Continuity of velocity gradients in suspensions of rod–like molecules

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Abstract

We investigate the Doi model for suspensions of rod–like molecules in the dilute regime. For certain parameter values, the velocity gradient vs. stress relation defined by the stationary and homogeneous flow is not rank–one monotone. We then consider the evolution of possibly large perturbations of stationary flows. We prove that, even in absence of a microscopic cut–off, discontinuities in the velocity gradient cannot occur in finite time. The proof relies on a novel type of estimate for the Smoluchowski equation.

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1 Introduction

1.1 Summary

We consider the Doi model for suspensions of rod–like molecules in the dilute regime. This kinetic model couples a microscopic to a macroscopic equation. The macroscopic one is the Stokes equation for the fluid velocity, the microscopic equation is a Fokker–Planck (Smoluchowski) equation for the probability distribution of rod orientations in every point of physical space. Velocity gradients distort the isotropic equilibrium concentration; these deviations from isotropy in turn generate an additional macroscopic stress, which is elastic in nature and entropic in origin.

The model is characterized by two non–dimensional parameters: The Deborah number which relates the externally imposed time scale to the intrinsic relaxation time, and a non-dimensional measure of concentration which

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quantifies the relative importance of elastic vs. viscous stress. For sufficiently large values of these parameters, the strain rate vs. stress relation defined by the stationary and homogeneous flow is not rank–one monotone. This non–monotonicity has been related to the occurrence of transition layers in velocity gradients. We consider the evolution of flows that are (possibly large) perturbations of stationary homogeneous flows. We prove that even in the absence of a microscopic cut–off these discontinuities in the velocity gradients cannot occur in finite time. This is a confirmation of Doi model. The proof relies on a novel type of estimate for the Smoluchowski equation.

1.2 The Doi model

As a first approximation, we think of the identical liquid crystal molecules as inflexible rods of a thickness b which is much smaller than their length L, as illustrated in Figure 1. Let ν denote their constant number density. Following [5], we distinguish three regimes for the solution:

- Dilute regime. The rods are well separated, as expressed by $\nu \ll L^{-3}$.
- Concentrated regime. In this regime, the excluded volume effects reduce the entropy substantially. The theory by Onsager shows that this happens for $\nu \gtrsim b^{-1} L^{-2}$. For a critical value of the dimensionless number $\nu\, b\, L^2$, this leads to the isotropic nematic–phase transition [3, Section 2.2], [5, Section 10.2].
- Semi–dilute regime. On one hand, there is the kinetic effect that rods hinder themselves in their rotational movement. On the other hand, there is not yet an entropic effect: $L^{-3} \ll \nu \ll b^{-1} L^{-2}$.

We will focus on the dilute regime. We are interested in creeping flows, where the inertia of solvent (and rods) can be neglected.

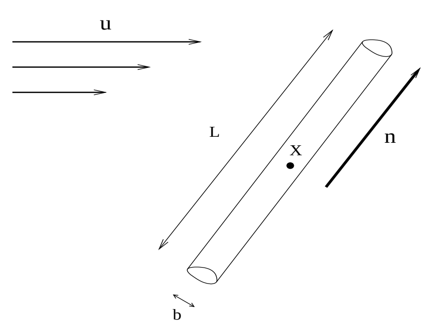

Figure 1: Rod–like molecule

Doi [4] introduced the model we will consider, see also [5, Chapter 8]. The system is described by a local *probability distribution* $f(x,t,n)\,dn$. It gives the time–dependent probability that a rod with center of mass at x has an axis n in the area element dn. The evolution of f is given by the Smoluchowski equation:

$$\begin{aligned}\partial_t f \;&=\; -\,u\cdot\nabla_x f \;-\; \nabla_n\cdot(P_{n^\perp}\nabla_x u\,n\,f) &(1)\\ &\quad\;+\,D\,\Delta_x f \;+\; D_r\,\Delta_n f. &(2)\end{aligned}$$

The two terms in (1) describe advection of the centers of mass by the velocity u respectively the rotation of the axes due to velocity gradients $\nabla_x u$. Here and in the sequel ∇_n, $\nabla_n\cdot$ and Δ_n denote the gradient, divergence and Laplacian on S^2. Finally, $P_{n^\perp}\nabla_x u\,n = \nabla_x u\,n - (n\cdot\nabla_x u\,n)\,n$ denotes the projection of the vector $\nabla_x u\,n$ on the tangent space in n.

The two terms in (2) describe the Brownian effects: translational diffusion respectively rotational diffusion. The Kirkwood theory [5, Appendix 8.1] derives asymptotic expressions for the diffusivities D and D_r from a microscopic theory. They scale as

$$D\;\sim\;\frac{k_B\,T}{\eta_s\,L}\quad\text{and}\quad D_r\;\sim\;\frac{k_B\,T}{\eta_s\,L^3} \tag{3}$$

(up to a logarithmic correction in $\frac{L}{b}$), where η_s denotes the viscosity of the solvent. The Kirkwood theory [5, Sec 8.3, App. 8.1] predicts that the longitudinal and transversal translational diffusion differ by an $O(1)$–factor. This difference is neglected here and the longitudinal and transversal diffusivities are taken equal; it will then turn out that the effect of translational diffusion is negligible. In the semi–dilute regime, the rotational diffusion would be hindered by the neighboring rods. This effect can be modeled by a mean–field *ansatz* on the level of the one–point statistics $f(t,x,n)\,dn$; it leads to a substantially reduced diffusivity $D_r(t,x,n)$. We also neglect this effect.

Diffusion can be seen as a gradient flow of the entropy functional

$$E[f]\;:=\;\nu\,k_B\,T\int_{\text{system}}\int_{S^2} f\,\ln f\,dn\,dx. \tag{4}$$

In the concentrated regime, the excluded volume effect would become important. Within a mean–field *ansatz*, this can be done on the level of the one–point statistics $f(t,x,n)\,dn$; it leads to the Onsager Potential. As we focus on the dilute regime, we neglect this term. As can be seen from (1), a velocity gradient $\nabla_x u$ distorts an isotropic distribution f which leads to an increase in entropy. Thermodynamic consistency [5, Section 8.6] requires that this is balanced by a stress tensor $\sigma(t,x)$ given by

$$\sigma(t,x) \;:=\; \nu\, k_B\, T \int_{S^2} (3\, n \otimes n - \mathrm{id})\, f(t,x,n)\, dn.$$

Notice that E plays the role of a stored energy functional and σ that of an elastic stress. The presence of the rod–like molecules gives also rise to a viscous stress which modifies the solvent viscosity. In the dilute and semi-dilute regimes, this additional viscous stress can be neglected. Hence the averaged continuity and momentum equations are given by

$$\nabla_x \cdot u \;=\; 0 \quad \text{and} \quad \nabla_x \cdot \left(\eta_s\, (\nabla_x + \nabla_x^t)\, u - p\, \mathrm{id} + \sigma\right) \;=\; 0. \tag{5}$$

Notice the coupling of the Smoluchowski equation (1) & (2) and the macroscopic equation (5) via the drift terms and the stress tensor σ. Together, they define an evolution for f.

We want to mimic a simple flow situation. The Doi model admits a special class of solutions that correspond to stationary flows driven by an externally imposed velocity gradient ∇u_{ext}, and we consider perturbations of such flows. For such flows there is a characteristic externally imposed time scale $\frac{1}{|\nabla_x u_{ext}|}$, and a macroscopic length scale L_{ext} related to the size of the perturbation. This evolution is a gradient flow of the entropy (4) and this will play a role in the analysis.

1.3 Non–dimensionalization

The problem has *three* characteristic time scales:

- The time scale related to rotational diffusion: $\frac{1}{D_r}$.
- A visco–elastic time scale $\frac{\eta_s}{k_B\, T\, \nu}$.
- An externally imposed time scale: $\frac{1}{|\nabla_x u_{ext}|}$.

We non–dimensionalize based on the visco–elastic time scale

$$t \;=\; \frac{\eta_s}{k_B\, T\, \nu}\, \hat{t}.$$

Since the translational diffusion has units of $\frac{\text{length}^2}{\text{time}}$, this gives rise to three length scales. In addition, there is the external length scale, which we use for non–dimensionalization:

$$x \;=\; L_{ext}\, \hat{x}.$$

This imposes the following non–dimensionalization of velocity, strain and stresses:

$$\begin{aligned} u &= L_{ext} \frac{k_B T \nu}{\eta_s} \hat{u}, \qquad \nabla_x u = \frac{k_B T \nu}{\eta_s} \nabla_{\hat{x}} \hat{u}, \\ \sigma &= k_B T \nu \, \hat{\sigma}, \qquad p = k_B T \nu \, \hat{p}. \end{aligned}$$

We are left with three non–dimensional parameters:

$$\begin{aligned} \hat{D}_r &= D_r \frac{\eta_s}{k_B T \nu} \overset{(3)}{\sim} (L^3 \nu)^{-1}, \\ \hat{D} &= D \frac{\eta_s}{k_B T \nu} L_{ext}^{-2} \overset{(3)}{\sim} (L L_{ext}^2 \nu)^{-1}, \\ \widehat{\nabla_x u_{ext}} &= \frac{\eta_s}{k_B T \nu} \nabla_x u_{ext}. \end{aligned}$$

Sometimes, it is more convenient to think in terms of the Deborah number $\widehat{\nabla_x u_{ext}}/\hat{D}_r = \nabla_x u_{ext}/D_r$, which relates the externally imposed time scale to the rotational relaxation time.

We collect the nondimensionalized equations (dropping the hats):

$$\partial_t f + \nabla_x f \cdot u + \nabla_n \cdot (P_{n\perp} \nabla_x u \, n \, f) - D_r \triangle_n f - D \triangle_x f = 0, \tag{6}$$

$$\int_{S^2} (3\, n \otimes n - \mathrm{id}) f \, dn = \sigma, \tag{7}$$

$$\nabla_x \cdot \big((\nabla_x u + \nabla_x^t u) - p \, \mathrm{id} + \sigma \big) = 0, \tag{8}$$

$$\nabla_x \cdot u = 0\,. \tag{9}$$

These form a system consisting of the transport equation (6) coupled with the Stokes system (8)-(9). The coupling is effected via (7) that determines the viscoelastic stresses as moments of the probability distribution f. The function $f(t, x, n)$ is a probability density on S^2,

$$f \geq 0\,, \qquad \int_{S^2} f(t, x, n) \, dn = 1\,. \tag{10}$$

This requirement is consistent with the evolution (6). Our system is supplemented with initial conditions

$$f(0, x, n) = f_0(x, n) \tag{11}$$

and one checks that property (10) is propagated from the initial data to solutions of (6).

The model (6)-(9) admits a special class of stationary steady states: Let $\nabla_x u_{ext}$ be a given traceless tensor, $\mathrm{tr}\nabla_x u_{ext} = 0$, then

$$u_{ext}(x) = (\nabla_x u_{ext})\, x \tag{12}$$

gives rise to an incompressible vector field. Define $f_{eq}(n)$ to be the unique solution of the stationary Fokker-Planck equation

$$\nabla_n \cdot (P_{n^\perp} \nabla_x u_{ext} n f - D_r \nabla_n f) = 0 \tag{13}$$

satisfying $f_{eq}(n) \geq 0$ and $\int_{S^2} f_{eq}(n) dn = 1$. Notice that $(f_{eq}(n), u_{ext}(x))$ is a stationary, steady solution of (6)-(9) associated to a constant pressure and with

$$\sigma_{eq} = \int_{S^2} (3n \otimes n - \mathrm{id}) f_{eq} dn\,.$$

This class plays an important role in our analysis. It will be used as a building block for constructing non-monotone spatially varying steady states, and we will study the evolution of (large) perturbations of $(f_{eq}(n), u_{ext}(x))$.

1.4 Non-monotonicity of steady states

Let $(f_{eq}(n), u_{ext}(x))$ be as defined in (12) & (13) and σ_{eq} be the associated moment in (7). By varying parametrically the imposed velocity gradient $\kappa = \nabla_x u_{ext}$ we define a mapping

$$\mathrm{End}(\mathbb{R}^3) \ni \kappa \mapsto \sigma_\kappa \in \mathrm{Sym}(\mathbb{R}^3), \tag{14}$$

taking strain-rates to elastic stresses and defined by (7). A necessary condition for structural stability of the homogeneous flow κx is that the mapping from deformation–rates to total stresses

$$\mathrm{End}(\mathbb{R}^3) \ni \kappa \mapsto (\kappa + \kappa^t) + \sigma_\kappa \in \mathrm{Sym}(\mathbb{R}^3) \tag{15}$$

be rank–one monotone at the κ under consideration. After appropriate rescaling with D_r, (14) is universal (see Definition 1). We will argue in Section 3.2 that it fails to be monotone along the shear direction (Lemmas 4 and 5). This implies that (15) fails to be monotone along the shear direction for sufficiently small D_r.

One effect of this non–monotonicity in the shear direction is that there exist spatially discontinuous solutions $(f(x, n), u(x))$ for vanishing translational diffusivity ($D = 0$), i. e. solutions of

$$\begin{aligned}
\nabla_x \cdot (f\, u) + \nabla_n \cdot (P_{n\perp} \nabla_x u\, n\, f) - D_r \triangle_n f &= 0, && (16)\\
\int_{S^2} (3\, n \otimes n - \mathrm{id}) f\, dn &= \sigma, && (17)\\
\nabla_x \cdot \big((\nabla_x u + \nabla_x^t u) - p\, \mathrm{id} + \sigma \big) &= 0, && (18)\\
\nabla_x \cdot u &= 0. && (19)
\end{aligned}$$

More precisely, we will show:

Theorem 1. *There exist $D_r > 0$ such that (16)–(19) admits a solution (in the distributional sense) with discontinuous $\nabla_x u$.*

This failure of ellipticity for (16)–(19) has been frequently seen as a deficiency of the Doi model. On the contrary, other schools have advocated the failure of ellipticity of steady states as the cause of the onset of instabilities in viscoelastic flows, and in particular as an explanation of the phenomenon of spurt. Spurt refers to a sudden increase of the volumetric flow rate at a critical stress which has been observed experimentally, see for instance [18]. Spurt has been connected in [11] to the non–monotonicity of the map (15), which allows for jumps in the steady strain rate when the driving pressure gradient exceeds a critical value. Such jumps can account for the sudden increase in the flow rate observed in experiments. This explanation of spurt motivated analytical results regarding existence of discontinuous steady states and their stability properties, accomplished for macroscopic models in the absence of translational diffusion D and for a 1–d geometry. The macroscopic model (Oldroyd B or Johnson–Segalman) can be seen as an exact closure of a kinetic model with Hookean springs instead of rigid rods. It has been shown that discontinuities in the strain rate $\nabla_x u$ form in infinite time, see [13, 12].

1.5 Continuity of velocity gradients

The main goal of this paper is to investigate on which time scale these near–discontinuities occur. We want to study a forced problem, and to this end we consider a solution that is a perturbation of the stationary steady state $(f_{eq}(n), u_{ext}(x))$ in (12)-(13). Our analysis is valid even for large perturbations and we find that the time scale can be bounded by below independently of the translational diffusion D, just in terms of the non–dimensional parameter D_r, and $\nabla_x u_{ext}$, see Theorem 2.

We now outline our strategy. Qualitatively speaking, we want to

control the modulus of continuity of $\nabla_x u$.

By Sobolev's embedding, this is a consequence of

$$\text{control of } \int_{\mathbb{R}^3} |\nabla_x^2 u|^p dx$$

for some fixed $3 < p < \infty$. In view of (8)&(9) and standard L^p–regularity theory for the Stokes system, this is a consequence of

$$\text{control of } \int_{\mathbb{R}^3} |\nabla_x \sigma|^p dx,$$

see Lemma 2. In view of (7), which yields

$$\partial_{x_i}\sigma \;=\; \int_{S^2} (3\, n\otimes n - \mathrm{id})\, \partial_{x_i} f\, dn, \tag{20}$$

this requires control of $\nabla_x f$. This control has to be the L^p–norm with respect to x but can be a weak norm with respect to n, for instance an $H^{-1}(S^2)$–norm. Recall that the $H^{-1}(S^2)$–norm of $\nabla_x f$ can be defined as

$$\|\nabla_x f\|_{H^{-1}(S^2)} := \left(\int_{S^2} |\nabla_n \phi|^2 dn\right)^{1/2},$$

where the potential $\phi = (\phi_1, \phi_2, \phi_3)$ is the solution of the Poisson problem for the Laplace operator

$$\partial_{x_i} f - \triangle_n \phi_i \;=\; 0.$$

For reasons intrinsic to the Fokker–Planck–like equation (16) (see the proof of Proposition 1), our choice is an f–dependent version of an $H^{-1}(S^2)$–norm of $\nabla_x f$:

$$\|\nabla_x f\|_{H_f^{-1}(S^2)} := \left(\int_{S^2} |\nabla_n \phi|^2 f\, dn\right)^{1/2},$$

where the potential $\phi = (\phi_1, \phi_2, \phi_3)$ is the solution of the following elliptic problem on S^2:

$$\partial_{x_i} f - \nabla_n \cdot (f \nabla_n \phi_i) \;=\; 0. \tag{21}$$

(Note that, for any tensor g, $|g|^2$ denotes the sum of the squares of the entries with respect to orthonormal bases.) This norm comes from a natural Riemannian structure of the space of probability densities f which was introduced in [14], see also [15, Section 3].
Accordingly, we define the quantities

$$w(t,x) \;=\; \int_{S^2} |\nabla_n \phi|^2\, f\, dn \tag{22}$$

and

$$W(t) := \int_{\mathbb{R}^3} w^{p/2}\, dx = \int_{\mathbb{R}^3} \left(\int_{S^2} |\nabla_n \phi|^2 f\, dn \right)^{p/2} dx\,, \tag{23}$$

and seek to establish control of $W(t)$.

A second ingredient is an identity for the relative entropy density

$$e(t,x) := \int_{S^2} (\ln \frac{f}{f_{eq}})\, f\, dn, \tag{24}$$

see Lemma 1 and [10], that yields differential control for the relative entropy

$$E(t) := \int_{\mathbb{R}^3} e(t,x)\, dx = \int_{\mathbb{R}^3} \int_{S^2} (\ln \frac{f}{f_{eq}})\, f\, dn dx\,. \tag{25}$$

We prove:

Theorem 2. *Let (f, u, p) be a solution of (6)–(9) (with $D = 0$ allowed), let (f_{eq}, u_{ext}) be as in* (12)-(13) *and assume that the data f_0 satisfy*

$$E(0) \;=\; \int_{\mathbb{R}^3} \int_{S^2} (\ln \frac{f_0}{f_{eq}})\, f_0\, dn\, dx < +\infty\,.$$

There exists a constant C only depending on $p \in (3, \infty)$ and a constant K only depending on $|\nabla_x u_{ext}|/D_r$ such that

$$\frac{dE}{dt} \;\le\; K\, E, \tag{26}$$

$$\frac{1}{p}\,\frac{dW}{dt} \;\le\; -D_r W + C\, \left(1 + |\nabla_x u_{ext}| + \ln E(t) + \ln W\right)\, W. \tag{27}$$

Remark 1. *Integrating the differential inequalities we obtain the bounds*

$$E(t) \le E(0) e^{K\,t} \tag{28}$$

$$W(t) \le \exp\left\{ (\ln W(0) + K)\, e^{K\,t} \right\} \tag{29}$$

Moreover, the following estimate

$$\begin{aligned} \int_{\mathbb{R}^3} |\nabla_x (u - u_{ext})|^2\, dx &\le \int_{\mathbb{R}^3} |\sigma - \sigma_{eq}|^2\, dx \\ &\le\; C \int_{\mathbb{R}^3} \left(\int_{S^2} |f - f_{eq}| dn \right)^2 dx < E(0)\, e^{Kt} \end{aligned} \tag{30}$$

is derived in Proposition 3 as a byproduct of the proof.

Let us comment only on the most pertinent mathematical literature: In [8], a purely macroscopic viscoelastic model is considered (Oldroyd–B). It can be interpreted as an exact closure of a kinetic model for Hookean springs instead of rigid rods. The existence of weak solutions is established by "propagation of compactness". This approach can be extended to our kinetic model [9]. Theorem 2 might be seen as a quantification of the more qualitative approach in [8].

In [6], a kinetic model for nonlinear springs is investigated (FENE). Among other things, sufficient conditions on the asymptotic stability of the homogeneous flow $\nabla_x u \equiv \nabla_x u_{ext}$ are given. A more careful analysis, to appear in [10], reveals that

$$\frac{dE}{dt} \;\le\; \Big(C\big(\frac{|\nabla_x u_{ext}|}{D_r}\big)^2 - C^{-1}\, D_r\, \exp\big(-C\,\frac{|\nabla_x u_{ext}|}{D_r}\big)\Big)\, E.$$

Hence also Theorem 2, in this extended version, yields a stability result in the regime of sufficiently small concentration $D_r \gg 1$ and sufficiently small Deborah number $|\nabla_x u_{ext}| \ll D_r$ (provided the initial perturbation $W(0)$ is sufficiently small). Finally, we refer to [2] for a recent global existence result, which is also valid in the concentrated regime, for flows that are asymptotically at rest at infinity driven by a body force. For comparison purposes, the present flow lies in the dilute regime but approaches any constant gradient flow at infinity.

2 Proof of Theorem 2

Theorem 2 is based on the following ingredients: an identity for the transport of the relative entropy density $e(t,x)$ defined in (24), a transport inequality for the norm $w(t,x)$ defined in (22), an L^∞ estimation for the Stokes system, and the derivation of differential inequalities for the quantities $E(t)$ and $W(t)$ in (25) and (23) respectively.

2.1 A relative entropy identity

Let $(u_{ext}, f_{eq}(n))$ be a stationary steady state as in (12)-(13) and let (f,u,p) be a solution of (6)-(9) which approaches at infinity $(u_{ext}, f_{eq}(n))$. The relative entropy density

$$e(t,x) := \int_{S^2} (\ln \frac{f}{f_{eq}})\, f\, dn, \tag{31}$$

serves as a measure of the distance between f_{eq} and f and satisfies the following identity.

Lemma 1. *Let* (f, u, p) *satisfy* (6)-(9)*, then*

$$
\begin{aligned}
&\big(\partial_t + u\cdot\nabla_x - D\triangle_x\big)e \\
&\qquad + D\int_{S^2} |\nabla_x(\ln\frac{f}{f_{eq}})|^2\, f\, dn + D_r\int_{S^2} |\nabla_n(\ln\frac{f}{f_{eq}})|^2\, f\, dn \\
&= \nabla_x(u-u_{ext}) : \left((\sigma-\sigma_{eq}) - \int_{S^2}\big(\nabla_n \ln f_{eq}\otimes n\big)(f-f_{eq})\right)\, dn\,.
\end{aligned}
$$

Proof of Lemma 1. Using the property that f_{eq} is independent of x and t, we derive from the Smoluchowski equation (6) the formula

$$
\begin{aligned}
&\big(\partial_t + u\cdot\nabla_x - D\triangle_x\big)\big(f\ln\frac{f}{f_{eq}}\big) + Df\big|\nabla_x \ln\frac{f}{f_{eq}}\big|^2 \\
&= \Big(1+\ln\frac{f}{f_{eq}}\Big)\Big(-\nabla_n\cdot(P_{n^\perp}\nabla_x u\, n\, f) + D_r\triangle_n f\Big) \\
&= -\Big(1+\ln\frac{f}{f_{eq}}\Big)\,\nabla_n\cdot\Big(P_{n^\perp}\nabla_x u\, n\, f - D_r\,\nabla_n f\Big),
\end{aligned}
$$

which after an integration over S^2 gives by integration by parts

$$
\begin{aligned}
&\big(\partial_t + u\cdot\nabla_x - D\triangle_x\big)e + D\int_{S^2}\big|\nabla_x \ln\frac{f}{f_{eq}}\big|^2\, f\, dn \\
&= \int_{S^2}\nabla_n \ln\frac{f}{f_{eq}}\cdot P_{n^\perp}\big(\nabla_x u - \nabla_x u_{ext}\big)\, n\, f\, dn \\
&\quad \int_{S^2}\nabla_n \ln\frac{f}{f_{eq}}\cdot\big(P_{n^\perp}\nabla_x u_{ext}\, n\, f - D_r\nabla_n f\big)\, dn \\
&=: J_1 + J_2.
\end{aligned}
\tag{32}
$$

We first treat J_2, by a classical formula for drift–diffusion equations. We write

$$
\begin{aligned}
&P_{n^\perp}\nabla_x u_{ext}\, n\, f - D_r\nabla_n f \\
&\quad = -D_r\, f_{eq}\,\nabla_n\frac{f}{f_{eq}} + \frac{f}{f_{eq}}\big(P_{n^\perp}\nabla_x u_{ext}\, n\, f_{eq} - D_r\nabla_n f_{eq}\big) \\
&\quad = -D_r\, f\,\nabla_n \ln\frac{f}{f_{eq}} + \frac{f}{f_{eq}}\big(P_{n^\perp}\nabla_x u_{ext}\, n\, f_{eq} - D_r\nabla_n f_{eq}\big),
\end{aligned}
$$

so that

$$\begin{aligned}
J_2 &= \int_{S^2} \nabla_n(\ln \frac{f}{f_{eq}}) \cdot \big(P_{n^\perp}\nabla_x u_{ext}\, n\, f - D_r \nabla_n f\big)\, dn \\
&= -D_r \int_{S^2} |\nabla_n(\ln \frac{f}{f_{eq}})|^2 f\, dn \\
&\quad + \int_{S^2} \frac{f}{f_{eq}} \nabla_n(\ln \frac{f}{f_{eq}}) \cdot \big(P_{n^\perp}\nabla_x u_{ext}\, n\, f_{eq} - D_r \nabla_n f_{eq}\big)\, dn. \qquad (33)
\end{aligned}$$

The last term in (33) vanishes by definition (13) of f_{eq}:

$$\begin{aligned}
&\int_{S^2} \frac{f}{f_{eq}} \nabla_n(\ln \frac{f}{f_{eq}}) \cdot \big(P_{n^\perp}\nabla_x u_{ext}\, n\, f_{eq} - D_r \nabla_n f_{eq}\big)\, dn \\
&= \int_{S^2} \nabla_n(\frac{f}{f_{eq}}) \cdot \big(P_{n^\perp}\nabla_x u_{ext}\, n\, f_{eq} - D_r \nabla_n f_{eq}\big)\, dn \\
&= -\int_{S^2} \frac{f}{f_{eq}} \nabla_n \cdot \big(P_{n^\perp}\nabla_x u_{ext}\, n\, f_{eq} - D_r \nabla_n f_{eq}\big)\, dn \;=\; 0.
\end{aligned}$$

Hence we have

$$J_2 \;=\; -D_r \int_{S^2} |\nabla_n(\ln \frac{f}{f_{eq}})|^2 f\, dn \qquad (34)$$

We now turn to J_1:

$$\begin{aligned}
J_1 &= \int_{S^2} \nabla_n \ln \frac{f}{f_{eq}} \cdot \nabla_x(u - u_{ext})\, n\, f\, dn \\
&= \nabla_x(u - u_{ext}) : \int_{S^2} \nabla_n \ln \frac{f}{f_{eq}} \otimes n\, f\, dn \\
&= \nabla_x(u - u_{ext}) : \Big(\int_{S^2} \nabla_n f \otimes n\, dn - \int_{S^2} \nabla_n f_{eq} \otimes n\, dn \\
&\qquad - \int_{S^2} (\nabla_n \ln f_{eq} \otimes n)\,(f - f_{eq})\, dn \Big). \qquad (35)
\end{aligned}$$

According to formula (95) in Appendix II and the definition (7) of σ we have

$$\begin{aligned}
&\int_{S^2} \nabla_n f \otimes n\, dn - \int_{S^2} \nabla_n f_{eq} \otimes n\, dn \\
&= \int_{S^2} (3\, n \otimes n - \mathrm{id}) f\, dn - \int_{S^2} (3\, n \otimes n - \mathrm{id}) f_{eq}\, dn \\
&= \sigma - \sigma_{eq}.
\end{aligned}$$

Hence J_1 can be rewritten as

$$J_1 \;=\; \nabla_x(u - u_{ext}) : \Big((\sigma - \sigma_{eq}) - \int_{S^2} (\nabla_n \ln f_{eq} \otimes n)(f - f_{eq})\, dn \Big). \qquad (36)$$

Lemma 1 follows from a combining of (32) with (34) and (36). $\square$

2.2 Transport inequality for the H_f^{-1}-norm

We introduce the H_f^{-1}-norm as defined by (22) and (21) and proceed to derive a differential inequality for w.

Proposition 1. *For any solution of* (6) *we have the partial differential inequality:*

$$\begin{aligned}
&\partial_t(\tfrac{1}{2}w) + \nabla_x(\tfrac{1}{2}w)\cdot u - D\,\triangle_x(\tfrac{1}{2}w)\\
&\qquad \le\ -D_r\,w + |\nabla_x u + \nabla_x^t u|\,w + |\nabla_x^2 u|\,w^{1/2}.
\end{aligned} \tag{37}$$

Proof of Proposition 1. We start by differentiating the defining equation (21) with respect to t:

$$\partial_{x_i}\partial_t f - \nabla_n\cdot(f\nabla_n\partial_t\phi_i) - \nabla_n\cdot(\partial_t f\nabla_n\phi_i)\ =\ 0. \tag{38}$$

Thus we have

$$\begin{aligned}
&\frac{d}{dt}\int_{S^2}\tfrac{1}{2}|\nabla_n\phi_i|^2\,f\,dn\\
&\quad= \int_{S^2}\big(\partial_t f\,\tfrac{1}{2}|\nabla_n\phi_i|^2 + f\,\nabla_n\phi_i\cdot\nabla_n\partial_t\phi_i\big)\,dn\\
&\quad= \int_{S^2}\big(\partial_t f\,\tfrac{1}{2}|\nabla_n\phi_i|^2 - \nabla_n\cdot(f\,\nabla_n\partial_t\phi_i)\,\phi_i\big)\,dn\\
&\quad\overset{(38)}{=} \int_{S^2}\big(\partial_t f\,\tfrac{1}{2}|\nabla_n\phi_i|^2 + \nabla_n\cdot(\partial_t f\,\nabla_n\phi_i)\,\phi_i - \partial_{x_i}\partial_t f\,\phi_i\big)\,dn\\
&\quad= \int_{S^2}\big(-\partial_t f\,\tfrac{1}{2}|\nabla_n\phi_i|^2 - \partial_{x_i}\partial_t f\,\phi_i\big)\,dn.
\end{aligned} \tag{39}$$

The contributions of the terms $\partial_t f$ and $\partial_{x_i}\partial_t f$ in (39) are calculated by invoking (6). We start with the contribution of the rotational diffusion term. It is given by

$$\begin{aligned}
&\int_{S^2}\big(-\triangle_n f\,\tfrac{1}{2}|\nabla_n\phi_i|^2 - \partial_{x_i}\triangle_n f\,\phi_i\big)\,dn\\
&\quad= \int_{S^2}\big(-\triangle_n f\,\tfrac{1}{2}|\nabla_n\phi_i|^2 - \partial_{x_i} f\,\triangle_n\phi_i\big)\,dn\\
&\quad\overset{(21)}{=} \int_{S^2}\big(-\triangle_n f\,\tfrac{1}{2}|\nabla_n\phi_i|^2 - \nabla_n\cdot(f\nabla_n\phi_i)\,\triangle_n\phi_i\big)\,dn\\
&\quad= \int_{S^2}\big(-\triangle_n(\tfrac{1}{2}|\nabla_n\phi_i|^2) + \nabla_n\phi_i\cdot\nabla_n\triangle_n\phi_i\big)\,f\,dn.
\end{aligned}$$

We now appeal to Bochner's formula

$$\triangle_n(\tfrac{1}{2}|\nabla_n\phi_i|^2) \;=\; \nabla_n\phi_i\cdot\nabla_n\triangle_n\phi_i + \mathrm{tr}(\mathrm{Hess}_n\phi_i\,\mathrm{Hess}_n^t\phi_i) + \nabla_n\phi_i\cdot\mathrm{Ric}\,\nabla_n\phi_i,$$

where $\mathrm{Hess}_n\phi_i$ denotes the Hessian (a covariant notion) and Ric the Ricci curvature tensor. We refer for instance to [16, Proposition 3.3, p. 175]. On S^2, Ric is just the metric tensor. Hence we obtain

$$-\triangle_n(\tfrac{1}{2}|\nabla_n\phi_i|^2) + \nabla_n\phi_i\cdot\nabla_n\triangle_n\phi_i \;\le\; -|\nabla_n\phi_i|^2\,,$$

and the contribution of rotational diffusion is

$$\sum_i\int_{S^2}\big(-\triangle_n f\,\tfrac{1}{2}|\nabla_n\phi_i|^2 - \triangle_n\partial_{x_i}f\,\phi_i\big)\,dn \;\le\; -\int_{S^2}|\nabla_n\phi|^2 f\,dn.$$

We now treat the term coming from the translational diffusion. In view of (39), it is given by

$$\begin{aligned}
&\int_{S^2}\big(-\triangle_x f\,\tfrac{1}{2}|\nabla_n\phi_i|^2 - \partial_{x_i}\triangle_x f\,\phi_i\big)\,dn\\
&\quad\overset{(21)}{=}\int_{S^2}\big(-\triangle_x f\,\tfrac{1}{2}|\nabla_n\phi_i|^2 - \triangle_x\nabla_n\cdot(f\nabla_n\phi_i)\,\phi_i\big)\,dn\\
&\quad=\int_{S^2}\big(-\triangle_x f\,\tfrac{1}{2}|\nabla_n\phi_i|^2 + \triangle_x(f\nabla_n\phi_i)\cdot\nabla_n\phi_i\big)\,dn.
\end{aligned}$$

The identities

$$\begin{aligned}
&-\triangle_x f\,\tfrac{1}{2}|\nabla_n\phi_i|^2 + \triangle_x(f\nabla_n\phi_i)\cdot\nabla_n\phi_i\\
&\quad=\triangle_x f\,\tfrac{1}{2}|\nabla_n\phi_i|^2 + 2\sum_j\partial_{x_j}f\partial_{x_j}\nabla_n\phi_i\cdot\nabla_n\phi_i + f\triangle_x(\nabla_n\phi_i)\cdot\nabla_n\phi_i\\
&\quad=\triangle_x f\,\tfrac{1}{2}|\nabla_n\phi_i|^2 + 2\sum_j\partial_{x_j}f\partial_{x_j}\tfrac{1}{2}|\nabla_n\phi_i|^2\\
&\qquad\quad+\sum_j\big(f\partial_{x_j}\big(\partial_{x_j}(\nabla_n\phi_i)\cdot\nabla_n\phi_i\big) - f\partial_{x_j}\nabla_n\phi_i\cdot\partial_{x_j}\nabla_n\phi_i\big)\\
&\quad=\triangle_x\left(f\tfrac{1}{2}|\nabla_n\phi_i|^2\right) - f\sum_j\partial_{x_j}\nabla_n\phi_i\cdot\partial_{x_j}\nabla_n\phi_i\\
&\quad=\triangle_x\left(f\tfrac{1}{2}|\nabla_n\phi_i|^2\right) - f|\nabla^2_{x,n}\phi_i|^2
\end{aligned}$$

show that the contribution is given by

$$\triangle_x\left(\int_{S^2}\tfrac{1}{2}|\nabla_n\phi|^2\,f\,dn\right) - \int_{S^2}|\nabla^2_{x,n}\phi|^2\,f\,dn.$$

For the inequality (37), we drop the non positive second term.

We now treat the contribution from the advection term in x. It splits into two parts

$$
\begin{aligned}
&\int_{S^2} \left(\nabla_x f \cdot u \, \tfrac{1}{2}|\nabla_n \phi_i|^2 + \partial_{x_i}(\nabla_x f \cdot u)\, \phi_i\right) \, dn \\
&\quad = \int_{S^2} \left(\nabla_x f \cdot u \, \tfrac{1}{2}|\nabla_n \phi_i|^2 + (\nabla_x \partial_{x_i} f \cdot u + \nabla_x f \cdot \partial_{x_i} u)\, \phi_i\right) \, dn \\
&\quad = \sum_j \int_{S^2} \left(\partial_{x_j} f \, \tfrac{1}{2}|\nabla_n \phi_i|^2 + \partial_{x_j}\partial_{x_i} f \, \phi_i\right) \, dn \; u_j \\
&\quad + \sum_j \partial_{x_i} u_j \int_{S^2} \partial_{x_j} f \, \phi_i \, dn \, .
\end{aligned}
$$

For the first term we observe

$$
\begin{aligned}
&\int_{S^2} \left(\partial_{x_j} f \, \tfrac{1}{2}|\nabla_n \phi_i|^2 + \partial_{x_j}\partial_{x_i} f \, \phi_i\right) \, dn \\
&\quad \overset{(21)}{=} \int_{S^2} \left(\partial_{x_j} f \, \tfrac{1}{2}|\nabla_n \phi_i|^2 + \partial_{x_j} \nabla_n \cdot (f \nabla_n \phi_i)\, \phi_i\right) \, dn \\
&\quad = \int_{S^2} \left(\partial_{x_j} f \, \tfrac{1}{2}|\nabla_n \phi_i|^2 - \partial_{x_j} (f \nabla_n \phi_i) \cdot \nabla_n \phi_i\right) \, dn \\
&\quad = -\int_{S^2} \partial_{x_j} (f \, \tfrac{1}{2}|\nabla_n \phi_i|^2) \, dn \\
&\quad = -\partial_{x_j} \left(\int_{S^2} \tfrac{1}{2}|\nabla_n \phi_i|^2 f \, dn \right).
\end{aligned}
$$

For the second term we notice

$$
\begin{aligned}
\sum_j \partial_{x_i} u_j \int_{S^2} \partial_{x_j} f \, \phi_i \, dn &\overset{(21)}{=} \sum_j \partial_{x_i} u_j \int_{S^2} \nabla_n \cdot (f \nabla_n \phi_j)\, \phi_i \, dn \\
&= -\sum_j \partial_{x_i} u_j \int_{S^2} \nabla_n \phi_j \cdot \nabla_n \phi_i \, f \, dn.
\end{aligned}
$$

Hence the contribution from advection in x is

$$
\begin{aligned}
&\sum_i \int_{S^2} \left(\nabla_x f \cdot u \, \tfrac{1}{2} |\nabla_n \phi_i|^2 + \partial_{x_i} (\nabla_x f \cdot u) \, \phi_i \right) \, dn \\
&\quad = \; - \sum_{i,j} \partial_{x_j} \left(\int_{S^2} \tfrac{1}{2} |\nabla_n \phi_i|^2 f \, dn \right) \, u_j \; - \sum_{i,j} \int_{S^2} \nabla_n \phi_j \cdot \nabla_n \phi_i \, f \, dn \, \partial_{x_i} u_j \\
&\quad = \; -\nabla_x \left(\int_{S^2} \tfrac{1}{2} |\nabla_n \phi|^2 f \, dn \right) \cdot u \\
&\qquad\qquad - \tfrac{1}{2} \sum_{i,j} \int_{S^2} \nabla_n \phi_j \cdot \nabla_n \phi_i \, f \, dn \, (\partial_{x_i} u_j + \partial_{x_j} u_i) \\
&\quad \leq \; -\nabla_x \left(\int_{S^2} \tfrac{1}{2} |\nabla_n \phi|^2 f \, dn \right) \cdot u \; + \; \tfrac{1}{2} \int_{S^2} |\nabla_n \phi|^2 \, f \, dn \, |\nabla_x u + \nabla_x^t u| .
\end{aligned}
$$

We finally come to the contribution from the drift term in n. We introduce the notation $b = P_{n^\perp} \nabla_x u \, n$ for the drift term:

$$
\begin{aligned}
&\int_{S^2} \left(\nabla_n \cdot (b \, f) \, \tfrac{1}{2} |\nabla \phi_i|^2 + \partial_{x_i} \nabla_n \cdot (b \, f) \, \phi_i \right) \, dn \\
&\quad = \; \int_{S^2} \left(\nabla_n \cdot (b \, f) \, \tfrac{1}{2} |\nabla \phi_i|^2 + \nabla_n \cdot (b \, \partial_{x_i} f + \partial_{x_i} b \, f) \, \phi_i \right) \, dn \\
&\quad \overset{(21)}{=} \; \int_{S^2} \left(\nabla_n \cdot (b \, f) \, \tfrac{1}{2} |\nabla \phi_i|^2 + \nabla_n \cdot (b \, \nabla_n \cdot (f \nabla_n \phi_i) + \partial_{x_i} b \, f) \; \phi_i \right) \, dn \\
&\quad = \; \int_{S^2} \left(-b \cdot \nabla_n (\tfrac{1}{2} |\nabla_n \phi_i|^2) + \nabla_n (b \cdot \nabla_n \phi_i) \cdot \nabla_n \phi_i - \partial_{x_i} b \cdot \nabla_n \phi_i \right) \, f \, dn
\end{aligned} \tag{40}
$$

We now use the formula

$$
\begin{aligned}
&-b \cdot \nabla_n (\tfrac{1}{2} |\nabla_n \phi_i|^2) + \nabla_n \phi_i \cdot \nabla_n (b \cdot \nabla_n \phi_i) \\
&\quad = \; -\nabla_n \phi_i \cdot \mathrm{Hess}_n \phi_i \, b + (b \cdot \mathrm{Hess}_n \phi_i \, \nabla_n \phi_i + \nabla_n \phi_i \cdot \mathrm{D}_n b \, \nabla_n \phi_i) \\
&\quad = \nabla_n \phi_i \cdot \mathrm{D}_n b \, \nabla_n \phi_i ,
\end{aligned} \tag{41}
$$

where $\mathrm{D}_n b$ denotes the covariant derivative of b on S^2. Since

$$
b \; = \; P_{n^\perp} \nabla_x u \, n \; = \; \nabla_x u \, n - (n \cdot \nabla_x u \, n) \, n \, ,
$$

we obtain for the component-wise derivative in a tangential direction $\tau \in n^\perp$

$$
\nabla_n b \, \tau \; = \; \nabla_x u \, \tau - (\tau \cdot \nabla_x u \, n) \, n - (n \cdot \nabla_x u \, \tau) \, n - (n \cdot \nabla_x u \, n) \, \tau
$$

and thus for the covariant derivative

$$
\mathrm{D}_n b \, \tau \; = \; P_{n^\perp} \nabla_n b \, \tau \; = \; (P_{n^\perp} \, \nabla_x u - (n \cdot \nabla_x u \, n) \, \mathrm{id}) \, \tau . \tag{42}
$$

Furthermore we have

$$\partial_{x_i} b \;=\; P_{n^\perp}\, \partial_{x_i} \nabla_x u\, n. \tag{43}$$

Inserting (43), (42) into (41) and (40), and since $\nabla_n \phi_i$ is on the tangent space of the sphere, we obtain

$$\begin{aligned}
&\int_{S^2} \big(\nabla_n \cdot (b\, f)\, \tfrac{1}{2}|\nabla \phi_i|^2 + \partial_{x_i} \nabla_n \cdot (b\, f)\, \phi_i\big)\; dn \\
&\quad = \int_{S^2} \nabla_n \phi_i \cdot (\nabla_x u - (n \cdot \nabla_x u\, n)\, \mathrm{id})\; \nabla_n \phi_i\, f\, dn \\
&\quad - \int_{S^2} \nabla_n \phi_i \cdot \partial_{x_i} \nabla_x u\, n\, f\, dn.
\end{aligned}$$

Thus the contribution from the drift term in n is

$$\begin{aligned}
&\sum_i \int_{S^2} \big(\nabla_n \cdot (b\, f)\, \tfrac{1}{2}|\nabla \phi_i|^2 + \partial_{x_i} \nabla_n \cdot (b\, f)\, \phi_i\big)\; dn \\
&\quad = \tfrac{1}{2} \sum_i \int_{S^2} \nabla_n \phi_i \cdot \big((\nabla_x u + \nabla_x^t u) - (n \cdot (\nabla_x u + \nabla_x^t u)\, n)\, \mathrm{id}\big)\; \nabla_n \phi_i\, f\, dn \\
&\quad - \int_{S^2} \nabla_n \phi_i \cdot \partial_{x_i} \nabla_x u\, n\, f\, dn \\
&\quad \le \tfrac{1}{2} \int_{S^2} |\nabla_n \phi|^2\, f\, dn\, |\nabla_x u + \nabla_x^t u| \;+\; \left(\int_{S^2} |\nabla_n \phi|^2\, f\, dn\right)^{1/2} |\nabla_x^2 u|.
\end{aligned}$$

2.3 Bounds on the Stokes system

Consider the Stokes system (8)&(9),

$$\nabla_x \cdot \big((\nabla_x u + \nabla_x^t u) - p\, \mathrm{id} + \sigma\big) \;=\; 0, \tag{44}$$

$$\nabla_x \cdot u \;=\; 0, \tag{45}$$

in $\mathbb{R}^3$. We need a standard and a not so standard regularity result.

Lemma 2. *There exists a constant C depending only on $p \in (1, \infty)$ with*

$$\int_{\mathbb{R}^3} |\nabla_x^2 u|^p dx \;\le\; C \int_{\mathbb{R}^3} |\nabla_x \sigma|^p\, dx.$$

Proposition 2. *There exists a constant C only depending on $p \in (3, \infty)$ such that*

$$\sup_x |\nabla_x u| \;\le\; C \left[1 + \ln\left(1 + \frac{\big(\int_{\mathbb{R}^3} |\sigma|^2 dx\big)^{\frac{1}{3}(1-\frac{3}{p})} \big(\int_{\mathbb{R}^3} |\nabla_x \sigma|^p dx\big)^{1/p}}{\big(\sup_x |\sigma|\big)^{\frac{2}{3}(1-\frac{3}{p})+1}}\right)\right] \sup_x |\sigma|.$$

Lemma 2 follows from standard regularity theory for the Stokes system; see [17, ChI, Prop 2.2]. Results of the type of Proposition 2 go back to Weigant & Kazhikov [19], see also [7, Appendix F]. We present a proof in Appendix I which is not based on a fundamental solution but on a dyadic decomposition in Fourier space.

2.4 Bound of the relative entropy

Given a stationary steady state $(u_{ext}, f_{eq}(n))$ and a solution (f, u, p) of (6)-(9) which is a (possibly large) perturbation of $(u_{ext}, f_{eq}(n))$, the relative entropy is defined by

$$E(t) := \int_{\mathbb{R}^3}\int_{S^2} (\ln \frac{f}{f_{eq}})\, f\, dndx\,. \tag{46}$$

Proposition 3. *Let (u_{ext}, f_{eq}) be as in (12)-(13) and (f, u, p) be a solution of (6)-(9) with data satisfying*

$$E_0 = \int_{\mathbb{R}^3}\int_{S^2} (\ln \frac{f_0}{f_{eq}})\, f_0\, dn\, dx < +\infty\,. \tag{47}$$

There exists a constant $K = K(|\nabla_x u_{ext}|/D_r)$ such that for $t \in (0, \infty)$

$$\frac{dE}{dt} \;\leq\; K\, E(t) \tag{48}$$

and

$$\int_{\mathbb{R}^3} |\nabla_x (u - u_{ext})|^2\, dx \;\leq\; \int_{\mathbb{R}^3} |\sigma - \sigma_{eq}|^2\, dx \;\leq\; C\, E_0\, e^{K\,t}\,, \tag{49}$$

where C denotes a universal constant.

A far more detailed estimation along the lines of Proposition 3 is derived in [10] and is used to study the stability of equilibria.

Proof.
The functions $u - u_{ext}$ and $\sigma - \sigma_{eq}$ satisfy

$$\begin{aligned} \triangle_x (u - u_{ext}) - \nabla_x p + \nabla_x \cdot (\sigma - \sigma_{eq}) &= 0, \\ \nabla_x \cdot (u - u_{ext}) &= 0\,. \end{aligned}$$

Therefore, we multiply by $(u - u_{ext})$ and integrate by parts to obtain

$$-\int_{\mathbb{R}^3} \nabla_x (u - u_{ext}) : (\sigma - \sigma_{eq})\, dx \;=\; \int_{\mathbb{R}^3} |\nabla_x (u - u_{ext})|^2 dx. \tag{50}$$

Combine next Lemma 1 with (25), (9) and (50) to obtain

$$\begin{aligned}
&\frac{d}{dt}\int_{\mathbb{R}^3} e\,dx + \int_{\mathbb{R}^3} |\nabla_x(u-u_{ext})|^2 dx \\
&\quad = \; -\int_{\mathbb{R}^3} \nabla_x(u-u_{ext}) : \int_{S^2} (\nabla_n \ln f_{eq} \otimes n)(f-f_{eq})\,dn\,dx \\
&\quad \leq \; K_1 \int_{\mathbb{R}^3} |\nabla_x(u-u_{ext})| \int_{S^2} |f-f_{eq}|\,dn\,dx,
\end{aligned} \tag{51}$$

where $K_1 = \sup_n |\nabla_n \ln f_{eq} \otimes n|$ is a constant that depends only on the quotient $|\nabla_x u_{ext}|/D_r$.

Next, we use the Kullback–Csiszar inequality, i. e.

$$\left(\int_{S^2} |f-f_{eq}|\,dn\right)^2 \;\leq\; 8 \int_{S^2} (\ln \frac{f}{f_{eq}})\, f\,dn \tag{52}$$

together with Young's inequality to obtain

$$\frac{dE}{dt} \;\leq\; K\,E$$

and thus

$$E(t) = \int_{\mathbb{R}^3} e(x,t)\,dx \leq E_0\, e^{K\,t}\,.$$

Observe next that (7) and (52) imply

$$\begin{aligned}
\int_{\mathbb{R}^3} |\sigma - \sigma_{eq}|^2\,dx &= \int_{\mathbb{R}^3} \Big| \int_{S^2} (3n\otimes n - \mathrm{id})(f-f_{eq}) dn \Big|^2 dx \\
&\leq C \int_{\mathbb{R}^3} \Big| \int_{S^2} |f-f_{eq}|\,dn \Big|^2 dx \\
&\leq C \int_{\mathbb{R}^3} e(t,x)\,dx\,,
\end{aligned}$$

hence, (49) follows from (50) and (48). □

2.5 Derivation of the differential inequality

Let w be defined in (22)-(21) and W be as in (23). We derive a differential inequality for W.

Proposition 4. *Let W be defined as in (23). There exists a constant C only depending on $p \in (3, \infty)$ such that*

$$\int_{\mathbb{R}^3} |\nabla_x^2 u|^p \, dx \;\; \leq \;\; C\, W, \tag{53}$$

$$\sup_x |\nabla_x u - \nabla_x u_{ext}| \;\; \leq \;\; C\left(1 + \ln E(t) + \ln W\right), \tag{54}$$

and W satisfies the differential inequality:

$$\frac{1}{p}\frac{dW}{dt} \leq \; -D_r W + C\Big(1 + \sup_x |\nabla_x u_{ext}| + \ln E(t) + \ln W\Big)\, W\,. \tag{55}$$

Proof. We evoke Proposition 1. With (37) as a starting point, we obtain for $p \geq 2$ the differential inequality

$$\begin{aligned} &\partial_t(w^{p/2}) + \nabla_x \cdot (u w^{p/2}) - D \,\triangle_x(w^{p/2}) \\ &\quad \leq \; -p\, D_r w^{p/2} + p|\nabla_x u + \nabla_x^t u|\, w^{p/2} + p|\nabla_x^2 u|\, w^{\frac{p-1}{2}}. \end{aligned} \tag{56}$$

Let us address the three terms on the right side of (56). The first term gives rise to

$$-D_r \int_{\mathbb{R}^3} w^{p/2}\, dx \;\; = \;\; -D_r\, W.$$

For the second term we notice

$$\int_{\mathbb{R}^3} w^{p/2}\, |\nabla_x u + \nabla_x^t u|\, dx \;\leq\; \sup_{\mathbb{R}^3} |\nabla_x u + \nabla_x^t u|\, W.$$

Finally, the last term is estimated with help of Hölder's inequality

$$\int_{\mathbb{R}^3} w^{\frac{p-1}{2}}\, |\nabla_x^2 u|\, dx \;\leq\; \left(\int_{\mathbb{R}^3} |\nabla_x^2 u|^p\, dx\right)^{1/p} W^{1-1/p}.$$

Combining these together gives

$$\frac{1}{p}\frac{dW}{dt} \leq \; \Big(-D_r + \sup_x |\nabla_x u + \nabla_x^t u|\Big)\, W + \left(\int_{\mathbb{R}^3} |\nabla_x^2 u|^p\, dx\right)^{1/p} W^{1-1/p}.$$

We next observe that there exists a universal constant C such that

$$\int_{\mathbb{R}^3} |\nabla_x \sigma|^p\, dx \;\leq\; C \int_{\mathbb{R}^3} \left(\int_{S^2} |\nabla_n \phi|^2 f\, dn\right)^{p/2} dx \;\; = \;\; C\, W. \tag{57}$$

Indeed, the starting point for deriving (57) is (20), written component-wise:

$$\partial_{x_i}\sigma_{kl} \;=\; \int_{S^2}(3\, n_k\, n_l - \delta_{kl})\, \partial_{x_i} f\, dn.$$

According to definition (21), we obtain

$$\partial_{x_i}\sigma_{kl} \;=\; -3\int_{S^2} \nabla_n(n_k\, n_l)\cdot\nabla_n\phi_i\, f\, dn$$

and thus

$$|\partial_{x_i}\sigma_{kl}|^2 \;\le\; 9\,\sup_n |\nabla_n(n_k\, n_l)|^2 \int_{S^2} |\nabla_n\phi_i|^2\, f\, dn.$$

It remains to sum over all i,k,l, raise to power $p/2$ and integrate over $\mathbb{R}^3$. This establishes (57). Estimate (53) now follows from Lemma 2 and, in turn, provides the differential inequality

$$\frac{1}{p}\frac{dW}{dt} \le\; -D_r W + 2\sup_x |\nabla_x u|\, W + C\, W\,. \tag{58}$$

Next, we observe that σ is uniformly bounded:

$$|\sigma|^2 \;\le\; 9\int_{S^2} |n\otimes n - \frac{1}{3}\,\mathrm{id}|^2\, f\, dn \;\le\; 6\int_{S^2} f\, dn \;=\; 6. \tag{59}$$

We also recall that $(u - u_{ext}, \sigma - \sigma_{eq})$ satisfies the Stokes system (44) &(45), and evoke Proposition 2. This implies

$$\begin{aligned}
\sup_x |\nabla_x u - \nabla_x u_{ext}| &\le C\left(1 + \ln\int_{\mathbb{R}^3} |\nabla_x\sigma|^p\, dx + \ln\int_{\mathbb{R}^3} |\sigma-\sigma_{eq}|^2\, dx\right)\\
&\overset{(57),(49)}{\le} C\left(1 + \ln W + \ln\int_{\mathbb{R}^3} e(t,x)\, dx\right)\\
&\le C\Big(1 + \ln W + \ln E(t)\Big)
\end{aligned}$$

which with (58) gives (55) and completes the proof. □

3 General properties of the Doi model

We list here certain properties of the Doi model: the invariance under rotations of the equations (6)-(9), and the non-monotonicity of steady states for steady shear flows (16)-(19).

3.1 Invariances of the Doi model

We consider the model (6)-(9) and will show that the system is invariant under rotations.

Proposition 5. *Let (f, u, p), with $f = f(t, x, n)$, $u = u(t, x)$ and $p = p(t, x)$, satisfy* (6)-(9). *Then $(\hat{f}, \hat{u}, \hat{p})$, defined by*

$$\begin{aligned} \hat{f}(t,x,n) &= f(t,Qx,Qn) \\ \hat{u}(t,x) &= Q^t u(t,Qx) \quad , \qquad Q \in \mathbb{O}(3)\,, \\ \hat{p}(t,x) &= p(t,Qx) \end{aligned} \tag{60}$$

satisfies (6)-(9). *Moreover,*

$$\hat{\sigma}(t,x) = Q^t \sigma(t,Qx)Q$$

The proof is based on invariance properties of the transport equation

$$\partial_t f + \nabla_x f \cdot u + \nabla_n \cdot (P_{n\perp} \nabla_x u\, n\, f) - D_r \triangle_n f - D \triangle_x f = 0 \tag{61}$$

in conjunction with well known invariances of the Stokes system. We use the notation

$$f_{u,\nabla_x u} = f_{u(t,x),\nabla_x u(t,x)}(t,x,n)$$

for the solution of (61) generated by the fields $u = u(t,x)$ and $\nabla_x u = \nabla_x u(t.x)$.

Lemma 3. *Let $f_{u,\nabla_x u}$ satisfy the transport equation* (61). *Then,*

$$\tilde{f}_{u,Q^t\nabla_x u Q}(t,x,n) := f_{u,\nabla_x u}(t,x,Qn)\,, \qquad Q \in \mathbb{O}(3) \tag{62}$$

$$\bar{f}_{R^t u(Rx),(\nabla_x u)(Rx)}(t,x,n) := f_{u,\nabla_x u}(t,Rx,n)\,, \qquad R \in \mathbb{O}(3) \tag{63}$$

$$\hat{f}_{R^t u(Rx),Q^t \nabla_x u(Rx) Q}(t,x,n) := f_{u,\nabla_x u}(t,Rx,Qn)\,, \quad Q,R \in \mathbb{O}(3) \tag{64}$$

satisfy transport equations (61) *with velocity and velocity-gradient fields as stated in* (62), (63), (64).

Proof of Lemma 3. This is a symmetry consideration. Let $f = f_{u,\nabla_x u}$ satisfy (61) with fields u and $\nabla_x u$, $Q \in \mathbb{O}(3)$, and define $\tilde{f}(n) := f(Q\,n)$. We then have $\nabla \tilde{f} = Q^t \nabla f(Qn)$ and

$$\begin{aligned} \nabla_n \tilde{f}(n) = P_{n^\perp} \nabla \tilde{f} &= \nabla \tilde{f} - (n \cdot \nabla \tilde{f})n \\ &= Q^t \big(\nabla f(Qn) - \big(Qn \cdot \nabla f(Qn)\big)Qn\big) \\ &= Q^t \nabla_n f(Qn) \end{aligned}$$

and

$$
\begin{aligned}
P_{n^\perp}\,(Q^t\,\nabla_x u\,Q)\,n &= (Q^t\,\nabla_x u\,Q)\,n - \big(n\cdot(Q^t\,\nabla_x u\,Q)\,n\big)\,n \\
&= Q^t\,\big(\nabla_x u\,(Q\,n) - (Q\,n)\cdot\nabla_x u\,(Q\,n)\,(Q\,n)\big) \\
&= Q^t\,\big(P_{n^\perp}\,\nabla_x u\,n\big)(Q\,n),
\end{aligned}
$$

so that

$$
\big(-\nabla_n\tilde f + P_{n^\perp}\,(Q^t\,\nabla_x u\,Q)\,n\,\tilde f\big)(n) \;=\; Q^t\,\big(-\nabla_n f + P_{n^\perp}\,\nabla_x u\,n f\big)(Q\,n).
$$

We infer

$$
\begin{aligned}
&\Big(-\triangle_n\tilde f + \nabla_n\cdot\big(P_{n^\perp}\,(Q^t\,\nabla_x u\,Q)\,n\,\tilde f\big)\Big)(n) \\
&\quad= \nabla_n\cdot\big(-\nabla_n\tilde f + P_{n^\perp}\,(Q^t\,\nabla_x u\,Q)\,n\,\tilde f\big)(n) \\
&\quad= \nabla_n\cdot\big(-\nabla_n f + P_{n^\perp}\,\nabla_x u\,n f\big)(Q\,n) \\
&\quad= \Big(-\triangle_n f + \nabla_n\cdot\big(P_{n^\perp}\,\nabla_x u\,n f\big)\Big)(Q\,n),
\end{aligned}
$$

and thus

$$
\begin{aligned}
&\partial_t\tilde f + u\cdot\nabla_x\tilde f + \nabla_n\cdot\big(P_{n^\perp}\,(Q^t\,\nabla_x u\,Q)\,n\,\tilde f\big) - D_r\triangle_n\tilde f - D\triangle_x\tilde f \\
&\quad= \Big(\partial_t f + u\cdot\nabla_x f + \nabla_n\cdot\big(P_{n^\perp}\,\nabla_x u\,n f\big) - D_r\triangle_n f - D\triangle_x f\Big)(t,x,Qn) \\
&\quad= 0\,.
\end{aligned}
$$

Next, again with $f = f_{u,\nabla_x u}$ and $R\in\mathbb{O}(3)$, set $\bar f = f(Rx)$. Observe that $\nabla_x\bar f = R^t(\nabla_x f)(Rx)$ and that $\triangle_x\bar f = (\triangle_x f)(Rx)$. We infer

$$
\begin{aligned}
&\partial_t\bar f + R^t u(Rx)\cdot\nabla_x\bar f + \nabla_n\cdot\big(P_{n^\perp}\,(\nabla_x u)(Rx)\,n\,\bar f\big) - D_r\triangle_n\bar f - D\triangle_x\bar f \\
&\quad= \Big(\partial_t f + u\cdot\nabla_x f + \nabla_n\cdot\big(P_{n^\perp}\,\nabla_x u\,n f\big) - D_r\triangle_n f - D\triangle_x f\Big)(t,Rx,n) \\
&\quad= 0\,.
\end{aligned}
$$

The last statement follows by combining the first two.

Proof of Proposition 5 Consider the function $(\hat f,\hat u,\hat p)$ defined by (60), and let $Q\in\mathbb{O}(3)$. We then have $\hat u = Q^t u(t,Qx)$,

$$
\nabla_x\hat u = Q^t\,(\nabla_x u)(t,Qx)\,Q\,,
$$

and, according to Lemma 3,

$$
\begin{aligned}
&\partial_t\hat f + \hat u\cdot\nabla_x\hat f + \nabla_n\cdot\big(P_{n^\perp}\,\nabla_x\hat u\,n\,\hat f\big) - D_r\triangle_n\hat f - D\triangle_x\hat f \\
&\quad= \Big(\partial_t f + u\cdot\nabla_x f + \nabla_n\cdot\big(P_{n^\perp}\,\nabla_x u\,n f\big) - D_r\triangle_n f - D\triangle_x f\Big)(t,Qx,Qn) \\
&\quad= 0\;\,.
\end{aligned}
$$

The transformation of viscoelastic stresses can be seen from (7). We have

$$\begin{aligned}\hat{\sigma}(t,x) &= \int_{S^2} (3\, n \otimes n - \mathrm{id}) \hat{f}\, dn \\ &= \int_{S^2} (3\, n \otimes n - \mathrm{id}) f(t, Qx, Qn)\, dn \\ &= \int_{S^2} (3\, Q^t n \otimes Q^t n - \mathrm{id}) f(t, Qx, n)\, dn \\ &= Q^t \sigma(t, Qx) Q\,.\end{aligned}$$

Moreover,

$$\nabla_x \cdot \hat{u} = (\nabla_x \cdot u)(t, Qx) = 0$$

and

$$\begin{aligned}&\nabla_x \cdot \big((\nabla_x \hat{u} + \nabla_x^t \hat{u}) - \hat{p}\, \mathrm{id} + \hat{\sigma} \big) \\ &\quad = Q^t \big[\nabla_x \cdot \big((\nabla_x u + \nabla_x^t u) - p\, \mathrm{id} + \sigma \big) \big](t, Qx) = 0\end{aligned}$$

that is $(\hat{f}, \hat{u}, \hat{p})$ satisfy (6)-(9).

3.2 Non–monotonicity and discontinuous solutions

In this section we prove Theorem 1. The proof is based on the properties of the normalized strain–rate to elastic stress mapping Σ which we now define.

Definition 1. *The map*

$$\Sigma \colon \mathrm{End}(\mathbb{R}^3) \ni \kappa \;\mapsto\; \sigma \in \mathrm{Sym}(\mathbb{R}^3)$$

is defined via

$$\sigma \;=\; \int_{S^2} (3\, n \otimes n - \mathrm{id})\, f_\kappa\, dn,$$

where f_κ is the unique solution of

$$\nabla_n \cdot (P_{n^\perp} \kappa\, n\, f) - \triangle_n f \;=\; 0 \tag{65}$$

with $f \geq 0$ and $\int_{S^2} f\, dn = 1$.

We denote by κ_s the gradient of a normalized shear flow, i. e.

$$\kappa_s \;=\; \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Hence x_1 is the flow direction, x_2 the shear direction and x_3 the vorticity direction. We will need the following three properties for $\Sigma(\dot{\gamma}\kappa_s)$:

Lemma 4.

$$\frac{d}{d\dot\gamma}_{|\dot\gamma=0} \Sigma_{12}(\dot\gamma\,\kappa_s) \;>\; 0.$$

Lemma 5.

$$\lim_{\dot\gamma\to\infty} \Sigma_{12}(\dot\gamma\,\kappa_s) \;=\; 0.$$

Lemma 6.

$$\Sigma_{23}(\dot\gamma\,\kappa_s) \;=\; 0.$$

Proof of Lemma 4. We start with remarking that the components of $3n \otimes n - \mathrm{id}$, i. e.

$$3\,n_i\,n_j - \delta_{ij},$$

are surface spherical harmonics of order 2. This means that they are harmonic polynomials on $\mathbb{R}^3$ of order 2, restricted to S^2. It is well known that surface spherical harmonics are eigenfunctions of the Laplacian on S^2. Their eigenvalue is $-\ell(\ell+1)$, where ℓ is the order [1, Appendix E]. Hence

$$\triangle_n(3\,n_i\,n_j - \delta_{ij}) \;=\; -6\,(3\,n_i\,n_j - \delta_{ij}). \tag{66}$$

This observation yields an alternative representation of the map Σ:

$$\begin{aligned} \Sigma(\kappa) \;&=\; \int_{S^2} (3n\otimes n - \mathrm{id})\, f_\kappa\, dn \\ &\overset{(66)}{=}\; -\frac{1}{6}\int_{S^2} \triangle_n \left(3\frac{n}{|n|}\otimes\frac{n}{|n|} - \mathrm{id}\right) f_\kappa\, dn \\ &=\; -\frac{1}{2}\int_{S^2} n\otimes n\,\triangle_n f_\kappa\, dn \\ &\overset{(65)}{=}\; -\frac{1}{2}\int_{S^2} n\otimes n\,\nabla_n\cdot(P_{n^\perp}\kappa n\, f_\kappa)\, dn. \end{aligned} \tag{67}$$

According to (67), we have in particular

$$\Sigma_{12}(\dot\gamma\,\kappa_s) \;=\; -\frac{\dot\gamma}{2}\int_{S^2} n_1\,n_2\,\nabla_n\cdot(P_{n^\perp}\kappa_s n f_{\dot\gamma\kappa})\, dn.$$

Hence we obtain

$$
\begin{aligned}
\frac{d}{d\dot\gamma}_{|\dot\gamma=0}\Sigma_{12}(\dot\gamma\,\kappa_s) &= -\frac{1}{2}\int_{S^2} n_1\, n_2\, \nabla_n\cdot(P_{n^\perp}\kappa_s n f_0)\, dn \\
&= -\frac{1}{8\pi}\int_{S^2} n_1\, n_2\, \nabla_n\cdot(P_{n^\perp}\kappa_s n)\, dn \\
&= \frac{1}{8\pi}\int_{S^2} \nabla_n(n_1\, n_2)\cdot P_{n^\perp}\kappa_s n\, dn \\
&= \frac{1}{8\pi}\int_{S^2} P_{n^\perp}\begin{pmatrix} n_2 \\ n_1 \\ 0\end{pmatrix}\cdot P_{n^\perp}\begin{pmatrix} n_2 \\ 0 \\ 0\end{pmatrix} dn \\
&= \frac{1}{8\pi}\int_{S^2} P_{n^\perp}\begin{pmatrix} n_2 \\ n_1 \\ 0\end{pmatrix}\cdot \begin{pmatrix} n_2 \\ 0 \\ 0\end{pmatrix} dn \\
&= \frac{1}{8\pi}\int_{S^2} (1-2\,n_1^2)\, n_2^2\, dn.
\end{aligned}
$$

By symmetry we have

$$\int_{S^2}(1-2\,n_1^2)n_2^2\, dn \;=\; \int_{S^2}(1-n_1^2-n_3^2)\, n_2^2\, dn \;=\; \int_{S^2} n_2^4\, dn,$$

so that the above turns into

$$\frac{d}{d\dot\gamma}_{|\dot\gamma=0}\Sigma_{12}(\dot\gamma\,\kappa_s) \;=\; \frac{1}{8\pi}\int_{S^2} n_2^4\, dn \;>\; 0.$$

Proof of Lemma 5. According to the definition of Σ, we have to show

$$\lim_{\dot\gamma\uparrow\infty}\int_{S^2} n_1\, n_2\, f_{\dot\gamma\kappa_s}\, dn \;=\; 0.$$

Because of Jensen

$$\left|\int_{S^2} n_1\, n_2\, f_{\dot\gamma\kappa_s}\, dn\right|^3 \;\le\; \int_{S^2} |n_1\, n_2|^3\, f_{\dot\gamma\kappa_s}\, dn$$

and the inequality

$$|n_1\, n_2|^3 \;\le\; |n_2|^3 \;\le\; (n_2^2+n_3^2)\,|n_2| \;=\; (1-n_1^2)\,|n_2|,$$

it suffices to show

$$\lim_{\dot\gamma\uparrow\infty}\int_{S^2}(1-n_1^2)\,|n_2|\, f_{\dot\gamma\kappa_s}\, dn \;=\; 0. \tag{68}$$

We now argue in favor of (68). According to (65), we have for any test function ζ

$$\int_{S^2} \left(\nabla_n \zeta \cdot P_{n^\perp} \kappa_s\, n + \dot\gamma^{-1} \triangle_n \zeta\right)\, f_{\dot\gamma \kappa_s}\, dn \;=\; 0. \tag{69}$$

We now make a special *ansatz* for ζ. We fix a smooth function $\varphi(\hat n_2)$ with

$$\varphi(\hat n_2) \;=\; 1 \;\text{ for } \hat n_2 \;\geq 1 \quad \text{and} \quad \varphi(\hat n_2) \;=\; -1 \;\text{ for } \hat n_2 \;\leq -1.$$

For given $\lambda > 0$ to be optimized later, we consider

$$\zeta_\lambda(n) \;=\; n_1\, \varphi(\frac{n_2}{\lambda}),$$

which we think of as an approximation of $n_1\, \mathrm{sign}(n_2)$ for $\lambda \ll 1$. On one hand we have

$$|\triangle_n \zeta_\lambda| \;\leq\; C\, \frac{1}{\lambda^2} \tag{70}$$

with a universal generic constant $C < \infty$. On the other hand, we have

$$\begin{aligned}
\nabla_n \zeta_\lambda \cdot P_{n^\perp} \kappa_s\, n \;&=\; P_{n^\perp} \begin{pmatrix} \varphi(\frac{n_2}{\lambda}) \\ \frac{n_1}{\lambda}\, \varphi'(\frac{n_2}{\lambda}) \\ 0 \end{pmatrix} \cdot P_{n^\perp} \begin{pmatrix} n_2 \\ 0 \\ 0 \end{pmatrix} \\
&=\; \begin{pmatrix} \varphi(\frac{n_2}{\lambda}) \\ \frac{n_1}{\lambda}\, \varphi'(\frac{n_2}{\lambda}) \\ 0 \end{pmatrix} \cdot \begin{pmatrix} n_2 - n_1^2\, n_2 \\ -n_1\, n_2^2 \\ -n_1\, n_2\, n_3 \end{pmatrix} \\
&=\; (1 - n_1^2)\, n_2\, \varphi\big(\frac{n_2}{\lambda}\big) - n_1^2\, \frac{n_2^2}{\lambda}\, \varphi'\big(\frac{n_2}{\lambda}\big).
\end{aligned} \tag{71}$$

Since

$$\begin{aligned}
\big|(1-n_1^2)\, n_2\, \varphi\big(\tfrac{n_2}{\lambda}\big) - (1-n_1^2)\, |n_2|\big| \;&\leq\; \lambda\, |\tfrac{n_2}{\lambda}|\, |\varphi\big(\tfrac{n_2}{\lambda}\big) - \mathrm{sign}\big(\tfrac{n_2}{\lambda}\big)| \;&\leq\; C\, \lambda, \\
\left|n_1^2\, \tfrac{n_2^2}{\lambda}\, \varphi'\big(\tfrac{n_2}{\lambda}\big)\right| \;&\leq\; \lambda\, \left|\big(\tfrac{n_2}{\lambda}\big)^2 \varphi'\big(\tfrac{n_2}{\lambda}\big)\right| \;&\leq\; C\, \lambda,
\end{aligned}$$

(71) yields

$$\big|\nabla_n \zeta_\lambda \cdot P_{n^\perp} \kappa_s n - (1-n_1^2)\, |n_2|\big| \;\leq\; C\, \lambda. \tag{72}$$

From (70) and (72) we obtain

$$\big|\nabla_n \zeta_\lambda \cdot P_{n^\perp} \kappa_s n + \dot\gamma^{-1} \triangle_n \zeta_\lambda - (1-n_1^2)\, |n_2|\big| \;\leq\; C\, \left(\lambda + \frac{1}{\dot\gamma\, \lambda^2}\right).$$

With the choice of $\lambda = \dot\gamma^{-1/3}$ this turns into

$$\big|\nabla_n \zeta_\lambda \cdot P_{n^\perp} \kappa_s n + \dot\gamma^{-1} \triangle_n \zeta_\lambda - (1-n_1^2)\, |n_2|\big| \;\leq\; C\, \dot\gamma^{-1/3}.$$

In view of (69) this yields

$$\left| \int_{S^2} (1-n_1^2)\, |n_2|\, f_{\dot\gamma\kappa_s}\, dn \right| \;\le\; C\, \dot\gamma^{-1/3},$$

which is a quantitative version of (68).

Proof of Lemma 6. This is an outcome of symmetry considerations. We notice that for any $Q \in \mathbb{O}(3)$,

$$f_{Q^t \kappa Q}(n) \;=\; f_\kappa(Q\, n). \tag{73}$$

Indeed, consider the transformation $\tilde f(n) := f(Q\, n)$. Proceeding as in the proof of Lemma 3 we obtain

$$\begin{aligned} &\Big(-\triangle_n \tilde f + \nabla_n \cdot \big(P_{n^\perp}\, (Q^t\, \kappa\, Q)\, n\, \tilde f \big) \Big)(n) \\ &\quad = \Big(-\triangle_n f + \nabla_n \cdot \big(P_{n^\perp}\, \kappa\, n f \big) \Big)(Q\, n). \end{aligned}$$

This identity implies (73) by uniqueness of (65).

We now notice that

$$Q \;:=\; \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \;\in\; \mathbb{O}(3) \quad \text{and} \quad Q^t\, (\dot\gamma k_s)\, Q \;=\; \dot\gamma k_s.$$

Hence by (73) we have

$$f_{\dot\gamma\kappa_s}(n_1, n_2, -n_3) \;=\; f_{\dot\gamma\kappa_s}(n_1, n_2, n_3),$$

which in turn yields

$$\begin{aligned} \Sigma_{23}(\dot\gamma\, \kappa_s) &= \int_{S^2} n_2\, n_3\, f_{\dot\gamma\kappa_s}(n_1, n_2, n_3)\, dn \\ &= \int_{S^2} n_2\, n_3\, f_{\dot\gamma\kappa_s}(n_1, n_2, -n_3)\, dn \\ &= -\int_{S^2} n_2\, n_3\, f_{\dot\gamma\kappa_s}(n_1, n_2, n_3)\, dn \\ &= -\Sigma_{23}(\dot\gamma\, \kappa_s). \end{aligned}$$

Proof of Theorem 1. According to Lemmas 4 and 5,

$$\mathbb{R} \ni \dot\gamma \;\mapsto\; \Sigma_{12}(\dot\gamma\kappa_s) \quad \text{is not monotone.}$$

Hence for sufficiently small D_r, also

$$\mathbb{R} \ni \dot\gamma \ \mapsto \ \dot\gamma + \Sigma_{12}\big(\frac{\dot\gamma\kappa_s}{D_r}\big) \quad \text{is not monotone.}$$

We fix such a D_r and select $\dot\gamma_\pm$ with

$$\dot\gamma_+ \ \neq \ \dot\gamma_- \quad \text{and} \quad \dot\gamma_+ + \Sigma_{12}\big(\frac{\dot\gamma_+\kappa_s}{D_r}\big) \ = \ \dot\gamma_- + \Sigma_{12}\big(\frac{\dot\gamma_-\kappa_s}{D_r}\big). \tag{74}$$

We introduce

$$\begin{aligned} f(x,n) \ &:= \ \left\{ \begin{array}{ll} f_{\dot\gamma_+\kappa_s}(n) & \text{for} \quad x_2 > 0 \\ f_{\dot\gamma_-\kappa_s}(n) & \text{for} \quad x_2 < 0 \end{array} \right\}, \\ u(x) \ &:= \ \left\{ \begin{array}{ll} \dot\gamma_+(x_2,0,0) & \text{for} \quad x_2 > 0 \\ \dot\gamma_-(x_2,0,0) & \text{for} \quad x_2 < 0 \end{array} \right\}, \\ p(x) \ &:= \ \left\{ \begin{array}{ll} \Sigma_{22}\big(\frac{\dot\gamma_+\kappa_s}{D_r}\big) & \text{for} \quad x_2 > 0 \\ \Sigma_{22}\big(\frac{\dot\gamma_-\kappa_s}{D_r}\big) & \text{for} \quad x_2 < 0 \end{array} \right\}, \end{aligned} \tag{75}$$

We notice that u is continuous with weak gradient

$$\nabla_x u(x) \ = \ \left\{ \begin{array}{ll} \dot\gamma_+\,\kappa_s & \text{for} \quad x_2 > 0 \\ \dot\gamma_-\,\kappa_s & \text{for} \quad x_2 < 0 \end{array} \right\}, \tag{76}$$

that $\nabla_x u$ is discontinuous and (19) is satisfied (in the weak sense).

We now argue that (18), which in view of (19) can be rewritten as

$$\nabla_x \cdot (\nabla_x u - p\,\mathrm{id} + \sigma) \ = \ 0 \tag{77}$$

holds in the weak sense. Indeed, because of (76), (75) and Definition 1 we have

$$\nabla_x u - p\,\mathrm{id} + \sigma \ = \ \left\{ \begin{array}{ll} \dot\gamma_+\,\kappa_s - \Sigma_{22}\big(\frac{\dot\gamma_+\kappa_s}{D_r}\big)\,\mathrm{id} + \Sigma\big(\frac{\dot\gamma_+\kappa_s}{D_r}\big) & \text{for} \quad x_2 > 0 \\ \dot\gamma_-\,\kappa_s - \Sigma_{22}\big(\frac{\dot\gamma_-\kappa_s}{D_r}\big)\,\mathrm{id} + \Sigma\big(\frac{\dot\gamma_-\kappa_s}{D_r}\big) & \text{for} \quad x_2 < 0 \end{array} \right\}.$$

Since this tensor is piecewise constant, it remains to show that

$$u_{i,2} - p\,\delta_{i2} + \sigma_{i2} \quad \text{is continuous across } \{x_2 = 0\} \ \text{ for } i = 1,2,3 \tag{78}$$

in order to conclude (77). For the flow direction $i = 1$ we have

$$u_{1,2} - p\,\delta_{12} + \sigma_{12} \ = \ \left\{ \begin{array}{ll} \dot\gamma_+ + \Sigma_{12}\big(\frac{\dot\gamma_+\kappa_s}{D_r}\big) & \text{for} \quad x_2 > 0 \\ \dot\gamma_- + \Sigma_{12}\big(\frac{\dot\gamma_-\kappa_s}{D_r}\big) & \text{for} \quad x_2 < 0 \end{array} \right\},$$

so that (78) follows from (74). For the shear direction $i = 2$ we notice that

$$u_{2,2} - p\,\delta_{22} + \sigma_{22} \; = \; 0$$

due to the definition (75) of the pressure. For the vorticity direction $i = 3$ we remark

$$u_{3,2} - p\,\delta_{32} + \sigma_{32} \; = \; \left\{ \begin{array}{ll} \Sigma_{23}\big(\frac{\dot\gamma_+\kappa_s}{D_r}\big) & \text{for} \quad x_2 > 0 \\ \Sigma_{23}\big(\frac{\dot\gamma_-\kappa_s}{D_r}\big) & \text{for} \quad x_2 < 0 \end{array} \right\},$$

which vanishes according to Lemma 6. Hence (78) is established.

The Smoluchowski equation (16) itself ist satisfied by definition (65) of $f_{\dot\gamma_\pm\,\kappa_s}$ and because of

$$\nabla_x \cdot (f u) \; = \; 0 \quad \text{distributionally},$$

since u has only a u_1–component and $f\,u$ depends on x only through x_2.

4 Appendix I.

Proof of Proposition 2. We select a φ in $\mathcal{S}(\mathbb{R}^3)$, the Schwartz space, such that its Fourier transform satisfies

$$\hat\varphi(k) \; = \; \frac{1}{(2\pi)^{3/2}} \quad \text{for} \;\; |k| \; \le \; 1. \tag{79}$$

The constant is chosen such that

$$\int_{\mathbb{R}^3} \varphi\,dx \; = \; 1. \tag{80}$$

We recall that u is periodic and that the Fourier symbol which relates σ to $\nabla_x u$ via the Stokes system (44) & (45) is given by

$$\hat u_{i,j}(k) \; = \; \frac{k_j}{|k|}\left(\frac{k_i}{|k|}\frac{k_\ell}{|k|} - \delta_{i\ell}\right)\frac{k_m}{|k|}\,\hat\sigma_{\ell m}(k), \tag{81}$$

where we sum over repeated indices. Thanks to (79),

$$\hat\psi_{ij\ell m}(k) \; = \; \left(\hat\varphi(\frac{k}{2}) - \hat\varphi(k)\right)\frac{k_j}{|k|}\left(\frac{k_i}{|k|}\frac{k_\ell}{|k|} - \delta_{i\ell}\right)\frac{k_m}{|k|}$$

defines a $\psi_{ij\ell m} \in \mathcal{S}(\mathbb{R}^3)$. We introduce the dyadically rescaled version of these Schwartz functions:

$$\varphi^{(\nu)}(x) \; = \; (2^\nu)^3\,\varphi(2^\nu x)\;, \quad \psi^{(\nu)}_{ij\ell m}(x) \; = \; (2^\nu)^3\,\psi_{ij\ell m}(2^\nu x)$$

for $\nu \in \{0, 1, \cdots\}$, and recall that $\widehat{\varphi^{(\nu)}}(k) = \hat{\varphi}(\frac{k}{2^\nu})$.

We now fix an $N \in \mathbb{N}$ which we will choose at the end. The decomposition of the right hand side σ into

$$\begin{aligned} \sigma_{\ell m} &= \sigma_{\ell m} - \varphi^{(N)} * \sigma_{\ell m} \\ &+ (\varphi^{(N)} - \varphi^{(N-1)}) * \sigma_{\ell m} + \cdots + (\varphi^{(1)} - \varphi^{(0)}) * \sigma_{\ell m} \\ &+ \varphi^{(0)} * \sigma_{\ell m} \end{aligned}$$

translates by definition of $\psi_{ij\ell m}$ into

$$\begin{aligned} u_{i,j} &= u_{i,j} - \varphi^{(N)} * u_{i,j} && (82) \\ &+ \psi^{(N-1)}_{ij\ell m} * \sigma_{\ell m} + \cdots + \psi^{(0)}_{ij\ell m} * \sigma_{\ell m} && (83) \\ &+ \varphi^{(0)} * u_{i,j}. && (84) \end{aligned}$$

Each of the terms in line (83) is easily estimated as follows

$$\begin{aligned} \sup_{x\in\mathbb{R}^3} |\psi^{(\nu)}_{ij\ell m} * \sigma_{\ell m}| &\le \int_{\mathbb{R}^3} |\psi^{(\nu)}_{ij\ell m}|\, dz \sup_{x\in\mathbb{R}^3} |\sigma_{\ell m}| \\ &= \int_{\mathbb{R}^3} |\psi_{ij\ell m}|\, d\hat{z} \sup_{x\in\mathbb{R}^3} |\sigma_{\ell m}| \\ &\le C \sup_x |\sigma|, \qquad (85) \end{aligned}$$

where C denotes a generic constant only depending on p.
For the term in line (84) we obtain

$$\begin{aligned} |\varphi^{(0)} * u_{i,j}(x)|^2 &\le \left(\int_{\mathbb{R}^3} |\varphi^{(0)}(x-y)|^2 dy\right) \left(\int_{\mathbb{R}^3} |u_{i,j}|^2\, dy\right) \\ &\le C \left(\int_{\mathbb{R}^3} |\sigma|^2\, dy\right). \qquad (86) \end{aligned}$$

We now address the term in line (82). We recall the Sobolev embedding theorem for functions in $W^{1,p}(\mathbb{R}^3)$,

$$|u_{i,j}(x) - u_{i,j}(y)| \le C\, |x-y|^{1-3/p} \left(\int_{\mathbb{R}^3} |\nabla u_{i,j}|^p\, dx\right)^{1/p}, \qquad (87)$$

and Lemma 2 with the $L^p(\mathbb{R}^3)$–estimate for the Stokes operator:

$$\left(\int_{\mathbb{R}^3} |\nabla^2 u|^p\, dx\right)^{1/p} \le C \left(\int_{\mathbb{R}^3} |\nabla \sigma|^p\, dx\right)^{1/p}. \qquad (88)$$

This allows to tackle the term in line (82):

$$
\begin{aligned}
&|(u_{i,j} - \varphi^{(N)} * u_{i,j})(x)| \\
&\quad \overset{(80)}{=} \quad \left| \int_{\mathbb{R}^3} \varphi^{(N)}(x-y)\,(u_{i,j}(x) - u_{i,j}(y))\,dy \right| \\
&\quad \overset{(87,88)}{\leq} \quad C \int_{\mathbb{R}^3} |\varphi^{(N)}(z)|\,|z|^{1-3/p}\,dz \left(\int_{\mathbb{R}^3} |\nabla u_{i,j}|^p\,dx \right)^{1/p} \\
&\quad = \quad C\,(2^{-N})^{1-3/p} \int_{\mathbb{R}^3} |\varphi(\hat{z})|\,|\hat{z}|^{1-3/p}\,d\hat{z} \left(\int_{\mathbb{R}^3} |\nabla \sigma|^p\,dx \right)^{1/p} \\
&\quad = \quad C\,2^{-N(1-3/p)} \left(\int_{\mathbb{R}^3} |\nabla \sigma|^p\,dx \right)^{1/p}.
\end{aligned} \tag{89}
$$

Combining (85), (86) & (89), we gather

$$
\begin{aligned}
\sup_{x\in\mathbb{R}^3} |\nabla u| \ \leq\ C \Big(& 2^{-N(1-3/p)} \left(\int_{\mathbb{R}^3} |\nabla \sigma|^p\,dx \right)^{1/p} \\
& + N \sup_{x\in\mathbb{R}^3} |\sigma| + \Big(\int_{\mathbb{R}^3} |\sigma|^2 dx \Big)^{1/2} \Big).
\end{aligned} \tag{90}
$$

The Stokes system (44)-(45) in $\mathbb{R}^3$ is invariant under the rescaling

$$
u_\ell(x) = \frac{1}{\ell^2} u(\ell x)\,, \quad \sigma_\ell(x) = \frac{1}{\ell}\sigma(\ell x)\,, \quad p_\ell(x) = \frac{1}{\ell} p(\ell x)
$$

We apply (90) to the rescaled functions u_ℓ, σ_ℓ and use the identities

$$
\|\sigma_\ell\|_{L^2(\mathbb{R}^3)} = \ell^{-\frac{5}{2}} \|\sigma\|_{L^2(\mathbb{R}^3)}\,, \quad \|\nabla_x \sigma_\ell\|_{L^p(\mathbb{R}^3)} = \ell^{-\frac{3}{p}} \|\nabla_x \sigma\|_{L^p(\mathbb{R}^3)}\,,
$$

to obtain

$$
\begin{aligned}
\sup_{x\in\mathbb{R}^3} |\nabla u| \ \leq\ C \Big(& 2^{-N(1-3/p)} \ell^{1-\frac{3}{p}} \|\nabla_x \sigma\|_{L^p(\mathbb{R}^3)} \\
& + N \sup_{x\in\mathbb{R}^3} |\sigma| + \ell^{-\frac{3}{2}} \|\sigma\|_{L^2(\mathbb{R}^3)} \Big).
\end{aligned} \tag{91}
$$

The interpolation estimate (91) depends on two parameters N and ℓ. We proceed to optimize their selection.

First choose $N \in \mathbb{N}$ such that

$$
2^{(N-1)(1-3/p)} \ \leq\ 1 + \frac{\ell^{1-3/p}\ \|\nabla_x \sigma\|_{L^p(\mathbb{R}^3)}}{\sup_x |\sigma|} \ \leq\ 2^{N(1-3/p)},
$$

so that

$$N \le C\left[1+\ln\Big(1+\frac{\ell^{1-3/p}\,\|\nabla_x\sigma\|_{L^p(\mathbb{R}^3)}}{\sup_x|\sigma|}\Big)\right].$$

Then (91) turns into

$$\begin{aligned}&\sup_{x\in\mathbb{R}^3}|\nabla u| \;\le\\ &\quad C\left[\Big[1+\ln\Big(1+\frac{\ell^{1-3/p}\,\|\nabla_x\sigma\|_{L^p(\mathbb{R}^3)}}{\sup_x|\sigma|}\Big)\Big]\sup_x|\sigma|+\ell^{-3/2}\|\sigma\|_{L^2(\mathbb{R}^3)}\right].\end{aligned} \tag{92}$$

Next we select

$$\ell=\left(\frac{\|\sigma\|_{L^2(\mathbb{R}^3)}}{\sup_x|\sigma|}\right)^{2/3}$$

in (92) and complete the proof of Proposition 2.

5 Appendix II.

The operator ∇_n satisfies certain elementary properties that are extensively used in this article: Let F be a vector-valued function and f, g be scalar-valued functions, then

$$\int_{S^2}(\nabla_n\cdot F)f\,dn=-\int_{S^2}F\cdot(\nabla_n f-2nf)dn \tag{93}$$

$$\int_{S^2}(\nabla_n\cdot\nabla_n f)g\,dn=\int_{S^2}(\nabla_n\cdot\nabla_n g)f\,dn \tag{94}$$

$$\int_{S^2}n\otimes\nabla_n f\,dn=\int_{S^2}\nabla_n f\otimes n\,dn=\int_{S^2}(3n\otimes n-\mathrm{id})f\,dn \tag{95}$$

A convenient way to prove such formulas is by expressing them to spherical coordinates, see [1, Appendix A.6 and E.6]. The change of variables for a point P with Cartesian coordinates (n_x,n_y,n_z) to spherical coordinates is

$$n_x=r\sin\theta\,\cos\varphi\,,\ n_y=r\sin\theta\,\sin\varphi\,,\ n_z=r\cos\theta$$

where $0<\theta<\pi$, $0\le\varphi<2\pi$. Let e_r, e_θ, e_φ be the orthonormal coordinate system associated to spherical coordinates and attached at P. It satisfies the derivative formulas

$$\begin{aligned}&\tfrac{\partial e_r}{\partial r}=0\,, && \tfrac{\partial e_r}{\partial\theta}=e_\theta\,, && \tfrac{\partial e_r}{\partial\varphi}=e_\varphi\,\sin\theta\,,\\ &\tfrac{\partial e_\theta}{\partial r}=0\,, && \tfrac{\partial e_\theta}{\partial\theta}=-e_r\,, && \tfrac{\partial e_\theta}{\partial\varphi}=e_\varphi\,\cos\theta\,,\\ &\tfrac{\partial e_\varphi}{\partial r}=0\,, && \tfrac{\partial e_\varphi}{\partial\theta}=0\,, && \tfrac{\partial e_\varphi}{\partial\varphi}=-e_r\,\sin\theta-e_\theta\,\cos\theta\,.\end{aligned} \tag{96}$$

We visualize the sphere S^2 as embedded in the Euclidean space. The operator ∇_n is related to the gradient operator ∇ through

$$\nabla_n = r(\mathrm{id} - n \otimes n) \cdot \nabla = e_\theta \frac{\partial}{\partial \theta} + e_\varphi \frac{1}{\sin\theta} \frac{\partial}{\partial \varphi}$$

For a scalar-valued function f

$$\begin{aligned} \nabla_n f &= e_\theta \frac{\partial f}{\partial \theta} + e_\varphi \frac{1}{\sin\theta} \frac{\partial f}{\partial \varphi} \\ \triangle_n f = \nabla_n \cdot \nabla_n f &= \frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2 f}{\partial \varphi^2} \end{aligned}$$

For a vector-valued function F, expressed in spherical coordinates in the form $F = F_r e_r + F_\theta e_\theta + F_\varphi e_\varphi$, we compute

$$\begin{aligned} \nabla_n \cdot F &= \left(e_\theta \frac{\partial}{\partial \theta} + e_\varphi \frac{1}{\sin\theta} \frac{\partial}{\partial \varphi} \right) \cdot \left(F_r e_r + F_\theta e_\theta + F_\varphi e_\varphi \right) \\ &\overset{(96)}{=} \frac{1}{\sin\theta} \frac{\partial}{\partial \theta} (\sin\theta F_\theta) + \frac{1}{\sin\theta} \frac{\partial F_\varphi}{\partial \varphi} + 2F_r \end{aligned}$$

Observe next that

$$\begin{aligned} \int_{S^2} (\nabla_n \cdot F) f dn &= \iint \left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} (\sin\theta F_\theta) + \frac{1}{\sin\theta} \frac{\partial F_\varphi}{\partial \varphi} + 2F_r \right) f \sin\theta \, d\theta d\varphi \\ &= -\iint \left(-2F_r f + F_\theta \frac{\partial f}{\partial \theta} + \frac{1}{\sin\theta} F_\varphi \frac{\partial f}{\partial \varphi} \right) \sin\theta \, d\theta d\varphi \\ &= -\int_{S^2} F \cdot (\nabla_n f - 2nf) dn \end{aligned}$$

gives (93). Formula (94) follows by applying (93) twice:

$$\begin{aligned} \int_{S^2} (\nabla_n \cdot \nabla_n f) g dn &= -\int_{S^2} \nabla_n f \cdot (\nabla_n g - 2ng) \, dn \\ &= -\int_{S^2} \nabla_n f \cdot \nabla_n g \, dn \\ &= \int_{S^2} f (\nabla_n \cdot \nabla_n g) dn \,. \end{aligned}$$

Finally, using integration by parts, we have the chain of identities

$$\begin{aligned}
&\int_{S^2} n \otimes \nabla_n f dn \\
&= \iint e_r \otimes \left(e_\theta \frac{\partial f}{\partial \theta} + e_\varphi \frac{1}{\sin\theta} \frac{\partial f}{\partial \varphi} \right) \sin\theta d\theta d\varphi \\
&= -\iint \left[\frac{\partial}{\partial \theta}(e_r \otimes e_\theta) + \frac{\cos\theta}{\sin\theta} e_r \otimes e_\theta + \frac{1}{\sin\theta} \frac{\partial}{\partial\varphi}(e_r \otimes e_\varphi) \right] f \sin\theta d\theta d\varphi \\
&\overset{(96)}{=} -\iint \left[e_\theta \otimes e_\theta + e_\varphi \otimes e_\varphi - 2 e_r \otimes e_r \right] f \sin\theta d\theta d\varphi \\
&= \int_{S^2} (3n \otimes n - \mathrm{id}) f dn
\end{aligned} \tag{97}$$

Since $(a \otimes b)^t = b \otimes a$ and the final equation in (97) is a symmetric tensor, we deduce (95).

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