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Macroscopic Limits and Phase Transition in a System of Self-propelled Particles

Pierre Degond · Amic Frouvelle · Jian-Guo Liu

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Abstract We investigate systems of self-propelled particles with alignment interaction. Compared to previous work (Degond and Motsch, Math. Models Methods Appl. Sci. 18:1193–1215, 2008a; Frouvelle, Math. Models Methods Appl. Sci., 2012), the force acting on the particles is not normalized, and this modification gives rise to phase transitions from disordered states at low density to aligned states at high densities. This model is the space-inhomogeneous extension of (Frouvelle and Liu, Dynamics in a kinetic model of oriented particles with phase transition, 2012), in which the existence and stability of the equilibrium states were investigated. When the density is lower than a threshold value, the dynamics is described by a nonlinear diffusion equation. By contrast, when the density is larger than this threshold value, the dynamics is described by a similar hydrodynamic model for self-alignment interactions as derived in (Degond and Motsch, Math. Models Methods Appl. Sci. 18:1193–1215,

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P. Degond (✉) · A. Frouvelle
Institut de Mathématiques de Toulouse, Université de Toulouse; UPS, INSA, UT1, UTM;
31062 Toulouse, France
e-mail: pierre.degond@math.univ-toulouse.fr

A. Frouvelle
e-mail: amic.frouvelle@math.univ-toulouse.fr

P. Degond · A. Frouvelle
Institut de Mathématiques de Toulouse UMR 5219; CNRS; 31062 Toulouse, France

J.-G. Liu
Department of Physics and Department of Mathematics, Duke University, Durham, NC 27708, USA
e-mail: jliu@phy.duke.edu

2008a; Frouvelle, Math. Models Methods Appl. Sci., 2012). However, the modified normalization of the force gives rise to different convection speeds, and the resulting model may lose its hyperbolicity in some regions of the state space.

Keywords Self-propelled particles · Alignment interaction · Vicsek model · Phase transition · Hydrodynamic limit · Nonhyperbolicity · Diffusion limit · Chapman–Enskog expansion

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1 Introduction

The context of this paper is that of Degond and Motsch (2008a) and is concerned with a kinetic model for self-propelled particles and its hydrodynamic or diffusion limits. The particles move with the same constant speed, and their velocity directions (which belong to the sphere $\mathbb{S}$) align to the local average orientation, up to the addition of some noise. This model has been proposed as a variant of the Vicsek particle model (Vicsek et al. 1995). In this paper, we remove the normalization of the force intensity which was performed in Degond and Motsch (2008a). This apparently minor modification leads to the appearance of phase transitions, which have been studied in the space-homogeneous setting in Frouvelle and Liu (2012). In Frouvelle and Liu (2012), it is proved that the equilibrium distribution function changes type according to whether the density is below or above a certain threshold value. Below this value, the only equilibrium distribution is isotropic in velocity direction and is stable. Any initial distribution relaxes exponentially fast to this isotropic equilibrium state. By contrast, when the density is above the threshold, a second class of anisotropic equilibria formed by von Mises–Fisher distributions of arbitrary orientation appears. The isotropic equilibria become unstable, and any initial distribution relaxes towards one of these anisotropic states with exponential speed of convergence. We would like to emphasize the connection of the presented alignment models to Doi and Edwards (1999), Onsager (1949) and Maier and Saupe (1958) models for phase transition in polymers. The occurrence of phase transitions makes a strong difference in the resulting macroscopic models as compared with the ones found in Degond and Motsch (2008a), Frouvelle and Liu (2012), where no such phase transitions were present.

In the present paper, we rely on this previous analysis to study the large-scale limit of the space-inhomogeneous system. In the regions where the density is below the threshold, the convection speed becomes zero and the large-scale dynamics becomes a nonlinear diffusion. On the other hand, in the region where the density is above the threshold, the large-scale dynamics is described by a similar hydrodynamic model for self-alignment interactions as derived in Degond and Motsch (2008a), Frouvelle (2012). However, the modified normalization of the force gives rise to different convection speeds, and the resulting model may lose its hyperbolicity in some regions of the state space.

The Vicsek model (Vicsek et al. 1995), among other phenomena, models the behavior of individuals in animal groups such as fish schools, bird flocks, herds of

mammalians, etc. (see also Aldana and Huepe 2003; Aoki 1982; Couzin et al. 2002; Grégoire and Chaté 2004). This particle model (also called the "individual-based model" or "agent-based model") consists of a discrete stochastic system for the particle positions and velocities. A time-continuous version of the Vicsek model and its kinetic formulation have been proposed in Degond and Motsch (2008a). The rigorous derivation of this kinetic model has been performed in Bolley et al. (2012).

Hydrodynamic models are more efficient than particle models for large numbers of particles, because they simply encode the different particle quantities into simple averages, such as the density or mean velocity. We refer to Chuang et al. (2007), D'Orsogna et al. (2006), Mogilner and Edelstein-Keshet (1999), Mogilner et al. (2003), Toner and Tu (1998), Topaz and Bertozzi (2004), Topaz et al. (2006) for other models of self-propelled particle interactions. Rigorous derivations of hydrodynamic models from kinetic ones for self-propelled particles are scarce; Degond and Motsch (2008a), Frouvelle (2012) are among the first ones (see also some phenomenological derivations in Kulinskii et al. (2005), Ratushnaya et al. (2006, 2007). Similar models have also been found in relation to the persistent turning walker model of fish behavior (Degond and Motsch 2008b, 2011). Diffusive corrections have also been computed in Degond and Yang (2010). We refer to Carrillo et al. (2009, 2010) for other macroscopic models of swarming particle systems derived from kinetic theory. In particular, we mention (Frouvelle 2012), where a vision angle and the dependence of alignment frequency upon local density have been investigated.

Here we consider N oriented particles in $\mathbb{R}^n$, described by their positions $X_1, \ldots, X_N$ and their orientation vectors $\omega_1, \ldots, \omega_N$ belonging to $\mathbb{S}$, the unit sphere of $\mathbb{R}^n$. We define the mean momentum J_k of the neighbors of the particle k by

$$J_k = \frac{1}{N} \sum_{j=1}^{N} K(X_j - X_k)\omega_j.$$

In this paper, the observation kernel K will be assumed isotropic (depending only on the distance $|X_j - X_k|$ between the particle and its neighbors), smooth and with compact support. Introducing a nonisotropic observation kernel as in Frouvelle (2012) would lead to the same conclusion, with a slightly different convection speed for the orientation in the macroscopic model, but the computations are more complicated. Therefore, we focus on an isotropic observation kernel for simplicity.

The particles satisfy the following system of coupled stochastic differential equations (which must be understood in the Stratonovich sense), for $k \in [\![1, N]\!]$:

$$\mathrm{d}X_k = \omega_k \,\mathrm{d}t, \tag{1.1}$$

$$\mathrm{d}\omega_k = (\mathrm{Id} - \omega_k \otimes \omega_k) J_k \,\mathrm{d}t + \sqrt{2d}(\mathrm{Id} - \omega_k \otimes \omega_k) \circ \mathrm{d}B_t^k. \tag{1.2}$$

The first equation expresses the fact that particles move at constant speed equal to unity, following their orientation ω_k. The terms B_t^k stand for N independent standard Brownian motions on $\mathbb{R}^n$, and the projection term $(\mathrm{Id} - \omega_k \otimes \omega_k)$ (projection orthogonally to ω_k) constrains the norm of ω_k to be 1. We have that $(\mathrm{Id} - \omega_k \otimes \omega_k) J_k = \nabla_\omega (\omega \cdot J_k)|_{\omega=\omega_k}$, where ∇_ω is the tangential gradient on the sphere. So the second equation can be understood as a relaxation (with a rate proportional to the norm of J_k)

towards a unit vector in the direction of J_k, subjected to a Brownian motion on the sphere with intensity $\sqrt{2d}$. We refer to Hsu (2002) for more details on Brownian motions on Riemannian manifolds.

The interaction term (first term of (1.2)) is the sum of smooth binary interactions. This model is an intermediate between the Cucker-Smale model (Cucker and Smale 2007), where there is no constraint on the velocity and no noise, and the time-continuous version of the Vicsek model proposed in Degond and Motsch (2008a), where the velocity is constant and noise is added. In Degond and Motsch (2008a), J_k is replaced by $\nu\Omega_k$, where $\Omega_k = \frac{J_k}{|J_k|}$ is the unit vector in the direction of J_k and the relaxation frequency ν is a constant. Therefore, in Degond and Motsch (2008a), the interaction term cannot be recast as a sum of binary interactions and has a singularity when J_k is close to 0. The model presented here brings a modification consisting in letting ν depend (linearly) on the norm of the velocity J_k. A related modification has previously been introduced in Frouvelle (2012), consisting in letting the relaxation parameter ν depend on a local density $\bar{\rho}_k$, but the modification considered here brings newer phase transition phenomena.

From the individual-based model (1.1), (1.2), we derive a mean-field limit as the number of particles N tends to infinity. We define the empirical distribution f^N by

$$f^N(x,\omega,t) = \frac{1}{N}\sum_{i=1}^{N} \delta_{(X_i(t),\omega_i(t))}(x,\omega),$$

where the Dirac distribution is defined by duality by $\langle \delta_{(X,\Omega)}, \varphi\rangle_{\mathbb{R}^n\times\mathbb{S}} = \varphi(X,\Omega)$ for any smooth function $\varphi \in C(\mathbb{R}^n \times \mathbb{S})$, the duality product $\langle\cdot,\cdot\rangle_{\mathbb{R}^n\times\mathbb{S}}$ extending the usual inner product of $L^2(\mathbb{R}^n \times \mathbb{S})$. For convenience, the integration measure is assumed to be of total mass equal to 1 on the sphere $\mathbb{S}$, and we have $\langle f^N, 1\rangle_{\mathbb{R}^n\times\mathbb{S}} = 1$. Denoting the convolution with respect to the space variable by $*$, and the duality product on the sphere by $\langle\cdot,\cdot\rangle_{\mathbb{S}}$, we get $J_k = \langle K * f^N(X_k), \omega\rangle_{\mathbb{S}}$. If there is no noise ($d = 0$), it is easy to see that f^N satisfies the following partial differential equation (in the sense of distributions):

$$\partial_t f^N + \omega\cdot\nabla_x f^N + \nabla_\omega\cdot\left((\mathrm{Id}-\omega\otimes\omega)\bar{J}_{f^N} f^N\right) = 0,$$

where $\nabla_\omega\cdot$ denotes the divergence operator on the unit sphere, and

$$\bar{J}_{f^N}(x,t) = \left\langle \left(K * f^N\right)(x),\omega\right\rangle_{\mathbb{S}}.$$

When noise is present ($d \neq 0$), the empirical distribution f^N tends to a probability density function f satisfying the following partial differential equation:

$$\partial_t f + \omega\cdot\nabla_x f + \nabla_\omega\cdot\left((\mathrm{Id}-\omega\otimes\omega)\bar{J}_f f\right) = d\Delta_\omega f, \tag{1.3}$$

with

$$\bar{J}_f(x,t) = \int_{\mathbb{S}} (K * f)(x,\omega,t)\,\omega\,\mathrm{d}\omega. \tag{1.4}$$

This result has been shown in Bolley et al. (2012), under the assumption that the kernel K is Lipschitz and bounded.

Equations (1.3), (1.4) are the starting point of our study. There is a competition between the alignment and diffusion terms; the alignment term is quadratic, whereas the diffusion term is linear. Thus, we expect that alignment wins over diffusion for high densities while at low densities, diffusion dominates. This is the source of the phase transition rigorously studied in the space-homogeneous setting in Frouvelle and Liu (2012). In this reference, it is proven that there is a unique isotropic equilibrium at low density, but beyond a certain density threshold, another family of nonisotropic equilibria in the form of von Mises–Fisher distributions arises. Above this threshold, the isotropic equilibria become unstable, and the anisotropic ones become the stable ones. Therefore, we expect different large-scale limits according to whether the density is lower or larger than this threshold.

We now make some preliminary remarks and assumptions. We suppose that the kernel K is integrable, and that its total weight $K_0 = \int_{\mathbb{R}^n} K(x)\,\mathrm{d}x$ is positive. Writing

$$\widetilde{f}(x,\omega,t) = f\left(\frac{1}{d}x,\omega,\frac{1}{d}t\right) \quad \text{and} \quad \widetilde{K}(x) = \frac{1}{K_0 d^n} K\left(\frac{1}{d}x\right),$$

we get that $\widetilde{f}$ satisfies (1.3) with $d = 1$ and K replaced by $\widetilde{K}$ in (1.4), and we have

$$\int_{\mathbb{R}^n} \widetilde{K}(x)\,\mathrm{d}x = 1.$$

So without loss of generality, we can suppose that $d = 1$ and that $K_0 = 1$.

We are now ready to investigate the large-scale behavior of (1.3), (1.4) in space and time. The derivation of the macroscopic limit proceeds as in Degond and Motsch (2008a), and closely follows the presentation of Frouvelle (2012). Thus, we only give a summary, focusing on the points which are specific to the present model, in particular the distinction between the ordered and disordered phases.

The outline of this paper is as follows. In Sect. 2, we investigate the properties of the rescaled mean-field model. We prove that there are two possibilities for a local equilibrium, depending on the value of its density ρ. Section 3 is devoted to the derivation of the diffusion model when the density ρ is below the threshold. In Sect. 4, we derive the hydrodynamic model for self-alignment interactions in the region where ρ is above the threshold and study its hyperbolicity. The conclusion is presented in Sect. 5. Two appendices are added. In Appendix A, we calculate a Poincaré constant which provides us with a fine estimate of the rate of convergence to the equilibrium states. In Appendix B some numerical computations of the coefficients of the model are given.

2 The Macroscopic Limit

In order to observe the system at large scales, we perform a hydrodynamic scaling. We introduce a small parameter ε, and the change of variables $x' = \varepsilon x$, $t' = \varepsilon t$. We write $f^\varepsilon(x',\omega,t') = f(x,\omega,t)$, and $K^\varepsilon(x') = \frac{1}{\varepsilon^n} K(x)$. Then f^ε satisfies

$$\varepsilon\left(\partial_t f^\varepsilon + \omega\cdot\nabla_x f^\varepsilon\right) = -\nabla_\omega\cdot\left((\mathrm{Id}-\omega\otimes\omega)\bar{J}^\varepsilon_{f^\varepsilon} f^\varepsilon\right) + \Delta_\omega f^\varepsilon, \tag{2.1}$$

with

$$\bar{J}^{\varepsilon}_{f^\varepsilon}(x,t) = \int_{\mathbb{S}} \big(K^\varepsilon * f^\varepsilon\big)(x,\omega,t)\,\omega\,\mathrm{d}\omega. \tag{2.2}$$

The purpose of this paper is to derive a formal limit of this rescaled mean-field model when the parameter ε tends to 0. The first effect of this hydrodynamic scaling is that, up to order 1 in ε, the equation becomes local. Indeed, supposing that f^ε does not present any pathological behavior as $\varepsilon \to 0$, we get the following expansion:

$$\bar{J}^{\varepsilon}_{f^\varepsilon}(t,x) = J_{f^\varepsilon}(t,x) + O\big(\varepsilon^2\big), \tag{2.3}$$

where the local flux J_f is defined by

$$J_f(x,t) = \int_{\mathbb{S}} f(x,\omega,t)\,\omega\,\mathrm{d}\omega. \tag{2.4}$$

The proof of this expansion is elementary and omitted here (see, e.g., Appendix A.1 of Frouvelle 2012). We also define the density ρ_f associated to f by

$$\rho_f(x,t) = \int_{\mathbb{S}} f(x,\omega,t)\,\mathrm{d}\omega. \tag{2.5}$$

Hence, Eq. (2.1) becomes, after dropping the $O(\varepsilon^2)$ term,

$$\varepsilon\big(\partial_t f^\varepsilon + \omega\cdot\nabla_x f^\varepsilon\big) = Q\big(f^\varepsilon\big), \tag{2.6}$$

with

$$Q(f) = -\nabla_\omega\cdot\big((\mathrm{Id}-\omega\otimes\omega)J_f f\big) + \Delta_\omega f. \tag{2.7}$$

This paper is concerned with the formal limit $\varepsilon \to 0$ of this problem.

We remark that the collision operator Q acts on the ω variable only. The derivation of the macroscopic model relies on the properties of this operator. An obvious remark is that

$$\int_{\omega\in\mathbb{S}} Q(f)\,\mathrm{d}\omega = 0, \tag{2.8}$$

which expresses the local conservation of mass.

The first step of the study consists in characterizing the equilibria, i.e., the functions f such that $Q(f)=0$. Indeed, when $\varepsilon\to 0$, $Q(f^\varepsilon)\to 0$ and the limit $f = \lim_{\varepsilon\to 0} f^\varepsilon$ belongs to the set of equilibria. For any unit vector $\Omega\in\mathbb{S}$, and $\kappa\geqslant 0$, we define the von Mises–Fisher distribution (Watson 1982) with concentration parameter κ and orientation Ω by

$$M_{\kappa\Omega}(\omega) = \frac{e^{\kappa\,\omega\cdot\Omega}}{\int_{\mathbb{S}} e^{\kappa\,\upsilon\cdot\Omega}\,\mathrm{d}\upsilon}. \tag{2.9}$$

We note that the denominator depends only on κ. $M_{\kappa\Omega}$ is a probability density on the sphere, and we will denote by $\langle\cdot\rangle_{M_{\kappa\Omega}}$ the average over this probability measure. For

functions γ depending only on $\omega \cdot \Omega$, the average $\langle \gamma(\omega \cdot \Omega)\rangle_{M_{\kappa\Omega}}$ does not depend on Ω and will be denoted by $\langle \gamma(\cos\theta)\rangle_{M_\kappa}$. Using spherical coordinates, this average is given by

$$\big\langle \gamma(\cos\theta)\big\rangle_{M_\kappa} = \frac{\int_0^\pi \gamma(\cos\theta) e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta}.$$

The flux of the von Mises–Fisher distribution is given by

$$J_{M_{\kappa\Omega}} = \langle\omega\rangle_{M_{\kappa\Omega}} = c(\kappa)\Omega, \tag{2.10}$$

where the order parameter $c(\kappa)$, which measures how the distribution $M_{\kappa\Omega}$ is concentrated about Ω, is such that $0 \leqslant c(\kappa) \leqslant 1$ and is defined by

$$c(\kappa) = \langle\cos\theta\rangle_{M_\kappa} = \frac{\int_0^\pi \cos\theta e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta}. \tag{2.11}$$

When $c(\kappa) = 0$, $M_{\kappa\Omega}$ is the uniform distribution $M_{\kappa\Omega} = 1$, and when $c(\kappa) \to 1$, we have $M_{\kappa\Omega} \to \delta_\Omega(\omega)$.

We remark that the dependence of $M_{\kappa\Omega}$ upon κ and Ω only appears through the product $\kappa\Omega$. In this way, we can consider M_J for any given vector $J \in \mathbb{R}^n$. We also note that $\nabla_\omega(M_J) = (\mathrm{Id} - \omega\otimes\omega)J\,M_J$. Therefore,

$$Q(f) = \nabla_\omega \cdot \left[M_{J_f} \nabla_\omega\left(\frac{f}{M_{J_f}}\right)\right].$$

Using Green's formula, we have

$$\int_{\mathbb{S}} Q(f)\frac{g}{M_{J_f}}\,\mathrm{d}\omega = -\int_{\mathbb{S}} \nabla_\omega\left(\frac{f}{M_{J_f}}\right)\cdot\nabla_\omega\left(\frac{g}{M_{J_f}}\right)M_{J_f}\,\mathrm{d}\omega,$$

and

$$\int_{\mathbb{S}} Q(f)\frac{f}{M_{J_f}}\,\mathrm{d}\omega = -\int_{\mathbb{S}}\left|\nabla_\omega\left(\frac{f}{M_{J_f}}\right)\right|^2 M_{J_f}\,\mathrm{d}\omega \leqslant 0. \tag{2.12}$$

Definition 2.1 A function $f(\omega)$ is said to be an equilibrium of Q if and only if $Q(f) = 0$.

Let f be an equilibrium. Using (2.12), we deduce that $\frac{f}{M_{J_f}}$ is a constant. Therefore, $f = \rho_f M_{J_f}$ is of the form $\rho M_{\kappa\Omega}$ with $\kappa \geqslant 0$ and $\Omega \in \mathbb{S}$ (we note that in the case $|J_f| = 0$, $\kappa = 0$ and we can take any $\Omega \in \mathbb{S}$ because f is then just the uniform distribution). Using (2.10), we get

$$\kappa\Omega = J_f = \rho J_{M_{\kappa\Omega}} = \rho c(\kappa)\Omega,$$

which leads to the following equation for κ (compatibility condition):

$$\rho c(\kappa) = \kappa. \tag{2.13}$$

The study of this condition and the classification of the equilibria can be found in Frouvelle and Liu (2012). The key point is to notice that the function $\kappa \mapsto \frac{c(\kappa)}{\kappa}$ is decreasing and tends to $\frac{1}{n}$ as $\kappa \to 0$. Therefore, there is no other solution than $\kappa = 0$ if $\rho \leqslant n$. By contrast, if $\rho > n$, there is a unique strictly positive solution in addition to the trivial solution $\kappa = 0$. This leads to the following proposition.

Proposition 2.2

(i) *If $\rho \leqslant n$, $\kappa = 0$ is the only solution to the compatibility relation (2.13). The only equilibria are the isotropic ones $f = \rho$, with arbitrary $\rho \geqslant 0$.*

(ii) *If $\rho > n$, the compatibility relation (2.13) has exactly two roots: $\kappa = 0$ and a unique strictly positive root denoted by $\kappa(\rho)$. The set of equilibria associated to the root $\kappa = 0$ consists of the isotropic equilibria $f = \rho$, with arbitrary $\rho > n$. The set of equilibria associated to the root $\kappa(\rho)$ consist of the von Mises–Fisher distributions $\rho M_{\kappa(\rho)\Omega}$ with arbitrary $\rho > n$ and arbitrary $\Omega \in \mathbb{S}$ and forms a manifold of dimension n.*

The rates of convergence to the equilibria have been studied in Frouvelle and Liu (2012) in the spatially homogeneous setting. We first recall these results and then provide better estimates of the convergence rates in the large time limit for the supercritical case $\rho > n$, using lemmas on Poincaré constants which are detailed in Appendix A. Denoting by $g^\varepsilon = f^\varepsilon / \rho_{f^\varepsilon}$ the velocity probability distribution function, we can rewrite (2.6) in the following form (omitting the superscripts ε for clarity and neglecting the $O(\varepsilon^2)$ term):

$$\varepsilon\big(\partial_t(\rho g) + \omega \cdot \nabla_x(\rho g)\big) = -(\rho)^2 \nabla_\omega \cdot \big((\mathrm{Id} - \omega \otimes \omega) J_g g\big) + \rho \Delta_\omega g.$$

In the spatially homogeneous setting, we let $\nabla_x(\rho g) = 0$ and get

$$\varepsilon \partial_t(\rho g) = -(\rho)^2 \nabla_\omega \cdot \big((\mathrm{Id} - \omega \otimes \omega) J_g g\big) + \rho \Delta_\omega g = Q(\rho g). \tag{2.14}$$

Integrating this equation with respect to ω and using (2.8), we find that $\partial_t \rho = 0$. Therefore, ρ is independent of t and can be canceled out. The homogeneous equation (2.14) therefore takes the form

$$\varepsilon \partial_t g = -\rho \nabla_\omega \cdot \big((\mathrm{Id} - \omega \otimes \omega) J_g g\big) + \Delta_\omega g. \tag{2.15}$$

We now recall the definitions of global and asymptotic rate.

Definition 2.3 Let $\mathcal{X}$ be a Banach space with norm $\|\cdot\|$ and let $f(t) : \mathbb{R}_+ \to \mathcal{X}$ be a function of t with values in $\mathcal{X}$. We say that $f(t)$ converges to f_∞ with global rate r if and only if there exists a constant C which only depends on $\|f_0\|$, such that

$$\big\|f(t) - f_\infty\big\| \leqslant C e^{-rt}. \tag{2.16}$$

We say that $f(t)$ converges to f_∞ with asymptotic rate r_∞ if and only if for all $r < r_\infty$ there exists a constant C depending on f_0 (but not only on $\|f_0\|$) such that (2.16) holds. Finally, we say that $f(t)$ converges to f_∞ with asymptotic algebraic rate α if and only if there exists a constant C depending on f_0, such that

$$\left\| f(t) - f_\infty \right\| \leqslant \frac{C}{t^\alpha}.$$

Now, concerning problem (2.15), we can state the following theorem.

Theorem 2.4 (Frouvelle and Liu 2012) *Suppose g_0 is a probability measure, belonging to $H^s(\mathbb{S})$. There exists a unique weak solution g to (2.15), with initial condition $g(0) = g_0$. Furthermore, this solution is a classical one, is positive for all time $t > 0$, and belongs to $C^\infty((0, +\infty) \times \mathbb{S})$.*

(i) *If $J_{g_0} \neq 0$, the large time behavior of the solution is given by one of the three cases below*:

- *Case $\rho < n$: g converges exponentially fast to the uniform distribution, with global rate*

$$r(\rho) = \frac{(n-1)(n-\rho)}{n\varepsilon}, \tag{2.17}$$

  in any H^p norm.
- *Case $\rho > n$: There exists $\Omega \in \mathbb{S}$ such that g converges exponentially fast to $M_{\kappa(\rho)\Omega}$, with asymptotic rate greater than*

$$r(\rho) = \frac{1}{\varepsilon}\big(\rho c\big(\kappa(\rho)\big)^2 + n - \rho\big)\Lambda_{\kappa(\rho)} > 0,$$

  in any H^p norm, where Λ_κ is the best constant for the following Poincaré inequality:

$$\big\langle |\nabla g|^2 \big\rangle_{M_{\kappa\Omega}} \geqslant \Lambda_\kappa \big\langle \big(g - \langle g \rangle_{M_{\kappa\Omega}}\big)^2 \big\rangle_{M_{\kappa\Omega}}. \tag{2.18}$$

  We have

$$r(\rho) \sim \frac{1}{\varepsilon} 2(n-1)\left(\frac{\rho}{n} - 1\right), \quad \text{when } \rho \to n. \tag{2.19}$$

- *Case $\rho = n$: g converges to the uniform distribution in any H^p norm, with algebraic asymptotic rate $1/2$.*

(ii) *If $J_{g_0} = 0$: Then (2.15) reduces to the heat equation on the sphere. So g converges to the uniform distribution, exponentially fast, with global rate $r = \frac{2n}{\varepsilon}$ in any H^p norm.*

Remark 2.1 That g_0 is a probability measure implies that $g_0 \in H^s(\mathbb{S})$ for all $s < -\frac{n-1}{2}$. However, the theorem holds for all s. So for $s \geqslant -\frac{n-1}{2}$, that $g_0 \in H^s(\mathbb{S})$ is not a mere consequence of being a probability measure, and it must be added to the hypothesis.

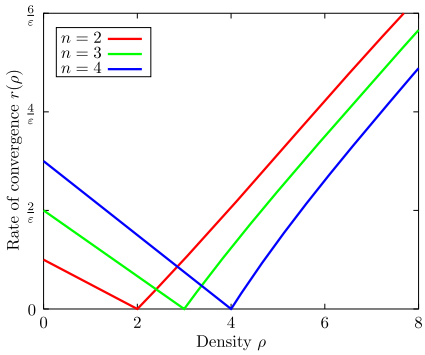

Fig. 1 Rates of convergence to equilibria in dimensions 2, 3, and 4, as functions of the density ρ

Now, we comment the results of this theorem.

First, in the supercritical case (when $\rho > n$), the uniform distribution is an unstable equilibrium: for any perturbation g of the uniform distribution such that $J_g \neq 0$, the associated solution converges to a given von Mises distribution, with a fixed concentration parameter $\kappa(\rho)$ defined by the compatibility condition (2.13). Second, the rates of convergence to the equilibrium are exponential. In the supercritical case, these rates are only asymptotic ones, but we can prove a uniform bound on these rates for ρ in any compact interval. A more precise study of the behavior of these rates is left to future work.

Therefore, when ε is small, the function f^ε converges rapidly to a given equilibrium, provided that the rate satisfies $r(\rho) \to \infty$ when $\varepsilon \to 0$. In the case $\rho < n$, from (2.17), this condition is equivalent to saying that $\varepsilon = o(n-\rho)$. In the case $\rho > n$, from (2.19), the condition $\varepsilon = o(n-\rho)$ implies that $r(\rho) \to \infty$ when $\varepsilon \to 0$ uniformly in any bounded ρ interval of the form $[n, A]$ with $A < \infty$. However, a uniform estimate from below of $r(\rho)$ is lacking when $\rho \to \infty$. But we can reasonably conjecture that away from a buffer region $|\rho - n| = O(\varepsilon)$, the convergence to the equilibrium is exponentially fast.

Some elements towards a uniform estimate of the rate $r(\rho)$ are provided in Appendix A. Furthermore, in Appendix B, we compute Λ_κ and then $r(\rho)$ numerically. The results are depicted in Fig. 1 for dimensions 2, 3, and 4.

We observe that for $\rho > n$, $r(\rho)$ grows linearly with ρ, which supports our conjecture.

Therefore, in the general space-inhomogeneous case, we will assume that the formal limit of f^ε as $\varepsilon \to 0$ is given by a function $f(x, \omega, t)$ which has a different velocity profile according to the position of the local density $\rho(x,t)$ with respect to the threshold value n. For this purpose, we define the disordered region $\mathcal{R}_d$ and the ordered region $\mathcal{R}_o$ as

$$\mathcal{R}_d = \big\{(x,t) \mid n - \rho^\varepsilon(x,t) \gg \varepsilon, \text{ as } \varepsilon \to 0\big\}, \tag{2.20}$$

$$\mathcal{R}_o = \big\{(x,t) \mid \rho^\varepsilon(x,t) - n \gg \varepsilon, \text{ as } \varepsilon \to 0\big\}. \tag{2.21}$$

We assume that as $\varepsilon \to 0$ we have

$$f^\varepsilon(x, \omega, t) \to \rho(x,t), \quad \forall (x,t) \in \mathcal{R}_d, \tag{2.22}$$

$$f^\varepsilon(x,\omega,t) \to \rho(x,t) M_{\kappa(\rho)\Omega(x,t)}, \quad \forall (x,t) \in \mathcal{R}_o, \tag{2.23}$$

and that the convergence is as smooth as needed.

The goal is now to derive evolution equations for $\rho(x,t)$ and $\Omega(x,t)$. This is the subject of the following two sections. We already note that, integrating (2.6) with respect to ω and using (2.8), we get the mass conservation equation

$$\partial_t \rho^\varepsilon + \nabla_x \cdot (J_{f^\varepsilon}) = 0. \tag{2.24}$$

3 Diffusion Model in the Disordered Region

We derive the macroscopic model in the disordered region $\mathcal{R}_d \subset \mathbb{R}^n$, using (2.22). With the mass conservation (2.24) and the fact that $J_{f^\varepsilon} \to J_f = 0$, this equation reduces to

$$\partial_t \rho = 0.$$

To obtain more precise information, we look for the next order in ε, using a Chapman–Enskog method, similarly as in the case of rarefied gas dynamics (see Degond 2004 for a review). We prove the following theorem.

Theorem 3.1 *When ε tends to zero, the (formal) first order approximation to the solution of the rescaled mean-field system (2.6), (2.7) in the disordered region $\mathcal{R}_d$ defined by (2.20) is given by*

$$f^\varepsilon(x,\omega,t) = \rho^\varepsilon(x,t) - \varepsilon \frac{n\,\omega \cdot \nabla_x \rho^\varepsilon(x,t)}{(n-1)(n-\rho^\varepsilon(x,t))}, \tag{3.1}$$

where the density ρ^ε satisfies the following diffusion equation:

$$\partial_t \rho^\varepsilon = \frac{\varepsilon}{n-1} \nabla_x \cdot \left(\frac{1}{n-\rho^\varepsilon} \nabla_x \rho^\varepsilon \right). \tag{3.2}$$

Proof We let $\rho^\varepsilon = \rho_{f^\varepsilon}$ and write $f^\varepsilon = \rho^\varepsilon(x,t) + \varepsilon f_1^\varepsilon(x,\omega,t)$ with $\int_{\mathbb{S}} f_1^\varepsilon \, \mathrm{d}\omega = 0$. Inserting this ansatz into (2.4), we get

$$J^\varepsilon_{f^\varepsilon} = \varepsilon J_{f_1^\varepsilon}(t,x),$$

and the model (2.6), (2.7) becomes

$$\partial_t \rho^\varepsilon + \omega \cdot \nabla_x \rho^\varepsilon + \varepsilon(\partial_t + \omega \cdot \nabla_x) f_1^\varepsilon = -\nabla_\omega \big((\mathrm{Id} - \omega \otimes \omega) J_{f_1^\varepsilon} \rho^\varepsilon \big) + \Delta_\omega f_1^\varepsilon - \varepsilon \nabla_\omega \big((\mathrm{Id} - \omega \otimes \omega) J_{f_1^\varepsilon} \rho^\varepsilon \big). \tag{3.3}$$

Additionally, (2.24) gives

$$\partial_t \rho^\varepsilon + \varepsilon \nabla_x \cdot (J_{f_1^\varepsilon}) = 0. \tag{3.4}$$

In particular, $\partial_t \rho^\varepsilon = O(\varepsilon)$. We need to compute f_1^ε to find the expression of the current. But, with this aim, we may retain only the terms of order 0 in (3.3). Since

$$\nabla_\omega\big((\mathrm{Id} - \omega \otimes \omega)A\big) = -(n-1)A \cdot \omega,$$

for any constant vector $A \in \mathbb{R}^n$, the equation for f_1^ε reads:

$$\Delta_\omega f_1^\varepsilon = \big(\nabla_x \rho^\varepsilon - (n-1)\rho^\varepsilon J_{f_1^\varepsilon}\big) \cdot \omega + O(\varepsilon).$$

This equation can be easily solved, since the right-hand side is a spherical harmonic of degree 1 (i.e., is of the form $A \cdot \omega$; we recall that $\Delta_\omega(A \cdot \omega) = -(n-1)A \cdot \omega$ and that $A \cdot \omega$ is of zero mean). Then:

$$f_1^\varepsilon = -\frac{1}{n-1}\big(\nabla_x \rho^\varepsilon - (n-1)\rho^\varepsilon J_{f_1^\varepsilon}\big) \cdot \omega + O(\varepsilon).$$

We immediately deduce, using that $\int_{\mathbb{S}} \omega \otimes \omega \, \mathrm{d}\omega = \frac{1}{n}\mathrm{Id}$,

$$J_{f_1^\varepsilon} = \frac{-1}{n(n-1)}\big(\nabla_x \rho^\varepsilon - (n-1)\rho^\varepsilon J_{f_1^\varepsilon}\big) + O(\varepsilon),$$

which implies that

$$J_{f_1^\varepsilon} = \frac{-1}{(n-1)(n-\rho^\varepsilon)}\big(\nabla_x \rho^\varepsilon + O(\varepsilon)\big).$$

Inserting this equation into (3.4) leads to the diffusion model (3.2) and ends the proof. □

Remark 3.1 The expression of f_1^ε, which is given by the $O(\varepsilon)$ term of (3.1) confirms that the approximation is only valid when $n - \rho^\varepsilon \gg \varepsilon$. The diffusion coefficient is only positive in the disordered region and it blows up as ρ^ε tends to n, showing that the Chapman–Enskog expansion loses its validity.

4 Hydrodynamic Model in the Ordered Region

4.1 Derivation of the Model

We now turn to the ordered region $\mathcal{R}_o \subset \mathbb{R}^n$ defined by (2.21). The purpose of this section is to give a formal proof of the following.

Theorem 4.1 *When ε tends to zero, the (formal) limit to the solution $f^\varepsilon(x, \omega, t)$ of the rescaled mean-field system (2.6), (2.7), in the ordered region $\mathcal{R}_o \subset \mathbb{R}^n$ defined by (2.21), is given by*

$$f(x, \omega, t) = \rho(x, t) M_{\kappa(\rho(x,t))\Omega(x,t)}(\omega), \tag{4.1}$$

where the von Mises–Fisher distribution $M_{\kappa\Omega}$ is defined at (2.9), and the parameter κ is the unique positive solution to the compatibility condition (2.13). Moreover, the

density $\rho > n$ and the orientation $\Omega \in \mathbb{S}$ satisfy the following system of first order partial differential equations:

$$\partial_t \rho + \nabla_x \cdot (\rho c \Omega) = 0, \tag{4.2}$$

$$\rho\big(\partial_t \Omega + \widetilde{c}(\Omega \cdot \nabla_x)\Omega\big) + \lambda(\mathrm{Id} - \Omega \otimes \Omega)\nabla_x \rho = 0, \tag{4.3}$$

where the coefficient $c = c(\kappa(\rho))$ is defined in (2.11), the coefficient $\widetilde{c} = \widetilde{c}(\kappa(\rho))$ will be defined later in (4.9), and the parameter $\lambda = \lambda(\rho)$ is given by

$$\lambda = \frac{\rho - n - \kappa\widetilde{c}}{\kappa(\rho - n - \kappa c)}. \tag{4.4}$$

Proof From now on, we will drop the dependence on ρ in the coefficients when no confusion is possible. With (2.23), $f^\varepsilon \to f$, where f is the stable local equilibrium (4.1). We now derive the evolution equations (4.2), (4.3) for ρ and Ω.

We recall that the concentration parameter κ satisfies the compatibility equation (2.13) where the order parameter c is defined by (2.11) and that we have $J_f = \rho c \Omega$. Therefore, Eq. (2.24), in the limit $\varepsilon \to 0$, reads

$$\partial_t \rho + \nabla_x \cdot (\rho c \Omega) = 0.$$

To compute the evolution equation for Ω, the method proposed originally in Degond and Motsch (2008a) consists in introducing the notion of generalized collisional invariant (GCI). This method has then been applied to Degond and Motsch (2011), Frouvelle (2012). The first step is the definition and determination of the GCIs. We define the linear operator $L_{\kappa\Omega}$ associated to a concentration parameter κ and a direction Ω as follows:

$$L_{\kappa\Omega}(f) = \Delta_\omega f - \kappa \nabla_\omega \cdot \big((\mathrm{Id} - \omega \otimes \omega)\Omega f\big) = \nabla_\omega \cdot \left[M_{\kappa\Omega} \nabla_\omega \left(\frac{f}{M_{\kappa\Omega}}\right)\right],$$

so that $Q(f) = L_{J_f}(f)$. We define the set $\mathcal{C}_{\kappa\Omega}$ of GCIs associated to $\kappa \in \mathbb{R}$ and $\Omega \in \mathbb{S}$ by

$$\mathcal{C}_{\kappa\Omega} = \left\{ \psi \,\middle|\, \int_{\omega\in\mathbb{S}} L_{\kappa\Omega}(f)\psi \,\mathrm{d}\omega = 0,\ \forall f \text{ such that } (\mathrm{Id} - \Omega \otimes \Omega)J_f = 0 \right\}.$$

Hence, if ψ is a GCI associated to κ and Ω, we have

$$\int_{\omega\in\mathbb{S}} Q(f)\psi \,\mathrm{d}\omega = 0, \quad \forall f \text{ such that } J_f = \kappa\Omega.$$

The determination of $\mathcal{C}_{\kappa\Omega}$ closely follows (Frouvelle 2012). We define the space

$$V = \left\{ g \,\middle|\, (n-2)(\sin\theta)^{\frac{n}{2}-2} g \in L^2(0,\pi),\ (\sin\theta)^{\frac{n}{2}-1} g \in H^1_0(0,\pi) \right\}, \tag{4.5}$$

and we denote by g_κ the unique solution in V of the elliptic problem

$$\widetilde{L}^*_\kappa g(\theta) = \sin\theta, \tag{4.6}$$

where

$$\widetilde{L}_\kappa^* g(\theta) = -(\sin\theta)^{2-n} e^{-\kappa\cos\theta} \frac{\mathrm{d}}{\mathrm{d}\theta}\left((\sin\theta)^{n-2} e^{\kappa\cos\theta}\frac{\mathrm{d}g}{\mathrm{d}\theta}(\theta)\right) + \frac{n-2}{\sin^2\theta} g(\theta). \tag{4.7}$$

Then defining h_κ by $g_\kappa(\theta) = h_\kappa(\cos\theta)\sin\theta$, we get

$$\mathcal{C}_{\kappa\Omega} = \left\{ h_\kappa(\omega\cdot\Omega) A\cdot\omega + C \,\middle|\, C\in\mathbb{R},\ A\in\mathbb{R}^n,\ \text{with } A\cdot\Omega = 0\right\}.$$

The set of GCIs $\mathcal{C}_{\kappa\Omega}$ is a vector space of dimension n, since A is a vector with $n-1$ independent components.

The next step consists in multiplying (2.6) by a GCI associated to κ^ε and Ω^ε such that $J_{f^\varepsilon} = \kappa^\varepsilon \Omega^\varepsilon$, and integrating it with respect to ω.

For any vector $A\in\mathbb{R}^n$, with $A\cdot\Omega^\varepsilon = 0$, we get

$$\int_{\omega\in\mathbb{S}} Q\big(f^\varepsilon\big) h_{\kappa^\varepsilon}\big(\omega\cdot\Omega^\varepsilon\big) A\cdot\omega\,\mathrm{d}\omega = 0.$$

So, the vector

$$X^\varepsilon = \frac{1}{\varepsilon}\int_{\omega\in\mathbb{S}} Q(f^\varepsilon) h_{\kappa^\varepsilon}\big(\omega\cdot\Omega^\varepsilon\big)\omega\,\mathrm{d}\omega$$

is parallel to Ω^ε, or equivalently $(\mathrm{Id} - \Omega^\varepsilon\otimes\Omega^\varepsilon)\, X^\varepsilon = 0$. Using (2.6), we get

$$X^\varepsilon = \int_{\omega\in\mathbb{S}} \big(\partial_t f^\varepsilon + \omega\cdot\nabla_x f^\varepsilon\big)\, h_{\kappa^\varepsilon}\big(\omega\cdot\Omega^\varepsilon\big)\omega\,\mathrm{d}\omega.$$

In the limit $\varepsilon\to 0$, we get

$$(\mathrm{Id} - \Omega\otimes\Omega)\, X = 0, \tag{4.8}$$

where

$$X = \int_{\omega\in\mathbb{S}} \big(\partial_t(\rho M_{\kappa\Omega}) + \omega\cdot\nabla_x(\rho M_{\kappa\Omega})\big) h_\kappa(\omega\cdot\Omega)\omega\,\mathrm{d}\omega.$$

Finally it has been proved in Frouvelle (2012) that (4.8) is equivalent to (4.3) with

$$\widetilde{c} = \langle\cos\theta\rangle_{\widetilde{M}_\kappa} = \frac{\int_0^\pi \cos\theta h_\kappa(\cos\theta) e^{\kappa\cos\theta}\sin^n\theta\,\mathrm{d}\theta}{\int_0^\pi h_\kappa(\cos\theta) e^{\kappa\cos\theta}\sin^n\theta\,\mathrm{d}\theta}, \tag{4.9}$$

$$\lambda = \frac{1}{\kappa} + \frac{\rho}{\kappa}\frac{\mathrm{d}\kappa}{\mathrm{d}\rho}(\widetilde{c} - c). \tag{4.10}$$

We can now compute a simpler expression of λ. We differentiate the compatibility condition (2.13) with respect to κ, and we get

$$c\frac{\mathrm{d}\rho}{\mathrm{d}\kappa} + \rho\frac{\mathrm{d}c}{\mathrm{d}\kappa} = 1.$$

We have

$$\begin{aligned}\frac{\mathrm{d}c}{\mathrm{d}\kappa} &= \frac{\mathrm{d}}{\mathrm{d}\kappa}\left(\frac{\int_0^\pi \cos\theta e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta}\right)\\ &= \frac{\int_0^\pi \cos^2\theta e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta} - \left(\frac{\int_0^\pi \cos\theta e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta}\right)^2\\ &= 1 - \frac{\int_0^\pi \sin^2\theta e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta} - c^2\\ &= 1 - (n-1)\frac{c}{\kappa} - c^2.\end{aligned}$$

Therefore, we get

$$c\frac{\mathrm{d}\rho}{\mathrm{d}\kappa} = \frac{\kappa}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}\kappa} = 1 - \rho\frac{\mathrm{d}c}{\mathrm{d}\kappa} = 1 - \rho\left(1 - (n-1)\frac{c}{\kappa} - c^2\right) = n - \rho + \kappa c, \quad (4.11)$$

and finally

$$\lambda = \frac{1}{\kappa} + \frac{\widetilde{c} - c}{n - \rho + \kappa c} = \frac{n - \rho + \kappa\widetilde{c}}{\kappa(n - \rho + \kappa c)},$$

which ends the proof of Theorem 4.1. □

The next part is devoted to the study of the properties of the model (4.2)–(4.3) in the ordered region.

4.2 Hyperbolicity of the Hydrodynamic Model in the Ordered Region

We first investigate the hyperbolicity of the hydrodynamic model (4.2)–(4.3). We recall some definitions. Let

$$\partial_t U + \sum_{i=1}^n A_i(U)\partial_{x_i} U = 0, \quad (4.12)$$

be a first order system where $x \in \mathbb{R}^n$, $t \geqslant 0$, $U = (U_1, \ldots, U_m)$ is an m-dimensional vector and $(A_i(U))_{i=1,\ldots,n}$ are n $m \times m$-dimensional matrices. Let $U_0 \in \mathbb{R}^m$. The constant and uniform state $U(x,t) = U_0$ is a particular solution of (4.12). The linearization of (4.12) about this constant and uniform state leads to the following linearized system:

$$\partial_t u + \sum_{i=1}^n A_i(U_0)\partial_{x_i} u = 0. \quad (4.13)$$

We look for solutions of (4.13) in the form of plane waves $u(x,t) = \bar{u}e^{i(k\cdot x - \omega t)}$, with $k \in \mathbb{R}^n$ and $\omega \in \mathbb{C}$. Such solutions exist if and only if $\omega/|k|$ is an eigenvalue of

the matrix $A(k/|k|)$ and $\bar{u}$ is the related eigenvector, where for a direction $\xi \in \mathbb{S}$, the matrix $A(\xi)$ is defined by

$$A(\xi) = \sum_{i=1}^{n} A_i(U)\xi_i. \tag{4.14}$$

The problem (4.12) is said to be hyperbolic about U_0, if only purely propagative plane waves with real ω can exist or equivalently, if $A(\xi)$ has real eigenvalues for any ξ. We also must rule out polynomially increasing in time solutions which could exist if the matrix would not be diagonalizable. This leads to the following definitions.

Definition 4.2

(i) Let $U_0 \in \mathbb{R}^m$. System (4.12) is hyperbolic about U_0 if and only if for all directions $\xi \in \mathbb{S}$, the matrix $A(\xi)$ is diagonalizable with real eigenvalues.
(ii) System (4.12) is hyperbolic, if and only if it is hyperbolic about any state U_0 in the domain of definition of the matrices $A_i(U)$.

The linearization of system (4.2)–(4.3) about a stationary uniform state (ρ_0, Ω_0) is obtained by inserting the following expansion:

$$\rho = \rho_0 + \delta r + o(\delta), \tag{4.15}$$

$$\Omega = \Omega_0 + \delta W + o(\delta), \tag{4.16}$$

where $\delta \ll 1$ is a small parameter and $r = r(x,t)$, $W = W(x,t)$ are the first order perturbations of ρ and Ω. Given that $|\Omega| = |\Omega_0| = 1$, we have $W \cdot \Omega_0 = 0$. Inserting (4.15), (4.16) into (4.2), (4.3) leads to the following linearized system:

$$\partial_t r + \gamma_0(\Omega_0 \cdot \nabla_x)r + \rho_0 c_0(\nabla_x \cdot W) = 0, \tag{4.17}$$

$$\partial_t W + \tilde{c}_0(\Omega_0 \cdot \nabla_x)W + \frac{\lambda_0}{\rho_0}(\mathrm{Id} - \Omega_0 \otimes \Omega_0)\nabla_x r = 0, \tag{4.18}$$

$$W \cdot \Omega_0 = 0, \tag{4.19}$$

with

$$\gamma(\rho) = c + \rho\frac{dc}{d\rho},$$

and $\gamma_0 = \gamma(\rho_0)$, $c_0 = c(\rho_0)$, $\tilde{c}_0 = \tilde{c}(\rho_0)$, and $\lambda_0 = \lambda(\rho_0)$.

Next, we show that system (4.17)–(4.19) is invariant under rotations. This will allow us to choose one arbitrary direction ξ in the definition (4.14) instead of checking all possible directions. For this purpose, let R be a rotation matrix of $\mathbb{R}^n$; i.e., R is an $n \times n$ matrix such that $R^T = R^{-1}$, where the exponent T denotes transposition. We introduce the change of variables $x = Rx'$ and define the new unknowns

$$r(x) = r'(x'), \qquad W(x) = RW'(x'), \qquad \Omega_0 = R\Omega_0'.$$

We note the following identities:

$$\Omega_0' \cdot W'(x') = \Omega_0 \cdot W(x) = 0,$$
$$\nabla_x r(x) = R \nabla_{x'} r'(x'),$$
$$\nabla_x W(x) = R \nabla_{x'} W'(x') R^T,$$
$$(\nabla_x \cdot W)(x) = (\nabla_{x'} \cdot W')(x'),$$
$$(\Omega_0 \cdot \nabla_x) W(x) = (\nabla_x W(x))^T \Omega_0 = R(\nabla_{x'} W(x'))^T \Omega_0' = R(\Omega_0' \cdot \nabla_{x'}) W'(x'),$$
$$(\Omega_0 \cdot \nabla_x) r(x) = (\Omega_0' \cdot \nabla_{x'}) r'(x').$$

With these identities, it is easy to show that (r', W') satisfies system (4.17)–(4.19) with Ω_0 replaced by Ω_0'.

The rotational invariance of (4.17)–(4.19) shows that, in order to check the hyperbolicity, it is enough to choose any particular direction ξ. Let us call this arbitrary direction z, with the unit vector in this direction denoted by e_z. To check the hyperbolicity of waves propagating in the z direction it is sufficient to look at the system where all unknowns only depend only on the space coordinate z and on the time t. Denoting by θ the angle between the z direction and Ω, we can write:

$$\Omega = \cos\theta e_z + \sin\theta v, \quad \theta \in [0, \pi], \ v \in \mathbb{S}_{n-2},$$

where $\mathbb{S}_{n-2}$ is the sphere of dimension $n-2$ collecting all unit vectors orthogonal to e_z. With these hypotheses, system (4.2)–(4.3) is written as follows:

$$\partial_t \rho + \partial_z(\rho c(\rho) \cos\theta) = 0, \tag{4.20}$$
$$\rho[\partial_t(\cos\theta) + \tilde{c}(\rho)\cos\theta \partial_z(\cos\theta)] + \lambda(1 - \cos^2\theta)\partial_z \rho = 0, \tag{4.21}$$
$$\partial_t v + \tilde{c}(\rho)\cos\theta \partial_z v = 0, \text{ with } |v| = 1 \text{ and } e_z \cdot v = 0. \tag{4.22}$$

In the special case of dimension $n = 2$, the system reduces to (4.20)–(4.21), with θ extended to $(-\pi, \pi)$ and $\Omega = \cos\theta\, e_z + \sin\theta\, v_0$, where v_0 is one of the two unit vectors orthogonal to e_z.

The hyperbolicity of this system depends on the sign of λ. Proposition 4.5 below shows that $\lambda < 0$ in the two limits $\rho \to n$ and $\rho \to \infty$. Additionally, the numerical computation of λ, displayed in Fig. 2, provides evidence that $\lambda < 0$ for all values of ρ, at least in dimensions $n = 2$, 3, and 4. Therefore, we assume that

$$\lambda < 0. \tag{4.23}$$

We first check the local hyperbolicity criterion.

Proposition 4.3 *We assume that we have* (4.23). *Then, the system* (4.20)–(4.22) *is hyperbolic about* (ρ, θ, v) *if and only if*

$$|\tan\theta| < \tan\theta_c := \frac{|\widetilde{c} - \frac{c}{n-\rho+\kappa c}|}{2\sqrt{-\lambda c}}. \tag{4.24}$$

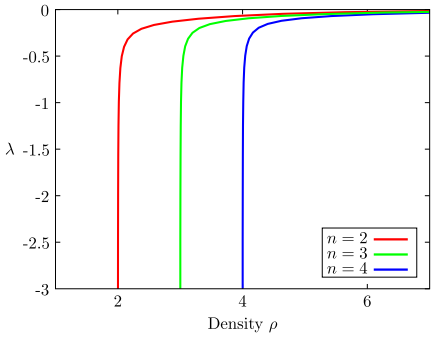

Fig. 2 Coefficient λ in dimensions 2, 3, and 4

Proof We apply (Frouvelle 2012) and find that the hyperbolicity criterion is written:

$$|\tan\theta| < \frac{|\widetilde{c} - \frac{\mathrm{d}}{\mathrm{d}\rho}(\rho c)|}{2\sqrt{-\lambda c}}.$$

Using the compatibility condition (2.13) and (4.11), Eq. (4.24) follows. □

As for global hyperbolicity, we have the following.

Proposition 4.4 *We assume* (4.23). *Then, system* (4.20)–(4.22) *is not hyperbolic.*

Proof It has been proved in Frouvelle (2012) that system (4.2)–(4.3) is hyperbolic if and only if $\lambda > 0$. As we assume (4.23), it follows that the system is not hyperbolic. □

We now provide asymptotic expansions of the coefficients which show that, at least when $\rho \to n$ or $\rho \to \infty$, we have $\lambda < 0$.

Proposition 4.5 *We have the following expansions.*

(i) *When* $\rho \to n$:

$$c = \frac{\sqrt{n+2}}{n}\sqrt{\rho - n} + O(\rho - n),$$
$$\widetilde{c} = \frac{2n-1}{2n\sqrt{n+2}}\sqrt{\rho - n} + O(\rho - n),$$
$$\lambda = \frac{-1}{4\sqrt{n+2}}\frac{1}{\sqrt{\rho - n}} + O(1),$$
$$\theta_c = \frac{\pi}{2} - \frac{2}{\sqrt{n+2}\sqrt{n}}\sqrt{\rho - n} + O(\rho - n).$$

(ii) *When* $\rho \to \infty$:

$$c = 1 - \frac{n-1}{2}\rho^{-1} + \frac{(n-1)(n+1)}{8}\rho^{-2} + O\big(\rho^{-3}\big),$$

$$\widetilde{c} = 1 - \frac{n+1}{2}\rho^{-1} - \frac{(n+1)(3n+1)}{24}\rho^{-2} + O\big(\rho^{-3}\big),$$
$$\lambda = -\frac{n+1}{6}\rho^{-2} + O\big(\rho^{-3}\big),$$
$$\theta_c = \arctan\left(\frac{\sqrt{n+1}\sqrt{6}}{4}\right) + O\big(\rho^{-1}\big).$$

Proof Using the compatibility condition (2.13), the expression (4.4) depends only on κ, c, and $\widetilde{c}$. With the asymptotic expansion of c and $\widetilde{c}$ as $\kappa \to 0$ and $\kappa \to \infty$ given in Frouvelle (2012), we can get an expansion for λ. We have

$$c = \begin{cases} \frac{1}{n}\kappa - \frac{1}{n^2(n+2)}\kappa^3 + O(\kappa^5) & \text{as } \kappa \to 0, \\ 1 - \frac{n-1}{2\kappa} + \frac{(n-1)(n-3)}{8\kappa^2} + O(\kappa^{-3}) & \text{as } \kappa \to \infty, \end{cases}$$
$$\widetilde{c} = \begin{cases} \frac{2n-1}{2n(n+2)}\kappa + O(\kappa^2) & \text{as } \kappa \to 0, \\ 1 - \frac{n+1}{2\kappa} + \frac{(n+1)(3n-7)}{24\kappa^2} + O(\kappa^{-3}) & \text{as } \kappa \to \infty. \end{cases}$$

We first compute an expansion of $\rho = \frac{\kappa}{c}$. We get

$$\rho = \begin{cases} n + \frac{1}{n+2}\kappa^2 + O(\kappa^4) & \text{as } \kappa \to 0, \\ \kappa + \frac{n-1}{2} + \frac{(n-1)(n+1)}{8\kappa} + O(\kappa^{-2}) & \text{as } \kappa \to \infty. \end{cases} \tag{4.25}$$

Using the definition (4.4), we then get

$$\lambda = \begin{cases} -\frac{1}{4\kappa} + O(1) & \text{as } \kappa \to 0, \\ -\frac{n+1}{6\kappa^2} + O(\kappa^{-3}) & \text{as } \kappa \to \infty. \end{cases}$$

We can also expand the threshold angle θ_c in terms of κ. We get

$$\theta_c = \begin{cases} \frac{\pi}{2} - \frac{2}{(n+2)\sqrt{n}}\kappa + O(\kappa^2) & \text{as } \kappa \to 0, \\ \arctan(\frac{\sqrt{n+1}\sqrt{6}}{4}) + O(\kappa^{-1}) & \text{as } \kappa \to \infty. \end{cases}$$

We can now reverse the expansion (4.25) to get an expansion of κ (and then of the other coefficients) in terms of the density ρ. We get

$$\kappa = \begin{cases} \sqrt{n+2}\sqrt{\rho - n} + O(\rho - n) & \text{as } \rho \to n, \\ \rho - \frac{n-1}{2} - \frac{(n-1)(n+1)}{8\rho} + O(\rho^{-2}) & \text{as } \rho \to \infty. \end{cases}$$

Inserting this expansion into the previous ones, we finally deduce the expressions stated in Proposition 4.5. □

When $\rho \sim n$, since $|\lambda| = -\lambda$ is large compared to ρ, which is large compared to $\rho\widetilde{c}$, the behavior of the orientation equation (4.3) can be compared to the behavior of

$$\partial_t \Omega = \frac{|\lambda|}{\rho}(\mathrm{Id} - \Omega \otimes \Omega)\nabla_x \rho,$$

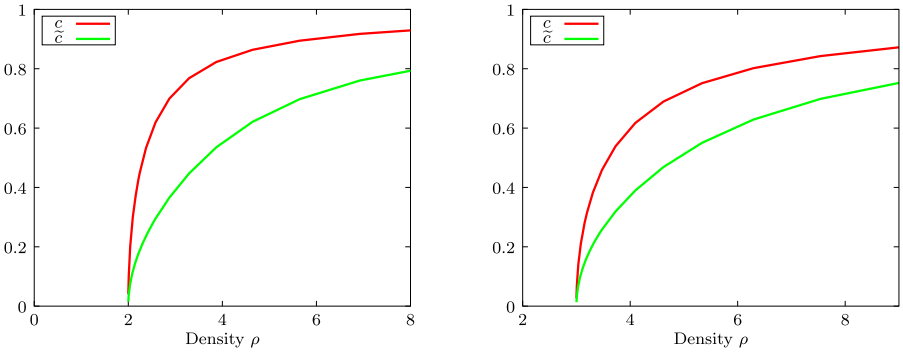

Fig. 3 The velocities c and $\widetilde{c}$ in dimension 2 (*left*) and 3 (*right*)

which relaxes Ω to the unit vector $\nabla_x\rho/|\nabla_x\rho|$, with rate

$$\frac{-\lambda}{\rho}|\nabla_x\rho| \sim \frac{1}{4n\sqrt{n+2}\sqrt{\rho-n}}|\nabla_x\rho|.$$

This actually makes sense only if the rate of convergence to the equilibrium (which is given by $\frac{1}{\varepsilon}r(\rho) \sim \frac{2n-1}{n\varepsilon}(\rho-n)$ in the neighborhood of n) is large compared to this relaxation rate. This requires $\varepsilon \ll (\rho-n)^{\frac{3}{2}}|\nabla_x\rho|$. In this case the leading behavior of the system is given by

$$\partial_t\rho + \nabla_x\cdot\left(\frac{\rho c}{|\nabla_x\rho|}\nabla_x\rho\right) = 0,$$

which is an ill-posed problem; it is some kind of nonlinear backwards heat equation. To stabilize this system, a possibility is to derive a first order diffusive correction to the model (4.2)–(4.3) using a Chapman–Enskog expansion. Such a correction has been derived in Degond and Yang (2010) for the model of Degond and Motsch (2008a), but leads to complicated terms. Another possibility is to add some contribution of the nonlocality of the interaction in the spirit of Degond et al. (2011).

When ρ is large, c and $\widetilde{c}$ are close to 1, and λ is small. In the intermediate regime, numerical computations (see Appendix B) show that there is a significant difference between c and $\widetilde{c}$. This means that the information about velocity orientation travels slower than the fluid. Figure 3 displays c and $\tilde{c}$ as functions of ρ, in dimensions 2 and 3.

Finally, when $\rho \to \infty$, the critical angle θ_c tends to a positive value $\arctan(\frac{\sqrt{n+1}\sqrt{6}}{4})$. Numerically, we see that θ_c is always larger than this limit value. Then, in the region where the angle θ between Ω and the direction of propagation is less than this limit value, system (4.20)–(4.22) is hyperbolic independently of the density ρ. Figure 4 summarizes the different types of macroscopic limits of the system in dimension 2, when the density ρ, and the angle θ between Ω and the propagation direction vary. The behavior of the system at the crossings, either between the hyperbolic and nonhyperbolic regions or between the ordered and disordered regions, remains an open problem. We note that nonhyperbolicity problems appear in

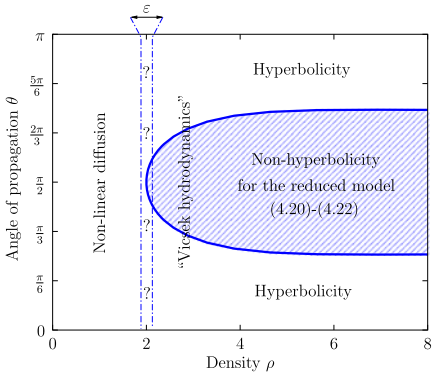

Fig. 4 Types of macroscopic limits in dimension 2. Around the threshold value $\rho = 2$, none of the diffusion or hydrodynamic limit is valid. The study of this transition is still open

other areas, such as the motion of an elastic string on a plane (Pego and Serre 1988). However, a simple modification of the alignment frequency with a dependence on the norm of the local average momentum removes the nonhyperbolicity problems, as shown in Degond et al. (2012).

5 Conclusion

In this paper, we have derived a macroscopic model for particles undergoing self-alignment interactions with phase transitions. This model is derived from a time-continuous version of the Vicsek model. We have identified two regimes. In the disordered regime, the macroscopic model is given by a nonlinear diffusion equation depending on the small parameter ε describing the ratios of the microscopic to macroscopic length scales. In the ordered regime, the model is given by a hydrodynamic model for self-alignment interaction which is not hyperbolic. Many problems remain open. Among others, a first one is to determine the evolution of the boundary between the ordered and disordered regions and to understand how the models in the two regions are connected across this boundary. A second problem is to understand how to cope with the nonhyperbolicity of the model in the ordered region and possibly modify it by adding small diffusive corrections. Numerical simulations of the particle model are in progress to understand the behavior of the model in the two regimes. Also, a simple modification of the collision frequency restores the hyperbolicity (Degond et al. 2012).

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Appendix A: Poincaré Constant

In this appendix, we prove the following.

Proposition A.1 *We have the following Poincaré inequality, for* $\psi \in H^1(\mathbb{S})$:

$$\left\langle |\nabla_\omega \psi|^2 \right\rangle_{M_{\kappa\Omega}} \geqslant \Lambda_\kappa \left\langle \left(\psi - \langle \psi \rangle_{M_{\kappa\Omega}}\right)^2 \right\rangle_{M_{\kappa\Omega}}. \tag{A.1}$$

The best constant Λ_κ *in this inequality is the smallest positive eigenvalue of the operator*

$$L^*_{\kappa\Omega} = -\frac{1}{M_{\kappa\Omega}} \nabla_\omega \cdot (M_{\kappa\Omega} \nabla_\omega). \tag{A.2}$$

We define the linear operator L^*_κ *by*

$$L^*_\kappa(g)(\theta) = -(\sin\theta)^{2-n} e^{-\kappa\cos\theta} \left((\sin\theta)^{n-2} e^{\kappa\cos\theta} g'(\theta)\right)'. \tag{A.3}$$

Then one of the following three possibilities is true:

(i) Λ_κ *is the smallest eigenvalue of the Sturm–Liouville problem*

$$L^*_\kappa(g) = \lambda g, \tag{A.4}$$

for $g \in C^2([0,\pi])$ *with Neumann boundary conditions* $(g'(0) = g'(\pi) = 0)$ *and such that* $\int_0^\pi (\sin\theta)^{n-2} e^{\kappa\cos\theta} g(\theta)\,\mathrm{d}\theta = 0$, *and the eigenspace of* $L^*_{\kappa\Omega}$ *associated to the eigenvalue* Λ_κ *is of dimension* 1, *spanned by* $\omega \mapsto h^0_\kappa(\omega \cdot \Omega)$, *where the function* $\theta \mapsto h_0(\cos\theta)$ *is smooth, positive for* $0 \leqslant \theta < \theta_0$, *and negative for* $\theta_0 < \theta \leqslant \pi$.

(ii) Λ_κ *is the smallest eigenvalue of the Sturm–Liouville problem*

$$\widetilde{L}^*_\kappa(g) = L^*_\kappa(g) + \frac{n-2}{\sin^2\theta} g(\theta) = \lambda g, \tag{A.5}$$

for $g \in C^2([0,\pi])$ *with Dirichlet boundary conditions* $(g(0) = g(\pi) = 0)$, *and the eigenspace of* $L^*_{\kappa\Omega}$ *associated to* Λ_κ *is of dimension* $n-1$, *consisting in the functions* ψ_A *of the form* $\psi_A(\omega) = h^1_\kappa(\omega \cdot \Omega) A \cdot \omega$ *for any vector* $A \in \mathbb{R}^n$ *such that* $\Omega \cdot A = 0$, *with* $\theta \mapsto h^1_\kappa(\cos\theta)$ *a smooth positive function for* $0 < \theta < \pi$.

(iii) *The two preceding Sturm–Liouville problems have the same smallest eigenvalue* Λ_κ, *and the eigenspace of* $L^*_{\kappa\Omega}$ *associated to* Λ_κ *is of dimension* n, *spanned by the two types of function of the above cases.*

Proof First of all, we have

$$\left\langle |\nabla_\omega \psi|^2 \right\rangle_{M_{\kappa\Omega}} \geqslant (\min M_{\kappa\Omega}) \int_{\mathbb{S}} |\nabla_\omega \psi|^2 \geqslant (\min M_{\kappa\Omega})(n-1) \int_{\mathbb{S}} \left(\psi - \int_{\mathbb{S}} \psi\right)^2, \tag{A.6}$$

and

$$\left\langle \left(\psi - \langle \psi \rangle_{M_{\kappa\Omega}}\right)^2 \right\rangle_{M_{\kappa\Omega}} \leqslant \left\langle \left(\psi - \int_{\mathbb{S}} \psi\right)^2 \right\rangle_{M_{\kappa\Omega}} \leqslant (\max M_{\kappa\Omega}) \int_{\mathbb{S}} \left(\psi - \int_{\mathbb{S}} \psi\right)^2. \tag{A.7}$$

The second inequality of (A.6) follows from the Poincaré inequality on the sphere:

$$\int_{\mathbb{S}}\left(\psi-\int_{\mathbb{S}}\psi\right)^2\leqslant\frac{1}{n-1}\int_{\mathbb{S}}|\nabla_\omega\psi|^2.$$

The first inequality of (A.7) follows from the fact that

$$\left\langle\left(\psi-\int_{\mathbb{S}}\psi\right)^2\right\rangle_{M_{\kappa\Omega}}-\left\langle\left(\psi-\langle\psi\rangle_{M_{\kappa\Omega}}\right)^2\right\rangle_{M_{\kappa\Omega}}=\left(\int_{\mathbb{S}}\psi-\int_{\mathbb{S}}\psi M_{\kappa\Omega}\right)^2\geqslant 0.$$

Equations (A.6) and (A.7) lead to the Poincaré inequality (A.1) with

$$\Lambda_\kappa\geqslant(n-1)\frac{\min M_{\kappa\Omega}}{\max M_{\kappa\Omega}}=(n-1)e^{2\kappa}.$$

We use the inner product $(\varphi,\psi)\mapsto\langle\varphi\psi\rangle_{M_{\kappa\Omega}}$, adapted to $M_{\kappa\Omega}$. We denote by $\dot{L}^2_\kappa(\mathbb{S})$ (resp. $\dot{H}^1_\kappa(\mathbb{S})$) the functions $\psi\in L^2(\mathbb{S})$ (resp. in $H^1(\mathbb{S})$) such that $\langle\psi\rangle_{M_{\kappa\Omega}}=0$.

The operator $L^*_{\kappa\Omega}$ given by (A.2) is self-adjoint since $\langle\nabla_\omega\psi\cdot\nabla_\omega\varphi\rangle_{M_{\kappa\Omega}}=\langle\psi L^*_{\kappa\Omega}\varphi\rangle_{M_{\kappa\Omega}}$. It is then easy to see, using the Lax-Milgram theorem, that if φ belongs to $\dot{L}^2_\kappa(\mathbb{S})$, then there is a unique solution $\psi\in\dot{H}^1_\kappa(\mathbb{S})$ to the equation $L^*_{\kappa\Omega}\psi=\varphi$. The so-obtained inverse operator is then compact and self-adjoint. By the spectral theorem, we get a basis of eigenfunctions, in the Hilbert space $\dot{L}^2_\kappa(\mathbb{S})$, which are also eigenfunctions of $L^*_{\kappa\Omega}$. If we denote Λ_κ^{-1} the largest eigenvalue of the inverse of $L^*_{\kappa\Omega}$, then it is easy to see that Λ_κ is the best constant for the following Poincaré inequality, in the space $\dot{H}^1_\kappa(\mathbb{S})$:

$$\left\langle|\nabla_\omega\psi|^2\right\rangle_{M_{\kappa\Omega}}\geqslant\Lambda_\kappa\left\langle\psi^2\right\rangle_{M_{\kappa\Omega}}\geqslant\Lambda_\kappa\left\langle\left(\psi-\langle\psi\rangle_{M_{\kappa\Omega}}\right)^2\right\rangle_{M_{\kappa\Omega}}.$$

Since the constants trivially satisfy this inequality, this shows that Λ_κ is the best constant for the Poincaré inequality (A.1) in $H^1(\mathbb{S})$.

The goal is now to reduce the computation of the eigenvalues to simpler problems, using separation of variables. We write $\omega=\cos\theta\,\Omega+\sin\theta\,v$, where v belongs to the unit sphere, orthogonal to Ω. We identify Ω with the last element of an orthogonal basis of $\mathbb{R}^n$, and we write $v\in\mathbb{S}_{n-2}$.

By spherical harmonic decomposition in an adapted basis (see for example Frouvelle and Liu 2012, Appendix A), we have a unique decomposition of the form

$$\psi(\omega)=\sum_{k,m}g^k_m(\theta)Z^k_m(v),\tag{A.8}$$

where $(Z^k_m(v))_{k\in[\![1,k_m]\!]}$ is a given orthonormal basis of the spherical harmonics of degree m on $\mathbb{S}_{n-2}$, for $m\in\mathbb{N}$, with $k_m=\binom{n+m-2}{n-2}-\binom{n+m-4}{n-2}$. If ψ is continuous, g^k_m is given by

$$g^k_m(\theta)=\int_{\mathbb{S}_{n-2}}\psi(\cos\theta\,\Omega+\sin\theta\,v)Z^k_m(v)\,\mathrm{d}v.\tag{A.9}$$

We now show that the decomposition (A.8) remains stable under the action of the operator $L_{\kappa\Omega}$, so that its spectral decomposition can be performed independently for each term of the decomposition.

First, we examine the case of dimension $n \geqslant 3$. Let $\psi(\omega) = g(\theta)Z(v)$. We have

$$\nabla_\omega \psi(\omega) = g'(\theta) e_\theta Z(v) + \frac{g(\theta)}{\sin\theta} \nabla_v Z(v),$$

where the unit vector e_θ is given by

$$e_\theta = \nabla_\omega \theta = -\frac{1}{\sin\theta}(\mathrm{Id} - \omega \otimes \omega)\Omega.$$

We take functions $\psi(\omega) = g_m^k(\theta) Z_m^k(v)$ and $\varphi(\omega) = \sum_{k,m} f_m^k(\theta) Z_m^k(v)$. Since the spherical harmonics are orthonormal, and are eigenfunctions of Δ_v for the eigenvalues $-m(m+n-3)$, we get:

$$\langle \nabla_\omega \psi \cdot \nabla_\omega \varphi \rangle_{M_{\kappa\Omega}} = \int_0^\pi \left[f_m^{k\prime}(\theta) g_m^{k\prime}(\theta) + \frac{m(m+n-3)}{\sin^2\theta} f_m^k(\theta) g_m^k(\theta) \right] \times (\sin\theta)^{n-2} e^{\kappa\cos\theta}\, \mathrm{d}\theta. \tag{A.10}$$

Suppose $m \geqslant 1$. Then, it is easy to see that the function ψ belongs to $\dot{H}^1_\kappa(\mathbb{S})$ if and only if $(\sin\theta)^{\frac{n}{2}-1} g' \in L^2(0,\pi)$ and $(\sin\theta)^{\frac{n}{2}-2} g' \in L^2(0,\pi)$. This condition is equivalent to the fact that $g \in V$, where V is defined by (4.5), and which we denote by V_κ^m for convenience:

$$V_\kappa^m = \left\{ g \,\middle|\, (\sin\theta)^{\frac{n}{2}-2} g \in L^2(0,\pi), (\sin\theta)^{\frac{n}{2}-1} g \in H_0^1(0,\pi) \right\}.$$

Suppose now that $m = 0$. Then Z_m^k is a constant, and the condition $\psi \in \dot{H}^1_\kappa(\mathbb{S})$ is equivalent to the first condition only: $(\sin\theta)^{\frac{n}{2}-1} g' \in L^2(0,\pi)$, under the constraint that $\int_0^\pi (\sin\theta)^{n-2} e^{\kappa\cos\theta} g(\theta)\, \mathrm{d}\theta = 0$. We will denote this space by V_κ^0:

$$V_\kappa^0 = \left\{ g \,\middle|\, (\sin\theta)^{\frac{n}{2}-1} g' \in L^2(0,\pi), \int_0^\pi (\sin\theta)^{n-2} e^{\kappa\cos\theta} g(\theta)\, \mathrm{d}\theta = 0 \right\}.$$

Formula (A.10) then suggests to define the operator $L^*_{\kappa,m} : V_\kappa^m \to (V_\kappa^m)^*$ by

$$\int_0^\pi f(\theta) L^*_{\kappa,m} g(\theta) (\sin\theta)^{n-2} e^{\kappa\cos\theta}\, \mathrm{d}\theta = \int_0^\pi \left[f' g' + \frac{m(m+n-3)}{\sin^2\theta} fg \right] (\sin\theta)^{n-2} e^{\kappa\cos\theta}\, \mathrm{d}\theta. \tag{A.11}$$

From (A.10), it follows that, if we decompose $\psi(\omega) = \sum_{k,m} g_m^k(\theta) Z_m^k(v)$, then

$$L^*_{\kappa\Omega} \psi(\omega) = \sum_{k,m} L^*_{\kappa,m} g_m^k(\theta) Z_m^k(v),$$

showing that $L^*_{\kappa\Omega}$ is block diagonal on each of these spaces V_κ^m (tensorized by the spherical harmonics of degree m on $\mathbb{S}_{n-2}$). So we can perform the spectral decomposition of $L^*_{\kappa\Omega}$ by means of the spectral decomposition of each of the $L^*_{\kappa,m}$. It is

indeed easy to prove, using the Lax-Milgram theorem, that the operators $L^*_{\kappa,m}$ have self-adjoint compact inverses for the dot product $(f,g)=\int_0^\pi fg(\sin\theta)^{n-2}e^{\kappa\cos\theta}\,\mathrm{d}\theta$. Therefore, the eigenfunctions and eigenvalues of $L^*_{\kappa\Omega}$ correspond to those of the operators $L^*_{\kappa,m}$, for all $m\in\mathbb{N}$. If we denote by $\lambda_{\kappa,m}$ the smallest eigenvalue of $L^*_{\kappa,m}$, we finally get

$$\Lambda_\kappa=\min\{\lambda_{\kappa,m},m\in\mathbb{N}\}.$$

We notice that

$$\lambda_{\kappa,m}=\inf\left\{\int_0^\pi f(\theta)L^*_{\kappa,m}f(\theta)(\sin\theta)^{n-2}e^{\kappa\cos\theta}\,\mathrm{d}\theta\;\middle|\;f\in V^m_\kappa,\ \int_0^\pi f^2(\theta)(\sin\theta)^{n-2}e^{\kappa\cos\theta}\,\mathrm{d}\theta=1\right\},$$

but since all the V^m_κ are the same for $m\geqslant 1$, and since

$$\int_0^\pi\frac{1}{\sin^2\theta}f^2(\sin\theta)^{n-2}e^{\kappa\cos\theta}\,\mathrm{d}\theta\geqslant\int_0^\pi f^2(\sin\theta)^{n-2}e^{\kappa\cos\theta}\,\mathrm{d}\theta,$$

we get

$$\lambda_{\kappa,m+1}\geqslant\lambda_{\kappa,m}+(m+1)(m+n-2)-m(m+n-3)=\lambda_{\kappa,m}+2m+n-2.$$

Finally, Λ_κ is the minimum between $\lambda_{\kappa,0}$ and $\lambda_{\kappa,1}$. The eigenfunctions for the operator $L^*_{\kappa\Omega}$ being smooth, this is also true for the operators $L^*_{\kappa,m}$, by formula (A.9). So we can transform the definitions (A.11) by integration by parts.

Indeed, if g_0 is an eigenfunction (in V^0_κ) associated to $L^*_{\kappa,0}$ and an eigenvalue λ, then g_0 is smooth and satisfies the Sturm–Liouville eigenvalue problem

$$L^*_\kappa g_0(\theta)=-(\sin\theta)^{2-n}e^{-\kappa\cos\theta}\big((\sin\theta)^{n-2}e^{\kappa\cos\theta}g'(\theta)\big)'=\lambda g_0(\theta).$$

Conversely, a smooth function with the condition $\int_0^\pi(\sin\theta)^{n-2}e^{\kappa\cos\theta}g(\theta)\,\mathrm{d}\theta=0$ belongs to V^0_κ. Actually, in dimension $n\geqslant 3$, we do not need to impose the Neumann boundary conditions: they appear naturally, since we have

$$L^*_\kappa g_0=-e^{-\kappa\cos\theta}\big(e^{\kappa\cos\theta}g_0'\big)'-\frac{n-2}{\tan\theta}g_0'=\lambda g_0.$$

Therefore, by continuity at $\theta=0$ and π, $g_0'(0)=g_0'(\pi)=0$. Then, using classical Sturm–Liouville oscillation theory (see Weidmann 1987, for example), we find that the first eigenspace of L^*_κ is of dimension 1, spanned by a function $g_{\kappa,0}(\theta)$, which is positive for $0\leqslant\theta<\theta_0$ and negative for $\theta_0<\theta\leqslant\pi$.

Similarly, if g_1 is an eigenfunction (in V^1_κ) associated to $L^*_{\kappa,1}$ and an eigenvalue λ, then g_1 is smooth, with $g_1(0)=g_1(\pi)=0$ and satisfies the Sturm–Liouville eigenvalue problem

$$\widetilde{L}^*_{\kappa,1}g_1(\theta)=L^*_\kappa g_1(\theta)+\frac{n-2}{\sin^2\theta}g_1(\theta)=\lambda g_1(\theta).$$

And conversely, if a function with Dirichlet boundary conditions is in $C^2([0,\pi])$, then it belongs to V^1_κ. Once again, if $n \geqslant 3$, we do not need to impose the Dirichlet boundary conditions in the $C^2([0,\pi])$ framework, since we have

$$L^*_\kappa g_1 = -e^{-\kappa\cos\theta}\left(e^{\kappa\cos\theta} g_1'\right)' - \frac{n-2}{\tan\theta} g_1' + \frac{n-2}{\sin^2\theta} g_1 = \lambda g_1.$$

So, by continuity at $\theta = 0$ and π, $g_1(0) = g_1(\pi) = 0$, and then a first order expansion shows that continuity holds, whatever the values of $g_0'(\theta)$ at the endpoints are. Again, using classical Sturm–Liouville theory, we find that the first eigenspace of L^*_κ is of dimension 1, spanned by a function $g_{\kappa,1}(\theta)$, which keeps the same sign on $(0,\pi)$.

The case $\lambda_{\kappa,0} < \lambda_{\kappa,1}$ corresponds to case (i) of the proposition. Since a spherical harmonic of degree 0 on the sphere $\mathbb{S}_{n-2}$ is a constant, introducing the function h^0_κ such that $h^0_\kappa(\cos\theta) = g_{\kappa,0}(\theta)$ allows us to state that the eigenspace of $L^*_{\kappa\Omega}$ associated to the lowest eigenvalue is spanned by $\omega \mapsto h^0_\kappa(\omega\cdot\Omega)$.

The case $\lambda_{\kappa,0} > \lambda_{\kappa,1}$ corresponds to case (ii) of the proposition. The spherical harmonics of degree 1 on the sphere $\mathbb{S}_{n-2}$ are the functions of the form $v \mapsto A\cdot v$, with $A\cdot\Omega = 0$. Introducing h^0_κ such that $h^0_\kappa(\cos\theta)\sin\theta = g_{\kappa,0}(\theta)$ allows us to state that the eigenspace of $L^*_{\kappa\Omega}$ associated to the lowest eigenvalue is of dimension $n-1$, consisting of the functions of the form $\omega \mapsto h^1_\kappa(\omega\cdot\Omega)A\cdot\omega$, with A any vector in $\mathbb{R}^n$ such that $A\cdot\Omega = 0$.

Finally, the case $\lambda_{\kappa,0} = \lambda_{\kappa,1}$ corresponds to case (iii) of the proposition, and this ends the proof in the case of dimension $n \geqslant 3$.

We now examine the special case of dimension $n = 2$. We identify $H^1(\mathbb{S})$ with the 2π-periodic functions in $H^1_{loc}(\mathbb{R})$. So, Λ_κ is the smallest eigenvalue of the periodic Sturm–Liouville problem

$$L^*_\kappa(g) = \widetilde{L}^*_\kappa(g) = -e^{-\kappa\cos\theta}\left(e^{\kappa\cos\theta} g'\right)' = \lambda g,$$

for functions g such that $\int_{-\pi}^{\pi} e^{\kappa\cos\theta} g(\theta)\,\mathrm{d}\theta = 0$. Here the decomposition corresponding to (A.8) is the even-odd decomposition (there are only two spherical harmonics on $\mathbb{S}_0$: the constant function of degree 0 and the odd function of degree 1). The odd part g_o of g can be identified with a function of $H^1_0(0,\pi)$, and it is easy to see that the odd part of $L^*_\kappa(g)$ is $L^*_\kappa(g_o)$, and similarly for the even part g_e. So, we can perform the spectral decomposition of L^*_κ separately on the spaces of even and odd functions.

Actually, if g is a solution of the Sturm–Liouville periodic problem, the function $\widetilde{g}$ defined by $\widetilde{g}(\theta) = e^{-\kappa\cos\theta}\partial_\theta g(\pi-\theta)$ is another solution with the same eigenvalue. Furthermore, if g is odd, then $\widetilde{g}$ is even and conversely. So the eigenvalues are the same for the odd and even spaces problems. Therefore, in dimension $n = 2$, Proposition A.1 can be refined, and we can state that case (iii) is the only possibility: the eigenspace of $L^*_{\kappa\Omega}$ associated to Λ_κ is of dimension 2, spanned by an odd function g^o_κ, positive on $(0,\pi)$, and an even function $g^e_\kappa = \widetilde{g}^o_\kappa$, positive for $0 < \theta < \theta_0$ and negative for $\theta_0 < \theta < \pi$. The proof of Proposition A.1 is complete. □

We can now state a conjecture, which refines Proposition A.1, if true, and which is based on numerical experiments.

Conjecture A.1

(i) *When* $\kappa > 0$ *and* $n \geqslant 3$, *only statement* (ii) *of Proposition A.1 is true.*
(ii) *The function* $\kappa \mapsto \Lambda_\kappa$ *is increasing.*

We also observe numerically that $\lambda_1 \sim \kappa$ when kappa is large.

Some investigations are in progress to prove the monotonicity of the eigenvalue with respect to κ, based on formal expansions similar to those used in Sect. 5 of Frouvelle (2012).

Remark A.1 At the end of the proof of Proposition A.1, we have seen that in dimension $n = 2$ only statement (iii) is true. The proof uses a transformation of the solution of an eigenvalue problem into the solution of another eigenvalue problem. We can try to find a similar transformation in dimensions $n \geqslant 3$: if f satisfies $L_{\kappa,0} f = \lambda f$ (with Neumann boundary conditions), then $\widetilde{f} = e^{-\kappa\cos\theta}\partial_\theta f(\pi - \theta)$ (with Dirichlet boundary conditions) satisfies

$$\int_0^\pi \widetilde{f} L_1 \widetilde{f} (\sin\theta)^{n-2} e^{\kappa\cos\theta}\,\mathrm{d}\theta = \lambda \int_0^\pi \widetilde{f}^2 (\sin\theta)^{n-2} e^{\kappa\cos\theta}\,\mathrm{d}\theta - \kappa(n-2)\int_0^\pi \cos\theta\, \widetilde{f}^2 (\sin\theta)^{n-2} e^{\kappa\cos\theta}\,\mathrm{d}\theta,$$

so if we can prove that $\int_0^\pi \cos\theta\, \widetilde{f}^2 (\sin\theta)^{n-2} e^{\kappa\cos\theta}\,\mathrm{d}\theta > 0$, we can deduce that $\lambda_0 > \lambda_1$. So far we have been unable to prove this estimate.

Appendix B: Numerical Computations of the Coefficients

We adopt a finite difference approach to compute the function g_κ associated to the GCIs and defined by (4.6). We consider the function f_κ such that $f_\kappa(\theta) = (\sin\theta)^{\frac{n}{2}-1} g_\kappa(\theta)$. In particular, since $g_\kappa \in V$ defined by (4.5), f_κ belongs to $H_0^1(0,\pi)$. Since g_κ satisfies (4.6), f_κ satisfies

$$-e^{-\kappa\cos\theta}\left(e^{\kappa\cos\theta} f_\kappa'\right)' + \left(\frac{n-2}{2\sin^2\theta}\left(1 + \frac{n-2}{2}\cos^2\theta\right) - \kappa\cos\theta\right) f_\kappa = \sin^{\frac{n}{2}}\theta.$$

We discretize the interval $(0,\pi)$ with $N+1$ points $\theta_i = \frac{1}{N} i\pi$, and denote by f_κ^i an approximation of f_κ at these points. Since $f_\kappa \in H_0^1(0,\pi)$, we have $f_\kappa^0 = f_\kappa^N = 0$. We define $e_\kappa^i = e^{\kappa\cos\theta_i}$. A second order approximation of $(e^{\kappa\cos\theta} f_\kappa')'$ at θ_i is then given by

$$\left(e^{\kappa\cos\theta} f_\kappa'\right)'(\theta_i) \approx \frac{N^2}{\pi^2}\left(e_\kappa^{i+\frac{1}{2}}\left(f_\kappa^{i+1} - f_\kappa^i\right) - e_\kappa^{i-\frac{1}{2}}\left(f_\kappa^i - f_\kappa^{i-1}\right)\right).$$

Introducing

$$d_\kappa^i = \frac{n-2}{2\sin^2\theta_i}\left(1 + \frac{n-2}{2}\cos^2\theta_i\right) - \kappa\cos\theta_i + \frac{N^2}{\pi^2}\frac{e_\kappa^{i-\frac{1}{2}} + e_\kappa^{i+\frac{1}{2}}}{e_k^i},$$

$$b_\kappa^i = -\frac{N^2}{\pi^2}\frac{e_\kappa^{i+\frac{1}{2}}}{e_k^i}, \quad \text{and} \quad \widetilde{b}_\kappa^i = -\frac{N^2}{\pi^2}\frac{e_\kappa^{i-\frac{1}{2}}}{e_k^i},$$

the vector $F = (f_\kappa^i)_{i\in[\![1,N-1]\!]}$ is the solution of the linear system $AF = S$, where the vector S is $(\sin^{\frac{n}{2}}\theta_i)_{i\in[\![1,N-1]\!]}$, and the tridiagonal matrix A is defined by

$$A = \begin{pmatrix} d_\kappa^1 & b_\kappa^1 & 0 & \cdots & \cdots & 0 \\ \widetilde{b}_\kappa^2 & d_\kappa^2 & b_\kappa^2 & \ddots & & \vdots \\ 0 & \widetilde{b}_\kappa^3 & d_\kappa^3 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & b_\kappa^{N-3} & 0 \\ \vdots & & \ddots & \widetilde{b}_\kappa^{N-2} & d_\kappa^{N-2} & b_\kappa^{N-2} \\ 0 & \cdots & \cdots & 0 & \widetilde{b}_\kappa^{N-1} & d_\kappa^{N-1} \end{pmatrix}. \tag{B.1}$$

We use the trapezoidal method to perform the integrations in the definitions (2.11) and (4.9) of c and $\widetilde{c}$. The other coefficients ρ, λ, and θ_c are then directly computed from c and $\widetilde{c}$. The numerical results provided in Figs. 3 and 4 have been obtained for $N = 3000$.

We now detail how we obtain an approximation of the Poincaré constant Λ_κ. By Appendix A, Λ_κ is the minimum between $\lambda_{\kappa,1}$ and $\lambda_{\kappa,0}$, which are the smallest eigenvalues of two Sturm–Liouville problems. Several algorithms exist to compute eigenvalues of singular Sturm–Liouville problems (which is the case here whenever $n \geqslant 3$) with a good precision (Bailey et al. 1991). However, we use a simpler method based on finite differences.

Actually, $\lambda_{\kappa,1}$ is the smallest eigenvalue associated to problem (A.5), with $g \in V$. So, considering once again the function f such that $f(\theta) = (\sin\theta)^{\frac{n}{2}-1}g(\theta)$, the vector AF, with A defined by (B.1), gives a second order approximation of $(\sin\theta)^{\frac{n}{2}-1}\widetilde{L}_\kappa^* g(\theta) = \lambda f(\theta)$ at the points θ_i. So we can take the smallest eigenvalue of A as an approximation of $\lambda_{\kappa,1}$.

We now look for an approximation of $\lambda_{\kappa,0}$.

Let g be a solution of the Sturm–Liouville problem (A.4) with Neumann boundary conditions. We introduce $G = (g_{i+\frac{1}{2}})_{i\in[\![0,N-1]\!]}$, the vector of approximations of g at the points $\theta_{i+\frac{1}{2}} = \frac{1}{N}(i+\frac{1}{2})\pi$. Introducing $m_\kappa^i = (\sin\theta)^{n-2}e^{\kappa\cos\theta_i}$, a second order approximation of $L_\kappa^* g$ at the point $\theta_{i+\frac{1}{2}}$, with $i \in [\![1, N-2]\!]$, is then given by

$$L_\kappa^* g(\theta_{i+\frac{1}{2}}) \approx \frac{N^2}{\pi^2 m_\kappa^{i+\frac{1}{2}}}\left(-m_\kappa^{i+1}\left(f_\kappa^{i+\frac{3}{2}} - f_\kappa^{i+\frac{1}{2}}\right) + m_\kappa^i\left(f_\kappa^{i+\frac{1}{2}} - f_\kappa^{i-\frac{1}{2}}\right)\right).$$

With the Neumann boundary conditions, the approximations at the points $\theta_{\frac{1}{2}}$ and $\theta_{N-\frac{1}{2}}$ are given by

$$L_\kappa^* g(\theta_{\frac{1}{2}}) \approx \frac{N^2}{\pi^2 m_\kappa^{\frac{1}{2}}} m_\kappa^1\left(f_\kappa^{\frac{3}{2}} - f_\kappa^{\frac{1}{2}}\right),$$

$$L_\kappa^* g(\theta_{N-\frac{1}{2}}) \approx -\frac{N^2}{\pi^2 m_\kappa^{N-\frac{1}{2}}} m_\kappa^{N-1}\big(f_\kappa^{N-\frac{1}{2}} - f_\kappa^{N-\frac{3}{2}}\big).$$

Introducing

$$d_\kappa^{i+\frac{1}{2}} = \frac{N^2}{\pi^2}\frac{m_\kappa^{i+1} + m_\kappa^i}{m_k^{i+\frac{1}{2}}},$$

$$b_\kappa^{i+\frac{1}{2}} = -\frac{N^2}{\pi^2}\frac{m_\kappa^{i+1}}{m_k^{i+\frac{1}{2}}}, \quad \text{and} \quad \widetilde{b}_\kappa^{i+\frac{1}{2}} = -\frac{N^2}{\pi^2}\frac{m_\kappa^i}{m_k^{i-\frac{1}{2}}},$$

a second order approximation of $L_\kappa^* g$ is given by BG, where the tridiagonal matrix B is defined by

$$B = \begin{pmatrix} -b_\kappa^{\frac{1}{2}} & b_\kappa^{\frac{1}{2}} & 0 & \cdots & \cdots & 0 \\ \widetilde{b}_\kappa^{\frac{3}{2}} & d_\kappa^{\frac{3}{2}} & b_\kappa^{\frac{3}{2}} & \ddots & & \vdots \\ 0 & \widetilde{b}_\kappa^{\frac{5}{2}} & d_\kappa^{\frac{5}{2}} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & b_\kappa^{N-\frac{5}{2}} & 0 \\ \vdots & & \ddots & \widetilde{b}_\kappa^{N-\frac{3}{2}} & d_\kappa^{N-\frac{3}{2}} & b_\kappa^{N-\frac{3}{2}} \\ 0 & \cdots & \cdots & 0 & \widetilde{b}_\kappa^{N-\frac{1}{2}} & -\widetilde{b}_\kappa^{N-\frac{1}{2}} \end{pmatrix}. \tag{B.2}$$

So we can take the smallest positive eigenvalue of B as an approximation of $\lambda_{\kappa,0}$ (excluding the constant functions). The computations of Fig. 1 have been performed with $N = 300$ points.

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