

A CONTINUUM MODEL FOR NEMATIC ALIGNMENT OF SELF-PROPELLED PARTICLES

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ABSTRACT. A continuum model for a population of self-propelled particles interacting through nematic alignment is derived from an individual-based model. The methodology consists of introducing a hydrodynamic scaling of the corresponding mean field kinetic equation. The resulting perturbation problem is solved thanks to the concept of generalized collision invariants. It yields a hyperbolic but non-conservative system of equations for the nematic mean direction of the flow and the densities of particles flowing parallel or anti-parallel to this mean direction. Diffusive terms are introduced under a weakly non-local interaction assumption and the diffusion coefficient is proven to be positive. An application to the modeling of myxobacteria is outlined.

1. Introduction. Systems of large numbers of self-propelled particles are commonly found in nature. In three space dimensions, well-known examples include fish schools, flocks of birds and insects [9, 11, 44]. In two space dimensions, typical examples are bacteria, such as myxobacteria and *Bacillus subtilis* [6, 35, 47, 51, 53]. However, the interest in such systems is not limited to biological examples. It has been found that the underlying principles also often apply to human walking behavior [32, 40] and physical systems, such as granular media [28, 42]. The main interest in these systems, both mathematically and from an application's point of view, stems from their emergent properties. Emergence refers to the fact that fairly local interaction rules between the agents like attraction, alignment, repulsion, etc. give rise to large scale collective behavior. Emergence is physically described as

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a phase transition to an ordered state (see e.g. the review [50]). Mathematical models often rely on a particle (agent) based description [1, 12, 14, 46]. Among these models, the time dependent Vicsek model [49] and variants of it have received much attention owing to its structural simplicity, while convincingly describing a wide range of phenomena. The general idea of the Vicsek model is to describe the agents as particles, moving with constant speed. At each time step each particle adjusts its direction towards the mean direction of the particles in its neighborhood subject to some random perturbation.

Whilst particle models are a good tool to reproduce and study the observed phenomena, the high number of agents involved make simulations computationally costly considering the amount of detail one is interested in. Hydrodynamic (macroscopic) models are typically easier to simulate and analyze and thereby offer a powerful alternative. Therefore a lot of effort has been made to formulate macroscopic equations starting from particle models [4, 7, 10, 13, 22, 25, 30, 39]. Mathematically one of the main challenges is the lack of conserved quantities, which is typically a key ingredient in the computation of the macroscopic limit (see again [50]). This lack of conservation is frequent in biological systems, which, as opposed to many physical systems, e.g. don't conserve momentum. One strategy to overcome this is the use of *generalized collision invariants (GCI)*, introduced for the first time in [25] to derive a hydrodynamic model of the Vicsek dynamics (later on referred to as the Self-Organized Hydrodynamic (SOH) model). The passage from individual-based to hydrodynamic models involves the construction of an intermediate kinetic model. For classical physical systems, momentum or energy conservation translates at the kinetic level into the concept of collision invariants. This is generalized to the GCI concept if the underlying system does not satisfy these conditions. The rigorous passage from kinetic to SOH models has been achieved in [41]. The GCI concept has been used in a variety of cases [18, 17, 21, 30] and even applied to a model of economics [23]. Modal analysis of the SOH model can be found in [27]. One important feature of the Vicsek model is the emergence of phase transitions. These are studied in the kinetic or macroscopic framework in [3, 7, 19, 20, 48]. Here, we concentrate on the derivation of macroscopic models and postpone the analysis of phase transitions to future works.

In this paper we want to apply this method to nematic alignment of polar, rod-shaped particles moving with constant speed in two space dimensions. Nematic alignment describes the situation where upon meeting, two particles either align if their mutual angle is acute or anti-align if their angle is obtuse. This nematic alignment rule typically results from volume exclusion and can be understood as an inelastic collision between polar particles. It differs from polar alignment of polar particles (which is akin to ferromagnetic interactions in spin systems, as is the case of the Vicsek model) and nematic alignment of apolar particles (active nematics, which is typically observed in liquid crystals [15], in fibrous tissues [16] or in systems of interacting disks [26]). Large collections of polar particles which nematically align have been observed to exhibit interesting macroscopic patterns such as high density traveling bands and their properties differ from the other types of alignment [31, 43]. Therefore the need for a hydrodynamic model derived from particle dynamics arises and this work suggests how to derive such a model. In the derivation we account for purely local interactions as well as weakly non-local interactions which leads to an additional diffusion term in the macroscopic limit.

To give an example how the nematic SOH model can be applied to biological systems, we consider the case of myxobacteria. Due to their ability to produce several macroscopic structures, such as waves, spirals and clusters [29, 35, 51], they have already received a lot of attention in terms of mathematical models [8, 33, 34, 52]. Since this type of bacteria can internally reverse its polarity, the model has to be complemented with a reaction term, describing these reversals. We demonstrate how such a term can be incorporated in a systematic way into the original model.

The rest of the document is structured as follows. In Section 2 we describe the particle model for nematic alignment and the resulting mean field model. The derived alignment operator Q_{al}^0 is examined in Section 3. Whilst it shares some properties with its polar alignment counterpart, there are also some differences, e.g. the set of equilibria has dimension three (instead of two). Mathematically more unexpected, showing the existence and uniqueness of solutions of the related linear operator, which amounts to proving a Poincaré inequality, is slightly more complex than in the polar case [25]. The section finishes with explicitly characterizing the equilibria and generalized collision invariants of Q_{al}^0 . With these ingredients we derive the macroscopic model in Section 4 and prove its hyperbolicity. In Section 5 we assume weakly non-local interactions and derive the corresponding macroscopic model. Finally in Section 6 we apply both macroscopic models to the case of myxobacteria by additionally describing density dependent reversal at the particle level. In the macroscopic model this leads to a reaction term which structurally hints at interesting dynamics expected to take place.

2. Particle and mean field model.

2.1. Particle model. As a first step towards a macroscopic model, we start with the description of a time-continuous particle (or agent-based) model. The model's structure is similar to the time-continuous version of the Vicsek model presented in [25] and we will discuss similarities and differences. We image the particles to resemble stiff rods of equal length and describe the i -th particle ($i \in \mathcal{N} := \{1, \dots, N\}$) at time $t \geq 0$ by its center of mass $X_i(t) \in \mathbb{R}^2$ and its orientation $v(\Theta_i(t))$, where we define

$$v(\theta) = \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix}, \quad v^\perp(\theta) = \begin{pmatrix} -\sin \theta \\ \cos \theta \end{pmatrix}$$

as the polar vectors associated with the angle θ in a fixed reference frame and where $\Theta_i(t)$ is defined modulo 2π . All particles are assumed to move in the direction of their orientation with constant speed, v_0 . In particular this means that they cannot drift sideways (as opposed to the model in [5]). Under these hypotheses, the motion of the particles is supposed to satisfy the following system of stochastic differential equations

$$\frac{dX_i}{dt} = v_0 v(\Theta_i(t)), \tag{1}$$

$$d\Theta_i = -\nu \text{Sign}(\cos(\Theta_i - \bar{\Theta}_i)) \sin(\Theta_i - \bar{\Theta}_i) dt + (2d \cos^2(\Theta_i - \bar{\Theta}_i))^{1/2} dB_t^i. \tag{2}$$

Here $\bar{\Theta}_i = \bar{\Theta}_i(t)$ is the average nematic alignment direction. It is defined as follows. First define a mean ‘nematic’ current

$$J_i(t) = \sum_{k \in \mathcal{N}: |X_k(t) - X_i(t)| \leq R} v(2\Theta_k(t)),$$

where $R > 0$ is the interaction radius. Next define $\bar{\Theta}_i(t)$ as an angle of lines (i.e. an angle defined modulo π) such that:

$$v(2\bar{\Theta}_i(t)) = \frac{J_i(t)}{|J_i(t)|}. \quad (3)$$

We note that the definition of the vector on the left-hand side of [3](#) does not depend on the choice of the reference frame used to measure the angles Θ_i as $\bar{\Theta}_i(t)$ can be equivalently defined by

$$\sum_{k \in \mathcal{N}: |X_k(t) - X_i(t)| \leq R} \sin 2(\Theta_k(t) - \bar{\Theta}_i(t)) = 0,$$

and that this relation is invariant under a uniform translation of all angles. To obtain a unique representation of the angles, we will use the convention that the particle angles $\Theta_i(t)$ are taken in $[-\pi, \pi)$ and the nematic angles $\bar{\Theta}_i(t)$ are taken in $[-\pi/2, \pi/2)$. For simplicity, we will identify $[-\pi, \pi)$ with $\mathbb{R}/2\pi\mathbb{Z}$ and the unit circle \mathbb{S}^1 . The notation dB_t^i describes independent Brownian motions with intensity $d \cos^2(\Theta_i - \bar{\Theta}_i)$ where $d > 0$. We are aiming for a separation of the particles into two (locally defined) groups, one with $\cos(\Theta_i - \bar{\Theta}_i) > 0$ and the other one with $\cos(\Theta_i - \bar{\Theta}_i) < 0$. Therefore, diffusion must vanish near $\cos(\Theta_i - \bar{\Theta}_i) = 0$, to avoid particles crossing the boundary between these two angular regions. The factor $\cos^2(\Theta_i - \bar{\Theta}_i)$ is intended to avoid that the two groups mix. The first term in the velocity evolution describes alignment of the bacteria within the interaction radius $R > 0$ with an alignment frequency $\nu \text{Sign}(\cos(\Theta_i - \bar{\Theta}_i)) \sin(\Theta_i - \bar{\Theta}_i)$ and $\nu \geq 0$. Due to the factor $\text{Sign}(\cos(\Theta_i - \bar{\Theta}_i))$, alignment occurs parallel or anti-parallel to the mean angle $\bar{\Theta}_i$, depending on whether Θ_i is closer to $\bar{\Theta}_i$ or $\bar{\Theta}_i + \pi$. Note that $\text{Sign}(\cos(\Theta_i - \bar{\Theta}_i)) \sin(\Theta_i - \bar{\Theta}_i)$ is a π -periodic function and so, does not depend on the choice of $\bar{\Theta}_i$ or $\bar{\Theta}_i + \pi$ as the representative of the corresponding angle of lines.

Here, the stochastic differential equation [2](#) involves a noise intensity $(2d \cos^2(\Theta_i - \bar{\Theta}_i))^{1/2}$ which depends on the state of the particle Θ_i . Therefore, it is important to specify which sense is given to its product with the Wiener process dB_t^i as different conventions will lead to different dynamics. In mathematics, two conventions are usually used, the Ito convention and the Stratonovich one. However, as pointed out in [\[38\]](#), none is compatible with the thermodynamical formalism. Thus, we interpret the stochastic term $(2d \cos^2(\Theta_i - \bar{\Theta}_i))^{1/2} dB_t^i$ in the so-called isothermal convention as defined in [\[36, 37\]](#) (also known as the Backwards Ito formalism [\[2\]](#)) and we refer to [\[38\]](#) for its definition and formal properties. The major usage that we will make of this convention is for the probability distribution of the process in the form of the Fokker-Planck equation in the next section.

Remark 1. Also other notions of nematic alignment between several particles are possible. In [\[45\]](#) the nematic mean direction was defined as

$$\bar{\Theta}_i(t) = \arg \left(\sum_{k \in \mathcal{N}: |X_k(t) - X_i(t)| \leq R} \text{Sign}(\cos(\Theta_i(t) - \Theta_k(t))) v(\Theta_k) \right). \quad (4)$$

The main difference between this definition and [3](#) is that the nematic angle defined in [3](#) depends on the particle index i only via the position $X_i(t)$, but is independent of the direction of the i -th particle, Θ_i . The outcome of [4](#) on the other hand depends on both the position and the direction of the i -th particle. Whilst the definition from [\[45\]](#) might be closer to reality, if the dispersion around the mean angle is

small, both types of nematic alignment lead to the same behavior. However, the independence from Θ_i makes 3 mathematically much easier to handle.

2.2. Mean field model. We follow the usual procedure to derive the mean field limit as described for example in [25]. The procedure starts with the definition of the empirical distribution function $f^N(x, \theta, t)$, with $x \in \mathbb{R}^2$, $\theta \in \mathbb{R}$ (modulo 2π) and $t > 0$,

$$f^N(x, \theta, t) = \frac{1}{N} \sum_{i \in \mathcal{N}} \delta_{(X_i(t), \Theta_i(t))}(x, \theta),$$

where $\delta_{(X_i(t), \Theta_i(t))}(x, \theta)$ is the Dirac delta in (x, θ) space located at $(X_i(t), \Theta_i(t))$ at time t . In the absence of noise ($d = 0$), f^N is a deterministic measure that satisfies a first order kinetic equation if we assume that all (X_i, V_i) fulfill 1-3. If $d \neq 0$, f^N is a random measure whose law satisfies a second order kinetic equation. Then as $N \rightarrow \infty$, f^N approximates a distribution function $f(x, \theta, t)$, satisfying the following Kolmogorov-Fokker-Planck type equation (owing to the fact that we have defined the Stochastic Differential Equation for the particles with the isothermal convention [38]):

$$\partial_t f + v_0 \nabla_x \cdot (v(\theta) f) = \tilde{Q}_{\text{al}} f, \quad (5)$$

where the collision operator \tilde{Q}_{al} is given by

$$\tilde{Q}_{\text{al}} f = \partial_\theta \left[\nu \text{Sign}(\cos(\theta - \bar{\Theta}_f)) \sin(\theta - \bar{\Theta}_f) f + d \cos^2(\theta - \bar{\Theta}_f) \partial_\theta f \right], \quad (6)$$

and $\bar{\Theta}_f$ is given by

$$v(2\bar{\Theta}_f(x, t)) = \frac{J_f(x, t)}{|J_f(x, t)|}, \quad (7)$$

$$J_f(x, t) = \int_{|y-x| \leq R} \int_{-\pi}^{\pi} v(2\theta) f(y, \theta, t) dy d\theta. \quad (8)$$

We note from 7 that $\bar{\Theta}_f$ is an angle of lines, defined modulo π and a representative of $\bar{\Theta}_f$ will be chosen in $[-\pi/2, \pi/2)$. We also note that 7-8 can be equivalently written as

$$\int_{|y-x| \leq R} \int_{-\pi}^{\pi} \sin 2(\theta - \bar{\Theta}_f(x, t)) f(y, \theta, t) dy d\theta = 0.$$

At this point the alignment interaction is non-local which is reflected in the fact that the computations for $J_f(x, t)$ involve integrals over a ball centered around x . As a next step we introduce dimensionless variables. Since we are interested in macroscopic phenomena, we use a hydrodynamic scaling. In the following we will do the non-dimensionalization and the hydrodynamic scaling in one step. A more detailed description for a similar equation can be found in [22]. On a microscopic scale we use the reference time $t_0 = 1/\nu$ and reference length $x_0 = v_0 t_0$. We also introduce a scaled diffusion constant $D = d t_0$. On the macroscopic scale we want to use units $t'_0 = \frac{t_0}{\varepsilon}$ and $x'_0 = \frac{x_0}{\varepsilon}$, which are large compared to the microscopic ones. We introduce the new (dimensionless, macroscopic) variables $\hat{x} = \frac{x}{x'_0} = \varepsilon \frac{x}{x_0}$ and $\hat{t} = \frac{t}{t'_0} = \varepsilon \frac{t}{t_0}$ and set $\hat{f}(\hat{x}, \theta, \hat{t}) = \frac{f(x, \theta, t)}{(1/x'_0)^2} = \left(\frac{x_0}{\varepsilon}\right)^2 f(x, \theta, t)$. Additionally we scale $\hat{R} = \frac{R}{x'_0} = \varepsilon \frac{R}{x_0} = \varepsilon r$ with $r = \frac{R}{x_0} = \mathcal{O}(1)$. Note that the scaling of \hat{R} supposes that the interactions between the particles are local. Another scaling which takes better account of the non-locality of the interactions will be investigated later on

(see Section 5). With this scaling and dropping the hats for better readability we find that f^ε satisfies the problem:

$$\varepsilon(\partial_t f^\varepsilon + \nabla_x \cdot (v(\theta) f^\varepsilon)) = \tilde{Q}_{\text{al}}^\varepsilon f^\varepsilon, \quad (9)$$

with (omitting the variables x and t):

$$\tilde{Q}_{\text{al}}^\varepsilon f(\theta) = \partial_\theta \left[\text{Sign}(\cos(\theta - \bar{\Theta}_f^\varepsilon)) \sin(\theta - \bar{\Theta}_f^\varepsilon) f(\theta) + D \cos^2(\theta - \bar{\Theta}_f^\varepsilon) \partial_\theta f(\theta) \right], \quad (10)$$

and

$$v(2\bar{\Theta}_f^\varepsilon(x, t)) = \frac{J_f^\varepsilon(x, t)}{|J_f^\varepsilon(x, t)|}, \quad (11)$$

$$J_f^\varepsilon(x, t) = \int_{-\pi}^{\pi} \int_{|y-x| \leq \varepsilon r} v(2\theta) f(y, \theta, t) dy d\theta. \quad (12)$$

By Taylor expansion we get:

$$\bar{\Theta}_f^\varepsilon(x, t) = \bar{\theta}_f(x, t) + \mathcal{O}(\varepsilon^2),$$

where

$$v(2\bar{\theta}_f(x, t)) = \frac{j_f(x, t)}{|j_f(x, t)|}, \quad (13)$$

$$j_f(x, t) = \int_{-\pi}^{\pi} v(2\theta) f(x, \theta, t) d\theta. \quad (14)$$

Again, $\bar{\theta}_f$ is an angle of lines, defined modulo π and a representative of $\bar{\theta}_f$ is chosen in $[-\pi/2, \pi/2)$. As above, 13-14 can be equivalently written as

$$\int_{-\pi}^{\pi} \sin 2(\theta - \bar{\theta}_f(x, t)) f(x, \theta, t) d\theta = 0.$$

Dropping the terms of order ε^2 or smaller, we find that $f^\varepsilon(x, \theta, t)$ satisfies the perturbation problem:

$$\varepsilon(\partial_t f^\varepsilon + \nabla_x \cdot (v(\theta) f^\varepsilon)) = Q_{\text{al}}^0 f^\varepsilon, \quad (15)$$

$$Q_{\text{al}}^0 f = \partial_\theta \left[\text{Sign}(\cos(\theta - \bar{\theta}_f)) \sin(\theta - \bar{\theta}_f) f + D \cos^2(\theta - \bar{\theta}_f) \partial_\theta f \right], \quad (16)$$

where $\bar{\theta}_f$ is given by 13.

3. Properties of the alignment operator Q_{al}^0 .

3.1. Functional setting. Let $\kappa = 1/D$. We can write:

$$Q_{\text{al}}^0 f = D \partial_\theta \left\{ \cos^2(\theta - \bar{\theta}_f) \left[\kappa \frac{\text{Sign}(\cos(\theta - \bar{\theta}_f)) \sin(\theta - \bar{\theta}_f)}{\cos^2(\theta - \bar{\theta}_f)} f + \partial_\theta f \right] \right\}. \quad (17)$$

Now, we introduce

Definition 3.1. For any angle of lines $\theta_0 \in [-\pi/2, \pi/2)$, we define the Generalized von Mises (GVM) distribution with direction θ_0 and concentration parameter κ as:

$$M_{\theta_0}(\theta) = \frac{1}{Z_\kappa} \exp \left(- \frac{\kappa}{|\cos(\theta - \theta_0)|} \right), \quad \theta \in [-\pi, \pi), \quad (18)$$

where

$$Z_\kappa = \int_{\cos \theta > 0} \exp \left(- \frac{\kappa}{\cos \theta} \right) d\theta,$$

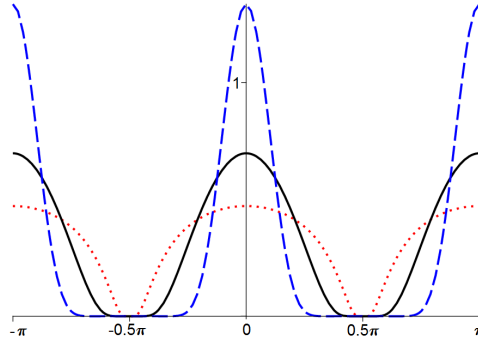


FIGURE 1. $M_0(\theta)$ for $\kappa = 0.5, 2, 10$ (red-dotted, black-solid, blue-dashed).

is the normalization coefficient such that

$$\int_{\cos \theta > 0} M_{\theta_0}(\theta) d\theta = \int_{\cos \theta < 0} M_{\theta_0}(\theta) d\theta = 1. \quad (19)$$

Figure 1 shows $M_0(\theta)$ for different values of κ . With this definition, we have

Lemma 3.2. *The alignment operator Q_{al}^0 can be written as:*

$$Q_{al}^0 f(\theta) = D \partial_\theta \left[\cos^2(\theta - \bar{\theta}_f) M_{\bar{\theta}_f} \partial_\theta \left(\frac{f}{M_{\bar{\theta}_f}} \right) \right].$$

Proof. Using 18 we calculate

$$\begin{aligned} M_{\bar{\theta}_f} \partial_\theta \left(\frac{f}{M_{\bar{\theta}_f}} \right) &= \partial_\theta f - f \partial_\theta (\log M_{\bar{\theta}_f}) \\ &= \partial_\theta f + \kappa f \partial_\theta \left(\frac{1}{|\cos(\theta - \bar{\theta}_f)|} \right) \\ &= \partial_\theta f + \kappa f \frac{\text{Sign}(\cos(\theta - \bar{\theta}_f)) \sin(\theta - \bar{\theta}_f)}{\cos^2(\theta - \bar{\theta}_f)}, \end{aligned}$$

which, upon multiplication by $\cos^2(\theta - \bar{\theta}_f)$, yields 17 and shows the claim. \square

We now give a more precise functional setting to define the collision operator Q_{al}^0 . For this purpose, we introduce the following.

Definition 3.3. (i) Let $\theta_0 \in [-\pi/2, \pi/2)$ be a given angle of lines. The linear operator \mathcal{L}_{θ_0} is defined as

$$\mathcal{L}_{\theta_0} \varphi = D \frac{1}{M_{\theta_0}} \partial_\theta (\cos^2(\theta - \theta_0) M_{\theta_0} \partial_\theta \varphi),$$

for any smooth function φ defined on $\mathbb{R}/(2\pi\mathbb{Z})$ with values in \mathbb{R} .

(ii) The space \mathcal{H}_{θ_0} is defined by

$$\mathcal{H}_{\theta_0} = \left\{ g : \mathbb{R}/2\pi\mathbb{Z} \rightarrow \mathbb{R}, \text{ measurable and } \int_{-\pi}^{\pi} |g(\theta)|^2 M_{\theta_0}(\theta) d\theta < \infty \right\}.$$

It is a Hilbert space when endowed with the inner product

$$(g, h)_{\mathcal{H}_{\theta_0}} = \int_{-\pi}^{\pi} g(\theta) h(\theta) M_{\theta_0}(\theta) d\theta,$$

and associated norm $\|g\|_{\mathcal{H}_{\theta_0}}^2 = (g, g)_{\mathcal{H}_{\theta_0}}$.

(iii) The space \mathcal{V}_{θ_0} is defined by

$$\mathcal{V}_{\theta_0} = \left\{ g \in \mathcal{H}_{\theta_0} : \sqrt{M_{\theta_0}(\theta)} |\cos(\theta - \theta_0)| \partial_{\theta} g(\theta) \in L^2(-\pi, \pi) \right\},$$

where $\partial_{\theta} g$ is defined in the distributional sense. It is a Hilbert space when endowed with the inner product

$$(g, h)_{\mathcal{V}_{\theta_0}} = (g, h)_{\mathcal{H}_{\theta_0}} + \int_{-\pi}^{\pi} \left(\sqrt{M_{\theta_0}(\theta)} |\cos(\theta - \theta_0)| \partial_{\theta} g(\theta) \right) \left(\sqrt{M_{\theta_0}(\theta)} |\cos(\theta - \theta_0)| \partial_{\theta} h(\theta) \right) d\theta,$$

and associated norm $\|g\|_{\mathcal{V}_{\theta_0}}^2 = (g, g)_{\mathcal{V}_{\theta_0}}$.

(iv) \mathcal{L}_{θ_0} defines a continuous mapping from \mathcal{V}_{θ_0} into the dual space \mathcal{V}'_{θ_0} of \mathcal{V}_{θ_0} by:

$$\begin{aligned} & \langle \mathcal{L}_{\theta_0} \varphi, \psi \rangle_{\mathcal{V}'_{\theta_0}, \mathcal{V}_{\theta_0}} \\ &= -D \int_{-\pi}^{\pi} \left(\sqrt{M_{\theta_0}(\theta)} |\cos(\theta - \theta_0)| \partial_{\theta} \varphi \right) \left(\sqrt{M_{\theta_0}(\theta)} |\cos(\theta - \theta_0)| \partial_{\theta} \psi \right) d\theta, \end{aligned} \quad (20)$$

for any $\varphi, \psi \in \mathcal{V}_{\theta_0}$. Here, $\langle \cdot, \cdot \rangle_{\mathcal{V}'_{\theta_0}, \mathcal{V}_{\theta_0}}$ denotes the duality bracket between \mathcal{V}_{θ_0} and its dual. This duality bracket extends the inner product of \mathcal{H}_{θ_0} , i.e. for $f \in \mathcal{H}_{\theta_0} \subset \mathcal{V}'_{\theta_0}$ and $g \in \mathcal{V}_{\theta_0}$, we have $\langle f, g \rangle_{\mathcal{V}'_{\theta_0}, \mathcal{V}_{\theta_0}} = \int f g M_{\theta_0} d\theta$. The operator \mathcal{L}_{θ_0} is formally self-adjoint, i.e. $\langle \mathcal{L}_{\theta_0} \varphi, \psi \rangle_{\mathcal{V}'_{\theta_0}, \mathcal{V}_{\theta_0}} = \langle \mathcal{L}_{\theta_0} \psi, \varphi \rangle_{\mathcal{V}'_{\theta_0}, \mathcal{V}_{\theta_0}}$ for all $\varphi, \psi \in \mathcal{V}_{\theta_0}$.

(v) The operator Q_{al}^0 is defined for functions $f \in L^1(-\pi, \pi)$ (which guarantees that θ_f is well-defined) such that $f/M_{\bar{\theta}_f} \in \mathcal{V}_{\bar{\theta}_f}$ by:

$$Q_{\text{al}}^0 f = M_{\bar{\theta}_f} \mathcal{L}_{\bar{\theta}_f} \left(\frac{f}{M_{\bar{\theta}_f}} \right). \quad (21)$$

By abuse of notation, we will simply write [20](#) as follows:

$$\langle \mathcal{L}_{\theta_0} \varphi, \psi \rangle_{\mathcal{V}'_{\theta_0}, \mathcal{V}_{\theta_0}} = -D \int_{-\pi}^{\pi} \partial_{\theta} \varphi \partial_{\theta} \psi M_{\theta_0}(\theta) \cos^2(\theta - \theta_0) d\theta.$$

Now we investigate the solvability of the equation

$$\mathcal{L}_{\theta_0} \varphi = \psi,$$

for a given function ψ . In view of [20](#), this problem can be recast into the following variational formulation:

$$\begin{aligned} & \varphi \in \mathcal{V}_{\theta_0}, \\ & -D \int_{-\pi}^{\pi} \partial_{\theta} \varphi \partial_{\theta} \chi M_{\theta_0} \cos^2(\theta - \theta_0) d\theta = \int_{-\pi}^{\pi} \psi \chi M_{\theta_0} d\theta \quad \forall \chi \in \mathcal{V}_{\theta_0}. \end{aligned} \quad (22)$$

For this variational formulation, we have the following

Proposition 1. (i) (Homogeneous problem) Suppose $\psi = 0$. Then, the unique solutions of [22](#), [23](#) are piecewise constant functions, i.e. there exist $C_{\pm} \in \mathbb{R}$ such that

$$\varphi(\theta) = \begin{cases} C_+ & \text{if } \cos(\theta - \theta_0) > 0, \\ C_- & \text{if } \cos(\theta - \theta_0) < 0. \end{cases} \quad (24)$$

(ii) (Nonhomogeneous problem) Let $\psi \in \mathcal{V}_{\theta_0}$. Then, there exists a solution to [22](#), [23](#) if and only if the following two solvability conditions hold simultaneously:

$$\int_{\cos(\theta-\theta_0)>0} \psi M_{\theta_0} d\theta = 0, \quad \int_{\cos(\theta-\theta_0)<0} \psi M_{\theta_0} d\theta = 0. \quad (25)$$

Under these solvability conditions, there exists a unique solution φ to [22](#), [23](#) which satisfies the additional conditions

$$\int_{\cos(\theta-\theta_0)>0} \varphi M_{\theta_0} d\theta = 0, \quad \int_{\cos(\theta-\theta_0)<0} \varphi M_{\theta_0} d\theta = 0, \quad (26)$$

and the general solution in \mathcal{V}_{θ_0} to [22](#), [23](#) is the sum of the unique solution satisfying [26](#) and the general solution [24](#) of the homogeneous problem.

(iii) (Invariance) Let $\theta_0 = 0$, $\psi_0 \in \mathcal{V}_0$ satisfying the solvability condition [25](#) and φ_0 be the unique solution to [22](#), [23](#) satisfying [26](#). Let now $\theta_0 \in [-\pi/2, \pi/2)$, $\theta_0 \neq 0$ and define ψ and φ such that $\psi(\theta) = \psi_0(\theta - \theta_0)$, $\varphi(\theta) = \varphi_0(\theta - \theta_0)$. Then, φ is the unique solution to [22](#), [23](#) satisfying [26](#) with that value of θ_0 .

Proof. We easily verify that we can choose $\theta_0 = 0$ and thus we drop the indices θ_0 in the definitions of the operators and spaces.

(i) We first verify that the function φ given by [24](#) belongs to \mathcal{V} and satisfies [22](#), [23](#) with $\psi = 0$. We clearly have $\varphi\sqrt{M} \in L^2(-\pi, \pi)$ and

$$\partial_\theta \varphi = (C_+ - C_-)(\delta_{-\pi/2} - \delta_{\pi/2}),$$

where $\delta_{\pm\pi/2}$ is the Dirac delta at $\theta = \pm\pi/2$. Since $|\cos\theta|\sqrt{M}$ is a C^∞ function which takes the value 0 at $\theta = \pm\pi/2$, we have $|\cos\theta|\sqrt{M}\partial_\theta\varphi = 0 \in L^2(-\pi, \pi)$ and φ satisfies [23](#) with right-hand side equal to zero. Now, we suppose that $\varphi \in \mathcal{V}$ is a function satisfying [23](#) with right-hand side equal to zero. Taking $\chi = \varphi$ as a test function in [23](#), we get $|\cos\theta|\sqrt{M}\partial_\theta\varphi = 0$. This implies that φ is constant on all connected components of the set $(|\cos\theta|\sqrt{M})^{-1}(\mathbb{R})$ and is 2π -periodic, which implies that φ is of the form [24](#).

(ii) Let $\psi \in \mathcal{V}$ be such that there exists a solution φ of the variational formulation [22](#), [23](#). Taking χ of the form [24](#), we get that ψ must satisfy the solvability conditions [25](#). Now, we denote by $\tilde{\mathcal{V}}$ the subspace of \mathcal{V} defined by

$$\tilde{\mathcal{V}} = \left\{ \varphi \in \mathcal{V} \text{ such that } \int_{\cos\theta>0} \varphi M d\theta = 0 \text{ and } \int_{\cos\theta<0} \varphi M d\theta = 0 \right\}.$$

Suppose that $\psi \in \mathcal{V}$ satisfies [25](#) and that φ is a solution of the following variational formulation:

$$\varphi \in \tilde{\mathcal{V}}, \quad (27)$$

$$D \int_{-\pi}^{\pi} \partial_\theta \varphi \partial_\theta \chi M \cos^2 \theta d\theta = - \int_{-\pi}^{\pi} \psi \chi M d\theta, \quad \forall \chi \in \tilde{\mathcal{V}}. \quad (28)$$

Then, we claim that φ is a solution of [22](#), [23](#). Indeed, let $\chi \in \mathcal{V}$. Define $\tilde{\chi} = \chi - \chi_0$ with χ_0 constructed according to [24](#) with the constants:

$$C_\pm = \int_{\pm \cos\theta>0} \chi M d\theta.$$

Then, $\tilde{\chi} \in \tilde{\mathcal{V}}$. Therefore, we can apply [28](#) with test function $\tilde{\chi}$. But since χ_0 is of the form [24](#) and ψ satisfies [25](#), the contribution of χ_0 to both the left and right-hand sides of [28](#) vanish. Consequently, φ satisfies [22](#), [23](#) as claimed.

We now show that the variational formulation 27-28 admits a unique solution. For this purpose, we apply Lax-Milgram's Lemma. First, we note that $\tilde{\mathcal{V}}$ is a closed subspace of \mathcal{V} . Indeed, it is obvious that the linear forms $\varphi \rightarrow \int_{\pm \cos \theta > 0} \varphi M \, d\theta$ are continuous. Therefore, $\tilde{\mathcal{V}}$ is a Hilbert space. Then, it is clear that the left-hand side of 28 defines a symmetric continuous bilinear form $a(\varphi, \chi)$ on $\tilde{\mathcal{V}}$ and that the right-hand side of 28 defines a continuous linear form $L(\chi)$ on $\tilde{\mathcal{V}}$. To apply Lax-Milgram's Lemma, it remains to prove that a is coercive. This amounts to proving a Poincaré inequality, i.e. that there exists a constant $C > 0$ such that for all $\varphi \in \tilde{\mathcal{V}}$ we have:

$$\int_{-\pi}^{\pi} |\partial_{\theta} \varphi|^2 M \cos^2 \theta \, d\theta \geq C \int_{-\pi}^{\pi} |\varphi|^2 M \, d\theta. \quad (29)$$

We show that

$$\int_{\cos \theta > 0} |\partial_{\theta} \varphi|^2 M \cos^2 \theta \, d\theta \geq C \int_{\cos \theta > 0} |\varphi|^2 M \, d\theta. \quad (30)$$

Obviously, if such a result is true, it is also true if the integration domains are changed to the set $\{\cos \theta < 0\}$ in both integrals, and this implies 29. We now concentrate on obtaining 30. Let $\psi \in \tilde{\mathcal{V}}$ and let θ_1 and θ_2 be such that $\cos \theta_1 > 0$, $\cos \theta_2 > 0$. We have:

$$\psi(\theta_2) - \psi(\theta_1) = \int_{\theta_1}^{\theta_2} \partial_{\theta} \psi(\theta) \, d\theta.$$

Multiplying by $M(\theta_1)$, integrating with respect to θ_1 on $(-\pi/2, \pi/2)$ and using that $\int_{\cos \theta_1 > 0} \psi(\theta_1) M(\theta_1) \, d\theta_1 = 0$ and $\int_{\cos \theta_1 > 0} M(\theta_1) \, d\theta_1 = 1$, we get:

$$\psi(\theta_2) = \int_{\cos \theta_1 > 0} \left(\int_{\theta_1}^{\theta_2} \partial_{\theta} \psi(\theta) \, d\theta \right) M(\theta_1) \, d\theta_1.$$

Taking the square, multiplying by $M(\theta_2)$ and integrating with respect to θ_2 on $(-\pi/2, \pi/2)$, it leads to:

$$\begin{aligned} & \int_{\cos \theta_2 > 0} |\psi(\theta_2)|^2 M(\theta_2) \, d\theta_2 \\ &= \int_{\cos \theta_2 > 0} \left| \int_{\cos \theta_1 > 0} \left(\int_{\theta_1}^{\theta_2} \partial_{\theta} \psi(\theta) \, d\theta \right) M(\theta_1) \, d\theta_1 \right|^2 M(\theta_2) \, d\theta_2, \end{aligned}$$

and by the Cauchy-Schwarz inequality with respect to the inner product on \mathcal{H} , again using that $\int_{\cos \theta_1 > 0} M(\theta_1) \, d\theta_1 = 1$, we obtain

$$\begin{aligned} & \int_{\cos \theta_2 > 0} |\psi(\theta_2)|^2 M(\theta_2) \, d\theta_2 \\ &\leq \int_{\cos \theta_1 > 0} \int_{\cos \theta_2 > 0} \left| \int_{\theta_1}^{\theta_2} \partial_{\theta} \psi(\theta) \, d\theta \right|^2 M(\theta_1) M(\theta_2) \, d\theta_1 \, d\theta_2 \\ &\leq I_1 + \dots + I_4, \end{aligned} \quad (31)$$

where I_1, \dots, I_4 are the integrals with respect to the sets Ω_1 to Ω_4 with $\Omega_1 = \{|\sin \theta_1| < 1/2, |\sin \theta_2| < 1/2\}$, $\Omega_2 = \{|\sin \theta_1| < 1/2, |\sin \theta_2| > 1/2\}$, $\Omega_3 = \{|\sin \theta_1| > 1/2, |\sin \theta_2| < 1/2\}$, $\Omega_4 = \{|\sin \theta_1| > 1/2, |\sin \theta_2| > 1/2\}$ respectively. For $|\sin \theta| < 1/2$, there exist constants C_1 and C_2 such that $0 < C_1 \leq M(\theta) \leq C_2$.

$C_2 < \infty$ and $0 < C_1 \leq \cos^2 \theta M(\theta) \leq C_2 < \infty$. So, for $(\theta_1, \theta_2) \in \Omega_1$, using Cauchy-Schwarz inequality, we have:

$$\int_{\theta_1}^{\theta_2} \partial_\theta \psi(\theta) d\theta \leq C \left(\int_{\cos \theta > 0} |\partial_\theta \psi(\theta)|^2 M(\theta) \cos^2 \theta d\theta \right)^{1/2}, \quad (32)$$

and consequently,

$$I_1 \leq C \int_{\cos \theta > 0} |\partial_\theta \psi(\theta)|^2 M(\theta) \cos^2 \theta d\theta, \quad (33)$$

where here and in the following, we denote by C generic constants. Take now $(\theta_1, \theta_2) \in \Omega_4$. Then, using Cauchy-Schwarz inequality, we have:

$$\begin{aligned} \int_{\theta_1}^{\theta_2} \partial_\theta \psi(\theta) d\theta &= \int_{\theta_1}^{\theta_2} |\cos \theta| \sqrt{M(\theta)} \partial_\theta \psi(\theta) (|\cos \theta| \sqrt{M(\theta)})^{-1} d\theta \\ &\leq \left(\int_{\theta_1}^{\theta_2} |\partial_\theta \psi(\theta)|^2 \cos^2 \theta M(\theta) d\theta \right)^{\frac{1}{2}} \left(\int_{\theta_1}^{\theta_2} \frac{d\theta}{\cos^2 \theta M(\theta)} \right)^{\frac{1}{2}}. \end{aligned} \quad (34)$$

Now, we remark that

$$\partial_\theta \left(\frac{1}{M(\theta)} \right) = \kappa \frac{1}{M(\theta)} \frac{\sin \theta}{\cos^2 \theta},$$

and deduce that

$$\begin{aligned} \int_{\theta_1}^{\theta_2} \frac{d\theta}{\cos^2 \theta M(\theta)} &= \frac{1}{\kappa} \int_{\theta_1}^{\theta_2} \partial_\theta \left(\frac{1}{M(\theta)} \right) \frac{1}{\sin \theta} d\theta \\ &= \frac{1}{\kappa} \left(\frac{1}{M(\theta_2) \sin \theta_2} - \frac{1}{M(\theta_1) \sin \theta_1} \right) + \frac{1}{\kappa} \int_{\theta_1}^{\theta_2} \frac{1}{M(\theta)} \frac{\cos \theta}{\sin^2 \theta} d\theta. \end{aligned} \quad (35)$$

Then, we have

$$\begin{aligned} &M(\theta_1) M(\theta_2) \int_{\theta_1}^{\theta_2} \frac{d\theta}{\cos^2 \theta M(\theta)} \\ &= \frac{1}{\kappa} \left(\frac{M(\theta_1)}{\sin \theta_2} - \frac{M(\theta_2)}{\sin \theta_1} \right) + \frac{1}{\kappa} \int_{\theta_1}^{\theta_2} \frac{M(\theta_1) M(\theta_2)}{M(\theta)} \frac{\cos \theta}{\sin^2 \theta} d\theta. \end{aligned} \quad (36)$$

The first term is bounded on Ω_4 . For the second term we remark that

$$\frac{M(\theta_1) M(\theta_2)}{M(\theta)} = \exp \left[\kappa \left(\frac{1}{\cos \theta} - \left(\frac{1}{\cos \theta_1} + \frac{1}{\cos \theta_2} \right) \right) \right].$$

Now, $1/\cos \theta$ is a convex function and $\theta \in [\theta_1, \theta_2]$. Assuming, without loss of generality, that $\theta_1 < \theta_2$, we have:

$$\frac{1}{\cos \theta} \leq \frac{\theta_2 - \theta}{\theta_2 - \theta_1} \frac{1}{\cos \theta_1} + \frac{\theta - \theta_1}{\theta_2 - \theta_1} \frac{1}{\cos \theta_2},$$

and we deduce that

$$\frac{1}{\cos \theta} - \left(\frac{1}{\cos \theta_1} + \frac{1}{\cos \theta_2} \right) \leq \frac{\theta_1 - \theta}{\theta_2 - \theta_1} \frac{1}{\cos \theta_1} + \frac{\theta - \theta_2}{\theta_2 - \theta_1} \frac{1}{\cos \theta_2} \leq 0.$$

Therefore, $M(\theta_1) M(\theta_2) / M(\theta) \leq 1$ and since $\frac{\cos \theta}{\sin^2 \theta}$ is also bounded for θ such that $\sin \theta > 1/2$, we deduce that the second term of [36](#) is also bounded. Consequently,

for $(\theta_1, \theta_2) \in \Omega_4$, we get

$$\left| \int_{\theta_1}^{\theta_2} \partial_\theta \psi(\theta) d\theta \right|^2 M(\theta_1) M(\theta_2) \leq C \int_{\cos \theta > 0} |\partial_\theta \psi(\theta)|^2 M(\theta) \cos^2 \theta d\theta, \quad (37)$$

which implies, upon integrating with respect to (θ_1, θ_2) , that

$$I_4 \leq C \int_{\cos \theta > 0} |\partial_\theta \psi(\theta)|^2 M(\theta) \cos^2 \theta d\theta. \quad (38)$$

Now, we take $(\theta_1, \theta_2) \in \Omega_2$ (obviously the case of $(\theta_1, \theta_2) \in \Omega_3$ can be treated similarly). In this case, I_2 is decomposed into $I_2 = I_2^1 + I_2^2$ where I_2^1 and I_2^2 correspond to integrals over the domains $\Omega_2^1 = (-\pi/6, \pi/6) \times (-\pi/2, -\pi/6)$ and $\Omega_2^2 = (-\pi/6, \pi/6) \times (\pi/6, \pi/2)$ respectively. We consider I_2^2 and a similar proof can be made for I_2^1 . For $(\theta_1, \theta_2) \in \Omega_2^2$, we can decompose:

$$\int_{\theta_1}^{\theta_2} \partial_\theta \psi(\theta) d\theta = \int_{\theta_1}^{\pi/6} \partial_\theta \psi(\theta) d\theta + \int_{\pi/6}^{\theta_2} \partial_\theta \psi(\theta) d\theta,$$

and consequently we have:

$$\left| \int_{\theta_1}^{\theta_2} \partial_\theta \psi(\theta) d\theta \right|^2 \leq 2 \left| \int_{\theta_1}^{\pi/6} \partial_\theta \psi(\theta) d\theta \right|^2 + 2 \left| \int_{\pi/6}^{\theta_2} \partial_\theta \psi(\theta) d\theta \right|^2. \quad (39)$$

Each of the terms will be evaluated separately. For the first term, we proceed as for I_1 and notice that $M(\theta)$ and $M(\theta) |\cos \theta|$ are bounded from above and from below away from zero, so that we can estimate it similarly to 32 and its contribution to I_2^2 leads to a similar estimate as 33. For the second term, we use 34 with θ_1 replaced by $\pi/6$ and likewise, we find 35 still with θ_1 replaced by $\pi/6$. We can keep on going through all the steps of the proof and we eventually get an estimate similar to 37 with θ_1 replaced by $\pi/6$. This shows that the second term of 39 leads to an estimate similar to 38. Therefore, we get

$$I_2 \leq C \int_{\cos \theta > 0} |\partial_\theta \psi(\theta)|^2 M(\theta) \cos^2 \theta d\theta. \quad (40)$$

Now, inserting 33, 38, 40 and its counterpart for I_3 into 31 leads to the Poincaré estimate 30 and eventually to 29, which ends the proof of the Poincaré estimate.

(iii) We restore the indices θ_0 . Then it is obvious that ψ and φ satisfy the conditions 25, 26 respectively and that they belong to \mathcal{V}_{θ_0} . So, they belong to $\tilde{\mathcal{V}}_{\theta_0}$. Furthermore, by the change of variable $\theta' = \theta + \theta_0$ in the variational formulation satisfied by φ_0 (i.e. with $\theta_0 = 0$), we easily see that φ satisfies the variational formulation 22, 23. Since the solution of this variational formulation in the space $\tilde{\mathcal{V}}_{\theta_0}$ is unique, φ is this solution. \square

3.2. Equilibria. We now define the notion of equilibria and characterize them:

Definition 3.4. An equilibrium is a function $f: \theta \in \mathbb{R}/(2\pi\mathbb{Z}) \mapsto f(\theta)$ such that $f \in L^1(-\pi, \pi)$, $f/M_{\bar{\theta}_f} \in \mathcal{V}_{\bar{\theta}_f}$ and $Q_{\text{al}}^0(f) = 0$. We denote by \mathcal{E} the set of equilibria of Q_{al}^0 .

We also introduce

Definition 3.5. Let ρ_+ , ρ_- be real numbers in $[0, \infty)$ and $\bar{\theta} \in [-\pi/2, \pi/2)$ be an angle of lines. The function $\bar{f}_{\rho_+, \rho_-, \bar{\theta}}$ is defined by

$$\bar{f}_{\rho_+, \rho_-, \bar{\theta}}(\theta) = \begin{cases} \rho_+ M_{\bar{\theta}}(\theta) & \text{for } \cos(\theta - \bar{\theta}) > 0, \\ \rho_- M_{\bar{\theta}}(\theta) & \text{for } \cos(\theta - \bar{\theta}) < 0. \end{cases} \quad (41)$$

It can also be written as:

$$\bar{f}_{\rho_+, \rho_-, \bar{\theta}} = M_{\bar{\theta}}(\theta) [\rho_+ \chi_{\bar{\theta}}^+ + \rho_- \chi_{\bar{\theta}}^-], \quad (42)$$

where $\chi_{\bar{\theta}}^{\pm}$ are the indicator functions:

$$\chi_{\bar{\theta}}^{\pm}(\theta) = \begin{cases} 1 & \text{if } \pm \cos(\theta - \bar{\theta}) > 0, \\ 0 & \text{if } \pm \cos(\theta - \bar{\theta}) < 0. \end{cases} \quad (43)$$

Now, with this definition and Proposition 1, we can state the

Lemma 3.6. *The set \mathcal{E} of equilibria of Q_{al}^0 is given by*

$$\mathcal{E} = \{\bar{f}_{\rho_+, \rho_-, \bar{\theta}} \mid (\rho_+, \rho_-) \in [0, \infty)^2, \bar{\theta} \in [-\pi/2, \pi/2)\}.$$

Proof. We use 21. Thanks to Proposition 1 (i), we first note that, for a given $\theta_0 \in [-\pi/2, \pi/2)$, we have

$$\begin{aligned} M_{\theta_0} \mathcal{L}_{\theta_0} \left(\frac{f}{M_{\theta_0}} \right) = 0 & \iff \frac{f}{M_{\theta_0}} \text{ is of the form 24} \\ & \iff \exists (\rho_+, \rho_-) \in [0, \infty)^2 \text{ s.t. } f = \bar{f}_{\rho_+, \rho_-, \theta_0}. \end{aligned}$$

Applying this statement with $\theta_0 = \bar{\theta}_f$, we deduce that if $f \in \mathcal{E}$, i.e. $Q_{al}^0 f = 0$, then f is necessarily written as $f = \bar{f}_{\rho_+, \rho_-, \bar{\theta}_f}$ and is consequently of the form 41. Conversely, for given $(\rho_+, \rho_-) \in [0, \infty)^2$, and $\bar{\theta} \in [-\pi/2, \pi/2)$, we consider $\bar{f}_{\rho_+, \rho_-, \bar{\theta}}$ and need to show that $Q_{al}^0 \bar{f}_{\rho_+, \rho_-, \bar{\theta}} = 0$. Since $\bar{f}_{\rho_+, \rho_-, \bar{\theta}}$ is such that $M_{\bar{\theta}} \mathcal{L}_{\bar{\theta}}(f/M_{\bar{\theta}}) = 0$ (by the equivalence shown above), it is enough to show that $\bar{\theta}_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}} = \bar{\theta}$, or equivalently, that:

$$\int_{-\pi}^{\pi} \sin 2(\theta - \bar{\theta}) \bar{f}_{\rho_+, \rho_-, \bar{\theta}} d\theta = 0.$$

But we can make the change of variables $\theta' = \theta - \bar{\theta}$ and use the periodicity to write:

$$\int_{-\pi}^{\pi} \sin 2(\theta - \bar{\theta}) \bar{f}_{\rho_+, \rho_-, \bar{\theta}} d\theta = \int_{-\pi}^{\pi} \sin 2\theta \bar{f}_{\rho_+, \rho_-, 0} d\theta,$$

and this last integral is clearly zero by symmetry. \square

3.3. Generalized collision invariants. We first define the notion of a collision invariant, thanks to the

Definition 3.7. A function $\theta \in \mathbb{R}/(2\pi\mathbb{Z}) \mapsto \Psi(\theta)$ is a collision invariant (CI) if and only if it satisfies

$$\int Q_{al}^0 f(\theta) \Psi(\theta) d\theta = 0 \quad \text{for all } f.$$

We deliberately leave the function setting vague as this notion will have to be enlarged later on. Clearly, the set of collision invariants is a vector space. At this point, however, we only have a one-dimensional space of collision invariants, spanned by the constant function $\Psi(\theta) = 1$, corresponding to mass conservation. Following the approach in [25], we therefore generalize the concept of a collision invariant and define a generalized collision invariant:

Definition 3.8. Given an angle of lines $\theta_0 \in [-\pi/2, \pi/2)$, a function $\Psi \in \mathcal{V}_{\theta_0}$ is a generalized collision invariant (GCI) associated with θ_0 if and only if

$$\langle \mathcal{L}_{\theta_0} \frac{f}{M_{\theta_0}}, \Psi \rangle_{\mathcal{V}'_{\theta_0}, \mathcal{V}_{\theta_0}} = 0 \quad \text{for all } f \in \mathcal{V}_{\theta_0} \cap L^1(-\pi, \pi) \quad \text{s.t. } \bar{\theta}_f = \theta_0. \quad (44)$$

Here the equality $\bar{\theta}_f = \theta_0$ is an equality of angles of lines, i.e. it holds modulo π . The set of GCI associated with θ_0 is a linear space denoted by \mathcal{G}_{θ_0} .

We note that for any $f \in \mathcal{V}_{\theta_0}$ such that $\mathcal{L}_{\theta_0} \frac{f}{M_{\theta_0}} \in \mathcal{H}_{\theta_0}$, the duality bracket $\langle \mathcal{L}_{\theta_0} \frac{f}{M_{\theta_0}}, \Psi \rangle_{\mathcal{V}'_{\theta_0}, \mathcal{V}_{\theta_0}}$ reduces to the classical integral, $\int \mathcal{L}_{\theta_0} \frac{f}{M_{\theta_0}}(\theta) \Psi(\theta) M_{\theta_0}(\theta) d\theta$. Since Ψ being a CI equivalently means that

$$\int \mathcal{L}_{\bar{\theta}_f} \frac{f}{M_{\bar{\theta}_f}}(\theta) \Psi(\theta) M_{\bar{\theta}_f}(\theta) d\theta = 0 \quad \text{for all } f,$$

we pass from the definition of a CI to that of a GCI by replacing the orientation $\bar{\theta}_f$ of f by an arbitrary orientation θ_0 and requesting that the integral is zero only for those functions f whose mean orientation $\bar{\theta}_f$ coincides with θ_0 . Because this means we restrict the set of functions f , we expect to find more Ψ , fulfilling the definition of a GCI as compared to that of a CI. We can reformulate the definition of a GCI in the following way:

Lemma 3.9. *Given an angle of lines $\theta_0 \in [-\pi/2, \pi/2)$, a function $\Psi \in \mathcal{V}_{\theta_0}$ is a GCI associated with θ_0 if and only if:*

$$\exists a \in \mathbb{R} \quad \text{such that} \quad \mathcal{L}_{\theta_0} \Psi(\theta) = a \sin 2(\theta - \theta_0) \quad \text{in } \mathcal{V}'_{\theta_0}. \quad (45)$$

Proof. We note that the constraint $\bar{\theta}_f = \theta_0$ can be equivalently rephrased as the linear constraint:

$$\int_{-\pi}^{\pi} \sin 2(\theta - \theta_0) f(\theta) d\theta = 0.$$

By a classical duality argument already used in [25], statement 44 is equivalent to the existence of a constant $a \in \mathbb{R}$ such that

$$\langle \mathcal{L}_{\theta_0} \frac{f}{M_{\theta_0}}, \Psi \rangle_{\mathcal{V}'_{\theta_0}, \mathcal{V}_{\theta_0}} = a \int_{-\pi}^{\pi} \sin 2(\theta - \theta_0) f(\theta) d\theta \quad \text{for all } f \in \mathcal{V}_{\theta_0} \cap L^1(-\pi, \pi).$$

Using the formal self-adjointness of \mathcal{L}_{θ_0} (see Definition 3.3 (iv)), this is equivalent to

$$\langle \mathcal{L}_{\theta_0} \Psi, \frac{f}{M_{\theta_0}} \rangle_{\mathcal{V}'_{\theta_0}, \mathcal{V}_{\theta_0}} = a \left(\sin 2(\theta - \theta_0), \frac{f}{M_{\theta_0}} \right)_{\mathcal{H}_{\theta_0}} \quad \text{for all } f \in \mathcal{V}_{\theta_0} \cap L^1(-\pi, \pi),$$

which implies that Ψ satisfies 45. The converse is obvious. \square

We now have the following result:

Proposition 2. (i) *Given an angle of lines $\theta_0 \in [-\pi/2, \pi/2)$, the space \mathcal{G}_{θ_0} of GCI associated with θ_0 is of dimension three and is spanned by $\chi_{\theta_0}^+$, $\chi_{\theta_0}^-$ and g_{θ_0} , with $\chi_{\theta_0}^{\pm}$ given by 43 and g_{θ_0} , the unique solution in \mathcal{V}_{θ_0} of the variational formulation 22, 23 with right-hand side $\psi(\theta) = \sin 2(\theta - \theta_0)$ and satisfying the cancellation condition 26.*

(ii) *The functions $\chi_{\theta_0}^{\pm}$ and g_{θ_0} can be written as:*

$$\chi_{\theta_0}^{\pm}(\theta) = \chi_0^{\pm}(\theta - \theta_0), \quad g_{\theta_0}(\theta) = g_0(\theta - \theta_0). \quad (46)$$

In the remainder, we will write χ^\pm and g for χ_0^\pm and g_0 . In addition, g satisfies the symmetry conditions:

$$g(-\theta) = -g(\theta), \quad g(\pi - \theta) = -g(\theta). \quad (47)$$

Proof. (i) First, we note that the solution space of Problem 45 is the linear space spanned by the solution of the same problem with $a = 1$. Therefore, we restrict ourselves to $a = 1$. Now, solving Problem 45 with $a = 1$ amounts to solving the variational formulation 22, 23 with right-hand side $\psi(\theta) = \sin 2(\theta - \theta_0)$. We apply Proposition 1 (ii). A necessary and sufficient condition for the existence of a solution is that the right-hand side satisfies the solvability condition 25, which in the present case, with $\psi = \sin 2(\theta - \theta_0)$ reads:

$$\int_{\cos(\theta - \theta_0) > 0} \sin 2(\theta - \theta_0) M_{\theta_0} d\theta = 0, \quad \int_{\cos(\theta - \theta_0) < 0} \sin 2(\theta - \theta_0) M_{\theta_0} d\theta = 0.$$

This condition is obviously satisfied by symmetry. Therefore, there exists a unique solution g_{θ_0} of the problem satisfying the cancellation condition 26 and all solutions of the problems differ from this one by the addition of a solution of the homogeneous problem, i.e. of the type 24. Such solutions are arbitrary linear combinations of $\chi_{\theta_0}^\pm$.

(ii) The statement is obvious for $\chi_{\theta_0}^\pm$. For g_{θ_0} , we simply apply Proposition 1 (iii). Finally, we remark that $\sin 2\theta$ satisfies the symmetry conditions 47. Therefore, using the uniqueness part of Proposition 1 (ii), we deduce that g satisfies the same symmetry conditions. \square

In the present simple two-dimensional case, we can have an explicit formula for g , given by the Lemma below and depicted in Figure 2.

Lemma 3.10. *For $\theta \in [0, \pi/2]$ we have*

$$g(\theta) = - \int_0^\theta \frac{\int_{\beta}^{\frac{\pi}{2}} \sin 2\alpha \exp(-\frac{\kappa}{\cos \alpha}) d\alpha}{\cos^2 \beta \exp(-\frac{\kappa}{\cos \beta})} d\beta, \quad (48)$$

and g is extended to $\mathbb{R}/(2\pi\mathbb{Z})$ by the symmetry conditions 47.

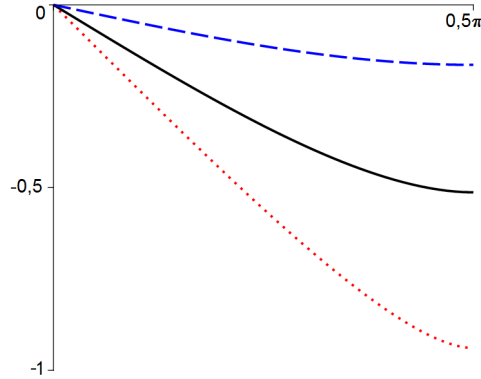
Proof. Solving for g consists of solving the following problem:

$$\frac{d}{d\theta} \left(\cos^2 \theta e^{-\frac{\kappa}{\cos \theta}} \frac{dg}{d\theta}(\theta) \right) = \sin 2\theta e^{-\frac{\kappa}{\cos \theta}}. \quad (49)$$

Eq. 49 can be solved explicitly for $\theta \in [0, \pi/2]$ and then extended using the symmetry conditions 47. Integration constants are determined by the cancellation conditions 26. \square

4. Hydrodynamic model.

4.1. Derivation. This section is concerned with the limit $\varepsilon \rightarrow 0$ in Problem 15-16. The first step is the observation that the dominant term $Q_{\text{al}}^0 f^\varepsilon = 0$ requires the limiting distribution to lie in the kernel of Q_{al}^0 , characterized by Lemma 3.6. To determine the equations satisfied by the macroscopic quantities $\rho_+(x, t)$, $\rho_-(x, t)$ and $\bar{\theta}(x, t)$, it is necessary to consider the terms of order ε in 15. This is done by multiplication with the three independent GCI given in Proposition 2 and subsequent integration over θ . The computations are similar to those in [25] and are described in more detail in the Appendix (Section 8.1). Here, we simply state the result:

FIGURE 2. $g(\theta)$ for $\kappa = 0.5, 2, 10$ (red-dotted, black-solid, blue-dashed).

Theorem 4.1. Taking the (formal) limit $\varepsilon \rightarrow 0$ in 15-16, we obtain

$$f^\varepsilon(x, \theta, t) \rightarrow \bar{f}_{\rho_+(x,t), \rho_-(x,t), \bar{\theta}(x,t)}(\theta),$$

where the macroscopic quantities $\rho_\pm(x, t)$ and $\bar{\theta}(x, t)$ have values in $[0, \infty)$ and $[-\pi/2, \pi/2)$ respectively and fulfill the following system of equations:

$$\partial_t \rho_+ + d_1 \nabla_x \cdot (\rho_+ v(\bar{\theta})) = 0, \quad (50)$$

$$\partial_t \rho_- - d_1 \nabla_x \cdot (\rho_- v(\bar{\theta})) = 0, \quad (51)$$

$$(\rho_+ + \rho_-) \partial_t \bar{\theta} + d_2 (\rho_+ - \rho_-) (v(\bar{\theta}) \cdot \nabla_x) \bar{\theta} + \mu v^\perp(\bar{\theta}) \cdot \nabla_x (\rho_+ - \rho_-) = 0, \quad (52)$$

where we recall that $v(\bar{\theta}) = (\cos \bar{\theta}, \sin \bar{\theta})$ and $v^\perp(\bar{\theta}) = (-\sin \bar{\theta}, \cos \bar{\theta})$. The coefficients d_1 , d_2 and μ are given by:

$$d_1 = \langle \cos \rangle_M, \quad d_2 = \frac{\langle g \frac{\sin}{\cos} \rangle_M}{\langle g \frac{\sin}{\cos^2} \rangle_M}, \quad \mu = \frac{1}{\kappa} \frac{\langle g \sin \rangle_M}{\langle g \frac{\sin}{\cos^2} \rangle_M}. \quad (53)$$

where g is the GCI defined in Proposition 2 and explicitly given by 48. For a function $\varphi(\theta)$, we denote by $\langle \varphi \rangle_M$ the following average:

$$\langle \varphi \rangle_M = 2 \int_0^{\pi/2} \varphi(\theta) M(\theta) d\theta = \frac{2}{Z_\kappa} \int_0^{\pi/2} \varphi(\theta) e^{-\frac{\kappa}{\cos \theta}} d\theta, \quad (54)$$

where M is $M_{\bar{\theta}}$ for $\bar{\theta} = 0$.

The proof can be found in the Appendix (Section 8.1).

As shown in the proof of Lemma 3.6, the macroscopic quantity $\bar{\theta}(x, t)$ is the local mean angle of lines as defined in 13 of the equilibrium distribution \bar{f} . The functions $\rho_+(x, t)$ and $\rho_-(x, t)$ describe the local densities of particles that point in direction $[\bar{\theta}(x, t) - \pi/2, \bar{\theta}(x, t) + \pi/2)$ and $[\bar{\theta}(x, t) + \pi/2, \bar{\theta}(x, t) + 3\pi/2)$ respectively. Eqs. 50 and 51 simply describe number density transport in the direction of $v(\bar{\theta})$ (for ρ_+) or $-v(\bar{\theta})$ (for ρ_-). These equations express local conservations of the number densities of the particles moving in the direction of $v(\bar{\theta})$ or $-v(\bar{\theta})$ respectively. Since GCI do not express local conservations (unless they are CI), in general one cannot expect that they will lead to conservation laws. Here, Eqs. 50 and 51 are conservation laws in spite of the fact that they are derived from using the GCI $\chi_{\theta_f}^\pm$. This unusual circumstance is due to the particular expression of the collision operator Q_{al}^0 .

Note that whenever $\rho_+ = \rho_-$, it follows that $\partial_t \bar{\theta} = 0$ and $\partial_t(\rho_+ + \rho_-) = 0$. An alternative formulation of System 50-52 can be obtained by defining $\rho = \rho_+ + \rho_-$ and $\delta = \rho_+ - \rho_-$. We get:

$$\partial_t \rho + d_1 \nabla_x \cdot (\delta v(\bar{\theta})) = 0, \quad (55)$$

$$\partial_t \delta - d_1 \nabla_x \cdot (\rho v(\bar{\theta})) = 0, \quad (56)$$

$$\rho \partial_t \bar{\theta} + d_2 \delta (v(\bar{\theta}) \cdot \nabla_x) \bar{\theta} + \mu (v(\bar{\theta})^\perp \cdot \nabla_x) \delta = 0. \quad (57)$$

It is instructive to compare with the Self-Organized Hydrodynamic (SOH) system derived in [25], which, in dimension two, takes the form:

$$\partial_t \rho + \tilde{d}_1 \nabla_x \cdot (\rho v(\bar{\theta})) = 0, \quad (58)$$

$$\rho (\partial_t \bar{\theta} + \tilde{d}_2 (v(\bar{\theta}) \cdot \nabla_x) \bar{\theta}) + \tilde{\mu} (v(\bar{\theta})^\perp \cdot \nabla_x) \rho = 0, \quad (59)$$

where the constants \tilde{d}_1, \tilde{d}_2 and $\tilde{\mu}$ depend on κ and the collision invariants of the corresponding alignment operator. This model is based on polar alignment. Here by contrast to System 50-52, $\bar{\theta}$ is an angle of vectors, i.e. $\bar{\theta} \in \mathbb{R}/(2\pi\mathbb{Z})$ and the particles are distributed according to a classical von Mises-Fisher distribution (i.e. their angular distribution is proportional to $e^{\kappa \cos(\theta - \bar{\theta})}$) and they move (with a certain dispersion described by κ) in the direction of $\bar{\theta}$.

The fact that the nematic alignment leads to an equilibrium *angle of lines* as opposed to an *angle of vectors* is reflected in the existence of two opposing local maxima at $\bar{\theta}$ and $\bar{\theta} + \pi$ of the GVM $M_{\bar{\theta}}(\theta)$, whilst the classical von Mises-Fisher distribution has only one. The factor $\cos^2(\theta - \bar{\theta}_f)$ in front of the diffusion operator in Q_{al}^0 allows for this separation into two groups and causes $M_{\bar{\theta}}(\theta) = 0$ for $\theta = \bar{\theta} \pm \pi/2$, i.e. in equilibrium there are no particles moving perpendicular to the equilibrium angle of lines. On the other hand, both the von Mises-Fisher distribution and the GVM share their general “bump-like” shape and the convergence to a Dirac delta for $\kappa \rightarrow \infty$. At the level of the macroscopic equations further similarities and differences become evident. In the nematic case both groups of particles have their own conservation law, consequently we have three instead of two macroscopic equations. The general structure remains the same: Transport equations for the density complemented by an equation describing the angle evolution, consisting of a time derivative, a convection term and a pressure term. However for the nematic SOH model both the convection and the pressure term depend on the local density difference δ . In the case where there is only one group of particles, e.g. $\rho_+ = \rho$ and $\rho_- = 0$ system 50-52 reduces to 58-59 (with different constants), since then the nematic character of the collisions does not play a role.

4.2. Hyperbolicity of the macroscopic model. An important property of the original SOH system 58-59 is its hyperbolicity. In [30] a variant of the SOH model was examined. It was found that in some regions hyperbolicity is lost, which affects the behavior of the solutions. Therefore, we examine the hyperbolicity of the macroscopic model 50-52. To simplify the analysis we rescale the system with $t \rightarrow d_1 t$. In the following we therefore abbreviate $\hat{d}_2 = d_2/d_1$ and $\hat{\mu} = \mu/d_1$.

Lemma 4.2. *The macroscopic system 50-52 is hyperbolic.*

Proof. We use the alternative formulation 55-57, which leads to simpler formulas. we define $u(x, t) = (\rho(x, t), \delta(x, t), \bar{\theta}(x, t))$ with $x = (x_1, x_2) \in \mathbb{R}^2$, yielding

$$\partial_t u + A \partial_{x_1} u + B \partial_{x_2} u = 0,$$

where

$$A(\rho, \delta, \bar{\theta}) = \begin{pmatrix} 0 & \cos \bar{\theta} & -\delta \sin \bar{\theta} \\ \cos \bar{\theta} & 0 & -\rho \sin \bar{\theta} \\ 0 & -\frac{\hat{\mu}}{\rho} \sin \bar{\theta} & \frac{\hat{d}_2 \delta}{\rho} \cos \bar{\theta} \end{pmatrix}, \quad B(\rho, \delta, \bar{\theta}) = A(\rho, \delta, \bar{\theta} - \pi/2).$$

To determine the hyperbolicity of the system, it suffices to show that the matrix A has real and distinct eigenvalues for all $\bar{\theta} \in [-\pi/2, \pi/2]$. The characteristic polynomial of A , $\text{charPoly}_A(z)$ is of third degree and has the shape

$$\begin{aligned} & \text{charPoly}_A(z) \\ &= z^3 - \frac{\delta}{\rho} \cos \theta \hat{d}_2 z^2 - (\hat{\mu} \sin^2 \theta + \cos^2 \theta) z - \frac{\delta}{\rho} \cos \theta (\mu \sin^2 \theta - \hat{d}_2 \cos^2 \theta). \end{aligned}$$

To understand its roots, we use the following definition of a discriminant of a third order polynomial: for $p(z) = a_3 z^3 + a_2 z^2 + a_1 z + a_0$ we define

$$\text{discr}_p = -27a_3^2 a_0^2 + 18a_3 a_0 a_1 a_2 + a_2^2 a_1^2 - 4a_3^3 a_0 - 4a_1^3 a_3.$$

Next we observe that the discriminant of the characteristic polynomial of A , which we define as $\Delta = \text{discr}_{\text{charPoly}_A}$, can be interpreted as a quadratic polynomial in $X = (\delta/\rho)^2$ with coefficients dependent on $c = \cos^2 \theta$, namely:

$$\Delta(X) = \alpha(c)X^2 + \beta(c)X + \gamma(c),$$

where

$$\begin{aligned} \alpha(c) &= 4\hat{d}_2^3 c^2 [c(\hat{d}_2 + \hat{\mu}) - \hat{\mu}], \\ \beta(c) &= c \left[\left(\hat{d}_2^2 \hat{\mu}^2 - 18\hat{d}_2 \hat{\mu}^2 - 27\hat{\mu}^2 - 36\hat{d}_2 \hat{\mu} - 8\hat{d}_2^2 - 20\hat{d}_2^2 \hat{\mu} \right) c^2 \right. \\ &\quad \left. + 2\hat{\mu} \left(-\hat{d}_2^2 \hat{\mu} + 18\hat{d}_2 + 10\hat{d}_2^2 + 27\hat{\mu} + 18\hat{\mu} \hat{d}_2 \right) c - \hat{\mu}^2 (18\hat{d}_2 - \hat{d}_2^2 + 27) \right], \\ \gamma(c) &= 4[c(1 - \hat{\mu}) + \hat{\mu}]^3. \end{aligned}$$

If $\Delta(X) > 0$ for all $c \in [0, 1]$ and all $X \in [0, 1]$ we have three distinct, real eigenvalues and the system is (strictly) hyperbolic. The roots of $\Delta(X)$ are given by

$$X_{1,2}(c) = \frac{-\beta(c) \pm \sqrt{\beta(c)^2 - 4\alpha(c)\gamma(c)}}{2\alpha(c)}.$$

Simple calculations show that for $c > \frac{9(\hat{\mu} + \hat{d}_2)}{9\hat{\mu} + \hat{\mu}\hat{d}_2 + 8\hat{d}_2}$ the discriminant $\Delta(X)$ has no real roots and is positive for all $X \in [0, 1]$. Otherwise we can distinguish between $c > s := \frac{\hat{\mu}}{\hat{\mu} + \hat{d}_2}$ and $0 \leq c \leq s$. In the first case both roots $X_{1,2}(c)$ are negative and are therefore not relevant. In the second case we lose hyperbolicity for $X > X_2(c)$. However a simple analysis shows that $X_2(c) \geq 1$ for all $0 \leq c \leq s$. In fact $X_2(c) \rightarrow \infty$ for $c \rightarrow 0^+$ and $c \rightarrow s^-$ and $\min_{c \in [0, s]} X_2(c) = 1$. Since $X \in [0, 1]$ this shows the hyperbolicity of the system. \square

5. Weakly non-local scaling. In this section we want to investigate how the model changes, if we allow for a relatively larger interaction radius. With the scaling choice below, this leads to interactions that are no longer local in the limit, but rather weakly non-local. This and other scaling choices for different models of self-propelled particles have been examined in [22]. In the scaling performed in

Section 2.2, we used $\hat{R} = \mathcal{O}(\varepsilon)$. If we use $\hat{R} = \mathcal{O}(\sqrt{\varepsilon})$ instead, namely $\hat{R} = \sqrt{\varepsilon} r$, we are led to the following expression for J_f^ε :

$$J_f^\varepsilon(x, t) = \int_{-\pi}^{\pi} \int_{|y-x| \leq \sqrt{\varepsilon} r} v(2\theta) f(y, \theta, t) dy d\theta,$$

and $\bar{\Theta}_f^\varepsilon$ is still given by 11. Then, we need to consider higher order terms in the Taylor expansion of J_f^ε and $\bar{\Theta}_f^\varepsilon$. These are given by the following:

Lemma 5.1. *We have*

$$J_f^\varepsilon(x, t) = \varepsilon \pi r^2 (j_f(x, t) + \varepsilon j_f^1(x, t) + \mathcal{O}(\varepsilon^2)), \quad (60)$$

$$j_f^1(x, t) = k \Delta_x j_f(x, t), \quad k = \frac{1}{4\pi r^2} \int_{|\xi| \leq r} |\xi|^2 d\xi = \frac{r^2}{8}, \quad (61)$$

$$\bar{\Theta}_f^\varepsilon = \bar{\theta}_f + \varepsilon \bar{\theta}_f^1 + \mathcal{O}(\varepsilon^2), \quad \bar{\theta}_f^1 = \frac{1}{2|j_f|} (j_f^1 \cdot v^\perp(2\bar{\theta}_f)), \quad (62)$$

and where $j_f, \bar{\theta}_f$ are given by 14 and 13 respectively.

Proof. We change variables to $y = x + \sqrt{\varepsilon} \xi$ and get

$$J_f^\varepsilon(x, t) = \varepsilon \int_{|\xi| \leq r} \int_{-\pi}^{\pi} v(2\theta) f(x + \sqrt{\varepsilon} \xi, \theta, t) d\xi d\theta.$$

By Taylor expansion of f with respect to $\sqrt{\varepsilon}$ and using cancellations of the order $\sqrt{\varepsilon}$ terms due to symmetry, we find 60, 61. Therefore, we get

$$\begin{aligned} \frac{J_f}{|J_f|} &= \frac{j_f}{|j_f|} + \varepsilon \frac{1}{|j_f|} \left(j_f^1 - (j_f^1 \cdot \frac{j_f}{|j_f|}) \frac{j_f}{|j_f|} \right) + \mathcal{O}(\varepsilon^2) \\ &= v(2\bar{\theta}_f) + \varepsilon \frac{1}{|j_f|} (j_f^1 \cdot v^\perp(2\bar{\theta}_f)) v^\perp(2\bar{\theta}_f) + \mathcal{O}(\varepsilon^2). \end{aligned} \quad (63)$$

Expanding $\bar{\Theta}_f$ according to the first equation of 62, we get

$$\frac{J_f}{|J_f|} = v(2\bar{\Theta}_f) = v(2\bar{\theta}_f) + 2\varepsilon \bar{\theta}_f^1 v^\perp(2\bar{\theta}_f) + \mathcal{O}(\varepsilon^2). \quad (64)$$

Identifying the coefficients of ε in 63 and 64, we get the second equation of 62. \square

From the expansion given in Lemma 5.1, we deduce an expansion of the operators $\tilde{Q}_{\text{al}}^\varepsilon f$. We recall that their expressions are given by 10. This expansion is given in the

Lemma 5.2. *We have*

$$\tilde{Q}_{\text{al}}^\varepsilon f = Q_{\text{al}}^0 f + \varepsilon Q_{\text{al}}^1 f + \mathcal{O}(\varepsilon^2), \quad (65)$$

where $Q_{\text{al}}^0 f$ is given by 16 and $Q_{\text{al}}^1 f$ is given by

$$\begin{aligned} Q_{\text{al}}^1 f &= \bar{\theta}_f^1 \partial_\theta \left[\left(2\delta(\cos(\theta - \bar{\theta}_f)) \sin^2(\theta - \bar{\theta}_f) - |\cos(\theta - \bar{\theta}_f)| \right) f \right. \\ &\quad \left. + 2D \cos(\theta - \bar{\theta}_f) \sin(\theta - \bar{\theta}_f) \partial_\theta f \right], \end{aligned} \quad (66)$$

where $\delta(\cos(\theta - \bar{\theta}_f))$ is the Dirac delta at $\cos(\theta - \bar{\theta}_f) = 0$.

Proof. Formula 65 follows from the first equation of 62 as well as

$$\theta - \bar{\Theta}_f^\varepsilon = \theta - \bar{\theta}_f - \varepsilon \bar{\theta}_f^1 + \mathcal{O}(\varepsilon^2).$$

Then, inserting this expansion in 10 and using elementary calculus, we are led to 66. \square

From the previous two lemmas, in the new scaling, the mean field kinetic equation 9 is written as:

$$\varepsilon \left(\partial_t f^\varepsilon + \nabla_x \cdot (v(\theta) f^\varepsilon) - Q_{\text{al}}^1 f^\varepsilon \right) = Q_{\text{al}}^0 f^\varepsilon + \mathcal{O}(\varepsilon^2), \quad (67)$$

and we will now drop the $\mathcal{O}(\varepsilon^2)$ term. The main theorem of this section is the following.

Theorem 5.3. *Taking the (formal) limit $\varepsilon \rightarrow 0$ in 67, we obtain*

$$f^\varepsilon(x, \theta, t) \rightarrow \bar{f}_{\rho_+(x,t), \rho_-(x,t), \bar{\theta}(x,t)}(\theta),$$

with $\bar{f}_{\rho_+, \rho_-, \bar{\theta}}$ given by 41. The macroscopic quantities ρ_\pm and $\bar{\theta}$ fulfill

$$\partial_t \rho_+ + d_1 \nabla_x \cdot (\rho_+ v(\bar{\theta})) = 0, \quad (68)$$

$$\partial_t \rho_- - d_1 \nabla_x \cdot (\rho_- v(\bar{\theta})) = 0, \quad (69)$$

$$\begin{aligned} (\rho_+ + \rho_-) \partial_t \bar{\theta} + d_2 (\rho_+ - \rho_-) (v(\bar{\theta}) \cdot \nabla_x) \bar{\theta} + \mu v(\bar{\theta})^\perp \cdot \nabla_x (\rho_+ - \rho_-) \\ = 2k \left(d_2 + d_3 - \mu - \frac{2}{\kappa} \right) \nabla_x \cdot ((\rho_+ + \rho_-) \nabla_x \bar{\theta}), \end{aligned} \quad (70)$$

where d_1 , d_2 and μ are given by 53 and

$$d_3 = 2 \frac{\langle g \frac{\sin^3}{\cos^3} \rangle_M}{\langle g \frac{\sin}{\cos^2} \rangle_M}. \quad (71)$$

The definition of $\langle \cdot \rangle_M$ can be found in 54.

The proof of this theorem is given in the Appendix (see Section 8.3). The weak non-locality of the interactions leads to the addition on a diffusion term on the right-hand side compared to purely local interactions. The sign of the diffusion constant depends on the sign of $\mathcal{D} = d_2 + d_3 - \mu - \frac{2}{\kappa}$. Lemma 5.4 shows that \mathcal{D} is positive.

Lemma 5.4. *Let the diffusion constant \mathcal{D} be defined by*

$$\mathcal{D} := d_2 + d_3 - \mu - \frac{2}{\kappa},$$

where d_2 and μ are given by 53 and d_3 given by 71. Then it holds that

$$\mathcal{D} \geq 0 \quad \text{for } \kappa \geq 0.$$

Proof. We start by rewriting

$$\begin{aligned} \mathcal{D} &= d_2 + d_3 - \mu - \frac{2}{\kappa} \\ &= \frac{\langle g \frac{\sin}{\cos} \rangle_M}{\langle g \frac{\sin}{\cos^2} \rangle_M} + 2 \frac{\langle g \frac{\sin^3}{\cos^3} \rangle_M}{\langle g \frac{\sin}{\cos^2} \rangle_M} - \frac{1}{\kappa} \frac{\langle g \sin \rangle_M}{\langle g \frac{\sin}{\cos^2} \rangle_M} - \frac{2}{\kappa} \\ &= \frac{1}{\kappa \langle g \frac{\sin}{\cos^2} \rangle_M} \left\langle g \left[\kappa \frac{\sin}{\cos} + 2\kappa \frac{\sin^3}{\cos^3} - \sin - 2 \frac{\sin}{\cos^2} \right] \right\rangle_M = \frac{A}{B}. \end{aligned} \quad (72)$$

Next, using the definition of $\langle \cdot \rangle_M$ given in 54, we examine the numerator A . Note that since Z_κ would appear in both A and B , we can omit it.

$$\begin{aligned} A &= \left\langle g \frac{\sin}{\cos^3} [\kappa (\cos^2 + 2 \sin^2) - \cos (\cos^2 + 2)] \right\rangle_M \\ &= \int_0^{\pi/2} g(\theta) \frac{\sin \theta}{\cos^3 \theta} e^{-\frac{\kappa}{\cos \theta}} [\kappa (\cos^2 \theta + 2 \sin^2 \theta) - \cos \theta (\cos^2 \theta + 2)] d\theta \\ &= \int_0^1 \frac{G(y)}{y^3} e^{-\frac{\kappa}{y}} [\kappa (2 - y^2) - y (y^2 + 2)] dy. \end{aligned} \quad (73)$$

In the last line we used the change of variable $y = \cos \theta$ and the definition

$$G(y) = g(\arccos(y)).$$

The last line 73 can be split into

$$\begin{aligned} A &= \int_0^1 \frac{G(y)}{y} \frac{d}{dy} \left(e^{-\frac{\kappa}{y}} \right) (2 - y^2) dy - \int_0^1 \frac{G(y)}{y^2} e^{-\frac{\kappa}{y}} (y^2 + 2) dy \\ &= A_1 + A_2. \end{aligned} \quad (74)$$

We start by rewriting A_1 using integration by parts. This yields

$$\begin{aligned} A_1 &= \frac{G(y)}{y} e^{-\frac{\kappa}{y}} (2 - y^2) \Big|_0^1 - \int_0^1 e^{-\frac{\kappa}{y}} \frac{d}{dy} \left(G(y) \frac{2 - y^2}{y} \right) dy \\ &= - \int_0^1 e^{-\frac{\kappa}{y}} \frac{2 - y^2}{y} \frac{d}{dy} G(y) dy - \int_0^1 e^{-\frac{\kappa}{y}} G(y) \frac{d}{dy} \left(\frac{2 - y^2}{y} \right) dy \\ &= A_1^1 + A_1^2, \end{aligned}$$

where the second equality is obtained by noting that the boundary term vanishes. Note that since $\frac{dg}{d\theta} \leq 0$ on $[0, \pi/2]$, which can be seen from its definition in 48, it also holds that

$$\frac{d}{dy} G(y) = - \frac{1}{\sqrt{1 - y^2}} \frac{dg}{d\theta}(\arccos(y)) \geq 0 \quad \text{for } y \in [0, 1]. \quad (75)$$

We continue by expanding A_1^2 :

$$A_1^2 = \int_0^1 e^{-\frac{\kappa}{y}} G(y) \left(\frac{2 + y^2}{y^2} \right) dy,$$

which shows that in fact $A_1^2 = -A_2$ as defined in 74. Using this and 75 we can conclude

$$A = A_1^1 = - \int_0^1 e^{-\frac{\kappa}{y}} \frac{2 - y^2}{y} \frac{d}{dy} G(y) dy \leq 0.$$

Finally, since $g \leq 0$ on $[0, \pi/2]$, we observe that the denominator B as defined in 72 (again omitting Z_κ) fulfills

$$B = \kappa \left\langle g \frac{\sin}{\cos^2} \right\rangle_M = \kappa \int_0^{\pi/2} g(\theta) e^{-\frac{\kappa}{\cos \theta}} \frac{\sin \theta}{\cos^2 \theta} d\theta \leq 0,$$

which shows the claim and finishes the proof. \square

6. Example: myxobacteria. In this section we want to give an example of how to use and adapt the derived nematic SOH model to a particular biological problem, the movement of myxobacteria. This type of rod-shaped bacteria can glide without the aid of flagella on surfaces. Under starvation conditions, prior to the formation of fruiting bodies, they go through a so-called *rippling phase*. During this stage traveling waves of high density bands are observed that seemingly pass through each other unaffected. However upon close examination it has been found that a large number of bacteria at the interface of two colliding waves in fact reverse their direction. These reversals can happen spontaneously, but a higher number of head-to-head contacts with other oppositely moving myxobacteria increases their likelihood [34, 51]. Biologically these reversals are quite fascinating, because they happen by the reorganization of the internal movement machinery as opposed to an actual turning process. The interaction of two bacteria that don't reverse can be described by nematic alignment. In terms of other communication between bacteria no diffusible chemotactic signal is known to coordinate their movement. At this point the nematic SOH model can describe the (nematic) alignment of two colliding bacteria, however the reversals still need to be included.

6.1. Particle and mean field model.

6.1.1. Particle Model. We complete the description of the particle model from Subsection 2.1 by assuming that particles reverse their direction of motion with a frequency, dependent on the density of oppositely moving bacteria ρ_{\pm}^i . So we let Θ_i be changed into $\Theta_i + \pi$ at Poisson random times with frequency $\lambda(\rho_{-\text{Sign} \cos(\Theta_i - \bar{\Theta}_i)}^i)$, where

$$\rho_{\pm}^i := \frac{1}{R^2 \pi} \text{Card}\{k \in \mathcal{N} \mid |X_k - X_i| \leq R \text{ and } \pm \cos(\Theta_k - \bar{\Theta}_i) \geq 0\},$$

where Card stands for the cardinal of a set. In other words, we have

$$\begin{aligned} & \text{Prob}\{\Theta_i(t+T) = \Theta_i(t) + \pi \mid \Theta_i(t+\tau) = \Theta_i(t) \forall \tau \text{ with } 0 \leq \tau < T\} \\ &= 1 - \exp\left(-\lambda(\rho_{-\text{Sign} \cos(\Theta_i - \bar{\Theta}_i)}^i) T\right). \end{aligned}$$

(assuming that $\rho_{-\text{Sign} \cos(\Theta_i - \bar{\Theta}_i)}^i = \rho_{-\text{Sign} \cos(\Theta_i - \bar{\Theta}_i)}^i(t)$ stays constant in the time interval $[t, t+T]$). In these formula, the function $\lambda(\rho_{\pm})$ is a reversal frequency. The way it depends on ρ_{\pm} will be discussed later.

6.1.2. Mean Field Model. The above considerations change Eq. 5 to

$$\partial_t f + v_0 \nabla_x \cdot (v(\theta) f) = \tilde{Q}_{\text{al}} f + \tilde{Q}_{\text{rev}} f,$$

where the collision operators \tilde{Q}_{al} is given by 6 and

$$\tilde{Q}_{\text{rev}} f(x, \theta, t) = \begin{cases} \lambda(\sigma_{f,+}) f(x, \theta + \pi, t) - \lambda(\sigma_{f,-}) f(x, \theta, t), & \text{for } \cos(\theta - \bar{\Theta}_f) > 0, \\ \lambda(\sigma_{f,-}) f(x, \theta + \pi, t) - \lambda(\sigma_{f,+}) f(x, \theta, t), & \text{for } \cos(\theta - \bar{\Theta}_f) < 0, \end{cases}$$

and where $\bar{\Theta}_f$ is given by 7-8 and $\sigma_{f,\pm}$ given by

$$\sigma_{f,\pm}(x, t) = \frac{1}{R^2 \pi} \int_{\pm \cos(\theta - \bar{\Theta}_f) \geq 0} \int_{|x-y| \leq R} f(y, \theta, t) dy d\theta.$$

To obtain local interactions, we assume as in Section 2.2 an interaction radius fulfilling $\hat{R} = \mathcal{O}(\varepsilon)$ and choose for the reversal frequency the scaling $\hat{\lambda}(\sigma_{\hat{f},\pm}) =$

$t'_0 \lambda(\sigma_{f,\pm}) = \frac{t_0}{\varepsilon} \lambda(\sigma_{f,\pm})$. The local density is then given by

$$\sigma_{f,\pm}^\varepsilon(x, t) = \frac{1}{\varepsilon^2 r^2 \pi} \int_{\pm \cos(\theta - \bar{\Theta}_f^\varepsilon) > 0} \int_{|x-y| \leq \varepsilon r} f(y, \theta, t) \, dy \, d\theta,$$

and it can be shown that

$$\sigma_{f,\pm}^\varepsilon(x, t) = \rho_{f,\pm}(x, t) + \mathcal{O}(\varepsilon^2),$$

where

$$\rho_{f,\pm}(x, t) = \int_{\pm \cos(\theta - \bar{\theta}_f) \geq 0} f(x, \theta, t) \, d\theta. \quad (76)$$

This changes Eq. 15 into

$$\varepsilon(\partial_t f^\varepsilon + \nabla_x \cdot (v(\theta) f^\varepsilon)) = Q_{\text{al}}^0 f^\varepsilon + \varepsilon Q_{\text{rev}}^0 f^\varepsilon, \quad (77)$$

where $Q_{\text{al}}^0 f$ is given by 16 and

$$Q_{\text{rev}}^0 f(x, \theta, t) = \begin{cases} \lambda(\rho_{f,+}) f(x, \theta + \pi, t) - \lambda(\rho_{f,-}) f(x, \theta, t) & \text{for } \cos(\theta - \bar{\theta}_f) > 0, \\ \lambda(\rho_{f,-}) f(x, \theta + \pi, t) - \lambda(\rho_{f,+}) f(x, \theta, t) & \text{for } \cos(\theta - \bar{\theta}_f) < 0, \end{cases} \quad (78)$$

where $\bar{\theta}_f$ and $\rho_{f,\pm}$ are given by 13 and 76 respectively.

Remark 2. In 77 the contributions from Q_{rev}^0 appear at the same scale as the transport operator, which is a consequence of the scaling choice for the reversal rate λ . Using $\hat{\lambda}(\sigma_{f,\pm}) = t_0 \lambda(\sigma_{f,\pm})$ instead, would lead to a different model, in which Q_{al}^0 and Q_{rev}^0 would be of the same order. Consequently also the shape of the equilibria and the macroscopic model would look very different. We leave this path for future work.

6.2. Hydrodynamic limits.

6.2.1. Macroscopic model - local scaling.

Proposition 3. Taking the (formal) limit $\varepsilon \rightarrow 0$ in 77-78, we obtain

$$f^\varepsilon(x, \theta, t) \longrightarrow \bar{f}_{\rho_+(x,t), \rho_-(x,t), \bar{\theta}(x,t)}(\theta),$$

where the macroscopic quantities $\rho_\pm(x, t)$ and $\bar{\theta}(x, t)$ have values in $[0, \infty)$ and $[-\pi/2, \pi/2)$ respectively and fulfill the following system of equations:

$$\partial_t \rho_+ + d_1 \nabla_x \cdot (\rho_+ v(\bar{\theta})) = \lambda(\rho_+) \rho_- - \lambda(\rho_-) \rho_+, \quad (79)$$

$$\partial_t \rho_- - d_1 \nabla_x \cdot (\rho_- v(\bar{\theta})) = \lambda(\rho_-) \rho_+ - \lambda(\rho_+) \rho_-, \quad (80)$$

$$(\rho_+ + \rho_-) \partial_t \bar{\theta} + d_2 (\rho_+ - \rho_-) (v(\bar{\theta}) \cdot \nabla_x) \bar{\theta} + \mu v(\bar{\theta})^\perp \cdot \nabla_x (\rho_+ - \rho_-) = 0, \quad (81)$$

where $v(\bar{\theta}) = (\cos \bar{\theta}, \sin \bar{\theta})$ and $v^\perp(\bar{\theta}) = (-\sin \bar{\theta}, \cos \bar{\theta})$. The coefficients d_1 , d_2 and μ are defined in 53.

The proof consists of some simple additions to the proof of Theorem 4.1 and is given in the Appendix (see Section 8.2).

6.2.2. *Macroscopic Model - Weakly Non-local Scaling.* To obtain the hydrodynamic limit of the myxobacteria model for the weakly non-local scaling described in Section 5, we note that in this scaling

$$\sigma_{f,\pm}^\varepsilon(x, t) = \frac{1}{\varepsilon r^2 \pi} \int_{\pm \cos(\theta - \bar{\Theta}_f^\varepsilon) > 0} \int_{|x-y| \leq \sqrt{\varepsilon} r} f(y, \theta, t) \, dy \, d\theta.$$

It holds that

$$\sigma_{f,\pm}^\varepsilon(x, t) = \rho_{f,\pm}(x, t) + \mathcal{O}(\varepsilon).$$

We observe that 67 is changed into

$$\varepsilon \left(\partial_t f^\varepsilon + \nabla_x \cdot (v(\theta) f^\varepsilon) - Q_{\text{al}}^1 f^\varepsilon - Q_{\text{rev}}^0 \right) = Q_{\text{al}}^0 f^\varepsilon + \mathcal{O}(\varepsilon^2),$$

with Q_{al}^1 and Q_{rev}^0 given by 66 and 78 respectively. The resulting limit is summarized in

Proposition 4. *Taking the (formal) limit $\varepsilon \rightarrow 0$ in 77-78, we obtain*

$$f^\varepsilon(x, \theta, t) \rightarrow \bar{f}_{\rho_+(x,t), \rho_-(x,t), \bar{\theta}(x,t)}(\theta),$$

with $\bar{f}_{\rho_+, \rho_-, \bar{\theta}}$ given by 41. The macroscopic quantities ρ_\pm and $\bar{\theta}$ fulfill

$$\begin{aligned} \partial_t \rho_+ + d_1 \nabla_x \cdot (\rho_+ v(\bar{\theta})) &= \lambda(\rho_+) \rho_- - \lambda(\rho_-) \rho_+, \\ \partial_t \rho_- - d_1 \nabla_x \cdot (\rho_- v(\bar{\theta})) &= \lambda(\rho_-) \rho_+ - \lambda(\rho_+) \rho_-, \\ (\rho_+ + \rho_-) \partial_t \bar{\theta} + d_2 (\rho_+ - \rho_-) (v(\bar{\theta}) \cdot \nabla_x) \bar{\theta} + \mu v(\bar{\theta})^\perp \cdot \nabla_x (\rho_+ - \rho_-) \\ &= 2k \left(d_2 + d_3 - \mu - \frac{2}{\kappa} \right) \nabla_x \cdot ((\rho_+ + \rho_-) \nabla_x \bar{\theta}), \end{aligned}$$

where d_1 , d_2 and μ are given by 53 and d_3 is given by 71. The definition of $\langle \cdot \rangle_M$ can be found in 54.

The proof is a simple combination of the proofs of Theorem 5.3 and Proposition 3.

One can observe that the additional reversal term leads to a reaction term on the right-hand side of Eqs. 79 and 80, with the precise shape depending on the choice of $\lambda(\rho)$. Motivated by biological findings we expect $\lambda(0) = \lambda_0 > 0$ to account for spontaneous reversals in the absence of other bacteria. Since head-to-head contacts increase the reversal frequency, $\lambda(\rho)$ should be an increasing function of ρ . To demonstrate what type of dynamics could be expected, we give an example, where we choose

$$\lambda(\rho) = \lambda_1 \rho^2 + \lambda_0, \tag{82}$$

with $\lambda_0, \lambda_1 > 0$. For a constant direction, $\bar{\theta}(x, t) \equiv \bar{\theta}$ and moving along the characteristics, the corresponding phase portrait is depicted in Figure 3. One can observe that wherever the total density $\rho_+ + \rho_- > 2\sqrt{\frac{\lambda_0}{\lambda_1}}$ one of the two groups dominates the other one, whilst for smaller values of $\rho_+ + \rho_-$ both attain the same number. This is similar to the waves observed in myxobacteria, where at the high density peaks of the waves, almost all bacteria move in the same directions, whilst in between the waves, there can be small numbers of bacteria moving in different directions.

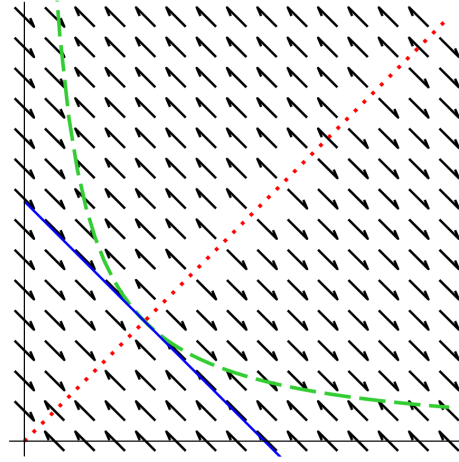


FIGURE 3. Local dynamics for $\lambda(\rho)$ given by 82. The arrows mark the flow field in the (ρ_+, ρ_-) plane. The red-dotted and green-dashed lines show the values for which $\lambda(\rho_+)\rho_- - \lambda(\rho_-)\rho_+ = 0$. The blue-solid line shows the threshold values $\rho_+ + \rho_- = 2\sqrt{\frac{\lambda_0}{\lambda_1}}$.

A detailed analytical and numerical analysis for this and other choices of $\lambda(\rho)$ will be examined in a forthcoming work [24], as well as the analysis and calibration of the model.

7. Conclusion. In this work we have derived the macroscopic equations for self-propelled, rod-shaped particles moving in two space dimensions starting at the particle level. The type of interaction considered is nematic alignment of polar particles, which is commonly found in biological and physical systems, but systematically derived hydrodynamic equations for this type of alignment are largely missing from the literature. In order to take the limit in the hydrodynamic scaling, we used the concept of generalized collision invariants. Two types of scalings have been examined: a local scaling and a weakly non-local scaling. The resulting macroscopic equations share some similarities with their polar alignment counterparts, but differ significantly in other aspects. A key difference is the splitting of the particles into two groups moving into opposite directions. Lastly, including density dependent reversals, we have demonstrated how the equations can be used to describe the behavior of myxobacteria. The research in the area of pattern formation and non-equilibrium states of large assemblies of particles is very active and more macroscopic models are needed to better understand the phase transitions and underlying causes. Several extensions of this work are possible. To describe a wider range of phenomena it could be generalized to three and more space dimensions. Further at this point the limits examined are on a formal level and lack a rigorous treatment. Extensive numerical experiments need to be conducted to compare the particle model with the macroscopic models and to characterize the different phases and states. To better understand the rippling behavior of myxobacteria different choices of reversal rates can be examined, both numerically and analytically.

8. Appendix: proofs.

8.1. Proof of Theorem 4.1.

8.1.1. *Formal limit* $\varepsilon \rightarrow 0$. All limits taken are formal. We suppose that f^ε converges to some f^0 when $\varepsilon \rightarrow 0$. From 15 we see that the limiting distribution has to fulfill $Q_{\text{al}} f^0 = 0$ and therefore, use of Lemma 3.6 leads us to

$$f^0(x, \theta, t) = \bar{f}_{\rho_+(x,t), \rho_-(x,t), \bar{\theta}(x,t)}(\theta). \quad (83)$$

To derive the equations determining $\rho_+(x, t)$, $\rho_-(x, t)$, $\bar{\theta}(x, t)$, we multiply 15 by the three GCI $\chi_{\bar{\theta}_{f^\varepsilon}}^\pm$ and $g_{\bar{\theta}_{f^\varepsilon}}$ associated to $\bar{\theta}_{f^\varepsilon}$ given by Proposition 2 and integrate with respect to θ .

8.1.2. *Use of GCI* $\chi_{\bar{\theta}_{f^\varepsilon}}^\pm$. We interpret the integral of $Q_{\text{al}}^0 f^\varepsilon$ against $\chi_{\bar{\theta}_{f^\varepsilon}}^\pm$ as follows:

$$\int Q_{\text{al}}^0 f^\varepsilon(\theta) \chi_{\bar{\theta}_{f^\varepsilon}}^\pm(\theta) d\theta = \langle \mathcal{L}_{\bar{\theta}_{f^\varepsilon}} \frac{f^\varepsilon}{M_{\bar{\theta}_{f^\varepsilon}}}, \chi_{\bar{\theta}_{f^\varepsilon}}^\pm(\theta) \rangle_{\mathcal{V}'_{\bar{\theta}_{f^\varepsilon}}, \mathcal{V}_{\bar{\theta}_{f^\varepsilon}}},$$

and, by Definition 3.8, this integral equals zero. Upon division by ε we are left with

$$\int_{\pm \cos(\theta - \bar{\theta}_{f^\varepsilon}) > 0} (\partial_t f^\varepsilon + v(\theta) \cdot \nabla_x f^\varepsilon) d\theta = 0.$$

Letting $\varepsilon \rightarrow 0$, using 83 and the fact that $\bar{\theta}_{f^\varepsilon} \rightarrow \bar{\theta}$, we are led to

$$\int_{\pm \cos(\theta - \bar{\theta}) > 0} (\partial_t + v(\theta) \cdot \nabla_x) \bar{f}_{\rho_+(x,t), \rho_-(x,t), \bar{\theta}(x,t)}(\theta) d\theta = 0. \quad (84)$$

Note that the integration domain depends on x and t . We calculate

$$\begin{aligned} (\partial_t + v(\theta) \cdot \nabla_x) \bar{f}_{\rho_+, \rho_-, \bar{\theta}}(\theta) &= M_{\bar{\theta}}(\theta) \left[(\partial_t + v(\theta) \cdot \nabla_x) \rho_\pm \right. \\ &\quad \left. \pm \frac{\kappa \rho_\pm}{\cos^2(\theta - \bar{\theta})} \sin(\theta - \bar{\theta}) (\partial_t + v(\theta) \cdot \nabla_x) \bar{\theta} \right] \text{ for } \pm \cos(\theta - \bar{\theta}) > 0, \end{aligned}$$

which can also be expressed as:

$$\begin{aligned} (\partial_t + v(\theta) \cdot \nabla_x) \bar{f}_{\rho_+, \rho_-, \bar{\theta}}(\theta) &= M_{\bar{\theta}}(\theta) \left[\chi_{\bar{\theta}}^+ (\partial_t + v(\theta) \cdot \nabla_x) \rho_+ \right. \\ &\quad \left. + \chi_{\bar{\theta}}^- (\partial_t + v(\theta) \cdot \nabla_x) \rho_- + \kappa \frac{\sin(\theta - \bar{\theta})}{\cos^2(\theta - \bar{\theta})} (\chi_{\bar{\theta}}^+ \rho_+ - \chi_{\bar{\theta}}^- \rho_-) (\partial_t + v(\theta) \cdot \nabla_x) \bar{\theta} \right]. \quad (85) \end{aligned}$$

We note that in spite of the presence of indicator functions in 42, $\bar{f}_{\rho_+, \rho_-, \bar{\theta}}$ is continuous (and even C^∞) across the points θ where $\cos(\theta - \bar{\theta}) = 0$, so that there is no delta distribution appearing at these points when we differentiate it. In the following we perform the calculations for the integral over θ such that $\cos(\theta - \bar{\theta}) > 0$, the case of $\cos(\theta - \bar{\theta}) < 0$ being treated in the same manner. The left-hand side of

84, denoted by L , is then equal to

$$\begin{aligned}
L &= \left(\int_{\cos(\theta-\bar{\theta})>0} M_{\bar{\theta}}(\theta) d\theta \right) \partial_t \rho_+ \\
&+ \left(\int_{\cos(\theta-\bar{\theta})>0} M_{\bar{\theta}}(\theta) v(\theta) d\theta \right) \cdot \nabla_x \rho_+ \\
&+ \kappa \rho_+ \left(\int_{\cos(\theta-\bar{\theta})>0} M_{\bar{\theta}}(\theta) \frac{\sin(\theta-\bar{\theta})}{\cos^2(\theta-\bar{\theta})} d\theta \right) \partial_t \bar{\theta} \\
&+ \kappa \rho_+ \left(\int_{\cos(\theta-\bar{\theta})>0} M_{\bar{\theta}}(\theta) \frac{\sin(\theta-\bar{\theta})}{\cos^2(\theta-\bar{\theta})} v(\theta) d\theta \right) \cdot \nabla_x \bar{\theta} \\
&= L_1 + \dots + L_4.
\end{aligned}$$

Thanks to the normalization condition 19, we have $L_1 = \partial_t \rho_+$. Using

$$v(\theta) = \cos(\theta - \bar{\theta}) v(\bar{\theta}) + \sin(\theta - \bar{\theta}) v^\perp(\bar{\theta}), \quad (86)$$

together with cancellations due to symmetries, L_2 simplifies into

$$\begin{aligned}
L_2 &= \int_{\cos(\theta-\bar{\theta})>0} M_{\bar{\theta}}(\theta) \left(\cos(\theta - \bar{\theta}) v(\bar{\theta}) \cdot \nabla_x + \sin(\theta - \bar{\theta}) v^\perp(\bar{\theta}) \cdot \nabla_x \right) \rho_+ d\theta \\
&= \left(\int_{\cos(\theta-\bar{\theta})>0} M_{\bar{\theta}}(\theta) \cos(\theta - \bar{\theta}) d\theta \right) (v(\bar{\theta}) \cdot \nabla_x) \rho_+ \\
&= \left(\int_{\cos \theta > 0} M(\theta) \cos \theta d\theta \right) (v(\bar{\theta}) \cdot \nabla_x) \rho_+ \\
&= d_1 (v(\bar{\theta}) \cdot \nabla_x) \rho_+,
\end{aligned}$$

where d_1 is defined in 53. We easily get $L_3 = 0$ by symmetry. Using again 86, cancellations due to symmetry and integration by parts, we find that

$$\begin{aligned}
L_4 &= \kappa \rho_+ \left(\int_{\cos(\theta-\bar{\theta})>0} M_{\bar{\theta}}(\theta) \frac{\sin^2(\theta - \bar{\theta})}{\cos^2(\theta - \bar{\theta})} d\theta \right) (v^\perp(\bar{\theta}) \cdot \nabla_x) \bar{\theta} \\
&= -\rho_+ \left(\int_{\cos(\theta-\bar{\theta})>0} \frac{dM_{\bar{\theta}}(\theta)}{d\theta} \sin(\theta - \bar{\theta}) d\theta \right) (v^\perp(\bar{\theta}) \cdot \nabla_x) \bar{\theta} \\
&= \rho_+ \left(\int_{\cos(\theta-\bar{\theta})>0} M_{\bar{\theta}}(\theta) \cos(\theta - \bar{\theta}) d\theta \right) (v^\perp(\bar{\theta}) \cdot \nabla_x) \bar{\theta} \\
&= d_1 \rho_+ (v^\perp(\bar{\theta}) \cdot \nabla_x) \bar{\theta}.
\end{aligned}$$

Finally, collecting the contributions from above, we get 50 and 51.

8.1.3. *Use of GCI $g_{\bar{\theta}_{f^\varepsilon}}$.* We start as in the previous section. We interpret the integral of $Q_{\text{al}}^0 f^\varepsilon$ against $g_{\bar{\theta}_{f^\varepsilon}}$ as

$$\int Q_{\text{al}}^0 f^\varepsilon(\theta) g_{\bar{\theta}_{f^\varepsilon}}(\theta) d\theta = \left\langle \mathcal{L}_{\bar{\theta}_{f^\varepsilon}} \frac{f^\varepsilon}{M_{\bar{\theta}_{f^\varepsilon}}}, g_{\bar{\theta}_{f^\varepsilon}}(\theta) \right\rangle_{\mathcal{V}'_{\bar{\theta}_{f^\varepsilon}}, \mathcal{V}_{\bar{\theta}_{f^\varepsilon}}},$$

and by Definition 3.8 this integral vanishes. Upon division by ε we get

$$\int (\partial_t f^\varepsilon + v(\theta) \cdot \nabla_x f^\varepsilon) g_{\bar{\theta}_{f^\varepsilon}} d\theta = 0.$$

Again, we assume that $f^\varepsilon \rightarrow \bar{f}_{\rho_+(x,t),\rho_-(x,t),\bar{\theta}(x,t)}$ and $\bar{\theta}_{f^\varepsilon} \rightarrow \bar{\theta}$ and find

$$0 = \int \left[(\partial_t + v(\theta) \cdot \nabla_x) \bar{f}_{\rho_+(x,t),\rho_-(x,t),\bar{\theta}(x,t)} \right] g_{\bar{\theta}} d\theta = X.$$

We use the calculations in 85 and split X into $X = X_1 + \dots + X_3$ with

$$\begin{aligned} X_1 &= \int \left[M_{\bar{\theta}(x,t)} (\chi_{\bar{\theta}}^+ \partial_t \rho_+ + \chi_{\bar{\theta}}^- \partial_t \rho_-) \right] g_{\bar{\theta}} d\theta, \\ X_2 &= \int M_{\bar{\theta}(x,t)} \left[v(\theta) \cdot (\chi_{\bar{\theta}}^+ \nabla_x \rho_+ + \chi_{\bar{\theta}}^- \nabla_x \rho_-) \right. \\ &\quad \left. + \kappa \frac{\sin(\theta - \bar{\theta})}{\cos^2(\theta - \bar{\theta})} (\chi_{\bar{\theta}}^+ \rho_+ - \chi_{\bar{\theta}}^- \rho_-) \partial_t \bar{\theta} \right] g_{\bar{\theta}} d\theta, \\ X_3 &= \kappa \int M_{\bar{\theta}(x,t)} \frac{\sin(\theta - \bar{\theta})}{\cos^2(\theta - \bar{\theta})} (\chi_{\bar{\theta}}^+ \rho_+ - \chi_{\bar{\theta}}^- \rho_-) (v(\theta) \cdot \nabla_x) \bar{\theta} g_{\bar{\theta}} d\theta. \end{aligned}$$

For the first integral inside the expression of X_1 we have

$$\int M_{\bar{\theta}(x,t)} \chi_{\bar{\theta}}^+ g_{\bar{\theta}} d\theta = 0.$$

Use the symmetry relations 47 and therefore $X_1 = 0$. For X_2 , using 86 and cancellations due to symmetry, we get:

$$\begin{aligned} X_2 &= \int M_{\bar{\theta}(x,t)} \left[\sin(\theta - \bar{\theta}) v^\perp(\bar{\theta}) \cdot (\chi_{\bar{\theta}}^+ \nabla_x \rho_+ + \chi_{\bar{\theta}}^- \nabla_x \rho_-) \right. \\ &\quad \left. + \kappa \frac{\sin(\theta - \bar{\theta})}{\cos^2(\theta - \bar{\theta})} (\chi_{\bar{\theta}}^+ \rho_+ - \chi_{\bar{\theta}}^- \rho_-) \partial_t \bar{\theta} \right] g_{\bar{\theta}} d\theta. \end{aligned}$$

Now, it turns out that the integrals with respect to θ on the two sets $\cos(\theta - \bar{\theta}) > 0$ and $\cos(\theta - \bar{\theta}) < 0$ are opposite by symmetry and we get

$$X_2 = \langle g \sin \rangle_M v^\perp(\bar{\theta}) \cdot \nabla_x (\rho_+ - \rho_-) + \kappa \left\langle g \frac{\sin}{\cos^2} \right\rangle_M (\rho_+ + \rho_-) \partial_t \bar{\theta}.$$

Finally for X_3 we again use 86 and cancellations due to symmetry and get:

$$\begin{aligned} X_3 &= \kappa \int M_{\bar{\theta}(x,t)} \frac{\sin(\theta - \bar{\theta})}{\cos(\theta - \bar{\theta})} (\chi_{\bar{\theta}}^+ \rho_+ - \chi_{\bar{\theta}}^- \rho_-) (v(\bar{\theta}) \cdot \nabla_x) \bar{\theta} g_{\bar{\theta}} d\theta \\ &= \kappa \left\langle g \frac{\sin}{\cos} \right\rangle_M (\rho_+ - \rho_-) (v(\bar{\theta}) \cdot \nabla_x) \bar{\theta}, \end{aligned}$$

since now, the integrals with respect to θ on the two sets $\cos(\theta - \bar{\theta}) > 0$ and $\cos(\theta - \bar{\theta}) < 0$ are equal by symmetry. Combining these equalities, we get

$$\begin{aligned} 0 &= \kappa \left\langle g \frac{\sin}{\cos^2} \right\rangle_M (\rho_+ + \rho_-) \partial_t \bar{\theta} + \kappa \left\langle g \frac{\sin}{\cos} \right\rangle_M (\rho_+ - \rho_-) (v(\bar{\theta}) \cdot \nabla_x) \bar{\theta} \\ &\quad + \langle g \sin \rangle_M v^\perp(\bar{\theta}) \cdot \nabla_x (\rho_+ - \rho_-). \end{aligned}$$

Dividing this equation by $\kappa \left\langle g \frac{\sin}{\cos^2} \right\rangle_M$, we get 52 with the coefficients defined by 53.

8.2. Proof of Proposition 3.

Proof. The proof consists of some straightforward extensions to the proof of Theorem 4.1. First of all we note that the limiting distribution f^0 still has to fulfill $Q_{\text{al}}^0 f^0 = 0$. Therefore we get

$$f^0(x, \theta, t) = \bar{f}_{\rho_+(x,t),\rho_-(x,t),\bar{\theta}(x,t)}(\theta)$$

and we are left with determining the integral of 78 against the generalized collision invariants $\chi_{\bar{\theta}_{f\epsilon}}^{\pm}$ and $g_{\bar{\theta}_{f\epsilon}}$. We start by noting that

$$Q_{\text{rev}}^0 \bar{f}_{\rho_+, \rho_-, \bar{\theta}}(\theta) = \begin{cases} (\lambda(\rho_+) \rho_- - \lambda(\rho_-) \rho_+) M_{\bar{\theta}}(\theta) & \text{for } \cos(\theta - \bar{\theta}) > 0, \\ (\lambda(\rho_-) \rho_+ - \lambda(\rho_+) \rho_-) M_{\bar{\theta}}(\theta) & \text{for } \cos(\theta - \bar{\theta}) < 0. \end{cases}$$

With this it follows easily that

$$\int Q_{\text{rev}}^0 \bar{f}_{\rho_+(x,t), \rho_-(x,t), \bar{\theta}(x,t)} \chi_{\bar{\theta}_{f\epsilon}}^{\pm} d\theta = \pm (\lambda(\rho_+) \rho_- - \lambda(\rho_-) \rho_+).$$

Finally following the same arguments as in Section 8.1.3 about X_1 , we find that

$$\int Q_{\text{rev}}^0 \bar{f}_{\rho_+(x,t), \rho_-(x,t), \bar{\theta}(x,t)} g_{\bar{\theta}} d\theta = 0,$$

which finishes the proof. \square

8.3. Weakly non-local scaling: proof of Theorem 5.3.

Proof. Compared to the proof of Theorem 4.1, we need to compute the contributions of

$$T_1^{\pm} = \int Q_{\text{al}}^1 \bar{f}_{\rho_+, \rho_-, \bar{\theta}}(\theta) \chi_{\bar{\theta}}^{\pm}(\theta) d\theta, \quad T_2 = \int Q_{\text{al}}^1 \bar{f}_{\rho_+, \rho_-, \bar{\theta}}(\theta) g_{\bar{\theta}}(\theta) d\theta.$$

We first compute:

$$\dot{j}_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}} = \rho_+ \int_{\cos(\theta - \bar{\theta}) > 0} v(2\theta) M_{\bar{\theta}}(\theta) d\theta + \rho_- \int_{\cos(\theta - \bar{\theta}) < 0} v(2\theta) M_{\bar{\theta}}(\theta) d\theta.$$

Thanks to

$$v(2\theta) = \cos(2(\theta - \bar{\theta})) v(2\bar{\theta}) + \sin(2(\theta - \bar{\theta})) v^{\perp}(2\bar{\theta}),$$

and cancellations by symmetry, we get

$$\begin{aligned} \dot{j}_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}} &= (\rho_+ + \rho_-) \left(\int_{\cos \theta > 0} \cos(2\theta) M(\theta) d\theta \right) v(2\bar{\theta}) \\ &= (\rho_+ + \rho_-) \langle \cos(2\cdot) \rangle_M v(2\bar{\theta}), \end{aligned}$$

and consequently

$$|\dot{j}_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}}| = (\rho_+ + \rho_-) \langle \cos(2\cdot) \rangle_M,$$

since $\langle \cos(2\cdot) \rangle_M > 0$. Now we get:

$$\begin{aligned} \dot{j}_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}}^1 &= k \Delta_x \dot{j}_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}} \\ &= k \langle \cos(2\cdot) \rangle_M \Delta_x ((\rho_+ + \rho_-) v(2\bar{\theta})) \\ &= k \langle \cos(2\cdot) \rangle_M \left(\Delta_x (\rho_+ + \rho_-) v(2\bar{\theta}) + 4 \nabla_x (\rho_+ + \rho_-) \cdot \nabla_x \bar{\theta} v^{\perp}(2\bar{\theta}) \right. \\ &\quad \left. + 4(\rho_+ + \rho_-) (\Delta_x \bar{\theta} v^{\perp}(2\bar{\theta}) - |\nabla_x \bar{\theta}|^2 v(2\bar{\theta})) \right), \end{aligned}$$

and finally

$$\begin{aligned}
\bar{\theta}_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}}^1 &= \frac{1}{2|j_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}}^1|} (j_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}}^1 \cdot v^\perp(2\bar{\theta}_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}})) \\
&= \frac{2k}{\rho_+ + \rho_-} (\nabla_x(\rho_+ + \rho_-) \cdot \nabla_x \bar{\theta} + (\rho_+ + \rho_-) \Delta_x \bar{\theta}) \\
&= \frac{2k}{\rho_+ + \rho_-} \nabla_x \cdot ((\rho_+ + \rho_-) \nabla_x \bar{\theta}).
\end{aligned} \tag{87}$$

Now we have

$$\begin{aligned}
&Q_{\text{al}}^1 \bar{f}_{\rho_+, \rho_-, \bar{\theta}}(\theta) \\
&= \bar{\theta}_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}}^1 \partial_\theta \left[\left(2 \delta(\cos(\theta - \bar{\theta})) \sin^2(\theta - \bar{\theta}) - |\cos(\theta - \bar{\theta})| \right) M_{\bar{\theta}}(\rho_+ \chi_{\bar{\theta}}^+ + \rho_- \chi_{\bar{\theta}}^-) \right. \\
&\quad \left. + 2D \cos(\theta - \bar{\theta}) \sin(\theta - \bar{\theta}) \partial_\theta \left(M_{\bar{\theta}}(\rho_+ \chi_{\bar{\theta}}^+ + \rho_- \chi_{\bar{\theta}}^-) \right) \right].
\end{aligned}$$

However,

$$\delta(\cos(\theta - \bar{\theta})) M_{\bar{\theta}} = 0, \tag{88}$$

and similarly

$$\partial_\theta \left(M_{\bar{\theta}}(\rho_+ \chi_{\bar{\theta}}^+ + \rho_- \chi_{\bar{\theta}}^-) \right) = (\rho_+ \chi_{\bar{\theta}}^+ + \rho_- \chi_{\bar{\theta}}^-) \partial_\theta M_{\bar{\theta}}.$$

Together with

$$\partial_\theta M_{\bar{\theta}}(\theta) = -\kappa \frac{\sin(\theta - \bar{\theta})}{\cos^2(\theta - \bar{\theta})} \text{Sign}(\cos(\theta - \bar{\theta})) M_{\bar{\theta}}(\theta),$$

we find (noting that $\kappa D = 1$):

$$\begin{aligned}
&Q_{\text{al}}^1 \bar{f}_{\rho_+, \rho_-, \bar{\theta}}(\theta) \\
&= -\bar{\theta}_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}}^1 \partial_\theta \left[\left(|\cos(\theta - \bar{\theta})| + 2 \frac{\sin^2(\theta - \bar{\theta})}{|\cos(\theta - \bar{\theta})|} \right) (\rho_+ \chi_{\bar{\theta}}^+ + \rho_- \chi_{\bar{\theta}}^-) M_{\bar{\theta}} \right].
\end{aligned}$$

We first compute T_1^+ (the computation is obviously similar for T_1^-). We have

$$\begin{aligned}
T_1^+ &= \int_{\cos(\theta - \bar{\theta}) > 0} Q_{\text{al}}^1 \bar{f}_{\rho_+, \rho_-, \bar{\theta}}(\theta) d\theta \\
&= -\bar{\theta}_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}}^1 \left[\left(|\cos(\theta - \bar{\theta})| + 2 \frac{\sin^2(\theta - \bar{\theta})}{|\cos(\theta - \bar{\theta})|} \right) (\rho_+ \chi_{\bar{\theta}}^+ + \rho_- \chi_{\bar{\theta}}^-) M_{\bar{\theta}} \right]_{\theta - \bar{\theta} = -\pi/2}^{\theta - \bar{\theta} = +\pi/2} = 0,
\end{aligned}$$

because the contact of $M_{\bar{\theta}}$ to 0 at $\theta - \bar{\theta} = \pm\pi/2$ is infinite order and compensates for the blow up $|\cos(\theta - \bar{\theta})|$ at the denominator.

We are left with the computation of T_2 . Using [46](#) and [88](#), we can write:

$$\begin{aligned}
T_2 &= \int_{-\pi}^{\pi} Q_{\text{al}}^1 \bar{f}_{\rho_+, \rho_-, \bar{\theta}}(\theta) g_{\bar{\theta}}(\theta) d\theta \\
&= -\bar{\theta}_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}}^1 \int_{-\pi}^{\pi} \partial_\theta \left[\left(|\cos \theta| + 2 \frac{\sin^2 \theta}{|\cos \theta|} \right) (\rho_+ \chi^+ + \rho_- \chi^-) M \right] g(\theta) d\theta \\
&= -\bar{\theta}_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}}^1 \int_{-\pi}^{\pi} \partial_\theta \left[\left(|\cos \theta| + 2 \frac{\sin^2 \theta}{|\cos \theta|} \right) M \right] g(\theta) (\rho_+ \chi^+ + \rho_- \chi^-) d\theta.
\end{aligned}$$

We have

$$\begin{aligned} & \partial_\theta \left[\left(|\cos \theta| + 2 \frac{\sin^2 \theta}{|\cos \theta|} \right) M \right] \\ &= \left\{ \text{Sign}(\cos \theta) \left(\sin \theta + 2 \frac{\sin \theta}{\cos^2 \theta} \right) - \kappa \left(\frac{\sin \theta}{\cos \theta} + 2 \frac{\sin^3 \theta}{\cos^3 \theta} \right) \right\} M. \end{aligned}$$

We note that this expression is changed into its opposite under the change $\theta \rightarrow \pi - \theta$. Since gM is also changed into its opposite under this transformation, it follows that the factors of ρ_+ and ρ_- are equal, which leads to:

$$\begin{aligned} T_2 = -\bar{\theta}_{\bar{f}_{\rho_+, \rho_-, \bar{\theta}}}^{-1} & \left[\langle \sin \theta g \rangle_M + 2 \left\langle \frac{\sin \theta}{\cos^2 \theta} g \right\rangle_M \right. \\ & \left. - \kappa \left(\left\langle \frac{\sin \theta}{\cos \theta} g \right\rangle_M + 2 \left\langle \frac{\sin^3 \theta}{\cos^3 \theta} g \right\rangle_M \right) \right] (\rho_+ + \rho_-). \end{aligned}$$

Finally, inserting 87 into this expression leads to 70, which ends the proof. \square

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