Derivation of the viscoelastic stress in Stokes flows induced by non-spherical Brownian rigid particles through homogenization

Richard M. Höfer ∗1, Marta Leocata†2, and Amina Mecherbet ‡1

1 Institut de Mathématiques de Jussieu – Paris Rive Gauche, Université de Paris, France
2 Luiss University, Rome, Italy

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Abstract

We consider a microscopic model of \( n \) identical axis-symmetric rigid Brownian particles suspended in a Stokes flow. We rigorously derive in the homogenization limit of many small particles a classical formula for the viscoelastic stress that appears in so-called Doi models which couple a Fokker-Planck equation to the Stokes equations. We consider both Deborah numbers of order \( 1 \) and very small Deborah numbers. Our microscopic model contains several simplifications, most importantly, we neglect the time evolution of the particle centers as well as hydrodynamic interaction for the evolution of the particle orientations.

The microscopic fluid velocity is modeled by the Stokes equations with given torques at the particles in terms of Stratonovitch noise. We give a meaning to this PDE in terms of an infinite dimensional Stratonovitch integral. This requires the analysis of the shape derivatives of the Stokes equations in perforated domains, which we accomplish by the method of reflections.

Keywords: Homogenization, Stokes flows, viscoelasticity, Doi model, Brownian particles

MSC: 76M50, 76D07, 35R60, 35Q70

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∗hoefer@imj-prg.fr
†mleocata@luiss.it
‡mecherbet@imj-prg.fr
1. Introduction

Suspensions of non-spherical rigid Brownian particles in viscous fluids are prototypes of viscoelastic fluids. It is classical (see e.g. [DE88; KK13; Gra18]) to model such complex fluids by an effective system consisting of a Fokker-Planck equation coupled to the Navier-Stokes equations which feature a viscoelastic stress $\sigma$ that depends on the particle density. In the
absence of external forces, such a model for rod-like particles reads in dimensionless form

\[
\begin{aligned}
\left\{ \begin{aligned}
\partial_t f + \text{div}(uf) + \text{div}(P_{\xi} \nabla_x u f) &= \frac{1}{\text{De}} \Delta \xi f + \frac{\lambda_1}{\text{De}} \text{div}_x((\text{Id} + \xi \otimes \xi) \nabla_x f), \\
\text{Re}(\partial_t u + (u \cdot \nabla) u) - \Delta u + \nabla p - \text{div} \sigma &= 0, \\
\sigma &= \sigma_v + \sigma_e = \lambda_2 \int_{S^2} (Du : \xi \otimes \xi) \xi \otimes \xi \, d\xi + \frac{\lambda_3}{\text{De}} \int_{S^2} (3\xi \otimes \xi - \text{Id}) f \, d\xi, \\
u(0, \cdot) &= u_0, \quad f(0, \cdot) = f_0.
\end{aligned} \right.
\]

(1.1)

Here \(u(t, x)\) and \(p(t, x)\) are the fluid velocity and pressure, and \(f(t, x, \xi)\) is the density of particles at time \(t \geq 0\), position \(x \in \mathbb{R}^3\) and orientation \(\xi \in S^2\). Moreover \(P_{\xi}\) denotes the orthogonal projection in \(\mathbb{R}^3\) to the subspace \(\xi^\perp\). Furthermore, \(\text{Re} \, \text{De}, \lambda_1, \lambda_2, \lambda_3\) are dimensionless parameters, where \(\text{Re}\) is the Reynolds number and \(\text{De}\) is the Deborah number which is the ratio between the observation time scale and the diffusion time scale for the particle orientation. The parameter \(\lambda_1 \ll 1\) depends only on the aspect ratio of the rod-like particles. The parameters \(\lambda_2, \lambda_3\) also depend on the diluteness of the suspension. It is usually argued that it is necessary for the validity of the Doi model that the particles can freely rotate which means \(n\ell^3 \ll 1\) (so-called dilute regime in the terminology of [GH11]), where \(n\) is the number density of the particles and \(\ell\) the length of the rod-like particles. In this dilute regime \(\lambda_2 \ll 1, \lambda_3 \ll 1\).

The two parts of the viscoelastic stress \(\sigma_v\) and \(\sigma_e\) are sometimes referred to as the viscous part and the elastic part, respectively. The viscous part already occurs for suspensions of non-Brownian spherical particles for which it was first studied theoretically by Einstein [Ein06] and later for ellipsoidal particles by Jeffery [Jef22]. The viscous stress \(\sigma_v\) as in (1.1) can be obtained from Jeffery’s computation as the leading order term for very elongated ellipsoids. Jeffery also computed the periodic orbits (Jeffery orbits) of such particles in constant shear flow by taking into account non-spherical inertialess particles are partly affected by pure straining motion of the fluid. In the case of rod-like particles the symmetric and skew-symmetric part of the gradient of the fluid velocity contribute equally to the particle rotation (asymptotically for infinite aspect ratio) as reflected by the full gradient in the third term in the Fokker-Planck equation in (1.1).

The elastic part of the stress only arises for Brownian non-spherical particles. Theoretical studies on such elastic stresses go back to the 1940s, see e.g. [Sim40; KK45; KR48] and also the later works [LH71; HL72; Bre74] and the references therein. To our knowledge the elastic stress \(\sigma_e\) has so far not been obtained rigorously from a corresponding microscopic model. On the contrary the scaling up has been described as mysterious by Constantin and Masmoudi in [CM08]. In the present paper, we provide such a mathematically rigorous derivation of the elastic stress starting from a simplified microscopic system. We will treat both the cases of Deborah numbers \(\text{De}\) of order one, and very small Deborah numbers.

1.1. Previous mathematical results

In the mathematical literature, the model (1.1) is often called Doi model and has attracted a lot of attention over the last years. Global well-posedness of such models have been studied in different contexts regarding the solution concept, the space dimension and the model for the fluid where in addition to the incompressible Navier-Stokes equations also the Stokes equations and the compressible Navier-Stokes equations have been considered. We refer to
[Con05; Con+07; CM08; OT08; CS09; CS10; BT12; BT13]. In [HO06; HT17] some further insights on rod-like suspensions are presented when effects of gravity are included. In [SS08b], [SS08a] a generalization of the Doi model for active particle is introduced. Existence of global weak entropy solution for this generalization of the Doi model is studied in [CL13] All the previously mentioned papers neglect the presence of the additional viscous stress $\sigma_v$, i.e., they pretend $\sigma = \sigma_e$. Global well-posedness for the Doi model including the full viscoelastic stress $\sigma$ is treated in [LM07; ZZ08; La19].

Regarding the derivation of the Doi model as a rigorous mean-field limit, there are only partial results so far. On the one hand, the viscous stress has been obtained in the quasistatic case. On the other hand, fully coupled systems have been obtained for non-Brownian spherical particles. In all these results the fluid is modeled by the stationary Stokes equations instead of the Navier-Stokes equations.

When the time evolution of the particles is neglected, the Stokes equations with a viscous stress corresponding to $\sigma_v$ above have recently been obtained rigorously as homogenization limits for spherical particles in [NS20] and subsequently for arbitrary shapes of the particles in [HW20]. These results have been refined in [Due20; DG20; GH20; GM20; DG21; GH21].

Dynamical models regarding the sedimentation of inertialess non-Brownian spherical particles have been rigorously derived in [JO04; Höf18; Mec19; HS21].

Another prominent example of viscoelastic fluids are suspensions of flexible polymers, which are typically modelled by chain of monomers connected by springs, see e.g. [BAHS87; Bir+87; DE88]. We refer to [LL07; LL12] for a mathematical introduction to the modelling of such fluids. The corresponding viscoelastic stress tensor $\sigma$ is given by the so-called Kramers expression which takes into account the polymer chain configurations and the force needed to extend or to compress the springs. In particular, two models can be found in the literature regarding the force modelling the polymers extension: the potential associated to Hooke’s law which states that the force is linear to the length of the chain and the FENE (Finitely Extensible Nonlinear Elastic) potential which takes into account the finite extensibility of the chain. A simplified model, the so-called dumbbell model, consists in assuming that the polymer is constituted of only two monomers, see [LL12, Subsections 2.3 and 2.4] for more details. We refer to [JLL02; JLL04; Jou+06] and the references therein for well posedness, long time behaviour and numerical investigations of such models.

Another popular model for the evolution of particles depending on their orientation are so-called Vicsek models. In these models, the particle evolution is also described by a (kinetic) Fokker-Planck equation. The particles (which might be microswimmers, but also birds, fish or pedestrians) move in the direction of their orientation. Moreover, the particles change their orientation due to Brownian motion and interaction with each other. This interaction is given in terms of an interaction kernel instead of the interaction through the fluid in the Doi model. Vicsek models have been studied mathematically including well-posedness, rigorous mean-field results and long-time behavior. One could refer for instance to [GK16; FKM18; BDM20].

1.2. Heuristics

Let us give a heuristic argument for the production of the elastic stress due to Brownian rod-like particles (general non-spherical particles are analogous). A similar argument can be found in [DE88, p. 309].
Figure 1.: Heuristic explanation of the viscoelastic stress arising from rotational Brownian motion

Consider a rod orientated in some direction as in Figure 1a. Since the rod is inertialess, the rod follows the fluid flow and consequently rotates if the surrounding fluid is rotating as well. However, as we see in the lower figure, it also rotates under purely straining motion of the fluid. This is the reason why the full gradient of $u$ appears in the third term of the Fokker-Planck equation in (1.1) and not only its skewsymmetric part.

This is directly related (though the symmetry of the resistance tensor, see Subsection 2.2) to the fact that a rigid rod-like particle subject to a torque needs to exert a stresslet on the fluid in order to maintain its shape. Therefore, Brownian torques on the particles arising from thermal noise lead to corresponding Brownian stresslets. It can then be argued that there is an average net stresslets at each of the particles as shown in Figure 1c which gives rise to the elastic stress $\sigma_e$. There is one additional subtlety in the above argument: By linearity of the Stokes equations, the instantaneous stresslet produced by a torque which corresponds to a rotation to the left (of a vertically oriented rod) is exactly the negative of the effect of a torque on the same rod corresponding to a rotation to the right. Due to the random nature, such torques occur with equal probability and therefore seem to cancel out.

However, since the random torques produce a Brownian motion of the particle orientation one has to take into account quadratic effects: One has to consider the stresslets produced by such torques after the rod has already started to rotate as visualized in Figure 1b. Summing these contributions leads indeed to the effective stresslet as in Figure 1c.

We summarize that there are three key ingredients that cause the elastic part of the stress: 1) The Brownian torque on the fluid; 2) the corresponding Brownian motion of the particle orientation; 3) the particle anisotropy.

We refer to Subsection 3.5 for a more formalized version of this heuristic argument.

1.3. Formal statement of the main results

The rigorous derivation of the complete system (1.1) from a microscopic description seems to be completely out of reach for the moment due to the highly singular interaction of the particles.
Instead, we consider a simplified microscopic model keeping those aspects that produce the viscoelastic stress: First, we model the fluid by the stationary Stokes equations with no-slip conditions and balance laws on each particle. Second, we freeze the time evolution of the particle centers and assume that there is no exchange of net force between the particles and the fluid. Third, we model the evolution of the particle orientation as if they were all alone in infinite fluid. Correspondingly, the Brownian torques at each particle are independent of each other. We also include an external torque acting on the particles which could be related to an external fluid flow, a magnetic force or chemotaxis. We mainly consider such a torque in order to have a nontrivial particle distribution for very small Deborah numbers $\text{De} \to 0$. For simplicity we do not include the effect of these torques on the fluid.

After non-dimensionalization, this leads to the system

\[
\begin{cases}
-\Delta u_n + \nabla p_n = 0 & \text{in } \mathbb{R}^3 \setminus \bigcup_{i=1}^n B_i(s), \\
\text{div} u_n = 0 & \text{in } \mathbb{R}^3 \setminus \bigcup_{i=1}^n B_i, \\
D u_n = 0 & \text{in } \bigcup_{i=1}^n B_i, \\
\int_{\partial B_i} \Sigma(u_n, p_n) \nu = 0, \\
\int_{\partial B_i} [\Sigma(u_n, p_n) \nu] \times (x - x_i) = \frac{\phi_n}{\pi} \sqrt{2} \gamma_{\text{rot}} \mathcal{R}_2(\xi_i(s)) \circ \hat{B}_i(s),
\end{cases}
\] (1.2a)

\[
\begin{cases}
d\xi_i(s) = \sqrt{2} \xi_i(s) \times \circ dB_i(s) + P_{\xi_i} h(s, \xi_i(s), x_i) \, ds, \\
\xi_i(0) = \xi_{i,0}.
\end{cases}
\] (1.2b)

Here, the particles $B_i$, $1 \leq i \leq n$, are obtained from an arbitrary axisymmetric reference particle (not necessarily rod-like) by translation, rotation and rescaling with a factor $r$ which only depends on the number of particles $n$. Moreover, $\phi_n = nr^3$ is the volume fraction of the particles, $x_i \in \mathbb{R}^3$, $\xi_i \in S^2$ the particle centers and orientations, $\mathcal{R}_2(\xi_i)$ and $\gamma_{\text{rot}}$ are related to the particle resistance to rotation, $D u_n$ is the symmetric gradient of $u_n$, $\Sigma(u_n, p_n)$ is the fluid stress, and $\nu$ the outer unit normal. Moreover, $B_i$ are Brownian motions, $\hat{B}_i$ corresponding white noise and $\circ$ indicates a product in the Stratonovitch sense. Finally $h$ is a given function related to an external torque.

We emphasize that the equation for the fluid (1.2a) implicitly depends on time trough the particle orientations as well as the random torques. The latter also prevent from an interpretation of this equation pointwise in time.

For details about the modeling we refer to Section 2 where we obtain this system (after non-dimensionalization) as a simplified version of a more physically accurate microscopic system. We refer to Subsection 3.6 for a discussion on the difficulties to treat such a more accurate system. A benefit of this simplified system is that it reveals very clearly that the elastic part of the stress arises because of the interplay of the rotational Brownian motion, the Brownian torque on the fluid and the particle anisotropy, as explained in the previous subsection.

We emphasize that the ratio between the viscoelastic time scale and the rotational diffusion time scale is of order of the volume fraction of the particles $\phi_n$ which corresponds to the parameter $\lambda_3$ in (1.1). Our methods restrict us to assume $\phi_n \to 0$ (see Subsection 3.1 for the precise assumptions). However, we emphasize that we consider in this paper two fundamental different scalings
(i). The case of Deborah numbers of order 1: Here we consider the observation timescale to be comparable to the diffusion time scale; hence the rescaled viscoelastic stress term is small whereas the rescaled diffusion coefficient is of order one (\(\gamma_{rot}\) is of order one). This case corresponds to the system (1.2) above.

(ii). Very small Deborah numbers, where we consider the observation timescale to be comparable to the viscoelastic time scale; hence the rescaled viscoelastic stress term is of order one whereas the rescaled diffusion coefficient is large, see (2.14a), (2.14b) for the corresponding microscopic system.

In the first case, we obtain that the empirical measure of the particles converges to the solution of the instationary Fokker-Planck equation

\[
\begin{align*}
\partial_t f + \text{div}_\xi (P_{\xi} h f - \nabla_\xi f) &= 0, \\
 f(0, \cdot) &= f_0.
\end{align*}
\] (1.3)

Since in this case, the total viscoelastic stress, which is the only source term for the fluid equation, is of order \(\phi_n\), we consider rescaled fluid velocities \(\phi_n^{-1} u_n\). We show that this rescaled sequence \(\phi_n^{-1} u_n\) converges to the Stokes equations with an additional viscoelastic stress, namely

\[
\begin{align*}
-\Delta u + \nabla p &= \text{div} \sigma, \\
\text{div} u &= 0, \\
\sigma(t, x) &= \hat{\gamma}_E (\text{Id} - 3\xi \otimes \xi) f(t, x, \xi) d\xi.
\end{align*}
\] (1.4)

The parameter \(\gamma_E \in \mathbb{R}\) depends only on the shape of the reference particle. We emphasize that the viscoelastic stress \(\sigma\) here corresponds to the elastic part \(\sigma_e\) in (1.1). The viscous part does not appear in this case because its effect is of order \(\phi_n^2\). It is classical that the viscous stress produced by the particles is proportional to their volume fraction to leading order. In our case however, since the elastic stress as the only source term is also of order \(\phi_n\), the total effect of the viscous stress is indeed quadratic in the volume fraction.

In the second case, which corresponds to very small Deborah numbers \(\text{De} \to 0\), we obtain in the limit the (quasi)-stationary Fokker-Planck equation for the particles

\[
\begin{align*}
\text{div}_\xi (P_{\xi} h f - \nabla_\xi f) &= 0, \\
\int f(t, \cdot) d\xi &= \int f_0 d\xi.
\end{align*}
\] (1.5)

In this case, the fluid velocity \(u_n\) itself converges to the solution to (1.4).

The Fokker-Planck equation (1.5) depends on time only through \(h\). Since the equation is elliptic, the initial configuration \(f_0\) only enters as a constraint on the spacial density \(\int f(t, \cdot) d\xi\) which is constant in time because the particles do not move in space. However, the solution \(f\) to (1.5) does in general not satisfy \(f(0, \cdot) = f_0\). This discrepancy in the initial data arises from the fast diffusion for very small Deborah numbers which creates an initial layer for the solution of the microscopic particle density. This initial layer can be related to the instationary Fokker Planck equation (1.3) in the sense that \(f(0, \cdot)\) is given as long-time limit \(\lim_{t \to \infty} \tilde{f}\) for the solution \(\tilde{f}\) to (1.3) with \(h\) replaced by \(\tilde{h}(t, \cdot) = h(0, \cdot)\).

We emphasize that already making sense of the equations for the fluid velocity \(u_n\) in (1.2) is non-trivial due to the Stratonovitch white noise in the torque that acts as a boundary condition.
for the Stokes equations. We overcome this issue by using the linearity of the problem in order to define $u_n$ through an Hilbert space valued Stratonovitch integral, see Subsection 3.1.

For the regularity in time of $u_n$ we obtain the optimal regularity $H^{-s}$, $s < \frac{1}{2}$, which corresponds to the regularity of white noise. For homogenization problems of the Stokes equations in perforated domains where the stresslets at the particles produce a nontrivial term in the limit, it is classical to obtains $L^p$-convergence in space of the fluid velocity for $p < 3/2$. Due to issues with Banach valued stochastic integrals, we will work in negative spaces $H^{-s}$, $s < \frac{1}{2}$, with respect to time and space.

Moreover, the Stratonovitch nature of the white noise makes it necessary to consider shape derivatives of the solution to the Stokes equations in perforated domains with prescribed torques. Such estimates and approximations for this solution will be obtained through the method of reflections that has already been used in several related works (e.g. [Höf18; Mec19; NS20]) but will here be used for the first time to estimate shape derivatives.

1.4. Organization of the rest of the paper

The rest of the paper is organized as follows

- **Section 2** is devoted to the modeling of the microscopic system that eventually leads to (1.2). After specifying the assumptions on the particle shape and recalling properties of the grand-resistance tensor for a single (axisymmetric) particle in Subsections 2.1 and 2.2, we introduce a full microscopic model of inertialess Brownian particles in a Stokes flow in Subsection 2.3. Subsequent simplifications and nondimensionalization in Subsections 2.4 and 2.5 then leads to (1.2).

- In Section 3 we first present the main assumptions on the initial particle configuration and specify the notion of solutions to (1.2). The main convergence results are then stated in Subsection 3.3. In Subsection 3.4 we introduce the main notations used in this paper. We summarize the key steps of the proof in Subsection 3.5 and we discuss about the limitations and possible generalizations of our approach in Subsection 3.6.

- Sections 4–6 are devoted to the proof of the main results. For a more detailed outline of these sections and the appendices, we refer to Subsection 3.5.

2. The microscopic model

2.1. The particles

We consider $n$ identical particles $B_i$ given by scaling, rotation and translation of a reference particle $B$. We assume that $0 \in B \subseteq B(0, 1)$ is a smooth compact set with rotational symmetry, i.e.

$$RB = B \quad \text{for all } R \in SO(3) \text{ with } Re_3 = e_3,$$

(2.1)

where $e_3 = (0, 0, 1) \in \mathbb{R}^3$.

We then consider $n$ identical particles $B_i = x_i + rR(\xi_i)B$, where $r > 0$ a scaling factor, $x_i \in \mathbb{R}^3$ is the position and $\xi_i \in S^2$ the orientation of the $i$-th particle. The rotation matrix $R(\xi_i) \in SO(3)$ is chosen such that $R(\xi_i)e_3 = \xi_i$. Note that this constraint does not characterize $R(\xi_i)$ uniquely, but due to the rotational symmetry of $B$, the choice of $R(\xi_i)$ does not affect $B_i$. 
2.2. The resistance tensor

For the setup of the model, we need to recall the notion of the (Stokes) resistance tensor. A detailed discussion on this topic can be found for example in [KK13, Chapter 5].

In the following $\text{Sym}_0(3)$ denotes the symmetric traceless matrices in $\mathbb{R}^{3 \times 3}$. For an arbitrary (smooth) bounded domain $A \subseteq \mathbb{R}^3$, the (grand) resistance tensor $R_A \in \mathbb{R}^{6 \times 6}$ relates the translational and angular velocities $V, \omega \in \mathbb{R}^3$ and the rate of strain $E \in \text{Sym}_0(3)$ of a particle in a quiescent Stokes flow to the force, torque and stresslet exerted on the fluid. More precisely, let $x_0 \in \mathbb{R}^3$ be a fixed reference point, and consider the solution $(v,p) \in (\dot{H}^1(\mathbb{R}^3), L^2(\mathbb{R}^3))$ (where $\dot{H}^1(\mathbb{R}^3)$ stands for the standard homogeneous Sobolev space) to the Stokes equations with some viscosity $\mu > 0$

$$
\begin{cases}
-\mu \Delta v + \nabla p = 0, & \text{div } v = 0 \quad \text{in } \mathbb{R}^3 \setminus A, \\
v = V + \omega \times (x - x_0) + E(x - x_0) \quad \text{in } A.
\end{cases}
$$

(2.2)

Then, the force and torque and stresslet exerted on the fluid by the particle are given as

\[
F = -\int_{\partial A} \Sigma[v,p] \nu, \\
T = -\int_{\partial A} \Sigma[v,p] \nu \times (x - x_0), \\
S = -\text{sym}_0 \left( \int_{\partial A} \Sigma[v,p] \nu \otimes (x - x_0) \right),
\]

with $\nu$ the outer normal at $\partial A$ and $\Sigma[v,p] = 2\mu Dv - p\text{Id}$ the fluid stress where $Dv = \text{sym}(\nabla v)$ and $\text{sym } B$ and $\text{sym}_0 B$ denote the symmetric and symmetric traceless part of a matrix $B \in \mathbb{R}^{d \times d}$, respectively.

Then, the resistance tensor is defined through

\[
\begin{pmatrix}
F \\
T \\
S
\end{pmatrix} = \mu R_A \begin{pmatrix}
V \\
\omega \\
E
\end{pmatrix}.
\]

(2.3)

By linearity of the Stokes equations, $R_A$ is well defined. Moreover, by some integration by parts, $R_A$ is symmetric and positive definite. We denote

\[
\mathcal{R} := R_B := \begin{pmatrix}
\mathcal{R}_1 & \mathcal{R}_{12} & \mathcal{R}_{13} \\
\mathcal{R}_{12}^T & \mathcal{R}_2 & \mathcal{R}_{23} \\
\mathcal{R}_{13}^T & \mathcal{R}_{23}^T & \mathcal{R}_3
\end{pmatrix},
\]

and find due to rotational symmetry

\[
\begin{align*}
\mathcal{R}_1 &= \gamma_\perp (\text{Id} - e_3 \otimes e_3) + \gamma_\parallel e_3 \otimes e_3, \\
\mathcal{R}_2 &= \gamma_{\text{rot}} (\text{Id} - e_3 \otimes e_3) + \gamma_{\text{rot},\parallel} e_3 \otimes e_3, \\
\mathcal{R}_{23}^T \omega &= \gamma_E \text{Sym }((\omega \times e_3) \otimes e_3),
\end{align*}
\]

\footnote{By linearity, one can replace the velocities $V, \omega, E$ by the corresponding quantities relative to prescribed velocities of the fluid at infinity, which we set equal to zero by imposing $v \in \dot{H}^1(\mathbb{R}^3)$. Considering nonzero velocities at infinity, $E$ might be nonzero even for a rigid particle.}
for some $\gamma_\perp, \gamma_\parallel, \gamma_{\text{rot}}, \gamma_{\text{rot.}} > 0$, $\gamma_E \in \mathbb{R}$. Formula for these quantities in the case of spheroids can be found in [KK13, Subsection 3.3]). In particular $\gamma_E \neq 0$ for all spheroids except for spheres. (We omit corresponding formula for $\bar{R}_3, \bar{R}_{12}, \bar{R}_{13}$ (see [KK13, Subsection 5.5]). In fact, $\bar{R}_{12} = \bar{R}_{13}$ according to [Gra18] by choosing $x_0$ as the so-called center of hydrodynamic reaction.)

By straightforward transformation arguments the resistance tensor of $B_i$ with respect to $x_i$ is given by

$$
R_{B_i} = \begin{pmatrix}
r^2R_1(\xi_i) & r^2R_{12}(\xi_i) & r^2R_{13}(\xi_i) \\
r^2R_{12}^T(\xi_i) & r^3R_2(\xi_i) & r^3R_{23}(\xi_i) \\
r^2R_{13}(\xi_i) & r^3R_{23}^T(\xi_i) & r^3R_3(\xi_i)
\end{pmatrix},
$$

where

$$
R_1(\xi_i) = \gamma_\perp (\text{Id} - \xi_i \otimes \xi_i) + \gamma_\parallel \xi_i \otimes \xi_i,
$$

$$
R_2(\xi_i) = \gamma_{\text{rot}} (\text{Id} - \xi_i \otimes \xi_i) + \gamma_{\text{rot.}} \parallel \xi_i \otimes \xi_i,
$$

$$
R_{23}^T(\xi_i) \omega = \gamma_E \text{Sym} ((\omega \times \xi_i) \otimes \xi_i).
$$

For an inertialess rigid particle, one is interested in the problem to determine the particle velocities $V, \omega$ as well as the stresslet $S$ when force and torque $F, T$ are given, as well as the rate of strain $E$ (which corresponds to the rate of strain of the fluid far from the particle). This is known as the mobility problem. We consider here only the case $E = 0, F = 0$. IN this case, we have

$$
\omega = \mu^{-1} r^{-3} R_2^{-1} T,
$$

$$
S = \mu r^3 (R_{23})^T \omega = R_{23}^T R_2^{-1} T
$$

The mapping $R_{23}^T R_2^{-1}$ which relates the torque to the stresslet will play an important role in the analysis of the viscoelastic stress, hence we introduce the following operator

$$
S : S^2 \rightarrow \mathcal{L}(\mathbb{R}^3, \text{Sym}_0(\mathbb{R}^3)),
\xi \mapsto R_{23}^T(\xi) R_2^{-1}(\xi).
$$

Note that $S$ is smooth. In particular, there exists a constant $C > 0$ such that

$$
\|S\|_{C^1(S^2; \mathcal{L}(\mathbb{R}^3, \text{Sym}_0(\mathbb{R}^3))} \leq C.
$$

2.3. The dynamics

We assume that the fluid satisfies the Stokes equations with no-slip condition at the particles:

$$
\begin{cases}
- \mu \Delta u_n + \nabla p_n = 0 & \text{in } \mathbb{R}^3 \setminus \bigcup_{i=1}^n B_i, \\
\text{div } u_n = 0 & \text{in } \mathbb{R}^3 \setminus \bigcup_{i=1}^n B_i, \\
u_n = v_i + \omega_i \times (x - x_i) & \text{in } B_i.
\end{cases}
$$

Here, $v_i, \omega_i \in \mathbb{R}^3$ are the translational and angular velocities on $B_i$. Neglecting the particle inertia, the velocities $v_i, \omega_i$ are not given but they are determined through the following
conditions, prescribing the total force and torque acting on each particle:

\[
\int_{\partial B_i} \Sigma(u_n, p_n) \nu = F_i, \\
\int_{\partial B_i} [\Sigma(u_n, p_n) \nu] \times (x - x_i) = T_i.
\]

Since the particles are inertialess, these forces and torques balance the forces and torques acting on the particles which are the sum of external forces and torques and of the random forces and torques acting on each particle due to collisions with fluid particles, \( F_i = F_i^E + F_i^B \) and \( T_i = T_i^E + T_i^B \).

According to the fluctuation-dissipation theorem, the random forces and torques are given by

\[
(F^B, T^B) = \sqrt{2 k_B \Theta \mu r^3} R^2 \circ dB_i, \quad (2.8)
\]

see e.g. [Rou92]. Here, \( k_B \) is the Boltzmann constant, \( \Theta \) the absolute temperature, \( B \) is a 6n-dimensional Brownian motion and \( F^B, T^B \in \mathbb{R}^{3n} \) are the vectors containing all the forces and torques \( F^B_i, T^B_i \). Moreover, \( \mathcal{R}_n \in \mathbb{R}^{6n \times 6n} \) is the resistance matrix of all the particles (excluding, stresslet/strain). More precisely, similar as in (2.3), \( \mathcal{R}_n \) relates given velocities \( v_i, \omega_i \) at all particles to forces and torques \( F_i, T_i \) by solving the corresponding \( n \) particle problem instead of (2.2). In particular \( \mathcal{R}_n \) depends on the positions and orientations of all the \( n \) particles.

The fluid equations are complemented by the equations of motion for the particles

\[
\begin{align*}
\dot{x}_i &= v_i, \\
\dot{\xi}_i &= \omega_i \times \xi_i.
\end{align*}
\]

### 2.4. Simplification of the model

As outlined in the introduction, deriving the Doi model from (2.7)–(2.10) seems presently out of reach. We now detail the simplifications that lead from (2.7)–(2.10) to the model (1.2a)–(1.2b).

Instead of (2.9) and (2.10), we fix the particle centers, and set the forces \( F_i \) equal to 0,

\[
\begin{align*}
\dot{x}_i &= 0, \\
F_i &= 0.
\end{align*}
\]

Moreover, instead of the equation of motion for the particle orientation (2.10), we assume

\[
d\xi_i(s) = \xi_i(s) \times \sqrt{2 k_B \Theta \mu r^{-3} R^{-1}_2} \circ dB_i(s) + P_{\xi_i} h(s, \xi_i(s), x_i) \, ds, \quad (2.11)
\]

where \( R_2 \) is as in (2.4). The first term on the right-hand side above corresponds to an angular velocity \( \omega_i \) caused by random collisions with fluid particles as if the particle \( B_i \) was alone in the fluid, i.e. \( \omega_i = \mu r^{-3} R^{-1}_2 T_i^B \) with \( T_i^B = \sqrt{2 k_B \Theta \mu r^3 R_2(\xi_i) \circ B_i} \). This is known as hydrodynamic decoupling and is at least formally justified for small particle volume fraction. Here, and in the following, \( B_i \) is brownian motion in \( \mathbb{R}^3 \). The additional term in (2.11) containing \( h \) could be understood as arising from an external torque for example associated to an external fluid flow, a magnetic field or chemotaxis. By an action reaction principle, a corresponding torque should act on the fluid as well, but we will omit this for the sake of simplicity. More precisely, regarding the fluid equations, we consider the random torques \( T_i^B \) as the only torques acting on the fluid.
Then, the simplified model at one glance is given by

\[
\begin{cases}
-\mu \Delta u_n + \nabla p_n = 0 & \text{in } \mathbb{R}^3 \setminus \bigcup_{i=1}^n B_i, \\
\text{div} u_n = 0 & \text{in } \mathbb{R}^3 \setminus \bigcup_{i=1}^n B_i, \\
D u_n = 0 & \text{in } \bigcup_{i=1}^n B_i,
\end{cases}
\]

\[\int_{\partial B_i} \Sigma(u_n, p_n) \nu = 0,\]

\[\int_{\partial B_i} \Sigma(u_n, p_n) \nu \times (x - x_i) = \sqrt{2k_B \Theta \mu r^{-3}} \hat{B}_i,\]

\[
\begin{cases}
d\xi_i(s) = \xi_i(s) \times \sqrt{2k_B \Theta \mu^{-1} r^{-3} \gamma_{\text{rot}}} \circ dB_i(s) + P_{\xi_i} h(s, \xi_i(s), x_i) ds, \\
\xi_i(0) = \xi_{i,0}, \\
x_i(s) = x_{i,0}.
\end{cases}
\]

(2.12a)

Here we used (2.5) and properties of the cross product to simplify the equation for \(\xi_i\). Moreover, for the ease of notation, we replaced the condition \(u_n = v_i + \omega_i \times (x - x_i)\) in \(B_i\) by the equivalent condition \(Du_n = 0\) in \(B_i\).

### 2.5. Nondimensionalization

We examine the expected order of magnitude of various terms and perform a nondimensionalization of the equation. A similar reasoning (for a model including translations and also gravity) can be found in [OT08].

We recall that we make the assumption that we are in the so-called dilute regime, meaning

\[
\phi_n := \frac{n}{L^3} \ll 1,
\]

where \(L\) is the characteristic length of the cloud of particles such that \(n/L^3\) is the number density. This assumption entails that the particles can freely rotate. Note that \(\phi_n\) is proportional to the particle volume fraction. For very elongated rods the reference particle \(B\) has a very small volume such that the particle volume fraction might be much less than \(\phi_n\). However, we fix the reference particle \(B\) to be independent of \(n\). Throughout the paper we will often simply refer to \(\phi_n\) as the particle volume fraction.

From (2.12b) we obtain a rotational diffusion constant

\[
D_r \sim \frac{k_B \Theta}{\mu \gamma_{\text{rot}}} r^3,
\]

this gives rise to a typical timescale for diffusion

\[
T_D = \frac{1}{D_r} \sim \frac{\mu r^3 \gamma_{\text{rot}}}{k_B \Theta}.
\]

On the other hand, we look at the viscoelastic stress \(\sigma\). Following the heuristic given in Subsection 1.2, we remind that a non-isotropic particle \(B_i\) induces a stresslet on the fluid proportional to the torque. The average stresslet produced by one particle arises then from
the variation of the stresslet with respect to changes of the orientation. Thus combining the
the formula for the torque from (2.12a) with the random part of the change of orientation in
(2.12b), formally leads to a stresslets of order
\[ |S_i| \sim \sqrt{k_B \Theta \mu^{-1} r^{-3} \sqrt{k_B \Theta \mu r^3}} = k_B \Theta, \]
for each individual particle. For a rigorous argument on how the individual stress arises, we
refer to Lemma 3.4. To obtain the total viscoelastic stress, we multiply with the number density
\[ |\sigma| \sim n L^3 \]
Since the induced fluid gradient is of order \( |\nabla u| \sim \frac{|\sigma|}{\mu} \), we arrive at the viscoelastic
timescale
\[ T_u = \frac{1}{|\nabla u|} \sim \frac{\mu \gamma \text{rot} L^3}{nk_B \Theta}. \]
In particular, we have
\[ \frac{T_D}{T_u} \sim \frac{n r^3}{L^3} = \phi_n \ll 1, \]
which means that the diffusion happens on a much faster timescale than the viscoelastic stress.
Consequently, when nondimensionalizing, we can choose to rescale to the diffusive timescale
\( T = T_D \) or to rescale to the viscoelastic timescale \( T = T_u \).

We first rescale (2.12) with the characteristic time \( T_D \) and the length \( L \). Keeping the same
symbols for the rescaled quantities, lengthy but straightforward calculations\(^2\) yield
\[
\begin{align*}
-\Delta u_n + \nabla p_n &= 0 \quad \text{in } \mathbb{R}^3 \setminus \bigcup_{i=1}^n B_i, \\
\text{div } u_n &= 0 \quad \text{in } \mathbb{R}^3 \setminus \bigcup_{i=1}^n B_i, \\
Du_n &= 0 \quad \text{in } \bigcup_{i=1}^n B_i, \\
\int_{\partial B_i} \Sigma(u_n, p_n) \nu &= 0, \\
\int_{\partial B_i} [\Sigma(u_n, p_n) \nu] \times (x - x_i) &= r^3 \sqrt{2 \gamma \text{rot} R_2(\xi_i(s))} \circ \dot{B}_i(s),
\end{align*}
\]
Note that from now on the nondimensional fluid stress is given as \( \Sigma(u_n, p_n) = 2Du_n - p_n \text{Id} \).
Note that due to the rescaling of the lengthscales with \( L \), the “volume fraction” \( \phi_n \) is now given by
\[ \phi_n = nr^3. \]
Finally, we remark that we dropped the trivial equation \( x_i(s) = x_{i,0} \), and we consider instead
the positions \( x_i \) as given time-independent quantities.
Similarly rescaling instead with the characteristic time \( T_u \) yields

\(^2\)Here one needs to use that the Brownian motion scales as \( B(Tt) \sim \sqrt{TB(t)} \).
\[-\Delta u_n + \nabla p_n = 0 \quad \text{in} \quad \mathbb{R}^3 \setminus \bigcup_{i=1}^n B_i,\]
\[\text{div} \, u_n = 0 \quad \text{in} \quad \mathbb{R}^3 \setminus \bigcup_{i=1}^n B_i,\]
\[Du_n = 0 \quad \text{in} \quad \bigcup_{i=1}^n B_i,\]
\[\int_{\partial B_i} \Sigma(u_n, p_n) \nu = 0,\]
\[\int_{\partial B_i} \Sigma(u_n, p_n) \nu \times (x - x_i) = \frac{1}{n} \sqrt{2^\gamma} \rho_n R_2(\xi_i(s)) \circ \dot{B}_i(s),\]
\[
\begin{cases}
  d \xi_i(s) = \xi_i(s) \times \frac{1}{\phi_n} \circ dB_i(s) + \frac{1}{\phi_n} P_{\xi_i} h(s, \xi_i(s), x_i) \, ds, \\
  \xi_i(0) = \xi_{i,0}.
\end{cases}
\]  

Clearly (2.13) can be recovered from (2.14) upon rescaling time with \(\phi_n\). Thus, in the limit \(n \to \infty\) with \(\phi_n \to 0\) one can interpret (2.13) as an initial layer of (2.14). We emphasize that in this sense, the function \(h\) in (2.13) corresponds to \(h(\phi_n t, \cdot)\) for \(h\) as in (2.14).

3. Main Results

3.1. Assumptions

We will impose the following assumptions for the rest of the paper. We work in the framework of a filtered probability space, denoted by \((\Omega, \mathcal{F}, \{\mathcal{F}_t\}, \mathbb{P})\). We recall that we consider \(n\) particles occupying \(B_i(\xi_i) = x_i + rR_i(\xi_i)B\), where \(B \subseteq \mathbb{R}^3\) is the reference particle specified in (2.1), the positions \(x_i \in \mathbb{R}^3\) are static random variables, the orientations \(\xi_i \in S^2\) are random and time-dependent, and the rotation matrix \(R_i(\xi_i) \in SO(3)\) is any matrix which satisfies \(R_i(\xi_i)e_3 = \xi_i\).

We emphasize that \(B_i, x_i, r, \xi_i\) all implicitly depend on \(n\).

We assume that the particle volume fraction \(\phi_n = nr^3\) tends to zero sufficiently fast, namely
\[
\lim_{n \to \infty} \phi_n \log n = 0.
\]  

Moreover, we assume that the particle centers \(x_i\) are well-separated in the sense that there exists \(c > 0\), independent of \(n\), such that
\[
d_{\text{min}} := \min_{i \neq j} |x_i - x_j| \geq cn^{-\frac{1}{3}}.
\]  

We remark that the above assumptions together imply in particular that there exists \(n_0 \in \mathbb{N}\) such that for all \(n \geq n_0\)

\[
\min_{i \neq j} \inf_{(\xi_i, \xi_j) \in S^2 \times S^2} \text{dist}(B_i, B_j) \geq cr.
\]  

We assume in addition that the particles are contained in a bounded domain uniformly in \(n\)
\[
\sup_n \max_{1 \leq i \leq n} |x_i| < +\infty.
\]  

We assume that \(B_i\) are independent \(\mathbb{R}^3\) valued Brownian motions, all independent of \(\xi_i, 0\), defined on the filtered probability space \((\Omega, \mathcal{F}, \{\mathcal{F}_t\}, \mathbb{P})\). Moreover, we assume that the initial
particle orientations $\xi_{i,0}$ are independent random variables and we assume the convergence of the initial empirical measure to some $f_0 \in \mathcal{P}_1(\mathbb{R}^3 \times S^2) \cap L^2(S^2 \times \mathbb{R}^3)$, i.e.

$$\lim_{n \to \infty} \mathbb{E} \left[ W_1 \left( f_0, \frac{1}{n} \sum_i \delta_{x_i, \xi_{i,0}} \right) \right]. \quad \text{(H4)}$$

Here, for two probability measures $g_1, g_2 \in \mathcal{P}_1(\mathbb{R}^3 \times S^2)$ with bounded first moment, we denote by $W_1(g_1, g_2)$ their 1-Wasserstein distance. It is well known that the $W_1$-distance metrizes weak convergence of measures.

Finally, we assume for simplicity that the external force $h$ is smooth, i.e.

$$h \in C^\infty([0, \infty) \times \mathbb{R}^3 \times S^2). \quad \text{(H5)}$$

### 3.2. Well-posedness of the microscopic system

We will now specify what the notion of solutions to the systems (2.14) and (2.13).

The uncoupled SDEs for the particle orientations are well known to be well-posed for $h$ as in (H5) (see Definition C.12 and Theorem C.15). Note that by introducing the diffusion matrix $\sigma_D$,

$$\sigma_D(\xi) := \sqrt{2} \begin{pmatrix} 0 & -\xi_3 & \xi_2 \\ \xi_3 & 0 & -\xi_1 \\ -\xi_2 & \xi_1 & 0 \end{pmatrix}, \quad \text{(3.2)}$$

and by the Ito-Stratonovich conversion, Remark C.14, we can rewrite (2.13b) and (2.14b) respectively as

$$d\xi_i = \sigma_D(\xi_i) dB_i - 2\xi_i ds + P_{\xi_i} h(s, \xi_i, x_i) ds, \quad \text{(3.3)}$$

$$d\xi_i(s) = \sqrt{\frac{1}{\phi_n} \sigma_D(\xi_i(s))} dB_i(s) - \frac{2}{\phi_n} \xi_i(s) ds + \frac{1}{\phi_n} P_{\xi_i} h(s, \xi_i(s), x_i) ds.$$

Since the fluid is modeled by the stationary Stokes equations, we can only expect the fluid velocity to be pathwise as (ir-)regular in time as the white noise that drives the fluid velocity through the prescribed torques. It is well known that white noise is in $H^{-s}$ for any $s > 1/2$.

To give a meaning to $u_n$ and to obtain this regularity, we write $u_n$ as the distributional derivative of a suitable stochastic integral. To this end, we first introduce the operator $L_n : \mathbb{R}^{3n} \to L(\mathbb{R}^{3n}, H^1(\mathbb{R}^3))$. For any fixed set of particle positions $(x_1, \ldots, x_n)$ it associates to every set of orientations $(\zeta_1, \ldots, \zeta_n)$ the solution to the Stokes system with given torques $(T_1, \ldots, T_n)$. More precisely,

$$v = L_n((\zeta_1, \ldots, \zeta_n))(T_1, \ldots, T_n), \quad \text{(3.4)}$$

\footnote{To see that for a given compactly supported function $f_0$, there exists $x_i, \xi_{i,0}$ which satisfy both assumptions (H2) and (H4), one might first generate i.i.d variables $\tilde{x}_i, \xi_{i,0}$ with law $f_0 dx$ and then define the positions $x_i \in n^{-1/3} \mathbb{Z}^3$ to be the closest points to $\tilde{x}_i$.}
is defined to be the solution to

\[
\begin{cases}
-\Delta v + \nabla q = 0 & \text{in } \mathbb{R}^3 \setminus \bigcup_{i=1}^n B_i, \\
\text{div } v = 0 & \text{in } \mathbb{R}^3 \setminus \bigcup_{i=1}^n B_i, \\
Dv = 0 & \text{in } \bigcup_{i=1}^n B_i, \\
\int_{\partial B_i} \Sigma(v, q) \nu = 0, \\
\int_{\partial B_i} [\Sigma(v, q) \nu] \times (x - x_i) = T_i,
\end{cases}
\]

(3.5)

where here (abusing the notation) \( B_i = x_i + r R(\xi_i) \). It is straightforward to see that for non-overlapping particles \( B_i \), the linear problem (3.4) admits a unique weak solution \( v \in \dot{H}^1(\mathbb{R}^3) \) (see e.g. [NS20]). In particular, \( L_n \) is well-defined for all particle configurations \( (y_1, \ldots, y_n) \) which satisfy (3.1).

This allows us to formally define

\[
U_n(t) := \frac{\sqrt{2} \gamma_{\text{rot}}}{n} \int_0^t L_n(\Xi(s)) \sqrt{\mathcal{R}_2(\Xi(s))} \circ d(B_1(s), \ldots, B_n(s)),
\]

(3.6)

where \( \Xi = (\xi_1, \ldots, \xi_n) \), \( \xi_i \) are the solutions to (2.14b), and \( \mathcal{R}_2(\Xi) \in \mathbb{R}^{3n \times 3n} \) is the block-diagonal matrix with blocks \( \mathcal{R}_2(\xi_i) \) (see (2.5)). Then, we define the (distributional) solution to (2.14a) \( u_n \) as the distributional derivative of \( U_n \),

\[
u_n := U_n'.
\]

(3.7)

Similarly, concerning the system (2.13), we set

\[
U_n(t) := r^3 \frac{\sqrt{2} \gamma_{\text{rot}}}{n} \int_0^t L_n(\Xi(s)) \sqrt{\mathcal{R}_2(\Xi(s))} \circ d(B_1(s), \ldots, B_n(s)),
\]

(3.8)

where \( \xi_i \) are the solutions to (2.13b).

To make these formal definition of \( u_n \) rigorous, we need to make sense of the stochastic integrals in (3.6) and (3.8). In Appendix C, we collect some statements about the definition and properties of such stochastic integrals with values in separable Hilbert spaces. Essentially, all standard results immediately carry over due to Itô isometry. Therefore, \( U_n \), and thereby \( u_n \), is well-defined provided we show that \( L_n \) is continuously differentiable with respect to the orientations \( \xi_i \).

We will show the following global well-posedness result of the microscopic dynamics.

**Theorem 3.1.** Let (H1)–(H2) be satisfied. Then, for all \( n \in \mathbb{N} \), there exists a unique solution \( (\xi_1, \ldots, \xi_n) \) to (2.13b) and (2.14b), respectively.

Moreover, there exists \( N_0 \in \mathbb{N} \) such that for all \( n \geq N_0 \) and all \( s > 1/2 \), the operator \( L_n \) defined through (3.4)–(3.5) satisfies \( L_n \in C^1((\mathbb{S}^2)^n; \mathcal{L}(\mathbb{H}^s, \mathbb{H}^{-s}(\mathbb{R}^3))) \), where \( \mathbb{H}^{-s}(\mathbb{R}^3) \) denotes the subspace of divergence free functions in \( \mathbb{H}^{-s}(\mathbb{R}^3) \).

In particular, the integral (3.6) (respectively (3.8)) is well defined and for all \( T > 0 \)

\[
u_n \in L^2(\Omega; \mathbb{H}^{-s}(0, T; \mathbb{H}^{-s}(\mathbb{R}^3)))).
\]
3.3. Convergence results

We are finally prepared to state the main results of our paper, the convergence to the mean-field limits for (2.14) and (2.13).

We denote by $S_n$ the empirical measure

$$S_n(t) := \frac{1}{n} \sum_{i} \delta_{x_i(t)},$$  \hspace{1cm} (3.9)

We first state the main result concerning system (2.13).

**Theorem 3.2.** Let assumptions (H1)–(H5) be satisfied. For $n \geq N_0$ as in Theorem 3.1, let $\xi_i$, $1 \leq i \leq n$ and $u_n$ be the unique solutions to (2.13). Then, for all $t > 0$ and all $s > 1/2$ the following convergence in probability holds:

$$\forall \varepsilon > 0 \lim_{n \to \infty} \mathbb{P} \left( \| \phi_n^{-1} u_n - u \|_{H^{-s/2}(0,t);H^{-s}(\mathbb{R}^3)} + \sup_{\tau \in [0,t]} \mathcal{W}_1(S_n(\tau),f(\tau)) > \varepsilon \right) = 0,$$

where $f \in C([0,\bar{t}],\mathcal{P}_1(\mathbb{R}^3 \times \mathbb{S}^2) \cap L^2(\mathbb{R}^3 \times \mathbb{S}^2))$ is the unique weak solution to (1.3) such that for almost all $x \in \mathbb{R}^3$, $f(\cdot,\cdot,x) \in L^2(0,t;H^1(\mathbb{S}^2))$, $f'(\cdot,\cdot,x) \in L^2(0,t;H^{-1}(\mathbb{S}^2))$ and $u \in L^2(0,t;H^1_s(\mathbb{R}^3))$ the unique weak solution to (1.4).

Similarly, we show the following convergence result for system (2.14).

**Theorem 3.3.** Let assumptions (H1)–(H5) be satisfied. For each $n \geq N_0$ as in Theorem 3.1, let $\xi_i$, $1 \leq i \leq n$ and $u_n$ be the unique solutions to (2.14). Then, for all $s_1 > 1/2, s_2 > 0, s_3 > 3/2$ the following convergence in probability holds:

$$\forall \varepsilon > 0 \lim_{n \to \infty} \mathbb{P} \left( \| u_n - u \|_{H^{-s_1}(0,t);H^{-s_2}(\mathbb{R}^3)} + \| S_n - f \|_{H^{-s_3}(0,t);H^{-s_3}(\mathbb{R}^3 \times \mathbb{S}^2)} > \varepsilon \right) = 0,$$

where $f \in L^2((0,t) \times \mathbb{S}^2 \times \mathbb{R}^3)$ is the unique weak solution to (1.5) such that for almost all $x \in \mathbb{R}^3$, $f(\cdot,\cdot,x) \in C^\infty((0,t) \times \mathbb{S}^2)$, and $u \in L^2(0,t;H^1_s(\mathbb{R}^3))$ the unique weak solution to (1.4).

3.4. Notation

- Throughout the paper we will often deal with vectors $V \in (\mathbb{R}^3)^n$, where $n \in \mathbb{N}$ is the number of particles. We will use the convention to denote the components $V_i \in \mathbb{R}^3$, $1 \leq i \leq n$ by Latin indices and use Greek indices to denote the components of these vectors, e.g. $V_{i,\alpha} \in \mathbb{R}$, $1 \leq \alpha \leq 3$. With this convention, we allow for the slight abuse to write $V \in \mathbb{R}^{3n}$ instead of $V \in (\mathbb{R}^3)^n$. In particular we denote by $e_{i,\alpha}$, $1 \leq i \leq n$, $1 \leq \alpha \leq 3$ the canonical basis of $\mathbb{R}^{3n}$.

Moreover, in the special case of the particle positions and orientations we will use capital letters to denote the collections $X = (x_1, \ldots, x_n) \in \mathbb{R}^{3n}$, and $\Xi = (\xi_1, \ldots, \xi_n) \in (\mathbb{S}^2)^n$ in order to avoid confusion with variables $x, \xi$ that appear in the limit systems.

- For any vector $T \in \mathbb{R}^3$, we set

$$[T]_M := \begin{pmatrix} 0 & -T_3 & T_2 \\ T_3 & 0 & -T_1 \\ -T_2 & T_1 & 0 \end{pmatrix},$$ \hspace{1cm} (3.10)
We allow for the abuse of notation

$$\|g\|_{W^{s,p}(\mathbb{R}^3)} \leq C,$$

to indicate that for all compact $K \subset \mathbb{R}^3$ there exists $C$ depending on $K$ such that

$$\|g\|_{W^{s,p}(K)} \leq C.$$
Similarly, we write \( g \in W^{s,p-}(U) \) and
\[
\|g\|_{W^{s,p-}(U)} \leq C,
\]
to indicate that for all \( 1 \leq q < p \) there exists \( C \) depending on \( q \) such that
\[
\|g\|_{W^{s,q}(U)} \leq C.
\]
The notation \( \|g\|_{W^{s,p-}(U)} \leq C \) should be understood analogously.

- For an open set \( O \subseteq \mathbb{R}^3 \), \( p \geq 1 \) and \( w \) as in (3.13), we introduce
\[
\|g\|_{L^p,2w,\mathcal{O}} := \|g\|_{L^p(O)} + \|g\|_{L^2(\mathbb{R}^3 \setminus \mathcal{O})},
\]
\[
L^p,2w,\mathcal{O} := \{ g \in L^1_{\text{loc}}(\mathbb{R}^3) : \|g\|_{L^p,2w,\mathcal{O}} < \infty \}.
\]

- We use an index \( s \) to denote subspaces of (distributionally) divergence free functions, i.e. we use the notation \( L^p_s(O) \), \( H^s(\mathcal{O}) \), \( H^s_{\text{div}}(\mathcal{O}) \), \( W^s_{\text{div}}(\mathcal{O}) \), \( W^s_{\text{sym}}(\mathcal{O}) \), \( L^p_{s,\text{div},\mathcal{O}} \) and all these subspaces are closed.

- Finally, in Sections 4 – 6 we will adopt the usual convention to denote by \( C > 0 \) any constant that might change from line to line and that might depend on certain quantities which are fixed like the reference particle or the constant appearing in (H2). We emphasize that the constant \( C \) will never depend on \( n \) though.

### 3.5. Outline of the proof of the main results

Starting from (2.13), the first step towards the derivation of the mesoscopic system (1.3), (1.4) is the following approximation for the fluid equations (2.13a):
\[
-\Delta u_{n,\text{app}} + \nabla \tilde{p}_{n,\text{app}} = \frac{\phi_n}{n} \sum_i ([T_i]_M + S(\xi_i)T_i) \nabla \delta_{x_i},
\]
where \( T_i = \sqrt{2\gamma_{\text{rod}}} \mathcal{R}_2(\xi_i) \circ \dot{B}_i \) and we recall that \( S(\xi_i) \) from (2.6) is the tensor that relates the torque to the stresslet and \( [T_i]_M \) is defined in (3.10). Thus the approximation (3.15) consists in a formal superposition principle of point torques and stresslets; each particle contributes to \( u_{n,\text{app}} \) as if it was alone in the fluid and only its total torque and stresslet acts on the fluid at the particle center.

The rigorous justification of this approximation is the content of Section 4. More precisely, Section 4 deals with the approximation of the solution \( L_n T \) to (3.5) by the solution \( L_{n,\text{app}} T \) to (3.15) for any given \( T \in \mathbb{R}^{3n} \) and any given collection of particle positions \( x_i \) and orientations \( \xi_i, 1 \leq i \leq n \) which satisfy assumption (H1)–(H3). To this end, we will first introduce an intermediate approximation \( L^m_{n,\text{app}} \) defined as the superposition of single particle problems, but with the full boundary conditions (no-slip and balance equations) for the single particle.

Estimates for approximations similar to (3.15) have been given for example in [Höf18; HV18; GH20; HW20; NS20; Ger21]. The main novelty here are estimates for \( \nabla \xi_i (L_n - L^m_{n,\text{app}}) T \), which are needed because of the Stratonovitch integral in (3.6). Since the fluid domain \( \mathbb{R}^3 \setminus \bigcup_i B_i \) depends on the particle orientations, we enter here the topic of shape derivatives. Such shape derivatives for the Stokes equations with different boundary conditions have been considered...
for example in [Sim91; BCD11]. Instead of identifying the boundary value problem solved by $\nabla \xi_i L_n$ as in [Sim91; BCD11], we rely on the method of reflections to analyze these shape derivatives in Subsection 4.2. The method of reflections has been used for related problems, see for example [Höf18; HV18; Mec19; GH20; HW20; Mec20; NS20]. It allows to express $L_n$ in terms of single particle problems only. Since these single particle operators have an explicit dependence on the particle orientation, this yields a useful expression for the shape derivative.

As reflected by the approximation (3.15) the given torques at each particle position $x_i$ perturb the fluid velocity in a singular way as $|x - x_i|^{-2}$. This is the reason why we only obtain sufficient estimates under the assumptions (H1)–(H2). Moreover, due to the singular nature of the perturbation, these estimates are locally only in $L^p$ for $p < 3/2$. Since the stochastic integral (3.6) does not seem compatible with such $L^p$ spaces (see e.g. [VVW15]), we work instead in weighted negative Sobolev spaces $H^{-s}_{w}(\mathbb{R}^3)$, $s > 1/2$, which are Hilbert spaces. In Appendix D, we show that $L^{p,2}_{w,K}$ (see (3.14)) embeds into $H^{-s}_{w}(\mathbb{R}^3)$ for a compact set $K$. Therefore, in Section 4, we will always work in the space $L^{p,2}_{w,K}$ where we choose $K$ to contain all the particles thanks to assumption H3.

The results in Section 4 immediately imply that the stochastic integral (3.6) that defines $u_n$ is well-defined which yields Theorem 3.1.

The approximation (3.15) suggests through an appropriate version of the Law of Large Numbers that the limit of $u_n$ is given in terms of the expectation of the torque and stresslet exerted on the fluid by each particle. The following lemma states that these expectation indeed correspond to the formula for the viscoelastic stress in (1.4). The proof of the lemma is a straightforward calculation which we postpone to Appendix B.

**Lemma 3.4.** Let $\xi_i$ be the solution to (2.13b). For any $A \in C^\infty_c((0,t),\text{Sym}_0(3))$ and $b \in C^\infty_c((0,t),\mathbb{R}^3)$ we have

\[
\mathbb{E} \left[ \int_0^t b(s) \cdot \sqrt{2} \xi_i(s) \circ dB_i(s) \right] = 0, \tag{3.16}
\]

\[
\mathbb{E} \left[ \int_0^t A(s) : S(\xi_i(s)) \sqrt{2} \xi_i(s) \circ dB_i(s) \right] = \frac{\gamma E}{\sqrt{2} \gamma_{\text{rot}}} \mathbb{E} \int_0^t [3\xi_i(s) \otimes \xi_i(s) - \text{Id}] : A(s) \, ds. \tag{3.17}
\]

The proof of the main convergence results, Theorems 3.2 and 3.3, is completed in Sections 5 and 6, respectively. Since the particle dynamics is uncoupled, we do not face here the problem of propagation of chaos as in classical mean field systems. However, a slight complication arises because the particle position are not assumed to be independent (which is impossible due to assumption (H2)). If they were independent, the law of each particle would be given by the Fokker-Planck equation (1.3) in the case of system (2.13b), and we would deduce convergence immediately by the Law of Large Numbers. Instead, we follow here a compactness approach used for example in [Oel85; Mél96; KL98; FLR21]. This approach is roughly described as follows. First, one shows tightness in a suitable functional spaces of the laws of the empirical measure $S_n$ and the fluid velocity $u_n$ in suitable spaces. Then one introduces functionals such that, on the one hand, $u_n$ and $S_n$ concentrate on the zeroes of these functionals, and on the other hand, these zeroes are precisely the unique solutions of the desired limit systems (1.4) together with (1.3) and (1.5), respectively.
The choice of the functionals correspond to distributional solutions of the limit system. We therefore need to show that such solutions are unique in the negative Sobolev spaces we use. The proof of these uniqueness results, which we give in Appendix A for completeness, is based on well-posedness and regularity of the corresponding dual problems. This is completely standard for the Stokes equations and the instationary Fokker-Planck equations. The slightly more involved proof for the stationary Fokker-Planck system we carry out in more detail.

### 3.6. Limitations and possible generalizations

In this subsection we comment on open questions related to limitations and possible generalizations of the analysis in this paper.

We dropped the evolution of the particle translations. It seems very challenging to include translations with the current techniques because they require well-separated particles in the sense of assumption (H2). Although this condition has been shown to propagate in time in [Höf18; Mec19; HS21] under suitable assumptions for sedimenting inertialess non-Brownian rigid spherical particles, the presence of Brownian forces and torques in the current model could break such propagation.

As discussed in Subsection 2.3 it seems physically more accurate to prescribe random forces and torques given by (2.8) and the evolution of the particle evolution through (2.10). For vanishing particle volume fraction as in assumption (H1), it seems not unrealistic to treat such a microscopic model (still ignoring the evolution of the particle centers). One might worry about rotations caused by hydrodynamic interactions between the particles which have a singularity like $|x|^{-3}$: a stresslet $S$ at a particle at $x_i$ creates a fluid velocity roughly like $\nabla \Phi(x - x_i) : S$ where $\Phi$ is the fundamental solution of the Stokes equations. The induced rotation at another particle then scales like the gradient of this function. However, as the viscoelastic stress is of smaller order than the diffusion rate by a factor $\phi_n$, this singular interaction could still be negligible if $\phi_n \rightarrow 0$. In the Doi model (1.1) this corresponds to $\lambda_2 = \lambda_3 = 0$ for $\phi_n \rightarrow 0$. The situation changes completely when one considers non vanishing volume fractions $\phi_n$. In that case, the singular interaction cannot be neglected. In fact, the critical singularity $|x|^{-3}$ of the interaction leaves little hope that one can pass to the formal mean-field limit that would give rise to the term $\text{div}_{\xi}(P_{\xi}^{-1} \nabla_{\xi} u_{\xi} f)$ in (a version of) the Doi model (1.1). Indeed, discrepancies between discrete and continuous convolutions which such singular convolution kernel have been studied in a related setting in [GH20].

On the technical side, we are restricted to vanishing volume fractions $\phi_n$, more precisely to assumption (H1), because of the factor $\phi_n \log n$ appearing in the estimates for the shape derivatives (see Proposition 4.3). It would be desirable to analyze whether this bound is optimal or could be improved under suitable assumptions on the particle configuration.

We dropped the fluid inertia and model the fluid by the stationary Stokes equations. An interesting question would be to investigate the instationary Navier-Stokes equations. Heuristically, the result should be unchanged since on the microscopic scale of the particles the fluid inertia does not matter. Mathematically though, already the problem of giving a meaning to the microscopic fluid velocity changes completely.

To our knowledge, even in the case of quasistatic non-Brownian particles, no rigorous homogenization results regarding the effective viscosity of suspensions are available for the Navier-Stokes equations. This has been obtained only for prescribed particle velocities (i.e. inertial particles) in [FNN16] where the effective equation contains the typical Brinkman term.
In this paper the particles are all obtained from (isotropic) rescaling of a fixed reference particle. In order to model rod-like particles, it would be interesting to consider particles which become more and more slender as $n \to \infty$. We refer to [HPS21] for the analysis of the evolution of such filaments in a fluid.

Finally, an important open problem is the rigorous derivation of models (expressions for the viscoelastic stress to begin with) of flexible polymers mentioned in the introduction. In the simplest setting one could start with a dumbbell model, where the flexible polymer is just modeled by two rigid balls connected by an (infinitesimally small) spring.

4. Approximation of the operator $L_n$

In this section, we study the solution operator $L_n$ which has been defined in Subsection 3.2 as the solution operator for the Stokes problem (3.5). Throughout this section, we denote by $x_i, \xi_i, 1 \leq i \leq n$, a generic (time-independent) collection of positions and orientations satisfying (H1)–(H3).

We introduce the following explicit approximate solution operator $L_{n,\text{app}}$:

$$L_{n,\text{app}} : \mathbb{R}^{3n} \to \mathcal{L}(\mathbb{R}^{3n}, L^{3/2}_{\text{loc}}(\mathbb{R}^3)), \quad \Xi := (\xi_1, \ldots, \xi_n) \mapsto L_{n,\text{app}}(\Xi),$$

defined for all $T := (T_1, \ldots, T_n) \in \mathbb{R}^{3n}$ by

$$(L_{n,\text{app}}((\xi_1, \ldots, \xi_n))T)(x) = \sum_i ([T_i]_M + S(\xi_i)T_i) : \nabla \Phi(x - x_i),$$

where $S(\xi_i)$ is defined in (2.6), $[T_i]_M$ is defined in (3.10) and

$$\Phi(x) = \frac{1}{8\pi} \left( \frac{1}{|x|} + \frac{x \otimes x}{|x|^3} \right),$$

is the fundamental solution of the Stokes equations. Moreover, in (4.1) and later on, we use the convention that for a matrix $M \in \mathbb{R}^{3 \times 3}$ we write

$$(M : \nabla \Phi)_{\alpha} = \sum_{\beta, \gamma} \partial_{x_j} M_{\gamma\beta} \Phi_{\alpha\gamma}.$$

From the definition, we seen that $v = L_{n,\text{app}}((\xi_1, \ldots, \xi_n))T$ is a distributional solution to

$$-\Delta v + \nabla p = \text{div} \left( \sum_i ([T_i]_M + S(\xi_i)T_i) \delta_{x_i} \right), \quad \text{div} v = 0, \text{ in } \mathbb{R}^3. \quad (4.2)$$

We emphasize that in contrast to $L_n$ the operator $L_{n,\text{app}}$ does only depend on the particle positions but not on the scaling factor $r$. The only dependence on the particle shape and orientations is through the function $S(\xi_i)$. Due to the asymptotic behavior of $\Phi$, $L_{n,\text{app}}T$ fails to be in $L^p$ for $p < 3/2$. To capture the decay at infinity we therefore consider $L^{3/2}_{s, \text{w}, B(0,M)}$ (see (3.14)) with weight $w$ as in (3.13) and for

$$M := \sup_n \max \left\{ 1, 2 \max_i |x_i|, 8r \right\}, \quad (4.3)$$

which is finite thanks to assumption (H3).

We make the following observation regarding $L_{n,\text{app}}$. 

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Lemma 4.1. Let $1 < p < 3/2$, $M$ be as in (4.3) and $w$ as in (3.13). Then, the operator $L_{n,\text{app}}$ satisfies $L_{n,\text{app}} \in C^1((\mathbb{S}^2)^n; \mathcal{L}(\mathbb{R}^{3n}, L^{p,2}_{s,w,B(0,M)}))$ with

$$\|L_{n,\text{app}}\|_{C^1((\mathbb{S}^2)^n; (L^{p,2}_{w,B(0,M)})^{3n})} \leq C\sqrt{n}.$$  

Remark 4.2. Note that we identified $\mathcal{L}(\mathbb{R}^{3n}, L^{p,2}_{s,w,B(0,M)})$ with $(L^{p,2}_{s,w,B(0,M)})^{3n}$ in order to clarify that we consider the norm $\|\cdot\|_{L^{p,2}_{w,B(0,M)}}$.

Proof. Since $S$ is a smooth function of $\xi$, the assertion follows immediately from the decay of $\nabla \Phi$ which implies $\nabla \Phi(\cdot - x_i) \in L^2_{\text{loc}}(\mathbb{R}^3)$ and $\nabla \Phi(\cdot - x_i) \in L^2_w(\mathbb{R}^3 \setminus B(0, M))$. \hfill \Box

The main result of this section is the following proposition.

Proposition 4.3. Let $M$ be as in (4.3) and $w$ as in (3.13). Then, there exists $N \in \mathbb{N}$ such that for all $n \geq N$ and all $1 < p < 3/2$ the operator $L_n$ defined in Subsection 3.2 satisfies $L_n \in C^1((\mathbb{S}^2)^n; \mathcal{L}(\mathbb{R}^{3n}, L^{p,2}_{s,w,B(0,M)}))$.

$$\|L_n - L_{n,\text{app}}\|_{C^1((\mathbb{S}^2)^n; (L^{p,2}_{w,B(0,M)})^{3n})} \leq C\sqrt{n}(\phi_n \log n + r^{-2+\frac{4}{p}}).$$

The proof of this proposition is given at the end of this section, see subsection 4.3. In subsection 4.3 we also show how this implies Theorem 3.1.

4.1. An intermediate semi-explicit approximation

For the proof of Proposition 4.3, we introduce yet another approximation for $L_n$ denoted $L^{\text{im}}_{n,\text{app}}$. For this approximation $L^{\text{im}}_{n,\text{app}}$, we neglect interactions between the particles, but we treat each particle by solving a Stokes problem in the exterior domain of that particle. In this sense, $L^{\text{im}}_{n,\text{app}}$ can be seen as intermediate between $L_n$ and $L_{n,\text{app}}$.

More precisely, we define $L^{\text{im}}_{n,\text{app}} : \mathbb{R}^{3n} \to \mathcal{L}(\mathbb{R}^{3n}, \dot{H}^1(\mathbb{R}^3))$ by

$$L^{\text{im}}_{n,\text{app}}(\xi_1, \ldots, \xi_n) T = \sum_i U_i[T_i], \quad (4.4)$$

where $U_i[T_i]$ is defined as the solution to

$$-\mu \Delta w_i + \nabla p_i = 0 \quad \text{in } \mathbb{R}^3 \setminus B_i,$$

$$\text{div } w_i = 0 \quad \text{in } \mathbb{R}^3 \setminus B_i,$$

$$Dw_i = 0 \quad \text{in } r B_i,$$

$$\int_{\partial B_i} \Sigma(w_i, p_i) \nu = 0,$$

$$\int_{\partial B_i} [\Sigma(w_i, p_i)] \times (x - x_i) = T_i. \quad (4.5)$$
The dependence on the particle orientation of $L_{n,\text{app}}^{im}$ can be made explicit. Indeed, consider the problem

$$
\begin{aligned}
-\mu \Delta w + \nabla p = 0, \quad & \text{in } \mathbb{R}^3 \setminus rB, \\
\text{div } w = 0 \quad & \text{in } \mathbb{R}^3 \setminus rB, \\
Dw = 0 \quad & \text{in } rB, \\
\int_{\partial rB} \Sigma(w, p) \nu = 0, \\
\int_{\partial rB} [\Sigma(w, p) \nu] \times x = T,
\end{aligned}
$$

where $T \in \mathbb{R}^3$ is a given torque. We denote by

$$(U[T], P[T])$$

the unique solution $(w, p) \in H^1_0(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$ to (4.6). Then, for $R_i \in SO(3)$ such that $R_i e_3 = \xi_i$, the solution $(U_i[T], P_i[T])$ to (4.5) is given by

$$(U_i[T](x), P_i[T](x)) = \left( R_i U[R_i^T T](R_i^T (x - x_i)), P[R_i^T T](R_i^T (x - x_i)) \right).$$

Indeed,

\begin{align*}
\int_{\partial rB} R_i \left[ \Sigma \left( U[R_i^T T], P[R_i^T T] \right) (R_i^T (x - x_i)) R_i^T \nu \right] \times (x - x_i) \\
= \int_{\partial rB} R_i \left[ \Sigma \left( U[R_i^T T], P[R_i^T T] \right) (y) \nu \right] \times (R_i y) \\
= T,
\end{align*}

where we used that the normal $\nu$ also gets rotated and that $(R_i a) \times (R_i b) = R_i (a \times b)$.

We show the following estimates between the explicit approximation $L_{n,\text{app}}^{im}$ and the semi-explicit approximation $L_{n,\text{app}}^{im}$.

**Proposition 4.4.** Let $i \in \{1, \cdots, n\}$ and $T_i \in \mathbb{R}^3$. Then, for all $1 < p < 3/2$, $U_i[T_i] \in C^1(S^2; L^p(B(0, M)))$ where $w$ and $M$ are as in (3.13) and (4.3), respectively, and for all $x \in \mathbb{R}^3 \setminus B_i$ and all $l \in \mathbb{N}$

$$
|\nabla^l (U_i[T_i])(x)| + |\nabla^l \nabla_{\xi_i} (U_i[T_i])(x)| \leq \frac{C|T_i|}{|x - x_i|^{l+2}},
$$

and

$$
\|U_i[T_i]\|_{C^1(S^2; L^p(B(0, M)))} \leq C|T_i|.
$$

In particular, $L_{n,\text{app}}^{im} \in C^1(S^2; L^p(B(0, M)))$ and

$$
\|L_{n,\text{app}}^{im} - L_{n,\text{app}}\|_{C^1(S^2; L^p(B(0, M)))} \leq C \sqrt{n} r^{-2+\frac{3}{p}}.
$$

The proof relies on the following expansion of $U[T]$ (see e.g. [HW20, Proposition 2.2.] for a similar result).
Proposition 4.5. There exists $\mathcal{H}[T]$ such that for and all $x \in \mathbb{R}^3 \setminus r\mathcal{B}$

$$U[T](x) = ([T]_M + S(e_3)T) : \nabla \Phi(x) + \mathcal{H}[T],$$

The error term satisfies for all $l \in \mathbb{N}$ and all $x \in \mathbb{R}^3 \setminus r\mathcal{B}$

$$\left| \nabla^l \mathcal{H}[T](x) \right| \leq C \frac{r|T|}{|x|^{l+1}}, \quad (4.11)$$

where the constant $C$ depends on $l$ and the reference particle $\mathcal{B}$.

Proof. By scaling, it suffices to show the assertion for $r = 1$. Let $|x| > 4$. Then, using the force free condition for $U[T]$ as well as that $T$ and $S$ are by definition the torque and stresslet associated to $U[T]$

$$U[T](x) = (T_M + S(e_3)) : \nabla \Phi(x)$$

$$= -\int_{\partial \mathcal{B}} \Sigma[U[T], P[T]](y) \nu \cdot (\Phi(x - y) - \Phi(x) - y \cdot \nabla \Phi(x)) \, dy$$

$$\leq 2 \|DU[T]\|_{L^2(\mathbb{R}^3)} \|D\psi\|_{L^2(\mathbb{R}^3)}$$

for any divergence free function $\psi \in \dot{H}^1(\mathbb{R}^3)$ with $\psi(y) = \Phi(x - y) - \Phi(x) - y \cdot \nabla \Phi(x)$ on $\partial \mathcal{B}$.

By Lemma 4.6 below and the decay of $\nabla^2 \Phi$, we find such a $\psi$ with

$$\|D\psi\|_{L^2(\mathbb{R}^3)} \leq C \frac{1}{|x|^3}.$$

Moreover, by some integration by parts, we have

$$2 \|DU[T]\|_{L^2(\mathbb{R}^3)}^2 = T \cdot R^{-1}_2 T \leq C.$$

Collecting these estimates yields the assertion for $|x| > 4$. On $\partial \mathcal{B}$, (4.11) holds as well since $U[T](x) = \omega \times x = (R^{-1}_2 T) \times x$ on $\partial \mathcal{B}$. Thus, by standard regularity theory, (4.11) also holds in $B(0, 4) \setminus \mathcal{B}$. \hfill $\square$

The following Lemma that we used above is standard. For spherical particles it can be found for example in [NS20, Lemma 4.4], and the proof given there also applies for general smooth particles considered here.

Lemma 4.6. Let $\varphi \in H^1_2(\mathcal{B})$. Then, there exists $\psi \in H^1_{s, 0}(B(0, 2))$ such that $D\psi = D\varphi$ in $\mathcal{B}$ and

$$\|D\psi\|_{L^2(B(0, 2))} \leq C \|D\varphi\|_{L^2(\mathcal{B})},$$

where $C$ depends only on $\mathcal{B}$.

Remark 4.7. By translation and scaling, the same statement holds for $\mathcal{B}$ replaced by $\mathcal{B}_i$, where the constant $C$ is independent of $i$.

Proof of Proposition 4.4. We focus on the estimates of derivatives in $\xi_i$ in (4.8), (4.9) and (4.10). The estimates for the functions themselves can be obtained analogously. The right-hand side of the representation (4.7) allows to view $U_i$ as dependent of $R_i$ instead of $\xi_i$. We recall that this is true since the right-hand side is the same for all $R_i \in SO(3)$ with $R_i e_3 = \xi_i$. It is
then sufficient to consider the derivative with respect to \( R_i \).

Fix \( 1 \leq i \leq n \) and let \( T_i \in \mathbb{R}^3 \). It suffices to consider the case \( x_i = 0 \). (Note that the weighted norm \( L^p_w(\mathbb{R}^3 \setminus B(0, M)) \) is not translation invariant. However, by definition of \( M \) in (4.3) we have \( |x - x_i| \geq \frac{1}{2}|x| \) for all \( x \in \mathbb{R}^3 \setminus B(0, M) \) and thus the position of \( x_i \) does not matter.)

Combining (4.7) and Proposition 4.5 and using how \( S \) and \( \Phi \) transform under rotations, we have

\[
U_i[T_i](x) - ([T_i]_M + S(\xi_i)T_i) : \nabla \Phi(x) = R_i H[R_i^T T_i](R_i^T x),
\]

and thus by the chain rule, (4.11)

\[
|\nabla_{\xi_i} ([T_i]_M + S(\xi_i)T_i) : \nabla \Phi(x) - U_i[T_i](x)| \leq C \frac{|T_i|}{|x|^3} \quad \text{in} \ \mathbb{R}^3 \setminus B_i. \tag{4.12}
\]

Using the decay of \( \nabla \Phi \), this implies (4.8) for \( l = 0 \). The estimate for \( l \geq 1 \) is analogous.

Estimate (4.12) directly implies \( \|\nabla_{\xi_i} U_i[T_i]\|_{L^2_w(\mathbb{R}^3 \setminus B(0, M))} \leq C|T_i| \). Moreover, we have

\[
U_i[T_i](x) = r^{-3}(R_2^{-1}T_i) \times x \in B_i,
\]

and thus

\[
|\nabla_{\xi_i} ([T_i]_M + S(\xi_i)T_i) : \nabla \Phi(x) - U_i[T_i](x)| \leq C \frac{|T_i|}{|x|^2} \quad \text{in} \ \mathbb{B}_i. \tag{4.13}
\]

This together with (4.8) implies \( \|\nabla_{\xi_i} U_i[T_i]\|_{L^p_w(\mathbb{B}(0, M))} \leq C|T_i| \) for \( p < 3/2 \) and therefore (4.9) holds.

It remains to show (4.10). By linearity of \( L_{n,\text{app}} \) and \( L_{n,\text{app}}^\text{im} \) in the particles it suffices to show

\[
\|U_i[T_i] - ([T_i]_M + S(\xi_i)T_i) : \nabla \Phi\|_{C^1(S^2, L^p_w(B(0, M)))} \leq C r^{-2+3/p}|T_i|. \tag{4.14}
\]

However, the pointwise estimates (4.12)–(4.13) directly imply (4.14). \( \square \)

### 4.2. Estimates for \( L_n - L_{n,\text{app}}^\text{im} \) through the method of reflections

In order to estimate \( L_n - L_{n,\text{app}}^\text{im} \), we write \( L_n \) in terms of single particle operators only, relying on the so-called method of reflections similarly as in [Höf18; Höf19]. We emphasize that \( L_n - L_{n,\text{app}}^\text{im} \) can be also estimated by energy and duality methods (see e.g. [GH21]). More precisely, arguing as in [GH21] one can show that

\[
\|(L_n - L_{n,\text{app}}^\text{im})\|_{L^p \text{loc}} \leq C \sum_i \|D L_{n,\text{app}}^\text{im} T_i\|_{L^1(\cup_i B_i)}. \tag{4.15}
\]

Using the decay estimate from Proposition 4.5 together with assumptions (H1),(H2), the right-hand side is bounded by \( \phi_n \log n \sum_i |T_i| \) which we recover through the method of reflections, see Proposition 4.9.

The reason why we rely on the method of reflections in this section are the derivatives with respect to the particle orientations \( \xi_i \). Here the method of reflections is very useful because the single particle problems occurring in the method of reflections have an explicit dependence on \( \xi_i \), giving direct access to these shape derivatives. More precisely, following the notation from

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To see this, observe that we might locally fix the choice of \( R_i \) such that \( R_i[\xi_i] \) is differentiable in \( \xi \) with \( |\nabla_{\xi_i} R| \leq C \).
[Höf18; Höf19], we introduce $Q_i$ as the solution operator that maps a function $w \in H^1_s(B_i)$ to the solution $v \in \dot{H}^1_s(\mathbb{R}^3)$ to

\[
\begin{aligned}
-\Delta v + \nabla p &= 0, \quad \text{div } v = 0 &\quad &\text{in } \mathbb{R}^3 \setminus B_i, \\
Dv &= Dw &\quad &\text{in } B_i, \\
0 &= \int_{\partial B_i} \Sigma[v, p] n = \int_{\partial B_i} \Sigma[v, p] n \times (x - x_i), &\quad &\text{for } 1 \leq i \leq n.
\end{aligned}
\]

(4.16)

Then, we claim that

\[
L_n = \lim_{k \to \infty} (1 - \sum_i Q_i^k) L^\text{im}_n, \quad (4.17)
\]

in the sense of convergence of operators $\mathbb{R}^{3n} \to \dot{H}^1_s(\mathbb{R}^3)$. Indeed, this has been proven for spherical particles in [Höf18] under the assumptions (H1),(H2) and in [Höf19] assuming only (H2). Since we impose (H1) in order to control the right-hand side of (4.15), we follow here the (simpler) approach of [Höf18]. The adaptation to non-spherical particles is rather straightforward, and based on the following decay estimates for $Q_i$.

**Lemma 4.8.** Let $w \in H^1_s(B_i)$ such that $\nabla w \in L^\infty(B_i)$. There exists a universal constant $C > 0$ such that for all $x \in \mathbb{R}^3 \setminus B(x_i, 2r)$

\[
|\nabla^l(Q_i w)(x)| \leq \frac{Cr^3}{|x - x_i|^{l + 2}} \|Dw\|_{L^\infty(B_i)}. \quad (4.18)
\]

Moreover,

\[
\|Q_i w\|_{\dot{H}^1(\mathbb{R}^3)} \leq Cr^{3/2} \|Dw\|_{L^\infty(B_i)}, \quad (4.19)
\]

and for all $p < 3/2$, with $w$ and $M$ as in (3.13) and (4.3), respectively,

\[
\|Q_i w\|_{L^p_{\omega, B(0,M)}} \leq Cr^3 \|Dw\|_{L^\infty(B_i)}. \quad (4.20)
\]

**Proof.** We observe that $Q_i w$ minimizes the $\dot{H}^1$ norm among all divergence free functions with $Dv = Dw$. By Lemma 4.6 we thus immediately obtain (4.19).

Now, let $p < 3/2$, $K \subseteq \mathbb{R}^3$ be compact and let $g \in L^{p'}$ with supp$g \subseteq K$. Let $\varphi$ be the solution to

\[
-\Delta \varphi + \nabla p = g, \quad \text{div } \varphi = 0 \quad \text{in } \mathbb{R}^3.
\]

Then, by standard regularity theory and Sobolev embedding

\[
\|\nabla \varphi\|_{L^\infty} \leq C_{K,p} \|g\|_{L^{p'}}.
\]

Consequently, using the equation that $Q_i w$ solves

\[
\int g \cdot Q_i w = \int D\varphi : DQ_i w
\]

\[
= \int_{B_i} D\varphi : DQ_i w + \int_{\mathbb{R}^3 \setminus B_i} D\varphi : DQ_i w
\]

\[
\leq Cr^3 \|Dw\|_{L^\infty(B_i)} \|g\|_{L^{p'}} + Cr^{3/2} \|Dw\|_{L^\infty(B_i)} \|D\psi\|_{L^2(B_i)}
\]

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for all \( \psi \in \dot{H}^1_3(\mathbb{R}^3) \) such that \( D\psi = D\varphi \) in \( B_i \). Appealing again to Lemma 4.6, such a function \( \psi \) exists with

\[
\|D\psi\|_{\dot{H}^1(\mathbb{R}^3)} \leq Cr^{3/2}\|D\varphi\|_{L^\infty(B_i)} \leq Cr^{3/2}\|g\|_{L^{p'}(\mathbb{R}^3)}.
\]

Combination of the above estimates with \( K = B(0, M) \) yields the \( L^p(B(0, M)) \) estimate in (4.20).

The proof of (4.18) is similar to the proof of Proposition 4.5 in the sense that we have for \( |x - x_i| \geq 2r \)

\[
|Q_iw(x)| \leq C \frac{r^{3/2}}{|x - x_i|^2}\|Dw\|_{L^2(B_i)}.
\]

In particular this yields the \( L^2_n(\mathbb{R}^3 \setminus B(0, M)) \) estimate in (4.20). Indeed since the above decay is valid for \( x \notin B(x_i, 2r) \), we have in particular \( |x - x_i| \geq \frac{1}{2}|x| \) for \( x \notin B(0, M), 1 \leq i \leq n \), this yields

\[
\|Q_iw\|_{L^2_n(\mathbb{R}^3 \setminus B(0, M))} \leq C r^3\|Dw\|_{L^\infty(B_i)} \left( \int_{\mathbb{R}^3 \setminus B(0, M)} \frac{(1 + |x|)\alpha}{|x|^4} dx \right)^{1/2}
\]

this concludes the proof since the above integral is finite for \( a < 1 \).

\[
\text{(4.21)}
\]

**Proposition 4.9.** There exists \( N_0 \in \mathbb{N} \) such that for all \( n \geq N_0 \)

\[
L_n = \lim_{k \to \infty} (1 - \sum_i Q_i)^k L_{n,\text{app}}
\]

in the sense of convergence of linear operators operators from \( \mathbb{R}^{3n} \) to \( \dot{H}^1_3 \). Moreover, with \( M \)

and \( w \) as in (3.3) and (3.13), respectively, for all \( 1 \leq p < 3/2, \)

\[
\|L_n - L_{n,\text{app}}\|_{C((\mathbb{R}^3)^n; (L^p(\mathbb{R}^3 \setminus B(0, M)))^3n)} \leq C \sqrt{n}\phi_n \log n.
\]

**Proof.** The convergence (4.21) can be proved exactly as in [Höf18]. We therefore only give the proof of (4.22).

Let \( p < 3/2 \) and \( T \in \mathbb{R}^{3n} \). We denote \( v = L_nT \) and \( v_k = (1 - \sum_i Q_i)^k L_{n,\text{app}}T \). To prove (4.22), we apply Lemma 4.8 to see that

\[
\|v_{k+1} - v_k\|_{L^2_3(\mathbb{R}^3 \setminus B(0, M))} + \|v_{k+1} - v_k\|_{L^p(B(0, M))} \leq \sum_i \|Q_i v_k\|_{L^p(B(0, M))} + \|Q_i v_k\|_{L^2_3(\mathbb{R}^3 \setminus B(0, M))}
\]

\[
\leq C \sum_i r^3\|Dv_k\|_{L^\infty(B_i)}.
\]

Now, using the fact that \( D(Q_i v_k) = Dv_k \) in \( B_i \) we get

\[
Dv_{k+1} = Dv_k - \sum_j DQ_j v_k = -\sum_{j \neq i} DQ_j v_k, \text{ in } B_i.
\]

Thus, using again Lemma 4.8 and assumption (H2), we get

\[
\sum_i \|Dv_{k+1}\|_{L^\infty(B_i)} \leq \sum_i \sum_{j \neq i} \|D(Q_j v_k)\|_{L^\infty(B_i)}
\]

\[
\leq \sum_i \sum_{j \neq i} \frac{r^3}{|x_i - x_j|^2}\|Dv_k\|_{L^\infty(B_i)}
\]

\[
\leq C\phi_n \log n \sum_j \|Dv_k\|_{L^\infty(B_i)}.
\]

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Hence, by iteration
\[ \sum_i \|Dv_k\|_{L^\infty(B_i)} \leq (C\phi_n \log n)^k \sum_i \|Dv_0\|_{L^\infty(B_i)}. \]  
(4.24)

By (4.4), we can write \( v_0 = \sum_i U_i(T_i) \), and thus the decay estimates from Proposition 4.5 yield
\[ \sum_i \|Dv_0\|_{L^\infty(B_i)} \leq C \sum_j \frac{T_j}{|x_i - x_j|^3} \leq \phi_n \log n |T|_{\mathcal{B}}. \]  
(4.25)

Combining (4.23), (4.24) and (4.25) yields
\[ \|v_{k+1} - v_k\|_{L^p_{\text{loc}}(\mathbb{R}^3)} + \|v_{k+1} - v_k\|_{L^2_{\infty}(\mathbb{R}^3 \setminus B(0,M))} \leq (C\phi_n \log n)^{k+1} |T|_{\mathcal{B}}. \]

Summing these errors in \( k \) yields (4.22). \( \square \)

We now turn to the derivatives in \( \xi_i \). We begin by estimating the derivative of \( Q_i \) with respect to \( \xi_i \).

**Lemma 4.10.** Let \( w \in H^2_r(B(x_i, 2r)) \) such that \( \nabla w \in W^{1,\infty}(B(x_i, 2r)) \). Then, \( \nabla_{\xi_i}(Q_iw) \in L^2_{\text{loc}}(\mathbb{R}^3) \) and for all \( x \in \mathbb{R}^3 \setminus B(x_i, 2r) \) and all \( l \in \mathbb{N} \)
\[ |\nabla^l \nabla_{\xi_i}(Q_iw)(x)| \leq C r^3 \left( \|Dw\|_{L^\infty(B_i)} + r \|\nabla Dw\|_{L^\infty(B_i)} \right). \]  
(4.26)

Moreover, for all \( p < 3/2 \) and with \( M \) and \( w \) as in (4.3) and (3.13), respectively,
\[ \|\nabla_{\xi_i}Q_iw\|_{L^p_{\text{loc}}(\mathbb{R}^3 \setminus B(0,M))} \leq C r^3 \left( \|Dw\|_{L^\infty(B_i)} + r \|\nabla Dw\|_{L^\infty(B_i)} \right). \]  
(4.27)

**Proof.** We begin by dropping all indices \( i \) and assume \( x_i = 0 \). Moreover, we set \( Q = Q[\xi] \) to denote the dependence on \( \xi \). By considering the defining equation for \( Q \), (4.16), we observe that for any \( R \in SO(3) \) with \( R\xi = e_3 \)
\[ (Q[\xi]w)(x) = R(Q[e_3]\bar{w})(R^T x), \]  
(4.28)

where \( \bar{w}(x) = R^T w(Rx) \). Note that this corresponds to the way how \( U_i \) is obtained from \( U \) in (4.7). Analogously, as argued at the beginning of the proof of Proposition 4.4, it suffices to view \( Q \) as a function of \( R \) to derive estimates for the derivative.

By the assumptions on \( w \) and the chain rule \( \nabla_{\xi}\bar{w} \in H^1(B(0,2r)) \) with
\[ |\nabla_{\xi}D_x\bar{w}(x)| \leq C |\nabla w|(x) + C|x||\nabla^2 w|(x). \]  
(4.29)

Consequently, since \( w \in H^2(B(0,2r)) \) and \( Q \) is a linear operator with values in \( \dot{H}^1 \), the representation (4.28) implies that \( \nabla_{\xi}(Q[\xi]w) \in L^2_{\text{loc}}(\mathbb{R}^3) \). Moreover, we can combine (4.28) and (4.29) with Lemma 4.8 to obtain for \( x \in \mathbb{R}^3 \setminus B(0,2r) \)
\[ |\nabla_{\xi}(Qw)(x)| \leq C |\nabla^l(Q[e_3]\bar{w})(R^T x)| + C|x||\nabla(Q[e_3]\bar{w})(R^T x)| + C|Q[e_3]|(\nabla_{\xi}\bar{w})(R^T x)| \]  
\[ \leq C r^3 \left( \|Dw\|_{L^\infty(B_i)} + C r^4 \|\nabla Dw\|_{L^\infty(B_i)} \right). \]  
(4.30)
This establishes (4.26) for \( l = 0 \) and the \( L^2_w(\mathbb{R}^3 \setminus B(0, M)) \) estimate in (4.27). The estimate for \( l \geq 1 \) is analogous.

Moreover, (4.30) implies
\[
\|\nabla_\xi (Qw)(x)\|_{L^p(B(0, M) \setminus B(0, 2r))} \leq C r^3 \|Dw\|_{L^\infty(B_i)} + C r^4 \|\nabla Dw\|_{L^\infty(B_i)}.
\]

It remains to estimate the \( L^p \) norm inside of \( B(0, 2r) \). We note that the first inequality in (4.30) also holds for all \( x \in B(0, 2r) \). Together with Lemma 4.8 and (4.29), it implies for all \( p < 3/2 \)
\[
\|\nabla_\xi (Qw)\|_{L^p(B(0, 2r))} \leq C r^3 \|D\bar{w}\|_{L^\infty(B(0,2r))} + \|x\|_{L^p(B(0, 2r))} \|\nabla Qw\|_{L^2(\mathbb{R}^3)} + r^3 \|\nabla Dw\|_{L^\infty(B_i)}.
\]

This finishes the proof.

To estimate \( \nabla_\xi (L_n - L_{n, \text{app}}^m) \) the idea is to proceed similarly as in Proposition 4.9. However, this is more delicate due to the loss of regularity when taking the derivative in \( \xi \). More precisely, by Lemma 4.10 we only have that \( \nabla_\xi (Q_i w) \) lies in \( L^2_{\text{loc}} \). In fact it is easy to see that \( \nabla_\xi (Q_i w) \) will in general not possess a weak derivative regardless how much regularity we impose on \( w \).

A consequence of this loss of regularity is that \( Q_\xi \nabla_\xi Q_j \) is not defined a priori since \( Q_\xi \) needs data in \( H^1(B_i) \). However Lemma 4.10 ensures that \( Q_\xi \nabla_\xi Q_j \) is well defined for \( i \neq j \). On the other hand, one can exploit that \( Q_i Q_j = Q_i \) to avoid any appearance of \( Q_i \nabla_\xi Q_i \). To this end, we rewrite the series expansion (4.17). Namely, adopting the notation \( v_k = (1 - \sum_i Q_i)^k L_{n, \text{app}}^m T \), we have
\[
v_k = v_0 - \sum_{i_1} Q_{i_1} v_0 + \sum_{i_1} \sum_{i_2 \neq i_1} Q_{i_2} Q_{i_1} v_0 - \sum_{i_1} \sum_{i_2 \neq i_1} \sum_{i_3 \neq i_2} Q_{i_3} Q_{i_2} Q_{i_1} v_0 + \ldots
\]
\[
+ (-1)^k \sum_{i_1} \sum_{i_2 \neq i_1} \ldots \sum_{i_k \neq i_{k-1}} Q_{i_k} Q_{i_{k-1}} \ldots Q_{i_1} v_0. \tag{4.31}
\]

This representation can be directly deduced from (4.17) by just using \( Q_i Q_i = Q_i \) (see [HV18, Section 2] for details).

**Proposition 4.11.** There exists \( N_0 \in \mathbb{N} \) such that for all \( n \geq N_0 \) the following holds. Let \( M \) be as in (4.3) and \( w \) as in (3.13), \( 1 < \alpha \leq n \) and \( 1 < \alpha \leq 3 \). Then, for all \( 1 < p < 3/2 \), \( L_n e_{i, \alpha} \) is differentiable in \( \xi_j \) for all \( 1 \leq j \leq n \) as a function in \( L^p_{\text{loc}, B(0, M)} \) and we have
\[
\|\nabla_\xi (L_n - L_{n, \text{app}}^m) e_{i, \alpha}\|_{L^p_{\text{loc}, B(0, M)}} \leq C \phi_n \log n.
\]
Moreover, for \( j \neq i \)
\[
\|\nabla_\xi (L_n - L_{n, \text{app}}^m) e_{i, \alpha}\|_{L^p_{\text{loc}, B(0, M)}} \leq C \frac{\rho^3}{|x_i - x_j|^3}. \tag{4.32}
\]

**Proof.** In the following we will assume \( i = 1 \). Since the \( L^2_w(\mathbb{R}^3 \setminus B(0, M)) \) and \( L^p(B(0, M)) \) estimates are analogous we only treat below the \( L^p(B(0, M)) \) estimates.

Let \( v_k = (1 - \sum_i Q_i)^k L_{n, \text{app}}^m e_{1, \alpha} \), then by virtue of (4.31) we have
\[
v_{k+1} - v_k = (-1)^{k+1} \sum_{i_1 \neq 1} \sum_{i_2 \neq i_1} \ldots \sum_{i_{k+1} \neq i_k} Q_{i_{k+1}} Q_{i_k} \ldots Q_{i_1} v_0.
\]
Here we used that $Dv_0 = DL_{n,app}^m e_i, a = DU_{1[i, a]} = 0$ in $B_1$ to deduce that the first sum only runs over $i \neq 1$.

Thanks to $\nabla_{\xi_1} Q_i = 0$ for $i \neq 1$, taking the derivative in $\xi_1$ yields

$$\nabla_{\xi_1}(v_{k+1} - v_k) = \sum_{i_1 \neq 1, i_2 \neq i_1} \ldots \sum_{i_{k+1} \neq i_k} Q_{i_{k+1}} Q_{i_k} \ldots Q_{i_1} \nabla_{\xi_1} v_0$$

$$\sum_{l=2}^{k+1} (-1)^{k+1} \sum_{i_1 \neq 1, i_2 \neq i_1} \ldots \sum_{i_{l-1} \neq 1, i_{l+1} \neq i_{l-1}} \sum_{i_{l+1} \neq i_{l-2}} Q_{i_{l+1}} \ldots Q_{i_{l-1}} Q_{i_l} \nabla_{\xi_1} Q_{i_l} \ldots Q_{i_1} v_0$$

$$=: \Psi_{k,1} + \Psi_{k,2}.$$  

Although the right-hand side looks very complicated, it can be estimated analogously as in the proof of Proposition 4.9. Indeed, inductive application of Lemma 4.8 and eventually application of Proposition 4.4 yields

$$\|\Psi_{k,1}\|_{L^p_{loc}} \leq Cr^3 \sum_{i_1 \neq 1, i_2 \neq i_1} \ldots \sum_{i_{k+1} \neq i_k} \|DQ_{i_k} \ldots Q_{i_1} \nabla_{\xi_1} v_0\|_{L^\infty(B_{k+1})}$$

$$\leq Cr^3 \sum_{i_1 \neq 1, i_2 \neq i_1} \ldots \sum_{i_{k+1} \neq i_k} \sum_{i_{l+1} \neq i_{l-2}} \|DQ_{i_{l+1}} \ldots Q_{i_1} \nabla_{\xi_1} v_0\|_{L^\infty(B_{k+1})}$$

$$\leq C r^3 (C \phi_n \log n)^k \sum_{i_1 \neq 1} \|D \nabla_{\xi_1} v_0\|_{L^\infty(B_{i+1})}$$

$$\leq C r^3 (C \phi_n \log n)^k \sum_{i_1 \neq 1} \frac{1}{|x_1 - x_{i+1}|^3}$$

$$\leq (C \phi_n \log n)^{k+1}.$$  

For the second term on the right-hand side of (4.33), we proceed similarly. We observe that the combination of Lemmas 4.8 and 4.10 implies for $i, j \neq 1$ and any function $\psi \in H^1(B_i)$ such that $\nabla \psi \in L^\infty(B_i)$.

$$\|D \nabla_{\xi_1} Q_i \psi\|_{L^\infty(B_j)} \leq C r^3 |x_j - x_1|^3 \left( \|DQ_i \psi\|_{L^\infty(B_1)} + r \|D \nabla Q_i \psi\|_{L^\infty(B_1)} \right)$$

$$\leq C \frac{r^3}{|x_j - x_1|^3} \left( 1 + \frac{r}{|x_j - x_1|^3} \right) \|D \psi\|_{L^\infty(B_j)}$$

$$\leq C \frac{r^3}{|x_j - x_1|^3} \|D \psi\|_{L^\infty(B_j)}.$$  

Similarly in the case $l = k + 1$ we have

$$\|\nabla_{\xi_1} Q_i \psi\|_{L^p_{loc}} \leq C \frac{r^3}{|x_1 - x_i|^3} \|D \psi\|_{L^\infty(B_i)}.$$  

In this way, we can estimate the second term on the right-hand side of (4.33) by

$$\|\Psi_{k,2}\|_{L^p_{loc}} \leq k (C \phi_n \log n)^{k+1}$$.
where the factor $k$ originates from the sum over $l$. Combining these estimates for $\Psi_{k,1}$ and $\Psi_{k,2}$ yields
\[
\|\nabla \xi_1 (v_{k+1} - v_k)\|_{L^p_{loc}} \leq (k + 1)(C \phi_n \log n)^{k+1}.
\]
Summation over $k$ yields the first assertion.

For the second estimate, we set $j = 2$ and remark that since $\nabla \xi_2 v_0 = \nabla \xi_2 U_1[e_\alpha] = 0$ we have
\[
\nabla \xi_2 (v_{k+1} - v_k) = \sum_{l=1}^{k+1} (-1)^{k+1} \sum_{i_k \neq i_{k+1}} \sum_{i_{k+1} \neq i_k} \sum_{i_{l+1} \neq i_{l-1}} Q_i v_{l+1} \ldots Q_i v_1 \nabla \xi_2 Q_i v_{l-1} \ldots Q_i v_0
\]
with the convention that for $l = 1$ the term corresponds to
\[
\sum_{i_2 \neq i_1} \ldots \sum_{i_{k+1} \neq i_k} Q_i v_{k+1} \ldots Q_i v_1 \nabla \xi_2 v_0.
\]
We have then
\[
\|\nabla \xi_2 (v_{k+1} - v_k)\|_{L^p_{loc}} \leq r^3 \sum_{l=1}^{k+1} \sum_{i_k \neq i_{k+1}} \sum_{i_{k+1} \neq i_k} \sum_{i_{l+1} \neq i_{l-1}} C \phi_n \log n)^{k-l+1} \sum_{i_2 \neq i_1} \ldots \sum_{i_{k+1} \neq i_k} \frac{C_r^3}{|x_{i_k+1} - x_{i_k}|^3} \frac{C_r^3}{|x_{i_{k+1}} - x_{i_{k+1}}|^3} \ldots \frac{C_r^3}{|x_{i_1} - x_1|^3}
\]
\[
\leq r^3 \sum_{l=1}^{k+1} \sum_{i_k \neq i_{k+1}} \sum_{i_{k+1} \neq i_k} \frac{C_r^3}{|x_{i_k+1} - x_{i_k}|^3} \frac{C_r^3}{|x_{i_{k+1}} - x_{i_{k+1}}|^3} \ldots \frac{C_r^3}{|x_{i_1} - x_1|^3} \leq \sum_{l=1}^{k+1} \frac{(C \phi_n \log n)^{k-l+1} I_{l-1}}{C_r^3}
\]
where for $l \geq 1$
\[
I_l := \sum_{i_k \neq i_{k+1}} \sum_{i_{k+1} \neq i_k} \sum_{i_{l+1} \neq i_{l-1}} \frac{C_r^3}{|x_{i_k+1} - x_{i_k}|^3} \frac{C_r^3}{|x_{i_{k+1}} - x_{i_{k+1}}|^3} \ldots \frac{C_r^3}{|x_{i_1} - x_1|^3},
\]
and $I_0 := \frac{C_r^3}{|x_2 - x_1|^3}$. Now we aim to show by induction that for some constant $\bar{C} > C$ we have
\[
I_l \leq (\bar{C} \phi_n \log n)^l \frac{C_r^3}{|x_1 - x_2|^3},
\]
indeed, for $l > 1$, we have by separating the term with $i_{l-1} = 2$
\[
I_l = \sum_{i_k \neq i_{k+1}} \sum_{i_{k+1} \neq i_k} \sum_{i_{l+1} \neq i_{l-1}} \frac{C_r^3}{|x_{i_k+1} - x_{i_k}|^3} \frac{C_r^3}{|x_{i_{k+1}} - x_{i_{k+1}}|^3} \ldots \frac{C_r^3}{|x_{i_1} - x_1|^3} + \sum_{i_k \neq i_{k+1}} \sum_{i_{k+1} \neq i_k} \sum_{i_{l+1} \neq i_{l-1}} \frac{C_r^3}{|x_{i_k+1} - x_{i_k}|^3} \frac{C_r^3}{|x_{i_{k+1}} - x_{i_{k+1}}|^3} \ldots \frac{C_r^3}{|x_{i_1} - x_1|^3}
\]
\[
\leq 8(C \phi_n \log n)I_{l-1} + (C \phi_n \log n)^2 I_{l-2},
\]

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where we used $\log n \geq 1$ (for $n \geq 3$) for the second term and for the first term that for any $i_i \neq 2 \neq i_{i-1}$ we have

$$\frac{1}{|x_2 - x_{i_i}|} \leq \frac{1}{|x_2 - x_{i_{i-1}}|} \left( \frac{1}{|x_2 - x_{i_i}|} + \frac{1}{|x_2 - x_{i_{i-1}}|} \right).$$

This yields (4.35) using the induction hypothesis and taking $8\bar{C}C + C^2 \leq \bar{C}^2$. Moreover, using the same arguments as above, one can show that the induction hypothesis is satisfied for $l = 0, 1$. Inserting (4.35) into (4.34) and summing over $k$ yields (4.32).

4.3. Proofs of Proposition 4.3 and Theorem 3.1

Proof of Proposition 4.3. The proof of Proposition is a direct consequence of Propositions 4.4, 4.9 and 4.11. Indeed we have thanks to Propositions 4.4 and 4.9 for all $1 < p < 3/2$

$$\|L_n - L_n,app\|_{C^1((S^2)^n; (H^s_w, B(0, M))^3n)} \leq C\sqrt{n}(\phi_n \log n + r^{\frac{3}{2} - 2}).$$

For the derivative we get from Proposition 4.11 for all $1 < p < 3/2$

$$\sum_{i,j,\alpha} \|\nabla_{\xi_i}(L_n - L_n,app)e_{j,\alpha}\|_{L^\infty((S^2)^n, (L^p_w, B(0, M)))}^2 \leq C\sum_{i,\alpha} \left( \sum_{j \neq i} \frac{r^6}{|x_i - x_j|^6} + (\phi_n \log n)^2 \right) \leq Cn\phi_n^2(1 + \log^2 n).$$

where we used that for all $i$, $\sum_{j \neq i} \frac{r^6}{|x_i - x_j|^6} \leq C \frac{r^6}{\min d} \leq C\phi_n^2$ thanks to assumption $H2$.

Combining again with Proposition 4.4 yields the assertion.

For the proof of Theorem 3.1, we first deduce the following corollary which is a direct consequence of Lemma 4.1 and Proposition 4.3 combined with Lemma D.1.

Corollary 4.12. For all $n$ sufficiently large and for all $1/2 < s < 1$ and $p = \frac{6}{3 + 2s}$

$$\|L_n\|_{C^1((S^2)^n; (H^s, H^{-s}(\mathbb{R}^3))^3n)} \leq C\sqrt{n},$$

$$\|L_n - L_n,app\|_{C^1((S^2)^n; (H^s, H^{-s}(\mathbb{R}^3))^3n)} \leq C\sqrt{n}(\phi_n \log n + r^{\frac{3}{2} - 2}).$$

Proof of Theorem 3.1. The assertion follows immediately from Corollary 4.12 combined with Proposition C.20 (see also Remark C.21).

5. Passage to the limit for Deborah numbers of order 1

In this section we prove Theorem 3.2. We recall the strategy from Subsection 3.5. First, we show that the laws of the empirical measure of the particles and of the fluid velocity field respectively are tight in suitable function spaces. For $S_n$ this is classical but we include the proof for completeness in Subsection 5.1. Tightness of $\phi_n^{-1}u_n$, which we show in Subsection
5.2, follows from the estimates in Section 4 which also allow us to replace \( u_n \) by more explicit functions \( u_{n,app} \).

The tightness of the laws implies weak convergence along subsequences by the Prokhorov Theorem. To conclude the proof of Theorem 3.2 we introduce certain functionals in Subsection 5.3. As we show later in Appendix A, these functionals vanish precisely on the solution of the desired limit system (1.3), (1.4). For the proof of Theorem 3.2 it therefore remains to show that the laws of the microscopic system concentrate on the zeroes of these functionals as \( n \to \infty \).

5.1. Tightness of \( S_n \)

**Lemma 5.1.** Let \( T > 0 \) and let \( S_n \) be the empirical measure defined in (3.9). Then, the family of laws \( \{Q^{S_n}\} \) of the empirical measures \( S_n \) is tight in the space \( C([0,T], \mathcal{P}_1(\mathbb{R}^3 \times S^2)) \).

**Proof.** By standard arguments, tightness follows from the uniform bounds

\[
E \left[ \sup_{t \in [0,T]} \int_{\mathbb{R}^3} \int_{S^2} ((|x| + |\xi|)S_n(t)(dx,d\xi)) \right] \leq C, \tag{5.1}
\]

\[
E \left[ \int_0^T \int_0^T W_1(S_n(t_1), S_n(t_2))^p \frac{dt_1 dt_2}{|t_1 - t_2|^{1 + sp}} \right] \leq C, \tag{5.2}
\]

for some \( s \in (0,\frac{1}{2}) \), \( p > s^{-1} \). Indeed, by the Ascoli-Arzelà theorem in metric spaces, the set

\[
\mathcal{K}_{M,R} = \left\{ f \in C([0,T], \mathcal{P}_1(\mathbb{R}^3 \times S^2)) \text{ s.t. } \sup_{t \in [0,T]} \int_{\mathbb{R}^3} \int_{S^2} ((|x| + |\xi|)f_t dx d\xi) \leq M, \right. \]

\[
\left. \int_0^T \int_0^T W_1(f(t_1), f(t_2))^p \frac{dt_1 dt_2}{|t_1 - t_2|^{1 + sp}} \leq R \right\}
\]

is relatively compact in \( C([0,T], \mathcal{P}_1(\mathbb{R}^3 \times S^2)) \). Indeed, for \( f \in \mathcal{K}_{M,R} \) and \( \varphi \in C^1(\mathbb{R}^3 \times S^2) \), we have for \( \theta = s - 1/p \) due to Sobolev inequality for fractional spaces (see e.g. [DPV12, Section 8])

\[
|\langle f(t), \varphi \rangle - \langle f(s), \varphi \rangle| \leq C|t - s|^\theta |\langle f, \varphi \rangle|_{s,p} \leq CR|t - s|^\theta \|
\]

Taking the supremum in \( \varphi \) yields equicontinuity and thus \( \mathcal{K}_{M,R} \) is compact.

For any \( \varepsilon > 0 \), by Chebyshev’s inequality and (5.1)–(5.2), choosing \( M \) and \( R \) big enough,

\[
Q^{S_n}(\mathcal{K}_{M,R}^c) < \varepsilon,
\]

which yields tightness of the laws \( \{Q^{S_n}\} \). Thus, it remains to show (5.1)–(5.2).

We recall that the particle positions \( x_i \) do not evolve in time and stay in a compact set \( K \subseteq \mathbb{R}^3 \) due to assumption (H3). Moreover the particle orientations lie on the sphere \( S^2 \) which is also compact, thus the first estimate (5.1) is trivial.

By definition of the Wasserstein distance, by Jensen inequality and by (3.3)

\[
E \left[ W_1(S_n(t_1), S_n(t_2))^p \right] \leq E \left[ \left( \frac{1}{n} \sum_{i=1}^n |\xi_i(t_1) - \xi_i(t_2)| \right)^p \right]
\]

\[
\leq C \frac{1}{n} \sum_{i=1}^n E \left[ \int_{t_1}^{t_2} \sigma_D(\xi_i(\tau)) dB_i(\tau)^p \right] + \left[ \int_{t_1}^{t_2} A(\tau, x_i, \xi_i(\tau)) d\tau \right]^p,
\]

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where \( A(t, x, \xi) := P_{\xi} h(t, \xi, x) - 2\xi \). Then, by the Burkholder-Davis-Gundy inequality, (see e.g. Theorem 3.28 in [KS12]) we deduce
\[
\mathbb{E} [\mathcal{W}_1(S_n(t_1), S_n(t_2))^p] \leq C \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} \left[ \left( \int_{t_1}^{t_2} \|\sigma_D(\xi_i(\tau))\|_{HS}^2 \, d\tau \right)^{p/2} \right] + C|t_1 - t_2|^p
\]
\[
\leq C|t_1 - t_2|^{p/2},
\]
where HS stands for the Hilbert-Schmidt norm. Therefore,
\[
\mathbb{E} \left[ \int_0^T \int_0^T \mathcal{W}_1(S_n(t_1), S_n(t_2))^p \frac{dt_1}{|t_1 - t_2|^{1+s_p}} \, dt_2 \right] \leq C \int_0^T \int_0^T |t_1 - t_2|^{p(1/2-s) - 1} \, dt_1 \, dt_2 \leq C_2
\]
since \( s < \frac{1}{2} \).

### 5.2. Tightness of \( u_n \)

Recall from (3.7)–(3.8) the definition of \( u_n \). Analogously, we define
\[
\begin{align*}
\text{u}_{n,\mathrm{app}} &:= U_{\text{n,app}}'', \\
U_{\text{n,app}}(t) &:= \frac{\phi_n \sqrt{\frac{2\gamma r_{\mathrm{rot}}}{n}}} \int_{0}^{t} L_{\text{n,app}}(\Xi(s)) \sqrt{g_{2}(\Xi(s))} \circ dB_{1}(s), \ldots, B_{n}(s),
\end{align*}
\]
where \( L_{n,\text{app}} \) is the operator defined at the beginning of Section 4.

**Lemma 5.2.** Let \( s > \frac{1}{2} \). Then, for all \( n \in \mathbb{N} \), the stochastic integral in (5.3) is well defined and \( u_{n,\text{app}} \in L^2(\Omega; H^{-s}(0, T; H^{-s}_{w}(\mathbb{R}^3))) \). Moreover, there exists \( N_0 \in \mathbb{N} \) such that for all for all \( n \geq N_0 \) and all \( s > \frac{1}{2} \)
\[
\mathbb{E} \left[ \left\| \phi_n^{-1} u_n \right\|_{H^{-s}(0,T;H^{-s}_{w}(\mathbb{R}^3))}^2 \right] \leq C, \quad \lim_{n\to\infty} \mathbb{E} \left[ \left\| \frac{1}{\phi_n} (u_n - u_{n,\text{app}}) \right\|_{H^{-s}(0,T;H^{-s}_{w}(\mathbb{R}^3))}^2 \right] = 0.
\]

**Proof.** To estimate the \( H^{-s}(0, T; H^{-s}_{w}(\mathbb{R}^3)) \) norm of \( u_n \) and \( u_n - u_{n,\text{app}} \), by (3.12), it suffices to estimate the corresponding \( H^{-s-1}(0, T; H^{-s}_{w}(\mathbb{R}^3)) \) norms of \( U_n \) and \( U_n - U_{n,\text{app}} \). Thus, by assumption (H1), to show (5.4)–(5.5), it suffices to prove
\[
\mathbb{E} \left[ \left\| \phi_n^{-1} U_{n,\text{app}} \right\|_{H^{1-s}(0,T;H^{-s}_{w}(\mathbb{R}^3))}^2 \right] \leq C, \quad \mathbb{E} \left[ \left\| \phi_n^{-1} (U_n - U_{n,\text{app}}) \right\|_{H^{1-s}(0,T;H^{-s}_{w}(\mathbb{R}^3))}^2 \right] \leq C(\phi_n \log n + r^{3/p-2}),
\]
for \( p = \frac{6}{3+2s} \).

To estimate these norms, we appeal to (C.11) and Remark C.21. To apply this estimate, we first recall from (2.13b) that for the vector \( \Xi = (\xi_1, \ldots, \xi_n) \),
\[
d\Xi(t) = \Sigma_D(\Xi(t)) \circ dB(t) + H(t, \Xi(t), x) \, dt
\]

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where $H(t, \Xi, x) = \left( P_{\xi_1} h(t, \xi_1, x_1), \ldots, P_{\xi_n} h(t, \xi_n, x_n) \right)$, $B = (B_1, \ldots, B_n)$ and $\Sigma_D(\Xi)$ is a block diagonal matrix in $\mathbb{R}^{3n \times 3n}$ whose blocks are $\sigma_D(\xi_3)$, defined in (3.2). In particular $\|\Sigma_D(\Xi)\|_{HS} \leq C\sqrt{n}$. Then, by (C.11) and Remark C.21

$$
\left( \mathbb{E} \left[ \left\| \phi_n^1 u_{n,app} \right\|_{H^{1-s((0,T);H^{s-\epsilon}((\mathbb{R}^3))}}^2 \right] \right)^{\frac{1}{2}} 
\leq \frac{C}{n} \left( \| L_{n,app} \|_{L^\infty((\mathbb{S}^2)^n; (H^{s-\epsilon}(\mathbb{R}^3))^{3n})} + \sqrt{n} \| \nabla L_{n,app} \|_{L^\infty((\mathbb{S}^2)^n; (H^{s-\epsilon}(\mathbb{R}^3))^{3n})} \right),
$$

Applying Corollary 4.12 yields (5.6). The proof of estimate (5.7) is completely analogous. \hfill \Box

**Lemma 5.3.** For all $s > 1/2$, the family of laws $\{Q^n\}$ of $u^n$, defined in (3.8), is tight in the space $H^{-s}((0, T), H_{s,\alpha}^{-\epsilon}(\mathbb{R}^3))$.

**Proof.** For $s > \frac{1}{2}$, let

$$
K_M = \{ v \in H^{-s}((0, T), H_{s,\alpha}^{-\epsilon}(\mathbb{R}^3)) : \|v\|_{H^{-s}((0, T), H_{s,\alpha}^{-\epsilon}(\mathbb{R}^3))} \leq M \}.
$$

By Lemma D.2 and [Ama00][Theorem 5.1], this set is relatively compact in $H^{-s}((0, T), H_{s,\alpha}^{-\epsilon}(\mathbb{R}^3))$. Thus, for all $\epsilon > 0$, by Chebyshev’s inequality, by Lemma 5.2 and choosing $M$ big enough,

$$
Q^n(K_M) = \mathbb{P} \left( \|u^n\|_{H^{-s}((0, T), H_{s,\alpha}^{-\epsilon}(\mathbb{R}^3))} > M \right) \leq \frac{\mathbb{E} \left[ \|u^n\|_{H^{-s}((0, T), H_{s,\alpha}^{-\epsilon}(\mathbb{R}^3))} \right]}{M} < \epsilon,
$$

which concludes the proof. \hfill \Box

### 5.3. Proof of Theorem 3.2

As outlined at the beginning of this Section, we now introduce functionals whose zeroes are the solutions of the system (1.3), (1.4). For $(v, g) \in H^{-s}((0, T); H_{s,\alpha}^{-\epsilon}((\mathbb{R}^3))) \times C((0, T]; P_1(\mathbb{R}^3 \times \mathbb{S}^2))$, we define for each $\varphi \in C_c^\infty((0, T) \times \mathbb{R}^3)$ with $\text{div} \varphi = 0$ and $\psi \in C_c^\infty([0, T] \times \mathbb{R}^3 \times \mathbb{S}^2)$,

$$
\Psi_\varphi(g) = \langle f_0, \psi(0) \rangle - \langle g(T), \psi(T) \rangle + \int_0^T \left( \langle g, \partial_t \psi + \nabla \xi \cdot P_{\xi} h + \Delta \xi \psi \rangle \right) dt,
$$

$$
\Phi_\varphi(v, g) = \langle v, \Delta \varphi \rangle - \gamma_E \langle g, (\text{Id} - 3\xi \otimes \xi) : \nabla \varphi \rangle.
$$

Note that $\langle \cdot, \cdot \rangle$ in (5.8) denotes the pairing in $\mathbb{R}^3 \times \mathbb{S}^2$ whereas the first pairing $\langle \cdot, \cdot \rangle$ in (5.9) denotes the pairing in $(0, T) \times \mathbb{R}^3$ and the second pairing $\langle \cdot, \cdot \rangle$ in (5.9) denotes the pairing in $(0, T) \times \mathbb{R}^3 \times \mathbb{S}^2$.

**Lemma 5.4.** For every test function $\psi \in C_c^\infty([0, T] \times \mathbb{R}^3 \times \mathbb{S}^2)$, the empirical measures $S_n$ satisfies the following identity,

$$
\Psi_\varphi(S_n) = \langle f_0 - S_n(0), \psi(0) \rangle - \int_0^T \frac{1}{n} \sum_{i=1}^n \nabla \psi(t, x_i(t)) \sigma_D(\xi_i(t)) dB_i(t)
$$

with $\sigma_D$ as in (3.2).
Proof. The proof follows by applying Ito’s formula (Lemma C.7) to \( \psi(t, x_t, \xi_t(t)) \) using (3.3). To avoid the issue of having to apply Ito’s formula on the manifold \( S^2 \), one might first extend \( \psi \) to a smooth function \( \tilde{\psi} \in C_\infty^\infty([0, T] \times \mathbb{R}^3) \) with \( \tilde{\psi} \equiv \psi \) on \( S^2 \), we find

\[
\tilde{\psi}(T, x_t, \xi_t(T)) = \tilde{\psi}(0, x_t, \xi_t(0)) + \int_0^T (\partial_t + P_{\xi \perp} h \cdot \nabla \xi - 2\xi \cdot \nabla \xi + P_{\xi \perp} : \nabla^2 \tilde{\psi})(t, x_t, \xi_t(t)) dt
\]

We then observe that

\[
P_{\xi \perp} : \nabla^2 \tilde{\psi} - 2\xi \cdot \nabla \tilde{\psi} = \text{div}(P_{\xi \perp} \nabla \tilde{\psi}) = \Delta_{S^2} \tilde{\psi},
\]

where \( \Delta_{S^2} \) is the Laplace-Beltrami operator. This concludes the proof. \( \square \)

**Proposition 5.5.** Denote by \( Q^n \) the law of \( (\phi_n^{-1} u_n, S_n) \) on the space \( H^{-s}((0, T), H_s^{-s}(\mathbb{R}^3)) \times C([0, T], \mathcal{P}_1(\mathbb{R}^3 \times S^2)) \). Then for all \( \delta > 0 \), all \( \varphi \in C_\infty^\infty((0, T), \mathbb{R}^3) \) with \( \text{div} \varphi = 0 \) and for all \( \psi \in C_\infty^\infty([0, T] \times \mathbb{R}^3 \times S^2) \)

\[
\lim_{n \to \infty} Q^n \left( (v, g) \in H^{-s}((0, T), H^{-s}_s(\mathbb{R}^3)) \times C([0, T], \mathcal{P}_1(\mathbb{R}^3 \times S^2)) : \right)
\]

\[
|\Phi_{\varphi}(v, g)| + |\Psi_\psi(g)| > \delta
\]

\( = 0. \)

Proof. By Chebyshev’s inequality, it suffices to show that

\[
\lim_{n \to \infty} \mathbb{E} \left[ |\Phi_{\varphi}(\phi_n^{-1} u_n, S_n)| + |\Psi_\psi(S_n)| \right] = 0. \quad (5.10)
\]

We start by studying the first term. With \( u_n, app \) as in (5.3) we have

\[
\langle \phi_n^{-1} u_n, \Delta \varphi \rangle = \phi_n^{-1} \int_0^T \langle U_{n, app}(t), \partial_t \Delta \varphi(t, \cdot) \rangle dt
\]

\[
= \frac{\sqrt{2\pi \text{rot}}}{n} \int_0^T \left( \int_0^t L_{n, app}(\Xi(s)) \sqrt{|\mathcal{P}_2(\Xi(s))|} \circ dB(s), \partial_t \Delta \varphi(t, \cdot) \right) dt.
\]

Now let us recall that since \( L := L_{n, app}(\Xi(s)) \sqrt{|\mathcal{P}_2(\Xi(s))|} \in \mathcal{L}(\mathbb{R}^{3n}, H) \) with \( H := H^{-s}_s(\mathbb{R}^3) \), we may identify \( \mathcal{L}(\mathbb{R}^{3n}, H) \) with \( H^{3n} \) through \( L_{i, \alpha} = L e_{i, \alpha} \) where \( e_{i, \alpha} \) denote the canonical basis vectors of \( \mathbb{R}^{3n} \). Then, with \( \langle \cdot, \cdot \rangle \) denoting the pairing between \( H^{-s}_s(\mathbb{R}^3) \) and \( H^s(\mathbb{R}^3) \), and \( \langle \cdot, \cdot \rangle \) the scalar product in \( H \), we use \( L_{i, \alpha} = \sum_k (L_{i, \alpha}, \epsilon_k) \epsilon_k \), where \( (\epsilon_k)_k \) is an orthonormal basis of \( H \), in order to get

\[
\sum_{i, \alpha} \left\langle \int_0^t L_{i, \alpha}(s) \circ dB_{i, \alpha}(s), h \right\rangle = \sum_{i, \alpha, k} \left\langle \int_0^t (L_{i, \alpha}(s), \epsilon_k) \epsilon_k \circ dB_{i, \alpha}(s), h \right\rangle
\]

\[
= \sum_{i, \alpha} \int_0^t \langle (L_{i, \alpha}(s), \epsilon_k) \epsilon_k, h \rangle \circ dB_{i, \alpha}(s)
\]

\[
= \sum_{i, \alpha} \int_0^t \langle L_{i, \alpha}(s), h \rangle \circ dB_{i, \alpha}(s).
\]

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Hence, this yields, with \( e_\alpha \) denoting the canonical basis vectors of \( \mathbb{R}^3 \),

\[
\langle \phi_n^{-1} u_{n,\text{app}}, \Delta \varphi \rangle = \frac{\sqrt{2} \gamma_{\text{rot}}}{n} \sum_{i,\alpha,\beta} \int_0^T \int_0^t \left( L_{n,\text{app}}(\Xi(s)) e_i, \partial_t \Delta \varphi(t,\cdot) \right) \frac{\sqrt{R_2(\xi_i(s))}}{\alpha,\beta} \circ dB_{i,\beta}(s) \, dt
\]

\[
= -\frac{\sqrt{2} \gamma_{\text{rot}}}{n} \sum_{i,\alpha,\beta} \int_0^T \int_0^t \left( [e_\alpha]_{\mathcal{M}} + S(\xi_i(s), e_\alpha) : \partial_t \nabla \varphi(t,x_i) \frac{\sqrt{R_2(\xi_i(s))}}{\alpha,\beta} \circ dB_{i,\beta}(s) \right) \, dt
\]

\[
= -\frac{\sqrt{2} \gamma_{\text{rot}}}{n} \sum_{i} \int_0^T \left( \int_0^t \partial_t D \varphi(t,x_i) : S(\xi_i(s)) \frac{\sqrt{R_2(\xi_i(s))}}{\alpha,\beta} \circ dB_{i}(s) + 2 \int_0^t \partial_t \nabla \varphi(t,x_i) : \frac{\sqrt{R_2(\xi_i(s))}}{\alpha,\beta} \circ dB_{i}(s) \right) \, dt
\]

\[
= \frac{\sqrt{2} \gamma_{\text{rot}}}{n} \sum_{i} \int_0^T D \varphi(t,x_i) : S(\xi_i(t)) \frac{\sqrt{R_2(\xi_i(t))}}{\alpha,\beta} \circ dB_{i}(t)
\]

\[
+ \frac{\sqrt{2} \gamma_{\text{rot}}}{n} \sum_{i} \int_0^T 2 \nabla \varphi(t,x_i) : \frac{\sqrt{R_2(\xi_i(t))}}{\alpha,\beta} \circ dB_{i}(t)
\]

where we used (4.2), (3.11) and an integration by parts formula for Stratonovitch integrals which follows from the chain rule, Remark C.11 (iii).

Thus,

\[
\Phi_{\varphi}(\phi_n^{-1} u_{n_k}, S_{n_k}) = \mathcal{I}_1 + \mathcal{I}_2,
\]

where

\[
\mathcal{I}_1 = \langle \phi_n^{-1} (u_{n_k} - u_{n,\text{app}}), \Delta \varphi \rangle,
\]

and

\[
\mathcal{I}_2 =: \frac{1}{n} \sum_i \mathcal{J}_i = \frac{1}{n} \sum_i \left( \frac{\sqrt{2} \gamma_{\text{rot}}}{n} \int_0^T 2 \nabla \varphi(t,x_i) : \frac{\sqrt{R_2(\xi_i(t))}}{\alpha,\beta} \circ dB_{i}(t) + \frac{\sqrt{2} \gamma_{\text{rot}}}{n} \int_0^T D \varphi(t,x_i) : S(\xi_i(t)) \frac{\sqrt{R_2(\xi_i(t))}}{\alpha,\beta} \circ dB_{i}(t) - \gamma_E \int_0^T (2 \xi_i \otimes \xi_i - \operatorname{Id}) : \nabla \varphi(t,x_i) \, dt \right).
\]

By Lemma 5.2, we have

\[
\lim_{n \to \infty} \mathbb{E}[|\mathcal{I}_1|] = 0.
\]

To estimate \( \mathcal{I}_2 \), we use Lemma 3.4, which implies \( \mathbb{E}[\mathcal{J}_i] = 0 \). Furthermore, since the particle orientations \( \xi_i \) are independent, also the terms \( \mathcal{J}_i \) are independent. Moreover, they have a bounded variance by the Itô Stratonovitch conversion formula, Remark C.11 (ii) and Itô isometry, Theorem C.4. Therefore,

\[
\mathbb{E}[\mathcal{I}_2^2] = \frac{1}{n^2} \sum_i \mathbb{E}[\mathcal{J}_i^2] \leq \frac{C}{n} \|
abla \varphi\|^2_{L^\infty}.
\]

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Inserting (5.12)-(5.13) in (5.11) yields
\[
\lim_{n \to \infty} \mathbb{E} \left[ |\Phi_{\psi}(\phi_n^{-1} u_{n_k}, S_{n_k})| \right] = 0. \tag{5.14}
\]
Regarding the second term of (5.10), Lemma 5.4 implies
\[
\Psi_{\psi}(S_n) - (f_0 - S_n(0), \psi(0)) = -\frac{1}{n} \sum_{i=1}^{\infty} \int_{0}^{T} \nabla \psi(t, x_i, \xi_i(t)) \sigma_D(\xi_i(t)) dB_i(t) =: \frac{1}{n} \sum_{i} \tilde{J}_i.
\]
Using assumption (H4), \(\mathbb{E}[|f_0 - S_n(0), \psi(0)|] \to 0\).
Combining this with independence of \(\tilde{J}_i\) and bounded variance as above, we conclude
\[
\lim_{n \to \infty} \mathbb{E} \left[ |\Psi_{\psi}(S_n)| \right] = 0. \tag{5.15}
\]
Combination of (5.14) and (5.15) yields (5.10) and the proof is completed. \(\square\)

To be in position to prove Theorem 3.2, we state the following uniqueness results which are proved in Appendix A.

**Theorem 5.6.** Let \(f_0 \in L^2(S^2 \times \mathbb{R}^3)\) and \(f \in C([0, T]; \mathcal{P}_1(\mathbb{R}^3 \times S^2))\) satisfying \(\Psi_{\psi}(f) = 0\) for all \(\psi \in C^\infty([0, T] \times \mathbb{R}^3 \times S^2)\). Then, \(f\) is the unique weak solution to (1.3) in \(C([0, T]; L^2(\mathbb{R}^3 \times S^2))\) such that for almost all \(x \in \mathbb{R}^3\), \(f(\cdot, \cdot, x) \in L^2(0, T; H^1(S^2))\) and \(f'(\cdot, \cdot, x) \in L^2(0, T; H^{-1}(S^2))\).

**Theorem 5.7.** Let \(f \in L^2((0, T) \times \mathbb{R}^3 \times S^2)\). Assume \(u \in H^{-s}((0, T), H^{-s}_x(\mathbb{R}^3))\) satisfies \(\Phi_{\psi}(u, f) = 0\) for all \(\varphi \in C^\infty((0, T), \mathbb{R}^3)\) with \(\text{div} \varphi = 0\). Then \(u\) is the unique weak solution in \(L^2(0, T; H^1_x(\mathbb{R}^3))\) to (1.4).

**Proof of Theorem 3.2.** By Lemmas 5.1 and 5.3, the law \(\{Q^n\}\) of \((S_n, u_n)\) is tight, and thus we can extract a convergent subsequence \(Q^{n_k}\) which converges weakly to some probability measure \(Q\) on \(H^{-s}((0, T); H^{-s}_x(\mathbb{R}^3) \times C([0, T]; \mathcal{P}_1(\mathbb{R}^3 \times S^2)))\). We will argue that \(Q = \delta_{(u, f)}\), where \((u, f)\) is the unique solution to (1.3)-(1.4). Then, by standard arguments, uniqueness of \((u, f)\) implies weak convergence of the whole sequence \(Q^n\), and, since \(Q\) is deterministic, we deduce convergence in probability of \((u_n, S_n)\) to \((u, f)\).

It thus remains to show that \(\delta_{(u, f)}\) is the only accumulation point of \(Q^n\). Let \(Q^{n_k}\) be a converging subsequence and \(Q\) its limit. First we observe that for all \(\varphi \in C^\infty((0, T) \times \mathbb{R}^3)\) with \(\text{div} \varphi = 0\) and all \(\psi \in C^\infty([0, T] \times \mathbb{R}^3 \times S^2)\) the functionals \(\Psi_{\psi}\) and \(\Phi_{\varphi}\) are continuous with respect to the topology of \(H^{-s}((0, T); H^{-s}_x(\mathbb{R}^3)) \times C([0, T]; \mathcal{P}_1(\mathbb{R}^3 \times S^2))\). Therefore, by Portmanteau theorem and Proposition 5.5, for all \(\delta > 0\)
\[
Q \left( ((v, g) : |\Phi_{\varphi}(v, g)| + |\Psi_{\psi}(g)| > \delta) \right) \leq \liminf_{k \to \infty} Q^{n_k} \left( ((v, g) : |\Phi_{\varphi}(v, g)| + |\Psi_{\psi}(g)| > \delta) \right) = 0,
\]
which implies
\[
Q \left( ((v, g) : |\Phi_{\varphi}(v, g)| + |\Psi_{\psi}(g)| = 0) \right) = 1.
\]
Since the functionals \(\Psi_{\psi}\) and \(\Phi_{\varphi}\) are also continuous with respect to \(\psi\) and \(\varphi\), a density argument yields
\[
Q \left( ((v, g) : |\Phi_{\varphi}(v, g)| + |\Psi_{\psi}(g)| = 0, \forall \varphi \in C^\infty((0, T), \mathbb{R}^3) \text{ with } \text{div} \varphi = 0, \psi \in C^\infty([0, T] \times \mathbb{R}^3 \times S^2) \right) = 1.
\]
Thus, Theorem 5.6 implies that the law of \(S^n\) concentrates indeed on \(f\). Finally, by Theorem 5.7 we conclude \(Q = \delta_{(u, f)}\). \(\square\)

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6. Passage to the limit for very small Deborah numbers

In this section, we prove Theorem 3.3, i.e. the passage to the quasi-stationary system (1.5), (1.4) starting from the microscopic dynamics (2.14a)–(2.14b). Large parts of the proof are analogous to the the proof of Theorem 3.2 given in the previous section.

The main difference concerns the tightness of the law of the empirical measure $S_n$ (defined in (3.9)). Indeed, we cannot expect tightness in $C([0,T]; P_1(\mathbb{R}^3 \times \mathbb{S}^2))$ since the solution to the limit problem (1.5) is discontinuous at time 0. This discontinuity arises from the fast diffusion that induces a boundary layer at the initial time. This fast diffusion also makes tightness in $C([\delta,T]; P_1(\mathbb{R}^3 \times \mathbb{S}^2))$ difficult to obtain. We therefore work in a weaker space instead, namely $H^{0,-}((0,T); H^{-3/2,-}(\mathbb{R}^3 \times \mathbb{S}^2))$.

**Lemma 6.1.** Let $T > 0$ and let $S_n$ be the empirical measure defined in (3.9). Then, the family of laws $\{Q^n_s\}$ of the empirical measures $S_n$ is tight in the space $H^{0,-}((0,T); H^{-3/2,-}(\mathbb{R}^3 \times \mathbb{S}^2))$.

**Proof.** We note that since $H^{3/2,+}(\mathbb{R}^3 \times \mathbb{S}^2)$ is compactly embedded into $C^0(\mathbb{R}^3 \times \mathbb{S}^2)$, we have that $S_n$ is uniformly bounded in $L^\infty((0,T); H^{-3/2,-}(\mathbb{R}^3 \times \mathbb{S}^2))$ and thus compactly embedded in $H^{0,-}((0,T); H^{-3/2,-}(\mathbb{R}^3 \times \mathbb{S}^2))$.

Since the fast diffusion is balanced by the different scaling of $u_n$, tightness of the law of $u_n$ is completely analogous as in the previous section.

**Lemma 6.2.** Let

$$u_{n,\text{app}} := U_{n,\text{app}}',$$

$$U_{n,\text{app}} (t) := \frac{\sqrt{2\gamma_0} \phi_n}{n} \int_0^t L_{n,\text{app}}(\Xi(s)) \sqrt{\mathcal{R}_2(\Xi(s))} \, d(B_1(s), \ldots, B_n(s)).$$

Then, $u_{n,\text{app}} \in L^2(\Omega; H^{-s}(0,T; H^{-s}_\#(\mathbb{R}^3)))$ is well-defined and there exists $N_0 \in \mathbb{N}$ such that for all $s > \frac{1}{2}$ and all $n \geq N_0$

$$\mathbb{E} \left[ ||u_n||_{H^{-s}((0,T); H^{-s}_\#(\mathbb{R}^3))}^2 \right] \leq C,$$

$$\lim_{n \to \infty} \mathbb{E} \left[ ||u_n - u_{n,\text{app}}||_{H^{-s}((0,T); H^{-s}_\#(\mathbb{R}^3))}^2 \right] = 0.$$

In particular, the family of laws $\{Q^n_s\}$ of $u^n$, defined through (3.6)–(3.7), is tight in the space $H^{-s}(0,T; H^{-s}_\#(\mathbb{R}^3))$.

In order to pass to the limit, we consider again functionals $\tilde{\Psi}_\phi(g), \Phi_\phi(v, g), \Theta_\theta(g)$ for $(v, g) \in H^{-s}(0,T; H^{-s}_\#(\mathbb{R}^3)) \times H^{0,-}((0,T); H^{-3/2,-})$ and $\varphi \in C^\infty_c((0,T) \times \mathbb{R}^3)$ with $\text{div} \varphi = 0$, $\psi \in C^\infty_c((0,T) \times \mathbb{R}^3 \times \mathbb{S}^2)$ and $\theta \in C^\infty((0,T) \times \mathbb{R}^3)$. Here, $\Phi_\phi$ is still given by (5.9), $\tilde{\Psi}_\phi$ and $\Theta_\theta$ are defined as

$$\tilde{\Psi}_\phi(g) := \langle g, \Delta \xi \psi + \nabla \xi \psi \cdot P_{\xi \cdot h} \rangle,$$

$$\Theta_\theta(g) := \langle f_0 - g, \theta \otimes 1 \rangle.$$

Correspondingly to Lemma 5.4, we have the following.
Lemma 6.3. For every test function $\psi \in C_c^\infty((0,T) \times \mathbb{R}^3 \times S^2)$, the empirical measures $S_n$ satisfies the following identity,

$$
\tilde{\Psi}_\psi(S_n) = -\phi_n \int_0^T (S_n(t), \partial_t \psi(t,x,\xi)) - \int_0^T \frac{1}{n} \sum_{i=1}^n \nabla \psi(t,x,\xi(t)) \sigma_D(\xi(t)) dB_i(t),
$$

with $\sigma_D$ as in (3.2).

The following proposition is the analogous version of Proposition 5.5.

Proposition 6.4. For each $\delta > 0$, for each $\varphi \in C_c^\infty((0,T), \mathbb{R}^3)$ with $\text{div} \, \varphi = 0$, $\psi \in C_c^\infty((0,T) \times \mathbb{R}^3 \times S^2)$ and $\theta \in C_c^\infty((0,T) \times \mathbb{R}^3)$

$$
\lim_{n \to \infty} Q^n \left( (v,g) \in H^{-s}((0,T); H^{-s}_g((\mathbb{R}^3)) \times H^{0-}((0,T); H^{-3/2-}((\mathbb{R}^3 \times S^2))) : \\
|\Phi_\varphi(v,g)| + |\tilde{\Psi}_\psi(g)| + |\Theta_\theta(g)| > \delta \right) = 0.
$$

Proof. The proof is analogous to the one of Proposition 5.5. Note in particular that Lemma 3.4 has to be adapted accordingly since $\Xi$ satisfies (2.14b) instead of (2.13b) which yields the appearance of a factor $\sqrt{\phi_n}^{-1}$ in (3.17) that will be compensated by the factor $\sqrt{\phi_n}$ appearing in the definition of $U_{n,\text{app}}$, see (6.1). To deal with the additional functional $\Theta_\theta$, we notice that

$$
\Theta_\theta(S_n) = \int_0^T \left( \frac{1}{n} \sum_{i=1}^n \delta_{x_i,0} - f_0(t, \cdot) \otimes 1 \right) dt,
$$

and therefore this functional can be handled due to assumption (H4).

Proof of Theorem 3.3. The proof is completely analogous to the proof of Theorem 3.2. The only difference is that regarding the uniqueness, we rely on Theorem 6.5 below instead of Theorem 5.6.

Theorem 6.5. Let $f_0 \in L^2(S^2 \times \mathbb{R}^3)$ and $g \in H^{0-}((0,T); H^{-3/2-})$ satisfy $\tilde{\Psi}_\psi(g) = 0$, $\Theta_\theta(g) = 0$ for all $\psi \in C_c^\infty((0,T) \times \mathbb{R}^3 \times S^2)$ and $\theta \in C_c^\infty((0,T) \times \mathbb{R}^3)$. Then, $g$ is the unique weak solution to (1.5) in $L^2((0,T) \times \mathbb{R}^3)$ such that for almost all $x \in \mathbb{R}^3$, $f(\cdot,\cdot,x) \in C^\infty((0,T) \times \mathbb{S}^2)$.

A. Uniqueness results for the Stokes and Fokker-Planck equations in negative Sobolev spaces

In this appendix we show the uniqueness results for solutions of the Stokes and the (in-)stationary Fokker-Planck equations as stated in Theorems 5.7, 5.6 and 6.5.

A.1. Proof of Theorem 5.7

Proof of Theorem 5.7. Well-posedness of (1.4) in $L^2((0,T); \dot{H}^1(\mathbb{R}^3))$ is classical. By linearity, it therefore remains to show that there is at most one function $u \in H^{-s}((0,T), H^{-s}(\mathbb{R}^3))$ that satisfies $\Phi_\varphi(u,0) = 0$ for all $\varphi \in C_c^\infty((0,T), \mathbb{R}^3)$ with $\text{div} \, \varphi = 0$.

Let $g \in C_c^\infty((0,T) \times \mathbb{R}^3)$ and define the pair $v_g \in C_c^\infty((0,T); H_0^{2+s}(\mathbb{R}^3) \cap \dot{H}^2(\mathbb{R}^3))$, $p_g \in C_c^\infty((0,T); H^{1+s}(\mathbb{R}^3) \cap \dot{H}^1(\mathbb{R}^3))$ to be the solution to the Stokes equations

$$
-\Delta v_g + \nabla p_g = g, \quad \text{div} \, v_g = 0.
$$
Then, by density of divergence free function of $C^\infty_\infty(R^3)$ in $\dot{H}^{2+s}_s(R^3) \cap H^2_s(R^3)$, we have
\[ 0 = \Phi_{vg}(u,0) = \langle u, g \rangle, \]
which finishes the proof. \hfill \square

A.2. Proof of Theorem 5.6

Proof of Theorem 5.6. Let $\varphi \in C^\infty([0,T] \times R^3 \times S^2)$ and let $\psi \in C^\infty([0,T] \times R^3 \times S^2)$ be the unique classical solution to the backwards parabolic equation
\[
\begin{cases}
-\partial_t \psi - \Delta_\xi \psi - P_{\xi \perp} h \cdot \nabla \psi = \varphi, \\
\psi(T,\cdot) = 0.
\end{cases}
\]
By standard regularity theory for parabolic equations, $\psi$ is well-defined.

Thus, for $f$ as in the statement
\[ 0 = \Psi_\psi(f) = \langle f_0, \psi(0) \rangle - \int_0^T \langle f, \varphi \rangle \, dt. \]
Since $f_0$ is given, this identity characterizes $f$ uniquely, and therefore $f$ must coincide with the unique classical solution to (1.3). \hfill \square

A.3. Proof of Theorem 6.5

The proof of Theorem 6.5 relies on the following theorem regarding the elliptic operator
\[ L v = - \text{div}(\nabla v - \tilde{h} v), \]
where $\tilde{h} \in C^\infty(S^2; R^3)$ with
\[ \xi \cdot \tilde{h} = 0 \quad \text{for all } \xi \in S^2. \tag{A.1} \]
The condition (A.1) ensures that $h(t,\cdot,x)$ takes values in the tangent space $TS^2$.

We denote the formal adjoint by
\[ L^* v := -\Delta v - \tilde{h} \cdot \nabla v. \]

In what follows we will often deal with functions $h$ depending on a parameter $z \in R^m$ and denote by $L_z$ and $L_z^*$ the corresponding operators as above.

Theorem A.1. (i). Let $\tilde{h} \in C^\infty(S^2; R^3)$ satisfy (A.1). Then $\dim \ker L = 1$ and all elements in $\ker L$ have a sign. In particular, there exists a unique classical solution $f$ to
\[ -L f = 0, \quad \int_{S^2} f = 1. \tag{A.2} \]
Furthermore, this solution $f$ depends smoothly on $h$. More precisely, let for a smooth family $(z,\xi) \in R^m \times S^2 \mapsto \tilde{h}_z(\xi)$, $z \in R^m$ be smooth such that $h_z$ satisfies (A.1) for all $z \in R^m$, then the family of solutions $z \mapsto f_z$ is smooth.
(ii). Let \((z, \xi) \in \mathbb{R}^m \times S^2 \mapsto h_z(\xi)\) be as above. Then, for all \(K \in \mathbb{R}^m\), \(k \in \mathbb{N}\) there exists \(C > 0\) such that for all \(z \in K\) and all \(\psi \in (\ker L_z)^\perp\), the unique solution \(v \in H^1(S^2)\) to 
\[ L_z^* v = \psi \quad \text{with} \quad \int v = 0 \] 
satisfies
\[ \|v\|_{H^{k+2}} \leq C \|\psi\|_{H^k}. \] (A.3)

In particular, if \(\varphi \in C_c^\infty(\mathbb{R}^m \times S^2)\), and \(v(z, \cdot)\) is the unique solution with \(\int v(z, \cdot) = 0\) to 
\[ L_z^* v(z, \cdot) = \varphi(z, \cdot) \], then \(v \in C_c^\infty(\mathbb{R}^m \times S^2)\).

**Proof.** We rely on classical results concerning elliptic PDEs on compact manifolds, for which we refer to [Tay11].

Existence and uniqueness for the problem (A.2) is classical, see e.g. [Zee88]. We give a short proof for completeness. The operator \(L\) is a compact perturbation of the selfadjoint operator \(-\Delta\). Thus, the index of \(L\) is 0, i.e.

\[ \dim \ker L = \dim \ker L^*. \]

Since \(L^*\) contains no zero-order terms, the maximum principle implies \(\ker L^* = \{\text{const}\}\). In particular \(\dim \ker L = \dim \ker L^* = 1\). It is easy to see that \(g \in \ker L\) implies that also the positive and negative parts \(g_+, g_-\) lie in \(\ker L\). Thus, \(g = g_+\) or \(g = g_-\), otherwise \(g_+\) and \(g_-\) would be linearly independent, contradicting \(\dim \ker L = 1\).

The proof of the assertion that \(\tilde{f}_z\) depends smoothly on \(z\) is similar to the proof of (ii) which we prove first.

Let \(v, \psi\) be as in the statement. From standard elliptic regularity theory it follows that
\[ \|v\|_{H^{k+2}} \leq C(\|v\|_{L^2} + \|\psi\|_{H^k}). \] (A.4)
for a constant \(C\) independent of \(z\) in \(K\). For (A.3), it remains to show that
\[ \|v\|_{L^2} \leq C \|\psi\|_{L^2}. \]

Assume for the sake of contradiction that there exists no such constant. Then, there exists a sequence \(z_n \in K\), \(\psi_n \in (\ker L_{z_n})^\perp\), \(v_n \in H^1(S^2)\) such that \(L^* v_n = \psi_n\), \(\int v_n = 0\), \(\|v_n\|_{L^2} = 1\) and \(\|\psi_n\|_{L^2} \leq 1/n\).

By (A.4), \(v_n\) is bounded in \(H^2(S^2)\), thus by taking a suitable subsequence \(v_n \to v_k\) in \(H^1(S^2)\) and \(z_n \to z_k\) for some \(v_k \in H^2(S^2)\), \(z_k \in K\). Note that by the smoothness assumption on \(h\), we have \(h_{z_k} \cdot \nabla v_k \to \nabla h_{z_k} \cdot v_k\) in \(L^2\). Thus, \(L_{z_k}^* v_k = 0\). Since \(\int v_k = 0\) and \(\|v_k\|_{L^2} = 1\) this contradicts \(\ker L_{z_k}^* = \{\text{const}\}\). This establishes (A.3).

For the second part of (ii), let \(\varphi \in C_c^\infty(\mathbb{R}^m \times S^2)\), and \(v(z, \cdot)\) be the unique solution with 
\[ \int v(z, \cdot) = 0 \] to 
\[ L_z^* v(z, \cdot) = \varphi(z, \cdot) \]. Note that \(v(z, \cdot) = 0\) if \(\varphi(z, \cdot) = 0\). Moreover, for \(z_1, z_2 \in \mathbb{R}^m\), we have
\[ L_{z_1}^* (v(z_1, \cdot) - v(z_2, \cdot)) = (h_{z_2} - h_{z_1}) \cdot \nabla v(z_2, \cdot) + \varphi(z_1, \cdot) - \varphi(z_2, \cdot). \]

Thus, by (A.3), we have
\[ \|v(z_1, \cdot) - v(z_2, \cdot)\|_{H^{k+2}(S^2)} \leq C \|h_{z_1} - h_{z_2}\|_{W^{k,\infty}(S^2)} \|\nabla v(z_2, \cdot)\|_{H^k(S^2)} \]
\[ + \|\varphi(z_1, \cdot) - \varphi(z_2, \cdot)\|_{H^k(S^2)} \leq C|z_1 - z_2|. \]
Thus, $v \in W^{1,\infty}(\mathbb{R}^m; H^k(S^2))$. Differentiating the equation with respect to $z_j$ leads to

$$L^* \tilde{v} = \tilde{\phi} + \tilde{h} \cdot \nabla v,$$

where $\tilde{v} = \partial_{z_j} v, \tilde{\phi} = \partial_{z_k} \phi$. Note that $\int \tilde{v}(z, \cdot) = 0$. Thus, repeating the above argument, we find that $\tilde{v} \in W^{1,\infty}(\mathbb{R}^m; H^k(S^2))$ and by induction $v \in C_c^\infty(\mathbb{R}^m \times S^2)$.

To see that $\bar{f}_z$ as in the second part of assertion (i) depends smoothly on $z$, we proceed analogously: Similarly as before, we observe that for any $\psi \in (\ker L_z)^\perp$ the unique solution to $L_z v = \psi$ with $\int v = 0$ satisfies

$$\|v\|_{H^{k+2}} \leq C\|\psi\|_{H^k}, \quad (A.5)$$

where $C$ depends only on $k$, uniformly on compact sets $K \subseteq \mathbb{R}^m$. Note that the only difference of this estimate to (A.3) is that $\int v = 0$ is not equivalent to $v \in \ker L_z^\perp$. However, inspection of the proof above reveals that we never used orthogonality but only that

$$\{v \in \ker L_z : \int v = 0\} = \{0\}. \quad (A.6)$$

This still holds true, since $\dim \ker L_z = 1$ and $\tilde{f}_z \in \ker L_z$ with $\int \tilde{f}_z = 1$. Thus, (A.5) holds.

Next, we observe that $\tilde{f}_z$ satisfies

$$\|\tilde{f}_z\|_{H^k} \leq C \quad (A.7)$$

uniformly on compact sets $z \in K$. Indeed, by elliptic regularity corresponding to (A.4), it suffices to treat the case $k = 0$. Observe that

$$\tilde{f}_z = \frac{\tilde{f}_z}{\int \tilde{f}_z \, d\xi}$$

for the normalized unique non-negative eigenvector $\tilde{f}_z \in \ker L_z$ with $\|\tilde{f}_z\|_2 = 1$. Thus, it suffices to show that

$$\int \tilde{f}_z \, d\xi \geq c,$$

uniformly on compact sets $z \in K$. Again, we argue by contradiction. Indeed, if such an estimate was not true, we would find a sequence $z_n \to z_*$ such that $\tilde{f}_{z_n} \to \tilde{f}_* \in H^1(S^2)$ with $\int \tilde{f}_* = 0$. But then, $f_* \in \ker L_{z_*}$ with $\|f_*\|_2 = 1$ which contradicts (A.6). This proves (A.7).

Finally, for $z_1, z_2 \in \mathbb{R}^m$ we have

$$L_{z_1}(\tilde{f}_{z_1} - \tilde{f}_{z_2}) = \text{div}((h_{z_1} - h_{z_2})\tilde{f}_{z_2}).$$

Using (A.7), the right-hand side is bounded by $C|z_1 - z_2|$ in $H^k$ and thus (A.5) implies Lipschitz estimates in $z$ as before and we conclude again by differentiation and iteration. \qed

**Proof of Theorem 6.5.** We denote by $L_{t,x}$ the operator corresponding to $\tilde{h}_{t,x}(\xi) = P_{\xi^1} h(t, x, \xi)$, and by $\tilde{f}_{t,x}$ the corresponding unique solution to (A.2).

We claim that $\bar{\Psi}_\psi(g) = 0$ for all $\psi \in C_c^\infty((0, T) \times \mathbb{R}^3 \times S^2)$ implies

$$g = \frac{1}{\|f_*\|_{L^2}^2} \bar{f}_* \mu. \quad (A.8)$$

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for some $\mu \in (C^\infty_c((0, T) \times \mathbb{R}^3))^*$ in the sense that
\[ \langle g, \psi \rangle = \langle \mu, \frac{1}{\|f\|_2^2} \int_{S^2} \tilde{f}(\xi)\psi(\cdot, \xi) \, d\xi \rangle \]

Note that this is well-defined since $(t, x, \xi) \mapsto \tilde{f}_{t,x}(\xi)$ is smooth by Theorem A.1 (i).

From this identity, $\int_{S^2} \tilde{f}_{t,x}(\xi) \, d\xi = 1$ and $\Theta_{\theta}(g) = 0$ for all $\theta \in C^\infty_c((0, T) \times \mathbb{R}^3)$, we immediately deduce
\[ \mu = \|\tilde{f}_{t,x}\|_2^2 \int_{S^2} f_0(x, \xi) \, d\xi, \]
which yields uniqueness and smoothness in $(t, x, \xi) \in (0, T) \times S^2$ of the solution for almost all $x \in \mathbb{R}^3$.

It remains to prove (A.8). Let $\psi \in C^\infty_c(\mathbb{R}^3 \times S^2)$ and let
\[ \varphi(t, x, \xi) = \psi(t, x, \xi) - \frac{1}{\|f_{t,x}\|_2^2} \int_{S^2} \tilde{f}_{t,x}(\xi)\psi(t, x, \xi) \, d\xi \tilde{f}_{t,x}(\xi). \]

Then, $\varphi(t, x, \cdot) \in (\ker L_{t,x})^\perp$. Hence, by Theorem A.1 (ii), there exists $\tilde{\varphi}(t, x, \xi) \in C^\infty_c((0, T) \times \mathbb{R}^3 \times S^2)$ such that $L_{t,x}^* \tilde{\varphi}(t, x, \xi) = \varphi(t, x, \xi)$ and $\int_{S^2} \varphi(t, x, \xi) \, d\xi = 0$. Thus, $\langle g, \varphi \rangle = \Psi_{\tilde{\varphi}}(g) = 0$ and hence
\[ \langle g, \psi \rangle = \langle g, \frac{1}{\|f_{t,x}\|_2^2} \int_{S^2} \tilde{f}(\xi)\psi(\cdot, \xi) \, d\xi \tilde{f}. \]
which yields the claim with
\[ \langle \mu, v \rangle = \langle g, \frac{1}{\|f_{t,x}\|_2^2} \tilde{f}, v \rangle. \]

This concludes the proof of the Theorem. \qed

**B. Proof of Lemma 3.4**

**Proof.** We drop the index $i$ in the proof. Let $b \in C^\infty_c((0, t), \mathbb{R}^3)$. Recalling (3.3), we appeal to the Itô Stratonovitch conversion formula (C.5) (after extending the occurring functions of $\xi$ to the whole space $\mathbb{R}^3$) to deduce with $R = \sqrt{R_2}$
\[ \mathbb{E} \left( \int_0^t b(s) \cdot \sqrt{R_2(\xi(s))} \, dB(s) \right) = \mathbb{E} \left( \int_0^t R(\xi(s))b(s) \, dB(s) \right) = \mathbb{E} \left( \frac{1}{2} \int_0^t tr(\nabla_\xi R(\xi(s))b(s)\sigma D(\xi(s))) \, ds \right) \]
where we used that the expectation of Itô integrals vanish. From (2.5), we have
\[ \nabla_\xi \sqrt{R_2(\xi)}b = (\sqrt{\gamma_{rot}} - \sqrt{\gamma_{rot}})[(\xi \cdot b)1d + \xi \otimes b] \]
\[ \frac{1}{2} \int_0^t tr(\nabla_\xi R(\xi(s))b(s)\sigma D(\xi(s))) \, ds \]
\[ \mathbb{E} \]
and we recall from (3.2) that \( \sigma_D = \sqrt{2}[\xi]_M \) (with the notation (3.10)). In particular, since \( \sigma_D \) is skew-symmetric,

\[
tr(\nabla_\xi \mathcal{R}(\xi)b\sigma_D(\xi)) = (\sqrt{\gamma_{\text{rot}}} - \sqrt{\gamma_{\text{rot}}}) tr((\xi \otimes b)\sigma_D(\xi)) = \sqrt{2}((\xi \otimes a_\alpha) \cdot b)(\xi \cdot a_\alpha)
\]

for any orthonormal basis \((a_\alpha)\) of \( \mathbb{R}^3 \). Since \( \xi \times a_\alpha(\xi \cdot a_\alpha) = \xi \times \xi = 0 \), we conclude (3.16).

Let \( A \in C_\infty^0((0,t),\text{Sym}_0(3)) \). From (2.5) and (2.6) we deduce that for any \( T \in \mathbb{R}^3 \)

\[
A : \left( S(\xi)\sqrt{\mathcal{R}_2(\xi)}(T) \right) = \gamma_E\gamma_{\text{rot}}^{-\frac{1}{2}} A : (T \times \xi) = \gamma_E\gamma_{\text{rot}}^{-\frac{1}{2}} ([\xi]_M A) \cdot T,
\]

\[
\nabla_\xi ([\xi]_M A) = [\xi]_M A - [A\xi]_M
\]

where we used, for the first line, that for any \( u, v, w \in \mathbb{R}^3 \),

\[
[u]_M v = u \times v, \quad u \cdot (v \times w) = v \cdot (w \times u)
\]

Thus, analogously as above

\[
\mathbb{E} \left( \int_0^t A(s) : S(\xi(s))\sqrt{\mathcal{R}_2(\xi(s))} d\xi(s) \right)
\]

\[
= \frac{\gamma_E}{\sqrt{2\gamma_{\text{rot}}}} \int_0^t tr\left( ([\xi]_M A(s) - [A(\xi(s))]_M) \xi(s)\right) d\xi(s)
\]

Using (B.1) and \( [v]_M = -[v]_M \) for any \( v \in \mathbb{R}^3 \), we get for any orthonormal basis \((a_\alpha)\) of \( \mathbb{R}^3 \)

\[
tr\left( ([\xi]_M A - [A\xi]_M) \xi \right) = \left( ([\xi]_M a_\alpha) \cdot ([A\xi]_M a_\alpha) - ([\xi]_M a_\alpha) \cdot ([\xi]_M a_\alpha)\right)
\]

\[
= (\xi \times a_\alpha) \cdot ([A\xi]_M a_\alpha) - [A\xi]_M (\xi \times a_\alpha) \cdot (\xi \times a_\alpha)
\]

\[
= A : \xi \otimes (\xi \times a_\alpha) - A : (\xi \times a_\alpha) \otimes (\xi \times a_\alpha)
\]

\[
= A : (2\xi \otimes \xi) + A : (\xi \otimes \xi - \text{Id})
\]

For the last line, we choose \( a_1 = \xi \) to get \( a_\alpha \times (\xi \times a_\alpha) = \xi \) for \( \alpha = 2,3 \) and

\[
\sum_\alpha (a_\alpha \times \xi) \otimes (\xi \times a_\alpha) = \xi \otimes \xi - \text{Id}
\]

which yields the desired result.

\[\square\]

C. Stochastic calculus

In this appendix we gather some theory on stochastic integrals that we rely on. In Subsection C.1, we collect standard definitions and results on stochastic calculus in Euclidean space. We mostly follow [Kuo06] and keep the setting as simple as possible. For further results, one could for instance refer to [KS12].

At the end of Subsection C.1, we also precise the notion of solutions to the SDEs for the particle orientations \( \xi_i \) in (2.13b) and (2.14b) which are SDEs on the manifold \( \mathbb{S}^2 \). Instead of dealing with SDEs on manifolds in an abstract way (see for instance [Hsu02]), we follow a more
pedestrian approach. Namely, we just consider corresponding SDEs in the ambient space \( \mathbb{R}^3 \) and show a posteriori that the solutions stay on \( S^2 \).

Finally, Subsection C.2 is devoted to stochastic calculus in infinite dimensions. Stochastic calculus in infinite dimensional Hilbert spaces is quite well developed, see for instance the monograph [DZ14] where stochastic integrals of the form \( \int f(s) dB(s) \) are considered for Hilbert-valued Brownian motions \( B(s) \in E \) and functions \( f \) such that \( f(s): E \to H \) is a Hilbert-Schmidt operator to another Hilbert space \( H \). Corresponding stochastic integrals in a Stratonovich sense are used for instance in [MMS19].

For our purpose, it is sufficient to consider the case where \( E = \mathbb{R}^d \) and \( H \) is an infinite dimensional separable Hilbert space. This case is considerably easier than the general framework. Therefore, we choose to present here the necessary theory in a self-contained way based only on the finite dimensional stochastic calculus in the preceding section.

### C.1. Reminder on stochastic calculus in finite dimensional space

In what follows we consider a probability space \( (\Omega, \mathcal{A}, P) \) and recall that a continuous-time stochastic process is a map \( t \mapsto X(t) \), \( t \in \mathbb{R}^+ \) such that \( X(t) \) is a random variable. We recall first the definition of a Brownian motion

**Definition C.1** (Brownian Motion). A continuous-time stochastic process \( B: \mathbb{R}^+ \times \Omega \to \mathbb{R} \), \( t \geq 0 \) is called a Brownian motion if and only if

(i). \( B(0, \omega) = a \) for each \( \omega \in \Omega \).

(ii). For any partition \( 0 \leq t_0 < t_1 < \cdots < t_n \), the increments \( B(t_{i+1}) - B(t_i) \) are independent random variables with distribution \( B(t_{i+1}) - B(t_i) \sim N(0, t_{i+1} - t_i) \)

(iii). \( P \)-almost every sample path \( t \mapsto B(t, \omega) \) is continuous.

An \( \mathbb{R}^d \)-valued stochastic process \( B(t, \omega) = (B_1(t, \omega), \cdots, B_d(t, \omega)) \) is called a multi-dimensional Brownian motion if and only if the components are independent one-dimensional Brownian motions.

In order to recall the definition of stochastic integrals, we introduce first filtrations and the notion of adapted processes.

**Definition C.2** (Filtrations and adapted processes). Let \( (\Omega, \mathcal{A}, P) \) be a probability space.

- A continuous-time filtration on \( (\Omega, \mathcal{A}) \) is a family \( (\mathcal{F}_t)_{t \geq 0} \), indexed by time, of increasing \( \sigma \)-algebras \( \mathcal{F}_t \subseteq \mathcal{A} \), that is, satisfying \( \mathcal{F}_t \subseteq \mathcal{F}_s \) for \( t \leq s \).

- A real-valued stochastic process \( M \) on \( (\Omega, \mathcal{A}, P) \) is adapted with respect to \( (\mathcal{F})_{t \geq 0} \) if \( M(t) \) is \( \mathcal{F}_t \) measurable for all \( t \geq 0 \).

- The natural (canonical) filtration \( (\mathcal{F}_s)_{s \geq 0} \) generated by a stochastic process \( M \), denoted by \( \sigma(M) \), is the filtration formed, for each \( t \), by the smallest \( \sigma \)-algebra for which the maps \( \omega \mapsto M(s, \omega) \), are measurable functions for all \( 0 \leq s \leq t \).

**Definition C.3** (Martingale). A stochastic process \( M \) adapted to a filtration \( (\mathcal{F}_t)_{t \geq 0} \) is a martingale if the following conditions hold:

- \( E[M(t)] < +\infty \) for all \( t \geq 0 \).
- \( E[M(t)\mathcal{F}_s] = M(s) \) for all \( 0 \leq s \leq t \)
Itô integral with respect to Brownian motion and Itô formula

We consider below a Brownian Motion and a filtration $(\mathcal{F}_t)_{t \geq 0}$ such that

- For all $t \geq 0$, $B(t)$ is $\mathcal{F}_t$ measurable.
- For all $0 \leq s \leq t$, the random variable $B(t) - B(s)$ is independent of the $\sigma$-algebra $\mathcal{F}_s$.

We recall the construction of the Itô integral in the same way as the Riemann integral, proceeding first for step stochastic processes given by

$$f(\omega) = \sum_{i=0}^{n} A_i(\omega) 1_{[s_i, s_{i+1})},$$

for a given decomposition $s_0 = 0 < s_1 < \cdots < s_n = T$ of $[0, T]$ such that $A_i$ is $F_{s_i}$-measurable and $E[A_i^2] < +\infty$. We set

$$I(f) = \sum_{i=0}^{n} A_i(B(s_{i+1}) - B(s_i)).$$

This defines a linear mapping $I$ and moreover we have $EI(f) = 0$ and

$$E(I(f)^2) = \int_0^T E([f(t)]^2) \, dt.$$ \hfill (C.1)

for each step stochastic process, see [Kuo06, Lemma 4.3.2]. Next, the idea is to extend this definition for each stochastic process in the space $f \in L^2_{\text{ad}}([0, T] \times \Omega)$ defined as the space of stochastic processes $f$ satisfying

- $\int_0^T E[f(s)]^2 \, ds < +\infty$
- $f$ adapted to the filtration $(\mathcal{F}_s)_{0 \leq s \leq T}$.

Indeed, each stochastic process $f \in L^2_{\text{ad}}([0, T] \times \Omega)$ can be approximated by a sequence of step stochastic processes $(f_k)_k$ in the following sense

$$\lim_{k \to \infty} \int_0^T E[f(s) - f_k(s)]^2 \, dt = 0,$$

see [Kuo06, Lemma 4.3.3]. According to this, one can define the Itô integral as the limit

$$I(f) = \lim_{k \to \infty} I(f_k)$$ \hfill (C.2)

where the limit does not depend on the choice of the sequence $(f_k)_k$. In particular, thanks to (C.1), $I: L^2_{\text{ad}}([0, T] \times \Omega) \to L^2(\Omega)$ is an isometry. We gather below additional properties, see [Kuo06, Theorem 4.3.5, Theorem 4.6.1 and Theorem 4.6.2].

**Theorem C.4** (Itô Isometry). Let $f \in L^2_{\text{ad}}([0, T] \times \Omega)$. The stochastic process corresponding to the Itô integral $I(f)$ defined in (C.2) and denoted by

$$X(t) = \int_0^t f(s) dB(s), \quad 0 \leq t \leq T,$$

is a continuous martingale with respect to the filtration $(\mathcal{F}_t)_{0 \leq t \leq T}$ such that $E[X(t)] = 0$ and

$$E \left[ \int_0^t f(s) dB(s) \right]^2 = \int_0^t E[f(s)]^2 \, ds.$$
Remark C.5. The definition of Itô integrals and the Itô isometry extends straightforwardly to the multidimensional case: For \( d \) independent Brownian motions \( B_i, 1 \leq i \leq d \) and \( \sigma \in L^2_{ad}([0, t] \times \Omega) \) a \( d \times d \) valued function,

\[
\int_0^t \sigma(s) dB(s) \in L^2_{ad}([0, t] \times \Omega)
\]

where \( \|A\|_{HS} = \sqrt{\text{Tr}(A^T A)} \) denotes the Hilbert-Schmidt norm of a matrix \( A \in \mathbb{R}^{d \times d} \).

Following [Kuo06, Subsection 7.5] we recall the multidimensional Itô formula.

**Definition C.6 (Ito process).** Let \( \sigma \in L^2_{ad}([0, T] \times \Omega) \) a \( d \times d \) valued function, \( b \in L^2_{ad}([0, T] \times \Omega) \) a \( \mathbb{R}^d \) valued function. Then, the stochastic process

\[
X(t) = X_0 + \int_0^t \sigma(s) dB(s) + \int_0^t b(s) ds
\]

is called Itô process with drift \( b \) and diffusion \( \sigma \).

**Lemma C.7 (Itô formula).** Let \( \phi \in C(\mathbb{R} \times \mathbb{R}^d; \mathbb{R}^d) \) with continuous partial derivatives \( \partial_t \phi, \nabla_x \phi, \nabla^2_x \phi \). Then \( \phi(t, X(t)) \) is also an Itô process satisfying

\[
\phi(t, X(t)) = \phi(0, X(0)) + \int_0^t \nabla \phi(s, X(s)) \sigma(s) dB(s)
+ \int_0^t \left[ \partial_t \phi(s, X(s)) + b(s) \cdot \nabla_x \phi(s, X(s)) + \frac{1}{2} \sigma(s) \sigma(s)^\top : \nabla^2_x \phi(s, X(s)) \right] ds.
\]

**Stratonovich Integral**

We now turn to the definition of the Stratonovich integral. We first recall the definition of quadratic variance and covariance.

**Definition C.8 (Quadratic variation and covariation).** The quadratic variation of a real-valued stochastic process \( M \) is the process written as \( [M] \) and defined as the following limit in probability, if it exists

\[
[M](t) = \lim_{\|P\| \to 0} \sum_{i} (M(t_i) - M(t_{i-1}))^2,
\]

where \( P = \{t_0, t_1, \cdots, t_n\} \) is any partition of \( [0, t] \) and \( \|P\| = \max_{1 \leq i \leq n} |t_i - t_{i-1}| \). Moreover, for two real-valued stochastic processes \( X, Y \), the covariation, denoted by \( [X, Y] \), is defined as

\[
[X, Y](t) = \lim_{\|P\| \to 0} \sum_{i} (X(t_i) - X(t_{i-1}))(Y(t_i) - Y(t_{i-1})).
\]

**Remark C.9.** (i). The quadratic variation exists for all continuous finite variation processes, and is zero.

(ii). The quadratic variation exists for all right continuous, square integrable martingale with left-hand limits, see [Kuo06, Formula (6.4.4)]
(iii). If $B$ and $W$ are two independent Brownian motions, $f \in L^2_{ad}([0,t] \times \Omega)$ and $X(t) = \int f(s) dB(s)$ then $[X,W](t) = 0$ and $[X,B](t) = \int f(s) ds$.

**Definition C.10** (Stratonovich integral). Let $X \in L^2_{ad}([0,T] \times \Omega)$ such that $[X]$ exists. The Stratonovich integral is defined as

$$
\int_0^t X(s) \circ dB(s) = \int_0^t X(s) dB(s) + \frac{1}{2} [X,B](t).
$$

**Remark C.11.** (i). In particular, if $X$ is given as an Itô process of the form (C.3), independence of $B_i, B_j$ for $i \neq j$ and Remark C.9 iii) yield

$$
\int_0^t X(s) \circ dB(s) = \int_0^t X(s) dB(s) + \frac{1}{2} \sum_i \left[ \int_0^t \sigma_{ij}(s) dB_j, B_i \right](t)
$$

$$
= \int_0^t X(s) dB(s) + \frac{1}{2} \int_0^t \text{tr}(\sigma(s) ds).
$$

(ii). One can extend the above formula to all $g \in C^1([0,T] \times \mathbb{R}^d; \mathbb{R}^d)$ in the following way

$$
\int_0^t g(s, X(s)) \circ dB(s) = \int_0^t g(s, X(s)) dB(s) + \frac{1}{2} \int_0^t \text{tr}(\nabla g \sigma) ds. \quad (C.5)
$$

where we used Itô formula (C.4) in the case $g \in C^2$ and a density argument in the case $g \in C^1$.

(iii). The chain rule holds for Stratonovich integrals. More precisely, if $\sigma \in L^2_{ad}([0,T] \times \Omega; \mathbb{R}^{d \times d})$ and $Y(t) := \int_0^t \sigma(s) \circ dB(s)$ and $\phi : [0,T] \times \mathbb{R}^d \to \mathbb{R}$ is a smooth function, then

$$
\phi(T, Y(T)) = \phi(0, Y(0)) + \int_0^T \partial_t \phi(t, Y(t)) dt + \int_0^T \nabla \phi(t, Y(t)) \sigma(t) \circ dB(t).
$$

**Stochastic differential equations**

Following [Kuo06, Subsection 10.3], we summarize existence and uniqueness result for SDEs of the form

$$
dX(s) = \sigma(s, X(s)) dB(s) + b(s, X(s)) ds, \quad 0 \leq s \leq T, \ X(0) = X^0,
$$

which must be interpreted as the stochastic integral equation

$$
X(t) = X^0 + \int_0^t \sigma(s, X(s)) dB(s) + \int_0^t b(s, X(s)) ds. \quad (C.6)
$$

**Definition C.12.** We say that a jointly measurable stochastic process $X$ on $[0,T]$, is a solution of the SDE (C.6) if

(i). The stochastic process $\sigma(s, X(s))$ lies in $L^2_{ad}([0,T] \times \Omega)$ and $\int_0^t \sigma(s, X(s)) dB(s)$ is an Itô integral for each $t \in [0,T]$.

(ii). Almost all sample paths of the stochastic process $b(s, X(s))$ belong to $L^1(0,T)$.
(iii). For each \( t \in [0, T] \), equation (C.6) holds true almost surely.

A global existence and uniqueness result can be obtained, in a similar way as for ODEs, in the case where both \( \sigma(t, \cdot) \) and \( b(t, \cdot) \) satisfy a global Lipschitz property on \( \mathbb{R}^d \).

**Theorem C.13.** Let \((t,x) \mapsto (\sigma_{ij})_{1 \leq i,j \leq d}, (t,x) \mapsto (b_{i})_{1 \leq i \leq d} \) measurable on \([0, T] \times \mathbb{R}^d \) satisfying a global Lipschitz property on \( \mathbb{R}^d \) uniformly on \([0, T] \). Assume that \( X^0 \) is an \( \mathcal{F}_0 \) measurable random variable with \( \mathbb{E}[\|X^0\|^2] < \infty \). Then the SDE (C.6) has a unique continuous solution \( X \in L_{ad}^2([0, T] \times \Omega) \).

We end this subsection by making the following observations regarding SDEs on a smooth compact submanifold \( M \subseteq \mathbb{R}^d \). In this case, it is convenient to consider Stratonovitch SDEs which read in integral form

\[
X(t) = X^0 + \int_0^t \sigma(s, X(s)) \circ dB(s) + \int_0^t b(s, X(s))dt, \quad t \in [0, T].
\]

(C.7)

for \((\sigma, b) : [0, T] \times M \rightarrow (\mathbb{R}^{d \times d}, \mathbb{R}^d)\)

We first remark how such a Stratonovitch SDE may be transformed to an Ito SDE:

**Remark C.14.** If \( \sigma \in C^1([0, T] \times M) \) and \( X \) solves the Ito SDE

\[
X(t) = X^0 + \int_0^t \sigma(s, X(s))dB(s) + \int_0^t b(s, X(s))dt + \frac{1}{2} \sigma(s, X(s)) : \nabla \sigma(s, X(s))ds,
\]

where \((\sigma : \nabla \sigma)_i = \sum_k \sigma_k \cdot \nabla \sigma_{ki}\), then, \( X \) satisfies (C.7) almost surely.

Indeed, this follows immediately from (C.5) with \( g = \sigma \).

**Theorem C.15.** Assume that \( X^0 : \Omega \rightarrow M \) is \( \mathcal{F}_0 \) measurable, \( \sigma \in C^2([0, T] \times M; \mathbb{R}^{d \times d}) \) and \( b \in C^1([0, T] \times M; \mathbb{R}^d) \) satisfy \( b(s, x) \in T_x M \) and \( \sigma(s, x)v \in T_x M \) for all \((s, x) \in [0, T] \times M\) and for all \( v \in \mathbb{R}^d \). Then, there exists a unique solution \( X \) to (C.7).

**Proof.** For simplicity we restrict to the case \( M = \mathbb{S}^{d-1} \).

Since \( M \subseteq \mathbb{R}^d \) is compact and smooth, there exist extensions \( \tilde{\sigma} \in C^2([0, T] \times \mathbb{R}^d) \) and \( \tilde{b} \in C^1([0, T] \times \mathbb{R}^d) \) such that \((\tilde{\sigma}, \tilde{b})|_M = (\sigma, b)\). By Theorem C.13 (and the remark above), there exists a unique solution to the SDE (C.7) with \( M \) replaced by \( \mathbb{R}^d \) and \( \sigma \) replaced by \( \tilde{\sigma} \).

By the Stratonovitch chain rule, Remark C.11 (iii), and the assumptions on \( \sigma \) and \( b \) we have

\[
d||X||^2 = 0,
\]

which ensures that \( X \) takes values in \( M = \mathbb{S}^d \). Thus, \( X \) is a solution to (C.7).

Conversely, every solution to (C.7) also satisfies the Ito SDE with \( \tilde{\sigma} \) on \( \mathbb{R}^d \) for which we already know uniqueness.

**C.2. Extension to infinite dimensions**

Let \( H \) an infinite dimensional separable Hilbert space, and let \((e_k)_k\) be an orthonormal basis of \( H \). Let \((\Omega, \mathcal{A}, P)\) a probability space and \((\mathcal{F}_t)_t\) a filtration as in the previous subsection. Let us denote by \( L_{ad}^2([0, T] \times \Omega; \mathcal{L}(\mathbb{R}^d, H)) \) the space of operator valued adapted processes \( X : [0, T] \times \Omega \rightarrow \mathcal{L}(\mathbb{R}^d, H) \) such that

\[
\|X\|_{L_{ad}^2([0, T] \times \Omega; \mathcal{L}(\mathbb{R}^d, H))} := \mathbb{E} \int_0^T \|X(t)\|^2_H dt < \infty
\]
where
\[ \|X\|_{HS}^2 = \text{tr}(XX^*) = \sum_k \|X^* e_k\|_{\mathbb{R}^d}^2 = \sum_l \|X a_l\|_H^2 \]
for the standard basis \((a_l)_l\) of \(\mathbb{R}^d\). Note that we can identify \(L(\mathbb{R}^d, H) = H^d\) through \(Ab = \sum_i A_i b_i\) for \(A \in L(\mathbb{R}^d, H), b \in \mathbb{R}^d\), where \(A_i = A a_i\). Then \(A^* e_k = \sum_i (A_i, e_k) a_i\).

We extend the definition of the Itô integral in the following way

**Definition C.16.** Let \(B\) be a \(d\)-dimensional Brownian motion and \(X \in L^2_{ad}(\emptyset, \mathcal{F}; L(\mathbb{R}^d, H))\). Then, for \(0 \leq t \leq T\)
\[
\int_0^t X(s) dB(s) := \sum_{k \in \mathbb{N}} \sum_{l=1}^d \left( \int_0^t (X_i(s), e_k) dB_i(s) \right) e_k. \tag{C.8}
\]

By density, we have that this is well defined and the Itô isometry carries over.

**Proposition C.17.** Let \(B\) and \(X\) be as above. Then \(\int_0^t X(s) dB(s) \in L^2(\Omega; H)\) and for all \(0 \leq t \leq T\)
\[
E \left\| \int_0^t X(s) dB(s) \right\|_H^2 = \int_0^t E \left\| X(s) \right\|_{HS}^2 \, ds. \tag{C.9}
\]

**Proof.** We observe that
\[
\int_0^t X(s) dB(s) = \sum_k \lambda_k e_k,
\]
\[
\lambda_k = \sum_i \int_0^t (X_i(s), e_k) dB_i(s).
\]
Then, by Theorem C.4
\[
E \lambda_k^2 = \sum_{i=1}^d \int_0^t E \left| (X_i(s), e_k) \right|^2 \, ds = \int_0^t E \left| (X(s), e_k) \right|^2 \, ds,
\]
and thus
\[
E \sum_k \lambda_k^2 = \int_0^t E \left\| X(s) \right\|_{HS}^2 \, ds.
\]
Therefore, by Parseval’s identity and dominated convergence theorem, the integral (C.8) is well-defined and (C.9) holds.

Similarly, we can define the Stratonovitch integral as follows.

**Definition C.18.** Let \(B\) be a \(d\)-dimensional Brownian motion and \(X \in L^2_{ad}(\emptyset, \mathcal{F}; L(\mathbb{R}^d, H))\). Moreover, assume that
\[
\sum_{k \in \mathbb{N}} \sum_{i=1}^d E \left[ [(X_i, e_k), B_i]^2(T) \right] < \infty.
\]
Then, we define the Stratonovitch integral for \(0 \leq t \leq T\)
\[
\int_0^t X(s) \circ dB(s) := \sum_{k \in \mathbb{N}} \sum_{l=1}^d \left( \int_0^t (X_i(s), e_k) dB_i(s) + [(X_i, e_k), B_i](t) \right) e_k.
\]
Remark C.19. Clearly Proposition C.17 implies that under the assumptions of this definition, the Stratonovitch integral is well-defined and satisfies

$$
E \left\| \int_0^t X(s) \circ dB(s) \right\|_H^2 \leq 2 \int_0^t E \| X(s) \|_H^2 \, ds + \frac{1}{2} \sum_{k \in \mathbb{N}} E \left[ \left( \sum_{i=1}^d [(X_i, e_k), B_i](t) \right)^2 \right].
$$

We are especially concerned with Stratonovitch integrals when the integrand is of the form $X(s) = g(Y(s))$, where $Y$ is an Itô process.

**Proposition C.20.** Let $0 < t \leq T$, let $B$ be a $d$-dimensional Brownian motion, and let $g \in C^1(\mathbb{R}^d; L(\mathbb{R}^d, H))$ with $\|g\|_{C^1(\mathbb{R}^d; L(\mathbb{R}^d, H))} < \infty$, $\sigma \in L^2_{ad}(\mathbb{R}^d \times \Omega; \mathbb{R}^{d \times d})$ and $b \in L^2_{ad}(\mathbb{R}^d \times \Omega; \mathbb{R}^d)$. Let $Y: \Omega \times [0, T] \to \mathbb{R}^d$ be the Itô process

$$
Y(t) = Y(0) + \int_0^t \sigma(s) \, dB(s) + \int_0^t b(s) \, ds.
$$

Then $g \circ Y$ satisfies the assumptions of Definition C.18 and

$$
Z(t) := \int_0^t g(Y(s)) \circ dB(s) = \int_0^t g(Y(s)) \, dB(s) + \sum_{i=1}^d \sum_{j=1}^d \frac{1}{2} \int_0^t \partial_j g_i(Y(s)) \sigma_{ij} \, ds. \quad (C.10)
$$

Moreover, $Z \in H^{\frac{1}{2}} - ((0, T) \times H)$ and

$$
E \left[ \| Z \|_{H^{\frac{1}{2}} - ((0, T) \times H)}^2 \right] \leq C_T \left( \|g\|_{L^\infty(\mathbb{R}^d; H^d)} + \|\sigma\|_{L^\infty(\mathbb{R}^d; H)} \|\nabla g\|_{L^\infty(\mathbb{R}^d; H)} \right). \quad (C.11)
$$

for a constant $C_T$ that depends only on $T$.

**Proof.** Clearly $g \circ Y \in L^2_{ad}(\mathbb{R}^d \times \Omega; L(\mathbb{R}^d, H))$. Moreover, for all $1 \leq i \leq d$ and all $k \in \mathbb{N}$ Definition C.10 and (C.5) imply

$$
\sum_{i=1}^d [(g_i \circ Y, e_k), B_i](t) = \sum_{i=1}^d \sum_{j=1}^d \int_0^t (\partial_j g_i(Y(s)), e_k) \sigma_{ij} \, ds.
$$

In particular,

$$
\sum_{k \in \mathbb{N}} E \left[ \sum_i [(g \circ Y, e_k), B_i]^2(t) \right] \leq t^2 \sum_{i,j=1}^d E \left[ \| \sigma_{ij} \partial_j g_i \circ Y \|_{L^\infty(\mathbb{R}^d; H)}^2 \right] \leq t^2 \|\nabla g\|_{L^\infty(\mathbb{R}^d; H)}^2 \|\sigma\|_{L^\infty(\mathbb{R}^d; H)}^2. \quad (C.12)
$$

Thus, $Z$ is well-defined and satisfies (C.10).

For $s \in (0, 1)$, recall

$$
\|f\|_{H^s(0,T);H}^2 = \|f\|_{L^2(0,T);H}^2 + \left( \int_0^T \int_0^T \frac{\|f(t_1) - f(t_2)\|_H^2}{|t_1 - t_2|^{1+2s}} \, dt_1 \, dt_2 \right)^{\frac{1}{2}}.
$$

Thus, (C.11) follows from (C.9) and (C.12) (adapted to $(t_1, t_2)$).
Remark C.21. This proposition can be directly extended to the case, when $M \subseteq \mathbb{R}^d$ is a smooth submanifold, $g \in C^1(M;\mathcal{L}(\mathbb{R}^d, H))$ with $\|g\|_{C^1(M;\mathcal{L}(\mathbb{R}^d, H))} < \infty$ and $Y: \Omega \times [0,t] \to M$ is the Itô process as above with the constraint $\sigma(s)v \in TV(s)M$ for all $v \in \mathbb{R}^d$ (which is in fact a necessary condition for $Y$ to stay in $M$).

Indeed, we can find $\tilde{g} \in C^1(\mathbb{R}^d;\mathcal{L}(\mathbb{R}^d, H))$ such that $g = \tilde{g}$ on $M$ and apply the above proposition. Due to the condition $\sigma(s)v \in TV(s)M$, we have $\sum_i \sum_j \partial_i \tilde{g}_j \sigma_{i,j} = \sum_j D_{\sigma_j} g_j$, where $D_{\sigma_j}$ is the derivative in the direction $\sigma_j = (\sigma_{ij})_i \in TYM$. Therefore (C.10) becomes

$$Z(t) := \int_0^t g(Y(s)) \circ dB(s) = \int_0^t g(Y(s))dB(s) + \sum_j \frac{1}{2} \int_0^t D_{\sigma_j} g_j(Y(s))ds,$$

and (C.11) still holds true.

D. Some embeddings in weighted Sobolev spaces

In this appendix we show some embeddings for the weighted fractional Sobolev space introduced in Subsection 3.4.

Lemma D.1. Let $K$ be an open bounded set in $\mathbb{R}^3$. Consider the non-negative function $w(x) = (1 + |x|^a)$ with $a \geq 0$. Then, for $p \geq \frac{6}{\sigma + 2a}$, we have the continuous embedding

$$L^{b,2}_{w,K} \hookrightarrow H^{-s}_w(\mathbb{R}^3).$$

Proof. By recalling the definition of the $H^s(K)$ norm and $H^s_w(K)$ norm and noting that $w$ is bounded below on $K$, we have

$$\|f\|_{H^s(K)} \leq \|f\|_{H^s_w(\mathbb{R}^3)}.$$

By Sobolev embedding we have that $H^s(K) \hookrightarrow L^{p'}(K)$ since $p' \leq \frac{6}{3-2s}$. Hence,

$$H^s_w(\mathbb{R}^3) \hookrightarrow H^s(K) \hookrightarrow L^{p'}(K) \quad \text{(D.1)}$$

Moreover, since $1/w \leq 1$, it is straightforward to prove that

$$H^s_w(\mathbb{R}^3) \hookrightarrow L^2_{1/w}(\mathbb{R}^3 \setminus K). \quad \text{(D.2)}$$

Now we observe that we can identify $L^{b,2}_{w,K} = L^2_w(\mathbb{R}^3 \setminus K) \times L^p(K)$ and thus the dual $(L^{b,2}_{w,K})^* = L^2_w(\mathbb{R}^3 \setminus K) \times L^{p'}(K)$. Combining (D.1) and (D.2) we get that

$$H^s_{1/w}(\mathbb{R}^3) \hookrightarrow L^2_{1/w}(\mathbb{R} \setminus K) \times L^{p'}(K).$$

Since $V \hookrightarrow W$ implies $W^* \hookrightarrow V^*$ and $(L^2_{1/w}(\mathbb{R}^3 \setminus K) \times L^{p'}(K))^* = L^2_{w}(\mathbb{R}^3 \setminus K) \times L^p(K)$ we conclude the desired embedding.

Lemma D.2. For $z > s > \frac{1}{2}$, the embedding $H^{-s}_w(\mathbb{R}^3) \hookrightarrow H^{-z}(\mathbb{R}^3)$ is compact.
Proof. By Schauder’s Theorem, it suffices to show compactness of the embedding $H^2(\mathbb{R}^3) \hookrightarrow H^s_{1/w}(\mathbb{R}^3)$.

To this end, we will prove that the unit ball of radius in $H^2(\mathbb{R}^3)$ is precompact in $H^s_{1/w}(\mathbb{R}^3)$. Fixed $L > 0$, we introduce $B(0, L)$, a ball of radius $L$ in $\mathbb{R}^3$ and a cut-off function $\eta : \mathbb{R}^3 \to \mathbb{R}$ such that $||\eta||_{C^3(\mathbb{R}^3)} \leq C$ and

$$\eta(x) = \begin{cases} 1 & \text{if } x \in B(0, L), \\ 0 & \text{if } x \in B(0, L + 2). \end{cases}$$

Let $\phi \in H^2(\mathbb{R}^3)$. Then,

$$||\phi\eta||_{H^s(\mathbb{R}^3)} \leq C ||\phi||_{H^s(\mathbb{R}^3)} ||\eta||_{C^3(\mathbb{R}^3)}, \quad (D.3)$$

Indeed,

$$||\phi\eta||_{H^s(\mathbb{R}^3)}^2 = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} |(\phi\eta)(x) - (\phi\eta)(y)|^2 \, dx \, dy$$

$$\leq 2 ||\eta||_{C^3(\mathbb{R}^3)}^2 [\phi]_{H^s(\mathbb{R}^3)}^2 + 2 \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|\phi(y)|^2 |\eta(x) - \eta(y)|^2}{|x - y|^{3+2s}} \, dx \, dy,$$

and the second term is further estimated as

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|\phi(y)|^2 |\eta(x) - \eta(y)|^2}{|x - y|^{3+2s}} \, dx \, dy \leq ||\eta||_{C^3(\mathbb{R}^3)}^2 \int_{\mathbb{R}^3} \int_{|x - y| \leq 1} \frac{|\phi(y)|^2}{|x - y|^{1+2s}} \, dx \, dy$$

$$+ ||\eta||_{C^3(\mathbb{R}^3)}^2 \int_{\mathbb{R}^3} \int_{|x - y| > 1} \frac{|\phi(y)|^2}{|x - y|^{3+2s}} \, dx \, dy$$

$$\leq C ||\eta||_{C^3(\mathbb{R}^3)}^2 ||\phi||_{L^2(\mathbb{R}^3)}^2.$$

Moreover,

$$||\phi(1 - \eta)||_{H^s_{1/w}(\mathbb{R}^3)}^2 = \int_{B(0,L)^c} \frac{[\phi(x)(1 - \eta(x))]^2}{w(x)} \, dx$$

$$+ \int_{B(0,L)^c} \int_{B(0,L)^c} \frac{|(\phi(1 - \eta))(x) - (\phi(1 - \eta))(y)|^2}{|x - y|^{3+2s}w(x)w(y)} \, dx \, dy$$

$$\leq \int_{\mathbb{R}^3} [\phi(x)(1 - \eta(x))]^2 \frac{1}{(1 + L)^a} \, dx$$

$$+ \frac{1}{(1 + L)^{2a}} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|(\phi(1 - \eta))(x) - (\phi(1 - \eta))(y)|^2}{|x - y|^{3+2s}} \, dx \, dy$$

$$\leq ||\phi(1 - \eta)||_{H^s(\mathbb{R}^3)}^2 \frac{1}{(1 + L)^a}.$$

Let $\varepsilon > 0$. Since $H^s_{\delta}(B(0, L + 2))$ is compactly embedded into $H^s_{\delta}(B(0, L + 2))$, there exists $N \in \mathbb{N}$ and functions $u_i \in H^s_{\delta}(B(0, L + 2))$, $1 \leq i \leq N$, such that

$$B_{H^s_{\delta}(B(0,L+2))}(0, C) \subseteq \bigcup_{i=1}^{N} B_{H^s_{\delta}(B(0,L+2))}(\varepsilon, u_i),$$

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where $C$ is the constant from (D.3). Thus, (extending the functions $u_i$ by 0 to functions in $H^2(\mathbb{R}^3)$ that vanish in $\mathbb{R}^3 \setminus B(0, L + 2)$, for each $v \in H^2(\mathbb{R}^3)$ with $\|v\|_{H^2(\mathbb{R}^3)} \leq 1$, there exists $1 \leq i \leq N$ such that

$$\|v - u_i\|_{H^1/2(\mathbb{R}^3)} \leq \|\eta v - u_i\|_{H^1(\mathbb{R}^3)} + \|(1 - \eta)v\|_{H^1(\mathbb{R}^3)} \leq \varepsilon + \frac{C}{(1 + L)^{s/2}}.$$  

Choosing $L$ sufficiently large finishes the proof. □

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