus we list some properties of Q as an operator acting on functions of (p, q) only, which are essential in the derivation of the limit equation.

2.4. **Properties of Q .** Note that the operator $Q(f)$ has the following properties

- The operator can be written as a conservative form

$$Q(f) = 2\zeta k_B T \left[\frac{1}{4} \nabla_p \cdot \left(M \nabla_p \left(\frac{f}{M} \right) \right) + \nabla_q \cdot \left(M \nabla_q \left(\frac{f}{M} \right) \right) \right].$$

- The conservation form leads to

$$\int Q(f) dpdq = 0$$

for every $f \in L^1(dp dq)$. This relation expresses the physical laws of mass conservation during the action of Q .

Moreover, this is the only such conservation law. This means that

$$\int Q(f) \psi dpdq = 0, \quad \forall f \Leftrightarrow \psi \in \text{span}\{1\}.$$

- Dissipation. There is a nonnegative function $\eta(f)$ that is an entropy for the operator Q . This means that for $\eta(f) \in L^1(dp dq)$ we have

$$\int \eta'(f) Q(f) \leq 0,$$

whose vanishing characterizes the local equilibrium of Q . For flexible polymers, $\eta'(f) = f/M$ since

$$\begin{aligned} D^Q(f) &= \int Q(f) \frac{f}{M} dpdq \\ &= -2k_B T \int M \left[\frac{1}{4} \left(\nabla_p \left(\frac{f}{M} \right) \right)^2 + \left(\nabla_q \left(\frac{f}{M} \right) \right)^2 \right] dpdq \leq 0. \end{aligned}$$

- Existence of equilibria. From the above dissipation property we see that the function $f(p, q)$ such that $Q(f) = 0$ forms a space identified through

$$\frac{f}{M} \in \text{span}\{1\}.$$

This equilibrium is unique up-to a constant multiplier. We normalize the density function then

$$f_{eq} = \left[\int M dpdq \right]^{-1} M.$$

2.5. Asymptotic limit as $\epsilon \downarrow 0$. Equipped with these properties we now investigate the asymptotic limit. Define

$$\begin{aligned} \rho^\epsilon(t, x) &= \int f dpdq, \\ J_1^\epsilon(t, x) &= \frac{1}{\epsilon} \int p f dpdq, \\ J_2^\epsilon(t, x) &= \frac{1}{\epsilon} \int q f dpdq. \end{aligned}$$

Then integration of (13) together with conservation property of Q yields

$$\partial_t \rho^\epsilon + \nabla_x \cdot J_1 + \nabla_n \cdot J_2 = 0, \quad \forall \epsilon > 0. \quad (15)$$

We suppose that as $\epsilon \downarrow 0$ the limit of f is identified by f^0 . It follows from the equation (13) that

$$f^0 \in Q^{-1}(0).$$

This implies that $f^0 = M(p, q)\rho^0(t, x, n)$, for the operator Q does not act on (t, x, n) . Hence the probability density function f takes the following form

$$f^\epsilon(t, x, n; p, q) = \rho^\epsilon(t, x, n)M(p, q) + \epsilon g^\epsilon,$$

where

$$\lim_{\epsilon \downarrow 0} \rho^\epsilon(t, x, n) = \rho^0(t, x, n).$$

Note that $\int p M dpdq = \int q M dpdq = 0$, we thus have

$$J_1^\epsilon = \frac{1}{\epsilon} \int p f^\epsilon dpdq = \int p g^\epsilon dpdq, \quad (16)$$

$$J_2^\epsilon = \frac{1}{\epsilon} \int q f^\epsilon dpdq = \int q g^\epsilon dpdq. \quad (17)$$

The limit of these flux functions depends only on the limit of g^ϵ .

Linearity of the operator Q and $Q(M) = 0$ leads to

$$Q(f^\epsilon) = Q(\rho^\epsilon(t, x, n)M(p, q) + \epsilon g^\epsilon) = \epsilon Q(g^\epsilon).$$

Using the equation (13) we obtain

$$\begin{aligned} Q(g^\epsilon) &= \frac{1}{\epsilon} Q(f^\epsilon) \\ &= \epsilon \partial_t f^\epsilon + \nabla_x \cdot (p f^\epsilon) + \nabla_n \cdot (q f^\epsilon) + \nabla_p \cdot (\zeta u(x) f^\epsilon) \\ &\quad + \nabla_q \cdot ((\zeta n \cdot \nabla_x u - 2F) f^\epsilon) \\ &= \nabla_x \cdot (p M \rho^\epsilon) + \nabla_n \cdot (q M \rho^\epsilon) + \nabla_p \cdot (\zeta u(x) \rho^\epsilon M) \\ &\quad + \nabla_q \cdot ((\zeta n \cdot \nabla_x u - 2F) M \rho^\epsilon) + O(\epsilon). \end{aligned}$$

Let $g^\epsilon \rightarrow g^0$ as $\epsilon \rightarrow 0$, then it is clear that

$$Q(g^0) = p \cdot \nabla_x \rho^0 M + q \cdot \nabla_n \rho^0 M + \zeta \rho^0 u(x) \cdot \nabla_p M + \rho^0 (\zeta n \cdot \nabla_x u - 2F) \cdot \nabla_q M.$$

Again note that Q is a linear operator, we may assume the ansatz for g^0 as follows.

$$g^0 = a \cdot \nabla_x \rho^0 + b \cdot \nabla_n \rho^0 + \zeta \rho^0 c \cdot u(x) + \rho^0 (\zeta n \cdot \nabla_x u - 2F) \cdot d.$$

In comparison with the expression of $Q(g^0)$ above, we see that it is sufficient to find a, b, c, d such as

$$\begin{aligned} Q(a) &= pM, \\ Q(b) &= qM, \\ Q(c) &= \nabla_p M, \\ Q(d) &= \nabla_q M. \end{aligned}$$

These relations are understood in the sense that the operator acts on each component of the underlying vector. In order to identify (a, b, c, d) we state the following lemma:

Lemma 2.2. *Let Q be the collision operator and $g \in L^2(\mathbb{R}^p \times \mathbb{R}^q)$ such that $\int g dpdq = 0$. The problem*

$$Q(\psi) = g, \tag{18}$$

has a unique weak solution in $\Lambda = \{\psi, \int \psi dpdq = 0, \psi \in H^1\}$.

This lemma, following from applying the Lax-Milgram theorem to the corresponding variational formulation, ensures that there exists unique a, b, c, d in the space $\{\phi | \int \phi dpdq = 0\}$ since

$$\int \{pM, qM, \nabla_p M, \nabla_q M\} dpdq = 0.$$

We also note that from

$$\nabla_p M = -\frac{2}{k_B T} pM, \quad \nabla_q M = -\frac{1}{2k_B T} qM,$$

it follows

$$c = -\frac{2a}{k_B T}, \quad d = -\frac{b}{2k_B T}.$$

It remains to determine only a and b . Let $a = \alpha M p$ we have

$$Q(a) = -\alpha \zeta pM = pM,$$

which gives $\alpha = -\frac{1}{\zeta}$, leading to $a = -\frac{1}{\zeta} pM$. Similarly we obtain $b = -\frac{1}{\zeta} qM$.

Clearly we see that

$$\int \{b, d\} \cdot p dpdq = 0, \quad \int \{a, c\} \cdot q dpdq = 0.$$

These enable us to determine the asymptotic limits of the fluxes.

$$\begin{aligned} J_1^0 &= \int p g^0 dpdq \\ &= \int (a \cdot \nabla_x \rho^0) p + \int (b \cdot \nabla_n \rho^0) p + \zeta \rho^0 \int (c \cdot u(x)) p + \\ &\hspace{15em} + \rho^0 \int d \cdot (\zeta n \cdot \nabla_x u - 2F) p \\ &= \int a \cdot \left(\nabla_x \rho^0 - \frac{2\zeta u(x) \rho^0}{k_B T} \right) p dpdq \\ &= -\left(\nabla_x \rho^0 - \frac{2\zeta u(x) \rho^0}{k_B T} \right) \frac{k_B T}{2\zeta} \int M dpdq. \end{aligned}$$

$$\begin{aligned}
J_2^0 &= \int qg^0 dpdq \\
&= \int (a \cdot \nabla_x \rho^0)q + \int b \cdot \nabla_n \rho^0 q + \zeta \rho^0 \int (c \cdot u(x))q + \\
&\quad + \rho^0 \int d \cdot (\zeta n \cdot \nabla_x u - 2F)q \\
&= \int b \cdot \left(\nabla_n \rho^0 - \frac{\rho^0}{2k_B T} (\zeta n \cdot \nabla_x u - 2F) \right) q dpdq \\
&= - \left(\nabla_n \rho^0 - \frac{\rho^0}{2k_B T} (\zeta n \cdot \nabla_x u - 2F) \right) \frac{2k_B T}{\zeta} \int M dpdq.
\end{aligned}$$

Now the equation (15) divided by $\int M dpdq$ asymptotically converges to

$$\partial_t \rho^0 + \nabla_x \cdot (u(x)\rho^0) + \nabla_n \cdot \left((n \cdot \nabla_x u - \frac{2F}{\zeta})\rho^0 \right) = \frac{k_B T}{2\zeta} \Delta_x \rho^0 + \frac{2k_B T}{\zeta} \Delta_n \rho^0.$$

This is exactly the equation (12) derived from ignoring inertial forces.

Remark 2. With these kinetic equations for Dumbell like polymers, it is natural to understand how these polymers contribute to the macroscopic flow governed by a coupled Navier-Stokes system

$$\partial_t u + (u \cdot \nabla_x u)u + \nabla_x p = \frac{\gamma}{Re} \Delta_x u + \frac{1-\gamma}{ReDe} \nabla_x \cdot \tau, \quad \nabla_x \cdot u = 0,$$

with the stress determined by

$$\tau = \int (n \otimes F) f dn dpdq.$$

Here De is called Deborah number, which is the most important parameter in non-Newtonian fluids. Re and γ are the Reynolds number and viscosity ratio, respectively. The tensor force follows the case when inertial force is ignored, the derivation of the tensor force with inclusion of inertial effects is beyond the scope of this work.

Remark 3. The spring force is determined by a potential function U through $F = -\nabla_n U$. Different potential leads to different models. Two choices are commonly used:

	Force	Potential
Hookean spring	Hn	$\frac{1}{2}Hn^2$
FENE spring	$\frac{Hn}{1-(n/n_0)^2}$	$-\frac{1}{2}Hn_0^2 \ln(1 - (n/n_0)^2)$

where n_0 is the maximum extension of the beads connector.

3. Rigid rod-like polymers. Though many polymers are flexible, there is still a large class of polymers which are not flexible and assume a rod-like structure. Rod-like polymers have some peculiar properties and have attracted a great deal of attention.

We consider rod-like molecules in concentrated regime. Rod-like polymers can have only two kinds of motion, i.e., translation and rotation. The translational Brownian motion is the random motion of the position vector x of the center of mass, and the rotational Brownian motion is the random motion of the unit vector n ($|n| = 1$) which is parallel to the polymer. We shall build a kinetic model for

the probability distribution of orientational motions of rod in every point of phase space (x, p) . This serves as a microscopic equation, which is expected to be coupled with the macroscopic equation (the Navier-Stokes equation) for the fluid velocity.

For the convenience of calculations in what follows, we introduce a local coordinate on the sphere S^2 as $q = (\theta, \phi)$, and set $n = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ with $\theta \in [0, \pi)$ and $\phi \in [0, 2\pi)$. The unit vector $e_\theta = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta)$ and $e_\phi = (-\sin\phi, \cos\phi, 0)$. We note that $\frac{\partial n}{\partial \theta} = e_\theta$, $\frac{\partial n}{\partial \phi} = \sin\theta e_\phi$. Thus, any tangent vector on the sphere is written as

$$\dot{n} = \dot{\theta}e_\theta + \dot{\phi}\sin\theta e_\phi,$$

which gives

$$\omega = n \times \dot{n} = \dot{\theta}e_\phi - \sin\theta\dot{\phi}e_\theta.$$

The gradient is

$$\nabla_n = e_\theta\partial_\theta + \frac{e_\phi}{\sin\theta}\partial_\phi.$$

The rotational gradient is

$$\mathcal{R} = n \times \nabla_n = \left(-\frac{\cos\phi\cos\theta}{\sin\theta}\partial_\phi - \sin\phi\partial_\theta, -\frac{\cos\theta\sin\phi}{\sin\theta}\partial_\phi + \cos\phi\partial_\theta, \partial_\phi \right)^T. \quad (19)$$

Divergence of a vector $A = A_\theta e_\theta + A_\phi e_\phi$ is

$$\nabla_n \cdot A = \frac{1}{\sin\theta}\partial_\theta(\sin\theta A_\theta) + \frac{1}{\sin\theta}\partial_\theta A_\phi.$$

The gradient in terms of ω is defined only for a given n , and will be understood from now on as

$$n \cdot \nabla_\omega f = 0, \quad \forall f.$$

To be more specific, we regard the identical liquid crystal molecules as inflexible rods of a thickness b which is much smaller than their length L , as illustrated in Figure 2:

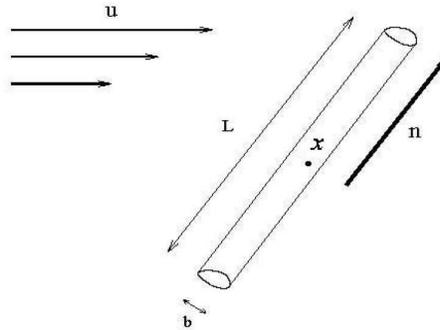


FIGURE 2. A rod like polymer

3.1. Translational Brownian motion. Let U be an interaction potential, the force thus induced is $-\nabla_x U$. The motion law is

$$m\ddot{x} = -\zeta_t(\dot{x} - u(x)) - \nabla_x U,$$

where ζ_t is the friction coefficient and $u(x)$ is the fluid velocity field. If f is the probability distribution in x , the Brownian force is expressed as $F_B = -\nabla_x(k_B T \ln f)$, where $-k_B T \ln f$ is the chemical potential. For nontrivial inertial force, the distribution needs to be accounted in an extended environment with inclusion of $p = \dot{x}$. The corresponding translational Brownian force thus reduces to

$$F_B = \nabla_p W, \quad W = -\frac{\zeta_t k_B T}{m} \ln f. \quad (20)$$

This can be justified by a similar derivation based on Brownian motions as that in Section 2. The scaled coefficient reflects balances between the friction force and the inertial force. Putting together we have the following translational motion law

$$\dot{x} = p, \quad (21)$$

$$\dot{p} = -\frac{\zeta_t}{m}(p - u(x)) - \frac{1}{m}\nabla_x U - \frac{\zeta_t}{m^2}\nabla_p(k_B T \ln f). \quad (22)$$

In what follows we shall conveniently use the chemical potential to describe the Brownian force.

3.2. Rotational Brownian motion. We consider a rod rotating with angular velocity ω , then the rotational motion can be described as

$$[J]\dot{\omega} = T,$$

where J is the moment of inertia and T is the total torque.

1. Rotational frictional force.

Consider a rod of length L placed in a viscous fluid with fluid velocity $u(x)$, where x is the center of mass of the rod.

The rod is parameterized by s , ranging from $-L/2$ to $L/2$, then the position vector of the s -point on this rod is written as

$$x(s) = x + ns, \quad x(0) = x, \quad -L/2 \leq s \leq L/2.$$

Let $v(s)$ and $F(s)$ be the velocity of this point, and forces acting on it. The velocity $v(s)$ is expressed by the angular velocity ω

$$v(s) = \omega \times (x(s) - x) = \omega \times (ns).$$

The frictional force at $x(s)$ is

$$F(s) = -\xi(s)(v(s) - u(x(s))),$$

where $\xi(s)$ is the frictional coefficient, being symmetric $\xi(s) = \xi(-s)$. Note that

$$u(x(s)) \simeq u(x) + \nabla_x u(x(s) - x(0)) = u(x) + s\nabla_x u \cdot n.$$

The frictional force thus reduces to

$$F(s) = -s\xi(s)(\omega \times n - \nabla_x u \cdot n) + \xi(s)u(x).$$

Thus the total torque induced by the frictional force acting on the rod is

$$\begin{aligned} T &= \frac{1}{L} \int_{-L/2}^{L/2} (x(s) - x) \times F(s) ds \\ &= -\xi_2 n \times (\omega \times n - \nabla_x u \cdot n) + \xi_1 n \times u(x), \end{aligned}$$

where

$$\xi_k = \frac{1}{L} \int_{-L/2}^{L/2} s^k \xi(s) ds, \quad k = 1, 2.$$

Symmetry of $\xi(s) = \xi(-s)$ leads to $\xi_1 = 0$. Then using $n \cdot \omega = 0$ we have

$$T = -\zeta_r [(Id - n \otimes n)\omega - n \times (\nabla_x u \cdot n)] = -\zeta_r [\omega - n \times (\nabla_x u \cdot n)],$$

where $\zeta_r = \xi_2$ denotes the rotational friction coefficient.

2. Thermodynamic potential force.

From $[J]\dot{\omega} = T$ it follows

$$\frac{d}{dt} E = T \cdot \omega, \quad E = \frac{1}{2} \omega^\top [J] \omega.$$

Let the potential be denoted by U . Then $d(E + U) = 0$ gives $dE = -dU = -\nabla_n U \cdot dn$.

Note that from $|n| = 1$ we have

$$\omega = n \times \dot{n},$$

which leads to

$$\omega dt = n \times dn.$$

We thus have

$$T \cdot (n \times dn) = T \cdot \omega dt = dE = -\nabla_n U \cdot dn.$$

Therefore $T \times n = -\nabla_n U$, i.e.,

$$T = -\mathcal{R}U, \tag{23}$$

where \mathcal{R} is the rotational gradient operator given by (19).

3. Rotational Brownian force.

The following property will be used on our derivation of forces below.

Lemma 3.1. *For a fixed vector a , let $x = a \times y$. Then for any function smooth g ,*

$$\nabla_y g = -a \times \nabla_x g$$

and

$$a \cdot \nabla_y g = 0, \quad \forall g.$$

Proof. Let ϵ_{ijk} as the usual permutation symbol, then $x_i = \sum_{j,k} \epsilon_{ijk} a_j y_k$. We thus have

$$\begin{aligned} (\nabla_y g)_m &= \sum_i \partial_{x_i} g \frac{\partial x_i}{\partial y_m} = \sum_i \partial_{x_i} g \sum_{j,k} \epsilon_{ijk} a_j \delta_{mk} \\ &= \sum_{i,j} \epsilon_{mij} \partial_{x_i} g a_j = - \sum_{i,j} \epsilon_{mji} a_j \partial_{x_i} g. \end{aligned}$$

This gives the desired relation. We now show the second claim.

$$\sum_m a_m \partial_{y_m} g = \sum_{mij} \epsilon_{mij} \partial_{x_i} g a_m a_j = - \sum_{mij} \epsilon_{mij} \partial_{x_i} g a_j a_m,$$

which ensures that $a \cdot \partial_y f = 0$ holds for any smooth function g □

Consider a rod again with center of mass at x , and momentum $p = 0$ at rest, the point vector of rod is $x(s) = x + sn$ with s ranging in $[-L/2, L/2]$. Correspondingly

$$p(s) = s\dot{n} = s\omega \times n.$$

From this we obtain that

$$\omega = \frac{1}{s}n \times p(s). \quad (24)$$

Also rod symmetry implies that

$$p(-s) = -p(s). \quad (25)$$

For any fixed s the associated Brownian force is calculated by

$$F_B(s) = \nabla_{p(s)}W, \quad W = -\frac{\zeta_r k_B T}{m} \ln f. \quad (26)$$

Note that for each fixed s and vector n , the mapping from $p(s)$ to ω is well-defined. The result in Lemma 3.1 gives

$$F_B(s) = \nabla_{p(s)}W = -\frac{1}{s}n \times \nabla_\omega W.$$

Thus the corresponding Brownian torque is determined by

$$T_B = \frac{1}{L} \int_{-L/2}^{L/2} sn \times F_B(s) ds,$$

which when combined with the above calculations leads to

$$\begin{aligned} T_B &= \frac{1}{L} \int_{-L/2}^{L/2} sn \times \left(-\frac{1}{s}n \times \nabla_\omega W \right) ds \\ &= -n \times (n \times \nabla_\omega W) \\ &= (Id - n \otimes n) \nabla_\omega W \\ &= -\frac{\zeta_r k_B T}{m} (Id - n \otimes n) \nabla_\omega (\ln f) \\ &= -\frac{\zeta_r k_B T}{m} \nabla_\omega (\ln f). \end{aligned}$$

Note that the moment of inertia for the rod is

$$[J] = j(Id - n \otimes n), \quad j = \frac{mL^2}{12}.$$

Using $\dot{\omega} \cdot n = 0$, we thus have

$$[J] \cdot \dot{\omega} = j\dot{\omega}.$$

This together with all forces involved leads to the following motion law

$$\dot{n} = \omega \times n, \quad (27)$$

$$\frac{mL^2}{12} \dot{\omega} = -\zeta_r (\omega - n \times (\nabla_x u) \cdot n) - \frac{\zeta_r k_B T}{m} \nabla_\omega (\ln f) - \mathcal{R}U, \quad (28)$$

where U is the interaction potential.

Remark 4. The potential can be defined as a generalized Onsager's potential:

$$U = \nu^2 k_B T b L^2 \int_{R_x} \int_{R_p} \int_{|n'|=1} \int_{n \cdot \omega=0} B(x, p; x', p') |n \times n'| f(t, x', p', n', \omega) dn' dx' dp' d_n \omega.$$

Here R_x and R_p is the configuration space for variables x and p . B is some localized kernel.

3.3. Kinetic equations. We shall derive a kinetic equation in the phase space (x, p, n, ω) with $(x, p) \in \mathbb{R}^3 \times \mathbb{R}^3$ and $(n, \omega) \in T\mathbb{S}^2$, where

$$T\mathbb{S}^2 := \{(n, \omega) \mid n \in \mathbb{S}^2, \omega \in T_n\mathbb{S}^2\}, \tag{29}$$

which is usually called the tangent bundle of the manifold \mathbb{S}^2 . We start from the continuity equation of a formal form

$$\partial_t f + \nabla_x \cdot (\dot{x}f) + \nabla_p \cdot (\dot{p}f) + \nabla_n \cdot (\dot{n}f) + \nabla_{\dot{n}} \cdot (\dot{\dot{n}}f) = 0. \tag{30}$$

This equation can be simplified when restricted on the tangent bundle: $(n, \omega) \in T\mathbb{S}^2$.

First we state the following

Lemma 3.2. *Let (n, ω) be any element of the tangent bundle $T\mathbb{S}^2$, mapped to another element $(m, \dot{n}) \in T\mathbb{S}^2$ such that*

$$m = n, \quad \dot{n} = \omega \times n,$$

then for any smooth function f we have

$$\nabla_n f = \nabla_m f - \omega \times \nabla_{\dot{n}} f, \quad \nabla_{\omega} f = n \times \nabla_{\dot{n}} f. \tag{31}$$

Proof. Let ϵ_{ijk} be the usual permutation symbol, then $\dot{n}_l = \sum_{jk} \epsilon_{ljk} \omega_j n_k$. Further we have

$$\begin{aligned} \partial_{n_i} f &= \partial_{m_i} f + \sum_l \partial_{\dot{n}_l} f \cdot \sum_{j,k} \epsilon_{ljk} \omega_j \delta_{ik} \\ &= \partial_{m_i} f + \sum_{l,j} \epsilon_{ilj} \partial_{\dot{n}_l} f \omega_j \\ &= \partial_{m_i} f - \sum_{l,j} \epsilon_{ijl} \omega_j \partial_{\dot{n}_l} f, \end{aligned}$$

where δ_{ij} is the Kronecker delta symbol. This gives the first relation in (31). The second relation follows from

$$\begin{aligned} \partial_{\omega_i} f &= \sum_l \partial_{\dot{n}_l} f \cdot \sum_{j,k} \epsilon_{ljk} \delta_{ij} n_k \\ &= \sum_{l,k} \epsilon_{lik} \partial_{\dot{n}_l} f n_k. \end{aligned}$$

□

Using similar arguments we have the following:

Lemma 3.3. *Let g be any smooth vector function, then*

$$(n \times \nabla_n) \cdot g = -\nabla_n \cdot (n \times g), \quad (n \times \nabla_{\omega}) \cdot g = -\nabla_{\omega} \cdot (n \times g). \tag{32}$$

Note from $\omega = n \times \dot{n}$ we have $\dot{\omega} = n \times \ddot{n}$ leading to $\dot{\omega} \cdot n = 0$. Also

$$\dot{n} = \omega \times n, \quad \ddot{n} = \dot{\omega} \times n - |\omega|^2 n.$$

Equipped with above lemmas and relations, we are able to reduce the equation (30). We only check the last two terms on the left-hand of (30). First,

$$\nabla_n \cdot (\dot{n}f) = \nabla_n \cdot (\omega \times n f) = \mathcal{R} \cdot (\omega f),$$

where $\mathcal{R} := n \times \nabla_n$ is the rotational gradient operator. For any smooth function g , Lemma 3.2 and Lemma 3.3 imply that

$$\nabla_{\dot{n}} g = -(n \times \nabla_\omega) g.$$

This enables us to simplify the last term in equation (30)

$$\begin{aligned} \nabla_{\dot{n}} \cdot (\dot{n} f) &= -(n \times \nabla_\omega) \cdot ((\dot{\omega} \times n - |\omega|^2 n) f) \\ &= \nabla_\omega \cdot (n \times (\dot{\omega} \times n - |\omega|^2 n) f) \\ &= \nabla_\omega \cdot ((Id - n \otimes n) \dot{\omega} f) \\ &= \nabla_\omega \cdot (\dot{\omega} f). \end{aligned}$$

Therefore the effective kinetic equation becomes

$$\partial_t f + \nabla_x \cdot (p f) + \nabla_p \cdot (\dot{p} f) + \mathcal{R} \cdot (\omega f) + \nabla_\omega \cdot (\dot{\omega} f) = 0, \quad (33)$$

where

$$\begin{aligned} \dot{p} &= -\frac{\zeta_t}{m} (p - u(x)) - \frac{1}{m} \nabla_x U - \frac{\zeta_t}{m^2} \nabla_p (k_B T \ln f), \\ \dot{\omega} &= -\frac{\zeta_r}{m} (\omega - n \times \nabla_x u(x) \cdot n) - \frac{1}{m} \mathcal{R} U - \frac{\zeta_r}{m^2} \nabla_\omega (k_B T \ln f). \end{aligned}$$

Note here the coefficient $L^2/12$ has been absorbed in both the ζ_r and the potential U , which is independent of both p and ω .

3.4. Scaling. We are interested in the solution behavior when inertia vanishes.

We now make the following scaling

$$m = \epsilon^2, \quad \epsilon p \rightarrow p, \quad \epsilon \omega \rightarrow \omega,$$

under this scaling the system (33) written into the new variables becomes

$$\begin{aligned} \epsilon \partial_t f + \nabla_x \cdot (p f) + \mathcal{R} \cdot (\omega f) + \zeta_t \nabla_p \cdot (u(x) f) \\ + \nabla_\omega \cdot ((\zeta_r n \times \nabla_x u \cdot n - \mathcal{R} \cdot U) f) = \frac{1}{\epsilon} Q(f), \end{aligned} \quad (34)$$

where

$$Q(f) = \zeta_t \nabla_p \cdot (p f + k_B T \nabla_p f) + \zeta_r \nabla_\omega \cdot (f \omega + k_B T \nabla_\omega f).$$

Our next task is to investigate the formal limit $\epsilon \rightarrow 0$ of this problem.

Theorem 3.4. *The limit $\epsilon \downarrow 0$ of the f^ϵ is given by $f^0 = \rho(t, x, n) M(p, \omega)$, where*

$$M = \exp \left(-\frac{p^2 + \omega^2}{2k_B T} \right) \quad (35)$$

satisfying $Q(M) = 0$ and $\rho(t, x, n)$ solves the following kinetic equation

$$\partial_t \rho + \nabla_x \cdot (u(x) \rho) + \mathcal{R} \cdot (n \times \nabla_x u \cdot \rho) = D_t \Delta_x \rho + D_r \mathcal{R} \cdot \left[\mathcal{R} \rho + \frac{\rho}{k_B T} \mathcal{R} U \right], \quad (36)$$

where

$$D_t = \frac{k_B T}{\zeta_t}, \quad D_r = \frac{k_B T}{\zeta_r}.$$

Remark 5. (i) When the coefficient $D_t = 0$, the equation (36) is the Doi’s kinetic model for rod-like polymers with inertial forces ignored. This equation is also called the Smoluchowski equation in literature.

(ii) If the translation diffusion has different strengths and U also depends on x , one needs to change $D_t \Delta_x \rho$ to

$$\nabla_x \cdot \left\{ [D_{\parallel} n \otimes n + D_{\perp} (Id - n \otimes n)] [\nabla_x \rho + \frac{\rho}{k_B T} \nabla_x U] \right\}.$$

The above justification procedure remains valid.

3.5. Properties of Q . The operator Q here acts on the augmented variables (p, ω) only and leaves other variables (t, x, n) as parameters. Thus we list some properties of Q as an operator acting on functions of (p, ω) only, which are essential in the derivation of the limit equation.

Set

$$M = \exp \left(-\frac{p^2 + \omega^2}{2k_B T} \right)$$

with ω satisfying $\omega \cdot n = 0$ for any fixed $n \in \mathbb{S}^2$.

This form enables us to conclude the following

Lemma 3.5. *The operator Q has the following properties:*

(i) *The operator Q can be written as*

$$Q(f) := \zeta_t k_B T \nabla_p \cdot \left(M \nabla_p \left(\frac{f}{M} \right) \right) + \zeta_r k_B T \nabla_{\omega} \cdot \left(M \nabla_{\omega} \left(\frac{f}{M} \right) \right). \quad (37)$$

(ii) *Conservation. For every $f \in L^1(dpd_n \omega)$,*

$$\int Q(f) dpd_n \omega = 0.$$

Moreover, this is the only such conservation laws. In other words, for any $f \in L^1(dpd_n \omega)$,

$$\int Q(f) \psi dpd_n \omega = 0, \quad \forall f \Leftrightarrow \psi \in \text{span}\{1\}.$$

(iii) *Dissipation. There is a nonnegative function $\eta(f)$ that is an entropy for the operator Q . This means that for $\eta(f) \in L^1(dpd_n \omega)$ we have*

$$D^Q(f) = \int Q(f) \eta'(f) dpd_n \omega \leq 0.$$

In the case of rod-like polymers, $\eta'(f) = f/M$ and the dissipation production is

$$-k_B T \left[\zeta_t \int M \left(\nabla_p \left(\frac{f}{M} \right) \right)^2 dpd_n \omega + \zeta_r \int M \nabla_{\omega} \left(\frac{f}{M} \right)^2 dpd_n \omega \right] \leq 0.$$

(iv) *Existence of equilibria. From the above dissipation property we see that the function $f(p, \omega)$ such that $Q(f) = 0$ if and only if*

$$\frac{f}{M} \in \text{span}\{1\}.$$

Proof of Lemma 3.5. (i) The conservation follows from a direct calculation. (ii) The conservation form in (i) leads to the null integration. Since the $\int Q(f)\psi dpd_n\omega = 0$ holds true for any f , we let $f = \psi M$ to have

$$\int Q(\psi M)\psi dpd_n\omega = 0.$$

The left-hand side of this relation is non-positive as

$$0 = -k_B T \left[\zeta_t \int M (\nabla_p \psi)^2 dpd_n\omega + \zeta_r \int M (\nabla_\omega \psi)^2 dpd_n\omega \right] \leq 0.$$

Thus ψ must satisfy both $\nabla_p \psi = 0$ and $\nabla_\omega \psi = 0$. Then one has $n \cdot \nabla_\omega \psi = 0$. These ensure that ψ must be independent of (p, ω) .

(iii) Dissipation property comes from integration by parts on the tangent plane.

(iv) From the dissipation inequality we see that if $Q(f) = 0$, then $D^Q(f) = 0$. The non-negativity of D^Q yields

$$\frac{f}{M} \in \text{span}\{1\}.$$

3.6. Asymptotic limit as $\epsilon \downarrow 0$. We now investigate the formal limit of the problem, assuming all involved functions are smooth and convergence holds true as needed.

We suppose that $f \rightarrow f^0$ as $\epsilon \rightarrow 0$. Then, from the scaled kinetic equation (34), $Q[f] = O(\epsilon)$ and we deduce that $Q(f^0) = 0$.

By property (ii) we have $f^0 = \rho M$, with $\rho = \rho(t, x, n) \geq 0$ and $n \in \mathbb{S}^2$. Note that Q acts only on (p, ω) , ρ are functions of (t, x, n) . To find this dependence, we use the generalized collisional invariants. We integrate the equation with respect to (p, ω) to find the continuity equation

$$\partial_t \rho^\epsilon + \nabla_x \cdot J_1^\epsilon + \mathcal{R} \cdot J_2^\epsilon = 0, \quad \forall \epsilon > 0,$$

where the density and fluxes are defined by

$$\begin{aligned} \rho^\epsilon(t, x, n) &= \int f dpd_n\omega, \\ J_1^\epsilon(t, x, n) &= \frac{1}{\epsilon} \int p f dpd_n\omega, \\ J_2^\epsilon(t, x, n) &= \frac{1}{\epsilon} \int \omega f dpd_n\omega. \end{aligned}$$

Here the integration over ω is interpreted as for any fixed n with $(n, \omega) \in TS^2$. In the limit $\epsilon \rightarrow 0$, $\rho^\epsilon \rightarrow C\rho^0$ and $J_i^\epsilon \rightarrow CJ_i^0$ ($i = 1, 2$) with $C = \int M dpd_n\omega$, and we obtain

$$\partial_t \rho^0 + \nabla_x \cdot J_1^0 + \mathcal{R} \cdot J_2^0 = 0. \quad (38)$$

Thus we may assume that

$$f^\epsilon = \rho^\epsilon(t, x, n)M(p, \omega) + \epsilon g^\epsilon(t, x, p, n, \omega),$$

which leads to

$$Q(f^\epsilon) = \epsilon Q(g^\epsilon).$$

To determine the limiting flux we need to explore the limit of g^ϵ . Using the kinetic equation (34) we have

$$\begin{aligned} Q(g^\epsilon) &= \frac{1}{\epsilon}Q(f^\epsilon) \\ &= \epsilon\partial_t f^\epsilon + \nabla_x \cdot (pf^\epsilon) + \mathcal{R} \cdot (\omega f^\epsilon) + \nabla_p \cdot (\zeta_t u(x)f^\epsilon) + \\ &\quad + \nabla_\omega \cdot ((\zeta_r n \cdot \nabla_x u - \mathcal{R}U)f^\epsilon) \\ &= \nabla_x \cdot (pM\rho^\epsilon) + \mathcal{R} \cdot (\omega M\rho^\epsilon) + \nabla_p \cdot (\zeta_t u(x)\rho^\epsilon M) \\ &\quad + \nabla_\omega \cdot ((\zeta_r n \cdot \nabla_x u - \mathcal{R}U)M\rho^\epsilon) + O(\epsilon). \end{aligned}$$

Let $g^\epsilon \rightarrow g^0$ as $\epsilon \rightarrow 0$, then it is clear that

$$\begin{aligned} Q(g^0) &= p \cdot \nabla_x \rho^0 M + \omega \cdot \mathcal{R} \rho^0 M + \zeta_t \rho^0 u(x) \cdot \nabla_p M + \\ &\quad + \rho^0 (\zeta_r n \times (\nabla_x u \cdot n) - \mathcal{R}U) \cdot \nabla_\omega M. \end{aligned}$$

Again note that $Q(f)$ is a linear operator, we may assume the ansatz for g^0 as follows.

$$g^0 = a \cdot \nabla_x \rho^0 + b \cdot \mathcal{R} \rho^0 + \zeta_t \rho^0 c \cdot u(x) + \rho^0 (\zeta_r n \times \nabla_x u \cdot n - \mathcal{R}U) \cdot d.$$

In comparison with the expression of $Q(g^0)$ above, we see that it is sufficient to find a, b, c, d such as

$$\begin{aligned} Q(a) &= pM, \\ Q(b) &= \omega M, \\ Q(c) &= \nabla_p M, \\ Q(d) &= \nabla_\omega M. \end{aligned}$$

In order to uniquely determine $\{a, b, c, d\}$ we state the following

Lemma 3.6. *Let $g \in L^2(dp d_n \omega)$ such that $\int g dp d_n \omega = 0$. The problem*

$$Q(\psi) = g, \tag{39}$$

has a unique weak solution in the space $H^1(dp d_n \omega)$.

Proof. For each fixed $n \in \mathbb{S}^2$, we apply the Lax-Milgram theorem to the following variational formulation of (39):

$$k_B T \int [\xi_t M \nabla_p \psi \cdot \nabla_p \phi + \xi_r M \nabla_\omega \psi \cdot \nabla_\omega \phi] dp d_n \omega = \int g \phi dp d_n \omega \tag{40}$$

for all $\phi \in H^1(dp d_n \omega)$. The function M is bounded from above and below on $\mathbb{R}_p^d \times T_n(\mathbb{S}^2)$, so the bilinear form at the left-hand side is continuous and coercive on $H^1(dp d_n \omega)$. The right-hand side is a continuous linear form on $H^1(dp d_n \omega)$ due to the zero average of g over $\mathbb{R}_p^d \times T_n(\mathbb{S}^2)$. \square

Lemma 3.6 ensures that there exists unique a, b, c, d in the space $\{\phi \mid \int \phi dp d_n \omega = 0\}$ since

$$\int \{pM, \omega M, \nabla_p M, \nabla_\omega M\} dp d_n \omega = 0.$$

Note also that from

$$\nabla_p M = -\frac{1}{k_B T} pM, \quad \nabla_\omega M = -\frac{1}{k_B T} \omega M,$$

it follows

$$c = -\frac{a}{k_B T}, \quad d = -\frac{b}{k_B T}. \tag{41}$$

It remains to determine only a and b . Let $a = \alpha Mp$ we have

$$Q(a) = -\alpha \zeta_t p M = p M,$$

which gives $\alpha = -\frac{1}{\zeta_t}$, leading to

$$a = -\frac{1}{\zeta_t} p M. \quad (42)$$

Similarly let $b = \beta M \omega$, then

$$\begin{aligned} Q(b) &= \zeta_r k_B T \nabla_\omega \cdot (\beta M) \\ &= \beta \zeta_r k_B T \nabla_\omega M \\ &= -\beta \zeta_r M \omega, \end{aligned}$$

which together with $Q(b) = M \omega$ gives $\beta = -1/\zeta_r$, thus

$$b = -\frac{1}{\zeta_r} \omega M. \quad (43)$$

It is straightforward to verify that

$$\int \{b, d\} \cdot p d p d_n \omega = 0, \quad \int \{a, c\} \cdot \omega d p d_n \omega = 0.$$

These enable us to determine the asymptotic limits of the fluxes.

$$\begin{aligned} J_1^0 &= \int p g^0 d p d_n \omega \\ &= \int (a \cdot \nabla_x \rho^0) p + \int (b \cdot R \rho^0) p + \zeta_t \rho^0 \int (c \cdot u(x)) p + \\ &\quad + \rho^0 \int d \cdot (\zeta_r n \cdot \nabla_x u - \mathcal{R}U) p \\ &= \int a \cdot \left(\nabla_x \rho^0 - \frac{\zeta_t u(x) \rho^0}{k_B T} \right) p d p d_n \omega, \end{aligned}$$

$$\begin{aligned} J_2^0 &= \int \omega g^0 d p d_n \omega \\ &= \int (a \cdot \nabla_x \rho^0) \omega + \int b \cdot R \rho^0 \omega + \zeta_t \rho^0 \int (c \cdot u(x)) \omega + \\ &\quad + \rho^0 \int d \cdot (\zeta_r n \cdot \nabla_x u - \mathcal{R}U) \omega \\ &= \int b \cdot \left(\mathcal{R} \rho^0 - \frac{\rho^0}{k_B T} (\zeta_r n \cdot \nabla_x u - \mathcal{R}U) \right) \omega d p d_n \omega. \end{aligned}$$

In order to further simplify the above fluxes, we state the following lemma:

Lemma 3.7. *Consider the space $p \in \mathbb{R}^3$ and $(n, \omega) \in TS^2$. For any vector A we have*

$$\int M(p \cdot A) p d p d_n \omega = k_B T A \int M d p d_n \omega, \quad (44)$$

$$\int M(\omega \cdot A) \omega d p d_n \omega = k_B T (Id - n \otimes n) A \int M d p d_n \omega. \quad (45)$$

Apply this lemma to the above expressions to obtain

$$J_1^0 = [\rho^0 u(x) - \frac{k_B T}{\zeta_t} \nabla_x \rho^0] \int M dp d_n \omega, \tag{46}$$

$$J_2^0 = (Id - n \otimes n) \left[-\frac{k_B T}{\zeta_r} \mathcal{R} \rho^0 + \frac{1}{\zeta_r} (\zeta_r n \times \nabla_x u \cdot n - \mathcal{R} U) \right] \int M dp d_n \omega. \tag{47}$$

A simple calculation shows for arbitrary A that

$$(Id - n \otimes n)(n \times A) = n \times A.$$

Therefore

$$J_2^0 = \left[-\frac{k_B T}{\zeta_r} \mathcal{R} \rho^0 + \left(n \times \nabla_x u \cdot n - \frac{1}{\zeta_r} \mathcal{R} U \right) \right] \int M dp d_n \omega.$$

Now the limiting equation (38) divided by $C = \int M dp d_n \omega$ reduces to

$$\begin{aligned} \partial_t \rho^0 + \nabla_x \cdot (u(x) \rho^0) + \mathcal{R} \cdot \left((n \times \nabla_x u \cdot n - \frac{\mathcal{R} U}{\zeta_r}) \rho^0 \right) &= \\ &= \frac{k_B T}{\zeta_t} \Delta_x \rho^0 + \frac{k_B T}{\zeta_r} \mathcal{R} \cdot \mathcal{R} \rho^0. \end{aligned}$$

Regrouping with ρ^0 replaced by ψ leads to

$$\partial_t \psi + \nabla_x \cdot (u(x) \psi) + \mathcal{R} \cdot (n \times \nabla_x u \cdot \psi) = D_t \Delta_x \psi + D_r \mathcal{R} \cdot \left[\mathcal{R} \psi + \frac{\psi}{k_B T} \mathcal{R} U \right],$$

where

$$D_t = \frac{k_B T}{\zeta_t}, \quad D_r = \frac{k_B T}{\zeta_r}.$$

This is exactly the equation derived for rod-like polymers with no inertial force.

Proof of Lemma 3.7. The integration is over ω from a tangent bundle with $(n, \omega) \in T\mathbb{S}^2$. We fix $n \in \mathbb{S}^2$ arbitrarily, it suffices to evaluate

$$\int_{n \cdot \omega = 0} e^{-\omega^2/a} (A \cdot \omega) \omega d_n \omega = \frac{a}{2} (Id - n \otimes n) A \int_{n \cdot \omega = 0} e^{-\omega^2/a} d_n \omega.$$

Let K be a rotational operator in \mathbb{R}^3 such that

$$n = K e_3, \quad K \in SO(3),$$

and use transform $\omega = K \omega'$, satisfying $|\omega|^2 = |\omega'|^2$.

Let $A = KB$, the transformation gives

$$\begin{aligned} \int_{n \cdot \omega = 0} e^{-\omega^2/a} (A \cdot \omega) \omega d_n \omega &= \int_{\omega'_3 = 0} e^{-(\omega')^2/a} (A \cdot K \omega') K \omega' d\omega' \\ &= K \int_{\omega'_3 = 0} e^{-((\omega'_1)^2 + (\omega'_2)^2)/a} (b_1 \omega'_1 + b_2 \omega'_2) \omega' d\omega'_1 d\omega'_2 \\ &= \frac{a}{2} K \begin{pmatrix} b_1 \\ b_2 \\ 0 \end{pmatrix} \int_{\omega'_3 = 0} e^{-((\omega'_1)^2 + (\omega'_2)^2)/a} d\omega'_1 d\omega'_2 \\ &= \frac{a}{2} K (B - e_3 b_3) \int_{n \cdot \omega = 0} e^{-\omega^2/a} d_n \omega \\ &= \frac{a}{2} (Id - n \otimes n) A \int_{n \cdot \omega = 0} e^{-\omega^2/a} d_n \omega. \end{aligned}$$

Here we have used the fact that

$$e_3 b_3 = K^{-1} n b_3 = n e_3^\top K^T A = K^{-1} n \otimes n A.$$

4. Concluding remarks. In this work we have derived novel kinetic equations for Dumbbell-like polymers as well as rod-like polymers. Inertial forces are taken care of by an augmented environment in an extended configuration space. In the case of rod-like polymers, the augmented space for orientation is just a tangent bundle of the usual sphere. We have also shown that the formal limit of the augmented equation recovers the usual inertia-free kinetic models explored in literature.

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