QUATERNIONS IN COLLECTIVE DYNAMICS*

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Abstract. We introduce a model of multiagent dynamics for self-organized motion; individuals travel at a constant speed while trying to adopt the averaged body attitude of their neighbors. The body attitudes are represented through unitary quaternions. We prove the correspondence with the model presented in [P. Degond, A. Frouvelle, and S. Merino-Aceituno, *Math. Models Methods Appl. Sci.*, 27 (2017), pp. 1005–1049], where the body attitudes are represented by rotation matrices. Differently from this previous work, the individual-based model introduced here is based on nematic (rather than polar) alignment. From the individual-based model, the kinetic and macroscopic equations are derived. The benefit of this approach, in contrast to that of the previous one, is twofold: first, it allows for a better understanding of the macroscopic equations obtained and, second, these equations are prone to numerical studies, which is key for applications.

Key words. body attitude coordination, quaternions, collective motion, nematic alignment, Q-tensor, Vicsek model, generalized collision invariant, dry active matter, self-organized hydrodynamics

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1. Introduction. In this paper we consider collective dynamics where individuals are described by their location in space and position of their body (body attitude). The body attitude is determined by a frame, i.e., three orthonormal vectors such that one vector indicates the direction of motion of the agent and the other two represent the relative position of the body around this direction. For this reason, the body frame of a given individual can be characterized by the rotation of a fixed reference frame. This rotation (and hence the body attitude) will be represented here by elements of the group of unitary quaternions, denoted by $\mathbb{H}_1$ (see Figure 1). There exist multiple ways of describing rotations in $\mathbb{R}^3$, as we will see in section 5.2. Here, we choose the quaternionic representation, as it is the one mostly employed in numerical simulations due to their efficiency in terms of memory usage and complexity of operations [39]. This is key to applying the results of the present work.

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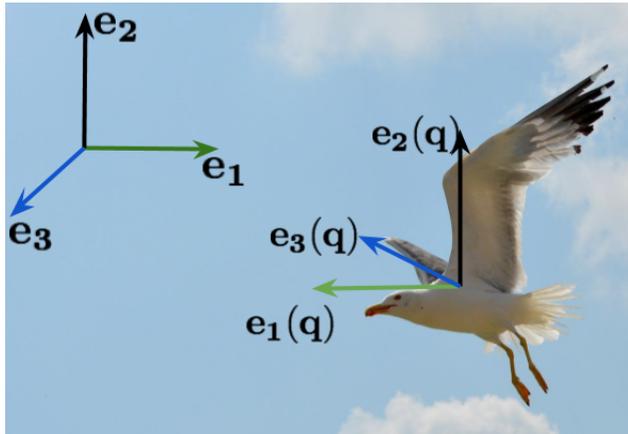
FIG. 1. *The reference frame given by the orthonormal basis* $\{\mathbf{e_1}, \mathbf{e_2}, \mathbf{e_3}\}$ *is rotated according to the unitary quaternion* $\mathbf{q}$ *and gives a new frame* $\{\mathbf{e_1}(\mathbf{q}), \mathbf{e_2}(\mathbf{q}), \mathbf{e_3}(\mathbf{q})\}$ *describing the body attitude of the bird (where* $\mathbf{e_i}(\mathbf{q})$ *denotes the rotation of the vector* $\mathbf{e_i}$ *by* $\mathbf{q} \in \mathbb{H}_1$*). The direction of motion is given by the vector* $\mathbf{e_1}(\mathbf{q})$*, while the pair* $(\mathbf{e_2}(\mathbf{q}), \mathbf{e_3}(\mathbf{q}))$ *gives the relative position of the body around this direction.*

Agents move at a constant speed while attempting to coordinate their body attitude with those of near neighbors. Here we present an individual-based model (particle model) for body attitude coordination. We derive the corresponding macroscopic equations from the associated mean-field equation, which we refer to as the Self-Organized Hydrodynamics based on Quaternions (SOHQ), by reference to the Self-Organized Hydrodynamics (SOH) derived from the Vicsek dynamics (see [21] and the discussion below). Our model is inspired by the one in [17] where the body attitude is represented by elements of the rotation group $SO(3)$. The macroscopic equations obtained in [17] present various drawbacks. First, some of the terms in the equations do not have a clear interpretation. Second, and most importantly, the macroscopic equations are impractical for numerical simulations due to their complexity, especially since some terms are defined implicitly (see (16)).

In the future, we aim to investigate and compare numerically the microscopic and macroscopic dynamics. The individual-based dynamics require great computational power given the large number of agents in the system. A quaternion formulation has better computational performance than a matrix formulation in terms of storage and computational efficiency. In terms of memory, quaternions only require 4 units of memory, while matrices require 9 units; i.e., for a given amount of memory, we can store more than double the number of agents with quaternions than with matrices. In terms of computational efficiency, at each time step, due to the accumulation of numerical error, we will need to orthogonalize the matrices to make sure that they belong to $SO(3)$, which is computationally expensive [13]. The equivalent operation for quaternions corresponds to just normalizing a 4-dimensional vector. Even though the rotation of a vector by a unitary quaternion is more expensive than by a matrix (17 additions and 24 multiplications versus 6 additions and 9 multiplications [26]), the savings in memory and in computational power required for the other operations largely outweigh this advantage of the matrix representation. Also, more specifically to our models, the individual-based model for matrices requires a polar decomposition to be performed at each time step for each agent (as will be seen in (101)). This is

in general computed using the singular value decomposition of the matrix, which makes this process computationally expensive [36]. A new method for computing the polar decomposition of a matrix is proposed in [33], which claims to be more efficient. This method is based on computing the corresponding Q matrix in quaternion form (see (20) below) and computing the leading eigenvector of this matrix. With the quaternion formulation, we do this directly without adding the extra computational costs required to convert back and forth into the matrix formulation. Analogously, the simulation of the macroscopic equations also benefits from the computational efficiency of the quaternions: each grid point will require less than half the memory to store the information of the system than is required when using matrices; we will avoid orthogonalizing matrices by just normalizing 4-dimensional vectors; and, importantly, all the terms in the quaternion formulation are explicit, while in the matrix formulation they are not and require the inversion of an operator (see (16)). In summary, by considering a quaternionic representation, we render the results in [17], which uses the matrix representation, amenable to a numerical study.

In contrast with the use of rotation matrices in [17], the use of the quaternion representation makes the modeling more difficult on the individual-based level; first, it is not clear how to define a mean body attitude based on quaternions and, second, we need to consider nematic alignment rather than polar alignment. However, the macroscopic equations obtained are easier to interpret than in [17] and provide the right framework to carry out numerical simulations. The *main contributions* of the present paper include (i) deriving the macroscopic equations, (ii) finding the right modeling at the individual-based level, and (iii) proving the equivalence of the models and results obtained here with those in [17] for the rotation-matrix representation.

There exist already a variety of models for collective behavior depending on the type of interaction between agents. In the case of body attitude coordination, apart from [17], other models have been proposed; see [40] and references therein. This has applications in the study of collective motion of biological systems such as sperm dynamics, or of animals such as birds and fish, and it is a stepping stone to modeling more complex agents formed by articulated bodies (corpora) [10, 11]. In the rest of the section we present related results in the literature and the structure of the document.

The literature on collective behavior is extensive. Such systems are ubiquitous in nature: fish schools, flocks of birds, herds [6, 7, 37], bacteria [4, 45], and human walking behavior [32] are some examples. The main benefit to studying collective motion and self-organization is to gain an understanding of their emergent properties: local interactions between a large number of agents give rise to large scale structures (see the review in [44]). Given the large number of agents, a statistical description of the system is more pertinent than an agent-based one. With this in mind, mean-field limits are devised when the number of agents tend to infinity. From them, macroscopic equations can be obtained using hydrodynamic limit techniques (as we explain below).

The body attitude coordination model presented here and the one in [17] are inspired by the Vicsek model. The Vicsek model is a particular type of model for self-propelled particles [1, 12, 30, 43] where agents travel at a constant speed while attempting to align their direction of motion with their neighbors. Other refinements and adaptations of the Vicsek model (at the particle level) or the SOH model (at the continuum level) have been proposed in the literature; we just mention a couple as examples: in [8] an individual-based model is proposed to better describe collective motion of turning birds; in [22] agents are considered to have the shape of discs, and volume exclusion is included in the dynamics.

One key difference in the modeling with respect to [21] is that we consider nematic

alignment rather than polar alignment: given $\mathbf{q} \in \mathbb{H}_1$, $\mathbf{q}$ and $-\mathbf{q}$ represent the same rotation. Collective dynamics based on nematic alignment is not, however, new; see, for example, [20, 22] and references therein. Nematic alignment also appears extensively in the literature of liquid crystals and colloids, like suspensions of polymers; see [20] and the reference book [25].

Our results are inspired by the SOH model (the continuum version of the Vicsek model) presented in [21], where we have substituted velocity alignment by body attitude coordination. The macroscopic equations are obtained from the mean-field limit equation, which takes the form of a Fokker–Planck equation.

To obtain the macroscopic equations, the authors in [21] use the well-known tools of hydrodynamic limits, first developed in the framework of the Boltzmann equation for rarefied gases [9, 14, 41]. Since its first appearance, hydrodynamic limits have been used in other contexts, including traffic flow modeling [3, 31] and supply chain research [2, 23]. However, in [21] a methodological breakthrough is introduced: the Generalized Collision Invariant (GCI), which will be essential to the present study (section 4.3). Typically, to obtain the macroscopic equations we would require as many conserved quantities in the kinetic equation as the dimension of the equilibria (see again [44]). In the mean-field limit of the Vicsek model this requirement is not fulfilled, and the GCI is used to sort out this problem. For other cases where the GCI concept has been used, see [15, 16, 17, 18, 19, 24, 27].

After this introduction, we discuss the main results in section 2. In section 3 we explain the derivation of the individual-based model for body coordination dynamics and show its equivalence to the model in [17] in section 5.2. Then in section 3.2 we give the corresponding (formal) mean-field limit for the evolution of the empirical measure when the number of agents goes to infinity.

The following part concerns the derivation of the macroscopic equations (Theorem 4.1) for the macroscopic density of the particles $\rho = \rho(t, x)$ and the quaternion of the mean body attitude $\bar{\mathbf{q}} = \bar{\mathbf{q}}(t, x)$. To obtain these equations we first study the rescaled mean-field equation ((27) in section 4.1), which is, at leading order, a Fokker–Planck equation. We determine its equilibria (see (31)). In section 4.3 we obtain the GCIs (Proposition 4.12), which are the main tools used to derive the macroscopic equations in section 4.4. Finally, in section 5 we prove the equivalence of our equations and results with the ones obtained in [17].

2. Discussion of the main results.

2.1. Preliminary on quaternions.
Some basic notions on quaternions are necessary to understand the main results of this paper. We introduce them here. The set of quaternions $\mathbb{H}$ is a field which forms a 4-dimensional algebra on $\mathbb{R}$ and whose elements are of the form

$$\mathbf{p} = p_0 + p_1 \vec{\imath} + p_2 \vec{\jmath} + p_3 \vec{k},$$

with $p_0, p_1, p_2, p_3 \in \mathbb{R}$, and where $\vec{\imath}, \vec{\jmath}, \vec{k}$, the fundamental quaternion units, satisfy $\vec{\imath}^2 = \vec{\jmath}^2 = \vec{k}^2 = \vec{\imath}\vec{\jmath}\vec{k} = -1$. From this, one can check that nonzero quaternions form a noncommutative group; particularly, it holds that

$$\vec{\imath}\vec{\jmath} = -\vec{\imath}\vec{\jmath} = \vec{k}, \quad \vec{\jmath}\vec{k} = -\vec{k}\vec{\jmath} = \vec{\imath}, \quad \vec{k}\vec{\imath} = -\vec{\imath}\vec{k} = \vec{\jmath}.$$

The zeroth element $p_0 = \mathrm{Re}(\mathbf{p})$ is called the real part of $\mathbf{p}$, and the first to third elements form the imaginary part $p_1 \vec{\imath} + p_2 \vec{\jmath} + p_3 \vec{k} = \mathrm{Im}(\mathbf{p})$.

The conjugate of $\mathbf{p} \in \mathbb{H}$ is defined as $\mathbf{p}^* = p_0 - p_1 \vec{\imath} - p_2 \vec{\jmath} - p_3 \vec{k}$. The inner product

corresponds to

$$(1) \qquad \mathbf{p} \cdot \mathbf{p}' = p_0 p_0' + p_1 p_1' + p_2 p_2' + p_3 p_3' = \mathrm{Re}(\mathbf{p}'\mathbf{p}^*),$$

which generates the norm $|\mathbf{p}|^2 = \mathrm{Re}(\mathbf{p}\mathbf{p}^*)$. Unitary quaternions are a subgroup of $\mathbb{H}$ defined as

$$\mathbb{H}_1 = \{\mathbf{q} \in \mathbb{H} \text{ such that } |\mathbf{q}| = 1\} \subset \mathbb{H}.$$

Notice that $\mathbb{H}_1$ can be parametrized as the 3-dimensional sphere $\mathbb{S}^3$ (see the proof of Proposition A.3). Unitary quaternions can be represented as follows:

$$(2) \qquad \mathbf{q} = e^{\frac{\theta}{2}(n_1\vec{\imath} + n_2\vec{\jmath} + n_3\vec{k})} = \cos\frac{\theta}{2} + \sin\frac{\theta}{2}\left(n_1\vec{\imath} + n_2\vec{\jmath} + n_3\vec{k}\right),$$

where $\mathbf{n} := (n_1, n_2, n_3)$ is a unitary vector in $\mathbb{R}^3$ and $\theta \in [0, 2\pi]$. With these notations, $\mathbf{q} \in \mathbb{H}_1$ represents a rotation in $\mathbb{R}^3$ around the axis given by $\mathbf{n}$ and of angle θ, counterclockwise. Specifically, for any vector $\mathbf{v} \in \mathbb{R}^3$, the corresponding rotated vector $\bar{\mathbf{v}} \in \mathbb{R}^3$ is obtained as follows (see remark below):

$$(3) \qquad \bar{\mathbf{v}} := \mathrm{Im}(\mathbf{q}\mathbf{v}\mathbf{q}^*).$$

The quaternions $\mathbf{q}$ and $-\mathbf{q}$ represent the same rotation. The product of unitary quaternions corresponds to the composition of rotations. The interested reader can find further information on the theory of quaternions in [34, 38]

Remark 2.1 (identification between purely imaginary quaternions and vectors in $\mathbb{R}^3$). Notice that in (3) we abuse notation: the product $\mathbf{q}\mathbf{v}\mathbf{q}^*$ must be understood in the quaternion sense (therefore we consider $\mathbf{v} = (v_1, v_2, v_3)$ as a quaternion which is purely imaginary, i.e., $\mathbf{v} = v_1\vec{\imath} + v_2\vec{\jmath} + v_3\vec{k}$). Conversely, $\bar{\mathbf{v}}$ is understood as a vector in $\mathbb{R}^3$ rather than a purely imaginary quaternion. This abuse of notation where we identify vectors in $\mathbb{R}^3$ with purely imaginary quaternions (and the converse) will be used throughout the text. The sense should be clear from the context. We will also use in general $\mathbf{q}$ to denote a unitary quaternion and $\mathbf{p}$ to denote an arbitrary quaternion.

2.2. Self-organized hydrodynamics based on quaternions (SOHQ). In section 3 we introduce an individual-based model for collective dynamics where individuals are described by their location in space and the position of their body (body attitude). Individuals move at a constant speed while trying to adopt the same body attitude, up to some noise; see (24)–(25). The body attitude is given by three orthonormal vectors, where one of the vectors indicates the direction of motion and the other two represent the relative position of the body around this direction. In this manner, the body frame of a given individual is characterized by the rotation of a fixed reference frame. This rotation will be represented here by elements of the group of unitary quaternions, denoted by $\mathbb{H}_1$ (see Figure 1). The main result of this paper is Theorem 4.1, which gives the macroscopic equations for these dynamics, i.e., the time-evolution equations for the macroscopic mass of agents $\rho = \rho(t, x)$ and the mean quaternion $\bar{\mathbf{q}} = \bar{\mathbf{q}}(t, x)$, which corresponds, as explained, to the mean body attitude. Here $t \geq 0$ is the time and $x \in \mathbb{R}^3$ denotes a point of the physical space. We will refer to this system as the Self-Organized Hydrodynamics based on Quaternions (SOHQ).

To discuss this result we first introduce the (right) relative differential operator on $\mathbb{H}_1$: for a function $\mathbf{q} = \mathbf{q}(t, x)$ where $\mathbf{q}(t, x) \in \mathbb{H}_1$ and for $\partial \in \{\partial_t, \partial_{x_1}, \partial_{x_2}, \partial_{x_3}\}$, let

$$(4) \qquad \partial_{\mathrm{rel}}\mathbf{q} := (\partial\mathbf{q})\mathbf{q}^* \left(= \mathrm{Im}((\partial\mathbf{q})\mathbf{q}^*) \right),$$

where $\partial\mathbf{q}$ belongs to the orthogonal space of $\mathbf{q}$, and the product has to be understood in the sense of quaternions. Notice that, effectively, $\partial_{\mathrm{rel}}\mathbf{q}$ is a purely imaginary quaternion, since $\mathrm{Re}((\partial\mathbf{q})\mathbf{q}^*) = \mathbf{q} \cdot \partial\mathbf{q} = 0$ by (1), and it can be identified with a vector in $\mathbb{R}^3$ (recall Remark 2.1).

With this notation the SOHQ corresponds to

$$\partial_t \rho + \nabla_x \cdot (c_1 \mathbf{e_1}(\bar{\mathbf{q}})\rho) = 0, \tag{5}$$

$$\rho\left(\partial_t\bar{\mathbf{q}} + c_2(\mathbf{e_1}(\bar{\mathbf{q}}) \cdot \nabla_x)\bar{\mathbf{q}}\right) + c_3\left[\mathbf{e_1}(\bar{\mathbf{q}}) \times \nabla_x\rho\right]\bar{\mathbf{q}}$$

$$+ c_4\rho\left[\nabla_{x,\mathrm{rel}}\bar{\mathbf{q}}\,\mathbf{e_1}(\bar{\mathbf{q}}) + (\nabla_{x,\mathrm{rel}} \cdot \bar{\mathbf{q}})\mathbf{e_1}(\bar{\mathbf{q}})\right]\bar{\mathbf{q}} = 0, \tag{6}$$

where $\mathbf{e_1}$ is a vector in $\mathbb{R}^3$ and $\mathbf{e_1}(\bar{\mathbf{q}})$ denotes the rotation of $\mathbf{e_1}$ by the quaternion $\bar{\mathbf{q}}$, that is,

$$\mathbf{e_1}(\bar{\mathbf{q}}) = \mathrm{Im}(\bar{\mathbf{q}}\mathbf{e_1}\bar{\mathbf{q}}^*), \tag{7}$$

and where we used the (right) relative space differential operators

$$\nabla_{x,\mathrm{rel}}\bar{\mathbf{q}} = (\partial_{x_i,\mathrm{rel}}\bar{\mathbf{q}})_{i=1,2,3} = ((\partial_{x_i}\bar{\mathbf{q}})\bar{\mathbf{q}}^*)_{i=1,2,3} \in (\mathbb{R}^3)^3 \subset \mathbb{H}^3, \tag{8}$$

$$\nabla_{x,\mathrm{rel}} \cdot \bar{\mathbf{q}} = \sum_{i=1,2,3}(\partial_{x_i,\mathrm{rel}}\bar{\mathbf{q}})_i = \sum_{i=1,2,3}((\partial_{x_i}\bar{\mathbf{q}})\bar{\mathbf{q}}^*)_i \in \mathbb{R}, \tag{9}$$

where $((\partial_{x_i}\bar{\mathbf{q}})\bar{\mathbf{q}}^*)_i$ indicates the ith component of $(\partial_{x_i}\bar{\mathbf{q}})\bar{\mathbf{q}}^*$. In (7) and in the last three terms of (6) we use the abuse of notation explained in Remark 2.1. The matrix product in the fourth term of (6) has to be understood as a matrix product, giving rise to a scalar product in $\mathbb{H}$:

$$\nabla_{x,\mathrm{rel}}\bar{\mathbf{q}}\,\mathbf{e_1}(\bar{\mathbf{q}}) = ((\partial_{x_i,\mathrm{rel}}\bar{\mathbf{q}}) \cdot \mathbf{e_1}(\bar{\mathbf{q}}))_{i=1,2,3}. \tag{10}$$

In (5)–(6), c_1, c_2, c_3, and c_4 are explicit constants (given in Theorem 4.1) that depend on the parameters of the model, namely, the rate of coordination and the level of the noise. The constants c_2, c_3, and c_4 depend on the Generalized Collision Invariant (GCI; see the introduction and section 4.3). Interestingly, c_1 had a special meaning as a "(polar) order parameter" in [17, 21] (see Remark 4.14). Here it has the same meaning, but as a "nematic" order parameter.

Equation (5) gives the continuity equation for the mass ρ and ensures mass conservation. The convection velocity is given by $c_1\mathbf{e_1}(\bar{\mathbf{q}})$, where the direction is given by $\mathbf{e_1}(\bar{\mathbf{q}})$, a unitary vector (since $\mathbf{e_1}$ is unitary), and the speed is c_1. Notice that the convection term is quadratic in $\bar{\mathbf{q}}$. This is a new structure with respect to [17, 21]. We consider next (6) for $\bar{\mathbf{q}}$. Observe first that all the terms in the equation belong to the tangent space at $\bar{\mathbf{q}}$ in $\mathbb{H}_1$, i.e., to $\bar{\mathbf{q}}^\perp$. This is true for the first term since $(\partial_t + c_2(\mathbf{e_1}(\bar{\mathbf{q}}) \cdot \nabla_x))$ is a differential operator (giving the transport of $\bar{\mathbf{q}}$), and it also holds for the rest of the terms since they are of the form $\mathbf{u}\bar{\mathbf{q}}$ with $\mathbf{u}$ purely imaginary (see Proposition A.2 in the appendices).

The term corresponding to c_3 gives the influence of $\nabla_x\rho$ (pressure gradient) on the body attitude $\bar{\mathbf{q}}$. It has the effect of rotating the body around the vector directed by $\mathbf{e_1}(\bar{\mathbf{q}}) \times \nabla_x\rho$ at an angular speed given by $\frac{c_3}{\rho}\|\mathbf{e_1}(\bar{\mathbf{q}}) \times \nabla_x\rho\|$, so as to align $\mathbf{e_1}(\bar{\mathbf{q}})$ with $-\nabla_x\rho$. Indeed the solution to the differential equation

$$\frac{d\mathbf{q}}{dt} + \gamma\mathbf{u}\mathbf{q} = 0,$$

when $\mathbf{u}$ is a constant purely imaginary unitary quaternion and γ a constant scalar, is given by $\mathbf{q}(t) = \exp(-\gamma\mathbf{u}t)\mathbf{q}(0)$, and $\exp(-\gamma\mathbf{u}t)$ is the rotation of axis $\mathbf{u}$ and angle

$-\gamma t$ (see (2)). Since c_3 is positive, the influence of this term consists of relaxing the direction of movement $\mathbf{e_1}(\bar{\mathbf{q}})$ toward $-\nabla_x \rho$, i.e., making the agents move from places of high concentration to low concentration. In this manner, the $\nabla_x \rho$ term has the same effect as a pressure gradient in classical hydrodynamics. In the present case the pressure gradient provokes a change in the full body attitude $\bar{\mathbf{q}}$. Finally, notice that in regions where $\rho > 0$ we can divide (6) by ρ, and this gives us the influence of each term depending on the local density. After division by ρ, we observe that the only term depending on the density ρ in (6) is the third term in the form

$$c_3 \left[\mathbf{e_1}(\bar{\mathbf{q}}) \times \frac{\nabla_x \rho}{\rho} \right] \bar{\mathbf{q}}.$$

Therefore, for small densities, this term may take large values and become dominant, while for large densities it becomes small and the other terms in the equation prevail for reasonably large $\nabla_x \rho$. The fact that agents tend to relax their direction of motion toward regions of lower concentration creates dispersion; this term is a consequence of the noise at the microscopic level. However, the relaxation becomes weaker once agents are in regions of high density or areas with small variations of density. The last two terms in (6) are unique to the body attitude coordination model and are the main difference with respect to the SOH equations for the Vicsek model.

Analogously to the discussions in [17, 21] for the body attitude model based on rotation matrices and for the Vicsek model, the SOHQ model bears some similarities to the compressible Euler equations, where (5) is the mass conservation equation and (6) is akin to the momentum conservation equation, where momentum transport is balanced by a pressure force. There are, however, major differences. First, the pressure term belongs to $\bar{\mathbf{q}}^\perp$ in order to ensure that $\bar{\mathbf{q}} \in \mathbb{H}_1$ for all times; in the Euler equations the velocity is an arbitrary vector, not necessarily normalized. Second, the convection speed c_2 is a priori different from the mass conservation speed c_1. This difference signals the lack of Galilean invariance of the system, which is a common feature of all dry active matter models (models for collective motion not taking place in a fluid); see [42]. Finally, the last two terms of (7) do not have a clear analogue to the compressible Euler equations: they seem quite specific to our model.

2.2.1. The equation as a relative variation. The (right) relative differential operator ∂_{rel} can be interpreted as the (right) relative variation of $\mathbf{q}$, i.e.,

$$\partial_{rel}\mathbf{q} = \partial\mathbf{q}\,\mathbf{q}^{-1},$$

where $\mathbf{q}^{-1} = \mathbf{q}^*$ is the inverse of $\mathbf{q}$ since $\mathbf{q}$ is unitary.

This expression would have a clear meaning in a commutative setting. For example, in the case of (unit) complex numbers (that is, if we consider rotations in two dimensions), we consider the analogous definition (for $z = z(t, x)$ a function with values in the group $\mathbb{U}$ of unitary complex numbers)

$$\partial_{rel,\mathbb{C}}z = \partial z\,z^{-1},$$

where z^{-1} is the inverse of z (which is also its complex conjugate). In this case, because $\mathbb{C}$ is commutative, we can write simply

$$\partial_{rel,\mathbb{C}}z = \frac{\partial z}{z}.$$

Equivalently, we can also recognize

$$\partial_{rel,\mathbb{C}}z = \partial\left(\log z\right),$$

and the interpretation in terms of a relative variation is standard.

Let us go back to quaternions. The logarithm is well defined on $\mathbb{H}_1 \setminus \{-1\}$, and for $\mathbf{q} \in \mathbb{H}_1 \setminus \{-1\}$, we have that $\log \mathbf{q} = \log(\exp(\theta \mathbf{n}/2)) = \theta \mathbf{n}/2$ with the notation of (2). But, because of the lack of commutativity of $\mathbb{H}$, it is not clear that the logarithm and the relative operator satisfy any relevant relation globally. Since such an interpretation cannot be, a priori, directly translated to quaternions, we propose the following *local* interpretation. Locally around a fixed point $(t_0, x_0) \in \mathbb{R}^+ \times \mathbb{R}^3$, we can write

$$(11) \qquad \mathbf{q}(t, x) = \mathbf{r}(t, x)\mathbf{q}(t_0, x_0),$$

where $\mathbf{r}(t, x) = \mathbf{q}(t, x)\mathbf{q}(t_0, x_0)^* \in \mathbb{H}_1$ represents the variation of $\mathbf{q}$ around $\mathbf{q}(t_0, x_0)$ with $\mathbf{r}(t_0, x_0) = 1$. Then, with this notation, it holds that

$$\partial_{\mathrm{rel}}\mathbf{q} = \left.(\partial \mathbf{r})\right|_{(t,x)=(t_0,x_0)}.$$

Remark 2.2. When $\partial = \partial_t$ is the time derivative, for a function $\mathbf{q} = \mathbf{q}(t, x)$ with values in $\mathbb{H}_1$, the vector $\partial_{t,\mathrm{rel}}\mathbf{q} = \partial_t \mathbf{q}\, \mathbf{q}^{-1}$ is half of the angular velocity of a solid of orientation represented by $\mathbf{q}$. By analogy, the vector $\partial_{x_i,\mathrm{rel}}\mathbf{q} = \partial_{x_i}\mathbf{q}\,\mathbf{q}^{-1}$ for $i = 1, 2, 3$ is half of the angular variation in space of a solid of orientation represented by $\mathbf{q}$.

Multiplying from the right the evolution equation (6) for $\bar{\mathbf{q}}$ by $\bar{\mathbf{q}}^*$, we obtain the following equivalent equation:

$$(12) \qquad \begin{aligned} &\rho\partial_{t,\mathrm{rel}}\bar{\mathbf{q}} + \rho c_2(\mathbf{e_1}(\bar{\mathbf{q}}) \cdot \nabla_{x,\mathrm{rel}})\bar{\mathbf{q}} + c_3\left[\mathbf{e_1}(\bar{\mathbf{q}}) \times \nabla_x\rho\right] \\ &\qquad + c_4\rho\left[\nabla_{x,\mathrm{rel}}\bar{\mathbf{q}}\,\mathbf{e_1}(\bar{\mathbf{q}}) + (\nabla_{x,\mathrm{rel}} \cdot \bar{\mathbf{q}})\mathbf{e_1}(\bar{\mathbf{q}})\right] = 0. \end{aligned}$$

In this equation we notice that all the differential operators naturally appear under their (right) relative form. Notice also that all other nonlinearities in $\bar{\mathbf{q}}$ are expressed in terms of $\mathbf{e_1}(\bar{\mathbf{q}})$. Therefore, the previous system can be interpreted as the evolution of the relative changes of $\bar{\mathbf{q}}$.

In terms of $\mathbf{r}$, the previous system can be recast into

$$\left.\left[\rho\partial_t\mathbf{r} + \rho c_2(\mathbf{e_1}(\mathbf{q}) \cdot \nabla_x)\mathbf{r} + c_3\mathbf{e_1}(\mathbf{q}) \times \nabla_x\rho + c_4\rho\left[\nabla_x\mathbf{r}\,\mathbf{e_1}(\mathbf{q}) + (\nabla_x \cdot \mathbf{r})\mathbf{e_1}(\mathbf{q})\right]\right]\right|_{(t_0,x_0)} = 0.$$

For an interpretation (again, *local*) in terms of $\mathbf{b} := \log \mathbf{r}$ we refer the reader to section 5.3.

2.3. Equivalence with the previous body attitude model. In [17] a model for body attitude coordination is presented where the body attitude is represented by a rotation matrix (element in $SO(3)$, orthonormal group) rather than by a quaternion. In section 5.2 we will prove the equivalence between the individual-based model presented in [17] and the one here, in the sense that the two stochastic processes are the same in law (Theorem 5.6).

In [17] also the macroscopic equations are obtained for the mean body attitude $\Lambda = \Lambda(t, x) \in SO(3)$ and spatial density of agents $\rho = \rho(t, x) \geq 0$, called self-organized hydrodynamics for body attitude coordination (SOHB):

$$(13)$$

$$\partial_t\rho + \nabla_x \cdot \left(\tilde{c}_1\rho\Lambda\mathbf{e_1}\right) = 0,$$

$$(14)$$

$$\rho\left(\partial_t\Lambda + \tilde{c}_2\left((\Lambda\mathbf{e_1}) \cdot \nabla_x\right)\Lambda\right)\Lambda^t + \left[(\Lambda\mathbf{e_1}) \times \left(\tilde{c}_3\nabla_x\rho + \tilde{c}_4\rho\,\mathbf{r}_x(\Lambda)\right) + \tilde{c}_4\rho\,\delta_x(\Lambda)\Lambda\mathbf{e_1}\right]_\times = 0,$$

with explicit constants $\tilde{c}_i$, $i = 1, \ldots, 4$, where Λ^t indicates the transpose matrix of Λ, and where for a vector $\mathbf{u} = (u_1, u_2, u_3)$ the antisymmetric matrix $[\mathbf{u}]_\times$ is defined by

$$(15) \qquad [\mathbf{u}]_\times := \begin{bmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{bmatrix}.$$

The scalar $\delta_x(\Lambda)$ and the vector $\mathbf{r}_x(\Lambda)$ are first order differential operators intrinsic to the dynamics. We define them next. For a smooth function $\Lambda = \Lambda(x)$ from $\mathbb{R}^3$ to $SO(3)$, we define the matrix $\mathscr{D}_x(\Lambda)$ by the equality

$$(16) \qquad \text{for all } \mathbf{w} \in \mathbb{R}^3, \quad (\mathbf{w} \cdot \nabla_x)\Lambda = [\mathscr{D}_x(\Lambda)\mathbf{w}]_\times \Lambda$$

(the matrix $\mathscr{D}_x(\Lambda)$ is well defined; see [17]). The first order operators $\delta_x(\Lambda)$ and $\mathbf{r}_x(\Lambda)$ are then defined by

$$(17) \qquad \delta_x(\Lambda) = \text{Tr}\left(\mathscr{D}_x(\Lambda)\right), \qquad [\mathbf{r}_x(\Lambda)]_\times = \mathscr{D}_x(\Lambda) - \mathscr{D}_x(\Lambda)^t.$$

Since the individual-based model formulated in terms of quaternions is equivalent (in law) to the one formulated with rotation matrices, we expect their respective macroscopic limits to also be equivalent. This is the case, as expressed in Theorem 5.13; i.e., if at time $t = 0$ $\Lambda(0)$ and $\bar{\mathbf{q}}(0)$ represent the same rotation, then $\Lambda(t)$ and $\bar{\mathbf{q}}(t)$ represent the same rotation for all t where the solutions are well defined.

There are, however, important differences between the SOHB and SOHQ macroscopic equations. On one hand, notice that the operators δ_x and $\mathbf{r}_x$ cannot be expressed under a simple explicit form, which makes the meaning of these operators less clear. In the quaternion case, all the elements in (5)–(6) are explicit. Moreover, quaternions give the right framework for numerical simulations (in terms of memory and operation efficiency), as explained in the introduction. On the other hand, when using rotation matrices, we obtain clear equations for the evolution of each one of the orthonormal vectors that define the body frame (see [17]). However, the expressions for these vectors in the quaternion formulation is complicated and not very revealing, due to the quadratic structure of the rotation (see (7)).

3. Modeling: The individual-based model and its mean-field limit.

3.1. The individual-based model. Consider a reference frame in $\mathbb{R}^3$ given by the orthonormal basis $\{\mathbf{e_1}, \mathbf{e_2}, \mathbf{e_3}\}$. Consider also N agents labeled by $k = 1, \ldots, N$ with position $X_k(t) \in \mathbb{R}^3$ and body attitude given by the unitary quaternion $\mathbf{q}_k(t) \in \mathbb{H}_1$. As explained in the introduction, the body frame of agent k corresponds to $\{\mathbf{e_1}(\mathbf{q}_k), \mathbf{e_2}(\mathbf{q}_k), \mathbf{e_3}(\mathbf{q}_k)\}$, where $\mathbf{e_i}(\mathbf{q}_k)$ denotes the rotation of $\mathbf{e_i}$ by $\mathbf{q}_k$ for $i = 1, 2, 3$. The vector $\mathbf{e_1}(\mathbf{q}_k)$ gives the direction of motion of agent k, and the other two vectors give the position of the body relative to this direction (see Figure 1). Our goal is to model collective dynamics where agents move at a constant speed while adopting the body attitude of their neighbors, up to some noise.

Evolution of the positions, $(X_k)_{k=1,\ldots,N}$. The fact that agent k moves in direction $\mathbf{e_1}(\mathbf{q}_k)$ at constant speed $v_0 > 0$ simply corresponds to the equation

$$\frac{\mathrm{d}X_k}{\mathrm{d}t} = v_0 \mathbf{e_1}(\mathbf{q}_k), \quad \mathbf{e_1}(\mathbf{q}_k) := \text{Im}(\mathbf{q}_k \mathbf{e_1} \mathbf{q}_k^*)$$

(recall (3) and Remark 2.1). Notice that the speed for all agents is constant and equal to $v_0 > 0$.

Evolution for the body attitudes, $(\mathbf{q}_k)_{k=1,\dots,N}$. Agents try to coordinate their body attitudes with those of their neighbors. To model this phenomenon, we need to first define an "average" body attitude around a given agent k and, second, express the relaxation of the body attitude of agent k towards this average.

Remark 3.1 (nematic alignment, sign invariance). The body attitude is uniquely defined by quaternions up to a sign since $\mathbf{q}_k$ and $-\mathbf{q}_k$ represent the same rotation. This implies, first, that the time evolution equation for $\mathbf{q}_k = \mathbf{q}_k(t)$ must be sign invariant and, second, that the average must take this sign invariance into account. This is called "nematic alignment" (as opposed to "polar" alignment), and it appears in other collective models [20, 22] and in liquid crystals [25]. Therefore, we cannot define the average analogously as in [21] since the alignment is polar in this case. For example, if one considers the normalized averaged quaternion defined in the same way as in the Vicsek model,

$$(18) \qquad \frac{\sum_{i=1}^{N} \mathbf{q}_i}{\left|\sum_{i=1}^{N} \mathbf{q}_i\right|} \in \mathbb{H}_1,$$

we obtain a unitary quaternion that can be interpreted as a rotation. However, the meaning of this rotation is unclear, and it is not invariant under changes of sign of any of the vectors $\mathbf{q}_i$. Nor can we use the nematic average used in [20] since it is valid only in $\mathbb{R}^2$.

We define (up to a sign) the average around $\mathbf{q}_k$ by

$$\bar{\mathbf{q}}_k := \text{unitary eigenvector of the maximal eigenvalue of } Q_k$$
$$(19) \qquad = \arg\max\{\mathbf{q} \cdot Q_k\mathbf{q},\ \mathbf{q} \in \mathbb{H}_1\},$$

with

$$(20) \qquad Q_k = \frac{1}{N}\sum_{i=1}^{N} K(|X_i - X_k|)\left(\mathbf{q}_i \otimes \mathbf{q}_i - \frac{1}{4}\text{Id}\right),$$

where the nonnegative-valued function K is a kernel of influence. It is in the definition that $\bar{\mathbf{q}}_k \in \mathbb{H}_1$; one can check that if $\bar{\mathbf{q}}_k$ is an average, so is $-\bar{\mathbf{q}}_k$ (so it is sign invariant); $\bar{\mathbf{q}}_k$ remains invariant under the change of sign of any of the arguments $\mathbf{q}_1, \dots, \mathbf{q}_N$; and $\bar{\mathbf{q}}_k$ maximizes over $\mathbb{H}_1$:

$$\mathbf{q} \mapsto \mathbf{q} \cdot Q_k\mathbf{q} = \frac{1}{N}\sum_{i=1}^{N} K(|X_i - X_k|)\left((\mathbf{q}_i \cdot \mathbf{q})^2 - \frac{1}{4}\right)$$
$$(21) \qquad = \frac{1}{N}\sum_{i=1}^{N} K(|X_i - X_k|)\left(\cos^2(\widehat{\langle \mathbf{q}_i, \mathbf{q}\rangle}) - \frac{1}{4}\right),$$

where $\widehat{\langle \mathbf{q}_i, \mathbf{q}\rangle}$ denotes the angle between $\mathbf{q}_i$ and $\mathbf{q}$ (seen as elements of the hypersphere $\mathbb{S}^3$).

Now to express the relaxation of $\mathbf{q}_k$ toward this average we define first

$$(22) \qquad F_k = \left(\bar{\mathbf{q}}_k \otimes \bar{\mathbf{q}}_k - \frac{1}{4}\text{Id}\right)\mathbf{q}_k$$

and write

$$(23) \qquad \frac{\mathrm{d}\mathbf{q}_k}{\mathrm{d}t} = P_{\mathbf{q}_{\mathbf{k}}^{\perp}} F_k \left(= \frac{1}{2} \nabla_{\mathbf{q}_k} (\mathbf{q}_k \cdot F_k) \right),$$

where $P_{\mathbf{q}_{\mathbf{k}}^{\perp}}$ indicates the projection on the orthogonal space to $\mathbf{q}_k$ (which corresponds to the tangent space of $\mathbf{q}_k$ in $\mathbb{H}_1$); $\nabla_{\mathbf{q}_k}$ indicates the gradient in $\mathbb{H}_1$ (the second equality in (23) is proven in Proposition A.1). Equation (23) relaxes $\mathbf{q}_k$ toward the maximizer of $\mathbf{q} \mapsto \mathbf{q} \cdot \left(\bar{\mathbf{q}}_k \otimes \bar{\mathbf{q}}_k - \frac{1}{4}\mathrm{Id} \right) \mathbf{q}$, which corresponds precisely to $\bar{\mathbf{q}}_k$ or $-\bar{\mathbf{q}}_k$.

Finally, putting everything together, we obtain the evolution equations:

$$(24) \qquad \frac{\mathrm{d}X_k}{\mathrm{d}t} = v_0 \mathbf{e_1}(\mathbf{q}_k), \quad \mathbf{e_1}(\mathbf{q}_k) := \mathrm{Im}(\mathbf{q}_k \mathbf{e_1} \mathbf{q}_k^*),$$

$$(25) \qquad \mathrm{d}\mathbf{q}_k = P_{\mathbf{q}_{\mathbf{k}}^{\perp}} \circ \left(\nu F_k \mathrm{d}t + \sqrt{D/2}\, \mathrm{d}B_t^k \right),$$

where $\nu > 0$ indicates the intensity of the relaxation. The evolution for the body attitudes results from two competing phenomena: body attitude coordination (the F_k-term) and noise due to errors that the agents make when trying to coordinate. The noise term is given by $(B_t^k)_{k=1,\dots,N}$ independent 4-dimensional Brownian motions. The constant $D > 0$ gives the intensity of the noise term (by modifying the variance of the Brownian motion). The projection $P_{\mathbf{q}_k^{\perp}}$ in (25) ensures that $\mathbf{q}_k(t) \in \mathbb{H}_1$ for all times t where the solution is defined. The stochastic differential equation (24)–(25) must be understood in the Stratonovich sense; see [35].

Remark 3.2. Some comments:
(i) Typically the noise term would be scaled by $\sqrt{2D}$, because then the generator of the process is the Laplacian with coefficient D. However, we chose the scaling $\sqrt{D/2}$ to make the model equivalent with the one based on rotation matrices in [17]. This will be discussed in section 5.2.
(ii) The operator Q_k in (20) corresponds to the de Gennes Q-tensor that appears in the theory of liquid crystal [25] and which is also related to the so-called nematic order coefficient. Notice that in the definition of Q_k in (20) the 1/4-factor could be ignored and the definition of the average $\bar{\mathbf{q}}_k$ would remain unchanged. Also in F_k in (22) the 1/4-factor can be ignored since that term disappears in the projection in (23). We keep it here for the parallelisms that it bears with the theory of liquid crystal and because it will appear when we define the equilibrium distribution in (31).
(iii) Notice that to define the average $\bar{\mathbf{q}}_k$ in (21), we assume that the maximal eigenvalue is *simple*. At the formal level, this assumption is reasonable since for general symmetric matrices the event of a multiple maximal eigenvalue is negligible. Of course, for a rigorous analysis, we would need to ensure carefully that this event can actually be neglected, or we would need to add an extra rule to determine uniquely the average.
(iv) Notice that we could have defined the relaxation F_k by considering directly $F_k = Q_k \mathbf{q}_k$ instead of (22), since, in this case, (23) relaxes also to $\bar{\mathbf{q}}_k$. However, for this case the relaxation is weaker. This is a modeling choice. We will prove in section 5.2 that our choice here is the one that corresponds to the model presented in [17], where the body attitude is described with rotation matrices.
(v) One can check that the particle system (24)–(25) is frame invariant in the sense that if $\tilde{X}_k = R_{\mathrm{frame}}(X_k)$ for $k = 1, \dots, N$, with R_{frame} the frame change associated to the quaternion q_{frame}, and $\tilde{q}_k = q_{\mathrm{frame}} q_k$, then the pair $(\tilde{X}_k, \tilde{q}_k)$ satisfies the same system (with the appropriate initial conditions).

3.2. Mean-field limit. We now obtain formally the mean-field limit for (24)–(25) as the number of particles $N \to \infty$. The rigorous mean-field limit has been proven for the Vicsek model in [5]. A key difference between the Vicsek model and the system (24)–(25) is the way we compute the average in (21). Consider the empirical distribution in $(x, \mathbf{q}) \in \mathbb{R}^3 \times \mathbb{H}_1$ over time

$$f^N(t, x, \mathbf{q}) := \frac{1}{N} \sum_{i=1}^{N} \delta_{(X_i(t), \mathbf{q}_i(t))}(x, \mathbf{q}),$$

where $(X_i(t), \mathbf{q}_i(t))_{i=1,\dots,N}$ satisfy (24)–(25).

Assume that f^N converges weakly to $f = f(t, x, \mathbf{q})$ as $N \to \infty$. It is standard to show (formally) that f satisfies

$$(26) \qquad \partial_t f + \nabla_x \cdot (v_0 \mathbf{e_1}(\mathbf{q}) f) + \nabla_{\mathbf{q}} \cdot (F_f f) = \frac{D}{4} \Delta_{\mathbf{q}} f,$$

$$F_f = \nu P_{\mathbf{q}^\perp} \bar{\mathbf{q}}_f^K \left(\bar{\mathbf{q}}_f^K \cdot \mathbf{q} \right) = \nu P_{\mathbf{q}^\perp} \left(\bar{\mathbf{q}}_f^K \otimes \bar{\mathbf{q}}_f^K \right) \mathbf{q},$$

$$\bar{\mathbf{q}}_f^K = \text{unitary eigenvector of the maximal eigenvalue of } Q_f^K$$

$$= \arg\max\{\mathbf{q} \mapsto \mathbf{q} \cdot Q_f^K \mathbf{q}\},$$

$$Q_f^K = \int_{\mathbb{R}^3} \int_{\mathbb{H}_1} K(|x - y|) \left(\mathbf{q} \otimes \mathbf{q} - \frac{1}{4} \text{Id} \right) f(t, y, \mathbf{q}) \, d\mathbf{q} \, dy,$$

where $\nabla_{\mathbf{q}}$ and $\Delta_{\mathbf{q}}$ denote the gradient and the Laplacian in $\mathbb{H}_1$, respectively, and $d\mathbf{q}$ is the Lebesgue measure on $\mathbb{H}_1$.

4. Hydrodynamic limit. The goal of this section is the derivation of the macroscopic equations for (26). After a dimensional analysis and a time and space scaling, described next in section 4.1, we recast (26) into

$$(27) \qquad \partial_t f^\varepsilon + \nabla_x \cdot (\mathbf{e_1}(\mathbf{q}) f^\varepsilon) = \frac{1}{\varepsilon} \Gamma(f^\varepsilon) + \mathcal{O}(\varepsilon),$$

$$(28) \qquad \Gamma(f) := -\nu \nabla_{\mathbf{q}} \cdot \left(P_{\mathbf{q}^\perp} \left((\bar{\mathbf{q}}_f \otimes \bar{\mathbf{q}}_f) \mathbf{q} \right) f \right) + \frac{D}{4} \Delta_{\mathbf{q}} f,$$

with $\bar{\mathbf{q}}_f$ defined by

$$\bar{\mathbf{q}}_f = \text{unitary eigenvector of the maximal eigenvalue of } Q_f$$

$$(29) \qquad = \arg\max\{\mathbf{q} \mapsto \mathbf{q} \cdot Q_f \mathbf{q}, \, \mathbf{q} \in \mathbb{H}_1\},$$

where

$$(30) \qquad Q_f = \int_{\mathbb{H}_1} f(t, x, \mathbf{q}) \left(\mathbf{q} \otimes \mathbf{q} - \frac{1}{4} \text{Id} \right) d\mathbf{q},$$

$d\mathbf{q}$ being the Lebesgue measure on $\mathbb{H}_1$. (Note that after the dimensional analysis and the rescaling the values of the parameters D and ν as well as the variables t and x have changed; see section 4.1 for details.)

We then analyze in section 4.2 the collisional operator Γ in (28); particularly, we determine its (von Mises–like) equilibria, given by (for $\bar{\mathbf{q}} \in \mathbb{H}_1$)

$$(31) \qquad M_{\bar{\mathbf{q}}}(\mathbf{q}) = \frac{1}{Z} \exp\left(\frac{2}{d} \left((\bar{\mathbf{q}} \cdot \mathbf{q})^2 - \frac{1}{4} \right) \right),$$

where d is a parameter given by

$$(32) \qquad d = \frac{D}{\nu},$$

and where Z is a normalizing constant (such that $\int_{\mathbb{H}_1} M_{\bar{\mathbf{q}}} \mathrm{d}\mathbf{q} = 1$). We then describe the structure of the *Generalized Collision Invariants* (GCIs) for Γ in section 4.3.

With this information we are ready to prove our main result.

THEOREM 4.1 ((formal) macroscopic limit). *When $\varepsilon \to 0$ in the kinetic equation* (27) *it holds (formally) that*

$$f^{\varepsilon} \to f = f(t, x, \mathbf{q}) = \rho M_{\bar{\mathbf{q}}}(\mathbf{q}), \quad \bar{\mathbf{q}} = \bar{\mathbf{q}}(t, x) \in \mathbb{H}_1, \, \rho = \rho(t, x) \geq 0.$$

Moreover, if the convergence is strong enough and the functions $\bar{\mathbf{q}}$ and ρ are regular enough, then they satisfy the system (5)–(6) *that we recall here:*

$$(33) \qquad \partial_t \rho + \nabla_x \cdot (c_1 \mathbf{e_1}(\bar{\mathbf{q}})\rho) = 0,$$

$$\rho \left(\partial_t \bar{\mathbf{q}} + c_2 (\mathbf{e_1}(\bar{\mathbf{q}}) \cdot \nabla_x)\bar{\mathbf{q}} \right) + c_3 \left[\mathbf{e_1}(\bar{\mathbf{q}}) \times \nabla_x \rho \right] \bar{\mathbf{q}}$$
$$(34) \qquad \qquad + c_4 \rho \left[\nabla_{x,\mathrm{rel}} \bar{\mathbf{q}} \, \mathbf{e_1}(\bar{\mathbf{q}}) + (\nabla_{x,\mathrm{rel}} \cdot \bar{\mathbf{q}})\mathbf{e_1}(\bar{\mathbf{q}}) \right] \bar{\mathbf{q}} = 0,$$

where the (right) relative differential operator $\nabla_{x,\mathrm{rel}}$ is defined in section 2.2, *where*

$$(35) \qquad \mathbf{e_1}(\bar{\mathbf{q}}) = \mathrm{Im}(\bar{\mathbf{q}}\mathbf{e_1}\bar{\mathbf{q}}^*),$$

and where c_i, $i = 1, \ldots, 4$, are explicit constants. To define them we use the following notation: For two real functions g, w consider

$$(36) \qquad \langle g \rangle_w := \int_0^\pi g(\theta) \frac{w(\theta)}{\int_0^\pi w(\theta')\mathrm{d}\theta'} \, \mathrm{d}\theta.$$

Then the constants are given by

$$(37) \qquad c_1 = \frac{2}{3} \langle 1/2 + \cos\theta \rangle_{m \, \sin^2(\theta/2)},$$

$$(38) \qquad c_2 = \frac{1}{5} \langle 1 + 4\cos\theta \rangle_{m \, \sin^4(\theta/2)h(\cos(\theta/2))\cos(\theta/2)},$$

$$(39) \qquad c_3 = \frac{d}{2},$$

$$(40) \qquad c_4 = \frac{1}{5} \langle 1 - \cos\theta \rangle_{m \, \sin^4(\theta/2)h(\cos(\theta/2))\cos(\theta/2)},$$

where d is given in (32), *where*

$$(41) \qquad m(\theta) := \exp\left(d^{-1} \left(\frac{1}{2} + \cos\theta \right) \right),$$

and where h is the solution of the differential equation (64).

We recall that in section 2 we provided a discussion of this main result. The proof is given in section 4.4. We conclude this study with section 5.3, where we compare the macroscopic limit obtained here with the corresponding one for the body attitude model with rotation matrices from [17].

4.1. Scaling and expansion. We assume that the kernel of influence K is Lipschitz, bounded, and such that

$$(42) \qquad K = K(|x|) \geq 0, \quad \int_{\mathbb{R}^3} K(|x|) \, dx = 1, \quad \int_{\mathbb{R}^3} |x|^2 K(|x|) \, dx < \infty.$$

We express the kinetic equation (26) in dimensionless variables. Let ν_0 be the typical interaction frequency, i.e., $\nu = \nu_0 \nu'$ with $\nu' = \mathcal{O}(1)$. We consider also the typical time and space scales t_0, x_0 with $t_0 = \nu_0^{-1}$ and $x_0 = v_0 t_0$. With this we define the nondimensional variables $t' = t/t_0$, $x' = x/t_0$. Consider also the dimensionless diffusion coefficient $D' = D/\nu_0$ and the rescaled influence kernel $K'(|x'|) = K(x_0|x'|)$. Skipping the primes, we get the same equation as (26) except that $v_0 = 1$, all the quantities are dimensionless, and D, ν, and K are assumed to be of order 1. Notice, in particular, that

$$d^{-1} = \frac{\nu}{D} = \frac{\nu'}{D'}$$

is the same before and after the dimensional analysis.

To perform the macroscopic limit we rescale space and time by $x' = \varepsilon x$ and $t' = \varepsilon t$. After skipping the primes we obtain

$$(43) \qquad \varepsilon\left[\partial_t f^\varepsilon + \nabla_x \cdot (\mathbf{e_1}(\mathbf{q}) f^\varepsilon)\right] + \nabla_\mathbf{q} \cdot (F_{f^\varepsilon}^\varepsilon f^\varepsilon) = \frac{D}{4} \Delta_\mathbf{q} f^\varepsilon,$$

$$F_f^\varepsilon = \nu P_{\mathbf{q}^\perp} \bar{\mathbf{q}}_f^\varepsilon \left(\bar{\mathbf{q}}_f^\varepsilon \cdot \mathbf{q}\right) = \nu P_{\mathbf{q}^\perp} \left(\bar{\mathbf{q}}_f^\varepsilon \otimes \bar{\mathbf{q}}_f^\varepsilon\right) \mathbf{q},$$

$$\bar{\mathbf{q}}_f^\varepsilon = \text{unitary eigenvector of the maximal eigenvalue of } Q_f^\varepsilon$$

$$(44) \qquad = \arg\max\{\mathbf{q} \mapsto \mathbf{q} \cdot Q_f^\varepsilon \mathbf{q}, \, \mathbf{q} \in \mathbb{H}_1\},$$

$$Q_f^\varepsilon = \frac{1}{\varepsilon^3} \int_{\mathbb{R}^3} \int_{\mathbb{H}_1} K\left(\frac{|x-y|}{\varepsilon}\right) \left(\mathbf{q} \otimes \mathbf{q} - \frac{1}{4}\text{Id}\right) f(t, y, \mathbf{q}) \, \mathrm{d}\mathbf{q}\mathrm{d}y.$$

LEMMA 4.2. *For any sufficiently smooth function f, we have the expansion*

$$Q_f^\varepsilon = \int f(t, x, \mathbf{q}) \left(\mathbf{q} \otimes \mathbf{q} - \frac{1}{4}\text{Id}\right) \, \mathrm{d}\mathbf{q} + \mathcal{O}(\varepsilon^2).$$

Proof. The result is obtained by a Taylor expansion in ε and by using that (recall (42))

$$\frac{1}{\varepsilon^3} \int K\left(\frac{|x|}{\varepsilon}\right) dx = 1, \qquad \frac{1}{\varepsilon^3} \int |x|^2 K(|x|) \, dx = \mathcal{O}(\varepsilon^2). \qquad \square$$

PROPOSITION 4.3. *For any sufficiently smooth function f, it holds that*

$$(45) \qquad \bar{\mathbf{q}}_f^\varepsilon = \left(\bar{\mathbf{q}}_f^\varepsilon \cdot \bar{\mathbf{q}}_f\right) \bar{\mathbf{q}}_f + \mathcal{O}(\varepsilon^2) \quad \text{as } \varepsilon \to 0.$$

In particular, we have

$$\bar{\mathbf{q}}_f^\varepsilon \otimes \bar{\mathbf{q}}_f^\varepsilon = \bar{\mathbf{q}}_f \otimes \bar{\mathbf{q}}_f + \mathcal{O}(\varepsilon^2) \quad \text{as } \varepsilon \to 0.$$

Proof. Let $\lambda_{max}^\varepsilon$, respectively, λ_{max}, be the maximal eigenvalue of Q_f^ε, respectively, Q_f (we assume them to be uniquely defined). From Lemma 4.2, we have

$$Q_f^\varepsilon = Q_f + \mathcal{O}(\varepsilon^2),$$

and, multiplying by $\bar{\mathbf{q}}_f^\varepsilon$ on both sides,

$$\lambda_{max}^\varepsilon = \bar{\mathbf{q}}_f^\varepsilon \cdot Q_f \bar{\mathbf{q}}_f^\varepsilon + \mathcal{O}(\varepsilon^2).$$

By maximality of λ_{max}, we have that $\bar{\mathbf{q}}_f^\varepsilon \cdot Q_f \bar{\mathbf{q}}_f^\varepsilon \leq \lambda_{max}$ so that

$$\lambda_{max}^\varepsilon \leq \lambda_{max} + \mathcal{O}(\varepsilon^2).$$

By symmetry, we also have $\lambda_{max} \leq \lambda_{max}^\varepsilon + \mathcal{O}(\varepsilon^2)$, and therefore

$$\lambda_{max}^\varepsilon - \lambda_{max} = \mathcal{O}(\varepsilon^2).$$

On the other hand, we have that

$$\begin{aligned}
(Q_f - \lambda_{max}\mathrm{Id})P_{\bar{\mathbf{q}}_f^\perp}\bar{\mathbf{q}}_f^\varepsilon &= (Q_f - \lambda_{max}\mathrm{Id})(\bar{\mathbf{q}}_f^\varepsilon - (\bar{\mathbf{q}}_f^\varepsilon \cdot \bar{\mathbf{q}}_f)\bar{\mathbf{q}}_f) \\
&= (Q_f - \lambda_{max}\mathrm{Id})\bar{\mathbf{q}}_f^\varepsilon - 0 \\
&= (Q_f^\varepsilon - \lambda_{max}^\varepsilon \mathrm{Id} + \mathcal{O}(\varepsilon^2))\bar{\mathbf{q}}_f^\varepsilon \\
&= \mathcal{O}(\varepsilon^2).
\end{aligned}$$

By our crucial assumption that λ_{max} is a single eigenvalue with eigenvector $\bar{\mathbf{q}}_f$, we can invert the matrix $(Q_f - \lambda_{max}\mathrm{Id})$ on the 3-dimensional space $\bar{\mathbf{q}}_f^\perp$. By a small abuse of notation we write its inverse $(Q_f - \lambda_{max}\mathrm{Id})^{-1}$ on $\bar{\mathbf{q}}_f^\perp$. Finally we have

$$(46) \qquad P_{\bar{\mathbf{q}}_f^\perp}\bar{\mathbf{q}}_f^\varepsilon = (Q_f - \lambda_{max}\mathrm{Id})^{-1}\mathcal{O}(\varepsilon^2) = \mathcal{O}(\varepsilon^2),$$

which proves (45). Taking the scalar product with $\bar{\mathbf{q}}_f^\varepsilon$ and using the fact that $\bar{\mathbf{q}}_f^\varepsilon$ is unitary, we have that

$$1 - (\bar{\mathbf{q}}_f \cdot \bar{\mathbf{q}}_f^\varepsilon)^2 = \mathcal{O}(\varepsilon^2),$$

so using (45) we can finally show that

$$\bar{\mathbf{q}}_f^\varepsilon \otimes \bar{\mathbf{q}}_f^\varepsilon = \bar{\mathbf{q}}_f \otimes \bar{\mathbf{q}}_f + \mathcal{O}(\varepsilon^2). \qquad \square$$

Using Proposition 4.3 we recast the rescaled kinetic equation (43) as (27).

4.2. Equilibrium solutions and Fokker–Planck formulation. Define $d = D/\nu$ and consider the generalization of the von Mises distribution in $\mathbb{H}_1$:

$$(47) \qquad M_{\bar{\mathbf{q}}}(\mathbf{q}) = \frac{1}{Z} \exp\left(\frac{2}{d}\left((\bar{\mathbf{q}} \cdot \mathbf{q})^2 - \frac{1}{4}\right)\right), \quad \int_{\mathbb{H}_1} M_{\bar{\mathbf{q}}}(\mathbf{q})\, d\mathbf{q} = 1, \quad \bar{\mathbf{q}} \in \mathbb{H}_1,$$

where Z is a normalizing constant. Observe that $Z < \infty$ is independent of $\bar{\mathbf{q}}$ since the volume element in $\mathbb{H}_1$ is left-invariant, i.e.,

$$\begin{aligned}
Z &= \int_{\mathbb{H}_1} \exp\left(\frac{2}{d}\left((\bar{\mathbf{q}} \cdot \mathbf{q})^2 - \frac{1}{4}\right)\right) d\mathbf{q} = \int_{\mathbb{H}_1} \exp\left(\frac{2}{d}\left((1 \cdot \mathbf{q}\bar{\mathbf{q}}^*)^2 - \frac{1}{4}\right)\right) d\mathbf{q} \\
&= \int_{\mathbb{H}_1} \exp\left(\frac{2}{d}\left((1 \cdot \mathbf{q})^2 - \frac{1}{4}\right)\right) d\mathbf{q}.
\end{aligned}$$

Note that we can recast

$$(48) \qquad M_{\bar{\mathbf{q}}}(\mathbf{q}) = \frac{m(\theta)}{4\pi \int_0^\pi m(\theta') \sin^2(\theta'/2)d\theta'}, \quad \text{with } \bar{\mathbf{q}} \cdot \mathbf{q} = \cos(\theta/2),$$

with $m(\theta)$ given by (41). Indeed,

$$M_{\bar{\mathbf{q}}}(\mathbf{q}) = \frac{1}{Z} \exp\left(\frac{2}{d}\left(\cos^2(\theta/2) - \frac{1}{4}\right)\right) = \frac{1}{Z} \exp\left(\frac{1}{d}\left(\cos(\theta) + \frac{1}{2}\right)\right) = \frac{1}{Z} m(\theta),$$

and by Proposition A.3,
(49)
$$Z = 4\pi \int_0^\pi \exp\left(\frac{2}{d}\left(\cos^2(\theta'/2) - \frac{1}{4}\right)\right) \sin^2(\theta'/2) \mathrm{d}\theta' = 4\pi \int_0^\pi m(\theta') \sin^2(\theta'/2) \mathrm{d}\theta'.$$

PROPOSITION 4.4 (properties of Γ). *The following hold:*
(i) *The operator Γ in (28) can be written as*

(50)
$$\Gamma(f) = \frac{D}{4} \nabla_{\mathbf{q}} \cdot \left(M_{\bar{\mathbf{q}}_f} \nabla_{\mathbf{q}}\left(\frac{f}{M_{\bar{\mathbf{q}}_f}}\right)\right),$$

and we have

(51)
$$\mathrm{H}(f) := \int_{\mathbb{H}_1} \Gamma(f) \frac{f}{M_{\bar{\mathbf{q}}_f}} \mathrm{d}\mathbf{q} = -\frac{D}{4} \int_{\mathbb{H}_1} M_{\bar{\mathbf{q}}_f} \left|\nabla_{\mathbf{q}}\left(\frac{f}{M_{\bar{\mathbf{q}}_f}}\right)\right|^2 \mathrm{d}\mathbf{q}.$$

(ii) *The equilibria, i.e., the functions $f = f(\mathbf{q}) \geq 0$ such that $\Gamma(f) = 0$, form a 4-dimensional manifold $\mathcal{E}$ given by*

$$\mathcal{E} = \{\rho M_{\bar{\mathbf{q}}}(\mathbf{q}) \,|\, \rho \geq 0,\, \bar{\mathbf{q}} \in \mathbb{H}_1\},$$

where ρ is the macroscopic mass, i.e.,

$$\rho = \int_{\mathbb{H}_1} \rho M_{\bar{\mathbf{q}}}(\mathbf{q}) \,\mathrm{d}\mathbf{q},$$

and $\bar{\mathbf{q}}$ is the eigenvector corresponding to the maximum eigenvalue of

$$\int_{\mathbb{H}_1} \mathbf{q} \otimes \mathbf{q} \, \rho M_{\bar{\mathbf{q}}}(\mathbf{q}) \,\mathrm{d}\mathbf{q}.$$

Furthermore, $\mathrm{H}(f) = 0$ if and only if $f = \rho M_{\bar{\mathbf{q}}}$ for some $\rho \geq 0$ and $\bar{\mathbf{q}} \in \mathbb{H}_1$.

Remark 4.5 (comparison with the equilibria considered in [17]). Thanks to (95), one can check that the equilibria $M_{\bar{\mathbf{q}}}$ represent the same equilibria as for the kinetic model corresponding to the body attitude model with rotation matrices in [17], which is given by

$$M_\Lambda(A) = \frac{1}{Z'} \exp\left(d^{-1}(A \cdot \Lambda)\right) \qquad \text{for } \Lambda, A \in SO(3)$$

(where Z' is a normalizing constant); i.e., as long as $\Lambda = \Phi(\bar{\mathbf{q}})$ and $A = \Phi(\mathbf{q})$ (Φ is defined in (90)), we have $Z' M_\Lambda(A) = Z M_{\bar{\mathbf{q}}}(\mathbf{q})$. Note that the normalizing constants Z and Z' are not equal since the measures chosen on $SO(3)$ and $\mathbb{H}_1$ are identical only up to a multiplicative constant.

Proof of Proposition 4.4.

Proof of point (i). Equation (50) is a consequence of the fact that

$$(\bar{\mathbf{q}} \cdot \mathbf{q})^2 = \mathbf{q} \cdot (\bar{\mathbf{q}} \otimes \bar{\mathbf{q}}) \, \mathbf{q}$$

and that (see Proposition A.1)

$$\frac{1}{2}\nabla_{\mathbf{q}}\left(\mathbf{q}\cdot(\bar{\mathbf{q}}\otimes\bar{\mathbf{q}})\mathbf{q}-\frac{1}{4}\right)=P_{\mathbf{q}^\perp}((\bar{\mathbf{q}}\otimes\bar{\mathbf{q}})\mathbf{q}).$$

A computation similar to [17, Lemma 4.3] allows us to conclude (50). Inequality (51) follows from (50) and the Stokes theorem in $\mathbb{H}_1$.

Proof of point (ii). From inequality (51), we have that if $\Gamma(f)=0$, then $\frac{f}{M_{\bar{\mathbf{q}}_f}}$ is constant in $\mathbf{q}$. We denote this constant by ρ (which is positive since f and $M_{\bar{\mathbf{q}}_f}$ are positive).

We are left with proving that $\bar{\mathbf{q}}$ is the eigenvector corresponding to the maximum eigenvalue of

$$\int_{\mathbb{H}_1}\mathbf{q}\otimes\mathbf{q}\,M_{\bar{\mathbf{q}}}(\mathbf{q})\,\mathrm{d}\mathbf{q}$$

(this will not change if multiplied by ρ since it is positive).

For any quaternion $\mathbf{p}_0\in\mathbb{H}$, the left multiplication by $\mathbf{p}_0$, that is, $\mathbf{p}\in\mathbb{H}\mapsto\mathbf{p}_0\mathbf{p}\in\mathbb{H}$, is an endomorphism on $\mathbb{H}$. We write $E^l(\mathbf{p}_0)$ the associated matrix, so that for all $\mathbf{p}\in\mathbb{H}$ the (quaternion) product $\mathbf{p}_0\mathbf{p}$ is equal to the (matrix) product $E^l(\mathbf{p}_0)\mathbf{p}$. Using the change of variable $\mathbf{q}'=\bar{\mathbf{q}}^*\mathbf{q}$, we compute

$$\int_{\mathbb{H}_1}\mathbf{q}\otimes\mathbf{q}M_{\bar{\mathbf{q}}}(\mathbf{q})\,\mathrm{d}\mathbf{q}=\int_{\mathbb{H}_1}(\bar{\mathbf{q}}\mathbf{q})\otimes(\bar{\mathbf{q}}\mathbf{q})M_1(\mathbf{q})\,\mathrm{d}\mathbf{q}$$

$$=\int_{\mathbb{H}_1}E^l(\bar{\mathbf{q}})(\mathbf{q}\otimes\mathbf{q})E^l(\bar{\mathbf{q}})^tM_1(\mathbf{q})\,\mathrm{d}\mathbf{q}$$

$$=E^l(\bar{\mathbf{q}})\left(\int_{\mathbb{H}_1}(\mathbf{q}\otimes\mathbf{q})M_1(\mathbf{q})\,\mathrm{d}\mathbf{q}\right)E^l(\bar{\mathbf{q}})^t.$$

To compute the value of the integral in the term above, first note that $M_1(\mathbf{q})$ depends only on $\mathrm{Re}\,\mathbf{q}$. We use a change of variable that switch q_i and q_j (for $i\neq j$) to check that the off-diagonal terms (i,j) and (j,i) are zero. Then we compute the diagonal terms: the zeroth diagonal term is clearly given by $\int_{\mathbb{H}_1}(\mathrm{Re}(\mathbf{q}))^2M_1(\mathbf{q})\,\mathrm{d}\mathbf{q}$, while with the same changes of variable that switch q_i and q_j (for $i\neq j$) we check that the first to third diagonal terms are identical and equal to $\frac{1}{3}\int_{\mathbb{H}_1}\mathrm{Im}^2(\mathbf{q})M_1(\mathbf{q})\,\mathrm{d}\mathbf{q}$. Using the fact that $\mathrm{Re}^2(\mathbf{q})+\mathrm{Im}^2(\mathbf{q})=1$, we obtain

$$\int_{\mathbb{H}_1}\mathbf{q}\otimes\mathbf{q}M_{\bar{\mathbf{q}}}(\mathbf{q})\,\mathrm{d}\mathbf{q}=E^l(\bar{\mathbf{q}})\left(\int_{\mathbb{H}_1}\mathrm{diag}\left[(\mathrm{Re}(\mathbf{q}))^2,\frac{1-(\mathrm{Re}(\mathbf{q}))^2}{3},\dots\right]M_1(\mathbf{q})\,\mathrm{d}\mathbf{q}\right)E^l(\bar{\mathbf{q}})^t$$

$$(52)\qquad=E^l(\bar{\mathbf{q}})\left(\mathrm{diag}\left[I^2,\frac{1-I^2}{3},\dots\right]\right)E^l(\bar{\mathbf{q}})^t,$$

where we defined

$$(53)\qquad\qquad I^2:=\int_{\mathbb{H}_1}(\mathrm{Re}(\mathbf{q}))^2M_1(\mathbf{q})\,\mathrm{d}\mathbf{q}>0.$$

Note that for any $\mathbf{p}\in\mathbb{H}$, we have $\mathbf{p}^tE^l(\bar{\mathbf{q}})^tE^l(\bar{\mathbf{q}})\mathbf{p}=\left(E^l(\bar{\mathbf{q}})\mathbf{p}\right)^tE^l(\bar{\mathbf{q}})\mathbf{p}=|\bar{\mathbf{q}}\mathbf{p}|^2=|\mathbf{p}|^2$. Therefore, $E^l(\bar{\mathbf{q}})^tE^l(\bar{\mathbf{q}})=\mathrm{Id}$, which implies, since $E^l(\bar{\mathbf{q}})$ is invertible (with inverse $E^l(\bar{\mathbf{q}}^*)$), that $E^l(\bar{\mathbf{q}})^t=E^l(\bar{\mathbf{q}})^{-1}=E^l(\bar{\mathbf{q}}^*)$.

Therefore, equality (52) is a diagonalization of the matrix $\int_{\mathbb{H}_1} \mathbf{q} \otimes \mathbf{q} M_{\bar{\mathbf{q}}}(\mathbf{q}) \, d\mathbf{q}$ in an orthonormal basis. It is direct to check that $\bar{\mathbf{q}}$ is an eigenvector corresponding to the first eigenvalue I^2. It is the maximum eigenvalue if and only if

$$I^2 > \frac{1 - I^2}{3},$$

that is, if and only if

$$(54) \qquad I^2 > \frac{1}{4}.$$

We compute (using Proposition A.3)

$$(55) \quad I^2 = \frac{\int_{\mathbb{H}_1} (\mathrm{Re}(\mathbf{q}))^2 \exp\left((\mathrm{Re}(\mathbf{q}))^2/d\right) d\mathbf{q}}{\int_{\mathbb{H}_1} \exp\left((\mathrm{Re}(\mathbf{q}))^2/d\right) d\mathbf{q}} = \frac{\int_0^\pi \cos^2\theta \exp(\cos^2\theta/d) \sin^2\theta d\theta}{\int_0^\pi \exp(\cos^2\theta/d) \sin^2\theta \, d\theta}$$

$$(56) \qquad = \frac{\int_{[-1,1]} r^2 \exp(r^2/d)(1-r^2)^{1/2} dr}{\int_{[-1,1]} \exp(r^2/d)(1-r^2)^{1/2} \, dr} =: \frac{I_1}{I_0},$$

and, writing $w(r) = (1-r^2)^{1/2} \exp\left(r^2/d\right)$, we have that

$$(57) \qquad \frac{\mathrm{d}}{\mathrm{d}d} I^2 = \frac{I_0 \frac{\mathrm{d}}{\mathrm{d}d} I_1 - I_1 \frac{\mathrm{d}}{\mathrm{d}d} I_0}{I_0^2}$$

$$(58) \qquad = \frac{-1}{d^2} \frac{1}{I_0^2} \left(\int_{-1}^1 w(r) \mathrm{d}r \int_{-1}^1 r^4 w(r) \mathrm{d}r - \left(\int_{-1}^1 r^2 w(r) \mathrm{d}r \right)^2 \right) < 0$$

by Jensen's inequality.

Therefore, we conclude that

$$(59) \qquad I^2 > \lim_{d \longrightarrow \infty} I^2.$$

By the dominated convergence theorem, and using an integration by parts, we have

$$(60) \qquad \lim_{d \longrightarrow \infty} I^2 = \frac{\int_0^\pi \cos^2\theta \sin^2\theta d\theta}{\int_0^\pi \sin^2\theta d\theta} = \frac{1}{4},$$

so that (54) holds true, which completes the proof. □

4.3. Generalized collision invariants.

4.3.1. Definition and characterization. Consider the rescaled kinetic equation (27)–(28). Formally, the limit f of f^ε as $\varepsilon \to 0$ belongs to the kernel of Γ, which, by Proposition 4.4, means that $f(t,x,\mathbf{q}) = \rho(t,x) M_{\bar{\mathbf{q}}(t,x)}(\mathbf{q})$ for some functions $\rho(t,x) \geq 0$ and $\bar{\mathbf{q}}(t,x) \in \mathbb{H}_1$. To obtain the macroscopic equations for ρ and $\bar{\mathbf{q}}$ we start by looking for conserved quantities of the kinetic equation; i.e., we want to identify functions $\psi = \psi(\mathbf{q})$ such that

$$\int_{\mathbb{H}_1} \Gamma(f)\psi \, d\mathbf{q} = 0 \quad \text{for all } f.$$

By Proposition 4.4, this can be rewritten as

$$0 = -\int_{\mathbb{H}_1} M_{\bar{\mathbf{q}}_f} \nabla_{\mathbf{q}} \left(\frac{f}{M_{\bar{\mathbf{q}}_f}} \right) \cdot \nabla_{\mathbf{q}} \psi \, d\mathbf{q},$$

which particularly holds for $\nabla_{\mathbf{q}}\psi = 0$, i.e., when ψ is a constant. Consequently, we only know one conserved quantity for our model corresponding to the macroscopic mass ρ. To obtain the macroscopic equation for $\bar{\mathbf{q}}$, a priori we would need three more conserved quantities. To sort out this problem, we use the method of the Generalized Collision Invariants (GCIs) introduced in [21].

Definition of the GCI. Define the operator

$$C(f, \bar{\mathbf{q}}) = \nabla_{\mathbf{q}} \cdot \left(M_{\bar{\mathbf{q}}} \nabla_{\mathbf{q}} \left(\frac{f}{M_{\bar{\mathbf{q}}}} \right) \right),$$

for a function f and $\bar{\mathbf{q}} \in \mathbb{H}_1$. Notice that

$$\Gamma(f) = C(f, \bar{\mathbf{q}}_f).$$

DEFINITION 4.6 (generalized collision invariant). *A function $\psi \in H^1(\mathbb{H}_1)$ is a generalized collision invariant (GCI) associated with $\bar{\mathbf{q}} \in \mathbb{H}_1$ if and only if*

$$\int_{\mathbb{H}_1} C(f, \bar{\mathbf{q}}) \psi \, \mathrm{d}\mathbf{q} = 0 \ \text{for all } f \text{ such that } P_{\bar{\mathbf{q}}^{\perp}} \left[\int (\mathbf{q} \otimes \mathbf{q}) f(\mathbf{q}) \, \mathrm{d}\mathbf{q} \, \bar{\mathbf{q}} \right] = 0.$$

We write $GCI(\bar{\mathbf{q}})$ to denote the set of GCIs associated with $\bar{\mathbf{q}}$.

If ψ exists for any given $\bar{\mathbf{q}} \in \mathbb{H}_1$, consider particularly $\psi_{\bar{\mathbf{q}}_{f^{\varepsilon}}}$, the GCI associated with $\bar{\mathbf{q}}_{f^{\varepsilon}}$ given by (44). It holds that

$$(61) \qquad \frac{1}{\varepsilon} \int_{\mathbb{H}_1} \Gamma(f^{\varepsilon}) \psi_{\bar{\mathbf{q}}_{f^{\varepsilon}}} \, \mathrm{d}\mathbf{q} = \frac{1}{\varepsilon} \frac{D}{4} \int_{\mathbb{H}_1} C(f^{\varepsilon}, \bar{\mathbf{q}}_{f^{\varepsilon}}) \psi_{\bar{\mathbf{q}}_{f^{\varepsilon}}} \, \mathrm{d}\mathbf{q} = 0,$$

since

$$P_{\bar{\mathbf{q}}_{f^{\varepsilon}}^{\perp}} \left[\int (\mathbf{q} \otimes \mathbf{q}) f^{\varepsilon} \, \mathrm{d}\mathbf{q} \, \bar{\mathbf{q}}_{f^{\varepsilon}} \right] = P_{\bar{\mathbf{q}}_{f^{\varepsilon}}^{\perp}} (\lambda_{max}^{\varepsilon} \bar{\mathbf{q}}_{f^{\varepsilon}}) = 0.$$

Therefore, after multiplying the kinetic equation (27) by $\psi_{\bar{\mathbf{q}}_{f^{\varepsilon}}}$ and integrating on $\mathbb{H}_1$, the right-hand side is of order ε.

Characterization of the GCI. The main result of this section is the following description of the set of GCIs.

PROPOSITION 4.7 (description of the set of GCIs). *Let $\bar{\mathbf{q}} \in \mathbb{H}_1$. Then*

$$(62) \qquad GCI(\bar{\mathbf{q}}) = span\left\{ 1, \cup_{\beta \in \bar{\mathbf{q}}^{\perp}} \psi^{\beta} \right\},$$

where, for $\beta \in \bar{\mathbf{q}}^{\perp}$, the function ψ^{β} is defined by

$$(63) \qquad \psi^{\beta}(\mathbf{q}) := (\beta \cdot \mathbf{q}) \, h(\mathbf{q} \cdot \bar{\mathbf{q}}),$$

with $h = h(r)$ the unique solution of the following differential equation on $(-1, 1)$:

$$(64) \qquad (1 - r^2)^{3/2} \exp\left(\frac{2r^2}{d} \right) \left(\frac{-4}{d} r^2 - 3 \right) h(r) + \frac{\mathrm{d}}{\mathrm{d}r} \left[(1 - r^2)^{5/2} \exp\left(\frac{2r^2}{d} \right) h'(r) \right]$$
$$= r (1 - r^2)^{3/2} \exp\left(\frac{2r^2}{d} \right).$$

Furthermore, the function h is odd, $h(-r) = -h(r)$, and it satisfies for all $r \geq 0$ $h(r) \leq 0$.

This proposition will be crucial to compute the hydrodynamical limit in section 4.4. The proof is done in the two subsections below.

4.3.2. Existence and uniqueness of GCI. We prove here the first characterization of the GCI.

PROPOSITION 4.8 (first characterization of the GCI). *Let $\bar{\mathbf{q}} \in \mathbb{H}_1$. We have that $\psi \in GCI(\bar{\mathbf{q}})$ if and only if*

(65) $\qquad$ *there exists $\beta \in \bar{\mathbf{q}}^\perp$ such that $\nabla_{\mathbf{q}} \cdot (M_{\bar{\mathbf{q}}} \nabla_{\mathbf{q}} \psi) = (\beta \cdot \mathbf{q})(\bar{\mathbf{q}} \cdot \mathbf{q}) M_{\bar{\mathbf{q}}}.$*

Proof of Proposition 4.8. We denote by $\mathcal{L}$ the linear operator $C(\cdot, \bar{\mathbf{q}})$ on $L^2(\mathbb{H}_1)$, and $\mathcal{L}^*$ its adjoint. We have the following sequence of equivalences, starting from Definition 4.6:

$$\psi \in GCI(\bar{\mathbf{q}}) \Leftrightarrow \int_{\mathbb{H}_1} \psi \mathcal{L}(f) \, d\mathbf{q} = 0 \quad \text{for all } f \text{ such that } P_{\bar{\mathbf{q}}^\perp}\left(\left[\int_{\mathbb{H}_1} \mathbf{q} \otimes \mathbf{q} f(\mathbf{q}) \, d\mathbf{q}\right] \bar{\mathbf{q}}\right) = 0$$

$$\Leftrightarrow \int_{SO(3)} \mathcal{L}^*(\psi) f \, d\mathbf{q} = 0 \quad \text{for all } f \text{ s.t. for all } \beta \in \bar{\mathbf{q}}^\perp, \ \beta \cdot \left[\int_{\mathbb{H}_1} \mathbf{q} \otimes \mathbf{q} f(\mathbf{q}) \, d\mathbf{q}\right] \bar{\mathbf{q}} = 0$$

$$\Leftrightarrow \int_{SO(3)} \mathcal{L}^*(\psi) f \, d\mathbf{q} = 0 \quad \text{for all } f \in \mathscr{F}_{\bar{\mathbf{q}}}^\perp$$

$$\Leftrightarrow \mathcal{L}^*(\psi) \in \left(\mathscr{F}_{\bar{\mathbf{q}}}^\perp\right)^\perp,$$

where

$$\mathscr{F}_{\bar{\mathbf{q}}} := \left\{f : \mathbb{H}_1 \to \mathbb{R}, \text{ with } f(\mathbf{q}) = (\beta \cdot \mathbf{q})(\bar{\mathbf{q}} \cdot \mathbf{q}) \text{ for some } \beta \in \bar{\mathbf{q}}^\perp\right\},$$

and $\mathscr{F}_{\bar{\mathbf{q}}}^\perp$ is the space orthogonal to $\mathscr{F}_{\bar{\mathbf{q}}}$ in $L^2(\mathbb{H}_1)$. Note that $\mathscr{F}_{\bar{\mathbf{q}}}$ is a vector subspace of L^2 isomorphic to $\bar{\mathbf{q}}^\perp$: indeed, if for some $\beta \in \bar{\mathbf{q}}^\perp$ we have that $f(\mathbf{q}) = (\beta \cdot \mathbf{q})(\bar{\mathbf{q}} \cdot \mathbf{q}) = 0$ for all $\mathbf{q} \in \mathbb{H}$, then $\beta \cdot \mathbf{q} = 0$ for all $\mathbf{q} \in \mathbb{H} \setminus \bar{\mathbf{q}}^\perp$, so that by continuity and density it is also true for all $\mathbf{q} \in \mathbb{H}$, which finally implies $\beta = 0$. Therefore, $\mathscr{F}_{\bar{\mathbf{q}}}$ is closed (finite-dimensional of dimension 3), and we have $(\mathscr{F}_{\bar{\mathbf{q}}}^\perp)^\perp = \mathscr{F}_{\bar{\mathbf{q}}}$. Therefore we get

$$\psi \in GCI(\bar{\mathbf{q}}) \Leftrightarrow \mathcal{L}^*(\psi) \in \mathscr{F}_{\bar{\mathbf{q}}} \Leftrightarrow \text{ there exists } \beta \in \bar{\mathbf{q}}^\perp \text{ such that } \mathcal{L}^*(\psi)(\mathbf{q}) = (\beta \cdot \mathbf{q})(\bar{\mathbf{q}} \cdot \mathbf{q}),$$

which ends the proof since the expression of the adjoint is $\mathcal{L}^*(\psi) = \frac{1}{M_{\bar{\mathbf{q}}}} \nabla_{\mathbf{q}} \cdot (M_{\bar{\mathbf{q}}} \nabla_{\mathbf{q}} \psi)$. $\quad \square$

We now verify that (65) in Proposition 4.8 has a unique solution in the space

$$H^1(\mathbb{H}_1) := \left\{\psi : \mathbb{H}_1 \to \mathbb{R} \,\middle|\, \int_{\mathbb{H}_1} |\psi|^2 \, d\mathbf{q} + \int_{\mathbb{H}_1} |\nabla_{\mathbf{q}} \psi|^2 \, d\mathbf{q} < \infty\right\}.$$

PROPOSITION 4.9 (existence and uniqueness of the GCI). *Let $\bar{\mathbf{q}} \in \mathbb{H}_1$, and let $\beta \in \bar{\mathbf{q}}^\perp$. Then (65) has a unique solution ψ (up to an additive constant) in $H^1(\mathbb{H}_1)$.*

Proof. To prove this proposition, we rewrite (65) in its weak formulation as

(66) $$\int_{\mathbb{H}_1} M_{\bar{\mathbf{q}}} \nabla_{\mathbf{q}} \psi \cdot \nabla_{\mathbf{q}} \varphi \, d\mathbf{q} = -\beta \cdot \int_{\mathbb{H}_1} \mathbf{q}(\mathbf{q} \cdot \bar{\mathbf{q}}) \varphi M_{\bar{\mathbf{q}}} \, d\mathbf{q}$$

for all test functions φ in $H^1(\mathbb{H}_1)$. Denote by $H_0^1(\mathbb{H}_1)$ the set of zero-mean functions in $H^1(\mathbb{H}_1)$, i.e.,

$$H_0^1(\mathbb{H}_1) = \left\{\psi \in H^1(\mathbb{H}_1) \,\middle|\, \int_{\mathbb{H}_1} \psi \, d\mathbf{q} = 0\right\}.$$

Note that, thanks to the Poincaré inequality on the sphere $\mathbb{H}_1$, the usual seminorm on $H^1(\mathbb{H}_1)$ given by $\psi \mapsto \int_{\mathbb{H}_1} |\nabla_{\mathbf{q}}\psi|^2 \, \mathrm{d}\mathbf{q}$ is a norm on $H^1_0(\mathbb{H}_1)$. The weak formulation (66) is equivalent on $H^1(\mathbb{H}_1)$ and on $H^1_0(\mathbb{H}_1)$; indeed, if ψ is a solution of (66) on $H^1_0(\mathbb{H}_1)$, then by a change of variable $\mathbf{q}' := \bar{\mathbf{q}}^*\mathbf{q}$ (and using $\beta \in \bar{\mathbf{q}}^\perp$),

$$\beta \cdot \int_{\mathbb{H}_1} \mathbf{q}(\mathbf{q} \cdot \bar{\mathbf{q}}) M_{\bar{\mathbf{q}}} \, \mathrm{d}\mathbf{q} = \beta \cdot \bar{\mathbf{q}} \int_{\mathbb{H}_1} \mathbf{q}(\mathrm{Re}\mathbf{q}) M_1(\mathrm{Re}\mathbf{q}) \, \mathrm{d}\mathbf{q} = 0,$$

so that (66) is also satisfied on the set of constant functions φ, and, by linearity, ψ solves (66) on $H^1(\mathbb{H}_1)$.

We want to apply the Lax–Milgram theorem to (66) in the Hilbert space $H^1_0(\mathbb{H}_1)$. The left-hand side of (66) is a bilinear operator in $(\psi, \varphi) \in (H^1_0(\mathbb{H}_1))^2$, which is continuous (thanks to a Cauchy–Schwarz inequality, using furthermore the fact that $M_{\bar{\mathbf{q}}}$ is upper bounded pointwise on $\mathbb{H}_1$) and coercive (by definition of the norm on $H^1_0(\mathbb{H}_1)$, and thanks to the fact that $M_{\bar{\mathbf{q}}}$ is lower bounded pointwise on $\mathbb{H}_1$). The right-hand side of (66) is a linear form in $\varphi \in H^1_0(\mathbb{H}_1)$, which is continuous (thanks to a Cauchy–Schwarz inequality, using again the pointwise upper bound for $M_{\bar{\mathbf{q}}}$).

We can therefore apply the Lax–Milgram theorem, which guarantees the existence of a unique solution $\psi_0 \in H^1_0(\mathbb{H}_1)$ of (65). We conclude by noticing that any function ψ in $H^1(\mathbb{H}_1)$ is a solution of (65) if and only if its zero-mean projection $\psi_0 := \psi - \frac{1}{2\pi^2} \int_{\mathbb{H}_1} \psi \, \mathrm{d}\mathbf{q}$ is also a solution of (65).   □

From all this we conclude the following.

COROLLARY 4.10. *Let $\bar{\mathbf{q}} \in \mathbb{H}_1$. Then*

$$\tag{67} GCI(\bar{\mathbf{q}}) = span\left\{1, \cup_{\beta \in \bar{\mathbf{q}}^\perp} \tilde{\psi}^\beta\right\},$$

where, for $\beta \in \bar{\mathbf{q}}^\perp$, the function $\tilde{\psi}^\beta$ is the unique solution in $H^1_0(\mathbb{H}_1)$ of (65).

Remark 4.11. The linear mapping $\beta \in \bar{\mathbf{q}}^\perp \mapsto \tilde{\psi}^\beta \in H^1_0(\mathbb{H}_1)$ is injective (by Proposition 4.9). Therefore, $GCI(\bar{\mathbf{q}})$ is a 4-dimensional vector space.

4.3.3. The nonconstant GCIs.

PROPOSITION 4.12. *Let $\bar{\mathbf{q}} \in \mathbb{H}_1$. Let ψ be a function of the form*

$$\psi(\mathbf{q}) = (\beta \cdot \mathbf{q}) h(\mathbf{q} \cdot \bar{\mathbf{q}})$$

for some $\beta \in \bar{\mathbf{q}}^\perp$ and some smooth (C^2) scalar function h. Then ψ is a solution of (65) in $H^1_0(\mathbb{H}_1)$ if and only if h is a solution of (64). Furthermore, the solution h of (64) exists and is unique, is an odd function, and satisfies $h(r) \leq 0$ for all $r \geq 0$.

Proof. Equation (65) is equivalent to

$$\tag{68} \nabla_{\mathbf{q}}(\log M_{\bar{\mathbf{q}}}) \cdot \nabla_{\mathbf{q}}\psi + \Delta_{\mathbf{q}}\psi = (\beta \cdot \mathbf{q})(\mathbf{q} \cdot \bar{\mathbf{q}}),$$

where we compute

$$\nabla_{\mathbf{q}}(\log M_{\bar{\mathbf{q}}}) = \frac{2}{d}\nabla_{\mathbf{q}}(\mathbf{q} \cdot \bar{\mathbf{q}})^2.$$

Next, we substitute $\psi = (\beta \cdot \mathbf{q}) h(\mathbf{q} \cdot \bar{\mathbf{q}})$ into (68). To carry out the computations we

will use the following expressions:

$$
\begin{aligned}
\nabla_{\mathbf{q}}\psi &= (\nabla_{\mathbf{q}}(\beta\cdot\mathbf{q}))\,h(\mathbf{q}\cdot\bar{\mathbf{q}}) + (\beta\cdot\mathbf{q})h'(\mathbf{q}\cdot\bar{\mathbf{q}})\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}}),\\
\Delta_{\mathbf{q}}[h(\mathbf{q}\cdot\bar{\mathbf{q}})] &= \nabla_{\mathbf{q}}\cdot(\nabla_{\mathbf{q}}[h(\mathbf{q}\cdot\bar{\mathbf{q}})]) = \nabla_{\mathbf{q}}\cdot(h'(\mathbf{q}\cdot\bar{\mathbf{q}})\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}}))\\
&= h''(\mathbf{q}\cdot\bar{\mathbf{q}})|\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}})|^2 + h'(\mathbf{q}\cdot\bar{\mathbf{q}})\Delta_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}}),\\
\Delta_{\mathbf{q}}\psi &= \Delta_{\mathbf{q}}(\beta\cdot\mathbf{q})h(\mathbf{q}\cdot\bar{\mathbf{q}}) + 2\nabla_{\mathbf{q}}(\beta\cdot\mathbf{q})\cdot\nabla_{\mathbf{q}}[h(\mathbf{q}\cdot\bar{\mathbf{q}})] + (\beta\cdot\mathbf{q})\Delta_{\mathbf{q}}[h(\mathbf{q}\cdot\bar{\mathbf{q}})]\\
&= \Delta_{\mathbf{q}}(\beta\cdot\mathbf{q})h(\mathbf{q}\cdot\bar{\mathbf{q}}) + 2\nabla_{\mathbf{q}}(\beta\cdot\mathbf{q})\cdot\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}})h'(\mathbf{q}\cdot\bar{\mathbf{q}})\\
&\quad + (\beta\cdot\mathbf{q})\left[h''(\mathbf{q}\cdot\bar{\mathbf{q}})|\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}})|^2 + h'(\mathbf{q}\cdot\bar{\mathbf{q}})\Delta_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}})\right].
\end{aligned}
$$

Substituting the previous expressions in (68), and grouping terms, we obtain that ψ satisfies (65) if and only if

$$
\begin{aligned}
&\left\{\frac{2}{d}\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}})^2\cdot\nabla_{\mathbf{q}}(\beta\cdot\mathbf{q}) + \Delta_{\mathbf{q}}(\beta\cdot\mathbf{q})\right\}h(\mathbf{q}\cdot\bar{\mathbf{q}})\\
&+\left\{\frac{2}{d}\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}})^2\cdot\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}})(\beta\cdot\mathbf{q}) + 2\nabla_{\mathbf{q}}(\beta\cdot\mathbf{q})\cdot\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}}) + \Delta_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}})(\beta\cdot\mathbf{q})\right\}h'(\mathbf{q}\cdot\bar{\mathbf{q}})\\
&+\left\{|\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}})|^2(\beta\cdot\mathbf{q})\right\}h''(\mathbf{q}\cdot\bar{\mathbf{q}})\\
&= (\beta\cdot\mathbf{q})(\mathbf{q}\cdot\bar{\mathbf{q}}).
\end{aligned}
$$
(69)

To compute this expression we will use the following identities:

$$
\begin{aligned}
\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}})\cdot\nabla_{\mathbf{q}}(\beta\cdot\mathbf{q}) &= P_{\mathbf{q}^\perp}(\bar{\mathbf{q}})\cdot P_{\mathbf{q}^\perp}(\beta) = -(\mathbf{q}\cdot\beta)(\mathbf{q}\cdot\bar{\mathbf{q}}),\\
\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}})^2 &= 2(\mathbf{q}\cdot\bar{\mathbf{q}})P_{\mathbf{q}^\perp}\bar{\mathbf{q}},\\
\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}})^2\cdot\nabla_{\mathbf{q}}(\beta\cdot\mathbf{q}) &= -2(\mathbf{q}\cdot\bar{\mathbf{q}})^2(\beta\cdot\mathbf{q}),\\
\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}})^2\cdot\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}}) &= 2(\mathbf{q}\cdot\bar{\mathbf{q}})\left[1-(\mathbf{q}\cdot\bar{\mathbf{q}})^2\right],\\
\Delta_{\mathbf{q}}(\beta\cdot\mathbf{q}) &= -3(\beta\cdot\mathbf{q}),\\
|\nabla_{\mathbf{q}}(\mathbf{q}\cdot\bar{\mathbf{q}})|^2 &= |P_{\mathbf{q}^\perp}(\bar{\mathbf{q}})|^2 = 1-(\mathbf{q}\cdot\bar{\mathbf{q}})^2,
\end{aligned}
$$

where we used that $\beta\cdot\bar{\mathbf{q}}=0$ and that in the sphere $\mathbb{S}^3$ it holds that $\Delta_{\mathbf{q}}(\mathbf{p}\cdot\mathbf{q}) = -3(\mathbf{p}\cdot\mathbf{q})$. Substituting the previous expressions into (69), we obtain that ψ solves (65) if and only if

$$
\begin{aligned}
&\left\{-\frac{4}{d}(\beta\cdot\mathbf{q})(\mathbf{q}\cdot\bar{\mathbf{q}})^2 - 3(\beta\cdot\mathbf{q})\right\}h(\mathbf{q}\cdot\bar{\mathbf{q}})\\
&+\left\{\frac{4}{d}(\beta\cdot\mathbf{q})(\mathbf{q}\cdot\bar{\mathbf{q}})\left[1-(\mathbf{q}\cdot\bar{\mathbf{q}})^2\right] - 3(\beta\cdot\mathbf{q})(\mathbf{q}\cdot\bar{\mathbf{q}}) - 2(\beta\cdot\mathbf{q})(\mathbf{q}\cdot\bar{\mathbf{q}})\right\}h'(\mathbf{q}\cdot\bar{\mathbf{q}})\\
&+\left\{(\beta\cdot\mathbf{q})(1-(\mathbf{q}\cdot\bar{\mathbf{q}})^2)\right\}h''(\mathbf{q}\cdot\bar{\mathbf{q}})\\
&= (\beta\cdot\mathbf{q})(\mathbf{q}\cdot\bar{\mathbf{q}}).
\end{aligned}
$$

When $\mathbf{q}$ ranges in $\mathbb{H}_1$, $r := (\mathbf{q}\cdot\bar{\mathbf{q}})$ ranges in $[-1,1]$. Therefore the previous equality can be rewritten (after factorizing out and simplifying the terms $(\beta\cdot\mathbf{q})$, using a continuity argument) as an equation in $r\in[-1,1]$:

$$
(70) \qquad \left(\frac{-4}{d}r^2 - 3\right)h + \left(\frac{4}{d}(1-r^2) - 5\right)r\,h' + (1-r^2)h'' = r.
$$

Finally, we recast this equation as shown in (64).

We define the Hilbert space

$$H_{(-1,1)} := \left\{ h : (-1,1) \longrightarrow \mathbb{R}, \text{ such that } \int_{-1}^{1} (1-r^2)^{3/2} h^2(r) \, \mathrm{d}r < \infty \text{ and} \right.$$

$$\left. \int_{-1}^{1} (1-r^2)^{5/2} \left(h'(r) \right)^2 \, \mathrm{d}r < \infty \right\}.$$

By a Lax–Milgram argument, we obtain the existence and uniqueness of the solution h in $H_{(-1,1)}$. By uniqueness of h, we see that h is an odd function of its argument. By a maximum principle, we furthermore obtain that $h(r) \leq 0$ for $r \geq 0$.

To conclude, it only remains to show that the solution h corresponds to a function $\psi \in H_0^1(\mathbb{H}_1)$. Since we know by Proposition 4.9 that the GCI exists and is unique in $H_0^1(\mathbb{H}_1)$, this proves that ψ given by (63) is the GCI. For that, we first compute the $L^2(\mathbb{H}_1)$ norm of gradient of ψ with

$$\int_{\mathbb{H}_1} |\nabla_{\mathbf{q}} \psi|^2 \mathrm{d}\mathbf{q} \leq 2 \int_{\mathbb{H}_1} |P_{\mathbf{q}^\perp} \beta|^2 h^2(\mathbf{q} \cdot \bar{\mathbf{q}}) \mathrm{d}\mathbf{q} + 2 \int_{\mathbb{H}_1} (\beta \cdot \mathbf{q})^2 |P_{\mathbf{q}^\perp} \bar{\mathbf{q}}|^2 (h'(\mathbf{q} \cdot \bar{\mathbf{q}}))^2 \mathrm{d}\mathbf{q}$$

$$= 2 \left[\int_{\mathbb{H}_1} |P_{(\mathbf{q}\bar{\mathbf{q}})^\perp} \beta|^2 h^2(\mathrm{Re}\mathbf{q}) \mathrm{d}\mathbf{q} + \int_{\mathbb{H}_1} (\beta \cdot (\mathbf{q}\bar{\mathbf{q}}))^2 |P_{(\mathbf{q}\bar{\mathbf{q}})^\perp} \bar{\mathbf{q}}|^2 (h'(\mathrm{Re}\mathbf{q}))^2 \mathrm{d}\mathbf{q} \right]$$

$$= 2 \left[\int_{\mathbb{H}_1} |P_{\mathbf{q}^\perp} (\beta \bar{\mathbf{q}}^*)|^2 h^2(\mathrm{Re}\mathbf{q}) \mathrm{d}\mathbf{q} + \int_{\mathbb{H}_1} (\beta \bar{\mathbf{q}}^* \cdot \mathbf{q})^2 (1 - \mathrm{Re}^2\mathbf{q})(h'(\mathrm{Re}\mathbf{q}))^2 \mathrm{d}\mathbf{q} \right]$$

$$= 2(\beta \bar{\mathbf{q}}^*) \cdot \int_{\mathbb{H}_1} (\mathrm{Id} - \mathbf{q} \otimes \mathbf{q}) h^2(\mathrm{Re}\mathbf{q}) \mathrm{d}\mathbf{q} \, (\beta \bar{\mathbf{q}}^*)$$

$$+ 2(\beta \bar{\mathbf{q}}^*) \cdot \int_{\mathbb{H}_1} (\mathbf{q} \otimes \mathbf{q})(1 - \mathrm{Re}^2\mathbf{q})(h'(\mathrm{Re}\mathbf{q}))^2 \mathrm{d}\mathbf{q} \, (\beta \bar{\mathbf{q}}^*).$$

We see directly that a sufficient condition for the first term of the last expression above to be finite is that

$$\tag{71} \int_{\mathbb{H}_1} h^2(\mathrm{Re}\mathbf{q}) \mathrm{d}\mathbf{q} < \infty.$$

Since $\mathrm{Re}(\beta \bar{\mathbf{q}}^*) = 0$ (remember that by definition $\beta \in \bar{\mathbf{q}}^\perp$), the second term is finite as soon as the 3×3 submatrix corresponding to the imaginary coordinate of the integral $\int_{\mathbb{H}_1} (\mathbf{q} \otimes \mathbf{q})(1 - \mathrm{Re}^2\mathbf{q})(h'(\mathrm{Re}\mathbf{q}))^2 \mathrm{d}\mathbf{q}$ is finite, that is, as soon as

$$\int_{\mathbb{H}_1} (\mathrm{Im}\mathbf{q} \otimes \mathrm{Im}\mathbf{q})(1 - \mathrm{Re}^2\mathbf{q})(h'(\mathrm{Re}\mathbf{q}))^2 \mathrm{d}\mathbf{q} < \infty,$$

that is, when the diagonal terms are finite (the off-diagonal elements being null by the changes of variables that change the sign of the coordinate q_i for $i = 1, 2, 3$), i.e.,

$$\int_{\mathbb{H}_1} q_i^2 (1 - \mathrm{Re}^2\mathbf{q})(h'(\mathrm{Re}\mathbf{q}))^2 \mathrm{d}\mathbf{q} < \infty.$$

Summing for $i = 1, 2, 3$ (all terms being nonnegative), this is true when

$$\tag{72} \int_{\mathbb{H}_1} (1 - \mathrm{Re}^2\mathbf{q})^2 (h'(\mathrm{Re}\mathbf{q}))^2 \mathrm{d}\mathbf{q} < \infty.$$

After a change of variable $r = \cos(\theta/2) = \mathrm{Re}\mathbf{q}$, using Proposition A.3, conditions (71) and (72) are rewritten as

$$(73) \qquad \int_{-1}^{1} (1 - r^2)^{1/2} h^2(r) \mathrm{d}r < \infty \quad \text{and} \quad \int_{-1}^{1} (1 - r^2)^{5/2} (h'(r))^2 \mathrm{d}r < \infty.$$

Since h is in $H_{(-1,1)}$, the second condition is true. Let us check the first condition. Using that h is in $H_{(-1,1)}$, we have that $h \in H^1(a,b)$ for all $-1 < a < b < 1$. By a Sobolev injection, this implies that h is continuous on $(-1,1)$. Now, since h is an odd and continuous function on $(-1,1)$, to obtain the first condition of (73) it is enough to show that

$$I_h := \int_{1/2}^{1} r(1 - r^2)^{1/2} h^2(r) \mathrm{d}r < \infty.$$

We compute, for some $\delta \in (0, 1/2)$, using an integration by parts and the inequality $2ab \leq a^2 + b^2$ for real numbers a and b,

$$\begin{aligned}
I_h(\delta) &:= \int_{1/2}^{1-\delta} r(1 - r^2)^{1/2} h^2(r) \mathrm{d}r \\
&= \left[-\frac{1}{3}(1 - r^2)^{3/2} h^2 \right]_{1/2}^{1-\delta} + \int_{1/2}^{1-\delta} \frac{2}{3}(1 - r^2)^{3/2} h h' \\
&\leq \frac{1}{3}\left(\frac{3}{4}\right)^{3/2} h^2(1/2) + \int_{1/2}^{1-\delta} \frac{2}{3}(1 - r^2)^{1/4} h (1 - r^2)^{5/4} h' \\
&\leq \frac{\sqrt{3}}{8} h^2(1/2) + \int_{1/2}^{1-\delta} \frac{1}{3}(1 - r^2)^{1/2} h^2 + \int_{1/2}^{1-\delta} \frac{1}{3}(1 - r^2)^{5/2}(h')^2 \\
&\leq \frac{\sqrt{3}}{8} h^2(1/2) + \frac{2}{3} I_h(\delta) + \int_{1/2}^{1} \frac{1}{3}(1 - r^2)^{5/2}(h')^2.
\end{aligned}$$

Therefore, taking the limit $\delta \longrightarrow 0$, the integral on $(0,1)$ is finite: $I_h = I_h(0) < \infty$. This proves conditions (73), so that $\nabla_{\mathbf{q}} \psi \in L^2(\mathbb{H}_1)$. Note that we have proved in particular that

$$(1 - r^2)^{5/4} h \in H^1(-1,1).$$

By a computation similar to that for $\nabla_{\mathbf{q}} \psi$, we see that

$$\begin{aligned}
\int_{\mathbb{H}_1} \psi \mathrm{d}\mathbf{q} &= \int_{\mathbb{H}_1} (\beta \cdot \mathbf{q}) \, h(\mathbf{q} \cdot \bar{\mathbf{q}}) \mathrm{d}\mathbf{q} \\
&= (\beta \bar{\mathbf{q}}^*) \cdot \int_{\mathbb{H}_1} \mathbf{q} \, h(\mathrm{Re}\mathbf{q}) \mathrm{d}\mathbf{q} = \mathrm{Re}\,(\beta \bar{\mathbf{q}}^*) \int_{\mathbb{H}_1} \mathrm{Re}\mathbf{q} \, h(\mathrm{Re}\mathbf{q}) \mathrm{d}\mathbf{q},
\end{aligned}$$

which is null since $\beta \in \bar{\mathbf{q}}^\perp$, so that ψ has mean zero on $\mathbb{H}_1$. $\qquad\square$

We are now ready to prove Proposition 4.7.

Proof of Proposition 4.7. The statement is a direct consequence of Proposition 4.9, Corollary 4.10, and Proposition 4.12. $\qquad\square$

4.4. The macroscopic limit. This section is devoted to the proof of Theorem 4.1. We will use the following.

LEMMA 4.13. *It holds that*

$$\int_{\mathbb{H}_1} \mathbf{e_1}(\mathbf{q}) M_{\bar{\mathbf{q}}}(\mathbf{q}) \mathrm{d}\mathbf{q} = c_1 \mathbf{e_1}(\bar{\mathbf{q}}), \tag{74}$$

where the positive constant c_1 is given in (37).

Remark 4.14 (comments on the constant c_1).
(i) The value for the constant c_1 obtained here is the same one as in the body attitude coordination model based on rotation matrices in [17]. This will allow us to prove the equivalence between the respective continuity equations (see section 5.3).
(ii) In the case of the Vicsek model in [21] and in the body attitude coordination model based on rotation matrices in [17], the constant c_1 played the role of "order parameter." Particularly, it holds that $c_1 \in [0, 1]$, and the larger its value, the more organized (coordinated/aligned) the dynamics are (and, conversely, the smaller c_1, the more disordered the dynamics are). The extreme cases take place, for example, when $D \to \infty$, and then $c_1 = 0$, and when $D \to 0$, giving $c_1 = 1$. Here we have the same properties and interpretations for c_1.

Proof of Lemma 4.13. We first make the change of variable $\mathbf{q}' = \mathbf{q}\bar{\mathbf{q}}^*$:

$$\int_{\mathbb{H}_1} \mathbf{e_1}(\mathbf{q}) M_{\bar{\mathbf{q}}}(\mathbf{q}) \mathrm{d}\mathbf{q} = \int_{\mathbb{H}_1} \mathbf{e_1}(\mathbf{q}\bar{\mathbf{q}}) M_1(\mathrm{Re}(\mathbf{q})) \mathrm{d}\mathbf{q},$$

where, for $\mathbf{q} = \cos(\theta/2) + \sin(\theta/2)\mathbf{n} \in \mathbb{H}_1$,

$$M_1(\mathrm{Re}(\mathbf{q})) = \frac{1}{Z} \exp\left(\frac{2}{d}\left((1 \cdot \mathbf{q})^2 - \frac{1}{4}\right)\right) = \frac{1}{Z} \exp\left(\frac{2}{d}\left(\mathrm{Re}(\mathbf{q})^2 - \frac{1}{4}\right)\right)$$

$$= \frac{1}{Z} \exp\left(\frac{2}{d}\left(\cos^2(\theta/2) - \frac{1}{4}\right)\right) = \frac{1}{Z} \exp\left(d^{-1}\left(\frac{1}{2} + \cos\theta\right)\right). \tag{75}$$

Then, defining $\bar{\mathbf{e}}_1 = \bar{\mathbf{q}}\mathbf{e_1}\bar{\mathbf{q}}^*$, we decompose

$$\mathbf{e_1}(\mathbf{q}\bar{\mathbf{q}}) = \mathrm{Im}(\mathbf{q}\bar{\mathbf{e}}_1\mathbf{q}^*) \tag{76}$$
$$= \left(2\mathrm{Re}^2(\mathbf{q}) - 1\right)\mathrm{Im}(\bar{\mathbf{e}}_1) + 2\mathrm{Re}(\mathbf{q})\left(\mathrm{Im}(\mathbf{q}) \times \mathrm{Im}(\bar{\mathbf{e}}_1)\right) + 2\left(\mathrm{Im}(\mathbf{q}) \otimes \mathrm{Im}(\mathbf{q})\right)\mathrm{Im}(\bar{\mathbf{e}}_1)$$
$$= \left(2\mathrm{Re}^2(\mathbf{q}) - 1\right)\mathbf{e_1}(\bar{\mathbf{q}}) + 2\mathrm{Re}(\mathbf{q})\left(\mathrm{Im}(\mathbf{q}) \times \mathbf{e_1}(\bar{\mathbf{q}})\right) + 2\left(\mathrm{Im}(\mathbf{q}) \otimes \mathrm{Im}(\mathbf{q})\right)\mathbf{e_1}(\bar{\mathbf{q}}),$$

where we used that, for $\mathbf{q}, \mathbf{r} \in \mathbb{H}_1$, it holds that $\mathrm{Re}(\mathbf{qr}) = \mathrm{Re}(\mathbf{r})\mathrm{Re}(\mathbf{q}) - \mathrm{Im}(\mathbf{q}) \cdot \mathrm{Im}(\mathbf{r})$ and $\mathrm{Im}(\mathbf{qr}) = \mathrm{Re}(\mathbf{q})\mathrm{Im}(\mathbf{r}) + \mathrm{Re}(\mathbf{r})\mathrm{Im}(\mathbf{q}) + \mathrm{Im}(\mathbf{q}) \times \mathrm{Im}(\mathbf{r})$.

We integrate against $M_1(\mathrm{Re}(\mathbf{q}))$: By arguments of parity the contribution of the second term vanishes (with a change of variable $\mathbf{q}' = \mathbf{q}^*$), and the contribution of the last term is diagonal (with the changes of variable that change the sign of q_i for $i = 1, 2, 3$), so that

$$\int_{\mathbb{H}_1} \mathbf{e_1}(\mathbf{q}) M_{\bar{\mathbf{q}}}(\mathbf{q}) \mathrm{d}\mathbf{q} = \int_{\mathbb{H}_1} \left[\left(2\mathrm{Re}^2(\mathbf{q}) - 1\right)\mathrm{Id} + 2\mathrm{diag}(q_1^2, q_2^2, q_3^2)\right] \mathbf{e_1}(\bar{\mathbf{q}}) M_1(\mathrm{Re}(\mathbf{q})) \mathrm{d}\mathbf{q}.$$

Using the changes of variable that switch the coordinates q_i and q_j for $i \neq j$, we see that the diagonal elements corresponding to q_i^2 for $i = 1, 2, 3$ give rise to the same value for the integral, and therefore

$$\int_{\mathbb{H}_1} \mathbf{e_1}(\mathbf{q}) M_{\bar{\mathbf{q}}}(\mathbf{q}) d\mathbf{q} = \int_{\mathbb{H}_1} \left[\left(2\mathrm{Re}^2(\mathbf{q}) - 1 \right) \mathrm{Id} + \frac{2}{3} |\mathrm{Im}(\mathbf{q})|^2 \mathrm{Id} \right] \mathbf{e_1}(\bar{\mathbf{q}}) \, M_1(\mathrm{Re}(\mathbf{q})) d\mathbf{q}$$

$$= \int_{\mathbb{H}_1} \left[\left(2\mathrm{Re}^2(\mathbf{q}) - 1 \right) + \frac{2}{3} (1 - \mathrm{Re}^2(\mathbf{q})) \right] \mathbf{e_1}(\bar{\mathbf{q}}) \, M_1(\mathrm{Re}(\mathbf{q})) d\mathbf{q},$$

so that equality (74) holds for

$$c_1 = \frac{1}{3} \left(\int_{\mathbb{H}_1} \left(4 \left(\mathrm{Re}(\mathbf{q}) \right)^2 - 1 \right) M_1(\mathrm{Re}(\mathbf{q})) d\mathbf{q} \right)$$

$$= \frac{2}{3} 4\pi \int_0^\pi \left(\frac{1}{2} + \cos\theta \right) \frac{m(\theta)}{Z} \sin^2(\theta/2) d\theta$$

$$= \frac{2}{3} \langle \frac{1}{2} + \cos\theta \rangle_{m \sin^2(\theta/2)},$$

where we used Proposition (A.3) on the volume element. $\qquad \square$

We are now ready to prove Theorem 4.1.

Proof of Theorem 4.1. By (27), we have that $\Gamma(f^\varepsilon) = \mathcal{O}(\varepsilon)$. Formally, the limit of f^ε as $\epsilon \to 0$ (if the limit exists) is in the kernel of Γ. Therefore, by Proposition 4.4, the limit has the form

$$(77) \qquad f(t, x, \mathbf{q}) = \rho(t, x) M_{\bar{\mathbf{q}}(t,x)}(\mathbf{q})$$

for some $\rho = \rho(t, x) \geq 0$ and $\bar{\mathbf{q}} = \bar{\mathbf{q}}(t, x) \in \mathbb{H}_1$. We integrate the kinetic (27) on $\mathbb{H}_1$ to obtain

$$(78) \qquad \partial_t \rho^\varepsilon + \nabla_x \cdot \left(\int_{\mathbb{H}_1} \mathbf{e_1}(\mathbf{q}) f^\varepsilon d\mathbf{q} \right) = \mathcal{O}(\varepsilon).$$

Taking the limit $\varepsilon \to 0$ and substituting the value of f with expression (77), we obtain the equation

$$(79) \qquad \partial_t \rho + \nabla_x \cdot \left(\rho(t, x) \int_{\mathbb{H}_1} \mathbf{e_1}(\mathbf{q}) M_{\bar{\mathbf{q}}(t,x)}(\mathbf{q}) d\mathbf{q} \right) = 0.$$

Lemma 4.13 gives us the value of the integral in the previous expression, from which we conclude the continuity equation (33).

We compute next the evolution equation for $\bar{\mathbf{q}} = \bar{\mathbf{q}}(t, x)$. We multiply the rescaled kinetic equation (27) by the GCI ψ associated with $\bar{\mathbf{q}}_{f^\varepsilon}$, that is, by Proposition 4.7,

$$\psi(\mathbf{q}) = (\beta \cdot \mathbf{q}) \, h(\mathbf{q} \cdot \bar{\mathbf{q}}_{f^\varepsilon}) \quad \text{for } \beta \in \bar{\mathbf{q}}^\perp,$$

and integrate over $\mathbb{H}_1$. We obtain (using (61))

$$\int_{\mathbb{H}_1} \left[\partial_t f^\varepsilon + \nabla_x \cdot (\mathbf{e_1}(\mathbf{q}) f^\varepsilon) \right] (\beta \cdot \mathbf{q}) \, h(\mathbf{q} \cdot \bar{\mathbf{q}}_{f^\varepsilon}) \, d\mathbf{q} = \mathcal{O}(\varepsilon).$$

Making $\varepsilon \to 0$ and using that (formally) $\bar{\mathbf{q}}_{f^\varepsilon} \to \bar{\mathbf{q}}$, the previous expression gives

$$\int_{\mathbb{H}_1} \left[\partial_t (\rho M_{\bar{\mathbf{q}}}) + \nabla_x \cdot (\mathbf{e_1}(\mathbf{q}) \rho M_{\bar{\mathbf{q}}}) \right] (\beta \cdot \mathbf{q}) \, h(\mathbf{q} \cdot \bar{\mathbf{q}}) \, d\mathbf{q} = 0 \quad \text{for all } \beta \in \bar{\mathbf{q}}^\perp.$$

Particularly, this implies that

$$\beta \cdot Y = 0 \quad \text{for all } \beta \in \bar{\mathbf{q}}^{\perp}$$

for

$$Y = \int_{\mathbb{H}_1} [\partial_t(\rho M_{\bar{\mathbf{q}}}) + \nabla_x \cdot (\mathbf{e_1}(\mathbf{q})\rho M_{\bar{\mathbf{q}}})] \, h(\mathbf{q} \cdot \bar{\mathbf{q}}) \, \mathbf{q} \, d\mathbf{q}.$$

This is equivalent to

$$X := P_{\bar{\mathbf{q}}^{\perp}} Y = P_{\bar{\mathbf{q}}^{\perp}} \int_{\mathbb{H}_1} [\partial_t(\rho M_{\bar{\mathbf{q}}}) + \nabla_x \cdot (\mathbf{e_1}(\mathbf{q})\rho M_{\bar{\mathbf{q}}})] \, h(\mathbf{q} \cdot \bar{\mathbf{q}}) \, \mathbf{q} \, d\mathbf{q} = 0.$$

Next we compute each term in the previous expression. We have that

$$\partial_t(\rho M_{\bar{\mathbf{q}}}) = (\partial_t \rho) M_{\bar{\mathbf{q}}} + \rho M_{\bar{\mathbf{q}}} \frac{4}{d} (\mathbf{q} \cdot \bar{\mathbf{q}})(\mathbf{q} \cdot \partial_t \bar{\mathbf{q}})$$

and

$$\nabla_x \cdot (\mathbf{e_1}(\mathbf{q})\rho M_{\bar{\mathbf{q}}}) = \mathbf{e_1}(\mathbf{q}) \cdot \left((\nabla_x \rho) M_{\bar{\mathbf{q}}} + \rho M_{\bar{\mathbf{q}}} \frac{4}{d} (\mathbf{q} \cdot \bar{\mathbf{q}}) \nabla_x (\mathbf{q} \cdot \bar{\mathbf{q}}) \right).$$

We define

(80) $$H(\mathbf{q} \cdot \bar{\mathbf{q}}) := M_{\bar{\mathbf{q}}}(\mathbf{q}) h(\mathbf{q} \cdot \bar{\mathbf{q}})(\mathbf{q} \cdot \bar{\mathbf{q}}),$$

which is even in its argument (recall that h is odd). We have that

$$X =: X_1 + X_2 + X_3 + X_4 = 0,$$

where

$$X_1 = P_{\bar{\mathbf{q}}^{\perp}} \int_{\mathbb{H}_1} (\partial_t \rho) M_{\bar{\mathbf{q}}} h(\mathbf{q} \cdot \bar{\mathbf{q}}) \, \mathbf{q} \, d\mathbf{q},$$

$$X_2 = P_{\bar{\mathbf{q}}^{\perp}} \int_{\mathbb{H}_1} \rho M_{\bar{\mathbf{q}}} \frac{4}{d} (\mathbf{q} \cdot \bar{\mathbf{q}})(\mathbf{q} \cdot \partial_t \bar{\mathbf{q}}) h(\mathbf{q} \cdot \bar{\mathbf{q}}) \, \mathbf{q} \, d\mathbf{q}$$

$$\quad = P_{\bar{\mathbf{q}}^{\perp}} \int_{\mathbb{H}_1} \rho \frac{4}{d} (\mathbf{q} \cdot \partial_t \bar{\mathbf{q}}) H(\mathbf{q} \cdot \bar{\mathbf{q}}) \, \mathbf{q} \, d\mathbf{q},$$

$$X_3 = P_{\bar{\mathbf{q}}^{\perp}} \int_{\mathbb{H}_1} \mathbf{e_1}(\mathbf{q}) \cdot (\nabla_x \rho) \, M_{\bar{\mathbf{q}}} h(\mathbf{q} \cdot \bar{\mathbf{q}}) \, \mathbf{q} \, d\mathbf{q},$$

$$X_4 = P_{\bar{\mathbf{q}}^{\perp}} \int_{\mathbb{H}_1} \mathbf{e_1}(\mathbf{q}) \cdot \left(\rho M_{\bar{\mathbf{q}}} \frac{4}{d} (\mathbf{q} \cdot \bar{\mathbf{q}}) \nabla_x (\mathbf{q} \cdot \bar{\mathbf{q}}) \right) h(\mathbf{q} \cdot \bar{\mathbf{q}}) \, \mathbf{q} \, d\mathbf{q}$$

$$\quad = P_{\bar{\mathbf{q}}^{\perp}} \int_{\mathbb{H}_1} \rho \frac{4}{d} \Big(\mathbf{q} \cdot (\mathbf{e_1}(\mathbf{q}) \cdot \nabla_x) \, \bar{\mathbf{q}} \Big) H(\mathbf{q} \cdot \bar{\mathbf{q}}) \, \mathbf{q} \, d\mathbf{q}.$$

Using the change of variable $\mathbf{q}' = \mathbf{q}\bar{\mathbf{q}}^*$ (and skipping the primes), we obtain

$$X_1 = P_{\bar{\mathbf{q}}^{\perp}} \int_{\mathbb{H}_1} (\partial_t \rho) M_1(\text{Re}(\mathbf{q})) h(\text{Re}(\mathbf{q})) \, \mathbf{q} \, d\mathbf{q} \, \bar{\mathbf{q}},$$

$$X_2 = P_{\bar{\mathbf{q}}^{\perp}} \int_{\mathbb{H}_1} \rho \frac{4}{d} (\mathbf{q} \cdot (\partial_t \bar{\mathbf{q}}) \bar{\mathbf{q}}^*) H(\text{Re}(\mathbf{q})) \, \mathbf{q} \, d\mathbf{q} \, \bar{\mathbf{q}},$$

$$X_3 = P_{\bar{\mathbf{q}}^{\perp}} \int_{\mathbb{H}_1} \mathbf{e_1}(\mathbf{q}\bar{\mathbf{q}}) \cdot (\nabla_x \rho) \, M_1(\text{Re}(\mathbf{q})) h(\text{Re}(\mathbf{q})) \, \mathbf{q} \, d\mathbf{q} \, \bar{\mathbf{q}},$$

$$X_4 = \rho \frac{4}{d} P_{\bar{\mathbf{q}}^{\perp}} \int_{\mathbb{H}_1} \Big(\mathbf{q}\bar{\mathbf{q}} \cdot (\mathbf{e_1}(\mathbf{q}\bar{\mathbf{q}}) \cdot \nabla_x) \, \bar{\mathbf{q}} \Big) H(\text{Re}(\mathbf{q})) \, \mathbf{q} \, d\mathbf{q}\bar{\mathbf{q}},$$

with $M_1(\mathbf{q})$ given by (75).

First notice the following: For any $\mathbf{q} \in \mathbb{H}$ and $\bar{\mathbf{q}} \in \mathbb{H}_1$ it holds that

$$
(81) \qquad P_{\bar{\mathbf{q}}^{\perp}}(\mathbf{q}\bar{\mathbf{q}}) = \mathbf{q}\bar{\mathbf{q}} - (\mathbf{q}\bar{\mathbf{q}} \cdot \bar{\mathbf{q}})\bar{\mathbf{q}} = \mathrm{Im}(\mathbf{q})\bar{\mathbf{q}}.
$$

The term X_1. We apply (81) on X_1:

$$
X_1 = \int_{\mathbb{H}_1} (\partial_t \rho) M_1(\mathrm{Re}(\mathbf{q})) h(\mathrm{Re}(\mathbf{q})) \, \mathrm{Im}(\mathbf{q}) \, \mathrm{d}\mathbf{q} \, \bar{\mathbf{q}},
$$

which gives an odd integral in $\mathrm{Im}(\mathbf{q})$, and hence $X_1 = 0$.

The term X_2. To compute X_2 we first apply (81) again:

$$
X_2 = \int_{\mathbb{H}_1} \rho \frac{4}{d} (\mathbf{q} \cdot (\partial_t \bar{\mathbf{q}})\bar{\mathbf{q}}^*) H(\mathrm{Re}(\mathbf{q})) \, \mathrm{Im}(\mathbf{q}) \, \mathrm{d}\mathbf{q} \, \bar{\mathbf{q}}.
$$

Now, it holds that

$$
(82) \qquad (\partial_t \bar{\mathbf{q}})\bar{\mathbf{q}}^* = \mathrm{Im}\left((\partial_t \bar{\mathbf{q}})\bar{\mathbf{q}}^*\right),
$$

since $\mathrm{Re}\left((\partial_t \bar{\mathbf{q}})\bar{\mathbf{q}}^*\right) = \partial_t \bar{\mathbf{q}} \cdot \bar{\mathbf{q}} = 0$ given that $\bar{\mathbf{q}} \perp \partial_t \bar{\mathbf{q}}$. Equation (82) implies, in particular, that $\mathbf{q} \cdot (\partial \bar{\mathbf{q}})\bar{\mathbf{q}}^* = \mathrm{Im}(\mathbf{q}) \cdot \mathrm{Im}((\partial_t \bar{\mathbf{q}})\bar{\mathbf{q}}^*)$. With all these considerations we conclude that

$$
(83) \qquad X_2 = \frac{4}{d}\rho \left[\left(\int_{\mathbb{H}_1} \mathrm{Im}(\mathbf{q}) \otimes \mathrm{Im}(\mathbf{q}) \, H(\mathrm{Re}(\mathbf{q})) \, \mathrm{d}\mathbf{q} \right) \mathrm{Im}\left((\partial_t \bar{\mathbf{q}})\bar{\mathbf{q}}^*\right) \right] \bar{\mathbf{q}}.
$$

Now observe that the off-diagonal elements in $\mathrm{Im}(\mathbf{q}) \otimes \mathrm{Im}(\mathbf{q})$ are odd in the components q_1, q_2, q_3 (where $\mathbf{q} = (q_0, q_1, q_2, q_3)$), and therefore the off-diagonal elements give integral zero. The diagonal elements corresponding to q_i^2 for $i = 1, 2, 3$ can be permuted, giving the same value for the integral. With these considerations in mind, we have that

$$
\begin{aligned}
\int_{\mathbb{H}_1} \mathrm{Im}(\mathbf{q}) \otimes \mathrm{Im}(\mathbf{q}) \, H(\mathrm{Re}(\mathbf{q})) \, \mathrm{d}\mathbf{q} &= \int_{\mathbb{H}_1} \frac{q_1^2 + q_2^2 + q_3^2}{3} \mathrm{Id} \, H(\mathrm{Re}(\mathbf{q})) \, \mathrm{d}\mathbf{q} \\
&= \int_{\mathbb{H}_1} \frac{1 - \mathrm{Re}^2(\mathbf{q})}{3} H(\mathrm{Re}(\mathbf{q})) \, \mathrm{d}\mathbf{q} \, \mathrm{Id} \\
(84) \qquad\qquad\qquad &=: C_2 \mathrm{Id}.
\end{aligned}
$$

We substitute (84) into (83) and conclude that

$$
(85) \qquad X_2 = \frac{4}{d} C_2 \rho \partial_t \bar{\mathbf{q}},
$$

with C_2 given in (84).

The term X_3. We apply (81) to obtain

$$
X_3 = \int_{\mathbb{H}_1} \mathbf{e_1}(\mathbf{q}\bar{\mathbf{q}}) \cdot (\nabla_x \rho) \, M_1(\mathrm{Re}(\mathbf{q})) h(\mathrm{Re}(\mathbf{q})) \, \mathrm{Im}(\mathbf{q}) \, \mathrm{d}\mathbf{q} \, \bar{\mathbf{q}}.
$$

Then we use the decomposition of $\mathbf{e_1}(\mathbf{q}\bar{\mathbf{q}})$ in (76) to compute

$$
X_3 := X_{3,1} + X_{3,2} + X_{3,3},
$$

where

$$X_{3,1} = \int_{\mathbb{H}_1} (2\mathrm{Re}^2(\mathbf{q}) - 1) \left[\mathbf{e_1}(\bar{\mathbf{q}}) \cdot \nabla_x \rho \right] M_1(\mathrm{Re}(\mathbf{q})) h(\mathrm{Re}(\mathbf{q})) \mathrm{Im}(\mathbf{q}) \, \mathrm{d}\mathbf{q} \, \bar{\mathbf{q}},$$

$$X_{3,2} = \int_{\mathbb{H}_1} 2\mathrm{Re}(\mathbf{q}) \left(\mathrm{Im}(\mathbf{q}) \times \mathbf{e_1}(\bar{\mathbf{q}}) \right) \cdot (\nabla_x \rho) \, M_1(\mathrm{Re}(\mathbf{q})) h(\mathrm{Re}(\mathbf{q})) \mathrm{Im}(\mathbf{q}) \, \mathrm{d}\mathbf{q} \, \bar{\mathbf{q}},$$

$$X_{3,3} = \int_{\mathbb{H}_1} 2 \left((\mathrm{Im}(\mathbf{q}) \otimes \mathrm{Im}(\mathbf{q})) \mathbf{e_1}(\bar{\mathbf{q}}) \right) \cdot (\nabla_x \rho) \, M_1(\mathrm{Re}(\mathbf{q})) h(\mathrm{Re}(\mathbf{q})) \mathrm{Im}(\mathbf{q}) \, \mathrm{d}\mathbf{q} \, \bar{\mathbf{q}}.$$

The integrands in the terms $X_{3,1}$ and $X_{3,3}$ are odd in $\mathrm{Im}(\mathbf{q})$, so $X_{3,1} = X_{3,3} = 0$. Next, using that $(\mathrm{Im}(\mathbf{q}) \times \mathbf{e_1}(\bar{\mathbf{q}})) \cdot \nabla_x \rho = (\mathbf{e_1}(\bar{\mathbf{q}}) \times \nabla_x \rho) \cdot \mathrm{Im}(\mathbf{q})$ we get

$$X_3 = X_{3,2} = 2 \left[\left(\int_{\mathbb{H}_1} \mathrm{Im}(\mathbf{q}) \otimes \mathrm{Im}(\mathbf{q}) \, H(\mathrm{Re}(\mathbf{q})) \, \mathrm{d}\mathbf{q} \right) (\mathbf{e_1}(\bar{\mathbf{q}}) \times \nabla_x \rho) \right] \bar{\mathbf{q}}$$
$$= 2C_2(\mathbf{e_1}(\bar{\mathbf{q}}) \times \nabla_x \rho) \bar{\mathbf{q}}$$

by using (84).

The term X_4. We first apply the projection

$$X_4 = \rho \frac{4}{d} P_{\bar{\mathbf{q}}^\perp} \int_{\mathbb{H}_1} \left(\mathbf{q}\bar{\mathbf{q}} \cdot (\mathbf{e_1}(\mathbf{q}\bar{\mathbf{q}}) \cdot \nabla_x) \, \bar{\mathbf{q}} \right) H(\mathrm{Re}(\mathbf{q})) \, \mathbf{q} \, \mathrm{d}\mathbf{q}\bar{\mathbf{q}}$$
$$= \rho \frac{4}{d} \int_{\mathbb{H}_1} \left(\mathbf{q}\bar{\mathbf{q}} \cdot (\mathbf{e_1}(\mathbf{q}\bar{\mathbf{q}}) \cdot \nabla_x) \, \bar{\mathbf{q}} \right) H(\mathrm{Re}(\mathbf{q})) \, P_{\bar{\mathbf{q}}^\perp} (\mathbf{q}\,\bar{\mathbf{q}}) \, \mathrm{d}\mathbf{q}$$
$$= \rho \frac{4}{d} \int_{\mathbb{H}_1} \left(\mathbf{q}\bar{\mathbf{q}} \cdot (\mathbf{e_1}(\mathbf{q}\bar{\mathbf{q}}) \cdot \nabla_x) \, \bar{\mathbf{q}} \right) H(\mathrm{Re}(\mathbf{q})) \, \mathrm{Im}\,(\mathbf{q}) \, \mathrm{d}\mathbf{q}\bar{\mathbf{q}}.$$

Now, note that, since $\partial_{x_j} \bar{\mathbf{q}} \in \bar{\mathbf{q}}^\perp$, we have, for all $\mathbf{q} \in \mathbb{H}_1$, that

$$((\mathrm{Re}(\mathbf{q})) \, \bar{\mathbf{q}}) \cdot ((\mathbf{e_1}(\mathbf{q}\bar{\mathbf{q}}) \cdot \nabla_x) \, \bar{\mathbf{q}}) = 0.$$

Therefore

$$X_4 = \rho \frac{4}{d} \int_{\mathbb{H}_1} \left(((\mathrm{Im}(\mathbf{q})) \, \bar{\mathbf{q}}) \cdot ((\mathbf{e_1}(\mathbf{q}\bar{\mathbf{q}}) \cdot \nabla_x) \, \bar{\mathbf{q}}) \right) H(\mathrm{Re}(\mathbf{q})) \, \mathrm{Im}\,(\mathbf{q}) \, \mathrm{d}\mathbf{q}\bar{\mathbf{q}}.$$

Then, using again the decomposition (76), we can write

$$X_4 = X_{4,a} + X_{4,b} + X_{4,c}.$$

We compute next

$$X_{4,a} = \rho \frac{4}{d} \int_{\mathbb{H}_1} \left(2\mathrm{Re}^2 \mathbf{q} - 1 \right) \left(\mathrm{Im}\,(\mathbf{q}) \, \bar{\mathbf{q}} \cdot (\mathbf{e_1}(\bar{\mathbf{q}}) \cdot \nabla_x) \, \bar{\mathbf{q}} \right) H(\mathrm{Re}(\mathbf{q})) \, \mathrm{Im}\,(\mathbf{q}) \, \mathrm{d}\mathbf{q} \, \bar{\mathbf{q}}$$
$$= \rho \frac{4}{d} \int_{\mathbb{H}_1} \left(2\mathrm{Re}^2 \mathbf{q} - 1 \right) \left(\mathrm{Im}\,(\mathbf{q}) \cdot [(\mathbf{e_1}(\bar{\mathbf{q}}) \cdot \nabla_x) \, \bar{\mathbf{q}}] \bar{\mathbf{q}}^* \right) H(\mathrm{Re}(\mathbf{q})) \, \mathrm{Im}\,(\mathbf{q}) \, \mathrm{d}\mathbf{q} \, \bar{\mathbf{q}}$$
$$= \rho \frac{4}{d} \int_{\mathbb{H}_1} \left(2\mathrm{Re}^2 \mathbf{q} - 1 \right) H(\mathrm{Re}(\mathbf{q}))(\mathrm{Im}(\mathbf{q})) \otimes (\mathrm{Im}(\mathbf{q}))[(\mathbf{e_1}(\bar{\mathbf{q}}) \cdot \nabla_x) \, \bar{\mathbf{q}}] \bar{\mathbf{q}}^* \mathrm{d}\mathbf{q} \, \bar{\mathbf{q}}$$
$$= \rho \frac{4}{3d} \int_{\mathbb{H}_1} \left(2\mathrm{Re}^2 \mathbf{q} - 1 \right) \left(1 - \mathrm{Re}^2 \mathbf{q} \right) H(\mathrm{Re}(\mathbf{q})) \mathrm{d}\mathbf{q} \, (\mathbf{e_1}(\bar{\mathbf{q}}) \cdot \nabla_x) \, \bar{\mathbf{q}},$$

where we use that the expression is odd in $\mathbf{q}_i$, $i = 1, \ldots, 3$, on the off-diagonal terms and the symmetry in $\mathbf{q}_i$ to group the diagonal terms, analogously to the computation of the term (84). Next, we have that

$$
\begin{aligned}
X_{4,b} &= \rho \frac{4}{d} \int_{\mathbb{H}_1} 2\mathrm{Re}(\mathbf{q}) \Big(((\mathrm{Im}(\mathbf{q}))\,\bar{\mathbf{q}}) \cdot ((\mathrm{Im}(\mathbf{q}) \times \mathbf{e_1}(\bar{\mathbf{q}})) \cdot \nabla_x)\,\bar{\mathbf{q}} \Big)\, H(\mathrm{Re}(\mathbf{q}))\,\mathrm{Im}\,(\mathbf{q})\,\mathrm{d}\mathbf{q}\bar{\mathbf{q}} \\
&= 0,
\end{aligned}
$$

since the integrand is odd in $\mathrm{Im}(\mathbf{q})$. Finally, we compute

$$
\begin{aligned}
X_{4,c} &= \rho \frac{4}{d} \int_{\mathbb{H}_1} 2\Big(((\mathrm{Im}(\mathbf{q}))\,\bar{\mathbf{q}}) \cdot (((\mathrm{Im}(\mathbf{q}) \otimes \mathrm{Im}(\mathbf{q}))\,\mathbf{e_1}(\bar{\mathbf{q}}) \cdot \nabla_x)\,\bar{\mathbf{q}}) \Big)\, H(\mathrm{Re}(\mathbf{q}))\,\mathrm{Im}\,(\mathbf{q})\,\mathrm{d}\mathbf{q}\bar{\mathbf{q}} \\
&= \rho \frac{4}{d} \int_{\mathbb{H}_1} 2(\mathrm{Im}(\mathbf{q}) \cdot \mathbf{e_1}(\bar{\mathbf{q}})) \Big(((\mathrm{Im}(\mathbf{q}))\,\bar{\mathbf{q}}) \cdot ((\mathrm{Im}(\mathbf{q}) \cdot \nabla_x)\,\bar{\mathbf{q}}) \Big)\, H(\mathrm{Re}(\mathbf{q}))\,\mathrm{Im}\,(\mathbf{q})\,\mathrm{d}\mathbf{q}\bar{\mathbf{q}} \\
&= \rho \frac{4}{d} \int_{\mathbb{H}_1} 2(\mathrm{Im}(\mathbf{q}) \cdot \mathbf{e_1}(\bar{\mathbf{q}})) \Big((\mathrm{Im}(\mathbf{q})) \cdot (((\mathrm{Im}(\mathbf{q}) \cdot \nabla_x)\,\bar{\mathbf{q}}\,\bar{\mathbf{q}}^*) \Big)\, H(\mathrm{Re}(\mathbf{q}))\,\mathrm{Im}\,(\mathbf{q})\,\mathrm{d}\mathbf{q}\bar{\mathbf{q}} \\
&= \rho \frac{4}{d} \int_{\mathbb{H}_1} 2(\mathrm{Im}(\mathbf{q}) \cdot \mathbf{e_1}(\bar{\mathbf{q}})) \Big((\mathrm{Im}(\mathbf{q})) \cdot (A(\bar{\mathbf{q}})\mathrm{Im}(\mathbf{q})) \Big)\, H(\mathrm{Re}(\mathbf{q}))\,\mathrm{Im}\,(\mathbf{q})\,\mathrm{d}\mathbf{q}\bar{\mathbf{q}},
\end{aligned}
$$

where $A(\bar{\mathbf{q}}) = \mathrm{Im}\,((\nabla_x\bar{\mathbf{q}})\bar{\mathbf{q}}^*)$, seen as a 3×3 matrix, that is,

$$(86) \qquad A(\bar{\mathbf{q}})_{i,j} := \big((\partial_{x_j}\bar{\mathbf{q}})\bar{\mathbf{q}}^*\big)_i = \big(\partial_{x_j,\mathrm{rel}}\bar{\mathbf{q}}\big)_i \qquad \text{for } i,\,j = 1,\,2,\,3.$$

We replace $A(\bar{\mathbf{q}})$ by its symmetrization $A^S(\bar{\mathbf{q}}) = \frac{1}{2}\,(A(\bar{\mathbf{q}}) + A^t(\bar{\mathbf{q}}))$ and diagonalize it in a orthogonal basis $A^S(\bar{\mathbf{q}}) = O^t D O$ with O an orthogonal 3×3 matrix and D a diagonal 3×3 matrix. Then, using a change of variable $\mathrm{Im}(\mathbf{q})' = O\mathrm{Im}(\mathbf{q})$, we have

$$
\begin{aligned}
X_{4,c} &= \rho \frac{4}{d} \int_{\mathbb{H}_1} 2(\mathrm{Im}(\mathbf{q}) \cdot \mathbf{e_1}(\bar{\mathbf{q}}))\,(\mathrm{Im}(\mathbf{q}) \cdot (O^t D O\mathrm{Im}(\mathbf{q})))\, H(\mathrm{Re}(\mathbf{q}))\,\mathrm{Im}\,(\mathbf{q})\,\mathrm{d}\mathbf{q}\bar{\mathbf{q}} \\
&= \rho \frac{4}{d} \int_{\mathbb{H}_1} 2(\mathrm{Im}(\mathbf{q}) \cdot O\mathbf{e_1}(\bar{\mathbf{q}}))\,(\mathrm{Im}(\mathbf{q}) \cdot (D\mathrm{Im}(\mathbf{q})))\, H(\mathrm{Re}(\mathbf{q}))\,O^t\mathrm{Im}\,(\mathbf{q})\,\mathrm{d}\mathbf{q}\bar{\mathbf{q}} \\
&= \rho \frac{4}{d} \left(O^t \int_{\mathbb{H}_1} 2(\mathrm{Im}(\mathbf{q}) \otimes \mathrm{Im}(\mathbf{q}))\,(\mathrm{Im}(\mathbf{q}) \cdot (D\mathrm{Im}(\mathbf{q})))\, H(\mathrm{Re}(\mathbf{q}))\,\mathrm{d}\mathbf{q}\,O\mathbf{e_1}(\bar{\mathbf{q}}) \right)\bar{\mathbf{q}}.
\end{aligned}
$$

Again, since the integrand is odd in q_i, $i = 1, \ldots, 3$, the off-diagonal terms in the integral are zero. We compute the ith diagonal term of the integral for $i \in \{1, 2, 3\}$:

$$
\begin{aligned}
&\left(\int_{\mathbb{H}_1} 2(\mathrm{Im}(\mathbf{q}) \otimes \mathrm{Im}(\mathbf{q}))\,(\mathrm{Im}(\mathbf{q}) \cdot (D\mathrm{Im}(\mathbf{q})))\, H(\mathrm{Re}(\mathbf{q}))\,\mathrm{d}\mathbf{q} \right)_{i,i} \\
&= \int_{\mathbb{H}_1} 2\mathbf{q}_i^2\,(\mathrm{Im}(\mathbf{q}) \cdot (D\mathrm{Im}(\mathbf{q})))\, H(\mathrm{Re}(\mathbf{q}))\,\mathrm{d}\mathbf{q} \\
&= \int_{\mathbb{H}_1} 2\left(d_i\mathbf{q}_i^4 + \Sigma_{j \neq i}d_j\mathbf{q}_i^2\mathbf{q}_j^2 \right)\, H(\mathrm{Re}(\mathbf{q}))\,\mathrm{d}\mathbf{q} \\
&= 2d_i \int_{\mathbb{H}_1} \mathbf{q}_1^4\,H(\mathrm{Re}(\mathbf{q}))\,\mathrm{d}\mathbf{q} + 2\Sigma_{j \neq i}d_j \int_{\mathbb{H}_1} \left(\mathbf{q}_1^2\mathbf{q}_2^2 \right)\,H(\mathrm{Re}(\mathbf{q}))\,\mathrm{d}\mathbf{q} \\
&= 2d_i \int_{\mathbb{H}_1} \mathbf{q}_1^2(\mathbf{q}_1^2 - \mathbf{q}_2^2)\,H(\mathrm{Re}(\mathbf{q}))\,\mathrm{d}\mathbf{q} + 2\mathrm{Tr}(D) \int_{\mathbb{H}_1} \mathbf{q}_1^2\mathbf{q}_2^2\,H(\mathrm{Re}(\mathbf{q}))\,\mathrm{d}\mathbf{q} \\
&= \left(2D \int_{\mathbb{H}_1} \mathbf{q}_1^2(\mathbf{q}_1^2 - \mathbf{q}_2^2)\,H(\mathrm{Re}(\mathbf{q}))\,\mathrm{d}\mathbf{q} + 2\mathrm{Tr}(D)\mathrm{Id} \int_{\mathbb{H}_1} \mathbf{q}_1^2\mathbf{q}_2^2\,H(\mathrm{Re}(\mathbf{q}))\,\mathrm{d}\mathbf{q} \right)_i.
\end{aligned}
$$

Inserting this expression into $X_{4,c}$, we have

$$
\begin{aligned}
X_{4,c} = \rho \frac{4}{d} \Bigg(O^t \Bigg(2D \int_{\mathbb{H}_1} \mathbf{q}_1^2 (\mathbf{q}_1^2 - \mathbf{q}_2^2)\, H(\mathrm{Re}(\mathbf{q}))\, \mathrm{d}\mathbf{q} \\
+ 2\mathrm{Tr}(D)\mathrm{Id} \int_{\mathbb{H}_1} \mathbf{q}_1^2 \mathbf{q}_2^2\, H(\mathrm{Re}(\mathbf{q}))\, \mathrm{d}\mathbf{q} \Bigg) O\mathbf{e_1}(\bar{\mathbf{q}}) \Bigg) \bar{\mathbf{q}} \\
= \rho \frac{4}{d} \Bigg(\Bigg(2A^S(\bar{\mathbf{q}}) \int_{\mathbb{H}_1} \mathbf{q}_1^2 (\mathbf{q}_1^2 - \mathbf{q}_2^2)\, H(\mathrm{Re}(\mathbf{q}))\, \mathrm{d}\mathbf{q} \\
+ 2\mathrm{Tr}(A(\bar{\mathbf{q}}))\mathrm{Id} \int_{\mathbb{H}_1} \mathbf{q}_1^2 \mathbf{q}_2^2\, H(\mathrm{Re}(\mathbf{q}))\, \mathrm{d}\mathbf{q} \Bigg) \mathbf{e_1}(\bar{\mathbf{q}}) \Bigg) \bar{\mathbf{q}}.
\end{aligned}
$$

Finally, we obtain

$$
X_4 = \rho \frac{4}{d} \Big[C_3\, (\mathbf{e_1}(\bar{\mathbf{q}}) \cdot \nabla_x)\, \bar{\mathbf{q}} + \big(2C_4 A^S(\bar{\mathbf{q}})\mathbf{e_1}(\bar{\mathbf{q}}) + 2C_5 \mathrm{Tr}(A(\bar{\mathbf{q}}))\mathbf{e_1}(\bar{\mathbf{q}}) \big)\, \bar{\mathbf{q}} \Big],
$$

with

$$
\begin{aligned}
C_3 &= \int_{\mathbb{H}_1} \frac{(2\mathrm{Re}^2\mathbf{q} - 1)}{3} \left(1 - \mathrm{Re}^2\mathbf{q} \right)\, H(\mathrm{Re}(\mathbf{q}))\mathrm{d}\mathbf{q}, \\
C_4 &= \int_{\mathbb{H}_1} \mathbf{q}_1^2 (\mathbf{q}_1^2 - \mathbf{q}_2^2)\, H(\mathrm{Re}(\mathbf{q}))\, \mathrm{d}\mathbf{q}, \\
C_5 &= \int_{\mathbb{H}_1} \mathbf{q}_1^2 \mathbf{q}_2^2\, H(\mathrm{Re}(\mathbf{q}))\, \mathrm{d}\mathbf{q}.
\end{aligned}
$$

Recall that $2A^S(\bar{\mathbf{q}}) = A(\bar{\mathbf{q}}) + A(\bar{\mathbf{q}})^t$ with $A(\bar{\mathbf{q}})$ defined in (86). We compute

$$
\begin{aligned}
A(\bar{\mathbf{q}})\mathbf{e_1}(\mathbf{q}) &= \left(\sum_j \left(\partial_{x_j, \mathrm{rel}}\bar{\mathbf{q}} \right)_i (\mathbf{e_1}(\bar{\mathbf{q}}))_j \right)_{i=1,\dots,3} = ((\mathbf{e_1}(\bar{\mathbf{q}}) \cdot \nabla_x)\, \bar{\mathbf{q}})\, \bar{\mathbf{q}}^*, \\
A^t(\bar{\mathbf{q}})\mathbf{e_1}(\mathbf{q}) &= \left(\sum_j \left(\partial_{x_i, \mathrm{rel}}\bar{\mathbf{q}} \right)_j (\mathbf{e_1}(\bar{\mathbf{q}}))_j \right)_{i=1,\dots,3} = \nabla_{x,\mathrm{rel}}\bar{\mathbf{q}}\, \mathbf{e_1}(\bar{\mathbf{q}}), \\
\mathrm{Tr}(A(\bar{\mathbf{q}})) &= \sum_i \left(\partial_{x_i, \mathrm{rel}}\bar{\mathbf{q}} \right)_i = \nabla_{x,\mathrm{rel}} \cdot \bar{\mathbf{q}},
\end{aligned}
$$

thanks to (8)–(10). Therefore, we have that

$$
X_4 = \rho \frac{4}{d} \Big[(C_3 + C_4)\, (\mathbf{e_1}(\bar{\mathbf{q}}) \cdot \nabla_x)\, \bar{\mathbf{q}} + (C_4\, \nabla_{x,\mathrm{rel}}\bar{\mathbf{q}}\, \mathbf{e_1}(\bar{\mathbf{q}}) + 2C_5\, (\nabla_{x,\mathrm{rel}} \cdot \bar{\mathbf{q}})\, \mathbf{e_1}(\bar{\mathbf{q}}))\, \bar{\mathbf{q}} \Big].
$$

End of the proof. Finally, we conclude that $X = X_1 + X_2 + X_3 + X_4 = 0$ is equivalent to

$$
\begin{aligned}
0 = X = &\frac{4}{d} C_2 \rho \partial_t \bar{\mathbf{q}} + 2C_2(\mathbf{e_1}(\bar{\mathbf{q}}) \times \nabla_x \rho)\bar{\mathbf{q}} \\
&+ \rho \frac{4}{d} \Big[(C_3 + C_4)\, (\mathbf{e_1}(\bar{\mathbf{q}}) \cdot \nabla_x)\, \bar{\mathbf{q}} + (C_4\, \nabla_{x,\mathrm{rel}}\bar{\mathbf{q}}\, \mathbf{e_1}(\bar{\mathbf{q}}) + 2C_5\, (\nabla_{x,\mathrm{rel}} \cdot \bar{\mathbf{q}})\, \mathbf{e_1}(\bar{\mathbf{q}}))\, \bar{\mathbf{q}} \Big],
\end{aligned}
$$

so that

$$\rho\left[\partial_t\bar{\mathbf{q}} + \frac{C_3+C_4}{C_2}\left(\mathbf{e_1}(\bar{\mathbf{q}})\cdot\nabla_x\right)\bar{\mathbf{q}}\right] + \frac{d}{2}(\mathbf{e_1}(\bar{\mathbf{q}})\times\nabla_x\rho)\bar{\mathbf{q}}$$
$$+ \rho\left[\left(\frac{C_4}{C_2}\nabla_{x,\mathrm{rel}}\bar{\mathbf{q}}\,\mathbf{e_1}(\bar{\mathbf{q}}) + 2\frac{C_5}{C_2}\left(\nabla_{x,\mathrm{rel}}\cdot\bar{\mathbf{q}}\right)\mathbf{e_1}(\bar{\mathbf{q}})\right)\bar{\mathbf{q}}\right] = 0.$$

It remains to compute each one of the constants C_i, $i=1,\ldots,5$. For this we will use repeatedly the change of variable of Proposition A.3 and the following:

$$4\pi\int_0^\pi f(\theta)H(\cos(\theta/2))\sin^2(\theta/2)\mathrm{d}\theta = \langle f(\theta)\cos(\theta/2)h(\cos(\theta/2))\rangle_{m\,\sin^2(\theta/2)},$$

which is a direct consequence of the definitions (80), (36), and of (48).

We now compute

$$C_2 = \int_{\mathbb{H}_1}\frac{1-\mathrm{Re}^2(\mathbf{q})}{3}H(\mathrm{Re}(\mathbf{q}))\,\mathrm{d}\mathbf{q}$$
$$= 4\pi\int_0^\pi\frac{\sin^2(\theta/2)}{3}H(\cos(\theta/2))\sin^2(\theta/2)\,\mathrm{d}\theta$$
$$= \frac{1}{3}\langle\sin^2(\theta/2)\cos(\theta/2)h(\cos(\theta/2))\rangle_{m\,\sin^2(\theta/2)};$$

$$C_3 = \int_{\mathbb{H}_1}\frac{\left(2\mathrm{Re}^2\mathbf{q}-1\right)}{3}\left(1-\mathrm{Re}^2\mathbf{q}\right)H(\mathrm{Re}(\mathbf{q}))\mathrm{d}\mathbf{q}$$
$$= 4\pi\int_0^\pi\frac{(2\cos^2(\theta/2)-1)}{3}\sin^2(\theta/2)H(\cos(\theta/2))\sin^2(\theta/2)\,\mathrm{d}\theta$$
$$= \frac{1}{3}\langle(2\cos^2(\theta/2)-1)\sin^2(\theta/2)\cos(\theta/2)h(\cos(\theta/2))\rangle_{m\,\sin^2(\theta/2)};$$

$$C_5 = \int_{\mathbb{H}_1}\mathbf{q}_1^2\mathbf{q}_2^2\,H(\mathrm{Re}(\mathbf{q}))\,\mathrm{d}\mathbf{q}$$
$$= \int_{\mathbb{S}^2}\int_0^\pi(\sin(\theta/2)n_1)^2(\sin(\theta/2)n_2)^2H(\cos(\theta/2))\sin^2(\theta/2)\mathrm{d}\theta\mathrm{d}\mathbf{n}$$
$$= \left(\int_0^\pi\sin^4(\theta/2)H(\cos(\theta/2))\sin^2(\theta/2)\,\mathrm{d}\theta\right)\left(\int_0^\pi\int_0^{2\pi}\cos^2\theta_2\sin^2\theta_2\cos^2\theta_3\sin\theta_2\mathrm{d}\theta_3\mathrm{d}\theta_2\right)$$
$$= \frac{4\pi}{15}\left(\int_0^\pi\sin^4(\theta/2)H(\cos(\theta/2))\sin^2(\theta/2)\,\mathrm{d}\theta\right)$$
$$= \frac{1}{15}\langle\sin^4(\theta/2)\cos(\theta/2)h(\cos(\theta/2))\rangle_{m\,\sin^2(\theta/2)};$$

$$C_4 = \int_{\mathbb{H}_1}\mathbf{q}_1^2(\mathbf{q}_1^2-\mathbf{q}_2^2)\,H(\mathrm{Re}(\mathbf{q}))\,\mathrm{d}\mathbf{q}$$
$$= \int_{\mathbb{H}_1}\mathbf{q}_1^4H(\mathrm{Re}(\mathbf{q}))\,\mathrm{d}\mathbf{q} - C_5$$
$$= \left(\int_{\mathbb{S}^2}n_1^4\mathrm{d}\mathbf{n}\right)\left(\int_0^\pi\sin^4(\theta/2)H(\cos(\theta/2))\sin^2(\theta/2)\,\mathrm{d}\theta\right) - C_5$$

$$= \left(\frac{4\pi}{5} - \frac{4\pi}{15} \right) \int_0^\pi \sin^4(\theta/2) H(\cos(\theta/2)) \sin^2(\theta/2) \, \mathrm{d}\theta$$

$$= \frac{8\pi}{15} \int_0^\pi \sin^4(\theta/2) H(\cos(\theta/2)) \sin^2(\theta/2) \, \mathrm{d}\theta$$

$$= 2C_5.$$

We finally compute

$$c_2 := \frac{C_3 + C_4}{C_2} = 3 \left\langle \frac{2\cos^2(\theta/2) - 1}{3} + \frac{2}{15}\sin^2(\theta/2) \right\rangle_{m \sin^4(\theta/2) h(\cos(\theta/2)) \cos(\theta/2)}$$

$$= \frac{1}{5} \langle 1 + 4\cos\theta \rangle_{m \sin^4(\theta/2) h(\cos(\theta/2)) \cos(\theta/2)};$$

$$c_4 := \frac{C_4}{C_2} = 2\frac{C_5}{C_2} = \frac{2}{5} \langle \sin^2(\theta/2) \rangle_{\sin^4(\theta/2) m h(\cos(\theta/2)) \cos(\theta/2)}$$

$$= \frac{1}{5} \langle 1 - \cos\theta \rangle_{\sin^4(\theta/2) m h(\cos(\theta/2)) \cos(\theta/2)}. \qquad \square$$

5. Comparison with the results in [17]. In this section we compare the models presented here with those obtained for the body attitude coordination model in [17]. The crucial difference between the two approaches is that, while in [17] the representation of body attitudes relies on rotation matrices in $SO(3)$, here it relies on unitary quaternions in $\mathbb{H}_1$ (which are more computationally efficient).

After an introductory presentation of the links between $SO(3)$ and $\mathbb{H}_1$ (section 5.1), we present the two main results of this section: the equivalence between the individual-based models (Theorem 5.6 in section 5.2) and the equivalence between the macroscopic models (Theorem 5.13 in section 5.3).

5.1. Relation between unitary quaternions and rotation matrices. We first introduce some notation. Rotations in $\mathbb{R}^3$ can be described mathematically in different ways. In this section we consider three particular descriptions, namely, the group of orthonormal matrices corresponding to the rotation group $SO(3)$; the description via unitary quaternions $\mathbf{q} \in \mathbb{H}_1$; and, finally, rotations described by the pair $(\theta, \mathbf{n}) \in [0, \pi] \times \mathbb{S}^2$, where $\mathbf{n}$ indicates the axis of rotation and θ the angle of rotation counterclockwise around $\mathbf{n}$. For $A \in SO(3)$, $\mathbf{q} \in \mathbb{H}_1$, and $(\theta, \mathbf{n}) \in [0, \pi] \times \mathbb{S}^2$ corresponding to the same rotation, we have the identities

$$(87) \qquad A = A(\theta, \mathbf{n}) = \mathrm{Id} + \sin(\theta)[\mathbf{n}]_\times + (1 - \cos\theta)[\mathbf{n}]_\times^2 = \exp(\theta[\mathbf{n}]_\times)$$
$$\text{(Rodrigues's formula)},$$

$$(88) \qquad \mathbf{q} = \mathbf{q}(\theta, \mathbf{n}) = \cos(\theta/2) + \sin(\theta/2)\mathbf{n},$$

$$(89) \qquad A\mathbf{v} = \mathrm{Im}(\mathbf{q}\bar{\mathbf{v}}\mathbf{q}^*) \quad \text{(rotation of } \mathbf{v}) \text{ for any } \mathbf{v} \in \mathbb{R}^3,$$

where $\bar{\mathbf{v}} \in \mathbb{H}$ with $\mathrm{Re}(\bar{\mathbf{v}}) = 0$ and $\mathrm{Im}(\bar{\mathbf{v}}) = \mathbf{v}$, and where we abuse notation in (88) and understand $\mathbf{n}$ as written in the Hamiltonian basis $\mathbf{n} = n_1\vec{\imath} + n_2\vec{\jmath} + n_3\vec{k}$ rather than in the canonical basis $\mathbf{n} = (n_1, n_2, n_3)$. Notice that when $\theta = 0$, the vector $\mathbf{n}$ is not defined, but this does not pose a problem in the sense that there is an unambiguous correspondence with $A = \mathrm{Id}$ and $\mathbf{q} = 1$.

Define the operator $\Phi : \mathbb{H}_1 \to SO(3)$ by

$$(90) \qquad \Phi : \mathbb{H}_1 \longrightarrow SO(3), \ \mathbf{q} \mapsto (\Phi(\mathbf{q}) : \mathbf{u} \in \mathbb{R}^3 \mapsto \mathrm{Im}(\mathbf{q}\mathbf{u}\mathbf{q}^*) \in \mathbb{R}^3).$$

This operator associates to each unitary quaternion $\mathbf{q} \in \mathbb{H}_1$ the corresponding rotation matrix $A = \Phi(\mathbf{q}) \in SO(3)$. In particular, the following identities hold for any $\mathbf{q}, \mathbf{r} \in \mathbb{H}_1$:

$$(91) \qquad \qquad \text{(i)} \quad \text{Id} = \Phi(1);$$

$$(92) \qquad \qquad \text{(ii)} \quad \Phi(\mathbf{q}) = \Phi(-\mathbf{q});$$

$$(93) \qquad \qquad \text{(iii)} \quad \Phi(\mathbf{q}^*) = [\Phi(\mathbf{q})]^t\,;$$

$$(94) \qquad \qquad \text{(iv)} \quad \Phi(\mathbf{q})\Phi(\mathbf{r}) = \Phi(\mathbf{qr}).$$

Identities (ii) and (iv) are consequences of (89); identity (iii) is a consequence of (iv), noticing that $\mathbf{q}^* = \mathbf{q}^{-1}$ and $A^t = A^{-1}$.

First, we show the relation between the inner products in $SO(3)$ and $\mathbb{H}_1$.

LEMMA 5.1. *Let $A, B \in SO(3)$ and $\mathbf{q}, \mathbf{r} \in \mathbb{H}_1$ to be such that $A = \Phi(\mathbf{q})$ and $B = \Phi(\mathbf{r})$. Then*

$$(95) \qquad \frac{1}{2} A \cdot B = (\mathbf{q} \cdot \mathbf{r})^2 - \frac{1}{4} = \mathbf{q} \cdot \left(\mathbf{r} \otimes \mathbf{r} - \frac{1}{4}\text{Id} \right) \mathbf{q},$$

where $A \cdot B = \text{Tr}(AB^t)/2$, with Tr denoting the trace.

Proof. To check (95), we recast the inner products in $SO(3)$ and $\mathbb{H}_1$ in the variables $(\theta, \mathbf{n}) \in [0, \pi] \times \mathbb{S}^2$. By (93)–(94), it holds that $AB^t = \Phi(\mathbf{qr}^*) \in SO(3)$. Let $(\theta, \mathbf{n}) \in [0, \pi] \times \mathbb{S}^2$ be the angle and rotation axis representing the same rotation as AB^t (and $\mathbf{qr}^*$). We have that

$$\mathbf{q} \cdot \mathbf{r} = \text{Re}(\mathbf{qr}^*) = 1 \cdot \mathbf{qr}^* = \cos(\theta/2),$$

$$A \cdot B = \frac{1}{2}\text{Tr}(AB^t) = \text{Id} \cdot AB^t = \text{Id} \cdot \left(\text{Id} + \sin\theta[\mathbf{n}]_\times + (1 - \cos\theta)[\mathbf{n}]_\times^2 \right) = \frac{1}{2} + \cos\theta,$$

so

$$(\mathbf{q} \cdot \mathbf{r})^2 - \frac{1}{4} = \cos^2(\theta/2) - \frac{1}{4} = \frac{1 + \cos\theta}{2} - \frac{1}{4} = \frac{1}{4} + \frac{\cos\theta}{2} = \frac{1}{2} A \cdot B.$$

The second equality in (95) is obtained directly using that $|\mathbf{q}| = 1$. $\qquad \square$

Next, we establish the correspondence between integrals in $SO(3)$ and $\mathbb{H}_1$.

LEMMA 5.2 (comparison of volume elements). *Consider $g : SO(3) \to \mathbb{R}$. Then*

$$(96) \qquad \int_{SO(3)} g(A)\,\mathrm{d}A = \frac{1}{2\pi^2} \int_{\mathbb{H}_1} g(\Phi(\mathbf{q}))\,\mathrm{d}\mathbf{q},$$

where $\mathrm{d}\mathbf{q}$ is the Lebesgue measure on the hypersphere $\mathbb{H}_1$ and $\mathrm{d}A$ is the normalized Lebesgue measure on $SO(3)$.

Proof. We apply Proposition A.3 to the (even) function $f(\mathbf{q}) := g(\Phi(\mathbf{q}))$, to get

$$\int_{\mathbb{H}_1} g(\Phi(\mathbf{q}))\,\mathrm{d}\mathbf{q} = \int_0^\pi \sin^2(\theta/2) \int_{\mathbb{S}^2} g(\Phi(\cos(\theta/2) + \sin(\theta/2)\mathbf{n}))\,\mathrm{d}\theta\mathrm{d}\mathbf{n}.$$

Using Rodrigues's formula (87), it yields

$$\int_{\mathbb{H}_1} g(\Phi(\mathbf{q}))\,\mathrm{d}\mathbf{q} = \int_0^\pi \sin^2(\theta/2) \int_{\mathbb{S}^2} \tilde{g}(\theta, \mathbf{n})\,\mathrm{d}\mathbf{n}\mathrm{d}\theta,$$

where $\tilde{g}(\theta, \mathbf{n}) := g(\exp(\theta[\mathbf{n}]_\times))$.

On the other hand, from [17], we know that

$$\int_{SO(3)} g(A)\,\mathrm{d}A = \frac{1}{2\pi^2}\int_0^\pi \sin^2(\theta/2)\int_{\mathbb{S}^2} \tilde{g}(\theta,\mathbf{n})\mathrm{d}\mathbf{n}\mathrm{d}\theta \tag{97}$$

holds, and this concludes the proof.   □

Finally, one can check that Φ is continuously differentiable on $\mathbb{H}_1$, given that it is a quadratic function on $\mathbb{H}_1$. The following holds.

PROPOSITION 5.3. *Denoting* $\mathrm{D}_{\mathbf{q}}\Phi : \mathbf{q}^\perp \longrightarrow T_{\Phi(\mathbf{q})}$ *the differential of* Φ *at* $\mathbf{q}\in\mathbb{H}_1$, *we have that for any* $\mathbf{q}\in\mathbb{H}_1$ *and any vector* $\mathbf{u}\in\mathbb{R}^3$,

$$\mathrm{D}_{\mathbf{q}}\Phi(\mathbf{uq}) = 2\,[\mathbf{u}]_\times\,\Phi(\mathbf{q}). \tag{98}$$

Equivalently, since the tangent space at $\mathbf{q}\in\mathbb{H}_1$ *is exactly the set* $\mathbf{q}^\perp = \{\mathbf{uq},\ \mathbf{u}\in\mathbb{R}^3\}$ *(see Proposition* A.2*), we have that*

$$\mathrm{D}_{\mathbf{q}}\Phi(\mathbf{p}) = 2\,[\mathbf{pq}^*]_\times\,\Phi(\mathbf{q}) \qquad \textit{for all } \mathbf{p}\in\mathbf{q}^\perp. \tag{99}$$

Remark 5.4. From this relation, we can deduce the links between the gradient, divergence, and Laplacian operators in $SO(3)$ and $\mathbb{H}_1$; see Propositions B.1–B.3 in Appendix B.

Proof. The operator Φ in (90) is quadratic and associated to the symmetric bilinear operator Φ_{BL} defined, for $\mathbf{p}_1,\mathbf{p}_2\in\mathbb{H}$ and for $\mathbf{v}\in\mathbb{R}^3$, by

$$\Phi_{\mathrm{BL}}(\mathbf{p}_1,\mathbf{p}_2)(\mathbf{v}) = \mathrm{Im}(\mathbf{p}_1\mathbf{v}\mathbf{p}_2^*).$$

Note that this operator is indeed symmetric since $\mathrm{Im}(\mathbf{p}_2\mathbf{v}\mathbf{p}_1^*) = -\mathrm{Im}((\mathbf{p}_2\mathbf{v}\mathbf{p}_1^*)^*)$ and $\mathbf{v}^* = -\mathbf{v}$. We then use Proposition A.1 to conclude that, for any $\mathbf{q}\in\mathbb{H}_1$, any $\mathbf{p}_1 = \mathbf{uq}\in\mathbf{q}^\perp$ (with $\mathbf{u}\in\mathbb{R}^3$), and any $\mathbf{v}\in\mathbb{R}^3$,

$$\begin{aligned}
[\mathrm{D}_{\mathbf{q}}\Phi\,(\mathbf{uq})](\mathbf{v}) &= 2\Phi_{\mathrm{BL}}(\mathbf{uq},\mathbf{q})(\mathbf{v}) = 2\mathrm{Im}(\mathbf{uqvq}^*)\\
&= 2\mathbf{u}\times\mathrm{Im}(\mathbf{qvq}^*) = 2[\mathbf{u}]_\times\Phi(\mathbf{q})\mathbf{v}. \qquad \square
\end{aligned}$$

5.2. Equivalence between individual-based models. In this section we check that the flocking dynamic considered in [17] corresponds with that of (24)–(25).

In [17] the authors describe an individual-based model for body attitude coordination given by the evolution over time of $(X_k, A_k)_{k=1,\dots,N}$ of N agents, where $X_k\in\mathbb{R}^3$ is the position of agent k and $A_k\in SO(3)$ is a rotation matrix giving its body attitude. The evolution of the system is given by the following equations:

$$\mathrm{d}\mathbf{X_k}(t) = v_0 A_k(t)\mathbf{e_1}\mathrm{d}t, \tag{100}$$

$$\mathrm{d}A_k(t) = P_{T_{A_k}}\circ\left[\nu\mathrm{PD}(M_k)\mathrm{d}t + 2\sqrt{D}\mathrm{d}W_t^k\right], \tag{101}$$

where the stochastic differential equation is in the Stratonovich sense (see [28]); W_t^k is the Brownian motion in the space of squared matrices; M_k is defined as

$$M_k(t) := \frac{1}{N}\sum_{i=1}^N K(|\mathbf{X}_i(t)-\mathbf{X_k}(t)|)A_i(t), \tag{102}$$

where K is a positive interaction kernel; ν, v_0, and D are positive constants; $\mathbf{e_1}$ is a vector; and P_{T_A} is the projection in $SO(3)$ to the tangent space to A. The term $PD(M)$ denotes the orthogonal matrix obtained from the polar decomposition of M, which is defined as follows.

LEMMA 5.5 (polar decomposition of a square matrix [29]). *Given a matrix $M \in \mathcal{M}$, if $\det(M) \neq 0$, then there exists a unique orthogonal matrix $A = PD(M)$ (given by $A = M(\sqrt{M^t M})^{-1}$) and a unique symmetric positive definite matrix S such that $M = AS$.*

The vector $A_k \mathbf{e_1}$ in (100) gives the direction of movement of agent k and is obtained as the rotation of the vector $\mathbf{e_1}$ by A_k. Equivalently, we can express it as $A_k \mathbf{e_1} = \mathbf{e_1}(\mathbf{q}_k)$ (in the notation of (24)) as long as A_k and $\mathbf{q}_k$ represent the same rotation. Therefore, (24) and (100) represent the same dynamics, and we are left to check that $\mathbf{q}_k = \mathbf{q}_k(t)$ and $A_k = A_k(t)$ in (25) and (101) represent the same rotation for each time t where the solutions are defined.

The goal of this section will be to prove that the solution to the stochastic differential equation (24)–(25) and the solution of the stochastic differential equation (100)–(101) are the same in law (in a precise way that will be given later).

The main result of this section is the following.

THEOREM 5.6 (equivalence in law). *The processes (24)–(25) and (100)–(101) are the same in law.*

The proof is done at the end of this section. First, we remark that in the absence of randomness (Brownian motion) the equations for the evolution of the body attitude are equivalent.

PROPOSITION 5.7. *Let $A_0 \in SO(3)$ and $\mathbf{q}_0 \in \mathbb{H}_1$ represent the same rotation. Consider the matrix M_k given in (102), the matrix Q_k given in (20), and $\bar{\mathbf{q}}_k \in \mathbb{H}_1$ given in (19). Then, if $\det(M_k) > 0$, the following two Cauchy problems are equivalent (in the sense that $A_k = A_k(t)$ and $\mathbf{q}_k = \mathbf{q}_k(t)$ represent the same rotation for all t where the solution is uniquely defined):*

$$\frac{\mathrm{d}A_k}{\mathrm{d}t} = P_{T_{A_k}}(PD(M_k)), \qquad A_k(0) = A_0,$$
$$\frac{\mathrm{d}\mathbf{q}_k}{\mathrm{d}t} = P_{\mathbf{q}_k^\perp}\left[\left(\bar{\mathbf{q}}_k \otimes \bar{\mathbf{q}}_k - \frac{1}{4}\mathrm{Id}\right)\mathbf{q}_k\right], \qquad \mathbf{q}_k(0) = \mathbf{q}_0.$$

Note that these two Cauchy problems can also be written, respectively, as

$$\frac{\mathrm{d}A_k}{\mathrm{d}t} = \nabla_A\left[PD(M_k) \cdot A\right]_{|A=A_k}, \qquad A_k(0) = A_0,$$
$$\frac{\mathrm{d}\mathbf{q}_k}{\mathrm{d}t} = \frac{1}{4}\nabla_\mathbf{q}\left[2\mathbf{q} \cdot \left(\bar{\mathbf{q}}_k \otimes \bar{\mathbf{q}}_k - \frac{1}{4}\mathrm{Id}\right)\mathbf{q}\right]_{|\mathbf{q}=\mathbf{q}_k}, \qquad \mathbf{q}_k(0) = \mathbf{q}_0,$$

where ∇_A and $\nabla_\mathbf{q}$ are the gradients in $SO(3)$ and $\mathbb{H}_1$, respectively.

To prove this proposition we first check that the average orientation of the neighbors is the same in the two models, in the sense described below.

LEMMA 5.8. *Let $A_i = \Phi(\mathbf{q}_i)$ for $i = 1, \ldots, N$. Then, for every $k \in \{1, \ldots, N\}$, it holds that*

(103) $$PD(M_k) \cdot A_k = 2\mathbf{q}_k \cdot F_k(\mathbf{q}_k),$$

as long as $\det(M_k) > 0$, where M_k is defined in (102) and F_k is given in (22).

Proof. Assume for simplicity that $K \equiv 1$ (the general case can be proven equally). First, notice that for $A = \Phi(\mathbf{q})$ ($\mathbf{q} \in \mathbb{H}_1$) it holds that

$$M_k \cdot A = \frac{1}{N} \sum_{i=1}^{N} A_i \cdot A = \frac{1}{N} \sum_{i=1}^{N} \Phi(\mathbf{q}_i) \cdot \Phi(\mathbf{q}) = 2\mathbf{q} \cdot \left(\frac{1}{N} \sum_{i=1}^{N} \left(\mathbf{q}_i \otimes \mathbf{q}_i - \frac{1}{4}\mathrm{Id} \right) \right) \mathbf{q} = 2\mathbf{q} \cdot Q_k \mathbf{q}$$

for Q_k given in (20) and where we used Lemma 5.1 to compute the inner product. Therefore, for any $\mathbf{q} \in \mathbb{H}_1$,

$$2\mathbf{q} \cdot Q_k \mathbf{q} = M_k \cdot \Phi(\mathbf{q}).$$

Now, the definition of $\bar{\mathbf{q}}_k$ implies that it maximizes $\mathbf{q} \mapsto \mathbf{q} \cdot Q_k \mathbf{q}$ in $\mathbb{H}_1$. Since $\mathbf{q} \cdot Q_k \mathbf{q} = \frac{1}{2} M_k \cdot A$, this implies that $\Phi(\bar{\mathbf{q}}_k)$ maximizes $A \mapsto M_k \cdot A$ in $SO(3)$, which is a property that characterizes the matrix $PD(M_k)$ (see [17, Prop. 3.1]). Therefore, it holds that $\Phi(\bar{\mathbf{q}}_k) = PD(M_k)$, as long as $\det(M_k) > 0$, and in this case, using again Lemma 5.1, we have

$$(104) \qquad PD(M_k) \cdot A_k = \Phi(\bar{\mathbf{q}}_k) \cdot \Phi(\mathbf{q}_k) = 2\mathbf{q}_k \cdot \left(\left(\bar{\mathbf{q}}_k \otimes \bar{\mathbf{q}}_k - \frac{1}{4}\mathrm{Id} \right) \mathbf{q}_k \right). \qquad \square$$

We are now ready to prove Proposition 5.7.

Proof of Proposition 5.7. The fact that we can rewrite the first pair of Cauchy problems as the second pair comes from the equalities

$$(105) \qquad P_{T_A}(PD(M)) = \nabla_A(PD(M) \cdot A), \qquad P_{\mathbf{q}^\perp} F(\mathbf{q}) = \frac{1}{4} \nabla_{\mathbf{q}}(2\mathbf{q} \cdot F(\mathbf{q})),$$

where

$$F(\mathbf{q}) := \left(\bar{\mathbf{q}}_k \otimes \bar{\mathbf{q}}_k - \frac{1}{4}\mathrm{Id} \right) \mathbf{q}.$$

We conclude the equivalence thanks to Lemma 5.8 and Proposition B.1. $\qquad \square$

To prove Theorem 5.6 we need the following result.

PROPOSITION 5.9. *Let $\sigma > 0$, and let H be a time-dependent tangent vector field on $\mathbb{H}_1$:*

$$H : \mathbb{H}_1 \times [0, \infty) \to \mathbb{H} \quad \text{with} \quad H(\mathbf{q}, t) \in \mathbf{q}^\perp \text{ for all} \mathbf{q} \in \mathbb{H}_1, \, t \geq 0.$$

Let $\tilde{\sigma} > 0$, and let $\tilde{H}$ be a time-dependent tangent vector field on $SO(3)$:

$$\tilde{H} : SO(3) \times [0, \infty) \to M_3 \quad \text{with} \quad \tilde{H}(A, t) \in T_A \text{ for all} A \in SO(3), \, t \geq 0.$$

Suppose that the following relations hold:

$$(106) \qquad \tilde{H}(\Phi(\mathbf{q})) = \mathrm{D}_{\mathbf{q}} \Phi \left(H(\mathbf{q}) \right) \qquad \text{for all } \mathbf{q} \in \mathbb{H}_1$$

and

$$(107) \qquad \tilde{\sigma} = \sqrt{8}\, \sigma.$$

Let $\tilde{p}_t$ be the law over time of a stochastic process in $SO(3)$ defined by

$$\mathrm{d}A = \tilde{H}(A, t)\mathrm{d}t + \tilde{\sigma} P_{T_A} \circ \mathrm{d}\tilde{B}_t$$

for $\tilde{B}_t$ a 9-dimensional Brownian motion. Then, if $\tilde{p}_t$ is an absolutely continuous measure, the absolutely continuous measure p_t defined by

$$(108) \qquad \tilde{p}_t(\Phi(\mathbf{q})) = 2\pi^2 p_t(\mathbf{q}) \quad \textit{for all } \mathbf{q} \in \mathbb{H}_1,\, t \geq 0,$$

is the law over time of a stochastic process in $\mathbb{H}_1$ defined by

$$(109) \qquad d\mathbf{q} = H(\mathbf{q}, t)dt + \sigma P_{\mathbf{q}^\perp} \circ dB_t$$

for B_t a 4-dimensional Brownian motion.

Proof. First, notice that for any Borel set $B \subset \mathbb{H}_1$ it holds that

$$\int_{\Phi(B)} \tilde{p}_t(A)\, dA = \int_B p_t(\mathbf{q})\, d\mathbf{q}$$

thanks to Lemma 5.2. Note that this is the reason why we introduce the factor $2\pi^2$ in (108), which allows us to have this equivalence of integrals. We start from the equation for $\tilde{p}_t$:

$$(110) \qquad \partial_t \tilde{p}_t(A) + \nabla_A \cdot \big(\tilde{H}(A, t)\, \tilde{p}_t(A) \big) = \frac{\tilde{\sigma}^2}{4} \Delta_A\, \tilde{p}_t(A).$$

Notice that the fact that we obtain a factor $\tilde{\sigma}^2/4$ is a consequence of considering the inner product $A \cdot B = \text{trace}(A^t B)/2$ (see [17]). By Proposition B.2 we have that

$$\nabla_A \cdot \big(\tilde{H}(\cdot, t)\, \tilde{p}_t \big)(\Phi(\mathbf{q})) = \nabla_{\mathbf{q}} \cdot \big(H(\mathbf{q}, t)\, 2\pi^2 p_t(\mathbf{q}) \big),$$

and by Proposition B.3 we have that

$$\Delta_A\, \tilde{p}_t(\Phi(\mathbf{q})) = \frac{1}{4} \Delta_{\mathbf{q}}\, (2\pi^2 p_t(\mathbf{q})).$$

Therefore, we recast (110) into

$$\partial_t p_t(\mathbf{q}) + \nabla_{\mathbf{q}} \cdot \big(H(\mathbf{q}, t)\, p_t(\mathbf{q}) \big) = \frac{\tilde{\sigma}^2}{16} \Delta_{\mathbf{q}}\, p_t(\mathbf{q}).$$

Consequently, p_t is the law of the process

$$d\mathbf{q} = H(\mathbf{q}, t)\, dt + \frac{\tilde{\sigma}}{\sqrt{8}} P_{\mathbf{q}^\perp} \circ dB_t,$$

which is exactly (109) thanks to (107). $\qquad\qquad\square$

Finally we are ready to prove Theorem 5.6.

Proof of Theorem 5.6. Using Proposition B.1, we deduce from (103) that

$$(111) \qquad \nabla_A\, (PD(M_k) \cdot A)|_{A=A_k} = D_{\mathbf{q}} \Phi \left(\frac{1}{2}\, \nabla_{\mathbf{q}}\, (\mathbf{q} \cdot F_k)|_{\mathbf{q}=\mathbf{q}_k} \right),$$

which, thanks to (105), can be rewritten as

$$(112) \qquad P_{T_{A_k}}\, (PD(M_k)) = D_{\mathbf{q}} \Phi \left(P_{\mathbf{q}_k^\perp} F_k \right).$$

The condition (106) in Proposition 5.9 is then satisfied with $\tilde{H}(A) = P_{T_A}\, (PD(M_k))$ and $H(\mathbf{q}) = P_{\mathbf{q}^\perp} F(\mathbf{q})$, so that, proceeding similarly as in Proposition 5.9 for the N-particles system, we conclude the result. $\qquad\square$

5.3. Comparison of the macroscopic model with (13)–(14). In this section we show the equivalence between the macroscopic system (33)–(34) (or, equivalently, (12) for the last expression), expressed in terms of unitary quaternions, and the system (13)–(14), expressed in term of rotation matrices from [17].

Recall Φ, the natural map between unitary quaternions and rotation matrices defined in (90). We first notice that if $\mathbf{q}$ and Λ represent the same rotation (that is, if $\Phi(\mathbf{q}) = \Lambda$), then

$$\Lambda \mathbf{e_1} = \mathbf{e_1}(\bar{\mathbf{q}}).$$

Therefore, the continuity equations (5) and (13) represent the same dynamics (it is direct from their definitions in (37) and in [17] that the constants c_1 and $\tilde{c}_1$ are identical). We are left with comparing the various differential operators in $\bar{\mathbf{q}}$ and Λ in (12) and (14).

5.3.1. Relation between the differential operators δ_x, $\mathbf{r}_x$, and ∂_{rel}.

PROPOSITION 5.10. *Let $\bar{\mathbf{q}} = \bar{\mathbf{q}}(t, x)$ be a function on $\mathbb{R}_+ \times \mathbb{R}^3$ with values in $\mathbb{H}_1$. We define $\Lambda = \Phi(\bar{\mathbf{q}})$ the matrix representation of the rotation represented by $\bar{\mathbf{q}}$. Let $\mathbf{v} = \mathbf{v}(t, x)$ be a vector field in $\mathbb{R}^3$. Then we have the following equalities (everywhere on $\mathbb{R}_+ \times \mathbb{R}^3$):*

$$(113) \qquad\qquad (\partial\Lambda)\,\Lambda^t = 2\Big[\partial_{\mathrm{rel}}\bar{\mathbf{q}}\Big]_\times \quad \text{for } \partial \in \{\partial_t, \partial_{x_1}, \partial_{x_2}, \partial_{x_3}\},$$

$$(114) \qquad\qquad \mathscr{D}_x(\Lambda) = 2(\nabla_{x,\mathrm{rel}}\bar{\mathbf{q}})^t,$$

$$(115) \qquad\qquad \delta_x(\Lambda) = 2\nabla_{x,\mathrm{rel}} \cdot \bar{\mathbf{q}},$$

$$(116) \qquad\qquad \mathbf{v} \times \mathbf{r}_x(\Lambda) = 2\,(\nabla_{x,\mathrm{rel}}\bar{\mathbf{q}})\,\mathbf{v} - 2\,(\mathbf{v} \cdot \nabla_{x,\mathrm{rel}})\,\bar{\mathbf{q}},$$

where the operators $\nabla_{x,\mathrm{rel}}$ and $\nabla_{x,\mathrm{rel}}\cdot$ are defined in (8)–(9).

Proof. Equation (113) is obtained by first differentiating the equality $\Lambda = \Phi(\bar{\mathbf{q}})$,

$$\partial\Lambda = \mathrm{D}_{\mathbf{q}}\Phi_{|\bar{\mathbf{q}}}(\partial\bar{\mathbf{q}}),$$

then using (99),

$$\partial\Lambda = 2\Big[(\partial\bar{\mathbf{q}})\,\bar{\mathbf{q}}^*\Big]_\times \Lambda = 2\Big[\partial_{\mathrm{rel}}\bar{\mathbf{q}}\Big]_\times \Lambda.$$

Let $\mathbf{w} \in \mathbb{R}^3$. We compute

$$\begin{aligned}
[(\nabla_{x,\mathrm{rel}}\bar{\mathbf{q}})^t\mathbf{w}]_\times \Lambda &= [((\mathbf{w} \cdot \nabla_x)\bar{\mathbf{q}})\bar{\mathbf{q}}^*]_\times \Lambda \\
&= \sum_{i=1,2,3} w_i\,[(\partial_{x_i}\bar{\mathbf{q}})\bar{\mathbf{q}}^*]_\times \Lambda \\
&= \frac{1}{2}\sum_{i=1,2,3} w_i\partial_{x_i}\Lambda \\
&= \frac{1}{2}(\mathbf{w} \cdot \nabla_x)\Lambda,
\end{aligned}$$

where we have used successively the definition of ∂_{rel}, the fact that in components $\mathbf{w} = (w_1, w_2, w_3)$, and (113). Recall that since $\partial_{x_i}\bar{\mathbf{q}}$ is orthogonal to $\bar{\mathbf{q}}$, the product $\partial_{\mathrm{rel},x_i} = (\partial_{x_i}\bar{\mathbf{q}})\bar{\mathbf{q}}^*$ is purely imaginary and can be identified with a vector in $\mathbb{R}^3$, so all the above terms make sense. Recall now the definition of $\mathscr{D}_x(\Lambda)$ in (16); we have just proved (114).

We now use (114) and the definitions of δ_x and $\mathbf{r}_x$ in (17) to verify

$$\delta_x(\Lambda) = \mathrm{Tr}\left(\mathscr{D}_x(\Lambda)\right) = 2\mathrm{Tr}\left(\nabla_{x,\mathrm{rel}}\bar{\mathbf{q}}\right) = 2\nabla_{x,\mathrm{rel}} \cdot \bar{\mathbf{q}}$$

and

$$\mathbf{v} \times \mathbf{r}_x(\Lambda) = -[\mathbf{r}_x(\Lambda)]_\times \mathbf{v} = -\mathscr{D}_x(\Lambda)\mathbf{v} + \mathscr{D}_x(\Lambda)^t\mathbf{v} = -2\left(\mathbf{v} \cdot \nabla_{x,\mathrm{rel}}\right)\bar{\mathbf{q}} + 2\left(\nabla_{x,\mathrm{rel}}\bar{\mathbf{q}}\right) \cdot \mathbf{v},$$

which concludes the result. $\square$

5.3.2. Interpretation in terms of a local vector b. In [17], an interpretation in terms of a locally defined vector field $\mathbf{b}$ was proposed for the operators $\delta_x(\Lambda)$ and $\mathbf{r}_x(\Lambda)$. We summarize it here: Let $(t_0, x_0) \in \mathbb{R}_+ \times \mathbb{R}^3$ be fixed. When $\Lambda = \Lambda(t,x)$ is smooth enough, we can write

(117) $$\Lambda(t,x) = \exp\left([2\mathbf{b}(t,x)]_\times\right)\Lambda(t_0,x_0),$$

with $\mathbf{b}(t,x)$ a uniquely defined vector in $\mathbb{R}^3$, smooth around (t_0, x_0), and with $\mathbf{b}(t_0,x_0) = 0$. Then
(118)
$$\delta_x(\Lambda)(t_0,x_0) = 2\left.\nabla_x \cdot \mathbf{b}(x)\right|_{|(t,x)=(t_0,x_0)} \quad \text{and} \quad \mathbf{r}_x(\Lambda)(t_0,x_0) = 2\left.\nabla_x \times \mathbf{b}(x)\right|_{|(t,x)=(t_0,x_0)},$$

where $\nabla_x \times$ is the curl operator.

We propose a similar interpretation for our model. Let $(t_0, x_0) \in \mathbb{R}_+ \times \mathbb{R}^3$ be fixed. We define $\mathbf{r} = \mathbf{r}(t,x)$ similarly as in (11):

(119) $$\bar{\mathbf{q}}(t,x) = \mathbf{r}(t,x)\bar{\mathbf{q}}(t_0,x_0).$$

Since $\mathbf{r} \in \mathbb{H}_1$, its logarithm is a purely imaginary quaternion $\mathbf{b} = \mathbf{b}(t,x)$ with $\mathbf{b}(t_0,x_0) = 0$. With this notation, we recast (119) into

$$\bar{\mathbf{q}}(t,x) = \exp(\mathbf{b}(t,x))\bar{\mathbf{q}}(t_0,x_0),$$

and differentiating with respect to any variable ($\partial \in \{\partial_t, \partial_{x_1}, \partial_{x_2}, \partial_{x_3}\}$), by definition of ∂_{rel},

(120) $$\partial_{\mathrm{rel}}\bar{\mathbf{q}}(t_0,x_0) = \left.(\partial \exp(\mathbf{b}))\right|_{(t,x)=(t_0,x_0)} = \left.(\partial\mathbf{b})\right|_{(t,x)=(t_0,x_0)}.$$

Note that if Λ and $\bar{\mathbf{q}}$ represent the same rotation, that is, if $\Lambda = \Phi(\bar{\mathbf{q}})$, applying the morphism Φ to (119), we end up with

$$\Lambda(t,x) = \Phi(\exp(\mathbf{b}(t,x)))\Lambda(t_0,x_0).$$

We have that $\mathbf{b} = \theta\mathbf{n}/2$ in the Euler axis-angle representation (see (2) and (87)), where $\theta \in [0,2\pi]$ and $\mathbf{n}$ is a unitary vector in $\mathbb{R}^3$. The unitary quaternion $\exp(\mathbf{b}) = \exp(\theta\mathbf{n}/2)$ represents the rotation of angle θ counterclockwise around the axis $\mathbf{n}$, whose matrix representation is the corresponding matrix formulation, given by Rodrigues's formula (equation (87)),

$$\Phi(\exp(\mathbf{b})) = \exp(2[\mathbf{b}]_\times),$$

which implies that

$$\Lambda(t,x) = \exp(2[\mathbf{b}]_\times)\Lambda(t_0,x_0),$$

and we recover (117).

Remark 5.11. The combination of (118) and (120) gives an alternative proof of (115) and (116).

5.3.3. Summary: Comparison between quaternions, matrices, and b.
We summarize the discussion of the two previous paragraphs in the following.

PROPOSITION 5.12. *Let $\rho = \rho(t,x)$ and $\bar{\mathbf{q}} = \bar{\mathbf{q}}(t,x)$ be two functions on $\mathbb{R}_+ \times \mathbb{R}^3$ with values in $\mathbb{R}_+$ and $\mathbb{H}_1$, respectively. We define $\Lambda = \Phi(\bar{\mathbf{q}})$ the matrix representation of the rotation represented by $\bar{\mathbf{q}}$. For any fixed $t_0 \in \mathbb{R}_+$, $x_0 \in \mathbb{R}^3$, we also define the vector field $\mathbf{b}^{t_0,x_0} = \mathbf{b}^{t_0,x_0}(t,x)$ as*

$$\mathbf{b}^{t_0,x_0}(t,x) = \log[\bar{\mathbf{q}}(t,x)\bar{\mathbf{q}}(t_0,x_0)^*].$$

Finally we define the velocity vector field

$$\mathbf{v} = \mathbf{e_1}(\bar{\mathbf{q}}) = \Lambda \mathbf{e_1}.$$

Then the following equivalence table holds:

i	Quaternion	Vector $\mathbf{b}$ locally at point (t_0,x_0)	Orthonormal matrix
1	$X_{\mathbf{q},1} := 2\rho\partial_{t,\mathrm{rel}}\bar{\mathbf{q}}$	$X_{\mathbf{b},1}^{t_0,x_0} := 2\rho\partial_t \mathbf{b}^{t_0,x_0}$	$X_{\Lambda,1} := \rho\,(\partial_t\Lambda)\,\Lambda^t$
2	$X_{\mathbf{q},2} := 2\rho(\mathbf{e_1}(\bar{\mathbf{q}})\cdot\nabla_{x,\mathrm{rel}})\bar{\mathbf{q}}$	$X_{\mathbf{b},2}^{t_0,x_0} := 2\rho\,(\mathbf{v}\cdot\nabla_x)\,\mathbf{b}^{t_0,x_0}$	$X_{\Lambda,2} := \rho\left(((\Lambda\mathbf{e_1})\cdot\nabla_x)\Lambda\right)\Lambda^t$
3	$X_{\mathbf{q},3} := \mathbf{e_1}(\bar{\mathbf{q}})\times\nabla_x\rho$	$X_{\mathbf{b},3}^{t_0,x_0} := \mathbf{v}\times\nabla_x\rho$	$X_{\Lambda,3} := [(\Lambda\mathbf{e_1})\times\nabla_x\rho]_\times$
4	$X_{\mathbf{q},4} := 2\rho\left(\nabla_{x,\mathrm{rel}}\bar{\mathbf{q}}\right)\mathbf{e_1}(\bar{\mathbf{q}})$	$X_{\mathbf{b},4}^{t_0,x_0} := 2\rho\left(\nabla_x\mathbf{b}^{t_0,x_0}\right)\mathbf{v}$	$X_{\Lambda,4} := \rho\left[(\Lambda\mathbf{e_1})\times\mathbf{r}_x(\Lambda)\right]_\times$ $\qquad +X_{\Lambda,2}$
5	$X_{\mathbf{q},5} := 2\rho\left(\nabla_{x,\mathrm{rel}}\cdot\bar{\mathbf{q}}\right)\mathbf{e_1}(\bar{\mathbf{q}})$	$X_{\mathbf{b},5}^{t_0,x_0} := 2\rho\left(\nabla_x\cdot\mathbf{b}^{t_0,x_0}\right)\mathbf{v}$	$X_{\Lambda,5} := [\rho\,\delta_x(\Lambda)\Lambda\mathbf{e_1}]_\times$

The equivalence is to be read in the following sense: For $i = 1,\ldots,5$, we have, everywhere on $\mathbb{R}_+ \times \mathbb{R}^3$,

(121) $$X_{\mathbf{q},i}(t_0,x_0) = X_{\mathbf{b},i}^{t_0,x_0}(t_0,x_0) \qquad \text{and} \qquad X_{\Lambda,i} = [X_{\mathbf{q},i}]_\times.$$

As a consequence, the following holds.

THEOREM 5.13. *Let $\rho_0 = \rho_0(x) \geq 0$. Let $\bar{\mathbf{q}}_0 = \bar{\mathbf{q}}_0(x) \in \mathbb{H}_1$ and $\Lambda_0 = \Lambda_0(x) \in SO(3)$ represent the same rotation, i.e., $\Lambda_0(x) = \Phi(\bar{\mathbf{q}}_0(x))$ for all $x \in \mathbb{R}^3$. Then the system (5)–(6) and the system (13)–(14) are equivalent (in the sense that any solution $(\rho,\bar{\mathbf{q}})$ of (5)–(6) gives a solution $(\rho,\Lambda = \Phi(\bar{\mathbf{q}}))$ of the system (13)–(14)).*

Proof. We already checked that the continuity equations (5) and (13) are equivalent. Using the notation of Proposition 5.12, we recast, after multiplying by 2, (12) for $\bar{\mathbf{q}}$ (which is equivalent to (6)) into

(122) $$X_{\mathbf{q},1} + c_2 X_{\mathbf{q},2} + 2\,c_3 X_{\mathbf{q},3} + c_4 X_{\mathbf{q},4} + c_4 X_{\mathbf{q},5} = 0,$$

and (14) for Λ into

(123) $$X_{\Lambda,1} + (\tilde{c}_2 - \tilde{c}_4)X_{\Lambda,2} + \tilde{c}_3 X_{\Lambda,3} + \tilde{c}_4 X_{\Lambda,4} + \tilde{c}_4 X_{\Lambda,5} = 0,$$

where (see [17])

$$\tilde{c}_3 = d,$$
$$\tilde{c}_2 = \tfrac{1}{5}\langle 2 + 3\cos\theta\rangle_{\widetilde{m}(\theta)\sin^2(\theta/2)},$$
$$\tilde{c}_4 = \tfrac{1}{5}\langle 1 - \cos\theta\rangle_{\widetilde{m}(\theta)\sin^2(\theta/2)},$$

and where the notation $\langle\cdot\rangle_{\widetilde{m}(\theta)\sin^2(\theta/2)}$ is given in (36). The function $\widetilde{m} : (0,\pi) \to (0,+\infty)$ is given by

$$(124) \qquad\qquad \widetilde{m}(\theta) := \sin^2\theta\, m(\theta)\, k(\theta),$$

where $m(\theta) = \exp\left(d^{-1}(\frac{1}{2} + \cos\theta)\right)$ is the same as in (41) and k is the solution of (142).

To check that (122)–(123) are equivalent, it suffices to show the correspondence between the constants since the equivalence of the terms is already given by (121). Therefore, we are left to check that $\tilde{c}_2 - \tilde{c}_4 = c_2$ and $\tilde{c}_4 = c_4$.

Recall the values of the constants

$$c_3 = \frac{d}{2},$$

$$c_2 = \frac{1}{5}\langle 1 + 4\cos\theta\rangle_{m(\theta)\sin^4(\theta/2)h(\cos(\theta/2))\cos(\theta/2)},$$

$$c_4 = \frac{1}{5}\langle 1 - \cos\theta\rangle_{m(\theta)\sin^4(\theta/2)h(\cos(\theta/2))\cos(\theta/2)}.$$

Using Proposition C.1, we have

$$(125) \qquad\qquad k(\theta) = 4\,\frac{h\left(\cos(\theta/2)\right)}{\cos(\theta/2)},$$

so that

$$\begin{aligned}
\widetilde{m}(\theta)\sin^2(\theta/2) &= \sin^2\theta\, m(\theta)\, k(\theta)\sin^2(\theta/2) \\
&= 4\,\frac{h\left(\cos(\theta/2)\right)}{\cos(\theta/2)}\sin^2\theta\, m(\theta)\,\sin^2(\theta/2) \\
&= 16\, h\left(\cos(\theta/2)\right)\cos(\theta/2)m(\theta)\,\sin^4(\theta/2).
\end{aligned}$$

Therefore, we have that

$$\langle\cdot\rangle_{\widetilde{m}(\theta)\sin^2(\theta/2)} = \langle\cdot\rangle_{m(\theta)\,\sin^4(\theta/2)\,h(\cos(\theta/2))\,\cos(\theta/2)}$$

(notice that the constant 16 is simplified), which allows us to conclude the equivalence of the constants, and hence of the equations. $\qquad\square$

6. Conclusion. In the present work we have introduced a flocking model for body attitude coordination where the body attitude is described through rotations represented by unitary quaternions. The deliberate choice of representing rotations by unitary quaternions is based on their numerical efficiency in terms of memory usage and operation complexity. This will be key for future applications of this model. At the modeling level, we introduce an individual-based model where agents try to coordinate their bodies' attitudes with those of their neighbors. To express this we needed to define an appropriate "averaged" quaternion based on nematic alignment. This average is related to the Gennes Q-tensor that appears in liquid crystal theory. From the individual-based model we have derived the macroscopic equations (SOHQ) via the mean-field equations. We also show the equivalence between the SOHQ and the macroscopic equations (SOHB) of [17] where the body attitude is expressed through rotation matrices. However, we observe that the SOHQ is simpler to interpret than the equivalent SOHB. In particular, all the terms in the SOHQ are explicit. We have also seen that the dynamics of the SOHQ system are more complex than those of the

SOH system (macroscopic equations corresponding to the Vicsek model). The body attitude coordination model presented here opens many questions and perspectives. We refer the reader to [17, Conclusions and open questions] for an exposition.

One may wonder why we did not consider translating the results in [17] for rotation matrices directly into quaternions. The answer is that, first, for the individual-based model, it is not possible to obtain a direct translation, in the sense that we need to consider some particular modeling choices (like the average in (21) and the relaxation in (23)) and check a posteriori the equivalence with the model in [17]. Second, the relation at the macroscopic level is not easy to obtain a priori. It is the macroscopic limit that gives us the necessary information and intuition to establish the link between both results.

In a future work, we will carry out simulations of the individual-based model and the SOHQ model, study the patterns that arise, and compare them with those of the Vicsek and SOH models.

Data statement. No new data was generated in the course of this research.

Conflict of interest. The authors declare that they have no conflict of interest.

Appendix A. Unitary quaternions: Some properties.

PROPOSITION A.1. *Let Q be a symmetric 4×4 matrix. For the function $\mathbf{q} \in \mathbb{H}_1 \mapsto (\mathbf{q} \cdot Q\mathbf{q})$, we have*

$$(126) \qquad \nabla_{\mathbf{q}}(\mathbf{q} \cdot Q\mathbf{q}) = 2P_{\mathbf{q}^\perp}(Q\mathbf{q}),$$

where $\nabla_{\mathbf{q}}$ is the gradient in $\mathbb{H}_1$.

Proof. Consider a path in $\mathbb{H}_1$ parametrized by $\varepsilon > 0$, $\mathbf{q} = \mathbf{q}(\varepsilon)$, where $\mathbf{q}(0) = \mathbf{q}$ and $\frac{d}{d\varepsilon}\mathbf{q}(\varepsilon)\big|_{\varepsilon=0} = \delta_{\mathbf{q}} \in T_{\mathbf{q}}$. Then

$$
\begin{aligned}
\partial_{\mathbf{q}}(\mathbf{q} \cdot Q\mathbf{q}) \cdot \delta_{\mathbf{q}} &= \lim_{\varepsilon \to 0} \frac{\mathbf{q}(\varepsilon) \cdot Q(\varepsilon)\mathbf{q}(\varepsilon) - \mathbf{q} \cdot Q\mathbf{q}}{\varepsilon} \\
&= \lim_{\varepsilon \to 0} \delta_{\mathbf{q}} \cdot Q\mathbf{q} + \mathbf{q} \cdot Q\delta_{\mathbf{q}} + \mathcal{O}(\varepsilon) \\
&= 2\delta_{\mathbf{q}} \cdot Q\mathbf{q},
\end{aligned}
$$

from which we conclude the result. □

PROPOSITION A.2. *Let $\mathbf{q} \in \mathbb{H}_1$. The tangent space $T_{\mathbf{q}}$ at $\mathbf{q}$ in $\mathbb{H}_1$ corresponds to $\mathbf{q}^\perp$ (the orthogonal space to $\mathbf{q}$). Particularly, it holds that*

$$(127) \qquad \mathbf{q}^\perp = \{\mathbf{v}\mathbf{q}, \ for \ \mathbf{v} \in \mathbb{R}^3\},$$

considering the abuse of notation explained in Remark 2.1.

Proof. The fact that $T_{\mathbf{q}} = \mathbf{q}^\perp$ can be seen by identifying $\mathbb{H}_1$ with the unit sphere $\mathbb{S}^3$. Since $\mathbf{q}$ is invertible, we have

$$\mathbb{H} = \{\mathbf{p}\mathbf{q} \text{ for } \mathbf{p} \in \mathbb{H}\},$$

and for any $\mathbf{p} \in \mathbb{H}$, we have

$$\mathbf{p}\mathbf{q} \in \mathbf{q}^\perp \iff (\mathbf{p}\mathbf{q}) \cdot \mathbf{q} = 0 \iff \operatorname{Re}(\mathbf{p}) = 0 \iff \mathbf{p} = \operatorname{Im}(\mathbf{p}) = \mathbf{v} \in \mathbb{R}^3. \qquad \square$$

PROPOSITION A.3 (decomposition of the volume form in $\mathbb{H}_1$). *Let $f = f(\mathbf{q})$ be a function on $\mathbb{H}_1$. Recall the parametrization in (2),*

$$\mathbf{q} = \cos\frac{\theta}{2} + \sin\frac{\theta}{2}\left(n_1\vec{\imath} + n_2\vec{\jmath} + n_3\vec{k}\right),$$

where $\mathbf{n} := (n_1, n_2, n_3)$ is a unitary vector in $\mathbb{R}^3$ and $\theta \in [0, 2\pi]$. Let

$$\bar{f}(\theta, \mathbf{n}) = f(\cos(\theta/2) + \sin(\theta/2)\mathbf{n}).$$

Then we have the following change of variable:

$$\int_{\mathbb{H}_1} f(\mathbf{q})\,\mathrm{d}\mathbf{q} = \int_0^{2\pi} \frac{\sin^2(\theta/2)}{2} \int_{\mathbb{S}^2} \bar{f}(\theta, \mathbf{n})\,\mathrm{d}\theta\mathrm{d}\mathbf{n},$$

where $\mathrm{d}\mathbf{q}$ is the Lebesgue measure on the hypersphere $\mathbb{H}_1$ and $\mathrm{d}\mathbf{n}$ is the Lebesgue measure on the sphere $\mathbb{S}^2$. In particular, if $f(\mathbf{q}) = f(-\mathbf{q})$, we have

$$\int_{\mathbb{H}_1} f(\mathbf{q})\,\mathrm{d}\mathbf{q} = \int_0^{\pi} \sin^2(\theta/2) \int_{\mathbb{S}^2} \bar{f}(\theta, \mathbf{n})\,\mathrm{d}\theta\mathrm{d}\mathbf{n},$$

and if furthermore $\bar{f}(\theta, \mathbf{n}) = \bar{f}(\theta)$ is independent of $\mathbf{n}$, we have

$$\int_{\mathbb{H}_1} f(\mathbf{q})\,\mathrm{d}\mathbf{q} = 4\pi \int_0^{\pi} \sin^2(\theta/2)\bar{f}(\theta)\,\mathrm{d}\theta.$$

Proof. We consider the following change of variables for $\mathbf{q} = (q_1, q_2, q_3, q_4)$ corresponding to the spherical coordinates on the 4-dimensional sphere:

$$\begin{aligned}
q_1 &= \cos(\theta/2), \\
q_2 &= \sin(\theta/2)\cos\theta_2, \\
q_3 &= \sin(\theta/2)\sin\theta_2\cos\theta_3, \\
q_4 &= \sin(\theta/2)\sin\theta_2\sin\theta_3
\end{aligned}$$

for $\theta \in [0, 2\pi]$, $\theta_2 \in [0, \pi]$, $\theta_3 \in [0, 2\pi)$. Then we have that

(128) $$\mathrm{d}\mathbf{q} = \frac{1}{2}\sin^2(\theta/2)\sin\theta_2\mathrm{d}\theta\mathrm{d}\theta_2\mathrm{d}\theta_3$$

by computing the Jacobian of this change of variables. However, $\mathbf{n} \in \mathbb{S}^2$ can be parametrized as

$$\mathbf{n} = \begin{bmatrix} 0 \\ \cos\theta_2 \\ \sin\theta_2\cos\theta_3 \\ \sin\theta_2\sin\theta_3 \end{bmatrix},$$

and $\mathrm{d}\mathbf{n} = \sin\theta_2\mathrm{d}\theta_2\mathrm{d}\theta_3$. Substituting this into (128), we conclude the proposition. $\square$

Appendix B. Differential operators on $SO(3)$ and on $\mathbb{H}_1$. The next three propositions explain the relation between the gradient, divergence, and Laplacian operators in $SO(3)$ and $\mathbb{H}_1$.

PROPOSITION B.1 (comparison of the gradient operator). *Consider a scalar function $g : SO(3) \to \mathbb{R}$ differentiable and define the function $f : \mathbb{H}_1 \to \mathbb{R}$ as $f(\mathbf{q}) = g(\Phi(\mathbf{q}))$. It holds that*

$$(129) \qquad (\nabla_A g)(\Phi(\mathbf{q})) = \frac{1}{4} D_{\mathbf{q}} \Phi(\nabla_{\mathbf{q}} f(\mathbf{q})),$$

or, equivalently, for any $\mathbf{u} \in \mathbb{R}^3$,

$$(130) \qquad \langle \nabla_{\mathbf{q}} f(\mathbf{q}), \mathbf{u}\mathbf{q} \rangle_{\mathbb{H}_1} = 2 \langle \nabla_A g(\Phi(\mathbf{q})), [\mathbf{u}]_\times \Phi(\mathbf{q}) \rangle_{SO(3)},$$

where $\langle \cdot, \cdot \rangle$ indicates the dot product and the subindex associated indicates to which space it corresponds.

Particularly, consider the following Cauchy problems for some $\mathbf{q}_0 \in \mathbb{H}_1$ and $A_0 = \Phi(\mathbf{q}_0)$:

$$(131) \qquad \frac{d\mathbf{q}}{dt} = \frac{1}{4} \nabla_{\mathbf{q}}(f(\mathbf{q})), \quad \mathbf{q}(0) = \mathbf{q}_0,$$

$$(132) \qquad \frac{dA}{dt} = \nabla_A(g(A)), \quad A(0) = A_0.$$

If $\mathbf{q} = \mathbf{q}(t)$ is a solution of (131) on some time interval $[0, T)$, then $A(t) := \Phi(\mathbf{q}(t))$ is a solution of (132) on the same time interval $[0, T)$.

Proof. To make the proof clearer we will use the notation $\langle \cdot, \cdot \rangle$ rather than the symbol "$\cdot$" to indicate the inner product (in the sense of matrices as well as in the sense of vectors and quaternions). We first check that (129) and (130) are equivalent: Indeed, since $D_{\mathbf{q}} \Phi(\nabla_{\mathbf{q}} f(\mathbf{q}))$ belongs to $T_{\Phi(\mathbf{q})} = \{[\mathbf{u}]_\times \Phi(\mathbf{q}), \mathbf{u} \in \mathbb{R}^3\}$, (129) can be rewritten as, for all $\mathbf{u} \in \mathbb{R}^3$,

$$(133) \qquad \langle (\nabla_A g)(\Phi(\mathbf{q})), [\mathbf{u}]_\times \Phi(\mathbf{q}) \rangle = \frac{1}{4} \langle D_{\mathbf{q}} \Phi(\nabla_{\mathbf{q}} f(\mathbf{q}), [\mathbf{u}]_\times \Phi(\mathbf{q}) \rangle.$$

By Proposition 5.3, the right-hand side is equal to

$$(134) \qquad \frac{1}{4} \langle D_{\mathbf{q}} \Phi(\nabla_{\mathbf{q}} f(\mathbf{q}), [\mathbf{u}]_\times \Phi(\mathbf{q}) \rangle = \frac{1}{2} \langle [(\nabla_{\mathbf{q}} f(\mathbf{q})) \mathbf{q}^*]_\times \Phi(\mathbf{q}), [\mathbf{u}]_\times \Phi(\mathbf{q}) \rangle$$

$$(135) \qquad\qquad\qquad\qquad = \frac{1}{2} \langle [(\nabla_{\mathbf{q}} f(\mathbf{q})) \mathbf{q}^*]_\times, [\mathbf{u}]_\times \rangle$$

$$(136) \qquad\qquad\qquad\qquad = \frac{1}{2} \langle (\nabla_{\mathbf{q}} f(\mathbf{q})) \mathbf{q}^*, \mathbf{u} \rangle$$

$$(137) \qquad\qquad\qquad\qquad = \frac{1}{2} \langle \nabla_{\mathbf{q}} f(\mathbf{q}), \mathbf{u}\mathbf{q} \rangle,$$

so that we recover (130).

We now prove (130): Fix some $\mathbf{q} \in \mathbb{H}_1$, $\mathbf{u} \in \mathbb{R}^3$ and let $\tilde{\mathbf{q}} = \tilde{\mathbf{q}}(s) \in \mathbb{H}_1$ be a differentiable path in $\mathbb{H}_1$ with

$$\tilde{\mathbf{q}}(0) = \mathbf{q},$$
$$\frac{d}{ds} \tilde{\mathbf{q}} \Big|_{s=0} = \mathbf{u}\mathbf{q}.$$

We compute

$$
\begin{aligned}
\langle \nabla_{\mathbf{q}} f(\mathbf{q}) \,, \mathbf{u}\mathbf{q} \rangle &= \left. \frac{\mathrm{d}}{\mathrm{d}s} f(\tilde{\mathbf{q}}(s)) \right|_{s=0} \\
&= \left. \frac{\mathrm{d}}{\mathrm{d}s} g(\Phi(\tilde{\mathbf{q}}(s))) \right|_{s=0} \\
&= \left\langle (\nabla_A g)(\Phi(\mathbf{q})), \left. \frac{\mathrm{d}}{\mathrm{d}s}\Phi(\tilde{\mathbf{q}}(s)) \right|_{s=0} \right\rangle \\
&= \langle (\nabla_A g)(\Phi(\mathbf{q})), \mathrm{D}_{\mathbf{q}}\Phi(\mathbf{u}\mathbf{q}) \rangle \\
&= 2\langle (\nabla_A g)(\Phi(\mathbf{q})), [\mathbf{u}]_\times \Phi(\mathbf{q}) \rangle,
\end{aligned}
$$

where we used Proposition 5.3 to compute $\mathrm{D}_{\mathbf{q}}\Phi$. This proves (130).

Let $\mathbf{q} = \mathbf{q}(t)$ be a solution of (131) on some time interval $(0,T)$, and let $A(t) := \Phi(\mathbf{q}(t))$ on $(0,T)$. For any $\mathbf{u} \in \mathbb{R}^3$, we compute

$$
\begin{aligned}
\left\langle \frac{\mathrm{d}A}{\mathrm{d}t}, [\mathbf{u}]_\times A(t) \right\rangle &= \left\langle \mathrm{D}_{\mathbf{q}}\Phi|_{\mathbf{q}(t)}\left(\frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t}\right), [\mathbf{u}]_\times A(t) \right\rangle \\
&= \langle \mathrm{D}_{\mathbf{q}}\Phi|_{\mathbf{q}(t)}(\mathbf{v}\mathbf{q}(t)), [\mathbf{u}]_\times A(t) \rangle \\
&= 2\langle [\mathbf{v}]_\times A(t), [\mathbf{u}]_\times A(t) \rangle \\
&= 2\langle \mathbf{v}, \mathbf{u} \rangle,
\end{aligned}
$$

where we note $\mathbf{v} = \mathbf{v}(t) := (\mathrm{d}\mathbf{q}/\mathrm{d}t)\mathbf{q}^*(t) \in \mathbb{R}^3$. On the other hand, we compute thanks to (130)

$$
\begin{aligned}
\langle \nabla_A g(A(t)), [\mathbf{u}]_\times A(t) \rangle &= \frac{1}{2}\langle \nabla_{\mathbf{q}} f(\mathbf{q}(t)), \mathbf{u}\mathbf{q}(t) \rangle \\
&= 2\langle \frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t}, \mathbf{u}\mathbf{q}(t) \rangle, \\
&= 2\langle \mathbf{v}, \mathbf{u} \rangle,
\end{aligned}
$$

so that

$$
(138) \qquad \left\langle \frac{\mathrm{d}A}{\mathrm{d}t}, [\mathbf{u}]_\times A(t) \right\rangle = \langle \nabla_A g(A(t)), [\mathbf{u}]_\times A(t) \rangle \qquad \text{for all } \mathbf{u} \in \mathbb{R}^3.
$$

This concludes the proof. $\qquad\qquad\square$

PROPOSITION B.2 (comparison of the divergence operator). *Let G be a vector field tangent to $SO(3)$ and H a vector field tangent to $\mathbb{H}_1$ such that*

$$
(139) \qquad\qquad G(\Phi(\mathbf{q})) = \mathrm{D}_{\mathbf{q}}\Phi\left(H(\mathbf{q})\right) \qquad \text{for all } \mathbf{q} \in \mathbb{H}_1.
$$

Then

$$
(140) \qquad\qquad (\nabla_{\mathbf{q}} \cdot H)(\mathbf{q}) = (\nabla_A \cdot G)(\Phi(\mathbf{q})) \qquad \text{for all } \mathbf{q} \in \mathbb{H}_1.
$$

Proof. Consider functions f, g with $f(\mathbf{q}) = g(\Phi(\mathbf{q}))$ and define $\mathbf{u} : \mathbb{H}_1 \to \mathbb{R}^3$ by

$$
\mathbf{u}(\mathbf{q}) = 2H(\mathbf{q})\mathbf{q}^* \qquad \text{for all } \mathbf{q} \in \mathbb{H}_1.
$$

By (139) and Proposition 5.3, we have

$$
G(\Phi(\mathbf{q})) = [\mathbf{u}(\mathbf{q})]_\times \Phi(\mathbf{q}) \qquad \text{for all } \mathbf{q} \in \mathbb{H}_1.
$$

Then we can compute

$$
\begin{aligned}
\int_{\mathbb{H}_1} f(\mathbf{q})\, \nabla_{\mathbf{q}} \cdot H(\mathbf{q})\, \mathrm{d}\mathbf{q} &= -\int_{\mathbb{H}_1} \langle \nabla_{\mathbf{q}} f(\mathbf{q}), H(\mathbf{q}) \rangle_{\mathbb{H}_1}\, \mathrm{d}\mathbf{q} \\
&= -\frac{1}{2} \int_{\mathbb{H}_1} \langle \nabla_{\mathbf{q}} f(\mathbf{q}), \mathbf{u}(\mathbf{q})\mathbf{q} \rangle_{\mathbb{H}_1}\, \mathrm{d}\mathbf{q} \\
&= -\int_{\mathbb{H}_1} \langle \nabla_A g(\Phi(\mathbf{q})), [\mathbf{u}(\mathbf{q})]_{\times}\Phi(\mathbf{q}) \rangle_{SO(3)}\, \mathrm{d}\mathbf{q} \\
&= -\int_{\mathbb{H}_1} \langle \nabla_A g(\Phi(\mathbf{q})), G(\Phi(\mathbf{q})) \rangle_{SO(3)}\, \mathrm{d}\mathbf{q} \\
&= -2\pi^2 \int_{\mathbb{H}_1} \langle \nabla_A g(A), G(A) \rangle_{SO(3)}\, \mathrm{d}A \\
&= 2\pi^2 \int_{\mathbb{H}_1} g(A)\, (\nabla_A \cdot G)(A)\, \mathrm{d}A \\
&= \int_{\mathbb{H}_1} g(\Phi(\mathbf{q}))\, (\nabla_A \cdot G)(\Phi(\mathbf{q}))\, \mathrm{d}\mathbf{q} \\
&= \int_{\mathbb{H}_1} f(\mathbf{q})\, (\nabla_A \cdot G)(\Phi(\mathbf{q}))\, \mathrm{d}\mathbf{q},
\end{aligned}
$$

where we have used integration by parts and (130). We conclude that

$$
\int_{\mathbb{H}_1} \left[\nabla_{\mathbf{q}} \cdot H(\mathbf{q}) - (\nabla_A \cdot G)(\Phi(\mathbf{q})) \right] f(\mathbf{q})\, \mathrm{d}\mathbf{q} = 0
$$

for all f such that $f(\mathbf{q}) = f(-\mathbf{q})$. This implies that (140) holds. $\qquad\square$

PROPOSITION B.3 (comparison of the Laplacians). *Consider a scalar function* $g : SO(3) \to \mathbb{R}$ *twice differentiable and define the function* $f : \mathbb{H}_1 \to \mathbb{R}$ *as* $f(\mathbf{q}) = g(\Phi(\mathbf{q}))$. *It holds that*

$$
(\Delta_A g)(\Phi(\mathbf{q})) = \frac{1}{4} \Delta_{\mathbf{q}} f(\mathbf{q}).
$$

Proof. By Proposition B.1, we have that (129) is true, so that (139) is true for $G := \nabla_A g$ and $H := \nabla_{\mathbf{q}} f / 4$. Applying Proposition B.2 gives the result. $\qquad\square$

Appendix C. Equivalence of the GCI equations.

PROPOSITION C.1. *Let h be a solution of* (64). *Then the function*

$$
(141) \qquad k(\theta) := 4\, \frac{h\left(\cos(\theta/2)\right)}{\cos(\theta/2)}
$$

is a solution of the equation

$$
(142) \quad \frac{1}{\sin^2(\theta/2)} \partial_\theta \left(\sin^2(\theta/2) m(\theta) \partial_\theta \left(\sin\theta\, k(\theta) \right) \right) - \frac{m(\theta)\sin\theta}{2\sin^2(\theta/2)} k(\theta) = \sin(\theta) m(\theta).
$$

Note: For P antisymmetric matrix and $\Lambda \in SO(3)$,

$$
\psi(A) = P \cdot (\Lambda^t A)\, \bar{k}(\Lambda \cdot A), \qquad A \in SO(3),
$$

is a generalized collision invariant in the body attitude coordination model based on rotation matrices from [17]. *In this case* $\bar{k}(\Lambda \cdot A) = \bar{k}\left(\frac{1}{2} + \cos(\theta)\right) =: k(\theta)$.

Proof. For convenience we introduce the notation

$$c := \cos(\theta/2), \qquad s := \sin(\theta/2),$$

so that

$$c^2 + s^2 = 1, \qquad \partial_\theta c = -s/2, \qquad \partial_\theta s = c/2, \qquad \cos\theta = c^2 - s^2, \qquad \sin\theta = 2cs.$$

We write

$$k(\theta) = 4\frac{h(c)}{c}.$$

We use the equivalent (70) for h and rewrite it in $r = c$ as

(143)
$$\left(\frac{-4}{d}c^2 - 3\right)h + \left(\frac{4}{d}s^2 - 5\right)ch' + s^2 h'' = c.$$

Finally by definition of m in (41),

$$m(\theta) = \exp\left(\frac{1}{d}\left(\frac{1}{2} + \cos\theta\right)\right), \qquad \partial_\theta m(\theta) = -\frac{2}{d}csm(\theta).$$

We want to check that k defined by (141) is a solution of (142). This is equivalent to showing that

$$D(\theta) := \partial_\theta[s^2 m(\theta)\partial_\theta(\sin\theta k(\theta))] - m(\theta)csk(\theta) = 2cs^3 m(\theta).$$

We first compute

$$\begin{aligned}
\partial_\theta\left(\sin(\theta)k(\theta)\right) &= \cos\theta k(\theta) + \sin\theta k'(\theta)\\
&= 4\cos\theta\frac{h(c)}{c} + 4\sin\theta\frac{s}{2c^2}h(c) + 4\frac{\sin\theta}{c}\frac{-s}{2}h'(c)\\
&= 4(c^2 - s^2)\frac{h(c)}{c} + 4cs\frac{s}{c^2}h(c) - 4s^2 h'(c)\\
&= 4ch(c) - 4s^2 h'(c).
\end{aligned}$$

Then, inserting this expression into $D(\theta)$, we have that

$$\begin{aligned}
D(\theta) &= 4\partial_\theta[s^2 m(\theta)\left(ch(c) - s^2 h'(c)\right)] - 4m(\theta)sh(\theta)\\
&= 4\partial_\theta[s^2 m(\theta)c]h(c) - 2cs^3 m(\theta)h'(c)\\
&\quad - 4\partial_\theta[s^4 m(\theta)]h'(c) - 4s^4 m(\theta)\frac{-s}{2}h''(c) - 4m(\theta)sh(\theta)\\
&= 4\left[scm(\theta)c - \frac{1}{2}s^3 m(\theta) - \frac{2}{d}c^2 s^3 m(\theta) - m(\theta)s\right]h(c)\\
&\quad + \left[-2cs^3 m(\theta) - 4[2cs^3 m(\theta) - \frac{2}{d}css^4 m(\theta)]\right]h'(c)\\
&\quad + 2s^5 m(\theta)h''(c)\\
&= 2s^3 m(\theta)\left\{2\left[c^2/s^2 - \frac{1}{2} - \frac{2}{d}c^2 - 1/s^2\right]h(c)\right.\\
&\quad \left. + \left[-c - 2\left[2c - \frac{2}{d}cs^2\right]\right]h'(c) + s^2 h''(c)\right\}\\
&= 2s^3 m(\theta)\left\{\left(-3 - \frac{4}{d}c^2\right)h(c) + \left(-5 + \frac{4}{d}s^2\right)ch'(c) + s^2 h''(c)\right\}.
\end{aligned}$$

Using (143), this last expression is equal to

$$(144) \qquad\qquad D(\theta) = 2s^3 m(\theta)c,$$

which concludes the proof.   □

<div align="center">REFERENCES</div>

[1] M. Aldana and C. Huepe, *Phase transitions in self-driven many-particle systems and related non-equilibrium models: A network approach*, J. Statist. Phys., 112 (2003), pp. 135–153.

[2] D. Armbruster, P. Degond, and C. Ringhofer, *A model for the dynamics of large queuing networks and supply chains*, SIAM J. Appl. Math., 66 (2006), pp. 896–920, https://doi.org/10.1137/040604625.

[3] A. Aw, A. Klar, T. Materne, and M. Rascle, *Derivation of continuum traffic flow models from microscopic follow-the-leader models*, SIAM J. Appl. Math., 63 (2002), pp. 259–278, https://doi.org/10.1137/S0036139900380955.

[4] E. Ben-Jacob, I. Cohen, and H. Levine, *Cooperative self-organization of microorganisms*, Adv. Phys., 49 (2000), pp. 395–554.

[5] F. Bolley, J. A. Cañizo, and J. A. Carrillo, *Mean-field limit for the stochastic Vicsek model*, Appl. Math. Lett., 25 (2012), pp. 339–343.

[6] J. Buhl, D. Sumpter, I. D. Couzin, J. J. Hale, E. Despland, E. R. Miller, and S. J. Simpson, *From disorder to order in marching locusts*, Science, 312 (2006), pp. 1402–1406.

[7] A. Cavagna, A. Cimarelli, I. Giardina, G. Parisi, R. Santagati, F. Stefanini, and M. Viale, *Scale-free correlations in starling flocks*, Proc. Natl. Acad. Sci. USA, 107 (2010), pp. 11865–11870.

[8] A. Cavagna, L. Del Castello, I. Giardina, T. Grigera, A. Jelic, S. Melillo, T. Mora, L. Parisi, E. Silvestri, M. Viale et al., *Flocking and turning: A new model for self-organized collective motion*, J. Statist. Phys., 158 (2014), pp. 601–627.

[9] C. Cercignani, R. Illner, and M. Pulvirenti, *The Mathematical Theory of Dilute Gases*, Appl. Math. Sci. 106, Springer Science & Business Media, 2013.

[10] P. Constantin, *The Onsager equation for corpora*, J. Comput. Theoret. Nanosci., 7 (2010), pp. 675–682.

[11] P. Constantin and A. Zlatoš, *On the high intensity limit of interacting corpora*, Commun. Math. Sci., 8 (2010), pp. 173–186.

[12] I. D. Couzin, J. Krause, R. James, G. D. Ruxton, and N. R. Franks, *Collective memory and spatial sorting in animal groups*, J. Theoret. Biol., 218 (2002), pp. 1–11.

[13] J. W. Daniel, W. B. Gragg, L. Kaufman, and G. W. Stewart, *Reorthogonalization and stable algorithms for updating the Gram-Schmidt factorization*, Math. Comp., 30 (1976), pp. 772–795.

[14] P. Degond, *Macroscopic limits of the Boltzmann equation: A review*, in Modeling and Computational Methods for Kinetic Equations, Springer, 2004, pp. 3–57.

[15] P. Degond, G. Dimarco, and T. B. N. Mac, *Hydrodynamics of the Kuramoto–Vicsek model of rotating self-propelled particles*, Math. Models Methods Appl. Sci., 24 (2014), pp. 277–325.

[16] P. Degond, G. Dimarco, T. B. N. Mac, and N. Wang, *Macroscopic models of collective motion with repulsion*, Commun. Math. Sci., 13 (2015), pp. 1615–1638.

[17] P. Degond, A. Frouvelle, and S. Merino-Aceituno, *A new flocking model through body attitude coordination*, Math. Models Methods Appl. Sci., 27 (2017), pp. 1005–1049.

[18] P. Degond and J. Liu, *Hydrodynamics of self-alignment interactions with precession and derivation of the Landau–Lifschitz–Gilbert equation*, Math. Models Methods Appl. Sci., 22 (2012), 1140001.

[19] P. Degond, J. Liu, and C. Ringhofer, *Evolution of wealth in a non-conservative economy driven by local Nash equilibria*, Phil. Trans. R. Soc. A, 372 (2014), 20130394.

[20] P. Degond, A. Manhart, and H. Yu, *A continuum model for nematic alignment of self-propelled particles*, Discrete Contin. Dyn. Syst. Ser. B, 22 (2017), pp. 1295–1327.

[21] P. Degond and S. Motsch, *Continuum limit of self-driven particles with orientation interaction*, Math. Models Methods Appl. Sci., 18 (2008), pp. 1193–1215.

[22] P. Degond and L. Navoret, *A multi-layer model for self-propelled disks interacting through alignment and volume exclusion*, Math. Models Methods Appl. Sci., 25 (2015), pp. 2439–2475.

[23] P. Degond and C. Ringhofer, *Stochastic dynamics of long supply chains with random breakdowns*, SIAM J. Appl. Math., 68 (2007), pp. 59–79, https://doi.org/10.1137/060674302.

[24] P. Degond and H. Yu, *Self-organized hydrodynamics in an annular domain: Modal analysis and nonlinear effects*, Math. Models Methods Appl. Sci., 25 (2015), pp. 495–519.

[25] M. Doi and S. F. Edwards, *The Theory of Polymer Dynamics*, Internat. Ser. Monogr. Phys. 73, Oxford University Press, 1988.

[26] D. Eberly, *Rotation Representations and Performance Issues*, Magic Software, Inc., Chapel Hill, NC, 2002.

[27] A. Frouvelle, *A continuum model for alignment of self-propelled particles with anisotropy and density-dependent parameters*, Math. Models Methods Appl. Sci., 22 (2012), 1250011.

[28] C. W. Gardiner, *Stochastic methods*, Springer-Verlag, Berlin, Heidelberg, New York, Tokyo, 1985.

[29] G. H. Golub and C. F. Van Loan, *Matrix Computations*, 4th ed., Johns Hopkins University Press, 2013.

[30] G. Grégoire and H. Chaté, *Onset of collective and cohesive motion*, Phys. Rev. Lett., 92 (2004), 025702.

[31] D. Helbing, *Traffic and related self-driven many-particle systems*, Rev. Modern Phys., 73 (2001), pp. 1067–1141.

[32] D. Helbing, A. Johansson, and H. Z. Al-Abideen, *Dynamics of crowd disasters: An empirical study*, Phys. Rev. E, 75 (2007), 046109.

[33] N. J. Higham and V. Noferini, *An algorithm to compute the polar decomposition of a 3×3 matrix*, Numer. Algorithms, 73 (2016), pp. 349–369.

[34] D. D. Holm, *Geometric Mechanics: Rotating, Translating and Rolling*, Vol. 2, Imperial College Press, 2008.

[35] E. P. Hsu, *Stochastic Analysis on Manifolds*, Grad. Stud. Math. 38, AMS, 2002.

[36] V. Klema and A. Laub, *The singular value decomposition: Its computation and some applications*, IEEE Trans. Automat. Control, 25 (1980), pp. 164–176.

[37] J. K. Parrish and W. M. Hamner, *Animal Groups in Three Dimensions: How Species Aggregate*, Cambridge University Press, 1997.

[38] L. Rodman, *Topics in Quaternion Linear Algebra*, Princeton University Press, 2014.

[39] E. Salamin, *Application of Quaternions to Computation with Rotations*, tech. report, Working Paper, 1979.

[40] A. Sarlette, R. Sepulchre, and N. E. Leonard, *Autonomous rigid body attitude synchronization*, Automatica, 45 (2009), pp. 572–577.

[41] Y. Sone, *Kinetic Theory and Fluid Dynamics*, Springer Science & Business Media, 2012.

[42] Y. Tu, J. Toner, and M. Ulm, *Sound waves and the absence of Galilean invariance in flocks*, Phys. Rev. Lett., 80 (1998), pp. 4819–4822.

[43] T. Vicsek, A. Czirók, E. Ben-Jacob, I. Cohen, and O. Shochet, *Novel type of phase transition in a system of self-driven particles*, Phys. Rev. Lett., 75 (1995), pp. 1226–1229.

[44] T. Vicsek and A. Zafeiris, *Collective motion*, Phys. Rep., 517 (2012), pp. 71–140.

[45] H. Zhang, A. Beer, E.-L. Florin, and H. L. Swinney, *Collective motion and density fluctuations in bacterial colonies*, Proc. Natl. Acad. Sci. USA, 107 (2010), pp. 13626–13630.