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Résumé

Cette thèse est consacrée à l'étude, à différentes échelles, de modèles cinétiques de particules en interaction, dont le vecteur vitesse est contraint à rester sur la sphère unité $\mathbb{S}$ de $\mathbb{R}^n$. Ces modèles interviennent dans la description du comportement d'individus dans des sociétés animales telles que des bancs de poissons ou des nuées d'oiseaux. En particulier, nous nous intéressons à des modèles avec une interaction d'alignement, comme le modèle de Vicsek [74] : les particules se déplacent à vitesse constante et modifient simultanément leur orientation en fonction de l'orientation moyenne des particules voisines.

Dans une première partie, nous commençons par étudier l'influence de deux modifications dans la version continue en temps du modèle de Vicsek proposée par P. Degond et S. Motsch dans [28], où un modèle macroscopique est obtenu, lorsque le système est observé à grande échelle en temps et en espace. En permettant aux paramètres du modèle individuel de dépendre de la densité locale de particules, et en introduisant de l'anisotropie dans les noyaux d'observation (cela peut modéliser un angle de vision restreint), nous montrons que le modèle macroscopique garde la même forme : une équation de conservation de la densité $\rho > 0$ de particules, et une équation non conservative pour leur orientation moyenne $\Omega \in \mathbb{S}$, données par

$$\partial_t \rho + \nabla_x \cdot (c_1 \rho \Omega) = 0. \tag{1}$$

$$\rho \, (\partial_t \Omega + c_2 (\Omega \cdot \nabla_x) \Omega) + \lambda \, (\mathrm{Id} - \Omega \otimes \Omega) \nabla_x \rho = 0. \tag{2}$$

La seule différence réside dans le fait que les coefficients du modèle ainsi obtenu dépendent de la densité, et nous montrons que cela peut entraîner la perte de l'hyperbolicité dans certains régimes. Nous établissons une méthode permettant de calculer un développement asymptotique, à tout ordre, des coefficients du modèle lorsque le paramètre de concentration tends vers 0 ou vers l'infini.

Nous étudions également une autre modification du modèle individuel, dans laquelle le taux de relaxation vers la direction moyenne des particules voisines est proportionnel à leur quantité de mouvement. Nous montrons qu'à grande échelle, ce modèle présente un phénomène de transition de phase lorsque la densité traverse un seuil, et nous dérivons un modèle macroscopique dans chacun des deux régimes. Nous obtenons un modèle de type diffusion dans la région de faible densité, où la distribution des vitesses des particules est isotrope. Quand la densité ρ est au dessus du seuil, la limite macroscopique est constituée du même système (1)-(2) d'équations aux dérivées partielles. Les développements asymptotiques des coefficients quand la densité est grande ou proche du seuil permettent de montrer que le système n'est pas hyperbolique dans ces régimes.

Finalement, nous introduisons un modèle, inspiré de la version continue en temps du modèle de Vicsek, où les particules se déplacent sur une variété Riemannienne générale (dans la plupart des simulations du modèle de Vicsek original, cela correspond au tore plat). Nous montrons que le système est bien défini, et qu'il possède la propriété de propagation du chaos, ce qui nous permet de dériver une limite de type champ moyen dans la limite d'un grand nombre de particules. Dans le cas de la sphère unité usuelle $\mathbb{S}_2$, nous effectuons des simulations numériques du système de particules obtenu.

Dans une seconde partie, nous analysons la dynamique de la version homogène en espace du modèle avec transition de phase introduit dans la première partie. Nous obtenons une équation de Fokker–Planck non linéaire, qui est en fait appelée équation de Doi [32] avec potentiel dipolaire. Cette équation apparaît dans l'étude de suspensions de polymères en forme de bâtonnets (elle peut être vue comme un flot-gradient de la fonctionnelle d'énergie libre d'Onsager [65]), et est habituellement étudiée avec le potentiel dit « de Maier–Saupe ». Nous montrons que le système est bien posé pour une condition initiale dans n'importe quel espace de Sobolev, et décrivons les solutions stationnaires en toute dimension. Nous obtenons l'existence d'un seuil pour l'intensité du bruit au-delà duquel l'unique équilibre est la distribution uniforme. En deçà de ce seuil, on obtient une variété d'équilibres indexés par une orientation $\Omega \in \mathbb{S}$. Nous montrons que toute solution converge dans tout espace de Sobolev vers un unique équilibre, et nous caractérisons les conditions initiales pour lesquelles la solution converge vers la distribution uniforme. Pour le cas sous-critique, nous construisons une nouvelle fonctionnelle d'entropie, à l'aide de décomposition en harmoniques sphériques, et cela nous donne un taux global exponentiel de convergence vers l'équilibre uniforme. Dans le cas surcritique, nous pouvons obtenir un taux local exponentiel de convergence vers l'équilibre, et dans le cas critique, nous prouvons que la convergence vers la distribution uniforme est algébrique en temps. Finalement, nous montrons que les outils que nous avons utilisés peuvent être appliqués à l'équation de Doi avec le potentiel de Maier–Saupe, et nous donnons des résultats de convergence vers un état stationnaire pour toute condition initiale en dimension 2.

Abstract

This thesis is devoted to the study, at different scales, of kinetic models of interacting particles whose velocity is constrained to stay on the unit sphere $\mathbb{S}$ of $\mathbb{R}^n$. These models aim to describe the behavior of individuals inside animal societies such as fish schools or flocks of birds. In particular, we are interested in models with alignment interaction, such as the Vicsek model [74]: particles move with constant speed and synchronously update their direction according to the mean orientation of their neighbors.

In a first part, we start by investigating the influence of two modifications in the time-continuous version of the Vicsek model proposed by P. Degond and S. Motsch in [28], where a macroscopic model is derived when the system is observed at large scale in time and space. Letting the parameters of the individual model depend on the local density, and introducing anisotropy in the observation kernels (this can model a restricted angle of vision), we prove that the macroscopic model has the same form: a conservative equation for the density $\rho > 0$, and a non-conservative equation for the mean orientation $\Omega \in \mathbb{S}$, given by

$$\partial_t \rho + \nabla_x \cdot (c_1 \rho \Omega) = 0. \tag{3}$$

$$\rho \, (\partial_t \Omega + c_2 (\Omega \cdot \nabla_x) \Omega) + \lambda \, (\mathrm{Id} - \Omega \otimes \Omega) \nabla_x \rho = 0. \tag{4}$$

The only difference is that the coefficients of the model depend on the density, and we show that this can lead to the loss of hyperbolicity in certain regimes. We provide a method to compute the expansion, up to any order, of the coefficients of the model when the concentration parameter goes to 0 or to ∞.

We also study another modification of the individual model, where the rate of relaxation towards the mean direction of the neighbors is proportional to their local momentum. We prove that, at large scale, this model presents a phenomenon of phase transition when the density goes across a threshold, and we derive a macroscopic model in each of the two regimes. We obtain a diffusive type model in the region of low density, where the distribution of the velocities of the particles is isotropic. When the density ρ is above the threshold, the macroscopic limit consists in the same system (3)-(4) of partial differential equations. Using the asymptotic expansions of the coefficients when the density is large or close to the threshold, we can prove that the system is not hyperbolic in these regimes.

We finally introduce a model inspired by the time-continuous version of the Vicsek model, where the positions of the particles live on a Riemannian manifold (instead of the flat torus which is the framework of most of the simulations of the Vicsek model). We prove its consistence, we show that it satisfies the propagation of chaos property, which allows to derive a mean-field limit as the number of particles goes to ∞. In the case of the 2-dimensional unit sphere $\mathbb{S}_2$, we perform some numerical simulations.

In a second part, we analyze the dynamics of the space homogeneous version of the model with phase transition introduced in the first part. We obtain a non-linear Fokker–Planck equation, actually called the Doi equation [32] with dipolar potential. This equation arises in the study of suspensions of rod-like polymers (as a gradient flow of the Onsager free energy functional [65]), and is usually studied with the so-called Maier–Saupe potential. We prove the

well-posedness of this system for an initial condition in any Sobolev space, and describe the steady-states in any dimension. We get that there is a threshold for the noise intensity over which the only equilibrium is the uniform distribution. Under this threshold, there is a manifold of equilibria indexed by an orientation $\Omega \in \mathbb{S}$. We prove that any solution converges in any Sobolev space to a unique equilibrium, and characterize the initial conditions leading to the uniform distribution. For the subcritical case, we construct a new entropy by a decomposition in spherical harmonics, which gives a global exponential rate of convergence to the uniform distribution. In the supercritical case, we are able to give a local exponential rate of convergence to the equilibrium, and in the critical case, we prove that the convergence to the uniform distribution is algebraic in time.

We finally show that the tools we used in the case of the dipolar potential can be applied to the Doi equation with Maier–Saupe potential, and give results of convergence to a steady-state for any initial condition in dimension 2.

Contents

Introduction générale

1 Motivation

Nous nous intéressons à l'étude de divers modèles de comportement collectif dans des systèmes comportant un grand nombre de particules, par exemple des modèles de déplacements de poissons à l'intérieur d'un banc, ou d'oiseaux dans une nuée. Ces modèles ont récemment donné lieu à de nombreuses questions, très stimulantes d'un point de vue mathématique [10]. Une des questions récurrentes sur ce sujet est la compréhension de la manière dont les comportements collectifs voient le jour sans meneur, par exemple à l'aide seulement d'interactions locales. De tels phénomènes sont courant dans la nature, on peut observer par exemple un alignement global des poissons dans un banc, ou la formation de structures et de motifs cohérents dans des nuées d'oiseaux, même si les individus semblent n'interagir qu'avec un nombre réduit de voisins.

Un modèle de déplacement très en vogue, proposé par Vicsek *et al.* [74], a été l'objet de beaucoup d'attention, au vu de sa capacité à reproduire ces phénomènes complexes et de son minimalisme. La règle d'interaction minimale était en fait déjà présente dans d'autres modèles [3, 67, 49, 23], appelés « modèles à trois zones », qui incluent de l'attraction à grande distance et de la répulsion à courte distance. Ces modèles ont pour but de décrire de façon réaliste le comportement d'animaux, tandis que le modèle de Vicsek se focalise sur les propriétés essentielles de l'interaction d'alignement, sans prétendre être aussi réaliste. Le modèle revient à considérer des particules se déplaçant à vitesse constante, et changeant simultanément leur orientation pour prendre (à un bruit angulaire près) l'orientation moyenne des particules voisines. Pour contourner le problème de confinement qui se pose alors, à la place d'introduire de l'attraction à grande distance par exemple, le modèle impose une condition de périodicité spatiale. D'un point de vue plus géométrique, la dynamique des particules a lieu sur le tore plat.

Dans ce cadre, un grand nombre de simulations de ce modèle et de variantes ont été effectués [46, 16, 62], qui montrent des phénomènes remarquables. La première chose que l'on observe est que, lorsque le bruit diminue, le système, dans son comportement global, est le siège d'un phénomène de transition de phase : quand le bruit est fort, les particules semblent se déplacer de façon aléatoire dans un état ambiant désordonné, et lorsque le bruit est faible, on peut observer la formation de structures cohérentes, et de fortes corrélations entre les orientations des particules. De nombreuses discussions se sont portées sur le fait de savoir si cette transition de phase est continue ou discontinue, la conclusion est que le nombre de particules dans

la simulation du modèle a une influence forte sur ce qui est observé, et la transition de phase devient nette lorsque le nombre de particules est important.

La seconde chose que l'on remarque est l'émergence, au bout d'un temps suffisamment long, de motifs cohérents. On peut observer des bandes à haute densité dans lesquelles le paramètre d'ordre est élevé, qui se déplacent dans une région désordonnée de faible densité. La direction de propagation de ces bandes est également reliée à la géométrie du domaine : les bandes se déplacent dans une direction de périodicité, et choisissent une direction avec plus de probabilité qu'une autre suivant la période spatiale du domaine dans ces directions.

À partir de là, trois axes d'études nous apparaissent importants d'un point de vue mathématique : premièrement, comprendre le comportement du système dans la limite d'un grand nombre de particules (dans le but d'une description mathématique du phénomène de transition de phase), deuxièmement, tenter d'expliquer, dans la limite d'un temps d'observation long, l'émergence de structures cohérentes et les lois qui les régissent, et finalement étudier le rôle joué par la géométrie de ces structures et du domaine.

L'étude mathématique de ce modèle, dans l'optique de ces trois axes, a été le point de départ du travail présenté ici, et poursuit le travail de Degond et Motsch [28].

2 Aperçu du sujet

Pour attaquer le problème de la description du comportement d'un système de particules lorsque le nombre de particules tend vers l'infini, la stratégie est de considérer la densité de probabilité de trouver une particule dans une position donnée, avec une vitesse donnée. La description cinétique du système limite est alors faite à travers la détermination de l'évolution temporelle de cette densité de probabilité. En général, cette évolution est donnée par une équation aux dérivées partielles, et c'est là qu'arrive le premier problème lorsqu'on cherche à étudier la limite du modèle de Vicsek quand le nombre de particules est grand. En effet, nous n'avons pas de description continue en temps du comportement des particules, les particules changeant seulement leur orientation de façon synchrone et régulière. C'est une des objections que l'on peut former à propos du modèle de Vicsek : même si, spatialement, il n'y a pas de meneur pour la dynamique, les interactions étant localisées en espace, ces dernières ne sont pas indépendantes en temps, il y a une synchronisation globale à travers une horloge qui donne des pas de temps réguliers. Deux approches peuvent permettre de contourner ce problème, tout en restant dans l'esprit du modèle minimal de Vicsek.

La première a été proposée par Pierre Degond et Sébastien Motsch dans l'article [28], l'idée est de remplacer le comportement discret en temps par une relaxation continue vers l'orientation des particules voisines. Au coût de l'ajout d'un nouveau paramètre ν (en fait, ce paramètre remplace le pas de temps qui est effectivement un paramètre du modèle original, et non un pas de temps de discrétisation), pouvant être vu comme une fréquence de relaxation vers l'orientation moyenne locale, ils ont pu dériver formellement un modèle cinétique de champ moyen, sous la forme d'une équation de type Fokker–Planck sur la densité de probabilité f des particules :

$$\partial_t f + \omega \cdot \nabla_x f + \nu \nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega) \bar{\Omega}_f \, f) = d \Delta_\omega f, \tag{2.1}$$

où la fonction f dépend du temps $t \geqslant 0$ et des variables d'espace $x \in \mathbb{R}^3$ et de vitesse $\omega \in S_2$. Le paramètre d représente l'intensité du bruit, et le vecteur $\bar{\Omega}_f \in \mathbb{S}_2$ désigne une direction cible, calculée à partir de f (de manière non locale), au point x. Enfin, $\nabla_\omega \cdot$ et Δ_ω sont les opérateurs de divergence et de Laplace–Beltrami sur la sphère, et la matrice $\mathrm{Id} - \omega \otimes \omega$ est la projection sur le plan orthogonal à ω. Cette méthode est le point de départ de la majeure partie de ce rapport.

Une autre approche pour régler ce problème de synchronisation globale est de donner à chaque particule une horloge propre pour son changement d'orientation, sous la forme d'un processus de Poisson de fréquence donnée ν (nous avons donc besoin également d'introduire un nouveau paramètre de fréquence), les horloges étant toutes indépendantes, ce qui permet de voir le modèle comme un processus de sauts. Un travail sur ce sujet a été entrepris avec Emmanuel Boissard et Sébastien Motsch lors d'une visite à l'Université du Maryland, mais n'est pas assez abouti pour prendre place dans ce rapport. Une remarque à faire sur cette approche est qu'elle peut permettre de définir un modèle de type Vicsek qui se situe dans un cadre unidimensionnel, et cela a été récemment proposé comme un modèle de déplacement d'essaims de criquets dans [34].

Le problème de trouver alors une description macroscopique du modèle continu en temps, lorsque l'on observe à une grande échelle temporelle, a également été traité dans le même article [28] par Pierre Degond et Sébastien Motsch. Nous résumons ici leurs résultats.

Une fois que l'équation cinétique (2.1) est obtenue (au moins formellement), ils s'agit toujours d'une description à petite échelle en temps et en espace, et nous ne pouvons donc pas observer les structures macroscopiques. L'idée est de faire un changement d'échelle en temps et en espace, appelé changement d'échelle hydrodynamique, à travers l'introduction d'un petit paramètre ε et l'étude des propriétés du modèle lorsque $\varepsilon \to 0$. Ce changement d'échelle a pour effet de rendre l'interaction locale en espace, et lorsque $\varepsilon \to 0$, la densité de probabilité f^ε est contrainte d'être un équilibre pour un certain opérateur Q, dans une variété de dimension 3 paramétrée par la densité locale de masse ρ et une orientation Ω appartenant à la sphère unité de $\mathbb{R}^3$ (la dynamique des particules ayant lieu dans $\mathbb{R}^3$) : les équilibres sont des la forme $\rho M_{\kappa\Omega}$, où $M_{\kappa\Omega}$ est la distribution de Von-Mises d'orientation Ω et de paramètre de concentration $\kappa = \frac{\nu}{d}$. Même si le bruit est grand, l'orientation de l'équilibre est bien définie, et on n'observe pas de phénomène de transition de phase avec cette limite hydrodynamique, contrairement aux observations dans les simulations de modèle de Vicsek.

L'étape suivante consiste à dériver les équations d'évolution pour la masse ρ et la direction Ω. La conservation de la masse donne une première équation, mais il n'y a pas d'autre relation de conservation évidente pour obtenir d'autre équation, et l'objet principal de [28] est d'introduire la notion d'invariants de collision généralisés qui permet d'obtenir l'équation d'évolution de Ω. Le modèle obtenu est le système non conservatif d'équations aux dérivées partielles du premier ordre suivant :

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (c_1 \rho \Omega) = 0. \\ \rho \left(\partial_t \Omega + c_2 (\Omega \cdot \nabla_x) \Omega \right) + \lambda \left(\mathrm{Id} - \Omega \otimes \Omega \right) \nabla_x \rho = 0. \end{cases} \tag{2.2}$$

où les coefficients c_1, c_2 et λ satisfont $0 < c_2 < c_1 < 1$ et $\lambda > 0$. Ce système est

hyperbolique. À notre connaissance, il s'agit du premier modèle qui a cette forme non conservative, dans le contexte de limites macroscopiques de systèmes constitués d'un grand nombre de particules en interaction. Ceci provient de la particularité de la contrainte de vitesse unité pour les particules, qui peut être naturelle dans la modélisation de phénomènes biologiques tels que des déplacements d'animaux, et qui a bien moins de sens lorsque l'on modélise les dynamiques microscopiques de gaz dilués, qui sont à la source de toute cette théorie cinétique.

Enfin, concernant le troisième axe de cette étude, c'est-à-dire l'analyse du rôle joué par la géométrie du domaine, il y a peu d'analyse mathématique rigoureuse à ce sujet, à notre connaissance. Les observations [16, 62] mettant en évidence des bandes se déplaçant, fortement ordonnées, sont toujours faites dans le cas du tore plat (conditions aux limites périodiques), et montrent que le mouvement a plutôt tendance à se faire le long de géodésiques de longueur minimale. Nous n'avons pas connaissance d'études sur une généralisation du modèle à d'autres configurations géométriques, comme la sphère unité (on pourrait par exemple décrire des individus se déplaçant à la surface de la Terre).

La première partie de ce rapport concerne la poursuite de l'étude de ces modèles de Vicsek continus en temps (nous nous plaçons également cette fois-ci en dimension $n \geqslant 2$ quelconque, et pas seulement dans le cas $n = 3$). En particulier, puisque le paramètre ν de relaxation a été introduite arbitrairement dans le modèle (un tel paramètre étant nécessaire pour définir proprement une relaxation), nous sommes libres de lui donner une forme plus générale. Dans l'article original [28], ce paramètre pouvait dépendre de l'angle entre la vitesse de la particule et sa direction cible. Dans le chapitre 1, nous laissons ν dépendre également d'une densité moyenne locale $\bar{\rho}$ et nous introduisons de l'anisotropie dans le noyau d'observation, c'est-à-dire que la façon dont chaque particule calcule sa direction cible par rapport aux particules voisines peut dépendre de son orientation. Ceci permet de modéliser par exemple un angle de vision restreint pour les individus, ou le fait que dans certaines espèces, les individus prennent plus en compte ceux situés en arrière, de façon à éviter de se faire manger (ces interactions sont appelées interactions de cannibalisme et observées dans [8] pour une espèce de criquets). Dans le chapitre 2, nous prenons ν proportionnel à la norme de la quantité de mouvement moyenne des voisins. Cela revient à dire que les individus ont tendance à s'orienter plus rapidement dans la direction moyenne de leurs voisins si ces derniers sont nombreux et fortement alignés. Cette rétroaction positive sur l'alignement entraîne l'apparition d'une transition de phase, et on retrouve les propriétés du modèle discret original, ce qui donne lieu à des questions très stimulantes. Enfin, l'objet principal du chapitre 3 est l'introduction d'une généralisation de modèle de Vicsek continu en temps lorsque les particules sont contraintes à se déplacer sur une variété Riemannienne, avec des simulations numériques dans le cas de la sphère unité bidimensionnelle. Ce modèle généralisé inclut le modèle de [28] et celui du chapitre 2, lorsque la variété est $\mathbb{R}^n$. Les détails et nos principales contributions à l'étude de ces généralisations du modèle de Vicsek continu en temps sont donnés dans la prochaine partie de cette introduction.

Le modèle introduit au chapitre 2 nous a mené à l'étude de sa version homogène en espace, sur la sphère unité $\mathbb{S}$ de $\mathbb{R}^n$, qui présente la même propriété de transition de phase. Lors de l'étude de ce problème, nous avons remarqué qu'il s'agissait d'un

cas particulier d'une classe plus large de modèles décrits par l'équation de Doi (aussi appelée équation de Smoluchowski), une équation non linéaire et non locale de la forme suivante :

$$\begin{cases} \partial_t f = \nabla_\omega \cdot (f \nabla \Psi_f) + \tau \Delta_\omega f, \\ \Psi_f(\omega, t) = \int_{\mathbb{S}} K(\omega, \bar{\omega})\, f(t, \bar{\omega})\, \mathrm{d}\bar{\omega}. \end{cases} \tag{2.3}$$

Cette équation a été introduite par Doi [32] comme un flot gradient pour la fonctionnelle d'énergie libre de Onsager :

$$\mathcal{F}(f) = \tau \int_{\mathbb{S}} f(.,\omega) \ln f(.,\omega) \mathrm{d}\omega + \tfrac{1}{2} \int_{\mathbb{S}\times\mathbb{S}} K(\omega,\bar{\omega}) f(.,\omega)\, f(.,\bar{\omega})\, \mathrm{d}\omega \mathrm{d}\bar{\omega}. \tag{2.4}$$

Cette fonctionnelle a été proposée par Onsager [65] pour décrire les états d'équilibre de suspensions de polymères en forme de bâtonnets, donnés par les points critiques de cette fonctionnelle. Dans le travail original de Onsager, le noyau était de la forme $K(\omega, \bar{\omega}) = |\omega \times \bar{\omega}|$, mais il existe une autre forme plus simple, introduite plus tard par Maier et Saupe [58], qui mène à des résultats similaires : $K(\omega, \bar{\omega}) = \frac{1}{n} - (\omega \cdot \bar{\omega})^2$. En particulier, on observe un phénomène d'hystérésis lorsque le paramètre τ, qui représente une température, varie en allant de grandes valeurs vers des petites puis retournant à des valeurs élevées.

Le modèle qui nous intéresse corresponds au cas où $K(\omega, \bar{\omega}) = -\omega \cdot \bar{\omega}$, appelé potentiel dipolaire, et peu d'études ont été faites concernant ce modèle seul. L'étude de ce modèle est l'objet du chapitre 2, motivée par une compréhension plus fine du modèle spatialement inhomogène, et nous a menés à l'étude de l'équation de Doi avec potentiel de Maier–Saupe, qui a récemment fait l'objet de nombreuses recherches du point de vue d'une rigoureuse analyse mathématique.

Nous présentons ici ce qui a été fait précédemment à propos de l'étude mathématique de cette équation.

La caractérisation des équilibres a commencé en 2004 en dimension $n = 2$ pour le potentiel de Maier–Saupe avec l'article [20] contenant un résultat partiel, qui a été ensuite complété par trois groupes indépendants [22, 38, 57] (de plus, une famille plus générale de noyaux est traitée dans [38], incluant le potentiel dipolaire, toujours en dimension $n = 2$). Dans le cas où la température τ est inférieure à $\frac{1}{4}$, la distribution uniforme est le seul état stationnaire, et quand $\tau < \frac{1}{4}$, il y a aussi une autre famille d'équilibres, qui sont non isotropiques, symétriques, et diffèrent l'un de l'autre par une simple rotation (ils sont appelés équilibres nématiques).

Le cas de la dimension 3 est un peu plus élaboré, puisque l'on a besoin tout d'abord de montrer que tout état stationnaire est axisymétrique. Après le résultat partiel [20], la caractérisation complète a été donnée en 2005, indépendamment dans [37, 55, 88]. On peut observer un phénomène fascinant d'hystérésis avec deux seuils pour la température : $\tau_c = \frac{2}{15}$ et $\tau^* > \tau_c$. Lorsque $\tau > \tau^*$, la distribution uniforme est l'unique état stationnaire ; lorsque τ est compris entre $\frac{2}{15}$ et τ^*, deux autres familles d'équilibres prolates (concentrés aux alentours de deux points antipodaux) voient le jour ; enfin lorsque $\tau > \frac{2}{15}$, une de ces familles se transforme en des équilibres oblates (concentrés autour d'un grand cercle). En analysant la stabilité au sens d'une minimisation locale de l'énergie libre de Onsager, cette dernière famille apparaît être instable pour $\tau < \tau^*$, ainsi que la distribution uniforme pour $\tau < \frac{2}{15}$.

Les autres équilibres sont stables, dans ce même sens. Ainsi, si l'on part d'une température τ élevée, le seul équilibre stable (la distribution uniforme) reste stable jusqu'à ce que τ atteigne $\frac{2}{15}$, et si l'on part d'une valeur faible, l'unique famille d'équilibre stable (une des deux familles d'équilibre nématiques prolates) reste stable jusqu'à ce que τ atteigne $\tau^* > \frac{2}{15}$, ce qui donne le phénomène d'hystérésis.

L'article [37] de Fatkullin et Slastikov considère également le cas du potentiel dipolaire en dimension 3 : quand $\tau \geqslant \frac{1}{3}$, la distribution uniforme est le seul équilibre, et une famille d'équilibres, qui diffèrent l'un de l'autre par une simple rotation, apparaît lorsque $\tau < \frac{1}{3}$, où l'équilibre uniforme devient instable, au sens où il ne minimise plus l'énergie libre.

Dans [89], un couplage entre les potentiels dipolaire et de Maier–Saupe est proposé, et les seuls équilibres stables sont alors nécessairement symétriques. Enfin, récemment, une caractérisation unifiée de ces équilibres dans de nombreux cas a été donnée [78], incluant le cas du potentiel de Maier–Saupe en dimension quelconque. L'idée principale est de prouver que le paramètre d'ordre tensoriel d'orientation est une matrice avec au plus deux valeurs propres distinctes, ce qui permet de réduire le problème.

Concernant la dynamique en temps, quelques résultats ont été donnés, pour le potentiel de Maier–Saupe seulement, en dimension 2 et 3. L'existence, l'unicité, la positivité et l'analyticité en espace d'une solution sont affirmées pour une condition initiale positive et continue dans [19, 21], qui montre aussi que le système est dissipatif dans une certaine classe de Gevrey de solutions. Récemment, l'existence de variétés inertielles a été établie [76, 77]. Mais cela ne fournit pas la preuve de la convergence vers un équilibre donné.

Un grand nombre de variantes ont été proposées et étudiées [80, 85, 87, 90, 75, 39] incluant des forces extérieures, d'élongation par exemple, ou un flot de cisaillement, ou modélisant des phénomènes plus complexes avec de la dépendance en espace. Enfin, très récemment, quelques résultats ont été donnés en dimension 2 permettant de comprendre un peu mieux le cas du noyau original de Onsager [18, 56, 79, 81], basé sur l'analyse des états stationnaires.

Notre principal apport dans ce domaine concerne la description dynamique du système lorsque le temps tends vers l'infini, qui a été peu traitée, et est détaillée dans la partie suivante.

3 Apports principaux

L'étude de différentes versions du modèle de Vicsek continu en temps a donné des résultats intéressants : l'introduction de modifications dans le modèle permettent de comprendre les caractéristiques importantes du modèle, qui présentent une sorte de robustesse par rapport à la limite macroscopique finale.

Dans le chapitre 1, le résultat principal est que le modèle macroscopique (2.2) est encore la limite formelle du modèle de champ moyen, même si le noyau d'observation n'est pas isotropique et si les paramètres ν et d dépendent de la densité locale $\bar{\rho}$. Cela confirme la capacité de ce modèle macroscopique à être un représentant naturel des modèles de déplacement de particules interagissant sur leur alignement,

avec une contrainte de vitesse unité, puisqu'il apparaît également comme limite d'un autre modèle de déplacement appelé « Persistent Turning Walker Model », lorsqu'une interaction d'alignement est prise en compte [30]. Toute l'information portée par les modifications qui ont été introduites apparaissent alors au travers des coefficients c_1, c_2, et λ. Par exemple, comme dans ce chapitre les paramètres du modèle dépende d'une densité locale, on obtient que les coefficients du modèle macroscopique dépendent de ρ.

Une des avancées de ce chapitre est également la position du problème dans n'importe quelle dimension $n \geqslant 2$ dans un cadre général. La méthode des invariants collisionnels généralisés est encore valide, et nous avons montré qu'ils ont une définition naturelle dans ce cadre.

Enfin, un résultat spécifique de ce chapitre concerne la présentation d'une méthode qui permet d'obtenir un développement asymptotique des coefficients du modèle, à tout ordre et en toute dimension, lorsque le paramètre de concentration $\kappa = \frac{\nu}{d}$ tend vers zéro ou vers l'infini. Cela permet d'étudier les propriétés des coefficients, même dans le modèle original, où nous pouvons voir que le coefficient c_2 est inférieur à c_1 dans les deux cas limites $\kappa \to 0$ et $\kappa \to \infty$. Cela permet également de montrer que dans certains cas, le modèle macroscopique n'est pas hyperbolique (le coefficient λ devenant négatif), et c'est une caractéristique nouvelle du modèle qui amène d'importantes questions.

Avec le modèle du chapitre 2, nous avons trouvé une manière d'obtenir une transition de phase à l'échelle macroscopique, tout en ayant un modèle continu en temps très proche du modèle discret. En utilisant des résultats du chapitre 4, ainsi qu'une analyse fine d'une constante de Poincaré spécifique, nous pouvons donner des arguments qui vont dans le sens d'une convergence en tout point, vers un équilibre local. Ce dernier peut être de deux types différents, soit la distribution uniforme, isotropique sur la sphère, si la densité ρ est inférieure au seuil critique $\rho^* = n$, ou une distribution avec une orientation donnée Ω dans le cas où $\rho > \rho^*$.

Le traitement mathématique de cette transition de phase consiste à dériver deux modèles différents, selon si la densité est en dessus ou au-dessous du seuil $\rho^* = n$. Nous obtenons au final un modèle macroscopique à deux phases, avec de la diffusion non linéaire dans la région de faible densité, et toujours le modèle macroscopique (2.2) dans la région de densité élevée. La description du comportement de la frontière entre ces deux régions reste un problème subtil. Encore une fois, le modèle se pose naturellement en toute dimension n, et les résultats sont donnés dans un cadre général.

La dernière chose importante à noter est que nous pouvons directement utiliser les résultats du chapitre 1 qui concernent les développements asymptotiques des coefficients, et nous obtenons que $\lambda < 0$ dans les deux cas limites. À l'aide d'approximations numériques, nous observons en fait que l'on a toujours $\lambda < 0$. Cela signifie que le modèle n'est pas hyperbolique dans toute la phase ordonnée. Toutefois, sous la contrainte d'une dynamique n'ayant lieu que le long d'une direction, nous obtenons une réduction du modèle qui présente un caractère moins pathologique, et on peut avoir de l'hyperbolicité dans certaines régions de l'espace des états.

L'introduction du modèle de Vicsek continu en temps sur une variété Riemannienne effectué dans le chapitre 3 est, à notre connaissance, quelque chose de ré-

ellement nouveau. Nous avons pu définir un modèle général qui inclut la plupart des modèles étudiés aux chapitres 1-2, ainsi que le modèle original [28]. Sous des restrictions de régularité du noyau d'observation et du coefficient ν du modèle, nous prouvons la propagation du chaos, en suivant le travail récent [13], et nous obtenons une limite de champ moyen qui correspond exactement à l'analogue de (2.1) sur une variété Riemannienne.

Les simulations numériques effectuées sur la sphère $\mathbb{S}_2$ donnent alors une nouvelle vision sur le mouvement collectif de particules se déplaçant à vitesse constante.

Passons maintenant à la description de notre apport principal à l'analyse des dynamiques dans l'équation (2.3).

La première chose à souligner est que nous avons fait un lien entre des sujets qui n'étaient pas reliés au premier abord. L'un vient de la biologie, l'autre de l'étude de suspensions de polymères en forme de bâtonnets, qui sont loin d'être des particules autopropulsées. Le point commun est que la dynamique se passe sur la sphère unité. En fait, pour être précis, dans le cadre des polymères en forme de bâtonnets, leur orientation est un élément de l'espace projectif, puisqu'on ne fait pas la distinction entre un bâtonnet et son opposé (il n'a pas de sens privilégié). Mais il est pratique de travailler avec des fonctions sur la sphère, qui sont donc considérées comme étant paires. Cette considération n'a alors pas de sens pour le potentiel dipolaire puisque, pour les fonctions paires, l'équation (2.3) avec potentiel dipolaire se ramène à l'équation de la chaleur.

Dans le cas du potentiel dipolaire, notre contribution constitue la majeure partie de son étude, à notre connaissance. Les équilibres avaient été seulement classifiés précédemment par Fatkullin et Slastikov en dimension 2 [38] et 3 [37]. Notre travail dans le chapitre 4 donne tout d'abord une classification complète des états stationnaire en toute dimension. Mais il inclut également des résultats d'existence, unicité, régularité instantanée, stricte positivité, et des bornes uniformes dans tout espace de Sobolev H^s pour une condition initiale positive dans un quelconque H^p, $p \in \mathbb{R}$. À partir de cela, nous obtenons une version du principe de LaSalle adaptée au problème, qui donne que la solution converges vers un unique ensemble d'équilibres. Nous développons alors l'énergie libre d'Onsager et son terme de dissipation autour d'un équilibre mobile adapté à f, et finalement, à l'aide d'un argument d'équation différentielle ordinaire, nous pouvons contrôler le déplacement de cet équilibre mobile. Notre travail montre que n'importe quelle solution converge vers un équilibre donné, à un taux exponentiel lorsque τ est différent de la valeur critique $\frac{1}{n}$, et à un taux algébrique pour $\tau = \frac{1}{n}$. En outre, nous pouvons déterminer le type d'équilibre de la limite selon la condition initiale : quand $\tau < \frac{1}{n}$, les seules conditions conditions initiales menant, en temps long, vers la distribution uniforme sont celles avec un premier moment nul.

En utilisant des harmoniques sphériques en dimension n, nous explicitons une étonnante relation de conservation mettant en jeu un opérateur appelé « Laplacien conforme ». Dans le cas où $\tau > \frac{1}{n}$, cette relation de conservation peut être vue comme la dissipation d'une nouvelle entropie, qui donne de la convergence avec un taux exponentiel global vers la distribution uniforme.

Dans le chapitre 5, nous utilisons les outils développés pour le cas du potentiel dipolaire dans le cadre plus étudié du potentiel de Maier–Saupe, ce qui donne une

compréhension nouvelle du cas de la dimension 2, qui est très similaire au cas du potentiel dipolaire : il y a convergence vers un équilibre donné pour n'importe quelle condition initiale, à un taux exponentiel lorsque $\tau \neq \frac{1}{4}$. Nous utilisons également ici une relation de conservation spéciale, qui a été observée dans [19] dans un cas particulier, mais pas utilisée de façon optimale. Nous pouvons donc aussi déterminer le type d'équilibre de la limite selon la condition initiale : quand $\tau < \frac{1}{4}$, les seules conditions initiales menant, en temps long, vers la distribution uniforme sont celles avec un second moment nul.

4 Présentation des résultats

Ch. 1 A continuum model for alignment of self-propelled particles with anisotropy and density-dependent parameters

Dans ce chapitre, nous étudions le modèle suivant, pour N particules dont les positions sont notées $X_k \in \mathbb{R}^n$ et les orientations $\omega_k \in \mathbb{S}$ (la sphère unité de $\mathbb{R}^n$), avec $k \in [\![1, N]\!]$, écrit sous la forme d'un système d'équation différentielles stochastiques couplées, dans la formulation de Stratonovich :

$$\begin{cases} \mathrm{d}X_k = \omega_k \mathrm{d}t, \\ \mathrm{d}\omega_k = \nu(\bar{\rho}_k)(\mathrm{Id} - \omega_k \otimes \omega_k)\bar{\omega}_k \,\mathrm{d}t + \sqrt{2d(\bar{\rho}_k)}\,(\mathrm{Id} - \omega_k \otimes \omega_k) \circ \mathrm{d}B_t^k, \end{cases} \tag{4.5}$$

où (B_t^k) sont des mouvements Browniens standards à valeurs dans $\mathbb{R}^n$. Ce système exprime le fait que les particules se déplacent à vitesse constante 1, suivant leur orientation, qui est relaxée vers l'orientation cible $\bar{\omega}$ à un taux $\nu(\bar{\rho})$ et soumise à un mouvement Brownien d'intensité $\sqrt{2d(\bar{\rho})}$ (le terme $\mathrm{Id} - \omega_k \otimes \omega_k$ est la projection sur l'hyperplan orthogonal à ω_k).

Les termes qui induisent un couplage sont la densité $\bar{\rho}_k$ et l'orientation cible $\bar{\omega}_k$, donnés par

$$\bar{\rho}_k = \frac{1}{N}\sum_{j=1}^{N} \widetilde{K}\left(|X_j - X_k|, \tfrac{X_j - X_k}{|X_j - X_k|} \cdot \omega_k\right),$$

$$\bar{\omega}_k = \frac{\bar{J}_k}{|\bar{J}_k|}, \text{ où } \bar{J}_k = \frac{1}{N}\sum_{j=1}^{N} K\left(|X_j - X_k|, \tfrac{X_j - X_k}{|X_j - X_k|} \cdot \omega_k\right)\omega_j,$$

où K et $\widetilde{K}$ sont des noyaux d'observations permettant de calculer par rapport aux voisins une valeur moyenne locale d'une quantité donnée. Par exemple pour prendre en compte seulement les voisins situés « devant », et à moins d'une certaine distance R, le noyau serait donné par $K(r, \gamma) = \mathbb{1}_{\{r \leqslant R\}}\mathbb{1}_{\{\gamma \geqslant 0\}}$.

Les fonctions positives ν et d sont arbitraires. Le choix de ν et d constant, et du fait que le noyau K dépend seulement de sa première variable, correspond exactement à la version continue en temps du modèle de Vicsek proposée dans [28].

Le but de ce chapitre est de dériver le modèle macroscopique suivant, à partir du système de particules (4.5) :

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (c_1(\rho)\rho\Omega) = 0, \\ \rho\ (\partial_t \Omega + c_2(\rho)(\Omega \cdot \nabla_x)\Omega) + \lambda(\rho)\,(\mathrm{Id} - \Omega \otimes \Omega)\nabla_x \rho = 0, \end{cases} \tag{4.6}$$

où les fonctions c_1, c_2, et λ seront définies en (4.9) et (4.10)-(4.11).

La première étape est d'écrire un modèle de champ moyen pour le système de particules, comme en (2.1), et de procéder ensuite à un changement d'échelle hydrodynamique, qui consiste à introduire un petit paramètre ε et écrire $f^\varepsilon(\varepsilon x, \omega, \varepsilon t) = f(x, \omega, t)$. Après quelques développements, on obtient

$$\varepsilon(\partial_t f^\varepsilon + \omega \cdot \nabla_x f^\varepsilon + \alpha\, P(f^\varepsilon) + \widetilde{\alpha}\, \widetilde{P}(f^\varepsilon)) = Q(f^\varepsilon) + O(\varepsilon^2)\,, \tag{4.7}$$

où les constantes α et $\widetilde{\alpha}$ dépendent seulement des noyaux d'observation K et $\widetilde{K}$. Ces constantes sont positives si le noyau est dirigé vers l'avant, et plus l'« angle de vision » est grand, plus la constante associée au noyau l'est. Les opérateurs P et $\widetilde{P}$ agissent sur f et sur ses dérivées spatiales, et Q est donné par

$$\begin{aligned} Q(f) =& -\nu(\rho_f)\nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega)\Omega_f f) + d(\rho_f)\Delta_\omega f, \\ \rho_f =& \int_{\omega \in \mathbb{S}} f(., \omega)\, \mathrm{d}\omega\,, \\ \Omega_f =& \frac{j_f}{|j_f|}, \text{ avec } j_f = \int_{\omega \in \mathbb{S}} \omega\, f(., \omega)\, \mathrm{d}\omega\,, \end{aligned}$$

Au vu de l'équation (4.7), lorsque $\varepsilon \to 0$, la fonction f^ε devient un équilibre, c'est-à-dire une fonction f^0 telle que $Q(f^0) = 0$. En introduisant la distribution de Von-Mises de paramètre de concentration $\kappa > 0$ et d'orientation $\Omega \in \mathbb{S}$:

$$M_{\kappa\Omega}(\omega) = \frac{e^{\kappa\, \omega \cdot \Omega}}{\int_{\mathbb{S}} e^{\kappa\, \upsilon \cdot \Omega}\, \mathrm{d}\upsilon}, \tag{4.8}$$

et en définissant l'opérateur linéaire $L_{\kappa\Omega}$ par

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

on remarque que l'opérateur $Q(f)$ s'écrit sous la forme $Q(f) = -d(\rho_f) L_{\kappa(\rho_f)\Omega_f}(f)$, avec $\kappa(\rho) = \frac{\nu(\rho)}{d(\rho)}$, et il est alors facile de voir que si $Q(f) = 0$, alors f est de la forme $\rho M_{\kappa(\rho)\Omega}$.

On a alors que $j_{M_{\kappa\Omega}} = c_1(\kappa)\Omega$, avec

$$c_1(\kappa) = \langle \cos\theta \rangle_{M_\kappa}, \quad \text{where} \langle \gamma(\cos\theta) \rangle_{M_\kappa} = \frac{\int_0^\pi \gamma(\cos\theta) e^{\kappa \cos\theta}\, \sin^{n-2}\theta\, \mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta}\, \sin^{n-2}\theta\, \mathrm{d}\theta}. \tag{4.9}$$

Si nous intégrons l'équation (4.7) sur la sphère, on obtient $\partial_t \rho + \nabla_x \cdot (j) = 0$, ce qui nous donne l'équation d'évolution de la densité :

$$\partial_t \rho + \nabla_x \cdot (c_1(\kappa)\rho\, \Omega) = 0.$$

Pour obtenir l'équation sur Ω, nous définissons les invariants collisionnels généralisés $\mathcal{C}_{\kappa\Omega}$ (associés à $\kappa > 0$ et $\Omega \in \mathbb{S}$) comme l'espace vectoriel suivant :

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

Nous trouvons alors qu'un invariant collisionnel généralisé est de la forme $C + h_\kappa(\omega\cdot\Omega)A\cdot\omega$, avec A arbitraire, orthogonal à Ω, et h_κ est une fonction positive et régulière (donnée comme la solution d'un problème elliptique). Nous pouvons alors multiplier (4.7) par $h_\kappa(\omega\cdot\Omega)A\cdot\omega$ et intégrer, on obtient que $A\cdot X = 0$ pour un vecteur X donné et pour tous les vecteurs A qui sont orthogonaux à Ω. Finalement X est aligné avec Ω, et écrire $(\mathrm{Id}-\Omega\otimes\Omega)X = 0$ donne exactement la deuxième équation de (4.6), avec

$$c_2 = \widetilde{c}_1 - \alpha\, d\,(n\,\widetilde{c}_1 + \kappa\,\langle\cos^2\theta\rangle_{\widetilde{M}_\kappa}),\ \text{avec}\quad \widetilde{c}_1 = \langle\cos\theta\rangle_{\widetilde{M}_\kappa}, \tag{4.10}$$

$$\lambda = \tfrac{1}{\kappa} + \rho\,\tfrac{\dot\kappa}{\kappa}\,[\,\widetilde{c}_1 - c_1 + \widetilde{\alpha}\,d\,(\kappa\,\langle\sin^2\theta\rangle_{\widetilde{M}_\kappa} - n\,\widetilde{c}_1)\,] + \tfrac{1}{2}\,\widetilde{\alpha}\,\rho\,\dot{d}\,(n-1+\kappa\,\widetilde{c}_1), \tag{4.11}$$

où le point est la dérivée par rapport à ρ, et avec la notation

$$\langle\gamma(\cos\theta)\rangle_{\widetilde{M}_\kappa} = \frac{\int_0^\pi \gamma(\cos\theta)h_\kappa(\cos\theta)e^{\kappa\cos\theta}\,\sin^n\theta\,\mathrm{d}\theta}{\int_0^\pi h_\kappa(\cos\theta)e^{\kappa\cos\theta}\,\sin^n\theta\,\mathrm{d}\theta}. \tag{4.12}$$

Enfin, dans une seconde partie, nous développons une méthode pour obtenir un développement asymptotique, à n'importe quel ordre, lorsque $\kappa \to 0$ ou $\kappa \to \infty$, d'expressions de la forme $\langle f(\theta)\rangle_{M_\kappa}$ et $\langle f(\theta)\rangle_{\widetilde{M}_\kappa}$. Ceci nous permet d'obtenir les développements des coefficients, et prouve que le coefficient λ peut devenir négatif, et le système (4.6) perd alors son hyperbolicité.

Ch. 2 Macroscopic limits and phase transition in a system of self-propelled particles

Dans ce chapitre, la modification du modèle individuel semble, au premier abord, être une simplification : on remplace $\nu\bar\omega_k$ dans (4.5), par $\nu\bar J_k$, c'est-à-dire que l'on ne divise pas par la norme. L'interaction est alors une somme d'interactions binaires, toujours interprétée comme une relaxation vers $\bar\omega_k$, mais à un taux proportionnel à $|\bar J_k|$. Le système prend la forme

$$\begin{cases} \mathrm{d}X_k = \omega_k \mathrm{d}t, \\ \mathrm{d}\omega_k = \nu(\mathrm{Id}-\omega_k\otimes\omega_k)\bar J_k\,\mathrm{d}t + \sqrt{2d}\,(\mathrm{Id}-\omega_k\otimes\omega_k)\circ\mathrm{d}B_t^k, \end{cases} \tag{4.13}$$

$$\bar J_k = \frac{1}{N}\sum_{j=1}^N K(X_j - X_k)\omega_j, \tag{4.14}$$

où (B_t^k) sont des mouvements Browniens indépendants à valeurs dans $\mathbb{R}^n$. La limite de champ moyen est alors donnée par

$$\begin{cases} \partial_t f + \omega\cdot\nabla_x f + \nu\nabla_\omega\cdot((\mathrm{Id}-\omega\otimes\omega)\bar J_f\, f) = d\Delta_\omega f \\ \bar J_f(x,t) = \int_{\mathbb{S}}(K*f)(x,\omega,t)\,\omega\,\mathrm{d}\omega, \end{cases} \tag{4.15}$$

où $*$ désigne la convolution par rapport à la variable d'espace. À l'aide d'un changement d'échelle en espace, en temps et en densité (en ne supposant plus que f est une densité de probabilité sur $\mathbb{R}^n \times \mathbb{S}$, mais simplement la densité d'une mesure finie), on peut supposer sans perte de généralité que $\nu = d = 1$ et que $\int_{\mathbb{R}^n} K(\xi)\mathrm{d}\xi = 1$. On peut noter que cette limite de champ moyen est plus facile à traiter, puisque la singularité en $\bar{J} = 0$, et la propagation du chaos a été effectivement prouvée récemment dans [13].

Le changement d'échelle hydrodynamique donne, si $K(\xi)$ dépend seulement de la norme $|\xi|$:

$$\varepsilon(\partial_t f^\varepsilon + \omega \cdot \nabla_x f^\varepsilon) = Q(f^\varepsilon) + O(\varepsilon^2), \tag{4.16}$$

avec

$$\begin{cases} Q(f) = -\nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega) J_f f) + \Delta_\omega f \\ J_f(x,t) = \int_{\mathbb{S}} f(x,\omega,t)\,\omega\,\mathrm{d}\omega. \end{cases} \tag{4.17}$$

Ici, les équilibres de Q sont toujours donnés par $\rho M_{\kappa\Omega}$, pour $\rho > 0$ et $\Omega \in \mathbb{S}$ arbitraires, où $M_{\kappa\Omega}$ est définie en (4.8), et où le paramètre de concentration κ satisfait la condition de compatibilité $\rho\kappa = c(\kappa)$, avec $c(\kappa)$ défini en (4.9). Nous avons alors l'alternative suivante :

Proposition 1. *Condition de compatibilité, équilibres.*

- *Si $\rho \leqslant n$, il y a une seule solution à la condition de compatibilité : $\kappa = 0$. Le seul équilibre est la fonction constante $f = \rho$.*
- *Si $\rho > n$, la condition de compatibilité a deux solutions : $\kappa = 0$ et une unique solution strictement positive, qui sera notée $\kappa(\rho)$. Mise à part la fonction constante $f = \rho$ (le cas $\kappa = 0$), les équilibres forment une variété de dimension n : les fonctions de la forme $f = \rho M_{\kappa(\rho)\Omega}$, où $\Omega \in \mathbb{S}$ est un vecteur unitaire arbitraire*

À l'aide d'arguments de stabilité et de taux de convergence vers l'équilibre pour la version homogène de (4.16) fournis par les résultats du chapitre 4, nous sommes amenés à considérer un modèle macroscopique constitué de deux zones : la limite formelle, lorsque $\varepsilon \to 0$ de la fonction f^ε est donnée par une fonction $f(x,\omega,t)$ qui satisfait

- $f(x,\omega,t) = \rho(x,t)$ avec $\rho(x,t) < n$, dans la région « désordonnée » $\mathcal{R}_d$ où l'on a $n - \rho^\varepsilon(x,t) \gg \varepsilon$,
- $f(x,\omega,t) = \rho(x,t) M_{\kappa(\rho)\Omega(x,t)}$ avec $\rho(x,t) > n$, dans la région « ordonnée » $\mathcal{R}_o$ où l'on a $\rho^\varepsilon(x,t) - n \gg \varepsilon$.

Dans la région de désordre, la limite formelle satisfait $\partial_t \rho = 0$, nous nous intéressons donc à une approximation à l'ordre un du modèle. Un développement de Chapman–Enskog mène à un modèle de diffusion non linéaire :

Proposition 2. *Modèle de diffusion dans la zone de désordre.*

Lorsque ε tend vers zéro, la correction (formelle) à l'ordre un de la solution du système de champ moyen mis à l'échelle hydrodynamique, dans la région $\mathcal{R}_d \subset \mathbb{R}^n$ où l'on a $n - \rho^\varepsilon(x,t) \gg \varepsilon$, est donnée par

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

où la densité ρ^ε satisfait l'équation de diffusion suivante :

$$\partial_t \rho^\varepsilon = \frac{\varepsilon}{n-1} \nabla_x \cdot \left(\frac{1}{n-\rho^\varepsilon} \nabla_x \rho^\varepsilon \right). \tag{4.18}$$

Dans la région ordonnée, la méthode des invariants collisionnels généralisés fonctionne et on peut dériver le modèle hydrodynamique (2.2) :

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (\rho \Omega) = 0, \\ \rho(\partial_t \Omega + \widetilde{c}(\Omega \cdot \nabla_x)\Omega) + \lambda(\mathrm{Id} - \Omega \otimes \Omega) = 0, \end{cases}$$

où la vitesse c dépendant de $\kappa(\rho)$ est définie en (4.9), la vitesse $\widetilde{c}$ est donnée par $\langle \cos\theta \rangle_{\widetilde{M}_{\kappa(\rho)}}$ avec la notation (4.12) et

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

La méthode de développement asymptotique introduite au chapitre 1 permet d'obtenir les développements suivants :

Proposition 3. *Développement des coefficients lorsque la densité est grande ou proche du seuil critique.*

On a les développements asymptotiques des coefficients c, $\widetilde{c}$, et λ suivants :

- *Lorsque la densité ρ est proche de n :*

$$\begin{aligned} c &= \tfrac{\sqrt{n+2}}{n}\sqrt{\rho - n} + O(\rho - n), \\ \widetilde{c} &= \tfrac{2n-1}{2n\sqrt{n+2}}\sqrt{\rho - n} + O(\rho - n), \\ \lambda &= \tfrac{-1}{4\sqrt{n+2}} \frac{1}{\sqrt{\rho - n}} + O(1). \end{aligned}$$

- *Lorsque la densité ρ tend vers l'infini :*

$$\begin{aligned} c &= 1 - \tfrac{n-1}{2}\rho^{-1} + \tfrac{(n-1)(n+1)}{8}\rho^{-2} + O(\rho^{-3}), \\ \widetilde{c} &= 1 - \tfrac{n+1}{2}\rho^{-1} - \tfrac{(n+1)(3n+1)}{24}\rho^{-2} + O(\rho^{-3}), \\ \lambda &= -\tfrac{n+1}{6}\rho^{-2} + O(\rho^{-3}). \end{aligned}$$

En particulier, on voit que puisque $\lambda < 0$ dans ces deux cas limites (numériquement, on peut observer que c'est toujours le cas), alors le système n'est pas hyperbolique.

Si nous contraignons les dynamiques à avoir lieu le long d'une seule direction, nous obtenons une condition d'hyperbolicité mettant en jeu l'angle entre Ω et cette direction de propagation, qui doit être inférieur à un angle critique θ_c qui satisfait :

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

Ch. 3 An individual time-continuous Vicsek model on a Riemannian manifold

Dans ce chapitre, nous étendons les dynamiques du modèle de Vicsek à une variété Riemannienne générale. La plupart des études numériques sur les dynamiques d'auto-organisation ont été faites sur le même espace géométrique : le tore plat, ou de façon équivalente un carré avec des conditions aux limites périodiques. Mais cette géométrie particulière a une influence sur les dynamiques. Pour cette raison, nous nous intéressons à une étude analytique et numérique du modèle de Vicsek sur une variété Riemannienne quelconque.

La première chose à faire est de décrire l'évolution d'une particule orientée (x, ω) sur une variété Riemannienne M donnée (de métrique g). À cet effet on introduit le fibré unitaire tangent UM associé à M :

$$UM := \{(x, \omega) \mid x \in M,\ \omega \in T_xM \ \text{ and } |\omega|_g = 1\},$$

où T_xM est l'espace tangent à M au point x. La variété UM est l'espace naturel à considérer pour l'évolution d'une particule orientée de vitesse unité.

Nous proposons d'abord un modèle décrivant la dynamique d'une seule particule (x, ω), se déplaçant à vitesse constante de norme un, dans un « champ de force orientationnel » η et dont l'orientation est soumise à un mouvement Brownien d'intensité $\sqrt{2d}$. En coordonnées locales, elle est donnée par une équation différentielle stochastique de Stratonovich :

$$\begin{cases} \mathrm{d}x^i = \omega^i \,\mathrm{d}t, \\ \mathrm{d}\omega^i = \eta^i \,\mathrm{d}t + \sqrt{2d} \sum_j (\sigma_{ij} - \omega^i \sum_{k,\ell} \omega^\ell \, g_{\ell k} \, \sigma_{kj}) \circ \mathrm{d}B_t^j - \sum_{j,k} \Gamma^i_{jk} \, \omega^j \, \omega^k \,\mathrm{d}t, \end{cases}$$

où B_t est un mouvement Brownien standard dans $\mathbb{R}^n$ (ou de façon équivalente, les B_t^i sont n mouvements Browniens réels standard indépendants), et (σ_{ij}) est l'inverse de la racine carrée (parmi les matrices symétriques définies positives) de la matrice (g_{ij}) donnant la métrique en coordonnées locales. Nous montrons que ce système est bien défini comme un processus stochastique à valeurs dans UM, et nous donnons l'équations aux dérivées partielles satisfaite par sa loi.

Nous donnons ensuite une formulation globale de ce système d'un point de vue extrinsèque, dans le cas où la variété M est plongée de manière isométrique dans $\mathbb{R}^m$, pour $m \geqslant n$:

$$\begin{cases} \mathrm{d}x = \omega \,\mathrm{d}t, \\ \mathrm{d}\omega = \eta \,\mathrm{d}t + \sqrt{2d}\, \pi_{x,\omega} \circ \mathrm{d}B_t + \mathrm{I\!I}_x(\omega, \omega) \,\mathrm{d}t, \end{cases}$$

où B_t est un mouvement Brownien standard dans $\mathbb{R}^{2m}$, où $\pi_{x,\omega}$ est la projection sur l'espace tangent $T_\omega \mathbb{S}_g^x$ à $\mathbb{S}_g^x$ (la sphère unité de l'espace tangent T_xM) en ω, et où $\mathrm{I\!I}_x(\omega, \omega)$ est la seconde forme fondamentale associée à la variété Riemannienne plongée.

Dans une deuxième partie, nous proposons une extension de la vitesse moyenne locale $\bar{J}$ en un point x de M à l'aide du transport parallèle le long des géodésiques. La dynamique de Vicsek continue en temps est alors simplement donnée comme

une relaxation de la vitesse d'une particule ω_k vers la direction portée par la vitesse moyenne $\bar{J}(x_k)$.

$$\partial_t f + g_x(\omega, \nabla_x^h f) + \nabla_\omega^x \cdot (\nu\, \pi_{x,\omega} J[f] f) = d\Delta_\omega^x f,$$

où le « gradient horizontal » $\nabla_x^h f$ correspond au gradient spatial de f, où $\nabla_\omega^x \cdot$ et $\nabla_\omega^x \cdot$ sont les opérateurs de divergence et de Laplace–Beltrami sur $\mathbb{S}_g^x$, la sphère unité de l'espace tangent $T_x M$, et où

$$J[f](x,\omega) = \int_{UM} K(x,\omega,x')\tau_{x,x'}(\omega') f(x',\omega')\,\mathrm{d}\mu(x',\omega'),$$

où $\tau_{x,x'}(\omega')$ est le transport parallèle de ω' le long de la géodésique joignant x à x', K est un noyau d'observation, et μ est la mesure naturelle sur UM, appelée mesure de Liouville ou cinématique.

Enfin, nous illustrons notre modèle par quelques simulations sur la sphère $\mathbb{S}_2$. Nous observons la formations de groupes se déplaçant dans la même direction. Mais en contraste avec le modèle de Vicsek sur le tore plat, il n'y a pas émergence d'une direction globale pour l'ensemble des particules.

Ch. 4 Dynamics in a kinetic model of oriented particles with phase transition

Dans ce chapitre, nous étudions la dynamique de l'équation de Doi (2.3) avec potentiel dipolaire, qui prend la forme suivante :

$$\begin{cases} \partial_t f = -\nabla_\omega \cdot ((\mathrm{Id} - \omega\otimes\omega) J[f] f) + \tau \Delta_\omega f, \\ J[f] = \int_{\mathbb{S}} \omega\, f(.,\omega)\,\mathrm{d}\omega. \end{cases} \tag{4.19}$$

Nous donnons tout d'abord des résultats d'existence et d'unicité d'une solution faible, pour une condition initiale dans un espace de Sobolev quelconque.

Theorem 1. *Étant donnée une mesure de probabilité initiale f_0 dans $H^s(\mathbb{S})$ (ce qui est toujours le cas pour $s < -\frac{n-1}{2}$), il existe une unique solution faible f de (4.19) telle que $f(0) = f_0$. Cette solution est globale en temps. De plus, $f \in C^\infty((0,+\infty)\times\mathbb{S})$, avec $f(t,\omega) > 0$ pour tout t strictement positif.*

Nous avons également les estimations suivantes, donnant de la régularité instantanée et des bornes uniformes (pour $m \in \mathbb{N}$, la constante C ne dépendant que de τ, m, s), pour tout $t > 0$:

$$\|f(t)\|_{H^{s+m}}^2 \leqslant C\left(1 + \frac{1}{t^m}\right)\|f_0\|_{H^s}^2.$$

En annexe, nous montrons de plus que la solution est analytique en espace.

En définissant l'énergie libre de Onsager $\mathcal{F}$ et son terme de dissipation $\mathcal{D}$ par

$$\mathcal{F}(f) = \tau \int_{\mathbb{S}} f \ln f - \tfrac{1}{2}|J[f]|^2,$$
$$\mathcal{D}(f) = \int_{\mathbb{S}} f |\nabla_\omega(\tau \ln f - \omega\cdot J[f])|^2,$$

nous obtenons, pour une solution f de l'équation de Doi (4.19), la relation de conservation suivante :

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F} + \mathcal{D} = 0.$$

Ceci nous permet de donner une adaptation du principe d'invariance de LaSalle à notre cadre d'équations aux dérivées partielles.

Proposition 4. *Principe d'invariance de LaSalle*

Soit f_0 une mesure de probabilité sur la sphère $\mathbb{S}$. Nous désignons par $\mathcal{F}_\infty$ la limite de $\mathcal{F}(f(t))$ quand $t \to \infty$, où f est la solution de l'équation de Doi (4.19) *avec condition initiale f_0.*

Alors l'ensemble $\mathcal{E}_\infty = \{f \in C^\infty(\mathbb{S})$ s.t. $\mathcal{D}(f) = 0$ and $\mathcal{F}(f) = \mathcal{F}_\infty\}$ est non vide.

De plus $f(t)$ converge dans toutes les normes H^s vers cet ensemble d'équilibres, au sens suivant :

$$\lim_{t\to\infty} \inf_{g\in\mathcal{E}_\infty} \|f(t) - g\|_{H^s} = 0.$$

Nous caractérisons alors les équilibres, de la forme $M_{\kappa\Omega}$ où κ satisfait la condition de compatibilité $c(\kappa) = \tau\kappa$.

Proposition 5. *Condition de compatibilité*

- *Si $\tau \geqslant \frac{1}{n}$, il n'y a qu'une solution à la condition de compatibilité : $\kappa = 0$. Le seul équilibre est la fonction constante $f = 1$.*
- *Si $\tau < \frac{1}{n}$, la condition de compatibilité a exactement deux solutions : $\kappa = 0$ et une unique solution strictement positive, que nous noterons $\kappa(\tau)$. Mise à part la fonction constante $f = 1$ (le cas $\kappa = 0$), les équilibres forment une variété de dimension $n - 1$: les fonctions de la forme $f = M_{\kappa(\tau)\Omega}$, où $\Omega \in \mathbb{S}$ est un vecteur unitaire arbitraire.*

À l'aide d'une analyse fine des harmoniques sphériques en dimension quelconque, nous obtenons une identité remarquable, pour une fonction h de moyenne nulle sur la sphère :

$$\int_{\mathbb{S}} \widetilde{\Delta}_{n-1} h \nabla_\omega h = 0,$$

où $\widetilde{\Delta}_{n-1}$ est le « Laplacien conforme »sur la sphère unité, donné, pour une harmonique sphérique Y^ℓ de degré ℓ, par $\widetilde{\Delta}_{n-1}Y^\ell = \ell(\ell+1)\dots(\ell+n-1)(\ell+n-2)Y^\ell$. C'est un opérateur différentiel quand n est impair, et pseudodifférentiel quand n est pair.

Cette identité remarquable mène à une nouvelle relation de conservation, pour une densité de probabilité f solution de (4.19), de la forme

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|f-1\|^2_{\widetilde{H}^{-\frac{n-1}{2}}} = -\tau\|f-1\|^2_{\widetilde{H}^{-\frac{n-3}{2}}} + \frac{1}{(n-2)!}|J[f]|^2,$$

où $\|\cdot\|_{\widetilde{H}^{-\frac{n-1}{2}}}$ et $\|\cdot\|_{\widetilde{H}^{-\frac{n-3}{2}}}$ sont des normes de Sobolev spécifiques associées au Laplacien conforme, équivalentes aux normes usuelles $H^{-\frac{n-1}{2}}$ et $H^{-\frac{n-3}{2}}$.

Dans le cas où $\tau > \frac{1}{n}$, cette loi de conservation peut être vue comme la dissipation d'une nouvelle entropie donnée par $\|f-1\|^2_{\widetilde{H}^{-\frac{n-1}{2}}}$, et on obtient la convergence globale vers l'équilibre uniforme, avec un taux $(n-1)(\tau - \frac{1}{n})$ dans cette norme faible, qui peut être ensuite étendue à toute norme H^s, avec $s > -\frac{n-1}{2}$.

Si $J[f_0] \neq 0$ nous montrons que $J[f(t)] \neq 0$ pour tout $t > 0$ (si $J[f_0] = 0$, l'équation se ramène à l'équation de la chaleur, et la solution converge exponentiellement vite vers la distribution uniforme). Dans le cas où $\tau < \frac{1}{n}$, nous pouvons alors définir le vecteur unitaire $\Omega(t)$ comme $\frac{J[f(t)]}{|J[f(t)]|}$. À l'aide du principe de LaSalle, nous obtenons que $f - M_{\kappa(\tau)\Omega(t)}$ converge vers zéro, nous pouvons alors développer $\mathcal{D}$ et $\mathcal{F}$ autour de $M_{\kappa(\tau)\Omega(t)}$ dans une « norme mobile » (un L^2 à poids donné par $M_{\kappa(\tau)\Omega(t)}$, qui dépend du temps). Nous obtenons alors la convergence exponentielle vers zéro de la différence $f - M_{\kappa(\tau)\Omega(t)}$. Enfin, en dérivant l'équation différentielle satisfaite par $\Omega(t)$, on peut contrôler sa dérivée par $\|f - M_{\kappa(\tau)\Omega(t)}\|$, ce qui donne que $\Omega(t)$ converge avec un taux exponentiel vers un certain $\Omega_\infty \in \mathbb{S}$. Avec de l'interpolation, on obtient le résultat suivant :

Proposition 6. *Si $\tau < \frac{1}{n}$, il existe un taux asymptotique de convergence exponentielle $r_\infty(\tau) > 0$, en norme H^p quelconque, vers un état d'équilibre donné.*

Plus précisément, pour tout $r < r_\infty(\tau)$, il existe $t_0 > 0$ (dépendant de f_0 et de p) tel que pour tout $t > t_0$, on a

$$\|f(t) - M_{\kappa\Omega_\infty}\|_{H^p} \leqslant e^{-rt}.$$

Lorsque τ est proche de $\frac{1}{n}$ on a $r_\infty(\tau) \sim 2(n-1)(\frac{1}{n} - \tau)$.

De la même manière, dans le cas critique $\tau = \frac{1}{n}$, on développe $\mathcal{D}$ et $\mathcal{F}$ autour de la distribution uniforme, et on obtient que le taux de convergence est donnée par $\frac{C}{\sqrt{t}}$.

Ch. 5 A note on the dynamics in the Doi equation with Maier–Saupe potential

Dans ce court chapitre, nous montrons que les outils utilisés dans le cas du potentiel dipolaire peuvent être adaptés pour obtenir des résultats dans le cas du potentiel de Maier–Saupe.

On considère l'équation aux dérivées partielles non locale sur $\mathbb{S}$ suivante, pour une densité de probabilité f sur la sphère :

$$\begin{cases} \partial_t f = \nabla_\omega \cdot (f \nabla_\omega \Psi_f) + \tau \Delta_\omega f, \\ \Psi_f(\omega, t) = \int_{\mathbb{S}} K(\omega, \bar{\omega})\, f(t, \bar{\omega})\, \mathrm{d}\bar{\omega}. \end{cases} \tag{4.20}$$

Le potentiel de Maier–Saupe est donné par $K(\omega, \bar{\omega}) = \frac{1}{n} - (\omega \cdot \bar{\omega})^2$.

Dans le cas général d'un noyau polynomial, nous donnons les même résultats d'existence et d'unicité, de stricte positivité et de régularité que dans le Théorème 1, et l'adaptation du principe d'invariance de LaSalle (Proposition 4) est toujours valide.

Nous définissons le paramètre d'ordre tensoriel d'orientation par

$$S[f] = \int_{\mathbb{S}} (\tfrac{1}{n}\mathrm{Id} - \omega \otimes \omega) f \mathrm{d}\omega,$$

et nous donnons une propriété d'instabilité dynamique de la distribution uniforme quand τ est en dessous de la valeur critique $\tau_c = \frac{2}{n(n+2)}$:

Proposition 7. *Instabilité de la distribution uniforme au-dessous d'un seuil.*

Si on a $S[f_0] = 0$*, alors* $S[f(t)] = 0$ *pour tout* $t \geqslant 0$*, et l'équation de Doi* (4.20) *devient l'équation de la chaleur sur la sphère. La solution converge exponentiellement vite vers la distribution uniforme.*

Si on a $S[f_0] \neq 0$*, alors* $S[f(t)] \neq 0$ *pour tout* $t \geqslant 0$*. De plus, dans le cas où* $\tau < \frac{2}{n(n+2)}$*, la solution ne peut pas converger vers la distribution uniforme.*

On montre enfin, en dimension 2, que l'on a les mêmes résultats de convergence que dans le cas du potentiel dipolaire, qui est très similaire.

General introduction

1 Motivation

We are interested in the study of various models of collective behavior in systems with a large number of particles, such as models of displacement of fish in schools, or birds in flocks for example. These models have recently given rise to many challenging issues, in a mathematical point of view [10]. One of the frequent question on this topic is the understanding of how collective behavior can occur without a leader, for example with only localized interactions. Such phenomena are recurrent in nature, for example the strong alignment of fish in a school, or the formation of coherent structures and patterns in flocks of birds, even if the individuals seem to interact only with a few number of neighbors [6].

A popular model of displacement proposed by Vicsek *et al.* [74] has attracted a lot of attention, with respect to its ability to reproduce these complex phenomena and to its minimalism. Actually the minimal interaction rule on the alignment was present in other models [3, 67, 49, 23], called "three-zone models", which include a long-range zone of attraction and a short-range zone of repulsion. These models aim at describing realistic behavior of animals, whereas the Vicsek model tries to focus on the essential properties of the alignment interaction, without claiming to be realistic. The model considers particles moving with constant speed and updating synchronously their orientation by taking (up to an angular noise) the mean orientation of their neighbors. If the particles can move freely in the whole plane, we cannot observe strong correlation since the diffusion implies that the particles go to infinity. Therefore in order to deal with this problem of confinement, instead of adding a long range attraction for example, the model impose the dynamics to be periodic in space. In a more geometric point of view, the particle dynamics take place on the flat torus.

In this framework, a lot of numerical simulations of this model and variants have been performed [46, 16, 62], showing striking phenomena. The first thing to remark is that, as the noise decreases, the global behavior of the system undergoes a phase transition phenomenon: when the noise is large, the particles seem to move randomly in a disordered ambient state, and when the noise is low, one can observe the formation of coherent structures, and strong correlations between the orientations of the particles. Whether this phase transition is continuous or discontinuous has raised a lot of discussions, the conclusion being that the number of particles in the simulation has a strong influence on what is observed, and the phase transition becomes sharper with a large number of particles.

The second observation is the emergence, in large time, of coherent patterns. One can observe large travelling bands of high density in which the order parameter is high, moving across a disordered region of low density. The direction of propagation of these bands is also closely related to the geometry of the domain: the bands travel in the direction of periodicity, and chose one direction more probably than one other depending on the space period of the domain along these directions.

From this, three axes of study appears in a mathematical point of view: first, understanding the behavior of the system in the limit of a large number of particles (in the aim of a mathematical description of the phase transition phenomena), second, trying to explain, at the limit of a long time observation, the emergence of coherent structures and their governing laws, and finally investigating the role played by the geometry of the coherent structures and of the domain.

The mathematical study of this model, in view of these three axes, was the starting point of the present work, following the work of Degond and Motsch [28].

2 Overview of the subject

Regarding the description of the behavior of a system of particles when the number of them goes to infinity, the usual strategy is to consider the probability to find a particle at a given location, with a given velocity. The kinetic description of the system is then done through the determination of the evolution in time of this density probability function. In general, this is given by a partial differential evolution equation, and this is where the first problem arises when we want to study the limit of the Vicsek model when the number of particles is large. Indeed, we do not have a continuous description in time of the behavior of the particles, which is only given by the synchronous update of the velocities. This is one of the objections we can raise about the Vicsek model: even if there is no spatial leader, and the interaction are local in space, they are not independent in time, a global synchronization is done through the clock of the time steps. Two approaches can be taken to overcome this problem, while staying in the spirit of the Vicsek minimal model.

The first one has been proposed by Pierre Degond and Sébastien Motsch in [28], the idea is to replace the discrete behavior by a continuous relaxation to the orientation of the neighbors. At the cost of introducing a new parameter ν (actually, this parameter replaces the time step, which is a parameter in the original Vicsek model, and not a discretization time step), viewed as a frequency of relaxation towards the local mean orientation, they are able to derive formally a mean-field kinetic equation of Fokker–Planck type for the density probability f of the particles, of the following form:

$$\partial_t f + \omega \cdot \nabla_x f + \nu \nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega)\bar{\Omega}_f f) = d\Delta_\omega f, \tag{2.1}$$

where the function f depends on the time $t \geqslant 0$, the space variable $x \in \mathbb{R}^3$, and the velocity variable $\omega \in \mathbb{S}_2$. The parameter d is the intensity of the noise, and the vector $\bar{\Omega}_f \in \mathbb{S}_2$ denotes a target orientation computed with respect to f (in a non-local way), at the point x. Finally, $\nabla_\omega \cdot$ and Δ_ω stand for the divergence and Laplace–Beltrami operators on the sphere, and the matrix $\mathrm{Id} - \omega \otimes \omega$ is the projection on the plane orthogonal to ω. This method is the starting point of the main part of

this report.

Another approach to overcome the problem of global synchronization is to give to each particle its own clock for the orientation updating, under the form of a Poisson process with a given frequency ν (so we also have to introduce a new parameter), all the clocks being independent and this allows to define a pure jump process. Some work on this topic has been done in collaboration with Emmanuel Boissard and Sébastien Motsch while visiting him in Maryland, but is not enough completed to take place in this report. One thing to remark is that this approach can also be used to define a Vicsek-like model which takes place in a one-dimensional framework, and have been recently proposed as a model for displacements of migratory locusts in [34].

The problem of finding then a macroscopic description of the model in large time has also been addressed by in the same paper [28] by Pierre Degond and Sébastien Motsch. Let us summarize here their results.

Once the kinetic equation (2.1) for the density probability function f is obtained (at least formally), it is still a description at a small scale in space and time, so we cannot observe the macroscopic structures. The idea is to perform a scaling in time and space, called hydrodynamic scaling, introducing a small parameter ε and investigating the properties of the model as $\varepsilon \to 0$. This scaling has the effect of localizing the interaction in space, and when $\varepsilon \to 0$, the probability density f^ε is constrained to be an equilibrium for a given operator Q, in a three-dimensional manifold parameterized by the local density of mass ρ and an orientation Ω belonging to the unit sphere of $\mathbb{R}^3$ (the dynamics of the particles take place in $\mathbb{R}^3$): the equilibria have the form $\rho M_{\kappa\Omega}$, where $M_{\kappa\Omega}$ is the Von-Mises distribution of orientation Ω and concentration parameter $\kappa = \frac{\nu}{d}$. Even if the noise is large, the orientation of the equilibrium is well defined, and we cannot observe a phenomenon of phase transition, in contrast with the observations in the simulations of the Vicsek Model.

The next step is to derive the evolution equations for the mass ρ and the direction Ω. The conservation of mass gives a first equation, but there is no other obvious conservation relation to get the remaining equation, and the main object of [28] is to introduce the notion of generalized collisional invariants which allows to get the evolution equation for Ω. The resulting model is the following non-conservative system of first order partial differential equations:

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (c_1 \rho \Omega) = 0. \\ \rho \left(\partial_t \Omega + c_2 (\Omega \cdot \nabla_x) \Omega \right) + \lambda \left(\mathrm{Id} - \Omega \otimes \Omega \right) \nabla_x \rho = 0. \end{cases} \tag{2.2}$$

where the coefficients c_1, c_2 and λ satisfy $0 < c_2 < c_1 < 1$ and $\lambda > 0$. This system is proved to be hyperbolic. As far as we know, this is the first model which has such a non-conservative form in the context of macroscopic limits of systems of large number of interacting particles. This comes from the particularity of unit speed constraint for the particles, which can be natural regarding to the modeling of biological phenomena such as animal displacements, and had much less sense when modeling the microscopic dynamics of dilute gases, from which all this kinetic theory comes.

Finally, regarding the third axe of study, namely the investigation of the role played by the geometry of the domain, there is not a lot of mathematical rigorous

analysis, to our knowledge. The observations [16, 62] of strongly ordered moving bands are always done in the case of a flat torus (periodic boundary conditions), showing that the movement is more likely to take place along a geodesic of minimal length. The generalization of the model to other geometrical configurations, such as the unit sphere (one can imagine for example the description of individuals moving on the surface of the Earth), has not been studied yet, as far as we know.

The first part of this report is then concerned with further study of these time-continuous Vicsek models (we also consider here dynamics in an arbitrary dimension $n \geqslant 2$ instead of the only case $n = 3$). In particular, since the parameter ν of relaxation was arbitrarily introduced in the model (and such a parameter is needed to define properly the relaxation), we are free to take a more general form for this parameter. In the original work [28], this parameter could depend on the angle between the velocity of the particle and its target direction. In Chapter 1, we let ν depend also on a local density $\bar{\rho}$ and we introduce anisotropy in the kernel of observation, that is to say that the way each particle compute the target orientation with respect to their neighbors may depend on the orientation of the particle. This enables to model for example a restricted angle of vision for the individuals, or the fact that in some species, the individuals take more into account the ones located behind, in order to avoid to be eaten (this is called a cannibalistic interaction and have been observed in [83] for a species of locust). In Chapter 2, we take ν proportional to the absolute value of the mean momentum of the neighbors. That is to say that the individuals tends to relax more rapidly to the direction of their neighbors if these last ones are numerous and strongly aligned. This positive feedback on the alignment strength leads to the apparition of phase transition, recovering the features of the original discrete model, which gives rise to challenging issues. Finally, the main object of Chapter 3 is the introduction of a generalization of the time-continuous Vicsek model, when the positions of the particles are constrained to live on a Riemannian manifold, with numerical simulations in the case of the 2-dimensional unit sphere. This generalized model includes the model of [28] and of Chapter 2, when the manifold is $\mathbb{R}^n$. The details of the main contributions brought by the study of these generalizations of the time-continuous Vicsek are given in the next section.

The model introduced in Chapter 2 led to the study of its spatial-homogeneous version on the unit sphere $\mathbb{S}$ of $\mathbb{R}^n$, which presents the same property of phase transition. When studying this problem, we remarked that this was a special case of a broad class of models described by the so called Doi equation (or Smoluchowski equation), a nonlinear and nonlocal equation of the following form:

$$\begin{cases} \partial_t f = \nabla_\omega \cdot (f \nabla \Psi_f) + \tau \Delta_\omega f, \\ \Psi_f(\omega, t) = \int_{\mathbb{S}} K(\omega, \bar{\omega})\, f(t, \bar{\omega})\, \mathrm{d}\bar{\omega}. \end{cases} \tag{2.3}$$

This equation was introduced by Doi [32] as a gradient flow equation for the Onsager free energy functional:

$$\mathcal{F}(f) = \tau \int_{\mathbb{S}} f(.,\omega) \ln f(.,\omega) \mathrm{d}\omega + \tfrac{1}{2} \int_{\mathbb{S}\times\mathbb{S}} K(\omega,\bar{\omega}) f(.,\omega)\, f(.,\bar{\omega})\, \mathrm{d}\omega \mathrm{d}\bar{\omega}. \tag{2.4}$$

This functional was proposed by Onsager [65] to describe the equilibrium states of suspensions of rod-like polymers, given by the critical points of this functional.

In the original work of Onsager, the kernel had the form $K(\omega, \bar{\omega}) = |\omega \times \bar{\omega}|$, but there is another form, introduced later by Maier and Saupe [58], which leads to similar quantitative results: $K(\omega, \bar{\omega}) = \frac{1}{n} - (\omega \cdot \bar{\omega})^2$. In particular, one observes a phenomenon of hysteresis when the parameter τ, which represents a temperature, goes from large to small values, and back to large values.

The model we were interested in corresponds to the case $K(\omega, \bar{\omega}) = -\omega \cdot \bar{\omega}$, called the dipolar potential, and few studies have been done concerning this model alone. The study of this model is the object of Chapter 4, motivated by the better understanding of the spatial inhomogeneous version of Chapter 2, and opened us to the study of the Doi equation with Maier–Saupe potential, which has received recent interest, from the point of view of rigorous mathematical analysis.

Let us review what have been done previously with respect to the mathematical study of this equation.

The characterization of equilibria started in 2004 in dimension $n = 2$ for the Maier–Saupe potential with the paper [20] containing a partial result, which was then completed by three independent groups in [22, 38, 57] (moreover, a whole family of different kernels is treated in [38] including the dipolar potential, still in dimension $n = 2$). In the case where the temperature τ is greater than or equal to $\frac{1}{4}$, the uniform distribution is the unique steady-state, and when $\tau < \frac{1}{4}$, there is also another family of equilibria, which are non-isotropic, symmetric, and differ from one to another by a simple rotation (called nematic equilibria).

The case of the dimension 3 is a little bit more elaborated, since we need first to show that any steady-state is axisymmetric. After the partial result [20], the complete characterization was provided in 2005, independently in [37, 55, 88]. One can observe a fascinating hysteresis phenomena with two thresholds for the temperature: $\tau_c = \frac{2}{15}$ and $\tau^* > \tau_c$. When $\tau > \tau^*$, the uniform distribution is the unique steady-state, when $\frac{2}{15} < \tau < \tau^*$, two other families of prolate (concentrated around two antipodal points) nematic equilibria appear, and when $\tau < \frac{2}{15}$, one of this families transforms into oblate equilibria (concentrated around a great circle). Analyzing stability as local minimization of Onsager free energy, this last family is proved to be unstable for $\tau < \tau^*$, as well as the uniform distribution for $\tau < \frac{2}{15}$. The other equilibria are stable in this sense. Hence, starting from a large τ, the only stable equilibrium (the uniform distribution) stays stable until τ reaches $\frac{2}{15}$, and starting from a small τ, the only family of stable equilibria (the prolate nematic equilibria) stays stable until τ reaches $\tau^* > \frac{2}{15}$, which gives the hysteresis phenomenon.

The paper [37] by Fatkullin and Slastikov also considers the case of the dipolar potential in dimension 3: when $\tau \geqslant \frac{1}{3}$, the uniform distribution is the only equilibrium, and a family of equilibria which differ from one to another by a is simple rotation is added when $\tau < \frac{1}{3}$, where the uniform equilibrium becomes unstable, in the sense of the minimization of the free energy.

In [89], a coupling between the Maier–Saupe and the dipolar potential is proposed, and the only stable equilibria are proved to be symmetric. And finally, recently, a unified characterization of these equilibria in many cases has been provided [78], including the case of the Maier–Saupe potential in any dimension. The main idea is to prove that the so-called orientational tensor order parameter is a matrix with at most two distinct eigenvalues, which allows to reduce the problem.

Regarding the dynamics in time, a few results were given, for the Maier–Saupe potential only, in dimension 2 and 3. Existence, uniqueness, non-negativity, and spatial-analyticity of a solution are claimed for a continuous nonnegative initial condition in [19, 21]. The system is proved to be dissipative in a certain Gevrey class of solution. Recently, the existence of inertial manifolds has been established [76, 77]. But this does not provide convergence in time to a given equilibrium.

A lot of variants were proposed and studied [80, 85, 87, 90, 75, 39] including external forces such as elongational force or shear flow, or modelling more complex phenomena with space dependence. And finally, very recently, some results were provided in dimension 2 to understand the case of the original Onsager kernel [18, 56, 79, 81], based on the analysis of the steady states.

Our main contributions to this field concerns the dynamical description of the system as time goes to infinity, which has not been treated a lot, and will be detailed in the next section.

3 Main contributions

The study of different time-continuous versions of the Vicsek model has given some interesting results: introducing modifications in the model let us understand the key features of the model, those which show some kind of robustness with respect to the final macroscopic limit.

In Chapter 1, the main result is that the macroscopic model (2.2) is still the formal limit of the mean-field model, even if the kernel of observation is non-isotropic, and if the parameters ν and d depend on a local density $\bar{\rho}$. This confirms this macroscopic model as a natural model arising as a model of displacement of a large number of particles interacting on their alignment and with a constraint of unit speed, since it appears also for another kind of model of displacement called "Persistent Turning Walker Model", when alignment interaction is taken in account [30]. All the information from the modifications which have been introduced appears through the coefficients c_1, c_2 and λ. For example, here, since the parameters of the model depend on a local density $\bar{\rho}$, so do the coefficients of the macroscopic model.

One of the advances that have been achieved in this chapter is also a clear statement of the problem in any dimension $n \geqslant 2$ in a unified framework. The methodology of generalized collisional invariants is still valid, and we have proved that they have a natural definition in this framework.

Finally, a specific result of this chapter is the presentation of a method which allows to have an asymptotic expansion of the coefficients of the model, up to any order, in any dimension, when the concentration parameter $\kappa = \frac{\nu}{d}$ tends to zero or to infinity. This allows to investigate the properties of the coefficients, even in the original model, where we see that the coefficient c_2 is always smaller than c_1 in the two limits $\kappa \to 0$ and $\kappa \to \infty$. This also proves that the macroscopic model can be non-hyperbolic, since the coefficient λ can be negative, and this is really a new feature of this model, which leads to important questions.

In the model of Chapter 2, we have found a way to get a macroscopic phase transition, while having a time-continuous model very close to the discrete one. Using

results of Chapter 4, together with a fine analysis of a specific Poincaré constant, we are able to provide arguments which confirm the convergence, at each point, to a local equilibrium. This last one can be of two different types, either the uniform distribution, isotropic on the sphere, if the density ρ is less than the critical threshold $\rho^* = n$, or a distribution with a given orientation Ω in the case where $\rho > \rho^*$.

The mathematical treatment of this phase transition consists in the derivation of two different models, depending whether the density is under or above the threshold $\rho^* = n$. We finally get a two-phase macroscopic model, with nonlinear diffusion in the region of low density, and still the macroscopic model (2.2) in the region of high density. The description of the behavior of the boundary between these two regions is a challenging problem. Once again, the model is naturally set in a n-dimensional framework, and the results are stated in a unified framework.

The last important thing to note is that we can directly use the results of Chapter 1 which concern the asymptotic expansions of the coefficients, and we get that $\lambda < 0$ in the two limit regimes. Using numerical computations, we see that we actually have $\lambda < 0$ in any case. This means that the system (2.2) is non-hyperbolic in all the ordered region of high density. However, under the constraint that the dynamics only take place along one direction, we obtain a reduced model which presents a less pathological behavior, and we have hyperbolicity in some regions of the states space.

The introduction of the time-continuous Vicsek model on a Riemannian manifold, done in Chapter 3, is, to our knowledge, a really new thing. We have been able to define a general model which includes most of the models studied in Chapters 1-2, and also the original continuous model of [28]. Under regularity restrictions on the kernel of observation and on the coefficient ν of the model, we prove the propagation of chaos, following the very recent work [13], and we obtain a mean-field limit which corresponds exactly to the analogous of (2.1) on a Riemannian manifold.

The numerical simulations performed on the sphere $\mathbb{S}_2$ give then a new vision on the collective motion of particles with unit speed.

We now turn to the description of our main contributions to the analysis of the dynamics in Doi equation (2.3).

The first thing to emphasize is that we have made a link between subjects which were not related at first glance. One of them comes from biology, the other from the study of suspensions of rod-like polymers, which are far to be self-propelled particles. The common point is that the dynamics take place on the unit sphere. Actually, to be precise, in the case of rod-like polymers, the orientation is an element of the projective space, since we do no distinguish between a rod and its opposite (the rod does not carry an arrow). But this is convenient to work with functions on the sphere, so the functions are considered to be even. This consideration makes no sense with the dipolar potential since, for even functions, the equation (2.3) with dipolar potential reduces to the heat equation.

In the case of the dipolar potential, our contribution constitutes the main part of the study, as far as we know. The equilibria had been classified before by Fatkullin and Slastikov in dimension 2 [38] and 3 [37]. Our work in Chapter 4 gives first a complete classification of the steady-states in any dimension. But it also includes results of existence and uniqueness, instantaneous regularity, positivity, and uniform bounds

on any Sobolev space H^s for an initial non-negative condition in any H^p, $p \in \mathbb{R}$. From this, we can then get an adapted version of LaSalle's principle which gives that the solution converges to a unique set of equilibria. Then, we expand the Onsager free energy and its dissipation term around a moving equilibrium adapted to f, and finally, using an ODE argument, we can control the displacement of this moving equilibrium. Our work gives that any solution converges to a given equilibrium, with exponential rate when τ is not the critical value $\frac{1}{n}$, and with algebraic rate when $\tau = \frac{1}{n}$. Moreover, we can classify the types of equilibria of the limit with respect to the initial condition: when $\tau < \frac{1}{n}$, the only initial conditions leading in long time to the uniform distribution are those with vanishing first moment.

Using spherical harmonics in dimension n, we provide an astonishing conservation relation involving the so-called conformal Laplacian. In the case where $\tau > \frac{1}{n}$, this conservation relation can be seen as a dissipation of a new entropy, which gives global exponential convergence towards the uniform distribution.

In Chapter 5, we use the tools developed for the dipolar potential in the framework of the more studied case of Maier–Saupe potential, giving new insight in the case of dimension 2, which is very similar to the dipolar potential : we have convergence to a given equilibrium for any initial condition, with exponential rate when $\tau \neq \frac{1}{4}$. We also use here a special cancellation, which had been observed in [19] in some special case, but not used to its maximal capacity. We can also classify the types of equilibria of the limit with respect to the initial condition: when $\tau < \frac{1}{4}$, the only initial conditions leading in long time to the uniform distribution are those with vanishing second moment.

4 Presentation of the results

Ch. 1 A continuum model for alignment of self-propelled particles with anisotropy and density-dependent parameters

In this chapter, we study the following model, for N particles with positions $X_k \in \mathbb{R}^n$ and orientations $\omega_k \in \mathbb{S}$ (the unit sphere of $\mathbb{R}^n$), with $k \in [\![1, N]\!]$, written as a system of coupled stochastic differential equations in the Stratonovich formulation:

$$\begin{cases} \mathrm{d}X_k = \omega_k \mathrm{d}t, \\ \mathrm{d}\omega_k = \nu(\bar{\rho}_k)(\mathrm{Id} - \omega_k \otimes \omega_k)\bar{\omega}_k \,\mathrm{d}t + \sqrt{2d(\bar{\rho}_k)}\,(\mathrm{Id} - \omega_k \otimes \omega_k) \circ \mathrm{d}B_t^k, \end{cases} \tag{4.5}$$

where (B_t^k) are independent standard Brownian motions on $\mathbb{R}^n$. This system expresses the fact that the particles move at constant speed 1, following their orientation, which relaxes to the target orientation $\bar{\omega}$ with rate $\nu(\bar{\rho})$ and subjected to a Brownian motion of intensity $\sqrt{2d(\bar{\rho})}$ (the term $\mathrm{Id} - \omega_k \otimes \omega_k$ is the projection on the hyperplane orthogonal to ω_k).

The coupling terms are the density $\bar{\rho}_k$ and the target orientation $\bar{\omega}_k$, given by

$$\bar{\rho}_k = \frac{1}{N}\sum_{j=1}^{N} \widetilde{K}\left(|X_j - X_k|, \tfrac{X_j - X_k}{|X_j - X_k|}\cdot \omega_k\right),$$
$$\bar{\omega}_k = \frac{\bar{J}_k}{|\bar{J}_k|}, \text{ where } \bar{J}_k = \frac{1}{N}\sum_{j=1}^{N} K\left(|X_j - X_k|, \tfrac{X_j - X_k}{|X_j - X_k|}\cdot \omega_k\right)\omega_j,$$

where K and $\widetilde{K}$ are observation kernels used to compute the local average of a quantity carried by the neighbors. For example, to take into account only the neighbors located "in front", and within a given radius R, of one particle, the kernel would be $K(r,\gamma) = \mathbb{1}_{\{r\leqslant R\}}\mathbb{1}_{\{\gamma\geqslant 0\}}$.

The positive functions ν and d are arbitrary. The choice of ν and d constant, together with the fact that the kernel K depends only on its first variable, correspond exactly to the time-continuous version of the Vicsek model proposed in [28].

The purpose of this chapter is to derive, from the individual particle system (4.5), the following macroscopic model:

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (c_1(\rho)\rho\Omega) = 0, \\ \rho\,(\partial_t \Omega + c_2(\rho)(\Omega\cdot\nabla_x)\Omega) + \lambda(\rho)\,(\mathrm{Id} - \Omega\otimes\Omega)\nabla_x\rho = 0, \end{cases} \tag{4.6}$$

where the functions c_1, c_2, and λ will be specified in (4.9) and (4.10)-(4.11).

The first step is to write a mean-field model of the particle system, as in (2.1), and then to perform a hydrodynamic scaling, which consists in introducing a small parameter ε and writing $f^\varepsilon(\varepsilon x, \omega, \varepsilon t) = f(x,\omega,t)$. After some expansions, we get

$$\varepsilon(\partial_t f^\varepsilon + \omega\cdot\nabla_x f^\varepsilon + \alpha\, P(f^\varepsilon) + \widetilde{\alpha}\,\widetilde{P}(f^\varepsilon)) = Q(f^\varepsilon) + O(\varepsilon^2)\,, \tag{4.7}$$

where the constants α and $\widetilde{\alpha}$ depend only on the observation kernels K and $\widetilde{K}$. These constants are positive if the kernel is directed forward, and the more acute the "angle of vision", the bigger the constant related to the kernel. The operators P and $\widetilde{P}$ act on f and its space derivatives, and Q is given by

$$\begin{aligned} Q(f) =& -\nu(\rho_f)\nabla_\omega\cdot((\mathrm{Id}-\omega\otimes\omega)\Omega_f f) + d(\rho_f)\Delta_\omega f, \\ \rho_f =& \int_{\omega\in\mathbb{S}} f(.,\omega)\,\mathrm{d}\omega\,, \\ \Omega_f =& \frac{j_f}{|j_f|}, \text{ with } j_f = \int_{\omega\in\mathbb{S}} \omega\, f(.,\omega)\,\mathrm{d}\omega\,, \end{aligned}$$

In view of (4.7), when $\varepsilon\to 0$, the function f^ε becomes an equilibrium, that is to say a function f^0 such that $Q(f^0) = 0$. Introducing the Von-Mises distribution of concentration parameter $\kappa > 0$ and orientation $\Omega\in\mathbb{S}$:

$$M_{\kappa\Omega}(\omega) = \frac{e^{\kappa\,\omega\cdot\Omega}}{\int_{\mathbb{S}} e^{\kappa\,\upsilon\cdot\Omega}\,\mathrm{d}\upsilon}, \tag{4.8}$$

and defining the linear operator $L_{\kappa\Omega}$ by

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

we remark that the operator $Q(f)$ can be written as $Q(f) = -d(\rho_f)L_{\kappa(\rho_f)\Omega_f}(f)$, with $\kappa(\rho) = \frac{\nu(\rho)}{d(\rho)}$, and hence it is easy to see that if $Q(f) = 0$, then f is of the form $\rho M_{\kappa(\rho)\Omega}$.

We have then that $j_{M_{\kappa\Omega}} = c_1(\kappa)\Omega$, with

$$c_1(\kappa) = \langle \cos\theta \rangle_{M_\kappa}, \quad \text{where} \langle \gamma(\cos\theta) \rangle_{M_\kappa} = \frac{\int_0^\pi \gamma(\cos\theta) e^{\kappa\cos\theta} \sin^{n-2}\theta \, \mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta} \sin^{n-2}\theta \, \mathrm{d}\theta}. \tag{4.9}$$

If we integrate equation (4.7) on the sphere, we get $\partial_t\rho + \nabla_x \cdot (j) = 0$, hence we have the equation for the evolution of mass:

$$\partial_t\rho + \nabla_x \cdot (c_1(\kappa)\rho\,\Omega) = 0.$$

To get the equation on Ω, we define the generalized collisional invariants $\mathcal{C}_{\kappa\Omega}$ (associated to $\kappa > 0$ and $\Omega \in \mathbb{S}$) as the following vector space:

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

We find that a generalized collisional invariant is of the form $C + h_\kappa(\omega\cdot\Omega)A\cdot\omega$, with A arbitrary, orthogonal to Ω, and h_κ a given smooth positive function (it is the solution to an elliptic problem). Hence we can multiply (4.7) by $h_\kappa(\omega\cdot\Omega)A\cdot\omega$ and integrate, we get that $A\cdot X = 0$ for a given vector X, and for all the vectors A which are orthogonal to Ω. So finally X is aligned with Ω, and writing $(\mathrm{Id} - \Omega\otimes\Omega)X = 0$ gives exactly the second equation of (4.6), with

$$c_2 = \widetilde{c}_1 - \alpha\, d\,(n\,\widetilde{c}_1 + \kappa\,\langle\cos^2\theta\rangle_{\widetilde{M}_\kappa}), \text{ with } \quad \widetilde{c}_1 = \langle\cos\theta\rangle_{\widetilde{M}_\kappa}, \tag{4.10}$$

$$\lambda = \tfrac{1}{\kappa} + \rho\,\tfrac{\dot\kappa}{\kappa}\,[\,\widetilde{c}_1 - c_1 + \widetilde{\alpha}\,d\,(\kappa\,\langle\sin^2\theta\rangle_{\widetilde{M}_\kappa} - n\,\widetilde{c}_1)\,] + \tfrac{1}{2}\,\widetilde{\alpha}\,\rho\,\dot{d}\,(n - 1 + \kappa\,\widetilde{c}_1), \tag{4.11}$$

where the dot denotes the derivative with respect to ρ, and with the notation

$$\langle\gamma(\cos\theta)\rangle_{\widetilde{M}_\kappa} = \frac{\int_0^\pi \gamma(\cos\theta) h_\kappa(\cos\theta) e^{\kappa\cos\theta} \sin^n\theta \,\mathrm{d}\theta}{\int_0^\pi h_\kappa(\cos\theta) e^{\kappa\cos\theta} \sin^n\theta \,\mathrm{d}\theta}. \tag{4.12}$$

Finally, in a second part, we develop a method to get an asymptotic expansion, up to any order, when $\kappa \to 0$ or $\kappa \to \infty$, of expressions of the form $\langle f(\theta)\rangle_{M_\kappa}$ and $\langle f(\theta)\rangle_{\widetilde{M}_\kappa}$. This enables us to compute the expansions of the coefficients, and to prove that the coefficient λ may become negative, and hence the system (4.6) loses its hyperbolicity.

Ch. 2 Macroscopic limits and phase transition in a system of self-propelled particles

In this chapter, the modification of the individual model seems, at first glance, to be a simplification: we replace $\nu\bar{\omega}_k$ in (4.5), by $\nu\bar{J}_k$, that is to say we do not divide by the norm. The interaction is then a sum of binary interactions, still understood

as a relaxation towards $\bar{\omega}_k$, but with rate proportional to $|\bar{J}_k|$. The system reads

$$\begin{cases} \mathrm{d}X_k = \omega_k \mathrm{d}t, \\ \mathrm{d}\omega_k = \nu(\mathrm{Id} - \omega_k \otimes \omega_k)\bar{J}_k \,\mathrm{d}t + \sqrt{2d}\,(\mathrm{Id} - \omega_k \otimes \omega_k) \circ \mathrm{d}B_t^k, \end{cases} \tag{4.13}$$

$$\bar{J}_k = \frac{1}{N}\sum_{j=1}^{N} K(X_j - X_k)\omega_j, \tag{4.14}$$

where (B_t^k) are independent standard Brownian motions on $\mathbb{R}^n$. The mean-field limit is then given by

$$\begin{cases} \partial_t f + \omega \cdot \nabla_x f + \nu \nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega)\bar{J}_f\, f) = d\Delta_\omega f \\ \bar{J}_f(x,t) = \int_{\mathbb{S}} (K * f)(x,\omega,t)\,\omega \,\mathrm{d}\omega, \end{cases} \tag{4.15}$$

where $*$ denotes the convolution with respect to the space variable. With a change of scale in space, time, and density (relaxing the fact that f is a probability density function on $\mathbb{R}^n \times \mathbb{S}$), we can assume without loss of generality that $\nu = d = 1$ and $\int_{\mathbb{R}^n} K(\xi)\mathrm{d}\xi = 1$. Let us notice that this mean-field limit is easy to treat, since we do not have the singularity at $\bar{J} = 0$, and propagation of chaos has been indeed shown recently in [13].

The hydrodynamic scaling gives, if $K(\xi)$ depends only on $|\xi|$:

$$\varepsilon(\partial_t f^\varepsilon + \omega \cdot \nabla_x f^\varepsilon) = Q(f^\varepsilon) + O(\varepsilon^2), \tag{4.16}$$

with

$$\begin{cases} Q(f) = -\nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega) J_f f) + \Delta_\omega f \\ J_f(x,t) = \int_{\mathbb{S}} f(x,\omega,t)\,\omega \,\mathrm{d}\omega. \end{cases} \tag{4.17}$$

Here, the equilibria of Q are still given by $\rho M_{\kappa\Omega}$, with arbitrary $\rho > 0$ and $\Omega \in \mathbb{S}$, where $M_{\kappa\Omega}$ is defined in (4.8), and where the concentration parameter κ satisfies the compatibility condition $\rho\kappa = c(\kappa)$, with $c(\kappa)$ defined in (4.9). We then have the following alternative:

Proposition 1. *Compatibility condition, equilibria.*

- *If $\rho \leqslant n$, there is only one solution to the compatibility condition: $\kappa = 0$. The only equilibrium is the constant function $f = \rho$.*
- *If $\rho > n$, the compatibility condition has exactly two solutions: $\kappa = 0$ and one unique positive solution, which will be denoted $\kappa(\rho)$. Apart from the constant function $f = \rho$ (the case $\kappa = 0$), the equilibria form a manifold of dimension n: the functions of the form $f = \rho M_{\kappa(\rho)\Omega}$, where $\Omega \in \mathbb{S}$ is an arbitrary unit vector.*

With arguments of stability and rate of convergence to the equilibrium for the space-homogeneous version of (4.16) provided by the results of Chapter 4, we shall consider a macroscopic model composed of two zones: the formal limit, as $\varepsilon \to 0$ of the function f^ε is given by a function $f(x,\omega,t)$ which satisfies

- $f(x,\omega,t) = \rho(x,t)$ with $\rho(x,t) < n$, in the "disordered" region $\mathcal{R}_d$ where we have $n - \rho^\varepsilon(x,t) \gg \varepsilon$,

- $f(x,\omega,t) = \rho(x,t) M_{\kappa(\rho)\Omega(x,t)}$ with $\rho(x,t) > n$, in the "ordered" region $\mathcal{R}_o$ where we have $\rho^\varepsilon(x,t) - n \gg \varepsilon$.

In the disordered region, the formal limit satisfies $\partial_t \rho = 0$, therefore we are interested in a first-order correction in ε of the model. A Chapman-Enskog expansion leads to a non-linear diffusion:

Proposition 2. *Diffusion model in the disordered zone.*

When ε goes to zero, the (formal) first order correction of the solution of the mean-field rescaled system, in the region $\mathcal{R}_d \subset \mathbb{R}^n$ where we have $n - \rho^\varepsilon(x,t) \gg \varepsilon$, is given by

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

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

$$\partial_t \rho^\varepsilon = \frac{\varepsilon}{n-1} \nabla_x \cdot \left(\frac{1}{n-\rho^\varepsilon} \nabla_x \rho^\varepsilon \right). \tag{4.18}$$

In the ordered region, the method of generalized collisional invariants works to derive the hydrodynamic model (2.2):

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (\rho \Omega) = 0, \\ \rho(\partial_t \Omega + \widetilde{c}(\Omega \cdot \nabla_x)\Omega) + \lambda(\mathrm{Id} - \Omega \otimes \Omega) = 0, \end{cases}$$

where the speed c depending on $\kappa(\rho)$ is defined in (4.9), the speed $\widetilde{c}$ is given by $\langle \cos\theta \rangle_{\widetilde{M}_{\kappa(\rho)}}$ with the notation (4.12) and

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

The method of asymptotic expansion introduced in Chapter 1 allows to get the following expansions:

Proposition 3. *Expansion of the coefficients when the density is large or close to the critical threshold.*

We have the following expansions for the coefficients c, $\widetilde{c}$, and λ.

- *When the density ρ is close to n:*

$$\begin{aligned} c &= \tfrac{\sqrt{n+2}}{n}\sqrt{\rho - n} + O(\rho - n), \\ \widetilde{c} &= \tfrac{2n-1}{2n\sqrt{n+2}}\sqrt{\rho - n} + O(\rho - n), \\ \lambda &= \tfrac{-1}{4\sqrt{n+2}} \frac{1}{\sqrt{\rho - n}} + O(1). \end{aligned}$$

- *When the density ρ tends to infinity:*

$$\begin{aligned} c &= 1 - \tfrac{n-1}{2}\rho^{-1} + \tfrac{(n-1)(n+1)}{8}\rho^{-2} + O(\rho^{-3}), \\ \widetilde{c} &= 1 - \tfrac{n+1}{2}\rho^{-1} - \tfrac{(n+1)(3n+1)}{24}\rho^{-2} + O(\rho^{-3}), \\ \lambda &= -\tfrac{n+1}{6}\rho^{-2} + O(\rho^{-3}). \end{aligned}$$

In particular, we see that since $\lambda < 0$ in these two limiting cases (numerically, we can see that this is always the case), then the system is not hyperbolic. If we constrain the dynamics to take place only along one direction, we get a condition of hyperbolicity involving the angle between Ω and this direction of propagation, which must be smaller than a critical angle θ_c which satisfies:

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

Ch. 3 An individual time-continuous Vicsek model on a Riemannian manifold

In this chapter, we extend the dynamics of the Vicsek model to a general Riemannian manifold. Most of the numerical studies on self-organized dynamics have been done on the same geometrical space: the flat torus, or equivalently a square box with periodic boundary conditions. But this particular geometry has an influence on the dynamics. For this reason, we would like to perform analytical and numerical studies of the Vicsek model on a general Riemannian manifold.

Our first goal is to write the evolution of an oriented particle (x, ω) on a given Riemannian manifold M with a metric g. To do so, we introduce the unit tangent bundle UM associated to the manifold M:

$$UM := \{(x, \omega) \mid x \in M,\ \omega \in T_xM \ \text{ and } |\omega|_g = 1\},$$

where T_xM is the tangent space of M at point x. The manifold UM is the natural space to consider for the evolution of an oriented particle with unit speed.

We first propose a model describing the dynamics of a single particle (x, ω) moving with unit speed, in an orientational force field η and whose orientation is submitted to a Brownian motion of intensity $\sqrt{2d}$. In local coordinates, it is given by a Stratonovich stochastic differential equation:

$$\begin{cases} \mathrm{d}x^i = \omega^i \,\mathrm{d}t, \\ \mathrm{d}\omega^i = \eta^i \,\mathrm{d}t + \sqrt{2d}\sum_j (\sigma_{ij} - \omega^i \sum_{k,\ell} \omega^\ell \, g_{\ell k} \, \sigma_{kj}) \circ \mathrm{d}B_t^j - \sum_{j,k} \Gamma^i_{jk} \, \omega^j \, \omega^k \,\mathrm{d}t, \end{cases}$$

where B_t is a standard Brownian motion in $\mathbb{R}^n$ (or equivalently, B_t^i are n independent real one-dimensional standard Brownian motions), and (σ_{ij}) is the inverse symmetric square root of the matrix (g_{ij}) of the metric in local coordinates. We prove that this system is well defined as a stochastic process with values in UM, and provide the partial differential equation satisfied by its law.

We then give a global formulation of this system in an extrinsic point of view, in the case where the manifold M is isometrically embedded in $\mathbb{R}^m$, for $m \geqslant n$:

$$\begin{cases} \mathrm{d}x = \omega \,\mathrm{d}t, \\ \mathrm{d}\omega = \eta \,\mathrm{d}t + \sqrt{2d}\,\pi_{x,\omega} \circ \mathrm{d}B_t + \mathrm{I\!I}_x(\omega, \omega) \,\mathrm{d}t, \end{cases}$$

where B_t is a standard Brownian motion in $\mathbb{R}^{2m}$, where $\pi_{x,\omega}$ is the projection onto the tangent space $T_\omega \mathbb{S}_g^x$ at ω of $\mathbb{S}_g^x$ (the unit sphere of the tangent space T_xM),

and where $\mathrm{I\!I}_x(\omega,\omega)$ is the second fundamental form associated to the embedded Riemannian manifold.

In a second part, we propose an extension of the local average velocity $\bar{J}$ at a point x in M using parallel transport along geodesics. Thus, the Vicsek dynamics on the manifold are simply given as a relaxation of a particle velocity ω_k towards the orientation of the local average velocity $\bar{J}(x_k)$. We prove the existence of a kinetic mean-field equation associated with this dynamics (proving the so-called propagation of chaos for the stochastic system), given by

$$\partial_t f + g_x(\omega, \nabla_x^h f) + \nabla_\omega^x \cdot (\nu\, \pi_{x,\omega} J[f] f) = d\Delta_\omega^x f,$$

where $\nabla_\omega^x\cdot$ and Δ_ω^x are the divergence and Laplace–Beltrami operators on $\mathbb{S}_g^x$, the unit sphere of the tangent space T_xM, where the "horizontal gradient" $\nabla_x^h f$ corresponds to the spatial gradient of f, and where

$$J[f](x,\omega) = \int_{UM} K(x,\omega,x')\tau_{x,x'}(\omega') f(x',\omega')\,\mathrm{d}\mu(x',\omega'),$$

where $\tau_{x,x'}(\omega')$ is the parallel transport of ω' along the geodesic from x to x', K is a kernel of observation, and μ is a natural measure on UM, called Liouville or kinematic measure.

Finally, we illustrate our model by performing some numerical simulations on the sphere $\mathbb{S}_2$. We observe the formations of groups moving in the same direction. But in contrast with the Vicsek model on the flat torus, there is no longer emergence of one global direction for the whole group of particles.

Ch. 4 Dynamics in a kinetic model of oriented particles with phase transition

In this chapter, we study the dynamics of the Doi equation (2.3) with the dipolar potential, which takes the following form:

$$\begin{cases} \partial_t f = -\nabla_\omega \cdot ((\mathrm{Id} - \omega\otimes\omega) J[f] f) + \tau \Delta_\omega f, \\ J[f] = \int_{\mathbb{S}} \omega\, f(.,\omega)\,\mathrm{d}\omega. \end{cases} \tag{4.19}$$

We first give results of existence and uniqueness of a weak solution, with an initial condition in an arbitrary Sobolev space.

Theorem 1. *Given an initial probability measure f_0 in $H^s(\mathbb{S})$ (which is always the case for $s < -\frac{n-1}{2}$), there exists a unique weak solution f to (4.19) such that $f(0) = f_0$. This solution is global in time. Moreover, $f \in C^\infty((0,+\infty)\times\mathbb{S})$, with $f(t,\omega) > 0$ for all positive t.*

We also have the following instantaneous regularity and uniform boundedness estimates (for $m \in \mathbb{N}$, the constant C depending only on τ, m, s), for all $t > 0$:

$$\|f(t)\|_{H^{s+m}}^2 \leqslant C\left(1 + \frac{1}{t^m}\right)\|f_0\|_{H^s}^2.$$

In appendix, we prove furthermore that the solution is analytic in space.

Defining the Onsager free energy $\mathcal{F}$ and its dissipation term $\mathcal{D}$ by

$$\mathcal{F}(f) = \tau \int_{\mathbb{S}} f \ln f - \tfrac{1}{2}|J[f]|^2,$$
$$\mathcal{D}(f) = \int_{\mathbb{S}} f|\nabla_\omega(\tau \ln f - \omega \cdot J[f])|^2,$$

we have, for a solution f of Doi equation (4.19), the following conservation relation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F} + \mathcal{D} = 0.$$

This allows us to give an adaptation of LaSalle's invariance principle to our PDE framework.

Proposition 4. *LaSalle's invariance principle*

Let f_0 be a probability measure on the sphere $\mathbb{S}$. We denote by $\mathcal{F}_\infty$ the limit of $\mathcal{F}(f(t))$ as $t \to \infty$, where f is the solution to Doi equation (4.19) with initial condition f_0.

Then the set $\mathcal{E}_\infty = \{f \in C^\infty(\mathbb{S})$ s.t. $\mathcal{D}(f) = 0$ and $\mathcal{F}(f) = \mathcal{F}_\infty\}$ is not empty.

Furthermore $f(t)$ converges in any H^s norm to this set of equilibria (in the following sense):

$$\lim_{t\to\infty} \inf_{g\in\mathcal{E}_\infty} \|f(t) - g\|_{H^s} = 0.$$

We then characterize the equilibria, of the form $M_{\kappa\Omega}$ where κ satisfies the compatibility condition $c(\kappa) = \tau\kappa$.

Proposition 5. *Compatibility condition*

- *If $\tau \geqslant \frac{1}{n}$, there is only one solution to the compatibility condition: $\kappa = 0$. The only equilibrium is the constant function $f = 1$.*
- *If $\tau < \frac{1}{n}$, the compatibility condition has exactly two solutions: $\kappa = 0$ and one unique positive solution, that we will denote $\kappa(\tau)$. Apart from the constant function $f = 1$ (the case $\kappa = 0$), the equilibria form a manifold of dimension $n-1$: the functions of the form $f = M_{\kappa(\tau)\Omega}$, where $\Omega \in \mathbb{S}$ is an arbitrary unit vector.*

Using fine analysis on spherical harmonics in any dimension, we obtain a special cancellation, for a function h with mean zero on the sphere:

$$\int_{\mathbb{S}} \widetilde{\Delta}_{n-1} h \nabla_\omega h = 0,$$

where $\widetilde{\Delta}_{n-1}$ is the so-called conformal Laplacian on the unit sphere, given, for a spherical harmonic Y^ℓ of degree ℓ, by $\widetilde{\Delta}_{n-1}Y^\ell = \ell(\ell+1)\dots(\ell+n-1)(\ell+n-2)Y^\ell$. This is a differential operator when n is odd, and a pseudodifferential operator when n is even.

This special cancellation leads to a new conservation relation, for a probability density f solution to (4.19), of the form

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|f-1\|^2_{\widetilde{H}^{-\frac{n-1}{2}}} = -\tau\|f-1\|^2_{\widetilde{H}^{-\frac{n-3}{2}}} + \frac{1}{(n-2)!}|J[f]|^2,$$

where $\|\cdot\|_{\widetilde{H}^{-\frac{n-1}{2}}}$ and $\|\cdot\|_{\widetilde{H}^{-\frac{n-3}{2}}}$ are special Sobolev norms associated to the conformal Laplacian, equivalent to the usual $H^{-\frac{n-1}{2}}$ and $H^{-\frac{n-3}{2}}$ norms.

In the case where $\tau > \frac{1}{n}$, this conservation law can be seen as the dissipation of a new entropy given by $\|f-1\|^2_{\widetilde{H}^{-\frac{n-1}{2}}}$, and we get global exponential convergence to the uniform equilibrium, with rate $(n-1)(\tau-\frac{1}{n})$ in this weak norm, which can then be extended to any H^s norm, with $s > -\frac{n-1}{2}$.

If $J[f_0] \neq 0$ we prove that $J[f(t)] \neq 0$ for all $t > 0$ (if $J[f_0] = 0$, the equation reduces to the heat equation, so the solution converges exponentially fast to the uniform distribution). In the case where $\tau < \frac{1}{n}$, we can then define the unit vector $\Omega(t)$ as $\frac{J[f(t)]}{|J[f(t)]|}$. Using LaSalle's principle, we get that $f - M_{\kappa(\tau)\Omega(t)}$ converges to zero, so we can expand $\mathcal{D}$ and $\mathcal{F}$ around $M_{\kappa(\tau)\Omega(t)}$ in a "moving norm" (a weighted L^2, with the weight $M_{\kappa(\tau)\Omega(t)}$, which depends on time). We then get exponential convergence to zero of the difference $f - M_{\kappa(\tau)\Omega(t)}$. Finally, deriving the ODE satisfied by $\Omega(t)$, we can control its derivative by $\|f - M_{\kappa(\tau)\Omega(t)}\|$, which gives that $\Omega(t)$ converges with exponential rate towards $\Omega_\infty \in \mathbb{S}$. Using interpolation, we get the following result:

Proposition 6. *If $\tau < \frac{1}{n}$, there is an asymptotic exponential rate $r_\infty(\tau) > 0$ of convergence, in any H^p norm, to a given equilibrium.*

More precisely, for all $r < r_\infty(\tau)$, there exists $t_0 > 0$ (depending on f_0 and p) such that for all $t > t_0$, we have

$$\|f(t) - M_{\kappa\Omega_\infty}\|_{H^p} \leqslant e^{-rt}.$$

When τ is close to $\frac{1}{n}$ we have that $r_\infty(\tau) \sim 2(n-1)(\frac{1}{n}-\tau)$.

In the same spirit, in the critical case $\tau = \frac{1}{n}$, we expand $\mathcal{D}$ and $\mathcal{F}$ around the uniform distribution, and we get that the rate of convergence is given by $\frac{C}{\sqrt{t}}$.

Ch. 5 A note on the dynamics in the Doi equation with Maier–Saupe potential

In this short chapter, we show that the tools we used in the case of the dipolar potential can be adapted to get results for the case of the Maier–Saupe potential.

We consider the following non-local partial differential equation on $\mathbb{S}$, for a probability density function f on the sphere:

$$\begin{cases} \partial_t f = \nabla_\omega \cdot (f \nabla_\omega \Psi_f) + \tau \Delta_\omega f, \\ \Psi_f(\omega, t) = \int_{\mathbb{S}} K(\omega, \bar{\omega})\, f(t, \bar{\omega})\, \mathrm{d}\bar{\omega}. \end{cases} \tag{4.20}$$

The Maier–Saupe potential is given by $K(\omega, \bar{\omega}) = \frac{1}{n} - (\omega \cdot \bar{\omega})^2$.

In the general case of a polynomial kernel, we provide the same results of existence and uniqueness, of positivity and regularity than Theorem 1, and the adaptation of LaSalle's invariant principle (Proposition 4) is still valid.

We define the orientational tensor order parameter by

$$S[f] = \int_{\mathbb{S}} (\tfrac{1}{n}\mathrm{Id} - \omega \otimes \omega) f \mathrm{d}\omega,$$

and we give a property of dynamical instability of the uniform distribution when τ is under the critical value $\tau_c = \frac{2}{n(n+2)}$:

Proposition 7. *Instability of the uniform distribution below a threshold.*

If we have $S[f_0] = 0$, then we have $S[f(t)] = 0$ for all $t \geqslant 0$, and the Doi equation (4.20) *becomes the heat equation on the sphere. The solution converges exponentially fast to the uniform distribution.*

If we have $S[f_0] \neq 0$, then we have $S[f(t)] \neq 0$ for all $t \geqslant 0$. Moreover, in the case where $\tau < \frac{2}{n(n+2)}$, the solution cannot converge to the uniform distribution.

We finally show that, in dimension 2, we have the same results of convergence as for the case of the dipolar potential.

Part I

Variations on time-continuous Vicsek models

Chapter 1

A continuum model for alignment of self-propelled particles with anisotropy and density-dependent parameters

This chapter has given an article [41] which is about to be submitted in Mathematical Models and Methods in Applied Sciences.

Abstract

We consider the macroscopic model derived by Degond and Motsch from a time-continuous version of the Vicsek model, describing the interaction orientation in a large number of self-propelled particles. In this chapter, we study the influence of a slight modification at the individual level, letting the relaxation parameter depend on the local density and taking in account some anisotropy in the observation kernel (which can model an angle of vision).

The main result is a certain robustness of this macroscopic limit and of the methodology used to derive it. With some adaptations to the concept of generalized collisional invariants, we are able to derive the same system of partial differential equations, the only difference being in the definition of the coefficients, which depend on the density. This new feature may lead to the loss of hyperbolicity in some regimes.

We provide then a general method which enables us to get asymptotic expansions of these coefficients. These expansions shows, in some effective situations, that the system is not hyperbolic. This asymptotic study is also useful to measure the influence of the angle of vision in the final macroscopic model, when the noise is small.

Key words: Vicsek model, orientation interaction, anisotropy, collisional invariants, non-hyperbolicity, asymptotic study.

AMS Subject classification: 35M30, 35Q70, 35Q80, 82C22, 82C70, 92D50.

1 Introduction

The study of complex particle systems has given rise to some challenging issues [10], in a mathematical point of view. One of the interesting problem is to understand how a collective behavior can emerge with only localized interactions.

The Vicsek model [74] has been proposed as a minimalist model describing the behavior of individuals inside animal societies such as fish schools or flocks of birds. It is a minimal version of a more complete and realistic model [3, 67, 49, 23] based on three zones (of repulsion, alignment, and attraction). The Vicsek model only considers the alignment behavior, getting around the problem of confining the particles in the same region by imposing spatial periodicity (particles move on the flat torus). All the particles have constant speed and synchronously update their direction according to their neighbors, their new orientation vector being given by the mean direction (subjected to some angular noise) of all particles at distance less than a given radius. As the noise decreases (or the density increases), one can observe a phenomenon of phase transition, from a regime of disordered particles, to an ordered phase with strong correlations between orientations of particles [74, 2, 46].

Two main difficulties arise when we try to derive a macroscopic limit of this individual based model. First of all, the system is discrete in time: the time step is fixed, and the model is not built in the goal of letting it tend to zero. The second problem is that, except for the total mass, there is no obvious conservation relation, so a good candidate for a macroscopic model would probably be a non-conservative system of partial differential equations, but we lack conservation relations to obtain any equation other than the conservation of mass.

In [28], Degond and Motsch have proposed an approach to handle these two complications. First, they provide a time-continuous version of the individual based model, introducing a rate of relaxation towards the local mean direction, under the form of a new parameter ν, which can be viewed as a frequency of interaction between a particle and its neighbors. It is therefore possible to derive a kinetic mean-field limit of this model. Then they develop a method, defining the notion of generalized collisional invariants, which allows to derive the formal limit of this kinetic mean-field model, at large scale in space and time. This continuum limit is a non-conservative system of PDE for the local mass and the local orientation. Moreover, this system is proved to be hyperbolic.

The goal of the present chapter is to confirm the ability of this type of macroscopic model to describe the large scale dynamics of systems of self-propelled particles with orientation alignment, and to show that the notion of generalized collisional invariants is well adapted to derive this model from the microscopic mechanism of alignment. This was shown in [30] for a different type of alignment, based on the curvature control (for a model of displacement introduced in [29], designed to fit biological experiments [45]): the method which uses the generalized collisional invariants is successful to derive a macroscopic model which is the same as the "Vicsek hydrodynamics" of [28], but for the definition of the coefficients in the model. We will show that this is also the case when we slightly modify the individual model, in order to be more coherent with some numerical observations, and to model the influence of an angle of vision.

One of the properties of the macroscopic model of [28] which fails to represent the numerical observations is that the local equilibria have a constant order parameter. This order parameter is indeed only related to the ratio between the frequency ν of interaction and the intensity d of the noise. In numerical experiments on the Vicsek model [16], the order parameter depends on the local density of particles: one can observe, at large time, formation of travelling bands of high density, strongly ordered, moving through a disordered area of low density.

The first refinement on the model will be to define the local density $\bar{\rho}$ in the particular model as the mean number of particles in a neighboring area, and to make the parameters ν and d depend on $\bar{\rho}$. In a modelling point of view, this could be interpreted as the fact that, due to some social pressure, it is more likely to move and update the direction when there is a large number of particles around (so ν increases with $\bar{\rho}$), and that the fluctuation in the estimation of the mean velocity is smaller when a lot of particles are taken in account in the neighborhood (so d decreases with $\bar{\rho}$, see for example the way the vectorial noise is defined in [46, 16]). This dependence on local parameters for the noise parameter has been introduced in other models of collective behavior [33, 83].

In [28], the parameter ν does also depend on the angle between one particle direction and its target direction. For convenience, we will not take this in account for most results, but some computations have been done and will be given in appendix.

Another property of the mean-field model of [28] is that the type of local equilibrium for the rescaled model is unique. The loss of this uniqueness could play a role to understand the formation of patterns such as the travelling bands [36], and in some models of rod-like particles, we have indeed bistability in some regime [55]. This is not the case here, and we will see in Section 3 that we still have a unique kind of equilibrium associated to a local density ρ and a local orientation Ω.

The second refinement is to take into account some "angle of vision" in the model. In the original Vicsek model, the target orientation for a given particle is chosen to be the mean orientation of the neighbors located in a ball centered on this particle. We will use here a more general kernel of observation which can be non-isotropic. This refinement has been proposed in various models of swarming [1, 54].

The main result of this chapter is that the formal macroscopic limit of this model take the same form as the previous "Vicsek Hydrodynamic model" of [28], consisting in a conservation equation for the local density of particles, and an evolution equation for the mean orientation, which is not conservative (the velocity is constrained to be on the unit sphere). This system of PDE is quite similar to the Euler equations for gas dynamics, but presents some specific issues, for example there are two different velocities of propagation. The difference between our model and the macroscopic model of [28] relies on the definition of the coefficients of this model, and on the fact that they depend on the local density. This last feature allows the model to lose the property of hyperbolicity.

In Section 2, we present the individual model and the final macroscopic model, focusing on how the two refinements are taken in account, and what are the consequences at the macroscopic level.

In Section 3, we provide elements of the derivation of this macroscopic model, following the method of [28], but emphasizing the details which are specific to this

study. We also give the method in a general n-dimensional framework (previously the method was only done in three dimensions). The case of the dimension 2 is special, since we are able to give an explicit expression of the coefficients.

In Section 4, we study the properties of the macroscopic model. We prove that when one of the coefficients is negative, then the system is not hyperbolic. We describe the region of hyperbolicity for a system which depends only on one space variable, and we discuss the influence of "angle of vision".

Finally, in Section 5, we provide a general method which gives an asymptotic expansion of the coefficients in any dimension, in the limit of a small or a large concentration parameter. With these expansions, we are able to study the qualitative influence of the "angle of vision" in the final macroscopic model, and to give examples for which the hyperbolicity is indeed lost.

2 Individual and continuum dynamics of a modified Vicsek model

We start by presenting the individual-based model and the continuum model we obtain in the limit of a large number of particles, when observed at large scale, in space and time. Elements of the derivation of this macroscopic model will be given in section 3.

2.1 Starting point: particle dynamics

Here, we briefly recall the time-continuous version of the Vicsek model, and introduce how we take into account the anisotropy of observation and the dependence on the local density for the rate of relaxation and the intensity of the noise.

We consider a system of N particles with positions X_k in $\mathbb{R}^n$ (with $k \in [\![1, N]\!]$) and orientations ω_k in the unit sphere $\mathbb{S}_{n-1}$, which we will simply write $\mathbb{S}$.

For each particle, we first define a local mean orientation $\bar{\omega}_k$ (considered as a target direction) and a local density $\bar{\rho}_k$. In the original model of Vicsek [74], the mean orientation $\bar{\omega}_k$ is computed on all the neighbors within a given radius R. Here we take the mean according to a kernel of observation K, which can be more general than the indicator function of the ball of radius R, as in the time-continuous version of [28]. The kernel therein depends only on the distance between the given particle and a given neighbor, so the refinement here is that it can also depend on (the cosine of) the angle between the orientation of the first particle and the right line joining the two particles:

$$\bar{\omega}_k = \frac{\bar{J}_k}{|\bar{J}_k|}, \text{ where } \bar{J}_k = \frac{1}{N}\sum_{j=1}^{N} K\left(|X_j - X_k|, \tfrac{X_j - X_k}{|X_j - X_k|} \cdot \omega_k\right) \omega_j. \tag{2.1}$$

For example, to take into account only the neighbors located "in front", and within a given radius R, of one particle, the kernel would be $K(r, \gamma) = \mathbb{1}_{\{r \leqslant R\}} \mathbb{1}_{\{\gamma \geqslant 0\}}$. We proceed in an analogous way to compute the local density $\bar{\rho}_k$, which may use

another kernel $\widetilde{K}$:

$$\bar{\rho}_k = \frac{1}{N}\sum_{j=1}^{N} \widetilde{K}\left(|X_j - X_k|, \tfrac{X_j - X_k}{|X_j - X_k|}\cdot\omega_k\right). \tag{2.2}$$

We now turn to the dynamics of the particle system. The k^{th} particle moves at constant speed 1, following its orientation ω_k. This last one relax towards the mean orientation $\bar{\omega}_k$ of its neighbors, with rate ν (depending in the local mean density $\bar{\rho}_k$), under the constraint that ω_k is of norm 1. Finally, this orientation ω_k is subjected to a Brownian motion (see [48] for more details on how to define such an object on a Riemannian manifold, such as the unit sphere here) of intensity d, which will also depend on the density $\bar{\rho}_k$. The model takes then the form of $2N$ coupled stochastic differential equations, which have to be understood in the Stratonovich sense:

$$\mathrm{d}X_k = \omega_k \mathrm{d}t, \tag{2.3}$$

$$\mathrm{d}\omega_k = \nu(\bar{\rho}_k)(\mathrm{Id} - \omega_k\otimes\omega_k)\bar{\omega}_k\,\mathrm{d}t + \sqrt{2d(\bar{\rho}_k)}\,(\mathrm{Id} - \omega_k\otimes\omega_k)\circ\mathrm{d}B_t^k, \tag{2.4}$$

where (B_t^k) are independent standard Brownian motions on $\mathbb{R}^n$.

Here we denote by $\mathrm{Id} - \omega_k\otimes\omega_k$ the projection on the plane orthogonal to ω_k, that is to say $(\mathrm{Id} - \omega\otimes\omega)\upsilon = \upsilon - (\upsilon\cdot\omega)\omega$. This projection is necessary to keep ω_k on the unit sphere. The term $(\mathrm{Id} - \omega_k\otimes\omega_k)\bar{\omega}_k$ can also be written $\nabla_\omega(\omega\cdot\bar{\omega}_k)|_{\omega=\omega_k}$, where ∇_ω is the tangential gradient on the unit sphere. The deterministic part of the SDE (2.4) can then be written $\frac{\mathrm{d}\omega_k}{\mathrm{d}t} = \nu(\bar{\rho}_k)\nabla_\omega(\omega\cdot\bar{\omega}_k)|_{\omega=\omega_k}$, which is indeed a relaxation towards $\bar{\omega}_k$ (where the function $\omega\mapsto\omega\cdot\bar{\omega}_k$ reaches its maximum), with rate $\nu(\bar{\rho}_k)$.

Since the local density $\bar{\rho}$ only appears through the functions ν and d, we can assume the following normalization for the kernel $\widetilde{K}$:

$$\int_{\xi\in\mathbb{R}^n} \widetilde{K}(|\xi|, \tfrac{\xi}{|\xi|}\cdot\omega)\mathrm{d}\xi = 1\,. \tag{2.5}$$

This normalization condition (which does not depend on $\omega\in\mathbb{S}$) means that the density is chosen to be 1 in the limit of a uniform distribution of the N particles in a region of unit volume. This is not necessary to take a similar condition for the kernel K, since $\bar{\omega}_k$, defined at equation (2.1), is independent of such a normalization.

In [28], the relaxation coefficient ν depends on (the cosine of) the angle between the orientation of one particle and the target direction, in order to take into account some "ability to turn". This would amount to replace $\nu(\bar{\rho}_k)$ by $\nu(\bar{\rho}_k, \omega_k\cdot\bar{\omega}_k)$ in (2.4). With our new features here, this would involve many more computations, but, following exactly the same method, this leads to the same conclusion. For simplicity here, we will work without this dependence. We will only present the final results with this dependence in some special cases, and add remarks to explain the difference in some steps of the derivation of the macroscopic model.

Some numerical simulations tend to show that this time-continuous individual based model present the same behavior at large scale as the discrete one (for example the formation of bands, as in [16]), in the case where ν and d are constant, and the observation kernel is isotropic, as in [28]. We can expect to observe the same behavior, even when ν and d depend on the local density $\bar{\rho}$. More precise investigations on the numerical comparison between the original discrete and the present time-continuous dynamical systems are in progress.

2.2 The continuum model

In this chapter, following the approach of [28], we derive, from the particle dynamics (2.3)-(2.4) introduced in the previous subsection, the following continuum model, the functions $\rho(x,t) > 0$ and $\Omega(x,t) \in \mathbb{S}$ describing the average density and particle direction at a given point $x \in \mathbb{R}^n$:

$$\partial_t \rho + \nabla_x \cdot (c_1(\rho)\rho\Omega) = 0, \tag{2.6}$$

$$\rho\,(\partial_t \Omega + c_2(\rho)(\Omega \cdot \nabla_x)\Omega) + \lambda(\rho)\,(\mathrm{Id} - \Omega \otimes \Omega)\nabla_x \rho = 0, \tag{2.7}$$

where the functions c_1, c_2, and λ will be specified later on: see (3.24) and (3.26)-(3.27).

This system of first order partial differential equations shows similarities with the Euler system of isothermal compressible gases, but also some important differences.

Equation (2.6) is the conservation of mass: the density ρ moves through direction Ω with velocity $c_1(\rho)$. We will see that this velocity, taking values between 0 and 1, plays the role of an order parameter: when the directions of the particles are strongly correlated (close to Ω), density moves with velocity close to 1. This order parameter depends only on the ratio between $\nu(\rho)$ (the alignment strength) and $d(\rho)$ (the noise intensity).

Equation (2.7) describes the evolution of the direction Ω, the norm of which is constrained to be constant (the projection $\mathrm{Id} - \Omega \otimes \Omega$ insures that the dynamics take place on the hyperplane orthogonal to Ω). This constraint implies that the equation is not conservative which is the counterpart of the fact that, at the microscopic level, the only conservative quantity is the mass. The perturbations of this vector travel with velocity $c_2(\rho)$, influenced by a term playing the role of pressure due to the density, of intensity $\lambda(\rho)$. It is important to see that in general (and contrary to the classical Euler system), the two convection speeds c_1 and c_2 are different, which means that the perturbations on the mean orientation do not travel at the same velocity as the "fluid".

This macroscopic model is the same as the "Vicsek hydrodynamics" of [28], except for the definitions of these speeds c_1 and c_2, and of the parameter λ. This confirms the ability of this model to describe the global dynamics of systems of self-propelled particles with constant speed and alignment interactions (this was also the result of [30]).

However, the parameters depend here on the density ρ, and their expressions are slightly different (due to this dependence and to the anisotropy of the kernel of observation). This leads to strong differences in their behavior, as we will see in Section 4, devoted to the investigation of the properties of (2.6)-(2.7). For example the parameter λ can be negative, which implies the loss of hyperbolicity. And because of the non isotropy of the observation kernel, the convection speed c_2 can take a large range of values, from negative if the kernel is strongly directed forward, to higher than c_1, if particles are more influenced by neighbors behind them than those in front of them (this has been observed in locust migratory bands [8], where the individuals have "cannibalistic interactions" and avoid to be eaten by those approaching from behind).

3 Elements of the derivation of the continuum model

This derivation proceeds like in [28] but there are significant differences due to the additional complexity. In this section, we briefly recall the method of Degond and Motsch and will focus on the points which are specific to the present study.

The derivation proceeds in several steps. The first one consists in writing a kinetic version of the particle dynamics.

3.1 Step 1: mean-field model

Let $f(x,\omega,t)$ be the probability density of finding one particle at position $x \in \mathbb{R}^n$, orientation $\omega \in \mathbb{S}$ and time $t \geqslant 0$. The mean-field version of (2.3)-(2.4) is given by

$$\partial_t f + \omega \cdot \nabla_x f + \nabla_\omega \cdot (Ff) = \nabla_\omega \cdot (\sqrt{d(\bar\rho)}\nabla_\omega \sqrt{d(\bar\rho)} f), \tag{3.8}$$

with

$$\begin{aligned}
F(x,\omega,t) &= \nu(\bar\rho)\,(\mathrm{Id} - \omega\otimes\omega)\bar\omega(x,\omega,t),\\
\bar\rho(x,\omega,t) &= \int_{y\in\mathbb{R}^n,\, v\in\mathbb{S}} \widetilde{K}\left(|y-x|, \tfrac{y-x}{|y-x|}\cdot\omega\right)\, f(y,v,t)\,\mathrm{d}y\,\mathrm{d}v\,,\\
\bar\omega(x,\omega,t) &= \frac{J(x,\omega,t)}{|J(x,\omega,t)|},\\
J(x,\omega,t) &= \int_{y\in\mathbb{R}^n,\, v\in\mathbb{S}} K\left(|y-x|, \tfrac{y-x}{|y-x|}\cdot\omega\right)\, v\, f(y,v,t)\,\mathrm{d}y\,\mathrm{d}v\,.
\end{aligned}$$

The first equation (3.8) is the so called Kolmogorov–Fokker–Planck equation. The force term $F(x,\omega,t)$ corresponds to the orientation interaction.

First of all, if there is no noise (that is $d(\bar\rho) = 0$ in equations (2.3)-(2.4), which become ordinary differential equations), the formal derivation of this system is easy: the usual methodology shows that the empirical distribution (see [71]) satisfies the equation (3.8), with $d = 0$.

When the noise is added, some difficulties appear. A method consisting in writing the BBGKY hierarchy (see [47], applied to the Cucker-Smale model of self-propelled particles) would not in that case reduce to a evolution equation involving only the one-particle and the two-particles distributions, since the interaction is not a sum of binary interactions.

We could slightly change our model to make the interaction as a sum of binary interactions, replacing $\bar\omega_k$ by $\bar J_k$ (defined in equation (2.1)) in the system of particles (2.3)-(2.4). In that case the model present an interesting phenomenon of phase transition and this is the object of Chapter 2 (in collaboration with P. Degond and J.-G. Liu, the homogeneous version being studied in Chapter 4, which is also a collaboration with J.-G. Liu). In that case, writing the BBGKY hierarchy and using exchangeability of particles gives a system of evolution equations, the first one involving only the one-particle and the two-particles distributions. The classical assumption of propagation of chaos amounts to consider the two-particles density as the tensor of the one-particle density f by itself (in the limit of a large number of

particles, two particles behave as if they were independent), and this gives exactly the evolution equation (3.8). Actually, it has been recently proved [13] that the mean-field limit of this model is the partial differential equation (3.8), where $\bar{\omega}$ is replaced by $\bar{J}$ in the definition of the force F (in the case where ν and d are constant). The main point to derive this limit is to adapt the classical theory of propagation of chaos [59, 73] in a framework of stochastic analysis in a Riemannian manifold (the unit sphere in the present case).

In the case of a non-linear diffusion, some results are given in [14] for other systems of self-propelled particles, under assumptions which would have to be adapted in our framework. We can expect to have conditions such as to be Lipschitz for the function $\sqrt{d}$, and to be Lipschitz and bounded for the kernel $\widetilde{K}$. Since we use the Stratonovich formulation in order to work on the unit sphere, we get the term $\nabla_\omega \cdot (\sqrt{d(\bar{\rho})}\nabla_\omega \sqrt{d(\bar{\rho})} f)$ (instead of $\Delta_v(d(\bar{\rho})f)$ when the velocity $v \in \mathbb{R}^d$ satisfies the SDE in the usual Itō formulation, see the sections 4.3.5 and 4.3.6 of [44] for the correspondence).

Finally, when the drift is not under the average form, it is sometimes possible to get a mean-field limit, under regularity assumptions on the coefficients [63], or with weaker assumptions, but assuming uniqueness of the solution of the mean-field model [61]. These results could to be adapted in the framework of stochastic differential equations on the sphere, but dealing with the singularity of $\bar{\omega}$ (when J is close to zero) seems to be slightly more complicated.

With these considerations in mind, it is however very reasonable that the limit of the particle system (2.3)-(2.4), when the number of particles is large, is given by the mean-field model (3.8). So we start with this model as a base for the derivation of the continuum model. A rigorous proof of the derivation of such a mean-field model from the individual dynamics is left to future work.

Remark 3.1. *If we want to take into account some "ability to turn", we just have to replace $\nu(\bar{\rho})$ by $\nu(\bar{\rho}, \omega \cdot \bar{\omega})$.*

The next step consists in observing this system at large scale, in both space in time.

3.2 Step 2: hydrodynamic scaling

The hydrodynamic scaling consists in the same rescaling for the time and space variable. We introduce a small parameter ε and we set $x' = \varepsilon x$, and $t' = \varepsilon t$. We define $f^\varepsilon(x', \omega, t') = f(x, \omega, t)$, and we rewrite the equation (3.8) in this new coordinates.

The kinetic equation has the same form, with a factor ε in front of each of the terms with space or time derivative:

$$\varepsilon(\partial_{t'} f^\varepsilon + \omega \cdot \nabla_{x'} f^\varepsilon) + \nabla_\omega \cdot (F^\varepsilon f^\varepsilon) = \nabla_\omega \cdot (\sqrt{d(\bar{\rho}^\varepsilon)}\nabla_\omega \sqrt{d(\bar{\rho}^\varepsilon)} f^\varepsilon),$$

with

$$F^\varepsilon(x', \omega, t') = \nu(\bar{\rho}^\varepsilon)\,(\mathrm{Id} - \omega \otimes \omega)\bar{\omega}^\varepsilon(x', \omega, t'),$$

where the local rescaled density and orientation are given by

$$\begin{aligned}
\bar{\rho}^\varepsilon(x',\omega,t') &= \int_{y\in\mathbb{R}^n,\, v\in\mathbb{S}} \widetilde{K}\left(|y-x'|, \tfrac{y-x'}{|y-x'|}\cdot\omega\right) f^\varepsilon(y,v,t')\,\tfrac{\mathrm{d}y}{\varepsilon^n}\,\mathrm{d}v\,,\\
\bar{\omega}^\varepsilon(x',\omega,t') &= \frac{J^\varepsilon(x',\omega,t')}{|J^\varepsilon(x',\omega,t')|},\\
J^\varepsilon(x',\omega,t') &= \int_{y\in\mathbb{R}^n,\, v\in\mathbb{S}} K\left(\tfrac{|y-x'|}{\varepsilon}, \tfrac{y-x'}{|y-x'|}\cdot\omega\right) v\, f^\varepsilon(y,v,t')\,\tfrac{\mathrm{d}y}{\varepsilon^n}\,\mathrm{d}v\,.
\end{aligned}$$

The important point is to realize that the average density $\bar{\rho}^\varepsilon$ and orientation $\bar{\omega}^\varepsilon$ now depend on ε, and can be easily expanded in terms of ε, the non-locality only appearing at high order. Omitting the primes for simplicity, we have the following expansions, the proofs of which are given in Lemma 1.3 of Appendix A.1:

$$\begin{aligned}
\bar{\omega}^\varepsilon(x,\omega,t) &= \Omega^\varepsilon(x,t) + \varepsilon\alpha\,(\omega\cdot\nabla_x)\,\Omega^\varepsilon(x,t) + O(\varepsilon^2)\,,\\
\bar{\rho}^\varepsilon(x,\omega,t) &= \rho^\varepsilon(x,t) + \varepsilon\widetilde{\alpha}\,\omega\cdot\nabla_x\rho^\varepsilon(x,t) + O(\varepsilon^2)\,,
\end{aligned}$$

where $\rho^\varepsilon = \rho_{f^\varepsilon}$ and $\Omega^\varepsilon = \Omega_{f^\varepsilon}$ are the local density and mean orientation associated to the function f^ε (these quantities, depending only on the space and time variables, are related to the first moments with respect to the variable ω) given by

$$\rho_f = \int_{\omega\in\mathbb{S}} f(.,\omega)\,\mathrm{d}\omega\,, \tag{3.9}$$

$$\Omega_f = \frac{j_f}{|j_f|},\ \text{with } j_f = \int_{\omega\in\mathbb{S}} \omega\, f(.,\omega)\,\mathrm{d}\omega\,, \tag{3.10}$$

and the constants α and $\widetilde{\alpha}$ depend only on the observation kernels K and $\widetilde{K}$. These constants are positive if the kernel is directed forward, and the more acute the "angle of vision", the bigger the constant related to the kernel.

Now we can introduce these expansions in the mean-field model, and after some easy algebra, the rescaled model can be written in the form

$$\varepsilon(\partial_t f^\varepsilon + \omega\cdot\nabla_x f^\varepsilon + \alpha\,P(f^\varepsilon) + \widetilde{\alpha}\,\widetilde{P}(f^\varepsilon)) = Q(f^\varepsilon) + O(\varepsilon^2)\,, \tag{3.11}$$

where Q, P and $\widetilde{P}$ are the operators given by the following equations (where $\dot{\nu}$ and $\dot{d}$ are the derivatives of ν and d with respect to ρ):

$$\begin{aligned}
Q(f) =& -\nu(\rho_f)\nabla_\omega\cdot((\mathrm{Id}-\omega\otimes\omega)\Omega_f f) + d(\rho_f)\Delta_\omega f,\\
P(f) =& \nu(\rho_f)\nabla_\omega\cdot((\mathrm{Id}-\omega\otimes\omega)((\omega\cdot\nabla_x)\,\Omega_f)f),\\
\widetilde{P}(f) =& \dot{\nu}(\rho_f)\nabla_\omega\cdot((\omega\cdot\nabla_x\rho_f)\,(\mathrm{Id}-\omega\otimes\omega)\Omega_f f)\\
&- \dot{d}(\rho_f)\nabla_\omega\cdot(\tfrac{1}{2}(\mathrm{Id}-\omega\otimes\omega)\nabla_x\rho_f f + (\omega\cdot\nabla_x\rho_f)\,\nabla_\omega f).
\end{aligned}$$

Notice that the operator Q (giving the only term of order 0 in ε) only acts on the variable ω, and the study of its properties will be important for the following.

Remark 3.2. *If ν also depends on $\omega\cdot\bar{\omega}$, the expression of the operator Q is the same with $\nu(\rho_f,\omega\cdot\Omega_f)$ instead of $\nu(\rho_f)$. But then the expressions of P and $\widetilde{P}$ complicate in a significant way, since there are also terms with the derivative of ν with respect to this second variable.*

Now we are ready to study this system when $\varepsilon\to 0$.

3.3 Step 3: limit as $\varepsilon \to 0$

This is the main step, where we give the link between the continuum limit (2.6)-(2.7) and the rescaled kinetic equation (3.11) of the particle dynamics.

Theorem 1.1. *The limit when $\varepsilon \to 0$ of f^ε is given (formally) by $f^0 = \rho M_{\kappa(\rho)\Omega}$ where $\rho = \rho(x,t) > 0$ is the total mass of f^0 and $\Omega = \Omega(x,t) \in \mathbb{S}$ its mean orientation:*

$$\rho(x,t) = \int_{\omega\in\mathbb{S}} f^0(x,\omega,t)\,\mathrm{d}\omega,$$
$$\Omega = \frac{j}{|j|}, \quad j(x,t) = \int_{\omega\in\mathbb{S}} f^0(x,\omega,t)\,\omega\,\mathrm{d}\omega,$$

where $M_{\kappa\Omega}$ is a given function of $\omega\cdot\Omega$ and $\kappa = \frac{\nu}{d}$ which will be specified later on (see (3.12)). Furthermore, $\rho(x,t)$ and $\Omega(x,t)$ satisfy the following system of first order partial differential equations:

$$\partial_t\rho + \nabla_x\cdot(c_1\rho\Omega) = 0.$$
$$\rho\,(\partial_t\Omega + c_2(\Omega\cdot\nabla_x)\Omega) + \lambda\,(\mathrm{Id} - \Omega\otimes\Omega)\nabla_x\rho = 0,$$

where the convection speeds c_1, c_2 and the parameter λ depend on ρ. Their expressions will be given in this section (see (3.24) and (3.26)-(3.27)).

The method to obtain this result follows closely [28], and is only summarized here. We will focus on the details which are specific to this study.

Equilibria

The first important point is to determine the null space $\mathcal{E}$ of Q, since it contains the limits of (3.11). We find, as in [28], that it is a n-dimensional manifold consisting of functions analogous to Maxwellian distributions in the classical Boltzmann theory:

$$\mathcal{E} = \{\rho M_{\kappa(\rho)\Omega}(\omega)\,|\,\rho > 0,\ \Omega\in\mathbb{S}\},$$

where

$$\kappa(\rho) = \frac{\nu(\rho)}{d(\rho)} > 0 \text{ and } M_{\kappa\Omega}(\omega) = \frac{e^{\kappa\,\omega\cdot\Omega}}{\int_{\mathbb{S}} e^{\kappa\,v\cdot\Omega}\,\mathrm{d}v}. \tag{3.12}$$

The main difference with [28] is the dependence on ρ for this equilibrium in a nonlinear way, coming from the dependence of ν and d on ρ. This will result in additional terms in the computations, and so in additional terms in the expressions of the constants in the macroscopic model.

The normalization constant $\int_{\mathbb{S}} e^{\kappa\,\omega\cdot\Omega}\,\mathrm{d}\omega$ depends only on κ (not on Ω) and so the total mass of $M_{\kappa\Omega}(\omega)$ is 1 and its mean direction is Ω, that is to say $\rho_{M_{\kappa\Omega}} = 1$ and $\Omega_{M_{\kappa\Omega}} = \Omega$. Indeed we can easily compute the flux $j_{M_{\kappa\Omega}}$ of this equilibrium, defined by (3.10), and we get:

$$j_{M_{\kappa\Omega}} = \langle\cos\theta\rangle_{M_\kappa}\,\Omega, \tag{3.13}$$

where for any function $\gamma(\cos\theta)$, the notation $\langle\gamma(\cos\theta)\rangle_{M_\kappa}$ stands for the mean of the function $\omega \mapsto \gamma(\omega\cdot\Omega)$ against the density $M_{\kappa\Omega}$, i.e.

$$\langle\gamma(\cos\theta)\rangle_{M_\kappa} = \int_{\omega\in\mathbb{S}} M_{\kappa\Omega}(\omega)\gamma(\omega\cdot\Omega)\,\mathrm{d}\omega = \frac{\int_{\mathbb{S}}\gamma(\omega\cdot\Omega)e^{\kappa\,\omega\cdot\Omega}\,\mathrm{d}\omega}{\int_{\mathbb{S}}e^{\kappa\,\omega\cdot\Omega}\,\mathrm{d}\omega}.$$

Notice that $\langle\gamma(\cos\theta)\rangle_{M_\kappa}$ depends only on κ, not on Ω:

$$\langle\gamma(\cos\theta)\rangle_{M_\kappa} = \frac{\int_0^\pi \gamma(\cos\theta)e^{\kappa\cos\theta}\,\sin^{n-2}\theta\,\mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta}\,\sin^{n-2}\theta\,\mathrm{d}\theta}. \tag{3.14}$$

Remark 3.3. *In the case where ν depends on ρ and $\omega\cdot\Omega$, we have to replace in all this point $\kappa\,\omega\cdot\Omega$ by $\widehat{\kappa}(\rho,\omega\cdot\Omega)$, where $\widehat{\kappa}(\rho,\mu) = \int_0^\mu \frac{\nu(\rho,\tau)}{d(\rho)}\mathrm{d}\tau$.*

Collisional invariants

The second important point is the determination of generalized collisional invariants. Indeed, since there is no other conservation relation than the conservation of mass, the collision invariants reduce to the constants, and the integration of the equation against these invariants only gives one equation, which is not sufficient to describe the behavior of the equilibrium (which lives on a n-dimensional manifold). The main idea in [28] was to overcome this problem with a generalization of the concept of collisional invariants.

A collision invariant is a function ψ such that for all function f of ω, the integration of $Q(f)$ against ψ is zero. So we ask for a generalized invariant to satisfy this definition only for a restricted subset of functions f. In the case where the dependence on ρ in the equilibria is linear, restricting to all functions with a given orientation Ω is sufficient to obtain the remaining equation. Here we also have to restrict to functions with a given density too (actually, we impose a given $\kappa(\rho)$). We will have then a set of generalized coefficients indexed by $\Omega\in\mathbb{S}$ and $\kappa>0$.

More precisely, to have a good definition, we have to work with linear operators (this point has been mentioned in [30], since the result given in [28], with the definition therein, was slightly incorrect). We first define the linear operator $L_{\kappa\Omega}$ by

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

and then the generalized collisional invariants $\mathcal{C}_{\kappa\Omega}$ (associated to $\kappa\in\mathbb{R}$ and $\Omega\in\mathbb{S}$) as the following vector space:

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

We remark that the operator $Q(f)$ can be written as $Q(f) = -d(\rho_f)L_{\kappa(\rho_f)\Omega_f}(f)$. Hence, for any generalized collisional invariant $\psi\in\mathcal{C}_{\kappa\Omega}$, we have

$$\forall f \text{ such that } \Omega_f=\Omega \text{ and } \kappa(\rho_f)=\kappa, \int_{\omega\in\mathbb{S}} Q(f)\,\psi\,\mathrm{d}\omega = 0, \tag{3.15}$$

and this is the only property of generalized collisional invariants we will need in the following.

The computation of the set of generalized collisional invariants has been done in [28] in dimension 3. We give here the general result in any dimension.

Proposition 3.1. *Structure of the generalized collisional invariants.*

Any generalized collisional invariant ψ associated to $\kappa \in \mathbb{R}$ and $\Omega \in \mathbb{S}$ has the following form:

$$\psi(\omega) = C + h_\kappa(\omega \cdot \Omega) A \cdot \omega,$$

where $C \in \mathbb{R}$ is a constant, the vector $A \in \mathbb{R}^n$ is orthogonal to Ω, and h_κ is a given positive function on $(-1, 1)$, depending on the parameter κ, which will be specified later on. In particular, the generalized collisional invariants form a vector space of dimension n.

Proof. We first rewrite the set $\{f |\, (\mathrm{Id} - \Omega \otimes \Omega) j_f = 0\}$ as the set of functions f such that for all $A \in \mathbb{R}^n$ with $A \cdot \Omega = 0$, we have that $\int_{\mathbb{S}} A \cdot \omega f \mathrm{d}\omega = 0$. Finally this is the orthogonal of the set $\{\omega \mapsto A \cdot \omega \text{ for } A \cdot \Omega = 0\}$, for the usual inner product on $L^2(\mathbb{S})$. We can then rewrite the set of generalized collisional invariants:

$$\begin{aligned}
\mathcal{C}_{\kappa\Omega} &= \left\{ \psi | \int_{\omega \in \mathbb{S}} f\, L^*_{\kappa\Omega}\, \psi \, \mathrm{d}\omega = 0,\ \forall f \in \{\omega \mapsto A \cdot \omega \text{ for } A \cdot \Omega = 0\}^\perp \right\} \\
&= \{\psi | L^*_{\kappa\Omega}\, \psi \in (\{\omega \mapsto A \cdot \omega \text{ for } A \cdot \Omega = 0\}^\perp)^\perp\} \\
&= \{\psi | L^*_{\kappa\Omega}\, \psi(\omega) = A \cdot \omega \text{ with } A \cdot \Omega = 0\},
\end{aligned}$$

the operator $L^*_{\kappa\Omega}$ being the adjoint of the operator $L_{\kappa\Omega}$, which can be written

$$L^*_{\kappa\Omega}\, \psi = -\Delta_\omega \psi - \kappa \Omega \cdot \nabla_\omega \psi = -\frac{1}{M_{\kappa\Omega}} \nabla_\omega \cdot (M_{\kappa\Omega} \nabla_\omega \psi). \tag{3.16}$$

It is then easy to show that the problem $L^*_{\kappa\Omega}\, \psi(\omega) = A \cdot \omega$, for $A \cdot \Omega = 0$ has a unique solution in the space $\dot{H}^1(\mathbb{S})$ (functions of $H^1(\mathbb{S})$ with mean zero), using Lax-Milgram theorem and the Poincaré inequality. Hence, if we show that this solution has the form $\psi(\omega) = h_\kappa(\Omega \cdot \omega) A \cdot \omega$, the solutions in the space $H^1(\mathbb{S})$ are equal to this solution plus a constant C.

We search a solution of this form. We identify Ω with the last element of an orthogonal basis of $\mathbb{R}^n$, and $\mathbb{S}_{n-2}$ with the elements on the unit sphere $\mathbb{S}$ which are orthogonal to Ω. We can then write $\omega = \cos\theta\, \Omega + \sin\theta\, v$, where $v \in \mathbb{S}_{n-2}$ and $\theta \in [0, \pi]$ (this decomposition is unique when ω is different from Ω and $-\Omega$). In this framework we try to find a solution of the form $\psi(\omega) = h_\kappa(\cos\theta) \sin\theta\, A \cdot v$.

For $\psi(\omega) = g(\theta) Z(v)$, we have, in dimension $n \geqslant 3$:

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

where the unit vector e_θ is $\nabla_\omega \theta = -\frac{1}{\sin\theta}(\mathrm{Id} - \omega \otimes \omega)\Omega$. A tangent vector field can always be written $a\, e_\theta + \mathcal{A}$ where $\mathcal{A}$ is a vector field tangent to the sphere $\mathbb{S}_{n-2}$, and we have

$$\nabla_\omega \cdot (a\, e_\theta + \mathcal{A}) = \sin^{2-n}\theta\, \partial_\theta(\sin^{n-2}\theta\, a) + \frac{1}{\sin\theta} \nabla_v \cdot \mathcal{A}\,.$$

Finally we get, using the second part of (3.16),

$$L^*_{\kappa\Omega}\, \psi = -\sin^{2-n}\theta e^{-\kappa\cos\theta} \tfrac{\mathrm{d}}{\mathrm{d}\theta}(\sin^{n-2}\theta e^{\kappa\cos\theta} g'(\theta)) Z(v) - \tfrac{1}{\sin^2\theta} g(\theta) \Delta_v Z(v).$$

In our case we have $Z(v) = A \cdot v$, so we get $\Delta_v Z = -(n-2)Z$ (this is a spherical harmonic of degree 1 on $\mathbb{S}_{n-2}$). So $L^*_{\kappa\Omega}\,\psi$ is also of the form $\widetilde{L}^*_\kappa g(\theta) Z(v)$, where

$$\widetilde{L}^*_\kappa g(\theta) = -\sin^{2-n}\theta e^{-\kappa\cos\theta}\tfrac{\mathrm{d}}{\mathrm{d}\theta}(\sin^{n-2}\theta e^{\kappa\cos\theta} g'(\theta)) + \tfrac{n-2}{\sin^2\theta} g(\theta). \tag{3.17}$$

Finally, solving $L^*_{\kappa\Omega}\,(h(\omega\cdot\Omega)A\cdot\omega) = A\cdot\omega$ comes down to solving

$$\widetilde{L}^*_\kappa g = \sin\theta, \quad \text{with} \quad g(\theta) = h(\cos\theta)\sin\theta. \tag{3.18}$$

When $A \neq 0$, it easy to see that the function $\omega \mapsto h(\omega\cdot\Omega)A\cdot\omega$ belongs to $H^1(\mathbb{S})$ if and only if the function $g : \theta \mapsto h(\cos\theta)\sin\theta$ belongs to the space V (a "weighted H^1_0") defined by

$$V = \{g \,|\, (n-2)(\sin\theta)^{\frac{n}{2}-2} g \in L^2(0,\pi),\ (\sin\theta)^{\frac{n}{2}-1} g \in H^1_0(0,\pi)\}. \tag{3.19}$$

Using again Lax-Milgram theorem in this space V, we get that the problem (3.18) has a unique solution, denoted g_κ, which is positive (by the maximum principle). Writing $h_\kappa(\mu) = (1-\mu^2)^{-\frac{1}{2}} g_\kappa(\arccos(\mu))$ gives that $\psi(\omega) = h_\kappa(\omega\cdot\Omega)\,A\cdot\omega$ is a solution to the partial differential equation $L^*_{\kappa\Omega}\,\psi(\omega) = A\cdot\omega$. We could write the elliptic equation on $(-1,1)$ satisfied by h_κ to have another definition, but this does not give a more elegant formulation.

In the case of dimension 2, we write $\psi(\omega) = g(\theta)A\cdot v_0$, where v_0 is one of the two unit vectors orthogonal to Ω and g is an odd 2π-periodic function in $H^1_{loc}(\mathbb{R})$, which can be identified with a function $g \in H^1_0(0,\pi) = V$. We still have that the elliptic problem $L^*_{\kappa\Omega}\,\psi(\omega) = A\cdot\omega$ is equivalent to (3.18) with $g \in V$, with the same definitions (3.17)-(3.19) of $\widetilde{L}_\kappa$ and V. But since this elliptic equation reduces to $(e^{\kappa\cos\theta} g'(\theta))' = -\sin\theta\, e^{\kappa\cos\theta}$, we now have the following explicit expression of g_κ:

$$g_\kappa(\theta) = \frac{\theta}{\kappa} - \frac{\pi}{\kappa}\frac{\int_0^\theta e^{-\kappa\cos\varphi}\mathrm{d}\varphi}{\int_0^\pi e^{-\kappa\cos\varphi}\mathrm{d}\varphi}\,. \tag{3.20}$$

□

Remark 3.4. *If we take into account the "ability to turn", we just replace $\kappa\cos\theta$ in equation (3.17) by $\widehat{\kappa}(\cos\theta)$. In dimension 2, we still have an explicit expression:*

$$g_{\widehat{\kappa}}(\theta) = g^0_{\widehat{\kappa}}(\theta) - \tfrac{g^0_{\widehat{\kappa}}(\pi)}{g^\infty_{\widehat{\kappa}}(\pi)} g^\infty_{\widehat{\kappa}}(\theta), \tag{3.21}$$

where

$$g^0_{\widehat{\kappa}}(\theta) = -\int_0^\theta \int_\varphi^\pi e^{\widehat{\kappa}(\cos\phi)-\widehat{\kappa}(\cos\varphi)}\sin\phi\,\mathrm{d}\phi\,\mathrm{d}\varphi, \tag{3.22}$$

$$g^\infty_{\widehat{\kappa}}(\theta) = \int_0^\theta e^{-\widehat{\kappa}(\cos\varphi)}\,\mathrm{d}\varphi\,. \tag{3.23}$$

Computation of the limit as $\varepsilon \to 0$

The third and final important point is taking the limit $\varepsilon \to 0$ in the equation (3.11), after integrating against the collision invariants. Since we do not have results of

existence, uniqueness and regularity of the solution, all the limits in this section have to be understood as formal limits. A rigorous proof of convergence is left to future work.

When $\varepsilon \to 0$, if we fix x and $t > 0$, we have that $Q(f^\varepsilon)$, as a function of ω, tends formally to zero, so f^ε tends to an equilibrium of the operator Q, of the form $\rho M_{\kappa(\rho)\Omega}$, where $\rho > 0$ and $\Omega \in \mathbb{S}$ are given functions of x and t. This is the first part of Theorem 1.1. So we have $\rho^\varepsilon \to \rho$, and $\Omega^\varepsilon \to \Omega$. When there is no possible confusion, we will write κ for $\kappa(\rho)$.

For the mass equation, we use the constant invariant: we have, since the operators Q, P and $\widetilde{P}$ are given as the divergence (with respect to ω) of a function,

$$\int_{\omega\in\mathbb{S}} Q(f^\varepsilon)\,\mathrm{d}\omega = \int_{\omega\in\mathbb{S}} P(f^\varepsilon)\,\mathrm{d}\omega = \int_{\omega\in\mathbb{S}} \widetilde{P}(f^\varepsilon)\,\mathrm{d}\omega = 0.$$

Hence, integrating the equation (3.11) with respect to ω, we get:

$$\partial_t \rho^\varepsilon + \nabla_x \cdot j^\varepsilon = O(\varepsilon).$$

Actually, we can even replace the $O(\varepsilon)$ by zero in this equation since in the original model (3.8) we have conservation of mass. We get in the $\varepsilon \to 0$ limit:

$$\partial_t \rho + \nabla_x \cdot (c_1(\kappa)\rho\,\Omega) = 0,$$

where (see (3.13)):

$$c_1(\kappa) = |j_{M_{\kappa\Omega}}| = \langle \cos\theta \rangle_{M_\kappa} = \frac{\int_0^\pi \cos\theta e^{\kappa\cos\theta}\,\sin^{n-2}\theta\,\mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta}\,\sin^{n-2}\theta\,\mathrm{d}\theta}. \tag{3.24}$$

This gives the second part of Theorem 1.1, with the equation on ρ and the definition of c_1.

To get the equation on Ω, we use the non-constant part of the collisional invariants. By Proposition 3.1 and using the result at equation (3.15), we get that for all A such that $A \cdot \Omega^\varepsilon = 0$, we have

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

So we have that the vector $X^\varepsilon = \int_{\omega\in\mathbb{S}} Q(f^\varepsilon) h_{\kappa(\rho^\varepsilon)}(\omega\cdot\Omega^\varepsilon)\,\omega\,\mathrm{d}\omega$ is orthogonal to A for all A orthogonal to Ω, that is to say that X^ε is in the direction of Ω^ε, which is equivalent to $(\mathrm{Id} - \Omega^\varepsilon \otimes \Omega^\varepsilon)\, X^\varepsilon = 0$. Using (3.11), we get that

$$X^\varepsilon = \varepsilon \int_{\omega\in\mathbb{S}} (\partial_t f^\varepsilon + \omega\cdot\nabla_x f^\varepsilon + \alpha P(f^\varepsilon) + \widetilde{\alpha}\widetilde{P}(f^\varepsilon))\, h_{\kappa(\rho^\varepsilon)}(\omega\cdot\Omega^\varepsilon)\,\omega\,\mathrm{d}\omega + O(\varepsilon^2).$$

Dividing by ε and taking the limit $\varepsilon \to 0$, we get $(\mathrm{Id} - \Omega\otimes\Omega)\,X = 0$, where

$$X = \int_{\omega\in\mathbb{S}} (\partial_t(\rho M_{\kappa\Omega}) + \omega\cdot\nabla_x(\rho M_{\kappa\Omega}) + \alpha P(\rho M_{\kappa\Omega}) + \widetilde{\alpha}\widetilde{P}(\rho M_{\kappa\Omega}))\, h_\kappa(\omega\cdot\Omega)\,\omega\,\mathrm{d}\omega\,. \tag{3.25}$$

The main point is then to compute $(\mathrm{Id} - \Omega\otimes\Omega)\,X$, in terms of ρ, Ω and their derivatives, using mainly the chain rule. The computation is similar to [28] for some terms, but some additional work is required for the terms coming from the nonlinearity of $M_{\kappa\Omega}$ in ρ and the operators P and $\widetilde{P}$. We give the result of the computations under the form of a proposition:

Proposition 3.2. $(\mathrm{Id} - \Omega \otimes \Omega)\, X = 0$, *where* X *is given in* (3.25), *is equivalent to*

$$\rho\ (\partial_t \Omega + c_2(\Omega \cdot \nabla_x)\Omega) + \lambda\, (\mathrm{Id} - \Omega \otimes \Omega)\nabla_x \rho = 0,$$

where

$$c_2 = \widetilde{c}_1 - \alpha\, d\, (n\, \widetilde{c}_1 + \kappa\, \langle \cos^2\theta \rangle_{\widetilde{M}_\kappa})\,, \quad \textit{with} \quad \widetilde{c}_1 = \langle \cos\theta \rangle_{\widetilde{M}_\kappa}\,, \tag{3.26}$$

$$\lambda = \tfrac{1}{\kappa} + \rho\, \tfrac{\dot{\kappa}}{\kappa}\, [\, \widetilde{c}_1 - c_1 + \widetilde{\alpha}\, d\, (\kappa\, \langle \sin^2\theta \rangle_{\widetilde{M}_\kappa} - n\, \widetilde{c}_1)\,] + \tfrac{1}{2}\, \widetilde{\alpha}\, \rho\, \dot{d}\, (n - 1 + \kappa\, \widetilde{c}_1)\,, \tag{3.27}$$

with the notation

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

This proposition is exactly the last part of Theorem 1.1, with a precise definition for coefficients c_2 and λ, and this ends the derivation of the continuum model (2.6)-(2.7).

The computations to get this result are given in Appendix A.2, the idea is to compute $(\mathrm{Id} - \Omega \otimes \Omega)\, X$ using the chain rule and the change of variable $\omega \rightsquigarrow (\theta, v)$ where $\omega = \cos\theta\, \Omega + \sin\theta\, v$, with v orthogonal to Ω, which simplifies a lot of terms.

Remark 3.5. *The computations have also been done in the case where* ν *depends on* $\omega \cdot \Omega$ *(and not on* ρ*) and where* d *is a constant. We get the same results, except that the constants are given (with analogous definitions) by:*

$$c_1 = \langle \cos\theta \rangle_{M_{\widehat{\kappa}}} \tag{3.28}$$

$$\begin{aligned} c_2 =& \langle \cos\theta \rangle_{\widetilde{M}_{\widehat{\kappa}}} - \alpha \langle \nu \cos^2\theta - \nu' \cos\theta \sin^2\theta \rangle_{\widetilde{M}_{\widehat{\kappa}}} \\ &- \alpha d \left\langle n\cos\theta + \tfrac{\nu'}{\nu}((n+2)\cos^2\theta - 1) - \tfrac{\nu''}{\nu}\cos\theta\sin^2\theta \right\rangle_{\widetilde{M}_{\widehat{\kappa}}}, \end{aligned} \tag{3.29}$$

$$\lambda = d \left\langle \tfrac{1}{\nu} \right\rangle_{\widetilde{M}_{\widehat{\kappa}}}, \tag{3.30}$$

where here we use the notation

$$\langle \gamma(\cos\theta) \rangle_{\widetilde{M}_{\widehat{\kappa}}} = \frac{\int_0^\pi \gamma(\cos\theta)\nu(\cos\theta) h_{\widehat{\kappa}}(\cos\theta) e^{\widehat{\kappa}(\cos\theta)}\, \sin^n\theta\, \mathrm{d}\theta}{\int_0^\pi \nu(\cos\theta) h_{\widehat{\kappa}}(\cos\theta) e^{\widehat{\kappa}(\cos\theta)}\, \sin^n\theta\, \mathrm{d}\theta}.$$

Since ν *is supposed to be positive, the constant* λ *is positive, and we will see in the next section that its possible change of sign with the dependence on* ρ *is important. This is why we focus on the dependence on* ρ *and not in* $\omega \cdot \Omega$ *in this chapter.*

4 Properties of the macroscopic model

4.1 Hyperbolicity

We recall here the macroscopic model (2.6)-(2.7):

$$\partial_t \rho + \nabla_x \cdot (c_1(\rho)\rho\Omega) = 0,$$
$$\rho\ (\partial_t \Omega + c_2(\rho)(\Omega \cdot \nabla_x)\Omega) + \lambda(\rho)\, (\mathrm{Id} - \Omega \otimes \Omega)\nabla_x \rho = 0,$$

where the functions c_1, c_2, and λ are given by (3.24) and (3.26)-(3.27). A first remark is that it is not possible to do another scaling to get rid of c_1, like in [28], because c_1 depends on ρ.

The main result about this model is that if d or ν depends on ρ, the coefficient λ can become negative in some regions of the state space, and in that case the system loses hyperbolicity. Let us first discuss here the interest and the problems due to the non-hyperbolicity.

The first thing to remark is that the model is not always well-posed. Indeed, in general, we cannot ensure that a solution will stay in the region of hyperbolicity for all time, even with smooth initial conditions in the hyperbolic region (actually, even with hyperbolicity everywhere, dealing with the discontinuities is a challenging issue, see [60]).

The property of hyperbolicity is linked with the fact that perturbations propagate with finite speed. Here the presence of a region of non-hyperbolicity means that we could have propagation with infinite speed across this region. This leads to a second remark: it may be possible to construct non-classical shocks, using the crossing of a zone of non-hyperbolicity, see [52], and [50]. The interest is that we may construct some travelling waves, as observed in [16]. Actually we did not manage to construct such solutions yet, this is part of our future work.

We should also construct models with formation of coherent structures from such non-hyperbolic models, if we could use stabilization with diffusion. But here the expansion at higher order in ε in the rescaled mean-field model (3.11), in order to obtain diffusion terms in the macroscopic model becomes too much complicated to perform some study (see [31] for the case of the original model of [28]).

We now turn to the description of the regions of non-hyperbolicity. We consider a system satisfying (2.6)-(2.7), but evolving only along one space direction $e_z \in \mathbb{S}$ (the density ρ and the orientation Ω depending only on $z = e_z \cdot x$ and t). We write then $\Omega = \cos\theta\, e_z + \sin\theta\, v$,where $v \in \mathbb{S}_{n-2}$ (identified to the set of unit vectors orthogonal to e_z). In this framework, the system is equivalent to

$$\partial_t \rho + \partial_z(\rho c_1(\rho)\cos\theta) = 0. \tag{4.31}$$

$$\rho[\partial_t(\cos\theta) + c_2(\rho)\cos\theta\,\partial_z(\cos\theta)] + \lambda\,(1-\cos^2\theta)\,\partial_z\rho = 0. \tag{4.32}$$

$$\partial_t v + c_2(\rho)\cos\theta\,\partial_z v = 0, \text{ with } |v| = 1 \text{ and } e_z \cdot v = 0. \tag{4.33}$$

In the special case of dimension 2, the system reduces to (4.31)-(4.32), with $\theta \in (-\pi, \pi)$ 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 general definition of a quasilinear hyperbolic system [70] gives that the system (2.6)-(2.7) is hyperbolic if and only if this system (4.31)-(4.33) is hyperbolic for all unit vector $e_z \in \mathbb{S}$. We give the result in the following statement:

Theorem 1.2. *Hyperbolicity.*

- *The system* (2.6)-(2.7) *is hyperbolic if and only if* $\lambda(\rho) > 0$.
- *The system* (4.31)-(4.33) *is hyperbolic if and only if*

$$\lambda(\rho) > 0 \text{ or } \begin{cases} |\tan\theta| < \frac{|c_2 - c_3|}{2\sqrt{-\lambda c_1}}, & \text{if } \lambda < 0, \\ \theta \neq \frac{\pi}{2} \text{ and } c_2 \neq c_3, & \text{if } \lambda = 0. \end{cases} \tag{4.34}$$

where $c_3(\rho) = \frac{\mathrm{d}}{\mathrm{d}\rho}(\rho c_1(\rho)) = c_1(\rho) + \rho\dot{\kappa}\left(\langle\cos^2\theta\rangle_{M_\kappa} - \langle\cos\theta\rangle^2_{M_\kappa}\right)$.

Proof. The system (4.31)-(4.33) can be written as the following first order quasilinear system of partial differential equations

$$\begin{pmatrix} \partial_t\rho \\ \partial_t\cos\theta \\ \partial_t v \end{pmatrix} + A(\rho,\cos\theta,v)\begin{pmatrix} \partial_z\rho \\ \partial_z\cos\theta \\ \partial_z v \end{pmatrix} = 0,$$

with

$$A(\rho,\cos\theta,v) = \begin{pmatrix} c_3(\rho)\cos\theta & c_1(\rho)\rho & 0 & \cdots & 0 \\ \frac{\lambda}{\rho}\sin^2\theta & c_2(\rho)\cos\theta & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & c_2(\rho)\cos\theta\,\mathrm{Id}_{n-2} & \\ 0 & 0 & & & \end{pmatrix},$$

and this system is hyperbolic in case $\lambda > 0$. The eigenvalues are $\gamma_\pm$ and γ_0 (of multiplicity $n-2$), given by

$$\gamma_0 = c_2\cos\theta, \quad \gamma_\pm = \frac{1}{2}\left[(c_2+c_3)\cos\theta \pm \left((c_2-c_3)^2\cos^2\theta + 4\lambda c_1\sin^2\theta\right)^{1/2}\right],$$

Now if $\lambda < 0$, asking $\gamma_\pm$ to be real and distinct is exactly equivalent to the equation (4.34). In this case the matrix A is diagonalizable. If $\gamma_+ = \gamma_-$, then A is diagonalizable only if its top left corner 2×2 submatrix is scalar (only one eigenvalue), which is not the case since $c_1(\rho)\rho > 0$. For the same reason, if $\lambda = 0$, we immediately get that A is diagonalizable if and only if the first two diagonal coefficients $c_2(\rho)\cos\theta$ and $c_3(\rho)\cos\theta$ are different, which ends the proof of the second statement.

Now we turn to the general case. If $\lambda > 0$, the system (4.31)-(4.33) is hyperbolic for all unit vector $e_z \in \mathbb{S}$, which gives that the system (2.6)-(2.7) is hyperbolic. Suppose now that the system (2.6)-(2.7) is hyperbolic in an open region of the state space, with $\lambda \leqslant 0$ at some point (ρ,Ω). Since $n \geqslant 2$ we can find e_z such that $e_z\cdot\Omega = 0$. Then we have $\cos\theta = 0$, which gives, by the condition (4.34) that (ρ,Ω) is in the region of non-hyperbolicity of the problem (4.31)-(4.33), and this is a contradiction. □

Actually, the positive functions d and ν being arbitrary, it is possible to have a lot of qualitatively different shapes for the region of non-hyperbolicity of the reduced system (4.31)-(4.33). We give here some examples in the case of dimension 2, where the coefficients are easy to compute numerically (using the explicit formulation (3.20) for g_κ).

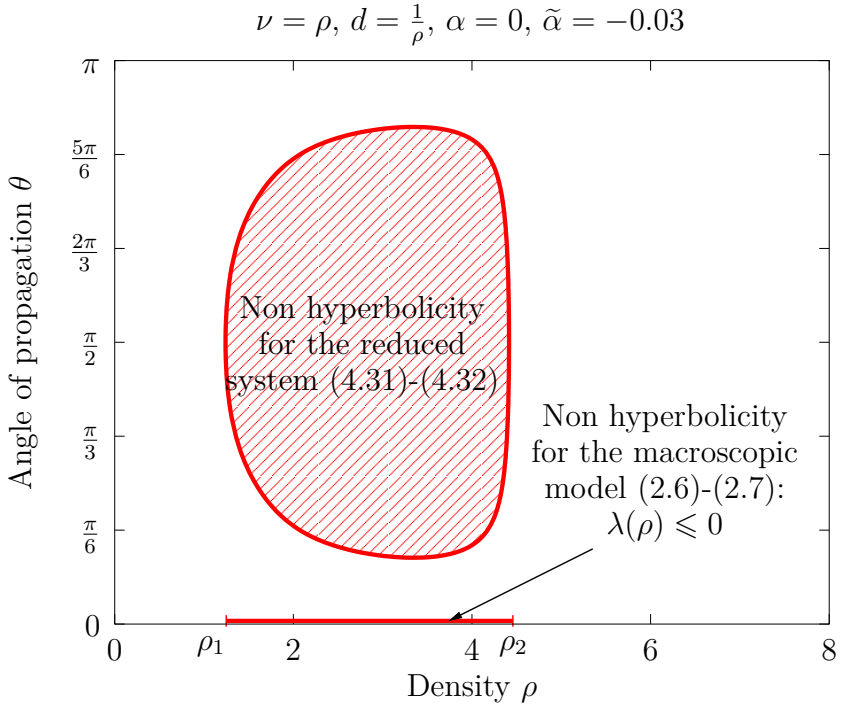

Figure 1.1: The region of hyperbolicity can be of the form $(0, \rho_1) \cup (\rho_2, +\infty)$

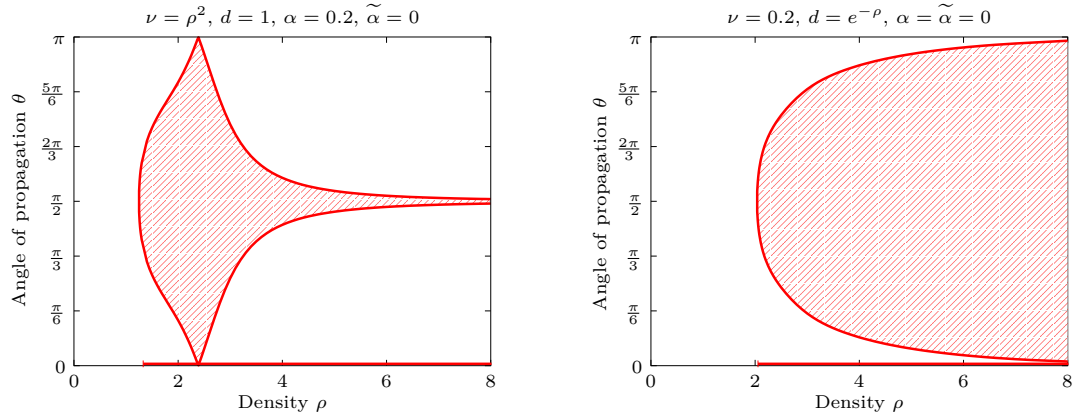

Figure 1.2: Other shapes for the zone of non-hyperbolicity

4.2 Influence of the anisotropy

On the final macroscopic model, the influence of the anisotropy in the observation kernels is only visible through the values of the speed c_2, and the coefficient λ.

We remark that the parameter α, which is related to the kernel K used to define the local orientation $\bar{\omega}$, only appears in the expression (3.26) of the velocity c_2, making it smaller when α is a large positive constant. The difference between c_1 and c_2, which is one of the differences between the macroscopic model (2.6)-(2.7) and the classical Euler system, is then enhanced when α is a large positive constant. This can be interpreted as follows: if the observation kernel is strongly directed forward, then the information on the orientation moves rapidly backward. This could be

compared to results on modelling of traffic flows, where the speed of a congested phase depends on the distance of anticipation of the drivers (see [4, 12, 25]).

The parameter $\widetilde{\alpha}$, related to the kernel $\widetilde{K}$ which is used to define the local density $\bar{\rho}$, only appears in λ, and obviously has an influence only if the relaxation frequency ν or the noise intensity d depends on this density (in the expression (3.27), we must have $\dot{\kappa} \neq 0$ or $\dot{d} \neq 0$). So the anisotropy of the kernel $\widetilde{K}$ can have an impact on the region of non-hyperbolicity for the system (2.6)-(2.7). The anisotropy of the kernel K does not play a role in this global hyperbolicity, but, through the condition (4.34), it can change the shape of the region of non-hyperbolicity for the one-dimensional reduction (4.31)-(4.33).

Since the expression (3.27) involves a lot of terms which can take different signs, it is not easy to directly quantify the influence of the parameter $\widetilde{\alpha}$ on the coefficient λ, as it was the case for α and c_2. In the next section, we perform an asymptotic study of the coefficients of the macroscopic model (2.6)-(2.7), as the concentration parameter κ tends to infinity (in the case of strong alignment, or low noise) or to zero (when the noise is high, or the frequency of alignment).

5 Asymptotic study of the coefficients

We want to obtain an asymptotic expansion of c_1, c_2 and λ given by the expressions (3.24), (3.26), (3.27) as the parameter κ tends to infinity or to zero.

Since we do not know explicitly the dependence on ρ for the coefficients ν and d, the only quantities we can study in the expressions of this coefficients are the averages $c_1 = \langle \cos\theta \rangle_{M_\kappa}$, $\widetilde{c_1} = \langle \cos\theta \rangle_{\widetilde{M}_\kappa}$, and $\langle \cos^2\theta \rangle_{\widetilde{M}_\kappa}$ (since the last average is $\langle \sin^2\theta \rangle_{\widetilde{M}_\kappa} = 1 - \langle \cos^2\theta \rangle_{\widetilde{M}_\kappa}$). The purpose of this section is to give a method to get the Taylor expansion up to any order in κ or $\frac{1}{\kappa}$ of the following averages:

$$\langle f(\theta) \rangle_{M_\kappa} = \frac{\int_0^\pi f(\theta) e^{\kappa\cos\theta} \sin^{n-2}\theta \,\mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta} \sin^{n-2}\theta \,\mathrm{d}\theta},$$
$$\langle f(\theta) \rangle_{\widetilde{M}_\kappa} = \frac{\int_0^\pi f(\theta) h_\kappa(\cos\theta) e^{\kappa\cos\theta} \sin^{n}\theta \,\mathrm{d}\theta}{\int_0^\pi h_\kappa(\cos\theta) e^{\kappa\cos\theta} \sin^{n}\theta \,\mathrm{d}\theta},$$

where h_κ is the function providing the generalized collisional invariants (see Proposition 3.1). We first give the method to obtain the expansion of the first type of average, and we apply it to get an expansion of c_1 in κ and $\frac{1}{\kappa}$.

5.1 Asymptotics of $\langle f(\theta) \rangle_{M_\kappa}$

The first expansion, when $\kappa \to 0$, is just a basic Taylor expansion. For a function f such that $f \sin^{n-2}\theta \in L^1(0,\pi)$, we define

$$b_p = \frac{1}{p!}\int_0^\pi f(\theta)\cos^p\theta \,\sin^{n-2}\theta \,\mathrm{d}\theta \quad \text{and} \quad a_p = \frac{1}{p!}\int_0^\pi \cos^p\theta \,\sin^{n-2}\theta \,\mathrm{d}\theta.$$

Then we get

$$\langle f(\theta) \rangle_{M_\kappa} = \frac{\sum_{p=0}^N b_p\kappa^p + O(\kappa^{N+1})}{\sum_{p=0}^N a_p\kappa^p + O(\kappa^{N+1})}. \tag{5.35}$$

If we take $f(\theta) = \cos\theta$, we have $b_p = (p+1)a_{p+1}$ and integrating by parts, we get the following induction relation: $(p+2)(p+n)a_{p+2} = a_p$. Since $a_1 = 0$, the odd terms vanish and we get

$$c_1 = \langle \cos\theta \rangle_{M_\kappa} = \frac{\frac{1}{n}\kappa + \frac{1}{2n(n+2)}\kappa^3 + O(\kappa^5)}{1 + \frac{1}{2n}\kappa^2 + O(\kappa^4)} = \frac{1}{n}\kappa - \frac{1}{n^2(n+2)}\kappa^3 + O(\kappa^5). \tag{5.36}$$

We now turn to the expansion of c_1 when $\kappa \to \infty$. We will use the following lemma, the proof of which is elementary, see [11] for examples and variants:

Lemma 1.1. *(Watson's Lemma)*

Let p be a function in $L^1(0,T)$, with $T > 0$, and let $I_\kappa(p) = \int_0^T p(t)e^{-\kappa t}\mathrm{d}t$. Suppose that, in the neighborhood of 0, we have $p(t) = t^\beta \left(\sum_{i=0}^{N-1} a_i t^i + O(t^N)\right)$, with $\beta > -1$.

Then $I_\kappa(p) = \kappa^{-\beta-1}\left(\sum_{i=0}^{N-1} a_i \Gamma(\beta+i+1)\kappa^{-i} + O(\kappa^{-N})\right)$ as $\kappa \to \infty$.

We use this lemma, after the change of variable $t = 1 - \cos\theta$, in the integrals of the form $[f(\theta)]_\kappa = \int_0^\pi f(\theta)e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta$. We get

$$[f(\theta)]_\kappa = e^\kappa \int_0^2 f(arccos(1-t))e^{-\kappa t}(2t-t^2)^{\frac{n-3}{2}}\,\mathrm{d}t.$$

So if we can expand the function $t \mapsto (2t-t^2)^{\frac{n-3}{2}} f(arccos(1-t))$ in the neighborhood of 0, we can apply directly Watson's Lemma to get an expansion of $[f(\theta)]_\kappa$, and then to $[1]_\kappa$, which gives finally the expansion of $\langle f(\theta)\rangle_{M_\kappa}$.

We take here the example of the function $f(\theta) = 1-\cos\theta$, so $f(arccos(1-t)) = t$. We want an expansion with two terms (since we have $c_1 = 1 - \langle f(\theta)\rangle_{M_\kappa}$ we will actually get three terms for c_1). We have

$$(2t-t^2)^{\frac{n-3}{2}} = 2^{\frac{n-3}{2}} t^{\frac{n-3}{2}}(1-\tfrac{1}{2}t)^{\frac{n-3}{2}} = 2^{\frac{n-3}{2}} t^{\frac{n-3}{2}}(1 - \tfrac{n-3}{4}t + O(t^2))$$

Applying directly Watson's Lemma to this function and to the same function multiplied by t, we get

$$\begin{aligned}
[1]_\kappa &= \frac{2^{\frac{n-3}{2}}e^\kappa}{\kappa^{\frac{n-1}{2}}}\left(\Gamma(\tfrac{n-1}{2}) - \tfrac{n-3}{4}\Gamma(\tfrac{n+1}{2})\frac{1}{\kappa} + O(\kappa^{-2})\right) \qquad (5.37)\\
[f(\theta)]_\kappa &= \frac{2^{\frac{n-3}{2}}e^\kappa}{\kappa^{\frac{n+1}{2}}}\left(\Gamma(\tfrac{n+1}{2}) - \tfrac{n-3}{4}\Gamma(\tfrac{n+3}{2})\frac{1}{\kappa} + O(\kappa^{-2})\right).
\end{aligned}$$

Since $\Gamma(p+1) = p\Gamma(p)$, we finally get

$$\begin{aligned}
\langle f(\theta)\rangle_{M_\kappa} = \frac{[f(\theta)]_\kappa}{[1]_\kappa} &= \frac{\Gamma(\frac{n+1}{2})}{\kappa\Gamma(\frac{n-1}{2})}\frac{1 - \frac{n-3}{4}\frac{n+1}{2}\frac{1}{\kappa}}{1 - \frac{n-3}{4}\frac{n-1}{2}\frac{1}{\kappa}} + O(\kappa^{-3})\\
&= \frac{n-1}{2\kappa} - \frac{(n-1)(n-3)}{8\kappa^2} + O(\kappa^{-3}).
\end{aligned}$$

In particular we get the expansion of c_1 as $\kappa \to \infty$:

$$c_1 = 1 - \frac{n-1}{2\kappa} + \frac{(n-1)(n-3)}{8\kappa^2} + O(\kappa^{-3}). \tag{5.38}$$

Using this method we can easily get the following lemma, which will be useful in the next subsection.

Lemma 1.2. *Estimation of* $\langle f(\theta)\rangle_{M_\kappa}$.

Suppose that $\theta \mapsto f(\theta)\sin^{n-2}\theta$ *belongs to* $L^1(0,\pi)$, *and that* $|f(\theta)| = O(\theta^{2\beta})$ *in the neighborhood of* 0, *with* $\beta > -\frac{n-1}{2}$. *Then* $\langle f(\theta)\rangle_{M_\kappa} = O(\kappa^{-\beta})$ *as* $\kappa \to \infty$.

We now turn to the method to compute averages of the form $\langle f(\theta)\rangle_{\widetilde{M}_\kappa}$.

5.2 Asymptotics of $\langle f(\theta)\rangle_{\widetilde{M}_\kappa}$

We first decompose $h_\kappa(\cos\theta)$ as a polynomial in κ or in κ^{-1} whose coefficients are polynomials of $\cos\theta$ plus a remainder which will be negligible.

Proposition 5.1. *Expansion of* h_κ.

We define the two linear operators L *and* D *on the space of polynomials by*

$$L(P) = -(1-X^2)P'' + (n+1)XP' + (n-1)P$$
$$D(P) = -(1-X^2)P' + XP.$$

We have the two following expansions:

$$h_\kappa(\cos\theta) = \sum_{p=0}^{N} H_p(\cos\theta)\kappa^p + R^N_{\kappa,0}(\cos\theta),$$
$$h_\kappa(\cos\theta) = \sum_{p=1}^{N} G^N_p(\cos\theta)\kappa^{-p} + R^N_{\kappa,\infty}(\cos\theta),$$

where the H_p *(resp.* G^N_p*) are the polynomials of degree* p *(resp. at most* $N-p$*) given by the following induction relations (the second one being in the neighborhood of* 0*):*

$$\begin{cases} L(H_0) = 1 \\ L(H_{p+1}) = -D(H_p) \end{cases} \quad \text{and} \quad \begin{cases} D(G^N_1)(\cos\theta) = 1 + O(\theta^{2N}) \\ (D(G^N_{p+1}) + L(G^N_p))(\cos\theta) = O(\theta^{2(N-p)}), \end{cases} \tag{5.39}$$

and where the remainders satisfy the following estimations, for any function f *such that* $\theta \mapsto f(\theta)\sin^{\frac{n}{2}}\theta$ *belongs to* $L^2(0,\pi)$ *and such that* $|f(\theta)| = O(\theta^{2\beta})$ *in the neighborhood of* 0*:*

$$\langle f(\theta)R^N_{\kappa,0}(\cos\theta)\sin^2\theta\rangle_{M_\kappa} = O(\kappa^{N+1}) \text{ as } \kappa \to 0,$$
$$\langle f(\theta)R^N_{\kappa,\infty}(\cos\theta)\sin^2\theta\rangle_{M_\kappa} = O(\kappa^{-\beta-N-2}) \text{ as } \kappa \to \infty.$$

The proof of this proposition is given in Appendix B.1. The first thing to do is to prove that the inductions relations (5.39) make sense to define the sequence of polynomials (an induction relation is given in Appendix B.1 to compute easily the polynomials G^N_p and H_p). The operators L and D are made so that

$$\widetilde{L}^*_\kappa(P(\cos\theta)\sin\theta) = (L(P) + \kappa D(P))(\cos\theta)\sin\theta,$$

where the operator $\widetilde{L}^*_\kappa$ is defined in (3.17). Since we have $\widetilde{L}^*_\kappa(h_\kappa(\cos\theta)\sin\theta) = \sin\theta$ by definition, we are then able to obtain the estimates on the remainders, using Poincaré inequalities in adapted spaces.

With this proposition, it is then easy to get an expansion for $\langle f(\theta)\rangle_{\widetilde{M}_\kappa}$, using expressions of the form $\langle g(\theta)\rangle_{M_\kappa}$, which can be expanded by the tools of the previous section:

$$\langle f(\theta)\rangle_{\widetilde{M}_\kappa} = \begin{cases} \dfrac{\sum_{p=0}^N \langle f(\theta) H_p(\cos\theta)\sin^2\theta\rangle_{M_\kappa}\kappa^p}{\sum_{p=0}^N \langle H_p(\cos\theta)\sin^2\theta\rangle_{M_\kappa}\kappa^p} + O(\kappa^{N+1}) & \text{as } \kappa\to 0, \\ \dfrac{\sum_{p=1}^N \langle f(\theta) G_p^N(\cos\theta)\sin^2\theta\rangle_{M_\kappa}\kappa^{-p}}{\sum_{p=1}^N \langle G_p^N(\cos\theta)\sin^2\theta\rangle_{M_\kappa}\kappa^{-p}} + O(\kappa^{-\beta-N}) & \text{as } \kappa\to\infty. \end{cases}$$

As an example, we can compute the first polynomials, we get

$$H_0 = \frac{1}{n-1}, \quad H_1 = \frac{-X}{2n(n-1)}, \quad G_1^2 = \frac{4-X}{3}, \quad G_2^2 = \frac{2(n-2)}{3}.$$

Hence,

$$\langle\cos\theta\rangle_{\widetilde{M}_\kappa} = \frac{\frac{1}{n-1}\langle\cos\theta\sin^2\theta\rangle_{M_\kappa} - \frac{\kappa}{2n(n-1)}\langle\cos^2\theta\sin^2\theta\rangle_{M_\kappa}}{\frac{1}{n-1}\langle\sin^2\theta\rangle_{M_\kappa} - \frac{\kappa}{2n(n-1)}\langle\cos\theta\sin^2\theta\rangle_{M_\kappa}} + O(\kappa^2),$$

$$\langle\cos\theta - 1\rangle_{\widetilde{M}_\kappa} = \frac{\frac{1}{3\kappa}\langle\cos\theta(4-\cos\theta)\sin^2\theta\rangle_{M_\kappa} + \frac{2(n-2)}{3\kappa^2}\langle\cos\theta\sin^2\theta\rangle_{M_\kappa}}{\frac{1}{3\kappa}\langle(4-\cos\theta)\sin^2\theta\rangle_{M_\kappa} + \frac{2(n-2)}{3\kappa^2}\langle\sin^2\theta\rangle_{M_\kappa}} - 1 + O(\kappa^{-3}).$$

As before, in the second equation, we computed $\langle\cos\theta - 1\rangle_{\widetilde{M}_\kappa}$ instead of $\langle\cos\theta\rangle_{\widetilde{M}_\kappa}$ in order to have a remainder of order 3 instead of 2.

Finally, we have to compute terms of the form $\langle\cos^\ell\theta\sin^2\theta\rangle_{M_\kappa}$. Instead of using the method of the previous subsection, we can actually express all these terms in function of $c_1 = \langle\cos\theta\rangle_{M_\kappa}$, by integrating by parts. We get

$$\langle\sin^2\theta\rangle_{M_\kappa} = \tfrac{n-1}{\kappa}c_1, \quad \langle\cos\theta\sin^2\theta\rangle_{M_\kappa} = \tfrac{n-1}{\kappa}(1-\tfrac{n}{\kappa}c_1)$$
$$\langle\cos^2\theta\sin^2\theta\rangle_{M_\kappa} = \langle\sin^2\theta\rangle_{M_\kappa} - \langle\sin^4\theta\rangle_{M_\kappa} = \tfrac{n-1}{\kappa}(c_1 - \tfrac{n+1}{\kappa}(1-\tfrac{n}{\kappa}c_1)).$$

Using the previous expansions (5.36) and (5.38), we finally get the expansions of $\widetilde{c_1}$:

$$\widetilde{c}_1 = \langle\cos\theta\rangle_{\widetilde{M}_\kappa} = \begin{cases} \frac{2n-1}{2n(n+2)}\kappa + O(\kappa^2) & \text{as } \kappa\to 0, \\ 1 - \frac{n+1}{2\kappa} + \frac{(n+1)(3n-7)}{24\kappa^2} + O(\kappa^{-3}) & \text{as } \kappa\to\infty. \end{cases} \tag{5.40}$$

In addition, we can compute an expansion of $\langle\sin^2\theta\rangle_{\widetilde{M}_\kappa}$, in order to get expansions for the coefficients c_2 and λ of the macroscopic model, given in equations (3.26)-(3.27). Using only H_0 and $G_1^1 = 1$, we get that

$$\langle\sin^2\theta\rangle_{\widetilde{M}_\kappa} = \begin{cases} \dfrac{\langle\cos^2\theta\sin^2\theta\rangle_{M_\kappa}}{\langle\sin^2\theta\rangle_{M_\kappa}} + O(\kappa) = \frac{n+1}{n+2} + O(\kappa) & \text{as } \kappa\to 0, \\ \dfrac{\langle\sin^4\theta\rangle_{M_\kappa}}{\langle\sin^2\theta\rangle_{M_\kappa}} + O(\kappa^{-2}) = \frac{n+1}{\kappa} + O(\kappa^{-2}) & \text{as } \kappa\to\infty. \end{cases}$$

So, using the expressions (5.36), (5.38) and (5.40), we get the following expansions:

$$c_1 = \begin{cases} \frac{1}{n}\kappa - \frac{1}{n^2(n+2)}\kappa^3 + O(\kappa^5) & \text{as } \kappa \to 0, \\ 1 - \frac{n-1}{2\kappa} + \frac{(n-1)(n-3)}{8\kappa^2} + O(\kappa^{-3}) & \text{as } \kappa \to \infty, \end{cases}$$

$$c_2 = \begin{cases} \frac{2n-1}{2n(n+2)}\kappa + O(\kappa^2) - \alpha\,\nu\,(\frac{2n+1}{2(n+2)} + O(\kappa)) & \text{as } \kappa \to 0, \\ 1 - \frac{n+1}{2}\,\kappa^{-1} + O(\kappa^{-2}) - \alpha\,\nu\,(1 - \kappa^{-1} + O(\kappa^{-2})) & \text{as } \kappa \to \infty, \end{cases}$$

$$\lambda = \begin{cases} \kappa^{-1} + \rho\,\frac{\dot\kappa}{\kappa}\,[\,-\frac{5}{2n(n+2)}\kappa + O(\kappa^2) + \widetilde{\alpha}\,\nu\,(\frac{3}{2(n+2)} + O(\kappa))\,] \\ \quad + \frac{1}{2}\,\widetilde{\alpha}\,\rho\,\frac{\dot d}{d}\,\nu\,((n-1)\kappa^{-1} + \frac{2n-1}{2n(n+2)}\kappa + O(\kappa^2)) & \text{as } \kappa \to 0, \\ \kappa^{-1}\,(1 + \rho\,\frac{\dot\kappa}{\kappa}\,[-1 + O(\kappa^{-1}) + \widetilde{\alpha}\,\nu\,(1 + O(\kappa^{-1}))\,]) \\ \quad + \frac{1}{2}\,\widetilde{\alpha}\,\rho\,\frac{\dot d}{d}\,\nu\,(1 + \frac{n-3}{2}\kappa^{-1} + O(\kappa^{-2})) & \text{as } \kappa \to \infty. \end{cases}$$

This shows that in any dimension, there are some simple cases were we actually have $\lambda < 0$ and the system loses hyperbolicity, even if $\widetilde{\alpha} = 0$ (for example if the kernel of observation $\widetilde{K}$ is isotropic). For example if we have $\kappa = \rho^\beta$ with $\beta > 0$, we have as $rho \to \infty$ that $\lambda(\rho) = (1-\beta)\rho^{-\beta} + O(\rho^{-2\beta})$, which gives that $\lambda(\rho) < 0$ if we take $\beta > 1$ and ρ sufficiently large.

These expansions also give a more precise estimation on the difference between c_1 and c_2 as the noise is small or large: when the kernel of observation is isotropic, we have $c_1 > c_2$ in the two expansions, in any dimension n. That means that the information on the orientation propagates slower than the "fluid".

Remark 5.1. *We can also do an expansion in the more general case where ν depends on ρ and $\omega \cdot \Omega$. When $d \to 0$, the expansion of the coefficients depends only on the local behavior of the function $x \mapsto \nu(\rho, x)$ near 1. In Appendix B.2 we give tips to perform this expansion. Here we only give the final expansion in the case where ν and d do not depend on ρ, so the coefficients are given by* (3.28)-(3.30)*. In this case we can suppose $\nu(1) = 1$ (up to a rescaling), and denote $\gamma = \nu'(1)$. We finally get, when $n = 2$:*

$$\begin{aligned} c_1 &= 1 - \tfrac{1}{2}d + O(d^2), \\ c_2 &= 1 - \alpha + ((1 + \tfrac{3}{2}\gamma)\alpha - \tfrac{3}{2})d + O(d^2), \\ \lambda &= d + \tfrac{3}{2}\gamma\, d^2 + O(d^3). \end{aligned}$$

6 Conclusion

In this chapter, we have seen that the introduction of a dependence on some local density for some parameters at the microscopic level implies a significant change in the macroscopic limit: the possible loss of hyperbolicity in some regimes. The introduction of a non-isotropic kernel of observation, without this dependence on the local density, is not sufficient to imply a strong difference of behavior for the continuum model. However, it enhances some properties, such as the difference between the velocity of the fluid and the velocity of the perturbations of the orientation.

It is important to note that the method introduced in [28] works to derive the macroscopic model. In particular the concept of generalized collisional invariants is still valid, with some adaptations, and we get the same macroscopic model, except for the definition of the coefficients.

Some questions are left open. The limit here is formal, and we are still looking for an appropriate functional framework to obtain more precise results of convergence. The rigorous derivation of the mean-field limit of the dynamical system of particles is also part of our future work.

Finally, the next step to this study consists in some numerical simulations, in order to see how the difference between c_2 and c_1 can be observed in simulations of the discrete dynamical system, or how the particles behave in the regions of non-hyperbolicity.

A Proof of some statements for section 3

A.1 Expansion of the local density and orientation

We recall the expressions of $\bar{\omega}^\varepsilon$ and $\bar{\rho}^\varepsilon$:

$$\bar{\omega}^\varepsilon(x,\omega,t) = \frac{\bar{J}^\varepsilon(x,\omega,t)}{|\bar{J}^\varepsilon(x,\omega,t)|}, \tag{A.41}$$

$$\bar{J}^\varepsilon(x,\omega,t) = \int_{y\in\mathbb{R}^n,\, v\in\mathbb{S}} K\left(\tfrac{|x-y|}{\varepsilon}, \tfrac{y-x}{|x-y|}\cdot\omega\right) v\, f^\varepsilon(y,v,t)\, \tfrac{\mathrm{d}y}{\varepsilon^n}\, \mathrm{d}v\,, \tag{A.42}$$

$$\bar{\rho}^\varepsilon(x,\omega,t) = \int_{y\in\mathbb{R}^n,\, v\in\mathbb{S}} \widetilde{K}\left(\tfrac{|x-y|}{\varepsilon}, \tfrac{y-x}{|x-y|}\cdot\omega\right) f^\varepsilon(y,v,t)\, \tfrac{\mathrm{d}y}{\varepsilon^n}\, \mathrm{d}v\,, \tag{A.43}$$

Lemma 1.3. *We have the following expansions:*

$$\bar{\omega}^\varepsilon(x,\omega,t) = \Omega^\varepsilon(x,t) + \varepsilon\alpha\,(\omega\cdot\nabla_x)\,\Omega^\varepsilon(x,t) + O(\varepsilon^2)\,,$$
$$\bar{\rho}^\varepsilon(x,\omega,t) = \rho^\varepsilon(x,t) + \varepsilon\widetilde{\alpha}\,\omega\cdot\nabla_x\rho^\varepsilon(x,t) + O(\varepsilon^2)\,.$$

where the constants α and $\widetilde{\alpha}$ depend only on the observation kernels K and $\widetilde{K}$, and

$$\Omega^\varepsilon(x,t) = \tfrac{j^\varepsilon(x,t)}{|j^\varepsilon(x,t)|},\ \textit{with } j^\varepsilon(x,t) = \int_{v\in\mathbb{S}} v\, f^\varepsilon(x,v,t)\,\mathrm{d}v\,,$$
$$\rho^\varepsilon(x,t) = \int_{v\in\mathbb{S}} f^\varepsilon(x,v,t)\,\mathrm{d}v\,.$$

Proof. After change of variable $y = x + \varepsilon\xi$, let us expand f at first order in ε in (A.42). We get

$$\bar{J}^\varepsilon(x,\omega,t) = \int_{\xi\in\mathbb{R}^n,\, v\in\mathbb{S}} K(|\xi|, \tfrac{\xi}{|\xi|}\cdot\omega)\, v\,(f^\varepsilon(x,v,t) + \varepsilon\,\xi\cdot\nabla_x f^\varepsilon(x,v,t) + O(\varepsilon^2))\,\mathrm{d}\xi\,\mathrm{d}v\,.$$

We have to compute

$$K_0(\omega) = \int_{\xi\in\mathbb{R}^n} K(|\xi|, \tfrac{\xi}{|\xi|}\cdot\omega)\mathrm{d}\xi \quad \text{and} \quad K_1(\omega) = \int_{\xi\in\mathbb{R}^n} K(|\xi|, \tfrac{\xi}{|\xi|}\cdot\omega)\,\xi\,\mathrm{d}\xi.$$

For any rotation R, the change of variable $\tilde{\xi} = R(\xi)$ gives on one hand

$$K_0(\omega) = K_0(R(\omega))\,,$$

and so K_0 does not depend on ω. On the other hand, we get

$$R(K_1(\omega)) = K_1(R(\omega))\,,$$

which shows that $K_1(\omega)$ is a vector invariant by any rotation which let ω invariant, so it is parallel to ω. Given a vector e of $\mathbb{S}$, we have $K_1(e) = k_1 e$. Then taking one rotation mapping ω to e, we get $R(K_1(\omega)) = K_1(e) = k_1 e = R(k_1\omega)$, so finally we get $K_1(\omega) = k_1\omega$ for all $\omega \in \mathbb{S}$. Let then $\alpha = \frac{k_1}{K_0}$, and we have

$$\begin{aligned}\frac{\bar{J}^\varepsilon(x,\omega,t)}{K_0} &= \int_{\upsilon\in\mathbb{S}} \upsilon\,(f^\varepsilon(x,\upsilon,t) + \varepsilon\,\alpha\,\omega\cdot\nabla_x f^\varepsilon(x,\upsilon,t))\,\mathrm{d}\upsilon + O(\varepsilon^2)\\ &= j^\varepsilon(x,t) + \varepsilon\,\alpha\,(\omega\cdot\nabla_x) j^\varepsilon(x,t) + O(\varepsilon^2)\,.\end{aligned}$$

Putting this expression into (A.41), we get

$$\left|\frac{\bar{J}^\varepsilon(x,\omega,t)}{K_0}\right|^2 = |j^\varepsilon(x,t)|^2 + 2\,\varepsilon\,\alpha\, j^\varepsilon(x,t)\cdot(\omega\cdot\nabla_x) j^\varepsilon(x,t) + O(\varepsilon^2)\,,$$

so

$$\left|\frac{\bar{J}^\varepsilon(x,\omega,t)}{K_0}\right|^{-1} = \frac{1}{|j^\varepsilon(x,t)|}\left(1 - \frac{\varepsilon\,\alpha}{|j^\varepsilon(x,t)|^2}\, j^\varepsilon(x,t)\cdot(\omega\cdot\nabla_x) j^\varepsilon(x,t)\right) + O(\varepsilon^2)\,,$$

and finally

$$\begin{aligned}\bar{\omega}^\varepsilon(x,\omega,t) &= \frac{j^\varepsilon(x,t)}{|j^\varepsilon(x,t)|}\\ &\quad + \varepsilon\,\alpha\left(\frac{(\omega\cdot\nabla_x) j^\varepsilon(x,t)}{|j^\varepsilon(x,t)|} - \frac{j^\varepsilon(x,t)}{|j^\varepsilon(x,t)|}\cdot\frac{(\omega\cdot\nabla_x) j^\varepsilon(x,t)}{|j^\varepsilon(x,t)|}\frac{j^\varepsilon(x,t)}{|j^\varepsilon(x,t)|}\right) + O(\varepsilon^2).\end{aligned}$$

But we also have

$$\begin{aligned}(\omega\cdot\nabla_x)\Omega^\varepsilon(x,t) &= \frac{(\omega\cdot\nabla_x) j^\varepsilon(x,t)}{|j^\varepsilon(x,t)|} + \left(\omega\cdot\nabla_x\left(\frac{1}{|j^\varepsilon(x,t)|}\right)\right) j^\varepsilon(x,t)\\ &= \frac{(\omega\cdot\nabla_x) j^\varepsilon(x,t)}{|j^\varepsilon(x,t)|} - \frac{1}{|j^\varepsilon(x,t)|^3}\left(((\omega\cdot\nabla_x) j^\varepsilon(x,t))\cdot j^\varepsilon(x,t)\right) j^\varepsilon(x,t)\,.\end{aligned}$$

Therefore

$$\bar{\omega}^\varepsilon(x,\omega,t) = \Omega^\varepsilon(x,t) + \varepsilon\alpha\,(\omega\cdot\nabla_x)\,\Omega^\varepsilon(x,t) + O(\varepsilon^2)\,,$$

and this is the first part of the lemma.

After the same change of variable $y = x + \varepsilon\xi$ and expansion in (A.43), and using the same techniques, and the normalization condition (2.5), we get

$$\begin{aligned}\bar{\rho}^\varepsilon(x,\omega,t) &= \int_{\upsilon\in\mathbb{S}} f^\varepsilon(x,\upsilon,t) + \varepsilon\,\widetilde{K_1}(\omega)\cdot\nabla_x f^\varepsilon(x,\upsilon,t)\,\mathrm{d}\upsilon + O(\varepsilon^2)\\ &= \rho^\varepsilon(x,t) + \varepsilon\,\widetilde{\alpha}\,\omega\cdot\nabla_x\rho^\varepsilon(x,t) + O(\varepsilon^2)\,.\end{aligned}$$

This is the second part of the lemma. □

A.2 Proof of Proposition 3.2

We have to compute $(\mathrm{Id} - \Omega \otimes \Omega)\, X$, where

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

For convenience, we will write ν, d for $\nu(\rho)$, $d(\rho)$ in the following. We first give some useful formulas to work on the unit sphere. For V a constant vector in $\mathbb{R}^n$, we have:

$$\begin{aligned} \nabla_\omega(\omega \cdot V) &= (\mathrm{Id} - \omega \otimes \omega)V, \\ \nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega)V) &= -(n-1)\, \omega \cdot V. \end{aligned}$$

Then we have that for any constant matrix A

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

where the notation ":" denotes the "contraction" of two operators (if $A = (A_{ij})$ and $B = (B_{ij})$ then $A : B = \sum_{i,j=1,\dots,n} A_{ij}B_{ij}$, this is the trace of AB^T). This can be shown when A is of the form $V_1 \otimes V_2$, using the previous formulas, and then extended by linearity.

We recall the definition of $M_{\kappa\Omega}$, given in equation (3.12):

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

We get, writing $\cos\theta$ for $\omega \cdot \Omega$, and using the notation $\langle \cdot \rangle_{M_\kappa}$ given in (3.14),

$$\begin{aligned} \nabla_\omega M_{\kappa\Omega} &= \kappa(\mathrm{Id} - \omega \otimes \omega)\Omega M_{\kappa\Omega}, \\ \nabla_\Omega M_{\kappa\Omega} &= \kappa(\mathrm{Id} - \Omega \otimes \Omega)\omega M_{\kappa\Omega}, \\ \partial_\kappa M_{\kappa\Omega} &= (\cos\theta - \langle \cos\theta \rangle_{M_\kappa}) M_{\kappa\Omega}. \end{aligned}$$

Using the chain rule, we then get

$$\begin{aligned} (\partial_t + \omega \cdot \nabla_x)(\rho M_{\kappa\Omega}) = (1 + (\cos\theta - \langle \cos\theta \rangle_{M_\kappa})\rho\dot{\kappa}) M_{\kappa\Omega}(\partial_t + \omega \cdot \nabla_x)\rho \\ + \rho\kappa(\mathrm{Id} - \Omega \otimes \Omega)\omega M_{\kappa\Omega} \cdot (\partial_t + \omega \cdot \nabla_x)\Omega, \end{aligned}$$

where $\dot{\kappa}$ is the derivative of κ with respect to ρ. Since Ω is of norm 1, we have that $(\partial_t + \omega \cdot \nabla_x)\Omega$ is orthogonal to Ω, and the term $\Omega \otimes \Omega$ vanishes. We get

$$\begin{aligned} (\partial_t + \omega \cdot \nabla_x)(\rho M_{\kappa\Omega}) = (1 + (\cos\theta - \langle \cos\theta \rangle_{M_\kappa})\rho\dot{\kappa}) M_{\kappa\Omega}(\partial_t \rho + \omega \cdot \nabla_x \rho) \\ + \rho\kappa M_{\kappa\Omega}(\omega \cdot \partial_t \Omega + \omega \otimes \omega : \nabla_x \Omega), \end{aligned}$$

where $\nabla_x\Omega$ is the gradient tensor of Ω that is to say $(\nabla_x\Omega)_{ij} = \partial_{x_i}\Omega_j$. We then have

$$\begin{aligned} P(\rho M_{\kappa\Omega}) &= \nu(\rho)\nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega)((\omega \cdot \nabla_x)\,\Omega)\rho M_{\kappa\Omega}), \\ &= \rho\nu(\rho)[\kappa\Omega \cdot (\mathrm{Id} - \omega \otimes \omega)((\nabla_x\Omega)^T\omega) + \nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega)(\nabla_x\Omega)^T\omega)]M_{\kappa\Omega}, \end{aligned}$$

where the notation ^{T} denotes the transpose of operators. Hence, using the fact that $(\nabla_x\Omega)^T\omega = (\omega\cdot\nabla_x)\,\Omega$ is orthogonal to Ω, and the formula given in the beginning of this section, with $A = (\nabla_x\Omega)^T$, and we get

$$\begin{aligned} P(\rho M_{\kappa\Omega}) &= \rho\nu(\rho)[-\kappa\cos\theta\,\omega\otimes\omega : (\nabla_x\Omega)^T + (\nabla_x\Omega)^T : (\mathrm{Id} - n\omega\otimes\omega)]M_{\kappa\Omega},\\ &= \rho\nu[\nabla_x\cdot\Omega - (n+\kappa\cos\theta)\,\omega\otimes\omega : \nabla_x\Omega]M_{\kappa\Omega}. \end{aligned}$$

Similarly, for the operator $\widetilde{P}$, we get

$$\begin{aligned} \widetilde{P}(\rho M_{\kappa\Omega}) &= \dot\nu(\rho)\nabla_\omega\cdot((\omega\cdot\nabla_x\rho)\,(\mathrm{Id}-\omega\otimes\omega)\Omega\rho M_{\kappa\Omega})\\ &\qquad - \dot d(\rho)\nabla_\omega\cdot(\tfrac12\rho M_{\kappa\Omega}(\mathrm{Id}-\omega\otimes\omega)\nabla_x\rho + (\omega\cdot\nabla_x\rho)\,\nabla_\omega\rho M_{\kappa\Omega}),\\ &= \rho(\dot\nu - \kappa\dot d)\nabla_\omega\cdot((\mathrm{Id}-\omega\otimes\omega)(\Omega\otimes\nabla_x\rho)\omega M_{\kappa\Omega})\\ &\qquad - \tfrac12\rho\dot d[\nabla_\omega\cdot((\mathrm{Id}-\omega\otimes\omega)\nabla_x\rho) + \kappa\Omega\cdot(\mathrm{Id}-\omega\otimes\omega)\nabla_x\rho]M_{\kappa\Omega}. \end{aligned}$$

But we have $\nu = \kappa d$, so $\dot\nu - \kappa\dot d = d\dot\kappa$. And we have

$$\begin{aligned} &\nabla_\omega\cdot((\mathrm{Id}-\omega\otimes\omega)(\Omega\otimes\nabla_x\rho)\omega M_{\kappa\Omega})\\ &\quad= \nabla_\omega\cdot((\mathrm{Id}-\omega\otimes\omega)(\Omega\otimes\nabla_x\rho)\omega)M_{\kappa\Omega} + \kappa\Omega\cdot(\mathrm{Id}-\omega\otimes\omega)(\Omega\otimes\nabla_x\rho)\omega]\\ &\quad= [(\Omega\otimes\nabla_x\rho) : (\mathrm{Id} - n\omega\otimes\omega) + \kappa(1-\cos^2\theta)\,\omega\cdot\nabla_x\rho]M_{\kappa\Omega}\\ &\quad= [\Omega\cdot\nabla_x\rho + (\kappa\sin^2\theta - n\cos\theta)\,\omega\cdot\nabla_x\rho]M_{\kappa\Omega}. \end{aligned}$$

Hence

$$\begin{aligned} \widetilde{P}(\rho M_{\kappa\Omega}) &= \rho d\dot\kappa[\Omega\cdot\nabla_x\rho + (\kappa\sin^2\theta - n\cos\theta)\,\omega\cdot\nabla_x\rho]M_{\kappa\Omega}\\ &\qquad + \tfrac12\rho\dot d[(\kappa\cos\theta + n - 1)\,\omega\cdot\nabla_x\rho - \kappa\Omega\cdot\nabla_x\rho]M_{\kappa\Omega}. \end{aligned}$$

Finally we can write $X = X_1 + X_2 + X_3$, where

$$\begin{aligned} X_1 &= \int_{\omega\in\mathbb{S}} h_\kappa(\cos\theta)\gamma_1(\cos\theta)\,\omega\,M_{\kappa\Omega}\mathrm{d}\omega,\\ X_2 &= \int_{\omega\in\mathbb{S}} h_\kappa(\cos\theta)\,\omega\otimes\omega(\gamma_2(\cos\theta)\,\nabla_x\rho + \rho\kappa\partial_t\Omega)\,M_{\kappa\Omega}\mathrm{d}\omega,\\ X_3 &= \int_{\omega\in\mathbb{S}} h_\kappa(\cos\theta)\gamma_3(\cos\theta)\,\omega(\omega\otimes\omega : \nabla_x\Omega)\,M_{\kappa\Omega}\mathrm{d}\omega, \end{aligned}$$

with (using the notation $c_1 = \langle\cos\theta\rangle_{M_\kappa}$)

$$\begin{aligned} \gamma_1(\cos\theta) &= (1 + (\cos\theta - c_1)\rho\dot\kappa)\partial_t\rho + \alpha\rho\nu\nabla_x\cdot\Omega + \widetilde\alpha\rho(d\dot\kappa - \tfrac12\dot d\kappa)\Omega\cdot\nabla_x\rho,\\ \gamma_2(\cos\theta) &= 1 + (\cos\theta - c_1)\rho\dot\kappa + \widetilde\alpha\rho(d\dot\kappa(\kappa\sin^2\theta - n\cos\theta) + \tfrac12\dot d\kappa(\kappa\cos\theta + n - 1)),\\ \gamma_3(\cos\theta) &= \rho\,\kappa - \alpha\rho\nu(n + \kappa\cos\theta). \end{aligned}$$

To do the computation we write $\omega = \cos\theta\,\Omega + \sin\theta\,v$, with $v\in\mathbb{S}_{n-2}$ (identified with the set of unit vectors which are orthogonal to Ω). We take the following convention: $\int_{v\in\mathbb{S}_{n-2}}\mathrm{d}v = 1$, and we have

$$\begin{gathered} \int_{\omega\in\mathbb{S}_{n-1}} a(\omega)\mathrm{d}\omega = \frac{1}{V_n}\int_0^\pi\int_{v\in\mathbb{S}_{n-2}} a(\theta,v)\sin^{n-2}\theta\,\mathrm{d}v\,\mathrm{d}\theta,\\ \int_{v\in\mathbb{S}_{n-2}} v\,\mathrm{d}v = 0,\ \text{and}\ \int_{v\in\mathbb{S}_{n-2}} v\otimes v\,\mathrm{d}v = \frac{1}{n-1}(\mathrm{Id}-\Omega\otimes\Omega), \end{gathered}$$

where V_n is a normalization constant (we will not need it in the following). These results are still valid when $n = 2$, with $\int_{v\in\mathbb{S}_0} \mathrm{d}v = \frac{1}{2}(a(v_0) + a(-v_0))$, v_0 being one of the two unit vectors orthogonal to Ω. Using these formulas, we get

$$\int_{\omega\in\mathbb{S}} \gamma(\cos\theta)\, M_{\kappa\Omega}\, \omega\, \mathrm{d}\omega = \langle \cos\theta\, \gamma(\cos\theta)\rangle_{M_\kappa}\, \Omega,$$

$$\int_{\omega\in\mathbb{S}} \omega\otimes\omega\, \gamma(\cos\theta)\, M_{\kappa\Omega}\, \mathrm{d}\omega = \langle \cos^2\theta\, \gamma\rangle_{M_\kappa} \Omega\otimes\Omega + \frac{\langle \sin^2\theta\, \gamma\rangle_{M_\kappa}}{n-1}(\mathrm{Id} - \Omega\otimes\Omega).$$

So we have (knowing that $\partial_t\Omega$ is orthogonal to Ω):

$$(\mathrm{Id} - \Omega\otimes\Omega)\, X_1 = 0,$$

$$(\mathrm{Id} - \Omega\otimes\Omega)\, X_2 = \frac{\langle \sin^2\theta\, \gamma_2 h_\kappa\rangle_{M_\kappa}}{n-1}(\mathrm{Id} - \Omega\otimes\Omega)\nabla_x\rho + \frac{\rho\kappa\langle \sin^2\theta\, h_\kappa\rangle_{M_\kappa}}{n-1}\partial_t\Omega.$$

To compute $(\mathrm{Id} - \Omega\otimes\Omega)\, X_3$, we first remark that

$$(\mathrm{Id} - \Omega\otimes\Omega)\, \omega(\omega\otimes\omega : \nabla_x\Omega) = \sin\theta\, v(\omega\cdot(\omega\cdot\nabla_x)\Omega) = \sin^2\theta\, v(v\cdot(\omega\cdot\nabla_x)\Omega),$$

since $(\omega\cdot\nabla_x)\Omega$ is orthogonal to Ω. But we have $\int_{v\in\mathbb{S}_{n-2}} v(v\otimes v : \nabla_x\Omega)\, \mathrm{d}v = 0$, because the integrand is odd with respect to v, and then we get

$$\begin{aligned}(\mathrm{Id} - \Omega\otimes\Omega)\, X_3 &= \langle \sin^2\theta\, \cos\theta\, \gamma_3\, h_\kappa\rangle_{M_\kappa} \int_{v\in\mathbb{S}_{n-2}} v\otimes v\, \mathrm{d}v\, (\Omega\cdot\nabla_x)\Omega \\ &= \frac{\langle \sin^2\theta\, \cos\theta\, \gamma_3\, h_\kappa\rangle_{M_\kappa}}{n-1}(\Omega\cdot\nabla_x)\Omega,\end{aligned}$$

since $(\Omega\cdot\nabla_x)\Omega$ is orthogonal to Ω.

So we have that $(\mathrm{Id} - \Omega\otimes\Omega)X = 0$ is equivalent to

$$\rho\kappa\langle \sin^2\theta\, h_\kappa\rangle_{M_\kappa}\partial_t\Omega + \langle \sin^2\theta\, \cos\theta\, \gamma_3\, h_\kappa\rangle_{M_\kappa}(\Omega\cdot\nabla_x)\Omega + \langle \sin^2\theta\, \gamma_2 h_\kappa\rangle_{M_\kappa}\nabla_x\rho = 0.$$

For any function $\gamma(\cos\theta)$, we denote by $\langle\gamma(\cos\theta)\rangle_{\widetilde{M}_\kappa}$ the mean of $\gamma(\cos\theta)$ following the "weight" $\sin^2\theta\, h_\kappa(\cos\theta)M_{\kappa\Omega}$, that is to say

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

We have

$$\langle\gamma(\cos\theta)\rangle_{\widetilde{M}_\kappa} = \frac{\langle \sin^2\theta\, h_\kappa(\cos\theta)\gamma(\cos\theta)\rangle_{M_\kappa}}{\langle \sin^2\theta\, h_\kappa(\cos\theta)\rangle_{M_\kappa}},$$

and so, dividing by $\kappa\langle \sin^2\theta h_\kappa(\cos\theta)\rangle_{M_\kappa}$ we finally get that $(\mathrm{Id} - \Omega\otimes\Omega)X = 0$ is equivalent to

$$\rho\,(\partial_t\Omega + c_2(\Omega\cdot\nabla_x)\Omega) + \lambda\,(\mathrm{Id} - \Omega\otimes\Omega)\nabla_x\rho = 0,$$

where the coefficients are given by

$$c_2(\rho) = \tfrac{1}{\kappa\rho}\langle\cos\theta\,\gamma_3(\cos\theta)\rangle_{\widetilde{M}_\kappa} \text{ and } \lambda(\rho) = \tfrac{1}{\kappa}\langle\gamma_2(\cos\theta)\rangle_{\widetilde{M}_\kappa}.$$

We finally get, writing $\widetilde{c}_1 = \langle\cos\theta\rangle_{\widetilde{M}_\kappa}$,

$$\begin{aligned} c_2 &= \widetilde{c}_1 - \alpha\, d\,(n\,\widetilde{c}_1 + \kappa\,\langle\cos^2\theta\rangle_{\widetilde{M}_\kappa})\,, \\ \lambda &= \tfrac{1}{\kappa} + \rho\,\tfrac{\dot\kappa}{\kappa}\,[\,(\,\widetilde{c}_1 - c_1 + \widetilde{\alpha}\, d\,(\kappa\langle\sin^2\theta\rangle_{\widetilde{M}_\kappa} - n\,\widetilde{c}_1)\,] + \tfrac{1}{2}\,\widetilde{\alpha}\,\dot{d}\,(\kappa\,\widetilde{c}_1 + n - 1)\,, \end{aligned}$$

which are exactly the expressions given in equations (3.26)-(3.27), and this ends the proof of Proposition 3.2.

B Asymptotics of the coefficients

B.1 Proof of Proposition 5.1

We recall that the two linear operators L and D on the space of polynomials are defined by

$$L(P) = -(1-X^2)P'' + (n+1)XP' + (n-1)P$$
$$D(P) = -(1-X^2)P' + XP.$$

We first give a preliminary lemma which will be helpful to construct the polynomials H_p and G_p^N.

Lemma 1.4. *Definition of the polynomials.*
Let Q be a polynomial and $N \in \mathbb{N}$. Then

- *There exists one unique polynomial P such that $L(P) = Q$.*
- *There exists one unique polynomial P^N of degree at most N such that*

$$D(P^N)(\cos\theta) = Q(\cos\theta) + O(\theta^{2(N+1)}) \text{ as } \theta \to \theta.$$

Proof. For the first point, if the leading term in a polynomial P is $a_k X^k$, with $a_k \neq 0$, then the leading term in $L(P)$ is $[k(k-1)+k(n+1)+(n-1)]a_k X^k$, and so $L(P) \neq 0$. So the linear operator L is injective from $\mathbb{R}_p[X]$ to $\mathbb{R}_p[X]$, and therefore it is bijective.

For the second point, the idea is to remark that

$$D((1-X)^k) = (2k+1)(1-X)^k + (k+1)(1-X)^{k+1},$$

so we write the polynomials in the basis $\{(1-X)^k, k \in \mathbb{N}\}$. We get that a polynomial R is such that $R(\cos\theta) = O(\theta^{2(N+1)})$ if and only if, in this basis, its first coefficients up to order $(X-1)^N$ are zero (because $1-\cos\theta = \frac{1}{2}\theta^2 + O(\theta^4)$ in the neighborhood of 0). We write $Q = \sum_{k=0}^{\infty} b_k(1-X)^k$ and $P^N = \sum_{k=0}^{N} a_k(1-X)^k$, and we get that

$$D(P^N)(\cos\theta) = Q(\cos\theta) + O(\theta^{2(N+1)}) \Leftrightarrow \begin{cases} a_0 = b_0 \\ (2k+1)a_k - ka_{k-1} = b_k \quad \forall k \in [\![1, N]\!]. \end{cases}$$

Since this induction relation defines in an unique way the coefficients a_k for $k \in [\![1, N]\!]$, this ends the proof. □

With this lemma, we can now define the following sequences of polynomials H_p and G_p^N, this last ones being of degree at most $N-p$:

$$\begin{cases} L(H_0) = 1 \\ L(H_{p+1}) = -D(H_p) \end{cases} \quad \text{and} \quad \begin{cases} D(G_1^N)(\cos\theta) = 1 + O(\theta^{2N}) \\ (D(G_{p+1}^N) + L(G_p^N))(\cos\theta) = O(\theta^{2(N-p)}). \end{cases}$$

Since the operator L is odd and D is even, it is easy to show that the polynomials H_p have the same parity as p. If we express the operator L in the basis $\{(1-X)^k, k \in \mathbb{N}\}$,

we are able to get the induction relation for the coefficients of the polynomials in this basis. We have

$$L((1-X)^k) = (n+k-1)(k+1)(1-X)^k - k(n+2k-1)(1-X)^{k-1},$$

So we have

$$H_p = \sum_{k=0}^{p} b_k^p (1-X)^k, \text{ and } G_p^N = \sum_{k=0}^{N-p} a_k^p (1-X)^k, \tag{B.44}$$

where a_k^p and b_k^p are given by the following induction relations for (with the convention that $b_{p+1}^p = b_{-1}^p = a_{-1}^p = 0$):

$$\begin{cases} b_0^0 = \frac{1}{n-1}, \\ (n+k-1)b_k^{p+1} - (n+2k+1)b_{k+1}^{p+1} = \frac{2k+1}{k+1}b_k^p - \frac{k}{k+1}b_{k-1}^p, \quad \forall p \in \mathbb{N}, \forall k = [\![0, p+1]\!]. \end{cases}$$

$$\begin{cases} a_k^0 = \frac{k!}{(2k+1)(2k-1)\ldots 3} = \frac{2^k (k!)^2}{(2k+1)!}, \\ \frac{2k+1}{k+1}a_k^{p+1} - \frac{k}{k+1}a_{k-1}^{p+1} = (n+k-1)a_k^p - (n+2k+1)a_{k+1}^p, \quad \forall p \in \mathbb{N}, \forall k \in \mathbb{N}. \end{cases}$$

We define then the remainders $R_{\kappa,0}^N$ and $R_{\kappa,\infty}^N$ by

$$R_{\kappa,0}^N(\mu) = h_\kappa(\mu) - \sum_{p=0}^{N} H_p(\mu)\kappa^p, \quad R_{\kappa,\infty}^N(\mu) = h_\kappa(\mu) - \sum_{p=1}^{N} G_p^N(\mu)\kappa^{-p}.$$

It is an easy matter to see that, for a given polynomial P, we have

$$\begin{aligned} \sin\theta \partial_\theta(P(\cos\theta)\sin\theta) &= D(P)(\cos\theta)\sin\theta, \\ -\partial_\theta(\sin^{n-2}\theta\partial_\theta(P(\cos\theta)\sin\theta)) + (n-2)\sin^{n-3}\theta P(\cos\theta) &= \sin^{n-1}\theta L(P)(\cos\theta), \end{aligned} \tag{B.45}$$

and then we get

$$\widetilde{L}_\kappa^*(P(\cos\theta)\sin\theta) = (L(P) + \kappa D(P))(\cos\theta)\sin\theta,$$

where the operator $\widetilde{L}_\kappa^*$ is defined in (3.17) by

$$\widetilde{L}_\kappa^* g(\theta) = -\sin^{2-n}\theta e^{-\kappa\cos\theta}\tfrac{\mathrm{d}}{\mathrm{d}\theta}(\sin^{n-2}\theta e^{\kappa\cos\theta}g'(\theta)) + \tfrac{n-2}{\sin^2\theta}g(\theta).$$

Since we have by definition $\widetilde{L}_\kappa^*(h_\kappa(\cos\theta)\sin\theta) = \sin\theta$, we get

$$\begin{aligned} \widetilde{L}_\kappa^*(R_{\kappa,0}^N(\cos\theta)\sin\theta) &= \sin\theta - \sum_{p=0}^{N}(L(H_p) + \kappa D(H_p))(\cos\theta)\sin\theta\kappa^p \\ &= -\kappa^{N+1}D(H_N)(\cos\theta)\sin\theta, \\ \widetilde{L}_\kappa^*(R_{\kappa,\infty}^N(\cos\theta)\sin\theta) &= \sin\theta - \sum_{p=1}^{N}(L(G_p^N) + \kappa D(G_p^N))(\cos\theta)\sin\theta\kappa^{-p} \\ &= -L(G_N^N)(\cos\theta)\sin\theta\kappa^{-N} + \sum_{p=0}^{N-1}\kappa^{-p}O(\theta^{2(N-p)})\sin\theta. \end{aligned}$$

To get estimations for the averages of the form $\langle f(\theta)R^N_{\kappa,\varepsilon}(\cos\theta)\sin^2\theta\rangle_{M_\kappa}$ (with ε standing for 0 or ∞) we first remark that, for a function g belonging to the space V (a "weighted H^1_0") defined in (3.19) by

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

we have the following Poincaré inequality:

$$\langle g(\theta)\widetilde{L}^*_\kappa g(\theta)\rangle_{M_\kappa} = \langle g'(\theta)^2\rangle_{M_\kappa} + (n-2)\langle \tfrac{1}{\sin^2\theta}g(\theta)^2\rangle_{M_\kappa} \geqslant (n-2)\langle (g(\theta))^2\rangle_{M_\kappa}.$$

Hence, for $n \geqslant 3$ and $g \in V$, using Cauchy-Schwarz inequality, we get that

$$\langle g(\theta)^2\rangle_{M_\kappa} \leqslant \frac{1}{n-2}\sqrt{\langle g(\theta)^2\rangle_{M_\kappa}\langle (\widetilde{L}^*_\kappa g(\theta))^2\rangle_{M_\kappa}}.$$

Since $g_\kappa(\theta) = h_\kappa(\cos\theta)\sin\theta$ belongs to V, we get that $g^N_{\kappa,\varepsilon}(\theta) = R^N_{\kappa,\varepsilon}(\cos\theta)\sin\theta$ also belongs to V.

We are now ready to do the estimations. For f such that $\theta \mapsto f(\theta)\sin^{\frac{n}{2}}\theta$ belongs to $L^2(0,\pi)$, we get, using Cauchy-Schwarz inequality,

$$\begin{aligned}
|\langle f(\theta)R^N_{\kappa,0}(\cos\theta)\sin^2\theta\rangle_{M_\kappa}| &\leqslant \sqrt{\langle (R^N_{\kappa,0}(\cos\theta))^2\sin^2\theta\rangle_{M_\kappa}\langle f(\theta)^2\sin^2\theta\rangle_{M_\kappa}} \\
&\leqslant \frac{1}{n-2}\sqrt{\langle (\widetilde{L}^*_\kappa R^N_{\kappa,0}(\cos\theta))^2\sin^2\theta\rangle_{M_\kappa}}\sqrt{\langle f(\theta)^2\sin^2\theta\rangle_{M_\kappa}} \\
&\leqslant \frac{1}{n-2}\kappa^{N+1}\sqrt{\langle (D(H_N)(\cos\theta))^2\sin^2\theta\rangle_{M_\kappa}}\sqrt{\langle f(\theta)^2\sin^2\theta\rangle_{M_\kappa}}.
\end{aligned}$$

Hence using the expansion as $\kappa \to 0$ given in (5.35), we get the final estimation:

$$\langle f(\theta)R^N_{\kappa,0}(\cos\theta)\sin^2\theta\rangle_{M_\kappa} = O(\kappa^{N+1}) \text{ as } \kappa \to 0. \tag{B.46}$$

Similarly, if $|f(\theta)| = O(\theta^{2\beta})$ in the neighborhood of 0, using Lemma 1.2, we get

$$\begin{aligned}
|\langle f(\theta)R^N_{\kappa,\infty}(\cos\theta)\sin^2\theta\rangle_{M_\kappa}|^2 &\leqslant \frac{1}{(n-2)^2}\langle f(\theta)^2\sin^2\theta\rangle_{M_\kappa} \\
&\quad\times \left\langle [L(G^N_N)(\cos\theta)\kappa^{-N} + \sum_{p=0}^{N-1}\kappa^{-p}O(\theta^{2(N-p)})]^2\sin^2\theta \right\rangle_{M_\kappa} \\
&\leqslant O(\kappa^{-2\beta-1}) \times O(\kappa^{-2N-1}),
\end{aligned}$$

which gives

$$\langle f(\theta)R^N_{\kappa,\infty}(\cos\theta)\sin^2\theta\rangle_{M_\kappa} = O(\kappa^{-\beta-N-1}) \text{ as } \kappa \to \infty.$$

Now, since we have the expression (B.44) of the polynomials G^N_p, we get, by definition of $R^N_{\kappa,\infty}$,

$$\begin{aligned}
R^N_{\kappa,\infty}(\mu) &= R^{N+1}_{\kappa,\infty}(\mu) + \sum_{p=0}^{N}(G^{N+1}_p - G^N_p)(\mu)\kappa^{-p} + G^{N+1}_{N+1}(\mu)\kappa^{-N-1} \\
&= R^{N+1}_{\kappa,\infty}(\mu) + \sum_{p=0}^{N+1} a^p_{N+1-p}(1-\mu)^{N+1-p}\kappa^{-p}.
\end{aligned}$$

Since $(1-\cos\theta)^k = O(\theta^{2k})$, we finally get, using Lemma 1.2,

$$\begin{aligned}\langle f(\theta)R^N_{\kappa,\infty}(\cos\theta)\sin^2\theta\rangle_{M_\kappa} &= \langle f(\theta)R^{N+1}_{\kappa,\infty}(\cos\theta)\sin^2\theta\rangle_{M_\kappa} + \sum_{p=0}^{N+1}\kappa^{-p}O(\kappa^{-\beta-1-N-1+p}) \\ &= O(\kappa^{-\beta-N-2}) \quad \text{as } \kappa\to\infty.\end{aligned}$$

This ends the proof of Proposition 5.1, in the case $n \geqslant 3$.

We suppose now that $n = 2$. The case $\kappa \to 0$ is easy, since we have the following Poincaré inequality:

$$\langle g(\theta)\widetilde{L}^*_\kappa g(\theta)\rangle_{M_\kappa} = \langle g'(\theta)^2\rangle_{M_\kappa} \geqslant \frac{e^{-\kappa}\int_0^\pi g'(\theta)^2\mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta}\mathrm{d}\theta} \geqslant \frac{e^{-\kappa}\int_0^\pi g(\theta)^2\mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta}\mathrm{d}\theta} \geqslant e^{-2\kappa}\langle g(\theta)^2\rangle_{M_\kappa}.$$

We get the same estimations, replacing $(n-2)$ by $e^{-2\kappa}$:

$$|\langle f(\theta)R^N_{\kappa,0}(\cos\theta)\sin^2\theta\rangle_{M_\kappa}| \leqslant e^{2\kappa}\kappa^{N+1}\sqrt{\langle (D(H_N)(\cos\theta))^2\sin^2\theta\rangle_{M_\kappa}\langle f(\theta)^2\sin^2\theta\rangle_{M_\kappa}},$$

which gives the estimate (B.46) since $e^{2\kappa} = O(1)$ when $\kappa \to 0$.

The case $\kappa \to \infty$ is different, since we are not able to get a better Poincaré constant. But we have an explicit expression for $g_\kappa(\theta) = h(\cos\theta)\sin\theta$, given by (3.20):

$$g_\kappa(\theta) = \frac{\theta}{\kappa} - \frac{\pi}{\kappa}\frac{\int_0^\theta e^{-\kappa\cos\varphi}\mathrm{d}\varphi}{\int_0^\pi e^{-\kappa\cos\varphi}\mathrm{d}\varphi}.$$

It is also easy to see that, in this case, the coefficients a_k^p appearing in the definition (B.44) of the polynomials G_p^N, are zero when $p \geqslant 1$. Therefore we get that $G_p^N = 0$ for $p \geqslant 1$.

We have $D(G_1^N)(\cos\theta) = 1 + O(\theta^{2N})$, so with the formula (B.45), we obtain

$$\partial_\theta(G_1^N(\cos\theta)\sin\theta) = 1 + O(\theta^{2N}),$$

so we get that $G_1^N(\cos\theta)\sin\theta = \theta + O(\theta^{2N+1})$ since $\theta \mapsto G_1^N(\cos\theta)$ is continuous as $\theta \to 0$. Actually, this is the Euler formula for arctan: if we write $t = \tan\frac{\theta}{2}$ we get $1-\cos\theta = \frac{2t^2}{1+t^2}$, $\sin\theta = \frac{2t}{1+t^2}$, and then, using the expression (B.44) of the polynomials G_1^N with $a_k = \frac{2^k(k!)^2}{(2k+1)!}$, we obtain

$$\arctan t = \frac{t}{1+t^2}\sum_{k=0}^{N}\frac{2^{2k}(k!)^2}{(2k+1)!}\frac{t^{2k}}{(1+t^2)^k} + O(t^{2N+1}).$$

Now, using the explicit expression of g_k, we have

$$\begin{aligned}R^N_{\kappa,\infty}(\cos\theta)\sin\theta &= g_\kappa(\theta) - G_1^N(\cos\theta)\sin\theta\,\kappa^{-1} \\ &= \kappa^{-1}(\theta - G_1^N(\cos\theta)\sin\theta) - \frac{\pi}{\kappa}\frac{\int_0^\theta e^{-\kappa\cos\varphi}\mathrm{d}\varphi}{\int_0^\pi e^{-\kappa\cos\varphi}\mathrm{d}\varphi} \\ &= \kappa^{-1}\,O(\theta^{2N+1}) - r^\infty_\kappa(\theta).\end{aligned}$$

We have

$$r^\infty_\kappa(\theta) \leqslant \frac{\pi^2}{\kappa}\frac{e^{-\kappa\cos\theta}}{\int_0^\pi e^{-\kappa\cos\varphi}\mathrm{d}\varphi},$$

and so, using the estimate (5.37) with $n = 2$, we get

$$\langle (r_\kappa^\infty(\theta))^2 \rangle_{M_\kappa} \leqslant \frac{\pi^4}{\kappa^2} \frac{\int_0^\pi e^{-2\kappa\cos\theta} e^{\kappa\cos\theta} \mathrm{d}\theta}{(\int_0^\pi e^{-\kappa\cos\varphi}\mathrm{d}\varphi)^2 \int_0^\pi e^{\kappa\cos\theta}\mathrm{d}\theta} \leqslant \frac{\pi^4}{\kappa^2 (\int_0^\pi e^{\kappa\cos\theta}\mathrm{d}\theta)^2} = O(\kappa^{-1}e^{-2\kappa}).$$

Therefore, using Cauchy-Schwarz inequality and Lemma 1.2,

$$|\langle f(\theta) r_\kappa^\infty(\theta)\sin\theta\rangle_{M_\kappa}| \leqslant \sqrt{\langle f(\theta)^2\sin^2\theta\rangle_{M_\kappa}\langle (r_\kappa^\infty(\theta))^2\rangle_{M_\kappa}} = O(\kappa^{-\beta-1}e^{-2\kappa}),$$

so we get the final estimate

$$\langle f(\theta) R_{\kappa,\infty}^N(\cos\theta)\sin^2\theta\rangle_{M_\kappa} = O(\kappa^{-\beta-N-2}) \text{ as } \kappa\to\infty,$$

and this ends the proof of Proposition 5.1.

B.2 Tips for the general case

Here we give some tips to perform an asymptotic study of the coefficients when ν depends also on $\omega\cdot\Omega$.

We will have to take averages against functions of the form $\theta\mapsto e^{\widehat{\kappa}(\rho,\cos\theta)}$, where

$$\widehat{\kappa}(\rho,\mu) = \frac{1}{d(\rho)}\int_0^\mu \nu(\rho,x)\mathrm{d}x.$$

We want to get for example an expansion as the noise d is large or small. So we are only interested in the dependence on $\cos\theta$, and we will drop the dependence on ρ for clarity. We suppose that the function $\theta\mapsto\nu(\cos\theta)$ is positive, smooth, bounded below and above, and we introduce the parameter $\kappa = \frac{1}{d}$, trying to expand with respect to κ. We write $\sigma(\mu) = \int_0^\mu \nu(x)\mathrm{d}x$, so we have $\widehat{\kappa}(\mu) = \kappa\,\sigma(\mu)$.

The first step consists in the expansion of $\langle f(\theta)\rangle_{\widehat{M}_\kappa}$ given by

$$\langle f(\theta)\rangle_{\widehat{M}_\kappa} = \frac{\int_0^\pi f(\theta)e^{\kappa\,\sigma(\cos\theta)}\sin^{n-2}\theta\,\mathrm{d}\theta}{\int_0^\pi e^{\kappa\,\sigma(\cos\theta)}\sin^{n-2}\theta\,\mathrm{d}\theta}.$$

As before, we can easily do a Taylor expansion when $\kappa\to 0$, and we get a result similar to (5.36) involving quantities of the form $\int_0^\pi f(\theta)\sigma(cos\theta)^p\mathrm{d}\theta$. Unless we know explicitly σ, we cannot say anything interesting.

When $\kappa\to\infty$, the strategy is the same: we do the change of variable, setting $t = \sigma(1)-\sigma(\cos\theta))$, and $a(t) = \sigma^{-1}(\sigma(1)-t)$, where σ^{-1} is the inverse function of σ (which is increasing since $\nu>0$, actually we have $a(t) = \cos\theta$). We get:

$$\int_0^\pi f(\theta)e^{\kappa\,\sigma(\cos\theta)}\sin^{n-2}\theta\,\mathrm{d}\theta = e^{\kappa\,\sigma(1)}\int_0^T \frac{f(\arccos a(t))e^{-\kappa t}}{\nu(a(t))(1-a(t)^2)^{\frac{n-3}{2}}}dt,$$

where $T = \sigma(1)-\sigma(-1)$. Since $a(0) = 1$, if we know the expansion of f around 0 and ν in the neighborhood of 1, it only remains to get a Taylor expansion of a around 0 to use Lemma 1.1 (Watson's Lemma). We can compute the derivatives of a by induction. We have

$$a'(t) = -\frac{1}{\nu(a(t))},$$

and this gives immediately $a^{(n)} = F_n(a(t))$, with the following induction relation for F_n

$$F_1(\mu) = -\frac{1}{\nu(\mu)}, \quad F_{n+1}(\mu) = -\frac{1}{\nu(\mu)}\frac{\mathrm{d}}{\mathrm{d}\mu}(F_n(\mu)).$$

This gives us the Taylor expansion of a at $t = 0$ up to order N:

$$a(t) = 1 + \sum_{n=1}^{N} f_n(1)\frac{t^n}{n!} + O(t^{N+1}).$$

Since we have $a'(0) < 0$, it is possible to get the analogous of Lemma 1.2: for a function f such that $f(\theta) = O(\theta^{2\beta})$, then $\langle f(\theta)\rangle_{\widehat{M}_\kappa} = O(\kappa^{-\beta})$ as $\kappa \to \infty$. Finally, we get an expansion of $\langle f(\theta)\rangle_{\widehat{M}_\kappa}$ which depend only on the first derivatives of ν at 1 and on the local behavior of f around 0.

The second step consists in expanding $\langle f(\theta)\widehat{g}_\kappa(\theta)\sin\theta\rangle_{\widehat{M}_\kappa}$, where $\widehat{L}^*_\kappa\widehat{g}_\kappa(\theta) = \sin\theta$, the operator $\widehat{L}^*_\kappa$ being defined by

$$\widehat{L}^*_\kappa g(\theta) = -\sin^{2-n}\theta e^{-\kappa\,\sigma(\cos\theta)}\tfrac{\mathrm{d}}{\mathrm{d}\theta}(\sin^{n-2}\theta e^{\kappa\,\sigma(\cos\theta)}g'(\theta)) + \tfrac{n-2}{\sin^2\theta}g(\theta).$$

It is easy to see that we have

$$\widetilde{L}^*_\kappa(P(\cos\theta)\sin\theta) = (L(P) + \kappa\nu(\cos\theta)D(P))(\cos\theta)\sin\theta,$$

so if we set $\widehat{g}_\kappa(\theta) = \widehat{h}_\kappa(\cos\theta)\sin\theta$, we can decompose $\widehat{h}_k$ in a way similar to Proposition 5.1:

$$\widehat{h}_\kappa(\cos\theta) = \sum_{p=0}^{N}\widehat{H}_p(\cos\theta)\kappa^p + \widehat{R}^N_{\kappa,0}(\cos\theta),$$
$$\widehat{h}_\kappa(\cos\theta) = \sum_{p=1}^{N}\widehat{G}^N_p(\cos\theta)\kappa^{-p} + \widehat{R}^N_{\kappa,\infty}(\cos\theta),$$

where $\widehat{H}_p$ are the functions (not necessarily polynomials) and $\widehat{G}^N_p$ the polynomials of degree at most $N - p$ given by the following induction relations:

$$\begin{cases} L(\widehat{H}_0) = 1 \\ L(\widehat{H}_{p+1})(\mu) = -\nu(\mu)D(\widehat{H}_p)(\mu) \end{cases}$$

$$\begin{cases} D(\widehat{G}^N_1)(\cos\theta) = 1 + O(\theta^{2N}) \\ (D(\widehat{G}^N_{p+1}) + \frac{1}{\nu(\cos\theta)}L(\widehat{G}^N_p))(\cos\theta) = O(\theta^{2(N-p)}). \end{cases}$$

Again, the remainders satisfy the following estimations, for any function f such that $\theta \mapsto f(\theta)\sin^{\frac{n}{2}}\theta$ belongs to $L^2(0,\pi)$ and such that $|f(\theta)| = O(\theta^{2\beta})$ in the neighborhood of 0:

$$\langle f(\theta)\widehat{R}^N_{\kappa,0}(\cos\theta)\sin^2\theta\rangle_{\widehat{M}_\kappa} = O(\kappa^{N+1}) \text{ as } \kappa \to 0,$$
$$\langle f(\theta)\widehat{R}^N_{\kappa,\infty}(\cos\theta)\sin^2\theta\rangle_{\widehat{M}_\kappa} = O(\kappa^{-\beta-N-2}) \text{ as } \kappa \to \infty,$$

and this allows to get an expansion of $\langle f(\theta)\widehat{h}_\kappa(\cos\theta)\sin^2\theta\rangle_{\widehat{M}_\kappa}$ when $\kappa \to 0$ and when $\kappa \to \infty$.

Chapter 2

Macroscopic limits and phase transition in a system of self-propelled particles

This chapter is the fruit of a collaboration with Pierre Degond and Jian-Guo Liu, and an article [27] is about to be submitted on this subject.

Abstract

We investigate a new time-continuous version of the Vicsek model, which describe the evolution of self-propelled particles with alignment interaction. This model takes the form of a system of coupled stochastic differential equations describing the evolution of the positions and orientations of the particles.

In the limit of a large number of particles, the model is described by a mean-field kinetic equation, which presents, when observed at large scale in space and time, a phenomenon of phase transition as the density crosses a threshold.

In this chapter, we derive the hydrodynamic limit of this mean-field model. When the density is under the threshold, the limit is given by a local isotropic distribution, the density of which, in a first order approximation, satisfies a non-linear diffusion equation. Over this threshold, we get the same "Vicsek hydrodynamics" as in Chapter 1: a non-conservative system of first-order partial differential equations describing the evolution of a local density and a local orientation, which turns out to be non-hyperbolic.

Key words: Vicsek model, phase transition, hydrodynamic limit, Chapman-Enskog expansion, non-hyperbolicity.

1 Introduction

In this chapter, following what have been done in Chapter 1, we investigate a new modification of the time continuous version of Vicsek model. This modification of the individual model seems, at first glance, to be a simplification: we replace $\bar{\omega}_k$ in equation (2.4) of Chapter 1 by $\bar{J}_k$, that is to say we do not divide by the norm: the particles evaluate only the local total momentum of their neighbors, not their local orientation. The interaction can then be recast as a sum of binary interactions, still understood as a relaxation towards the unit vector $\bar{\omega}_k$, but with rate proportional to the absolute value of the local total momentum of their neighbors $|\bar{J}_k|$. That is to say that the individuals tends to relax more rapidly to the direction of their neighbors if these last ones are numerous and strongly aligned. This positive feedback on the alignment strength leads to the apparition of phase transition, recovering the features of the original discrete model, which gives rise to challenging issues.

So, we have found a way to get a macroscopic phase transition, in agreement with the numerical simulations of the discrete Vicsek model, and with a time-continuous model still very close to the original discrete one. Using results of Chapter 4, together with a fine analysis of a specific Poincaré constant, we are able to provide arguments which confirm the convergence, at each point, to a local equilibrium. This last one can be of two different types, either the uniform distribution, isotropic on the sphere, if the density ρ is less than the critical threshold $\rho^* = n$, or a distribution with a given orientation Ω in the case where $\rho > \rho^*$.

The mathematical treatment of this phase transition consists in the derivation of two different models, depending whether the density ρ is above or under the threshold $\rho^* = n$. We finally get a two-phase macroscopic model, with nonlinear diffusion in the region of low density, and still the "macroscopic Vicsek" model in the region of high density. The description of the behavior of the boundary between these two regions is a challenging problem. Once again, as in Chapter 1, the model is naturally set in a n-dimensional framework, and the results are qualitatively the same in any dimension.

The last important thing to note is that we can directly use the results of Chapter 1 which concern the asymptotic expansions of the coefficients, and we get, in the ordered region, that the coefficient λ, playing the role of a pressure in the macroscopic model, is negative in the two limit cases, when ρ is large or close to the threshold n. Using numerical computations, we see that we actually have $\lambda < 0$ in any case. This means that the "macroscopic Vicsek" model we obtained is non-hyperbolic in all the ordered region of high density. However, under the constraint that the dynamics only take place along one direction, we obtain a reduced model which presents a less pathological behavior, and we have hyperbolicity in some regions of the states space.

The outline of this chapter is as follows.

In Section 2, we describe the individual model, and its mean-field limit when the number of particles is large.

In Section 3, 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.

The Section 4 is devoted to the derivation of a diffusion model in the case where the density ρ is less than n. This model is a non-linear obtained as a first order approximation in ε, given by the method of the Chapman-Enskog expansion.

Finally, in Section 5, we derive, with the method of the generalized collisional invariants, the hydrodynamic model in the region where $\rho > n$. The "macroscopic Vicsek" model is obtained, with coefficients which depend on the density ρ, and its properties are studied, in particular the non-hyperbolicity, with the help of the asymptotics expansions that have been done in Chapter 1.

2 System of particles and its mean-field limit

We consider N oriented particles in $\mathbb{R}^n$, described by their positions $X_1, \dots X_N$ and their orientation vectors $\omega_1, \dots, \omega_N$ 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 chapter, the kernel of observation K will be supposed to be isotropic (depending only on the distance $|X_j - X_k|$ between the particle and its neighbors), smooth and with compact support. Introducing a non-isotropic kernel of observation, as in Chapter 1 would lead to the same conclusion, with a slightly different speed of convection for the orientation in the macroscopic model, but the computations are more complicated, this is why we focus on a kernel of observation which is isotropic.

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

$$\mathrm{d}X_k = \omega_k \,\mathrm{d}t \tag{2.1}$$

$$\mathrm{d}\omega_k = (\mathrm{Id} - \omega_k \otimes \omega_k) J_k \,\mathrm{d}t + \sqrt{2d}(\mathrm{Id} - \omega_k \otimes \omega_k) \circ \mathrm{d}B_t^k, \tag{2.2}$$

The first equation expresses the fact that particles move at constant speed 1, 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 [48] for more details on how to define Brownian motion on a Riemannian manifold.

We remark that the interaction can be seen as a sum of smooth binary interactions. This model can then be viewed as an intermediate between the Cucker-Smale model [24] (where there is no constraint on the norm of the velocity and no noise) and the Vicsek model, where the velocity is constant and noise is added, but the interaction cannot be recast as a sum of binary interactions. Actually the only difference with the time-continuous version of the Vicsek model presented in [28] is that J_k is there 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 frequency of relaxation ν is constant (so the interaction term has a singularity when J_k is close to 0). The model presented here can then be viewed as a modification consisting in letting ν depend (linearly) on the norm of the velocity J_k, which can be compared to the modification introduced in Chapter 1, where this relaxation parameter ν depend on a local density $\bar{\rho}_k$.

The first step to investigate a macroscopic limit of this model is to get a mean-field limit of the system, as the number of particles tend to infinity. We define the empirical distribution of particles 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: $\langle \delta_{X,\Omega}, \varphi\rangle_{\mathbb{R}^n\times\mathbb{S}} = \varphi(X,\Omega)$ for a 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, we work with the uniform measure of total mass 1 on the sphere $\mathbb{S}$, so we have $\langle f^N, 1\rangle_{\mathbb{R}^n\times\mathbb{S}} = 1$. With this notations, we get that $J_k = \langle f^N, K_{X_k}\omega\rangle_{\mathbb{R}^n\times\mathbb{S}}$, where $K_{X_k}(x) = K(X_k - x)$. Denoting the convolution with respect to the space variable by $*$, we get $J_k = \langle K * f^N(X_k), \omega\rangle_{\mathbb{S}}$. It is then easy to see, in the case of no noise (when $d = 0$), that f^N satisfies the following partial differential equation (in the sense of distributions)

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

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

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

When the noise is added, some complications appear. We expect to get that the empirical distribution f^N tends to a probability density function f satisfying the following partial differential equation:

$$\partial_t f + \omega\cdot\nabla_x f + \nabla_\omega\cdot((\mathrm{Id} - \omega\otimes\omega)\bar{J}_f f) = d\Delta_\omega f, \tag{2.3}$$

with

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

This convergence is linked to the so-called property of "propagation of chaos", which amounts to consider that a given finite number k of particles behave as if they were independent and following the same law, when the total number of particles N tends to infinity. A classical way to prove this property, called the coupling method, consists in the introduction of artificial nonlinear processes, the law of which satisfies the equation (2.3), and which are a good approximation of the original system of particles. We refer to [73] for more details.

The main point is to adapt this theory in the framework of stochastic differential equations on a manifold (the sphere $\mathbb{S}$ here). This has actually been recently done for this system by Bolley, Cañizo, and Carrillo in [13]. Under the assumption that the kernel K is Lipschitz and bounded, they prove existence and uniqueness of the solution of the system (2.1)-(2.2) and of the artificial process associated to it. They

provide then estimates which ensure that the empirical distribution converges to a solution of the equation (2.3), called Kolmogorov–Fokker–Planck equation.

This equation is the starting point of our study. We see that there is a competition between the alignment term and the diffusion term. However, alignment term is quadratic with respect to f, whereas the diffusion term is linear. So we can expect that when f is small, the leading behavior is the diffusion in the direction variable ω, and when f is large, the alignment will be seen at the macroscopic level.

Let us point out that the study of the space-homogeneous version of the equation is exactly the object of Chapter 4, and the result is that there are indeed two regimes, one where the equilibrium is isotropic, and another where the equilibrium depend on an arbitrary direction Ω. This will also be the case here, and we will see that the macroscopic models we obtain are really different in each regime.

But before deriving these macroscopic models, we can make some remarks and assumptions on d and K. 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

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

we get that $\widetilde{f}$ satisfies the equation (2.3) with $d = 1$ and K replaced by $\widetilde{K}$ in (2), 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 behavior at large scale in space and time. The derivation of the model proceeds as in [28], and follows closely the presentation of Chapter 1, so 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.

3 The macroscopic limit

3.1 Hydrodynamic scaling

In order to observe the system at large scale, we perform a hydrodynamic scaling. We introduce a small parameter ε, and we will work with the new space and time variables $x' = \varepsilon x$, $t' = \varepsilon t$. We write $f^\varepsilon(x',\omega,t') = f(x,\omega,t)$, and $K^\varepsilon(x') = \frac{1}{\varepsilon^n}K(x)$. We can then write the equation satisfied by f^ε, if f is a solution of the Kolmogorov–Fokker–Planck equation (2.3). Omitting the primes for simplicity, we get

$$\varepsilon(\partial_t f^\varepsilon + \omega\cdot\nabla_x f^\varepsilon) = -\nabla_\omega\cdot((\mathrm{Id}-\omega\otimes\omega)\bar{J}^\varepsilon_{f^\varepsilon} f^\varepsilon) + \Delta_\omega f^\varepsilon, \tag{3.4}$$

with

$$\bar{J}^\varepsilon_{f^\varepsilon}(x,t) = \int_{\mathbb{S}} (K^\varepsilon * f^\varepsilon)(x,\omega,t)\,\omega\mathrm{d}\omega. \tag{3.5}$$

The purpose of this chapter 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:

$$\bar{J}^\varepsilon_{f^\varepsilon}(t,x) = J_{f^\varepsilon}(t,x) + O(\varepsilon^2),$$

where the local flux J_f is defined, for a function f of ω, by

$$J_f(x,t) = \int_{\mathbb{S}} f(x,\omega,t)\,\omega\,\mathrm{d}\omega. \tag{3.6}$$

The proof of this expansion is elementary and omitted here, we refer to Appendix A.1 of Chapter 1 for a detailed proof with a more general kernel, we use here the fact that $K(x)$ depends only on $|x|$, and the normalization $K_0 = 1$.

We also define the density ρ_f associated to f by

$$\rho_f(x,t) = \int_{\mathbb{S}} f(x,\omega,t)\,\mathrm{d}\omega. \tag{3.7}$$

Hence, the equation (3.4) becomes

$$\varepsilon(\partial_t f^\varepsilon + \omega\cdot\nabla_x f^\varepsilon) = Q(f^\varepsilon) + O(\varepsilon^2), \tag{3.8}$$

with

$$Q(f) = -\nabla_\omega\cdot((\mathrm{Id}-\omega\otimes\omega)J_f f) + \Delta_\omega f. \tag{3.9}$$

Remark 3.1. *Another way to get rid of the non-local term (and of the $O(\varepsilon^2)$ term in* (3.8) *in the same occasion) consists in making the scaling at the particular level, in the observation kernel. The so-called moderate interaction [64] concerns only $O(N^{1-\beta})$ particles, with $0<\beta<1$, and leads to the localization of the operator Q, in the limit of a large number of particles. The study of this scaling is left to future work.*

We remark that the "collision operator" Q only acts on the variable ω. The derivation of the macroscopic model relies on the properties of this operator. The first step consists in the characterization of the equilibria, that is to say the functions f such that $Q(f) = 0$, since when $\varepsilon \to 0$, we have $Q(f^\varepsilon) \to 0$. This is the purpose of the next subsection, we get that the equilibria are characterized by observable quantities, such as the density ρ, or a local direction Ω.

3.2 Equilibria

We define, for a unit vector $\Omega \in \mathbb{S}$, and $\kappa \geqslant 0$ the so-called Fisher-Von Mises distribution [82] with concentration parameter κ and orientation Ω by (note that the denominator depends only on κ):

$$M_{\kappa\Omega}(\omega) = \frac{e^{\kappa\,\omega\cdot\Omega}}{\int_{\mathbb{S}} e^{\kappa\,\upsilon\cdot\Omega}\,\mathrm{d}\upsilon}\,. \tag{3.10}$$

We have that $M_{\kappa\Omega}$ is a density probability function on the sphere, and we will denote by $\langle\cdot\rangle_{M_{\kappa\Omega}}$ the mean against this probability measure. We will often have to compute such means for functions γ depending only on $\omega\cdot\Omega$. In this case we have that the mean $\langle\gamma(\omega\cdot\Omega)\rangle_{M_{\kappa\Omega}}$ does not depend on Ω, so we will denote it $\langle\gamma(\cos\theta)\rangle_{M_\kappa}$. Using spherical coordinates, we can express this mean with simple integrals on $(0,\pi)$:

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

We have for example that the flux of the Fisher-Von Mises distribution is

$$J_{M_{\kappa\Omega}} = \langle\omega\rangle_{M_{\kappa\Omega}} = c(\kappa)\Omega, \tag{3.11}$$

where the order parameter $c(\kappa)$, taking values between 0 and 1, is defined by

$$c(\kappa) = \langle\cos\theta\rangle_{M_\kappa} = \frac{\int_0^\pi \cos\theta\, e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta}{\int_0^\pi e^{\kappa\cos\theta}\sin^{n-2}\theta\,\mathrm{d}\theta}. \tag{3.12}$$

This order parameter measures how the distribution $M_{\kappa\Omega}$ is concentrated around Ω. The case $c(\kappa) = 0$ corresponds to the uniform distribution, and $M_{\kappa\Omega}$ tends to the Dirac mass located at the point Ω when $c(\kappa)$ tends to 1.

We remark that the dependence on the two parameters κ and Ω in the definition of $M_{\kappa\Omega}$ is only visible through the vector $\kappa\Omega$, so we can consider M_J for a given vector J in $\mathbb{R}^n$. We have that $\nabla_\omega(M_J) = (\mathrm{Id} - \omega\otimes\omega)J\, M_J$, so we get that

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

If f is an equilibrium (that is to say $Q(f) = 0$), multiplying this equation by $\frac{f}{M_{J_f}}$ and integrating by part on the sphere $\mathbb{S}$, we get that $\frac{f}{M_{J_f}}$ is a constant ρ (which is the density of f). So f is of the form $\rho M_{\kappa\Omega}$ with $\kappa \geqslant 0$ and $\Omega \in \mathbb{S}$ (in the case where $|J_f| = 0$, then $\kappa = 0$ and we can take any $\Omega \in \mathbb{S}$, this is just the uniform distribution). Using (3.11), we get $\kappa\Omega = J_f = \rho J_{M_{\kappa\Omega}} = \rho c(\kappa)\Omega$, which gives the following compatibility condition:

$$\rho c(\kappa) = \kappa. \tag{3.13}$$

The study of this condition and the classification of the equilibria is done in Chapter 4. The key point is to prove that the function $\kappa \mapsto \frac{c(\kappa)}{\kappa}$ is decreasing and tends to $\frac{1}{n}$ as $\kappa \to 0$. We give the final results in the following proposition.

Proposition 3.1. *Compatibility condition, equilibria.*

- *If $\rho \leqslant n$, there is only one solution to the compatibility condition: $\kappa = 0$. The only equilibrium is the constant function $f = \rho$.*
- *If $\rho > n$, the compatibility condition has exactly two solutions: $\kappa = 0$ and one unique positive solution, which will be denoted $\kappa(\rho)$. Apart from the constant function $f = \rho$ (the case $\kappa = 0$), the equilibria form a manifold of dimension n: the functions of the form $f = \rho M_{\kappa(\rho)\Omega}$, where $\Omega \in \mathbb{S}$ is an arbitrary unit vector.*

In the next subsection, we provide arguments to determine a formal limit of f^ε as $\varepsilon \to 0$. They are based on the rates of convergence to equilibrium of the solution of the spatial homogeneous version studied in Chapter 4, as well as an argument of instability of the uniform equilibrium when $\rho > n$.

3.3 Rates of convergence to equilibrium

Let us first state here the results obtained in Chapter 4 for the convergence to equilibrium in the spatial homogeneous case.

Theorem 2.1. *Convergence to equilibrium in the spatial homogeneous case.*

Suppose g_0 is a probability measure, belonging to $H^s(\mathbb{S})$ (this is always the case for some $s < -\frac{n-1}{2}$).

Then there exists a unique weak solution g to the following equation (satisfying the initial condition $g(0) = g_0$):

$$\partial_t g = -\nabla_\omega \cdot ((Id - \omega \otimes \omega) J_g g) + \tau \Delta_\omega g. \tag{3.14}$$

Furthermore, this is a classical solution, positive for all time $t > 0$, and belonging to $C^\infty((0, +\infty) \times \mathbb{S})$.

If $J_{g_0} \neq 0$, then we have the three following cases, depending on τ.

- *If $\tau > \frac{1}{n}$, then g converges exponentially fast to the uniform distribution, with global rate $(n-1)(\tau - \frac{1}{n})$ in any H^p norm.*
- *If $\tau < \frac{1}{n}$, there exists a unique positive solution to the equation $c(\kappa) = \tau\kappa$. Then there exists $\Omega \in \mathbb{S}$ such that g converges exponentially fast to $M_{\kappa\Omega}$, with asymptotic rate greater than $r_\infty(\tau) = (c(\kappa)^2 + n\tau - 1)\Lambda_\kappa > 0$ for any H^p norm, where Λ_κ is the best constant for the following Poincaré inequality:*

$$\langle |\nabla g|^2 \rangle_{M_{\kappa\Omega}} \geqslant \Lambda_\kappa \langle (g - \langle g \rangle_{M_{\kappa\Omega}})^2 \rangle_{M_{\kappa\Omega}}, \tag{3.15}$$

  When τ is close to $\frac{1}{n}$ we have that $r_\infty(\tau) \sim 2(n-1)(\frac{1}{n} - \tau)$.

- *If $\tau = \frac{1}{n}$, then f converges to the uniform distribution in any H^p norm, with asymptotic rate $\sqrt{\frac{n(n-1)^{p-1}(n+2)}{2t}}$.*

If $J_{g_0} = 0$ the equation reduces to the heat equation on the sphere, so g converges to the uniform distribution, exponentially with global rate $2n\tau$ in any H^p norm.

In the view of getting an idea of what should be the rates of convergence to equilibrium, we will denote by g^ε the distribution of velocities corresponding to f^ε: this is the function such that $\rho^\varepsilon(x,t)g^\varepsilon(x,\omega,t) = f^\varepsilon(x,\omega,t)$, where $\rho^\varepsilon = \rho_{f^\varepsilon}$ is the local density, defined in equation (3.7), associated to the rescaled distribution f^ε. Hence $g^\varepsilon(x,\cdot,t)$ is a probability density function on the sphere. We can then rewrite the equation (3.8) under the following form:

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

Skipping the superscripts ε for the sake of clarity, neglecting the $O(\varepsilon^2)$ terms and those with a spatial derivative(this means, with the mass conservation (3.16) given later on that we can also drop the term $\partial_t \rho^\varepsilon$), and dividing by ρ^2, we finally get the following homogeneous equation

$$\frac{\varepsilon}{\rho}\, \partial_t g = -\nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega) J_g g) + \frac{1}{\rho}\, \Delta_\omega g,$$

which is nothing else than the equation (3.14), with $\rho = \frac{1}{\tau}$ and a time scaling factor.

The first result of Theorem 2.1 is that in the supercritical case (when $\tau < \frac{1}{n}$, or equivalently $\rho > n$), the uniform distribution is an unstable equilibrium: any perturbation on J_g making it non-zero implies that the density converges to a given Von-Mises distribution, with a fixed concentration parameter $\kappa(\rho)$ defined by the compatibility condition (3.13).

The second result is that we have exponential rates of convergence to the equilibrium. Notice that the rate r_∞ is an asymptotic rate, meaning that for any $r < r_\infty$, the norm of the difference between the solution and its limit is bounded by a constant $C_0(\kappa)$ times e^{-rt}. The fact that the constant C_0 depend on ρ is another difficulty, but at least we can have a uniform bounded on this constant when ρ is not too large. A more precise study of the behavior of this constant is left to future work.

With the time scaling factor, the rates have to be multiplied by $\frac{\rho}{\varepsilon}$ in our problem. They are given by $\frac{1}{\varepsilon} r(\rho)$, where

$$r(\rho) = \begin{cases} \frac{n-1}{n}(n-\rho) & \text{for } \rho < n \\ (n - \rho(1 - c(\kappa)^2))\Lambda_\kappa & \text{for } \rho > n. \end{cases}$$

It is then reasonable to expect, when ε is small, that the function f^ε converges rapidly to a given equilibrium, provided that the rate is large, that is to say that $r(\rho)$ is large compared to ε. In the case where $\rho < n$, the condition becomes $\varepsilon = o(n-\rho)$.

In the case where $\rho > n$, the asymptotic expansion given in Theorem 2.1 gives that $r(\rho) \sim 2\frac{n-1}{n}(\rho - n)$ in the neighborhood of n. But this does not ensure that the rate of convergence is bounded below on (n, ∞). We can prove that the Poincaré constant Λ_κ can be seen as the principal eigenvalue of a linear elliptic operator, but theoretically we have not been able to provide a sufficiently strong lower bound. Actually, we are able to reduce the problem, which comes down to finding the principal eigenvalue of two one-dimensional Sturm-Liouville problem. We provide the details in Appendix A. This allows to easily compute Λ_κ and then $r(\rho)$ numerically (see Appendix B), the results are depicted in Figure 2.1 for dimensions 2, 3, and 4.

We get that for $\rho > n$, the rate $r(\rho)$ grows linearly with ρ. And therefore, we get that $r(\rho)$ is large compared to ε if and only if $\varepsilon = o(n - \rho)$. It is then reasonable that the formal limit, as $\varepsilon \to 0$ of the function f^ε is given by a function $f(x, \omega, t)$ which satisfies

- $f(x, \omega, t) = \rho(x, t)$ with $\rho(x, t) < n$, in the "disordered" region $\mathcal{R}_d$ where we have $n - \rho^\varepsilon(x, t) \gg \varepsilon$,
- $f(x, \omega, t) = \rho(x, t) M_{\kappa(\rho)\Omega(x,t)}$ with $\rho(x, t) > n$, in the "ordered" region $\mathcal{R}_o$ where we have $\rho^\varepsilon(x, t) - n \gg \varepsilon$.

The goal is now to derive evolution equations for the density $\rho(x, t)$ and the orientation $\Omega(x, t)$. This is the object of the following two sections. Supposing that f^ε converges to such an equilibrium, the idea is to integrate the equation (3.8) against functions ψ such that the term of order zero in ε vanishes, and this gives evolution equations for the observable quantities. Such functions ψ are called collisional invariants.

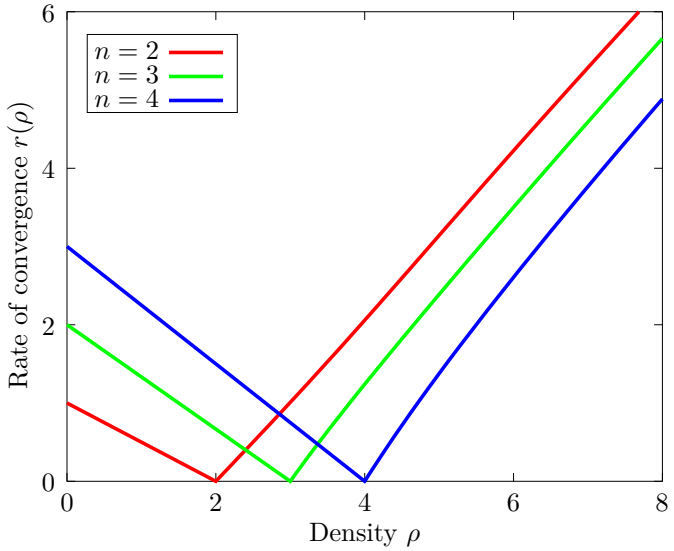

Figure 2.1: Rates of convergence in dimensions 2, 3, and 4.

For example, integrating the equation (3.8) against the constant function 1 on the sphere, we get

$$\partial_t \rho^\varepsilon + \nabla_x \cdot (J_{f^\varepsilon}) = O(\varepsilon). \tag{3.16}$$

This is the conservation of mass, which reflects that we have conservation of the number of particles in the individual model (actually we have an exact conservation of mass if we use the equation (3.4): the $O(\varepsilon)$ term vanishes, replacing the term J_{f^ε} by $\bar{J}^\varepsilon_{f^\varepsilon}$). In the limit $\varepsilon \to 0$, this gives an evolution equation for ρ. As in [28] and Chapter 1, the notion of collisional invariants must be generalized in the "ordered" region, where we lack conservation equations.

4 Diffusion in the "disordered" region

We consider a region $\mathcal{R}_d \subset \mathbb{R}^n$ where we have $n - \rho^\varepsilon(x,t) \gg \varepsilon$, and we suppose that f^ε converges to a function f of the form $f(x,\omega,t) = \rho(x,t)$.

With the conservation of mass (3.16), if we suppose that $J_{f^\varepsilon} \to J_f = 0$, we get that the mass ρ satisfies

$$\partial_t \rho = 0.$$

This means that we cannot see something interesting at this order, in the point of view of pattern formation. So we want a first order correction in ε of this stationary model. The derivation is based on the Chapman-Enskog method, similarly to the case of rarefied gas dynamics (see [26] for a review).

We write $f^\varepsilon = \rho^\varepsilon(x,t) + \varepsilon f_1^\varepsilon(x,\omega,t)$, so we have $\int_{\mathbb{S}} f_1^\varepsilon \mathrm{d}\omega = 0$ since ρ^ε is the local density of f^ε. We go back to the rescaled mean-field model (3.4), since we can have a better expansion than (3.5) for $\bar{J}^\varepsilon_{f^\varepsilon}$:

$$\bar{J}^\varepsilon_{f^\varepsilon} = \varepsilon \bar{J}^\varepsilon_{f_1^\varepsilon}(t,x) = \varepsilon J_{f_1^\varepsilon}(t,x) + O(\varepsilon^3).$$

This means that we have the same localized model as in equation (3.8), but with a correction of order ε^3 instead of ε^2. Dividing by ε, with this expansions, the model becomes:

$$\begin{aligned}\partial_t\rho^\varepsilon + \omega\cdot\nabla_x\rho^\varepsilon + \varepsilon(\partial_t+\omega\cdot\nabla_x)f_1^\varepsilon = -\nabla_\omega((\mathrm{Id}-\omega\otimes\omega)J_{f_1^\varepsilon}\rho^\varepsilon) + \Delta_\omega f_1^\varepsilon \\ - \varepsilon\nabla_\omega((\mathrm{Id}-\omega\otimes\omega)J_{f_1^\varepsilon}\rho^\varepsilon) + O(\varepsilon^2).\end{aligned} \tag{4.17}$$

First of all, integrating this equation on the sphere, we get a more precise conservation of mass than (3.16):

$$\partial_t\rho^\varepsilon + \varepsilon\nabla_x\cdot(J_{f_1^\varepsilon}) = O(\varepsilon^2), \tag{4.18}$$

which gives that $\partial_t\rho^\varepsilon$ is of order ε, and so we can look at the terms of order 0 in the model (4.17). Since $\nabla_\omega((\mathrm{Id}-\omega\otimes\omega)A) = -(n-1)A\cdot\omega$ for a constant vector $A\in\mathbb{R}^n$, we get

$$\Delta_\omega f_1^\varepsilon = (\nabla_x\rho^\varepsilon - (n-1)\rho^\varepsilon J(f_1^\varepsilon))\cdot\omega + O(\varepsilon).$$

We can directly solve this equation, since the term of order zero is a spherical harmonic of degree 1 (of the form $A\cdot\omega$, satisfying $\Delta_\omega(A\cdot\omega) = -(n-1)A\cdot\omega$):

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

Since we have $\int_{\mathbb{S}} f_1^\varepsilon \mathrm{d}\omega = 0$, we get that the constant C is of order ε. Integrating against the function ω the previous equality on the sphere, we get an equation for $J(f_1^\varepsilon)$: we have $\int_{\mathbb{S}}\omega\otimes\omega\mathrm{d}\omega = \frac{1}{n}\mathrm{Id}$ (by invariance by rotation, this must be a scalar matrix, the trace of which is $\int_{\mathbb{S}}|\omega|^2\mathrm{d}\omega = 1$), therefore we obtain

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

which gives that

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

We have then $f_1^\varepsilon = \frac{-n\omega\cdot\nabla_x\rho^\varepsilon + O(\varepsilon)}{(n-1)(n-\rho^\varepsilon)}$. We obtain here a confirmation that this approximation is only valid when $n-\rho^\varepsilon$ is large compared to ε. The final diffusion model given in the following proposition is obtained with the mass conservation equation (4.18).

Proposition 4.1. *Diffusion model in the disordered zone.*

When ε tends to zero, the (formal) first order correction of the solution of the mean-field rescaled system (3.4)*, in the region $\mathcal{R}_d\subset\mathbb{R}^n$ where we have $n-\rho^\varepsilon(x,t)\gg\varepsilon$, is given by*

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

where the density ρ^ε satisfies the following diffusion equation

$$\partial_t\rho^\varepsilon = \frac{\varepsilon}{n-1}\nabla_x\cdot\left(\frac{1}{n-\rho^\varepsilon}\nabla_x\rho^\varepsilon\right). \tag{4.19}$$

In any case, the sign of the diffusion coefficient shows that this model can only be valid in a region where $\rho^\varepsilon < n$, and moreover, this coefficient blows up as ρ^ε tends to n, where the Chapman-Enskog expansion is not valid.

5 Hydrodynamic model in the "ordered" region

We now turn to a region $\mathcal{R}_o \subset \mathbb{R}^n$ where we have $\rho^\varepsilon(x,t) - n \gg \varepsilon$, the purpose of this section is to derive and study the following model in this region.

Proposition 5.1. *Hydrodynamic model in the ordered region.*

When ε tends to zero, the (formal) limit of the solution $f^\varepsilon(x,\omega,t)$ of the mean-field rescaled system (3.4), in the region $\mathcal{R}_o \subset \mathbb{R}^n$ where we have $\rho^\varepsilon(x,t) - n \gg \varepsilon$, is given by

$$f^0(x,\omega,t) = \rho(x,t) M_{\kappa(\rho(x,t))\Omega(x,t)}(\omega),$$

where the Von Mises distribution $M_{\kappa\Omega}$ is defined in (3.10), and the parameter κ is the unique positive solution to the compatibility condition (3.13). Moreover, the density $\rho > n$ and the orientation $\Omega \in \mathbb{S}$ satisfy the following system of first order partial differential equations:

$$\partial_t \rho + \nabla_x \cdot (\rho c \Omega) = 0, \tag{5.20}$$

$$\rho(\partial_t \Omega + \widetilde{c}(\Omega \cdot \nabla_x)\Omega) + \lambda(\mathrm{Id} - \Omega \otimes \Omega) = 0, \tag{5.21}$$

where the coefficient c is defined in (3.12), the coefficient $\widetilde{c}$, depending on κ, will be defined later on in (5.25), and the parameter λ is given by

$$\lambda = \frac{\rho - n - \kappa\widetilde{c}}{\kappa(\rho - n - \kappa c)}. \tag{5.22}$$

The first part of this section is devoted to the derivation of this model.

5.1 Derivation of the model

With the arguments given at the end of section 3.3, we have formally that the limit of $f^\varepsilon(x,\omega,t)$ is given by the stable local equilibrium: $f = \rho(x,t) M_{\kappa(\rho(x,t))\Omega(x,t)}$. We want to derive the evolution equations for ρ and Ω.

We recall that the concentration parameter κ (we will drop the dependence on ρ in the notation when no confusion is possible) satisfies the compatibility condition (3.13): $\rho c = \kappa$, where the order parameter c is defined by (3.12):

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

We have that $J_f = \rho c \Omega$.

Integrating with respect to ω gives the conservation of mass (3.16), which, 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 [28] consists to introduce a generalized notion of the collisional invariants. This method has been successful in an other model of alignment of self-propelled particles [30], as well as in the refinement of the original model studied in Chapter 1.

The first step is the definition and the determination of the generalized collisional invariants. We define the linear operator $L_{\kappa\Omega}$ associated to a concentration parameter κ and a direction Ω as follows:

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

so we have that $Q(f) = -L_{J_f}(f)$. And we define the set of generalized collisional invariants $\mathcal{C}_{\kappa\Omega}$ (associated to $\kappa \in \mathbb{R}$ and $\Omega \in \mathbb{S}$) as the following vector space:

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

Hence, if ψ is a collisional invariant associated to κ and Ω, we have $\int_{\omega\in\mathbb{S}} Q(f)\,\psi\,\mathrm{d}\omega = 0$ for any function f such that $J_f = \kappa\Omega$.

The determination of $\mathcal{C}_{\kappa\Omega}$ has been done in Chapter 1. We define the space

$$V = \{ g \,|\, (n-2)(\sin\theta)^{\frac{n}{2}-2} g \in L^2(0,\pi),\ (\sin\theta)^{\frac{n}{2}-1} g \in H^1_0(0,\pi) \}, \tag{5.23}$$

and we denote by g_κ the unique solution in the space V of the elliptic problem $\widetilde{L}^*_\kappa g(\theta) = \sin\theta$, where

$$\widetilde{L}^*_\kappa g(\theta) = -\sin^{2-n}\theta e^{-\kappa\cos\theta} \tfrac{\mathrm{d}}{\mathrm{d}\theta}(\sin^{n-2}\theta e^{\kappa\cos\theta} g'(\theta)) + \tfrac{n-2}{\sin^2\theta} g(\theta). \tag{5.24}$$

Then if we take h_κ as the function such that $g_\kappa(\theta) = h_\kappa(\cos\theta)\sin\theta$, we get that the generalized collisional invariants associated to κ and Ω is a vector space of dimension n consisting in the functions $\omega \mapsto h_\kappa(\omega\cdot\Omega)A\cdot\omega + C$, with $C \in \mathbb{R}$, and $A \in \mathbb{R}^n$, with A orthogonal to Ω.

The next step consists in multiplying the rescaled kinetic model (3.8) by a collisional invariant associated to κ^ε and Ω^ε such as $J_{f^\varepsilon} = \kappa^\varepsilon\Omega^\varepsilon$, and to integrate on the sphere. We get, for any vector $A \in \mathbb{R}^n$, with $A\cdot\Omega^\varepsilon = 0$, that

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

So we have that the vector $X^\varepsilon = \frac{1}{\varepsilon}\int_{\omega\in\mathbb{S}} Q(f^\varepsilon) h_{\kappa^\varepsilon}(\omega\cdot\Omega^\varepsilon)\,\omega\,\mathrm{d}\omega$ is orthogonal to A for all A orthogonal to Ω, that is to say that X^ε is in the direction of Ω^ε, which is equivalent to $(\mathrm{Id} - \Omega^\varepsilon\otimes\Omega^\varepsilon)\,X^\varepsilon = 0$. Using (3.8), we get that

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

In the limit $\varepsilon \to 0$, we get $(\mathrm{Id} - \Omega\otimes\Omega)\,X = 0$, where

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

Finally it has been proved in Chapter 1 that $(\mathrm{Id} - \Omega\otimes\Omega)\,X = 0$ is equivalent to the following first order partial differential equation for Ω:

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

where

$$\widetilde{c} = \langle \cos\theta \rangle_{\widetilde{M}_\kappa} = \frac{\int_0^\pi \cos\theta h_\kappa(\cos\theta) e^{\kappa\cos\theta} \sin^n\theta \,\mathrm{d}\theta}{\int_0^\pi h_\kappa(\cos\theta) e^{\kappa\cos\theta} \sin^n\theta \,\mathrm{d}\theta}, \tag{5.25}$$

$$\lambda = \frac{1}{\kappa} + \frac{\rho}{\kappa}\frac{\mathrm{d}\kappa}{\mathrm{d}\rho}(\widetilde{c} - c). \tag{5.26}$$

We can now compute a more simple expression of λ. We differentiate the compatibility condition $\rho c = \kappa$ 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

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

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 Proposition 5.1.

The next part is devoted to the study of the properties of the model (5.20)-(5.21) in the ordered region.

5.2 Properties of the model

We first investigate the hyperbolicity of the hydrodynamic model. It has been proved in Chapter 1 that the system (5.20)-(5.21) is hyperbolic if and only if $\lambda > 0$. We see that, using the compatibility condition $\rho c = \kappa$, the expression (5.22) 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 Chapter 1, 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

$$\rho = \begin{cases} n + \frac{1}{n+2}\kappa^2 + O(\kappa^4) & \text{as } \kappa \to 0, \\ \kappa + \frac{n-1}{2} + \frac{(n-1)(n+1)}{8\kappa} + O(\kappa^{-2}) & \text{as } \kappa \to \infty. \end{cases} \tag{5.27}$$

Using the definition (5.22), we then get

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

Finally we have that the system is not hyperbolic in these two limits. Numerically, with the computations done in Appendix B, we see that λ is actually negative for all values of κ.

We now consider a system satisfying (5.20)-(5.21), but evolving only along one space direction $e_z \in \mathbb{S}$ (the density ρ and the orientation Ω depending only on t and $z = e_z \cdot x$). We write then $\Omega = \cos\theta\, e_z + \sin\theta\, v$,where $v \in \mathbb{S}_{n-2}$ (identified to the set of unit vectors orthogonal to e_z). In this framework, the system is equivalent to

$$\partial_t \rho + \partial_z(\rho c_1(\rho)\cos\theta) = 0. \tag{5.28}$$

$$\rho[\partial_t(\cos\theta) + c_2(\rho)\cos\theta\,\partial_z(\cos\theta)] + \lambda\,(1-\cos^2\theta)\,\partial_z\rho = 0. \tag{5.29}$$

$$\partial_t v + c_2(\rho)\cos\theta\,\partial_z v = 0, \text{ with } |v| = 1 \text{ and } e_z \cdot v = 0. \tag{5.30}$$

In the special case of dimension 2, the system reduces to (5.28)-(5.29), with $\theta \in (-\pi, \pi)$ and $\Omega = \cos\theta\, e_z + \sin\theta\, v_0$, where v_0 is one of the two unit vectors orthogonal to e_z.

For this constrained system, we have a weaker condition of hyperbolicity, given in Chapter 1: in the present case where $\lambda < 0$, we get that the system (5.28)-(5.30) is hyperbolic if and only if

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

In our case, we have $\rho c = \kappa$, using the formula $c\,\frac{\mathrm{d}\rho}{\mathrm{d}\kappa} = n - \rho + \kappa c$ obtained in the previous subsection, and we have that this reduced system is hyperbolic if and only if $\theta \in [0, \theta_c) \cup (\pi - \theta_c, \pi]$, where the critical angle θ_c is defined by

$$\theta_c = \arctan\left(\frac{|\widetilde{c} - \frac{c}{n-\rho+\kappa c}|}{2\sqrt{-\lambda c}}\right). \tag{5.31}$$

We can once again do an expansion 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 (5.27) to get an expansion of κ (and then of the other coefficients) in terms of the density ρ, which is more suitable to understand the behavior of the system as ρ is large or close to the critical threshold n. We get

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

Therefore, we can state the results under the form of a proposition.

Proposition 5.2. *Expansion of the coefficients when the density is large or close to the critical threshold.*

We have the following expansions for the coefficients c, $\widetilde{c}$, λ and θ_c.

- *When the density ρ is close to n, we have:*

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

- *When the density ρ tends to infinity, we have:*

$$\begin{aligned} c &= 1 - \tfrac{n-1}{2}\rho^{-1} + \tfrac{(n-1)(n+1)}{8}\rho^{-2} + O(\rho^{-3}), \\ \widetilde{c} &= 1 - \tfrac{n+1}{2}\rho^{-1} - \tfrac{(n+1)(3n+1)}{24}\rho^{-2} + O(\rho^{-3}), \\ \lambda &= -\tfrac{n+1}{6}\rho^{-2} + O(\rho^{-3}), \\ \theta_c &= \arctan(\tfrac{\sqrt{n+1}\sqrt{6}}{4}) + O(\rho^{-1}). \end{aligned}$$

This proposition allows us to investigate the features of this hydrodynamic model in the limit cases.

In the case where ρ is close to n, since $|\lambda| = -\lambda$ is large compared to ρ, which is large compared to $\rho\widetilde{c}$, the behavior of the orientation equation (5.21) can be compared to the behavior of

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

which is exactly a strong relaxation to the unit vector in the same direction as $\nabla_x\rho$, with rate

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

This actually makes sense only in the case where the rate of convergence to the equilibrium $\frac{1}{\varepsilon}r(\rho) \sim \frac{2n-1}{n\varepsilon}(\rho-n)$ in the neighborhood of n is large compared to this rate of relaxation, that is to say $\varepsilon \ll (\rho-n)^{\frac{3}{2}}|\nabla_x\rho|$. 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. A better understanding of the behavior of the macroscopic model in the case where ρ is close to n may be possible if we derive a first order correction in ε of the model (3.4). Such a correction has been established in [31] for the model of [28], but results in complicated terms. More investigations are in progress to see if we can get a simple first order correction in our case, which may also help to connect the two regions of order and disorder, since we already have the diffusion (4.19) in the disordered region.

When the density ρ large, the two speeds c and $\widetilde{c}$ are close to 1, and the parameter λ is small. But in the intermediate regime, the numerical computation of the coefficients (see Appendix B) gives that there is a significant difference between the two velocities c and $\widetilde{c}$. This means that the information on the orientation travels slower than the fluid. The figure 5.2 depicts this difference, in dimension 2 and 3.

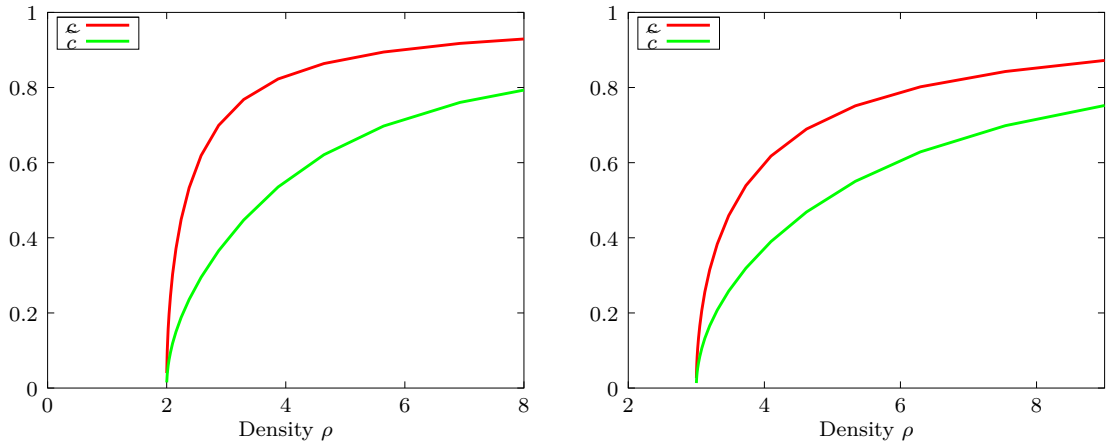

Figure 2.2: The velocities c and $\widetilde{c}$ in dimension 2 (left) and 3 (right).

Finally, we see that the critical angle θ_c tends to a positive value $\arctan(\frac{\sqrt{n+1}\sqrt{6}}{4})$. Numerically, we get that it is always greater than this limit value. Then, the reduced system (5.28)-(5.30) is hyperbolic in the region where the angle θ between Ω and the direction of propagation is less than this limit value, independently of the density ρ. The problem of crossing this zone of non-hyperbolicity appears in some other problems such as the motion a an elastic string on a plane [66].

In summary, in Figure 5.2, we depict the types of macroscopic limits of the system in dimension 2, described by a density ρ, and an angle θ in the case where ρ and θ depend only on one space dimension.

6 Conclusion

We have derived, from this time-continuous version of the Vicsek model, a macroscopic limit with two regimes.

In the disordered regime, the model is given by a nonlinear diffusion equation depending on a small parameter ε.

In the ordered regime, the model is given by the macroscopic Vicsek model, which confirms the ability of this model to describe the large scale behavior of general systems of self-propelled particles with alignment interaction. The interesting feature here is that this system of first-order partial differential equations is non-hyperbolic.

A lot of challenging issues arise from this study. The first one is to understand the evolution in the boundary region $\mathcal{R}_b$ where $\rho^\varepsilon(x,t) = n + O(\varepsilon)$, as well as the study of the evolution of the regions $\mathcal{R}_o$ and $\mathcal{R}_d$ in time. The second one is to have a better understanding of the implications of the non-hyperbolicity, in the ordered region.

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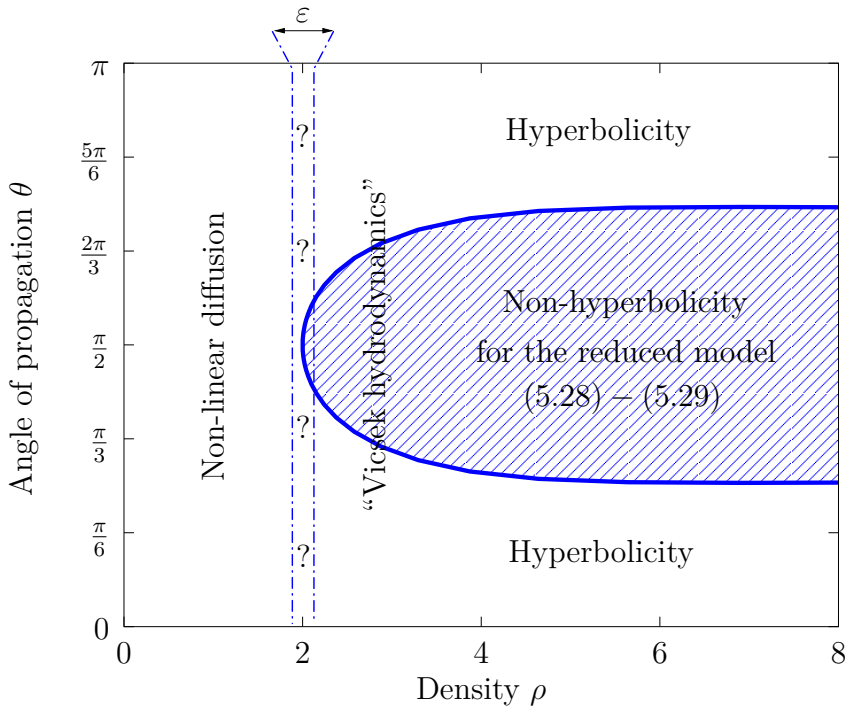

Figure 2.3: Types of macroscopic limits in dimension 2.

Numerical simulations of the particular model are in progress to understand the behavior of the model in the two regimes.

A Poincaré constant

Proposition A.1. *Study of the Poincaré constant Λ_κ.*

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

$$\langle |\nabla_\omega \psi|^2 \rangle_{M_{\kappa\Omega}} \geqslant \Lambda_\kappa \langle (\psi - \langle \psi \rangle_{M_{\kappa\Omega}})^2 \rangle_{M_{\kappa\Omega}}. \tag{A.32}$$

The best constant Λ_κ in this inequality is is the smallest positive eigenvalue of the operator $L^*_{\kappa\Omega} = -\frac{1}{M_{\kappa\Omega}} \nabla_\omega \cdot M_{\kappa\Omega} \nabla_\omega$.

We define the linear operator L^*_κ by

$$L^*_\kappa(g)(\theta) = -\sin^{2-n}\theta e^{-\kappa\cos\theta} (\sin^{n-2}\theta e^{\kappa\cos\theta} g'(\theta))'. \tag{A.33}$$

Then we have one of these three possibilities:

- *Λ_κ is the smallest eigenvalue of the Sturm-Liouville problem*

$$L^*_\kappa(g) = \lambda g,$$

for $g \in C^2([0,\pi])$ with Neumann boundary conditions ($g'(0) = g'(\pi) = 0$) and such that $\int_0^\pi \sin^{n-2}\theta e^{\kappa\cos\theta} g(\theta) \mathrm{d}\theta = 0$, 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 $\theta_0 < \theta \leqslant \pi$.

- *Λ_κ is the smallest eigenvalue of the Sturm-Liouville problem*

$$\widetilde{L}^*_\kappa(g) = L^*_\kappa(g) + \tfrac{n-2}{\sin^2\theta} g(\theta) = \lambda g,$$

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 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 $0 < \theta < \pi$.

- *The two above 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

$$\langle |\nabla_\omega \psi|^2 \rangle_{M_{\kappa\Omega}} \min M_{\kappa\Omega} \int_{\mathbb{S}} |\nabla_\omega \psi|^2 \geqslant \min M_{\kappa\Omega} (n-1) \int_{\mathbb{S}} (\psi - \textstyle\int_{\mathbb{S}} \psi)^2,$$

and

$$\langle (\psi - \langle \psi \rangle_{M_{\kappa\Omega}})^2 \rangle_{M_{\kappa\Omega}} \leqslant \langle (\psi - \textstyle\int_{\mathbb{S}} \psi)^2 \rangle_{M_{\kappa\Omega}} \leqslant \max M_{\kappa\Omega} \int_{\mathbb{S}} (\psi - \textstyle\int_{\mathbb{S}} \psi)^2,$$

which gives the Poincaré inequality (A.32) with $\Lambda_\kappa \geqslant (n-1)\frac{\min M_{\kappa\Omega}}{\max M_{\kappa\Omega}} = (n-1)e^{2\kappa}$.

We work with 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 $\langle \varphi\psi \rangle_{M_{\kappa\Omega}} = 0$.

We can remark that the operator $L^*_{\kappa\Omega} : \psi \mapsto -\frac{1}{M_{\kappa\Omega}} \nabla_\omega \cdot (M_{\kappa\Omega} \nabla_\omega \psi)$ is self-adjoint: we have $\langle \nabla_\omega \psi \cdot \nabla_\omega \varphi \rangle_{M_{\kappa\Omega}} = \langle \psi L^*_{\kappa\Omega} \varphi \rangle_{M_{\kappa\Omega}}$. It is then easy to see, using 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 inverse operator obtained 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 $\dot{H}^1_\kappa(\mathbb{S})$:

$$\langle |\nabla_\omega \psi|^2 \rangle_{M_{\kappa\Omega}} \geqslant \Lambda_\kappa \langle \psi^2 \rangle_{M_{\kappa\Omega}}.$$

This gives, adding the constants, that Λ_κ is the best constant for the following Poincaré inequality (A.32) in $H^1(\mathbb{S})$.

The goal is now to reduce the computation of the eigenvalues to more simple problems, using separation of variables: we write $\omega = \cos\theta\,\Omega + \sin\theta\, v$, where v is on 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 the appendix A of Chapter 4), we have a unique decomposition of the form

$$\psi(\omega) = \sum_{k,m} g^k_m(\theta) Z^k_m(v), \tag{A.34}$$

where $(Z_m^k(v))_{k\in[\![1,k_m]\!]}$ is a given orthonormal basis of the spherical harmonics of degree m on $\mathbb{S}_{n-2}$, for $m \in \mathbb{N}$. In the case where the function ψ is continuous, the coefficient function g_m^k is just given by

$$g_m^k(\theta) = \int_{\mathbb{S}_{n-2}} \psi(\cos\theta\Omega + \sin\theta v) Z_m^k(v)\mathrm{d}v. \tag{A.35}$$

We will see that the operator $L_{\kappa\Omega}$ stabilizes this decomposition, so we can do its spectral decomposition in these spaces.

In dimension $n \geqslant 3$, for $\psi(\omega) = g(\theta)Z(v)$, 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 $\nabla_\omega\theta = -\frac{1}{\sin\theta}(\mathrm{Id} - \omega\otimes\omega)\Omega$.

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

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

When $m \geqslant 1$, it is easy to see that the function ψ belongs to $\dot{H}^1_\kappa(\mathbb{S})$ if and only if $\sin^{\frac{n}{2}-1}\theta g' \in L^2(0,\pi)$ and $\sin^{\frac{n}{2}-2}\theta g' \in L^2(0,\pi)$. This condition is equivalent to the fact that $g \in V$, where the space V is defined by (5.23), and we will denote it V_κ^m for convenience:

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

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

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

We then define the operator $L^*_{\kappa,m} : V_\kappa^m \to (V_\kappa^m)^*$ by

$$\int_0^\pi f(\theta)L^*_{\kappa,m}g(\theta)\sin^{n-2}\theta e^{\kappa\cos\theta}\mathrm{d}\theta = \int_0^\pi [f'g' + \tfrac{m(m+n-3)}{\sin^2\theta}fg]\sin^{n-2}\theta e^{\kappa\cos\theta}\mathrm{d}\theta. \tag{A.36}$$

In this framework, if we have $\psi(\omega) = \sum_{k,m} g_m^k(\theta)Z_m^k(v)$, then we get

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

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

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

It is then easy to see that

$$\lambda_{\kappa,m} = \inf_{\substack{f\in V_\kappa^m \\ \int_0^\pi f^2(\theta)\sin^{n-2}\theta e^{\kappa\cos\theta}\mathrm{d}\theta=1}} \{\textstyle\int_0^\pi f(\theta)L^*_{\kappa,m}f(\theta)\sin^{n-2}\theta e^{\kappa\cos\theta}\mathrm{d}\theta\},$$

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

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

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 the formula (A.35). So we can transform the definitions (A.36) by integration by parts.

Indeed, if g_0 is an eigenfunction (in V_κ^0) associated to $L^*_{\kappa,0}$ and an eigenvalue λ, we get that g_0 is smooth and satisfies the Sturm-Liouville eigenvalue problem

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

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

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

therefore by continuity at $\theta = 0$ and π, we get that $g_0'(0) = g_0'(\pi) = 0$. The classical Sturm-Liouville oscillation theory gives then 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_κ^1) associated to $L^*_{\kappa,1}$ and an eigenvalue λ, we get that g_1 is smooth, with $g_1(0) = g_1(\pi) = 0$ and satisfies the Sturm-Liouville eigenvalue problem

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

And conversely, if a function with Dirichlet boundary conditions is in $C^2([0,\pi])$ it is easy to show that it belongs to V_κ^1. Once again, we do not need to impose the Dirichlet boundary conditions if we work in $C^2([0,\pi])$, since we have

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

so by continuity at $\theta = 0$ and π, we get that $g_1(0) = g_1(\pi) = 0$, and then a first order expansion shows that we have continuity, whatever the values of $g_0'(\theta)$ at the endpoints. The classical Sturm-Liouville theory gives then 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 $(0,\pi)$.

If $\lambda_{\kappa,0} < \lambda_{\kappa,1}$, we are in the first case of the proposition, and since a spherical harmonic of degree 0 on the sphere $\mathbb{S}_{n-2}$ is a constant, writing $h_k^0(\cos\theta) = g_{\kappa,0}(\theta)$ gives that the first eigenspace of $L^*_{\kappa\Omega}$ is spanned by $\omega \mapsto h^0_\kappa(\omega \cdot \Omega)$. If $\lambda_{\kappa,0} > \lambda_{\kappa,1}$, we are in the second case 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 $A \cdot \Omega = 0$. Writing $h_k^0(\cos\theta)\sin\theta = g_{\kappa,0}(\theta)$ gives that the first eigenspace of $L^*_{\kappa\Omega}$ is of dimension $n-1$, consisting in the functions of the form $\omega \mapsto h^1_\kappa(\omega\cdot\Omega)A\cdot\Omega$, with A any vector in $\mathbb{R}^n$ which is orthogonal to Ω. Finally, when $\lambda_{\kappa,0} = \lambda_{\kappa,1}$, we are in the third case of the proposition, and this ends the proof in the case where $n \geqslant 3$.

When $n = 2$, 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

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

for a function g such that $\int_{-\pi}^{\pi} e^{\kappa\cos\theta}g(\theta)\mathrm{d}\theta = 0$. Here the decomposition corresponding to (A.34) 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 do the spectral decomposition of L^*_κ separately on the even and odd functions.

Actually, if we have a solution g of the Sturm-Liouville periodic problem, we get that $\widetilde{g}(\theta) = e^{-\kappa\cos\theta}\partial_\theta g(\pi-\theta)$ 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 two distinct problems.

We are in the third case: 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 $\theta_0 < \theta < \pi$. □

Conjecture 2.1. *Behavior of* Λ_κ

- *When* $\kappa > 0$ *and* $n \geqslant 3$*, we only have the second case of the Proposition A.1.*
- *The function* $\kappa \mapsto \Lambda_\kappa$ *is increasing.*

We have seen in the end of the proof of Proposition A.1 that when $n = 2$ we are in the third case, using a transformation of a solution of an eigenvalue problem to a solution to another eigenvalue problem.

We can try to do the same in the case $n \geqslant 3$: if we have $L_{\kappa,0}f = \lambda f$ (with Neumann boundary conditions) then the function $\widetilde{f} = e^{-\kappa\cos\theta}\partial_\theta f(\pi-\theta)$ (with Dirichlet boundary conditions) satisfies

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

so if we can prove that $\int_0^\pi \cos\theta\widetilde{f}^2\sin^{n-2}\theta e^{\kappa\cos\theta}g(\theta)\mathrm{d}\theta > 0$, we get that $\lambda_0 > \lambda_1$. Actually, this is what we get numerically (see Appendix B) for the case $n \geqslant 3$, and we also get that $\lambda_1 \sim \kappa$ when κ is large.

Some investigations are in progress to prove the monotonicity of the eigenvalue with κ, based on formal expansions similar to those used in Section 5.1 of Chapter 1.

B Numerical computations of the coefficients

We adopt a finite difference approach to compute g_k. We consider the function f_κ such that $f_k(\theta) = \sin^{\frac{n}{2}-1}\theta g_\kappa(\theta)$. In particular since $g_\kappa \in V$ defined in (5.23), we get that $f_\kappa \in H_0^1(0,\pi)$. We have $\widetilde{L}_\kappa^*(g_k) = \sin\theta$ with the definition of $\widetilde{L}_\kappa^*$ given in (5.24), and it is easy to see that this is equivalent to

$$-e^{-\kappa\cos\theta}(e^{\kappa\cos\theta}f_k')' + (\tfrac{n-2}{2\sin^2\theta}(1+\tfrac{n-2}{2}\cos^2\theta) - \kappa\cos\theta)f = \sin^{\frac{n}{2}}\theta.$$

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

$$\frac{N^2}{\pi^2}(e_\kappa^{i+\frac{1}{2}}(f_\kappa^{i+1}-f_\kappa^i) - e_\kappa^{i-\frac{1}{2}}(f_\kappa^i - f_\kappa^{i-1})).$$

Writing

$$d_\kappa^i = \frac{n-2}{2\sin^2\theta_i}(1+\tfrac{n-2}{2}\cos^2\theta_i) - \kappa\cos\theta_i + \frac{N^2}{\pi^2}\frac{e_\kappa^{i-\frac{1}{2}} + e_\kappa^{i+\frac{1}{2}}}{e_k^i},$$
$$b_\kappa^i = -\frac{N^2}{\pi^2}\frac{e_\kappa^{i+\frac{1}{2}}}{e_k^i}, \quad \text{and} \quad \widetilde{b}_\kappa^i = -\frac{N^2}{\pi^2}\frac{e_\kappa^{i-\frac{1}{2}}}{e_k^i},$$

we get that 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

$$A = \begin{pmatrix} d_\kappa^1 & b_\kappa^1 & 0 & \dots & \dots & 0 \\ \widetilde{b}_\kappa^2 & d_\kappa^2 & b_\kappa^2 & \ddots & & \vdots \\ 0 & \widetilde{b}_\kappa^3 & d_\kappa^3 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & b_\kappa^{N-3} & 0 \\ \vdots & & \ddots & \widetilde{b}_\kappa^{N-2} & d_\kappa^{N-2} & b_\kappa^{N-2} \\ 0 & \dots & \dots & 0 & \widetilde{b}_\kappa^{N-1} & d_\kappa^{N-1} \end{pmatrix}. \tag{B.37}$$

We use then the trapezoidal method to perform the integrations in the definition (3.12)-(5.25) 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 Figures 5.2-5.2 have been obtained for $N = 3000$.

We now detail a little bit how we obtain the Poincaré constant Λ_κ. By Appendix A, we have that Λ_κ is the minimum between $\lambda_{\kappa,1}$ and $\lambda_{\kappa,0}$, which are the smallest eigenvalue of two Sturm-Liouville problems. Several algorithms exist to compute with a good precision this eigenvalues even for a singular Sturm-Liouville problem [5], which is the case here whenever $n \geqslant 3$, but we use here a simple method based on finite differences.

Actually we have that $\lambda_{\kappa,1}$ is the smallest eigenvalue associated to the problem $\widetilde{L}_\kappa^* g = \lambda g$, with $g \in V$. So considering once again the function f such that $f(\theta) = \sin^{\frac{n}{2}-1}\theta g(\theta)$, we have that the vector AF, with A defined by (B.37)

give a second order approximation of $\sin^{\frac{n}{2}-1}\theta \widetilde{L}^*_\kappa g(\theta) = \lambda f(\theta)$ at the points θ_i. So we can take the smallest eigenvalue of A as an an approximation of $\lambda_{\kappa,1}$.

We want an approximation of $\lambda_{\kappa,0}$. If g is an eigenfunction associated to λ for the problem $L^*_\kappa g = \lambda g$ with Neumann boundary conditions, then we write $G = (g_{i+\frac{1}{2}})_{i\in[\![0,N-1]\!]}$ an approximation of g at the points $\theta_{i+\frac{1}{2}} = \frac{1}{N}(i+\frac{1}{2})\pi$. If we write $m^i_\kappa = \sin^{n-2} e^{\kappa\cos\theta_i}$. A second order approximation of $L^*_\kappa g$ at the point $\theta_{i+\frac{1}{2}}$ is then given by, when $i \in [\![1, N-2]\!]$, by

$$\frac{N^2}{\pi^2 m_\kappa^{i+\frac{1}{2}}}(-m^{i+1}_\kappa(f_\kappa^{i+\frac{3}{2}} - f_\kappa^{i+\frac{1}{2}}) + m^i_\kappa(f_\kappa^{i+\frac{1}{2}} - f_\kappa^{i-\frac{1}{2}})).$$

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

$$\frac{N^2}{\pi^2 m_\kappa^{\frac{1}{2}}} m^1_\kappa (f_\kappa^{\frac{3}{2}} - f_\kappa^{\frac{1}{2}}) \quad \text{and} \quad -\frac{N^2}{\pi^2 m_\kappa^{N-\frac{1}{2}}} m^{N-1}_\kappa (f_\kappa^{N-\frac{1}{2}} - f_\kappa^{N-\frac{3}{2}}).$$

Writing

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

we get that a second order approximation of $L^*_\kappa g$ is given by BG, where the tridiagonal matrix B is defined by

$$B = \begin{pmatrix} -b_\kappa^{\frac{1}{2}} & b_\kappa^{\frac{1}{2}} & 0 & \dots & \dots & 0 \\ \widetilde{b}_\kappa^{\frac{3}{2}} & d_\kappa^{\frac{3}{2}} & b_\kappa^{\frac{3}{2}} & \ddots & & \vdots \\ 0 & \widetilde{b}_\kappa^{\frac{5}{2}} & d_\kappa^{\frac{5}{2}} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & b_\kappa^{N-\frac{5}{2}} & 0 \\ \vdots & & \ddots & \widetilde{b}_\kappa^{N-\frac{3}{2}} & d_\kappa^{N-\frac{3}{2}} & b_\kappa^{N-\frac{3}{2}} \\ 0 & \dots & \dots & 0 & \widetilde{b}_\kappa^{N-\frac{1}{2}} & -\widetilde{b}_\kappa^{N-\frac{1}{2}} \end{pmatrix}, \tag{B.38}$$

So we can take the smallest positive eigenvalue of B as an approximation of $\lambda_{\kappa,0}$ (so we exclude the constant functions). The computations for the rates of convergence (Figure 2.1) have been done with $N = 300$.

Chapter 3

An individual time-continuous Vicsek model on a Riemannian manifold

This chapter is an ongoing collaboration with Sébastien Motsch.

Abstract

We consider a generalization of the time-continuous version of the Vicsek model introduced by Degond and Motsch to the case where the particles are constrained to move on a general complete Riemannian manifold (the original model corresponding to the case of the Euclidean space or of the flat torus), the dynamics taking then place on its unit tangent bundle.

Using parallel transport to define a local average orientation, we are able to give a consistent model, under the form of coupled stochastic differential equations on the manifold. We prove the propagation of chaos property for this system, and derive a mean-field model in the limit of a large number of particles.

Finally, we perform some numerical simulations of this model in the case where the manifold is the two-dimensional unit sphere.

Key words: Unit tangent bundle, Vicsek model, stochastic process on a manifold, propagation of chaos.

1 Introduction

Self-organization in nature provides many astonishing phenomenon. "One out of many" is the gigantic flocks produced by birds. To understand this phenomenon, many models have been studied and in particular the so-called Vicsek model. One can observe that the Vicsek model leads to the formation of a large band of particles similar to a flock observed in nature. However, despite the abundance of numerical studies on the Vicsek model, all the simulations have been made on the same geometric space: a flat torus, in another words a square box with periodic boundary conditions. Since the geometry of the domain influences the global dynamics of the particles, we would like to study in this work in progress an extension of the Vicsek model on a general Riemannian manifold. Could we observe similar band formation when the geometric domain is a sphere and not a flat torus?

The Vicsek model is a simple model which describes how particles interact to align with their neighbors. Due to the simplicity of the model, this dynamics has drawn lot of attention [74, 16, 46, 28]. One of the main features of the Vicsek model is the emergence of large flocks through its dynamics. Although particles only interact locally in the model, they manage to align globally and produce a large "band" moving in one single direction [16, 62]. However, the emergence of such a band may not be entirely due to the dynamics of the Vicsek model, the geometry of the domain may play an important role. In the simulations of the Vicsek model in two dimensions, when a band appears, particles are more likely to move in one of the cardinal direction (East, West, North or South). In other words, the direction of the "band" is not uniform. This phenomenon can be explained by the geometry of the domain: the simulations are done on a flat torus (a square box with periodic boundary condition), therefore the two axis (East-West and North-South) are the two periodic geodesic with shortest length. Thus, the band formation minimizes the distance on the flat torus. But is this geometry essential for the formation of band? Does the Vicsek model lead to band formation in other geometry? Can we observe band formation when the domain is for example a sphere, or even the standard torus in $\mathbb{R}^3$ and not the flat one?

To answer these questions, the first task is to build a framework to describe the evolution of oriented particles on a manifold. To do so, we extend the notion of random perturbation in this context and we determine the dynamics of a particle on a manifold subjected to an external orientational force. As a result, the dynamics of a single particle on a manifold is written as a stochastic differential equation. We also prove that the law of such a particle satisfied a so-called Kolmogorov–Fokker–Planck equation.

Once the framework is settled, we have to extend the Vicsek model in this set-up. In other words, we would like to implement an alignment rule for particles moving on a manifold. To do so, we first define what is the local average velocity around the k^{th} particle (we cannot sum the velocities anymore since they do not belong to the same tangent space). Then, the model that we propose simply reads as the relaxation of the velocity of this particle towards the orientation of this local average. As for the Vicsek model in a "flat" domain, we can prove the existence of a kinetic equation associated with this dynamics (proving the so-called propagation of chaos for the

dynamics, in the spirit of what have been done in [13] for the model of Chapter 2).

To illustrate our theory, we run several numerical simulations of the model on the sphere $\mathbb{S}_2$. We observe that particles quickly align with their neighbors as for the Vicsek model on the flat torus. However, no global preferred direction emerges from the dynamics. Every direction seems to be equally chosen. A more intensive study has to be done to confirm this observation. Works are in progress in this direction.

Another line of work consists in finding explicit equilibrium of the Vicsek model on compact manifold such as the sphere $\mathbb{S}_2$. In [60], it has been observed that a "vortex" configuration was an equilibrium for macroscopic limit of the Vicsek model on the whole plane $\mathbb{R}^2$. However, this vertex configuration is no longer an equilibrium on the flat torus due to the periodic boundary conditions. Therefore, we cannot check numerically the emergence of a vertex configuration. In contrast, if we are able to find an explicit stationary state for the Vicsek dynamics on a compact manifold with axial symmetry, such as the unit sphere, it may be possible to predict the emergence of equilibria in the numerical simulations.

2 The individual-based model

2.1 Dynamics of a single particle on a manifold

We consider a complete Riemannian manifold M of dimension $n \geqslant 2$ with a metric g (we impose that M is complete in order for the particles to never reach a boundary). We would like to describe the evolution in time of an oriented particle on the manifold M. An oriented particle is described by a couple (x, ω), where x is the position of the particle ($x \in M$) and ω is the velocity of the particle belonging to the tangent space T_xM. Moreover, we assume that the particle is moving at a constant speed: $|\omega|_g = 1$ with $|\cdot|_g$ the induced norm on T_xM (see figure 3.1).

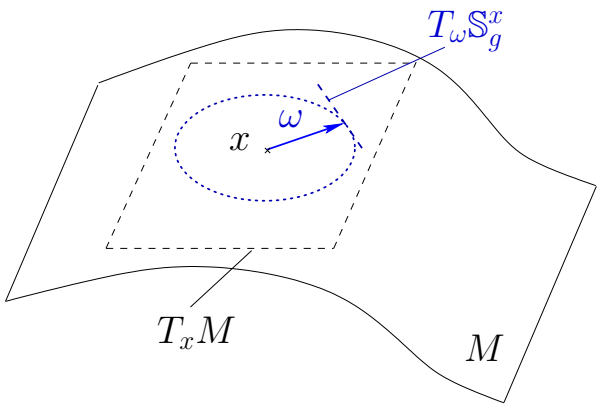

Figure 3.1: An oriented particle (x, ω) on a manifold M. The velocity ω belongs to the tangent space T_xM and we also impose that ω has a unit length (e.g. $|\omega|_g = 1$).

To simplify the notations, we introduce the unit tangent bundle UM:

$$UM := \{(x, \omega) \mid x \in M,\ \omega \in T_xM \ \text{ and } |\omega|_g = 1\}. \tag{2.1}$$

The manifold UM has a natural metric, called Sasaki metric, allowing to decompose the tangent space of UM at a point (x, ω) as a direct orthogonal sum of the horizontal space T_xM and the tangent space of the unit sphere $\mathbb{S}_g^x$ at the point ω denoted by $T_\omega \mathbb{S}_g^x$ (with $T_\omega \mathbb{S}_g^x \subset T_xM$). In other words, we can identify $T_{(x,\omega)}UM$ with $T_xM \bigoplus T_\omega \mathbb{S}_g^x$.

Hence, to define the dynamics of a particle, it is sufficient to give the variation of x in T_xM, and the variation of ω in $T_\omega \mathbb{S}_g^x$. We refer to [43] for an introduction to Riemannian geometry, and to [68, 69] for the natural Riemannian structure of the tangent and unit tangent bundles.

To illustrate the idea, we introduce a local coordinate neighborhood, that is to say an open subset $\mathcal{U}_M$ of M, diffeomorphic to $\mathcal{U} \subset \mathbb{R}^n$. We write the coordinates of $x \in M$ with this identification by $(x^i)_{i \in [\![1,n]\!]} \in \mathcal{U}$. If the components of a tangent vector $\omega \in T_xM$ with respect to the natural frame $(\frac{\partial}{\partial x^i})$ are written v^i, then we get local coordinates of TM, written $((x^i)_{i \in [\![1,n]\!]}, (v^i)_{i \in [\![1,n]\!]}) \in \mathcal{U} \times \mathbb{R}^n$.

Let us consider $(x(t), \omega(t))$ a curve in UM, given in the local coordinate neighborhood of TM by $((x^i)_{i \in [\![1,n]\!]}, (\omega^i)_{i \in [\![1,n]\!]}) \in \mathcal{U} \times \mathbb{R}^n$. Since ω belongs to the unit sphere $\mathbb{S}_g^x$, we first have:

$$|\omega|_g = \sum_{j,k} g_{jk}(x)\, \omega^j\, \omega^k = 1. \tag{2.2}$$

Moreover, the particle $(x(t), \omega(t))$ has to stay on the manifold UM, therefore its derivative in time has to satisfy:

$$\frac{\mathrm{d}x^i}{\mathrm{d}t} = v^i, \quad \frac{\mathrm{d}\omega^i}{\mathrm{d}t} = \eta^i - \sum_{j,k} \Gamma^i_{jk}\, \omega^j\, v^k, \tag{2.3}$$

where Γ^i_{jk} are the Christoffel symbols of g in the coordinates x^i. The sum in equation (2.3) expresses that ω has to stay in the tangent space of x. The vector η is the "internal" modification of the velocity ω, it will encode the interactions between the particles later on (see section 2.2). The vector η has to belong to the tangent space T_xM and it also has to be orthogonal to the velocity to preserve the unit length of ω (see figure 3.2):

$$\langle \eta, \omega \rangle_g = \sum_{j,k} g_{jk}(x)\, \eta^j\, \omega^k = 0. \tag{2.4}$$

Remark 2.1. *In our model, ω is the velocity of the particle (e.g. $\frac{\mathrm{d}x}{\mathrm{d}t} = \omega$). Therefore, one can replace v by ω in equations* (2.3) *and* (2.5)*.*

Remark 2.2. *If the vector η is zero, then the particle has a free movement, it follows the geodesic flow. Thus, the equation* (2.3)*, when $v^i = \omega^i$ and $\eta^i = 0$, is exactly the equation of a geodesic.*

We would like to introduce "noise" in the motion of the particle. More precisely, we want to add a Brownian motion of intensity $\sqrt{2d}$ to the dynamics of the orientation ω. We refer to [48] for an introduction to Brownian motion on Riemannian manifolds. We can first determine the stochastic differential equation satisfied by a Brownian motion on $\mathbb{S}_g^x$, the unit sphere of T_xM for the metric g at the point x, in the local coordinates.

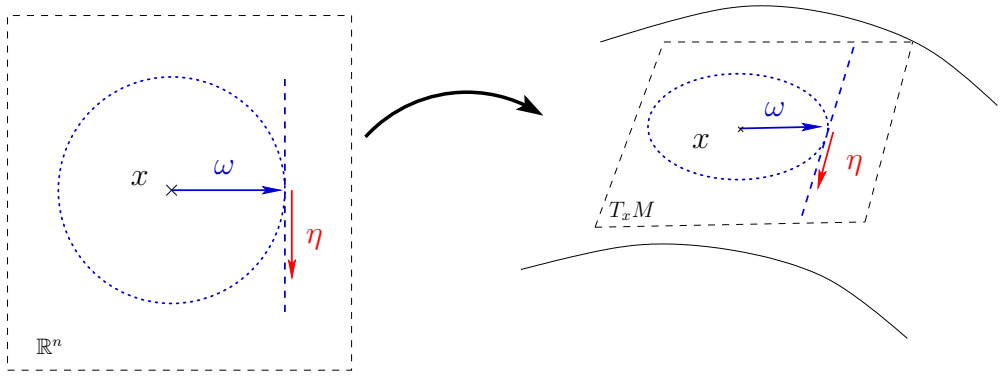

Figure 3.2: In local coordinates, the particles (x, ω) moves in the Euclidean space $\mathbb{R}^n$. Its tangential acceleration η has to be orthogonal to ω (2.4).

Lemma 3.1. *Brownian motion on $\mathbb{S}_g^x$, in local coordinates of T_xM.*

The stochastic differential equation for a Brownian motion W_t on $\mathbb{S}_g^x$, in the local coordinates of T_xM, is given (in the Stratonovich sense) by

$$\mathrm{d}W_t = \pi_{x,W_t}\, \sigma \circ \mathrm{d}B_t,$$

where σ is the positive definite symmetric square root of g in the local coordinates, $\pi_{x,\omega}$ is the projection at ω on the tangent space $T_\omega \mathbb{S}_g^x$ of the unit sphere $\mathbb{S}_g^x$, and B_t is a standard Brownian motion in $\mathbb{R}^n$.

Proof. The main point is to remark that, in the local coordinates of T_xM the (linear) map σ from $\mathbb{S}_{n-1}$ (the unit sphere of $\mathbb{R}^n$, with the canonical metric) to $\mathbb{S}_g^x$ (with the metric g) which maps (ω^i) to $(\sum_j \sigma_{ij}\, \omega^j)$ an isometry between Riemannian manifolds.

The Brownian motion $\widetilde{W}_t$ on $\mathbb{S}_{n-1}$ satisfies the following differential equation (in the Stratonovich sense):

$$\mathrm{d}\widetilde{W}_t = (\mathrm{Id} - \widetilde{W}_t \otimes \widetilde{W}_t) \circ \mathrm{d}B_t,$$

with B_t a standard Brownian motion on $\mathbb{R}^n$. Hence we get that $W_t = \sigma\, \widetilde{W}_t$ is a Brownian motion on $\mathbb{S}_g^x$, which satisfies the equation

$$\mathrm{d}W_t = \sigma\, (\mathrm{Id} - \sigma^{-1} W_t \otimes \sigma^{-1} W_t) \circ \mathrm{d}B_t.$$

Since $\sigma^{-1} = g\sigma$, we easily get that $(\mathrm{Id} - \sigma^{-1} W_t \otimes \sigma^{-1} W_t)v = \pi_{x,W_t} \sigma v$ (we recall that $\pi_{x,\omega} v$ for a vector $v \in T_xM$ is given by $v - g_x(\omega, v)\omega$), which ends the proof. □

Thus, we can finally write the dynamics as a stochastic differential equations. We suppose that $\eta(t)$ is a given function $UM \to TM$ satisfying (2.4) in the local coordinates[1]. The particle $(x(t), \omega(t))$ driven by η and subject to random noise of intensity $\sqrt{2d}$ on its velocity satisfies:

$$\begin{cases} \mathrm{d}x^i = \omega^i\, \mathrm{d}t, \\ \mathrm{d}\omega^i = \eta^i\, \mathrm{d}t + \sqrt{2d} \sum_j (\sigma_{ij} - \omega^i \sum_{k,\ell} \omega^\ell\, g_{\ell k}\, \sigma_{kj}) \circ \mathrm{d}B_t^j - \sum_{j,k} \Gamma^i_{jk}\, \omega^j\, \omega^k\, \mathrm{d}t, \end{cases} \tag{2.5}$$

[1]More precisely, for all x in M, $\eta_x(t)$ is given as a vector field on $\mathbb{S}_g^x$, the unit sphere for the inner product g in the tangent space T_xM.

where B_t is a standard Brownian motion in $\mathbb{R}^n$ (or equivalently, B_t^i are n independent real one-dimensional Brownian motions). We give a result on the law of one particle satisfying this system.

Theorem 3.1. *Law of one particle*

There is local existence up to time T, and pathwise uniqueness for the system (2.5) with initial condition x_0, ω_0 in UM, if the geodesic ball of radius T centered at x_0 is included in $\mathcal{U}_M$.

Moreover, if we denote by $f_t : UM \to \mathbb{R}$ the law of the process (x_t, ω_t), that is to say the density probability function with respect to the natural measure of UM, defined in (2.7), we get that f_t satisfies the following Kolmogorov–Fokker–Planck equation:

$$\partial_t f_t + g_x(\omega, \nabla_x^h f_t) + \nabla_\omega^x \cdot (\eta(x,\omega) f_t) = d\Delta_\omega^x f_t, \tag{2.6}$$

where $\nabla_\omega^x \cdot$ and Δ_ω^x are the divergence and Laplace–Beltrami operators on the unit sphere $\mathbb{S}_g^x$ of T_xM, and ∇_x^h is the projection on T_xM of the horizontal component of the gradient of f (on UM).More precisely, if we denote Ξ the (horizontal) vector field in UM given by the geodesic flow at the point (x,ω), and g^s is the Sasaki metric on $T_{x,\omega}UM$, we have $g_x(\omega, \nabla_x^h f_t) = g^s(\Xi, \nabla_{x,\omega} f)$.

The proof of this theorem is given in Appendix A. We recall that the unit tangent bundle UM has a natural measure μ (called Liouville or kinematic measure) defined, for a continuous function $h : UM \to \mathbb{R}$ with compact support, by

$$\int_{UM} h \, \mathrm{d}\mu = \int_M \left(\int_{\mathbb{S}_g^x} h(x,\omega) \mathrm{d}^x\omega \right) \mathrm{d}m(x), \tag{2.7}$$

where m is the Riemannian volume measure on M, given in local coordinates by $\sqrt{\det g}\mathrm{d}x^1 \dots \mathrm{d}x^n$, and the measure $\mathrm{d}^x\omega$ on $\mathbb{S}_g^x$ is the unique probability measure which is invariant under rotations, this is the volume measure of $\mathbb{S}_g^x$ with respect to the metric g_x (in the local coordinates, we can use as in Lemma 3.1 the isometry between $\mathbb{S}_g^x$ and $\mathbb{S}_{n-1}$ given by the multiplication by σ). This measure μ is invariant under the geodesic flow.

Let us do two remarks here: first of all we get that the system (2.5) is independent of the chart, in the sense that the law of the particle $(x,\omega) \in UM$ is independent of the choice of the Brownian motion and the local chart. So if the manifold does not present a pathological behavior, for example if we can find $T > 0$ such that around any point there is a local chart including the ball of radius T (the manifold is then said to have a positive radius of injectivity, which is the case when the manifold is compact), then we can define step by step the global dynamics for the particle.

Secondly, this expression of the dynamics can be very convenient in some cases, for example when the manifold is flat, and the Christoffel symbols are simple. Moreover, it involves only $2n$ variables, and a Brownian motion of dimension n, for dynamics taking place in a manifold UM of dimension $2n-1$. But for other cases, such as the unit sphere for example, the computations can be hard, even if the manifold has a "simple" expression, as an embedding for example.

With these remarks in mind, one can try to define the dynamics in an extrinsic point of view, at the cost of working in a higher-dimensional ambient space. This will

define global dynamics in time, without the need to change the chart. Indeed, by the celebrated embedding theorem of Nash, we can always consider the manifold M as a submanifold of $\mathbb{R}^m$, equipped with the canonical induced metric. In this framework, the equation for a geodesic is given by

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \omega, \quad \frac{\mathrm{d}\omega}{\mathrm{d}t} = \mathrm{I\!I}_x(\omega, \omega),$$

where $\mathrm{I\!I}_x(\omega, \omega)$ is the second fundamental form associated to the embedded Riemannian manifold.

So we can get the stochastic differential equation (in the Stratonovich sense) for the dynamics of $(x, \omega) \in \mathbb{R}^{2m}$, corresponding to (2.5):

$$\begin{cases} \mathrm{d}x = \omega \, \mathrm{d}t, \\ \mathrm{d}\omega = \eta \, \mathrm{d}t + \sqrt{2d} \, \pi_{x,\omega} \circ \mathrm{d}B_t + \mathrm{I\!I}_x(\omega, \omega) \, \mathrm{d}t, \end{cases} \tag{2.8}$$

where B_t is a standard Brownian motion in $\mathbb{R}^{2m}$. Finally, at the cost of working in higher dimensions, we get a simple formulation of the dynamics. A lot of information on the Brownian motion is lost by the projection $\pi_{x,\omega}$ on the orthogonal of ω (a space of dimension $n-1$) in the tangent space $T_x(M)$. Although the original Brownian motion has $2m$ components, we only get a diffusion of dimension $n-1$. The equation (2.5) is well-defined even if $\eta_{x,\omega}(t)$ is not a vertical component, and has a meaning for any initial condition on $\mathbb{R}^{2m}$, not necessarily in UM. Using Itō's formula, it is possible to show, following for example what have been done in the proof of Proposition 3.1, that the solution of the stochastic differential equation lives almost surely on UM if the initial condition is in UM and if for any $(x, \omega) \in UM$, $\eta_{x,\omega}(t)$ is in the tangent space $T_x(M)$, and orthogonal to ω.

Now we have all the tools to define a model of interacting particles on a manifold.

2.2 System of interacting particles

We consider a system of N particles (x_k, ω_k) belonging to UM, and satisfying the equation (2.8) (or (2.5) equivalently), where the Brownian motions used to define the dynamics of the particles are independent, and where η will be a coupling term depending on all the particles.

To specify the interaction, we first have to define a local mean velocity $\bar{J}(x)$ of the particles at a given point $x \in M$. This velocity will be taken as the target orientation for the particle located at x. Let suppose that the particle (x_j, ω_j) has to be taken in account in this local velocity, we must evaluate the "contribution" of ω_j in the tangent space T_xM. So we want to transport ω_j from x_j to x. We use for that the geodesic joining x_j and x (see figure 3.3).

Definition 2.1. *Let K an observation kernel, $K : M \times M \to \mathbb{R}$. We suppose that for all y in the support of the function $K(x, \cdot)$, there exists a unique geodesic joining x and y. Then the average velocity around the particle x is defined as:*

$$\bar{J}(x) = \frac{1}{N} \sum_{j=1}^{N} K(x, x_j) \tau_x(\omega_j),$$

where $\tau_x(\omega_j)$ is the parallel transport of ω_j along the geodesic from x_j to x, with respect to the Levi-Civita connection of M.

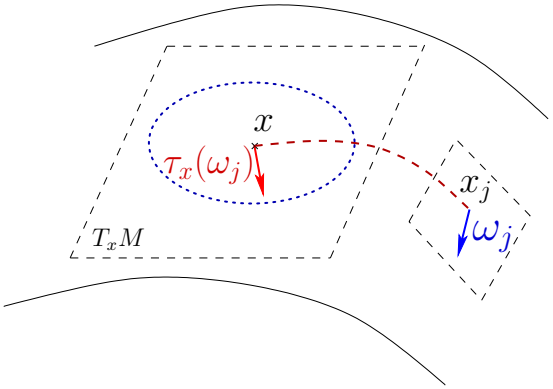

Figure 3.3: To compute the average velocity $\bar{J}$, each velocity ω_j is transported along a geodesic to x.

For example, to get the generalization of the model [28], we can consider a kernel K depending only on the geodesic distance between its two arguments. That is to say $K(x,y) = f(d(x,y))$, where d is the geodesic distance and f has compact support in $[0, r_0]$, with r_0 such that $d(x,y) \leqslant r_0$ implies that there is one unique geodesic joining x and y. When M is a compact Riemannian manifold, one can always find such a radius of injectivity $r_0 > 0$ (we also have relations between this radius and bounds on the curvature of the manifold, see [7] and Chapter 5 of [17] for some examples).

Remark 2.3. *We could also generalize this definition, in the spirit of Chapter 1, in order to model an angle of vision. That would imply to define a kernel $K : UM \times M \to \mathbb{R}$ depending also on an orientation ω at the point x:*

$$\bar{J}(x,\omega) = \frac{1}{N}\sum_{j=1}^{N} K(x,\omega,x_j)\tau_x(\omega_j),$$

where, for example, $K(x,\omega,y)$ depends only on the geodesic distance $d(x,y)$ and on $g_x(v_{x,y},\omega)$, where $v_{x,y} \in T_xM$ is the direction at x of the unique geodesic joining x and y.

We want the orientation to be relaxed to the unit vector with the same direction as $\bar{J}_k = \bar{J}(x_k)$, with rate $\nu(|\bar{J}_k|)$. We can take, as in the original time-continuous model [28], the case $\nu(r) = \frac{\nu_0}{r}$, or $\nu = 1$, as in the modification of Chapter 2. The idea is to see that the function $\omega \mapsto g_x(\omega, J)$ from $\mathbb{S}_g^x$ is maximal when ω is aligned in the same direction as J (by the equality case in the Cauchy-Schwarz inequality). The gradient (on $\mathbb{S}_g^x$) of this function at a point ω is given by $\pi_{x,\omega}J = J - g_x(\omega, J)\omega$ (this is exactly the projection on the orthogonal of ω for the inner product g_x, or equivalently $\pi_{x,\omega}$ is the orthogonal projection on $T_\omega\mathbb{S}_g^x$). So the dynamical system (in $\mathbb{S}_g^x$) $\frac{\mathrm{d}}{\mathrm{d}t}\omega = \alpha(J - g_x(\omega, J)\omega)$ is a relaxation towards the unit vector in the same

direction as J with rate $\alpha|J|$. So we choose the vertical component η in (2.3) to be equal to $\nu(|\bar{J}(x,\omega)|)\pi_{x,\omega}\bar{J}(x,\omega)$ (expressed in the local coordinates).

In summary, the dynamics of the particles are given by the following system of coupled stochastic differential equations (in $\mathbb{R}^{2mN}$), which have to be understood in the Stratonovich sense.

Definition 2.2. (Continuous Vicsek model on a manifold)
Let M be a complete manifold. The continuous Vicsek model for a system of N particles $(x_k,\omega_k)_{k\in[\![1,N]\!]}$ on the unit tangent bundle UM (2.1) is written as:

$$\begin{cases} \mathrm{d}x_k = \omega_k \mathrm{d}t \\ \mathrm{d}\omega_k = \nu(|\bar{J}_k|)\,\pi_{x_k,\omega_k}\bar{J}_k \mathrm{d}t + \sqrt{2d}\,\pi_{x_k,\omega_k}\circ \mathrm{d}B_t^k + \mathbb{I}_{x_k}(\omega_k,\omega_k)\mathrm{d}t, \end{cases} \tag{2.9}$$

$$\bar{J}_k = \bar{J}(x_k,\omega_k) = \frac{1}{N}\sum_{j=1}^{N} K(x_k,\omega_k,x_j)\tau_{x_k}(\omega_j), \tag{2.10}$$

where B_t^k are N independent Brownian motions in $\mathbb{R}^m$.

We illustrate the model (2.9),(2.10) in the figure 3.4.

Remark 2.4. *In the context of an embedded manifold, we can also propose another definition for the mean velocity $\bar{J}$, since we can now do a sum in the ambient space $\mathbb{R}^m$: we can replace $\Gamma_x(\omega_k)$ by ω_k, and consider any kernel $K:\mathbb{R}^m\times\mathbb{R}^m\to\mathbb{R}$, for example we can suppose that $K(x,y)$ depends only on the ambient metric distance. In this case, the vector $\bar{J}(x)$ may not stay on the tangent space T_xM, but this is not a problem since the vertical component $\eta=\nu(|\bar{J}(x,\omega)|)\pi_{x,\omega}\bar{J}(x,\omega)$ lies in $T_\omega\mathbb{S}_g^x$, if the orthogonal projection $\pi_{x,\omega}$ is extended from all the ambient tangent space of $\mathbb{R}^n$ to $T_\omega\mathbb{S}_g^x\subset T_xM$. The advantage of this system is that it is more convenient to perform numerical simulations, since we do not have to compute the parallel transport. The drawback is that this definition depends then on the embedding, and not only on the manifold M. However, one can expect that in a given scaling limit (when the radius of observation tends to 0 for example), we get that the two systems coincide, the two metrics being locally close, and the parallel transport being close to a translation in $\mathbb{R}^m$.*

When $M=\mathbb{R}^n$ and $m=n$, we get exactly the dynamics of [28] if $\nu(r)=\frac{\nu_0}{r}$ (or those of Chapter 1 when the kernel is non isotropic, but with no dependence on the local density), and the dynamics of Chapter 2 if $\nu=1$. When $M=\mathbb{T}^n$ is the flat torus (which is the framework of the original Vicsek model [74], and of all the numerical simulations based on it [16, 46, 60]) we get a formulation with $m=2n$, considering the identification $(\mathbb{S}_1)^n\subset\mathbb{R}^{2n}$. However, in that case, it is more convenient (and equivalent) to work in the local coordinates neighborhood system (2.5), since the metric is always the canonical metric of the local coordinates, and the Christoffel symbols vanish.

The next section is devoted to the derivation of a mean-field limit for this system of particles, as the number N tends to infinity.

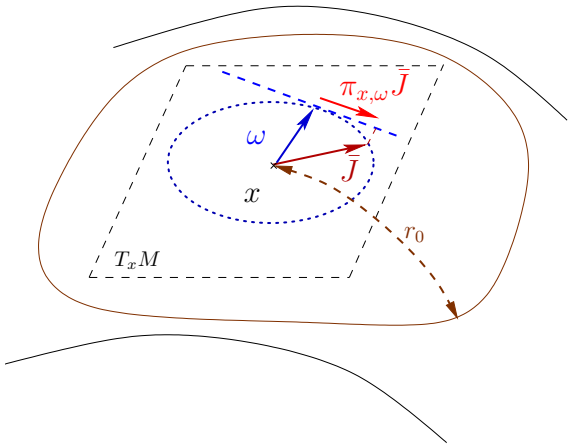

Figure 3.4: In the dynamics (2.9),(2.10), the particle tries to align with the local average velocity $\bar{J}$.

3 Propagation of chaos and mean-field limit

We define the empirical distribution f^N of the particles by

$$f^N(x,\omega) = \frac{1}{N}\sum_{k=1}^{N} \delta_{x_k,\omega_k}(x,\omega),$$

where the Dirac mass $\delta_{x,\omega}$ at the point (x,ω) is defined by duality against smooth functions $h : UM \to \mathbb{R}$ with compact support: $\int_{UM} \delta_{x,\omega} h \,\mathrm{d}\mu = h(x,\omega)$, where μ is the natural measure on UM, called Liouville or kinematic measure, defined in (2.7).

We can then reformulate $\bar{J}$ as a function of the empirical distribution $J[f^N]$, where

$$J[f](x,\omega) = \int_{UM} K(x,\omega,x')\tau_x(\omega') f(x',\omega')\,\mathrm{d}\mu(x',\omega'),$$

and we write $H[f] = \nu(|J[f]|)J[f]$.

The equation of the dynamics, in the framework where M is embedded isometrically in $\mathbb{R}^m$, is then given by the stochastic differential system:

$$\begin{cases} \mathrm{d}x_k = \omega_k\,\mathrm{d}t \\ \mathrm{d}\omega_k = \pi_{x_k,\omega_k} H[f^N](x_k,\omega_k)\,\mathrm{d}t + \sqrt{2d}\,\pi_{x_k,\omega_k} \circ \mathrm{d}B_t^k + \mathbb{I}_{x_k}(\omega_k,\omega_k)\,\mathrm{d}t, \end{cases} \tag{3.11}$$

The adaptation of what have been done in [13] for the model of Chapter 2 (which is itself an adaptation of the classical coupling argument of [73] in the case where the velocity belongs to the unit sphere) is then straightforward, in the special case where $\nu = 1$.

We introduce the artificial coupling processes $(\bar{x}_k, \bar{\omega}_k)$, solutions of a nonlinear stochastic differential equation, which are built in order to behave like the processes $(\bar{x}_k, \bar{\omega}_k)$ as $N \to \infty$:

$$\begin{cases} \mathrm{d}\bar{x}_k = \bar{\omega}_k \mathrm{d}t \\ \mathrm{d}\bar{\omega}_k = \pi_{\bar{x}_k,\bar{\omega}_k} H[\bar{f}_t](\bar{x}_k,\bar{\omega}_k)\mathrm{d}t + \sqrt{2d}\,\pi_{\bar{x}_k,\bar{\omega}_k} \circ \mathrm{d}B_t^k + \mathbb{I}_{\bar{x}_k}(\bar{\omega}_k,\bar{\omega}_k)\mathrm{d}t \\ \bar{f}_t = \mathrm{law}(\bar{x}_k,\bar{\omega}_k). \end{cases} \tag{3.12}$$

We remark the essential additional nonlinearity, through the condition that the law $\bar{f}_t$ at any time t must be the law of the process (x_k, ω_k). Actually we can see that there is no coupling here between the particles, so we can drop the subscript k and we get a nonlinear stochastic differential equation for a process with values in UM, of dimension $2n-1$ contrary to the system (3.11), which is a process living in $(UM)^N$, of dimension $N(2n-1)$.

Let us express what partial differential equation the law of such a process would satisfy, in view of Proposition 3.1:

$$\partial_t f_t + g_x(\omega, \nabla_x^h f_t) + \nabla_\omega^x \cdot (\pi_{x,\omega} H[f_t] f_t) = d\Delta_\omega^x f_t. \tag{3.13}$$

This non-linear (and non-local) Kolmogorov–Fokker–Planck equation is our mean-field model.

We have the following results, in the case where $\nu = 1$.

Theorem 3.2. *Existence and uniqueness for the stochastic and mean-field models.*

Let f_0 be a probability measure on UM such that it has a finite second moment in $x \in \mathbb{R}^m$ (when viewed, with the embedding of M, as a measure on $\mathbb{R}^m$). Let (x_k^0, ω_k^0) be N independent random variables in UM, with law f_0. Suppose moreover that the function K is bounded and sufficiently smooth, with the function τ_x sufficiently smooth on the support of $K(x, \omega, \cdot)$. Then

- *We have global existence and pathwise uniqueness for the particle system* (3.11) *with initial conditions $(x_k^0, \omega_k^0)_{k \in [\![1,N]\!]}$, which takes values in $(UM)^N$.*
- *For a given $k \in [\![1, N]\!]$, we have global existence and pathwise uniqueness for the artificial process* (3.12) *with initial condition (x_k^0, ω_k^0), which takes values in UM.*
- *There exists a unique weak solution to the nonlinear mean-field model* (3.13) *(which is global), with initial condition f_0. Moreover, it is the law of each of the processes $(\bar{x}_k, \bar{\omega}_k)$, solutions to* (3.12) *with initial condition (x_k^0, ω_k^0).*

The proof follows exactly [13], and will be omitted here. Let us remark that to deal with the case of a non-constant ν, we would need to have estimates on the regularity of $f \mapsto H[f]$ with respect to an appropriate Wasserstein distance. This point is the object of ongoing work. In the case where we do not have enough regularity, some recent results [53, 86] show that it is sometimes possible to give a sense to such a system of stochastic differential equations.

Once we have this results, the idea is then to take two solutions of (3.11)-(3.12), starting from the same initial conditions and driven by the same family of Brownian motions, and estimate the difference of behavior between them.

Theorem 3.3. *Estimates on the stochastic processes.*

Under the conditions of Theorem 3.2, we denote by (x_k^t, ω_k^t), and $(\bar{x}_k^t, \bar{\omega}_k^t)$ the solutions of (3.11) *and* (3.12) *with the same initial conditions and driven by the same Brownian motions. Then for all $T > 0$, there exists a constant $C > 0$, such that for all $t \in [0, T]$, for all $N \geqslant 1$ and $k \in [\![1, N]\!]$, we have*

$$\mathbb{E}[|x_k^t - \bar{x}_k^t|^2 + |\omega_k^t - \bar{\omega}_k^t|] \leqslant \frac{C}{N}.$$

Once again, the proof is omitted and proceeds as in [13], we get then that these estimates allows to show (see [73, 14], fore more details on this topic) that:

- Any of the processes (x_k^t, ω_k^t) converge in law, when k is fixed and $N \to \infty$, to f_t, satisfying (3.13).
- The system (3.11) has the propagation of chaos property : the law of k particles converges to the law of k independent particles of same law f_t (when $k = o(N)$ as $N \to \infty$).
- The empirical distribution f^N converges towards f_t at time t, when $N \to \infty$.

The study of a hydrodynamic limit of this mean-field model, in the spirit of [28] and Chapters 1-2 is left to future work. The first thing to do would be to define a proper scaling, since here the manifold is not invariant under dilatation (as it was the case for $\mathbb{R}^n$). Another approach (see Remark 3.1 of Chapter 2) would consist in doing the scaling at the microscopic individual level, the radius of the kernel of observation being dependent on N (this is called "moderate interaction"). This allows to have, when the number of particles tends to infinity, a limit which satisfies a localized version of (3.13). We refer to [64] for an introduction to this approach.

In the following section, we provide simulations of the stochastic process 3.11, in the case where M is the 2-dimensional sphere.

4 Simulations in the case of the sphere $\mathbb{S}_2$

We consider the special case of the 2-dimensional unit sphere $\mathbb{S}_2$, embedded in $\mathbb{R}^3$, so we have $n = 2$ and $m = 3$. The unit tangent bundle $U\mathbb{S}_2$ is composed of the elements $(x, \omega) \in \mathbb{S}_2 \times \mathbb{S}_2$ such that $x \cdot \omega = 0$ (we refer to [51] for a detailed study of this unit tangent bundle, isomorphic to $SO(3)$). In that case the geodesics are the great circles. The equation of such a geodesic is given by:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \omega, \quad \frac{\mathrm{d}\omega}{\mathrm{d}t} = -x,$$

so the second fundamental form is given by $\mathrm{I\!I}_x(\omega, \omega) = -x$. The projection Π_x on the tangent plane at the point x is the projection on the orthogonal of x, and on this plane the projection on the tangent line at the point ω is also the projection on the orthogonal of ω, so finally the projection $\pi_{x,\omega}$ is the orthogonal projection along the vector $x \times \omega$, that we will denote $\Pi_{x\times\omega}$. The system of particles (3.11) reads

$$\mathrm{d}x_k = \omega_k \, \mathrm{d}t \tag{4.14}$$

$$\mathrm{d}\omega_k = \Pi_{x\times\omega} \bar{H}_k \, \mathrm{d}t + \pi_{x\times\omega} \circ \mathrm{d}B_t^k - x \, \mathrm{d}t. \tag{4.15}$$

We adopt a finite-difference approach to compute numerical simulations of this system, with a given time interval $\Delta t > 0$.

The first thing to remark is that it is easy to simulate the Brownian motion on the circle. Indeed, if B_t is a Brownian motion of the line, then e^{iB_t} is a Brownian motion on the unit circle, seen as a subset of $\mathbb{C}$. Hence if θ is a random variable with normal

distribution, then the Brownian motion on the line has the same law at time Δt than $\theta\sqrt{\Delta t}$. and then the Brownian motion on the unit circle starting at $1 \in \mathbb{C}$ has the same law as $e^{i\theta\sqrt{\Delta t}}$. Then, we will see that all the elementary movements of the particles can be done with small rotations. If v is a vector belonging to $\mathbb{S}_2$ and $\alpha \in \mathbb{R}$, we denote by $R[v, \alpha]$ the rotation of angle α around the axis v, with the orientation given by the direction of v.

We first explain how we compute the mean velocity $\bar{J}_k$. First of all, we have that the parallel transport along the geodesic (that is to say a great circle) from y to x is given (whenever x and y are different and not antipodal) by the rotation of axis aligned with the vector $y \times x$ and of angle $\alpha \in (0, \pi)$, where $\cos\alpha = x \cdot y$, the orientation being given by the orientation of $y \times x$. So we get

$$\tau_x(\omega_k) = R[\tfrac{x_k \times x}{|x_k \times x|}, \arccos(x \cdot x_k)]\, \omega_k.$$

We will not use an angle of vision here, as in (2.10), so we chose that the function $K(x, y)$ depends only on the geodesic distance between x and y, which is given by $\arccos(x \cdot y)$. We finally get, writing $r_{ik} = \arccos(x_i \cdot x_k)$,

$$\bar{J}_k = \frac{1}{N} \sum_i \kappa(r_{ik}) R[\tfrac{x_i \times x_k}{|x_i \times x_k|}, r_{ik}]\, \omega_i.$$

In the simulations, we have taken $\kappa(r) = \mathbb{1}_{\{r \leqslant r_0\}}$, with $r_0 = .2$. That is to say that the sum is only computed for particles in the geodesic ball of radius r_0. When r_0 is small, all the rotation are close to the identity, and we can take an approximation of $\bar{J}_k$ by

$$\widetilde{J}_k = \frac{1}{N} \sum_{\substack{i \text{ such that} \\ x_i \cdot x_k \geqslant \cos(r_0)}} \omega_i,$$

and then taking as a definition $\bar{J}_k = (\mathrm{Id} - x_k \otimes x_k)\widetilde{J}_k$, the projection ensuring that $\bar{J}_k$ belongs to the tangent plane at the point x_k.

Finally we compute $\bar{H}_k = \nu(|\bar{J}_k|)\bar{J}_k$. In the present case, we have taken, as in [28], $\nu(r) = \frac{\nu_0}{r}$, with $\nu_0 = 2$.

We now turn to the simulation of the dynamics. Since the interaction on the orientation is done in the plane orthogonal to x_k, this is a rotation around x_k, so we update ω_k first since we have $\bar{J}_k$ in this plane. The contribution of the Brownian motion corresponds to a rotation of angle $\theta\sqrt{2d\Delta t}$, where θ is a random variable with normal distribution, and the angular speed of the local rotation corresponding to the relaxation is given by $(x_k \times \omega_k) \cdot \bar{H}_k$. For the update of the position, the transport of x along the great circle directed by ω with velocity 1 can be viewed as a rotation around the vector $x \times \omega$, with angular speed 1.

We denote by x_k^n, ω_k^n the positions and orientations of the particles at time $n\Delta t$. Our discrete simulation is then given by:

$$\begin{cases} \omega_k^{n+1} = R[x_k^n, (x_k^n \times \omega_k^n) \cdot \bar{H}_k^n \Delta t + \theta_{n,k}\sqrt{2d\Delta t}]\, \omega_k^n \\ x_k^{n+1} = R[x_k^n \times \omega_k^{n+1}, \Delta t]\, x_k^n, \end{cases}$$

where $\theta_{n,\kappa}$ are independent random variables with normal distribution. The following figures depict the numerical simulation for $d = .1$ and $\Delta t = .01$.

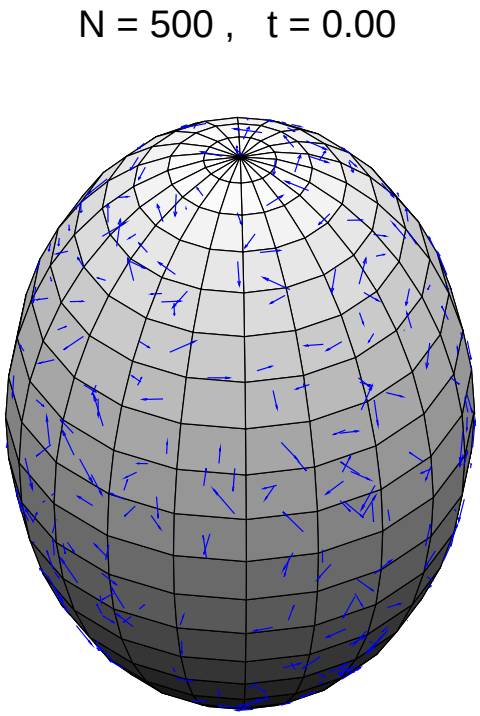

Figure 3.5: Initial position and orientation of particles.

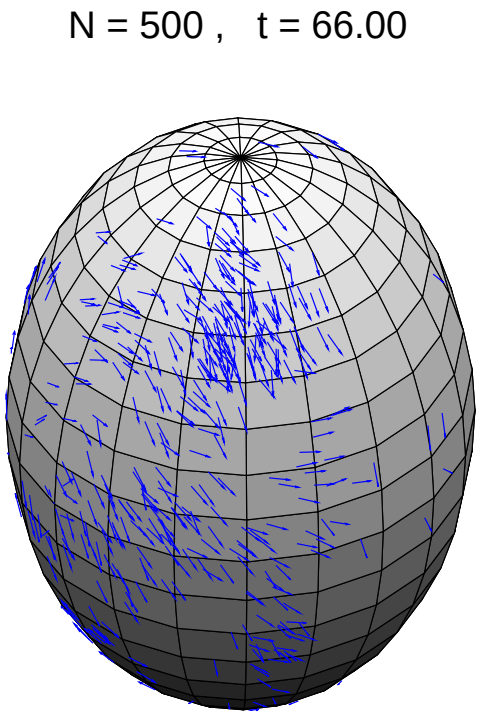

Figure 3.6: Position and orientation of particles at time $t = 66$.

A Law of one particle

This appendix is devoted to the proof of Theorem 3.1, which gives the consistence of the one particle model (2.5) and the evolution of its law. We recall the theorem here:

Theorem 3.1. *Law of one particle*

There is local existence up to time T, and pathwise uniqueness for the system (2.5) *with initial condition x_0, ω_0 in UM, if the geodesic ball of radius T centered at x_0 is included in $\mathcal{U}_M$.*

Moreover, if we denote by $f_t : UM \to \mathbb{R}$ the law of the process (x_t, ω_t), that is to say the density probability function with respect to the natural measure of UM, defined in (2.7)*, we get that f_t satisfies the following Kolmogorov–Fokker–Planck equation:*

$$\partial_t f_t + g_x(\omega, \nabla^h_x f_t) + \nabla^x_\omega \cdot (\eta(x,\omega) f_t) = d\Delta^x_\omega f_t, \tag{A.16}$$

where $\nabla^x_\omega \cdot$ and Δ^x_ω are the divergence and Laplace–Beltrami operators on the unit sphere $\mathbb{S}^x_g$ of T_xM, and ∇^h_x is the projection on T_xM of the horizontal component of the gradient of f (on UM).More precisely, if we denote Ξ the (horizontal) vector field in UM given by the geodesic flow at the point (x,ω), and g^s is the Sasaki metric on $T_{x,\omega}UM$, we have $g_x(\omega, \nabla^h_x f_t) = g^s(\Xi, \nabla_{x,\omega} f)$.

Proof. We first consider the more general system

$$\begin{cases} \mathrm{d}x^i = v^i \,\mathrm{d}t, \\ \mathrm{d}v^i = \widetilde{\eta}^i(x,\widetilde{\omega})\,\mathrm{d}t + \sqrt{2d}\,\widetilde{\pi}_{x,\widetilde{\omega}}\,\sigma \circ \mathrm{d}B_t - \sum_{j,k} \Gamma^i_{jk}\, v^j\, v^k \,\mathrm{d}t, \end{cases} \tag{A.17}$$

without the normalization condition (2.2) on v. The function $\widetilde{\omega}$ is chosen to be, for each x, a smooth function of $v \in T_xM$ such that, for $\frac{1}{2} \leqslant |v|_g \leqslant 2$, we have $\widetilde{\omega} = \frac{v}{|v|_g}$. We then take the function $\widetilde{\eta}$ as a sufficiently smooth extension of η given in TM and not only on UM, and we define $\widetilde{\pi}_{x,\widetilde{\omega}} u = u - g_x(\widetilde{\omega}, u)\widetilde{\omega}$.

We have local existence and pathwise uniqueness for this equation, and using Itō formula for a Stratonovich formulation, (see for example [48], Proposition 1.1.16), we get, for a function $f \in C^2(\mathcal{U} \times \mathbb{R}^n)$ and up to explosion time

$$\begin{aligned} \mathrm{d}h(x_t, v_t) = \sum_i [v^i \partial_{x^i} h + (\widetilde{\eta}^i - \sum_{j,k} \Gamma^i_{jk}\, v^j\, v^k) \partial_{v^i} h] dt \\ + \sqrt{2d} \sum_{i,j} (\sigma_{ij} - \widetilde{\omega}^i \sum_{k,\ell} \widetilde{\omega}^\ell\, g_{\ell k}\, \sigma_{kj}) \partial_{v^i} h \circ \mathrm{d}B^j_t. \end{aligned}$$

Let us take $h = \sum_{j,k} g_{jk}(x)\, v^j\, v^k = |v|^2_g$, therefore we have $\partial_{x^i} h = \sum_{j,k} \partial_{x^i} g_{jk}\, v^j\, v^k$ and $\partial_{v^i} h = 2 \sum_\ell g_{i\ell}\, v^\ell$. Hence, using the definition of the Christoffel symbols:

$$\Gamma^i_{jk} = \frac{1}{2} \sum_m g^{im} (\partial_{x^j} g_{km} + \partial_{x^k} g_{jm} - \partial_{x^m} g_{jk}),$$

where (g^{ij}) is the inverse matrix of (g_{ij}) (which is symmetric), we get that

$$\begin{aligned}\sum_{i,j,k} \Gamma^i_{jk}\, v^j\, v^k \partial_{v^i} h &= \sum_{i,j,k,\ell,m} g_{i\ell} g^{im} (\partial_{x^j} g_{km} + \partial_{x^k} g_{jm} - \partial_{x^m} g_{jk})\, v^j\, v^k\, v^\ell \\ &= \sum_{j,k,m} (\partial_{x^j} g_{km} + \partial_{x^k} g_{jm} - \partial_{x^m} g_{jk})\, v^j\, v^k\, v^m \\ &= \sum_{i,j,k} \partial_{x^i} g_{jk}\, v^j\, v^k\, v^m = \sum_i v^i \partial_{x^i} h,\end{aligned}$$

which is nothing else than the fact that the geodesic flow preserves the metric. Whenever $\frac{1}{2} \leqslant |v|_g \leqslant 2$, we have on one hand

$$\sum_i \widetilde{\eta}^i(x, \widetilde{\omega}) \partial_{v^i} h = \sum_{i,\ell} \eta^i(x, \tfrac{1}{|v|_g} v) g_{i\ell}\, v^\ell = 0,$$

in virtue of (2.4), and on the other hand

$$\begin{aligned}\sum_i \widetilde{\omega}^i \sum_{k,\ell} \widetilde{\omega}^\ell\, g_{\ell k}\, \sigma_{kj} \partial_{v^i} h &= 2 \frac{1}{|v|_g^2} \sum_{i,k,\ell,m} g_{\ell k}\, \sigma_{kj} g_{im}\, v^i\, v^m\, v^k\, v^\ell \\ &= 2 \sum_{k,\ell} g_{\ell k}\, \sigma_{kj}\, v^k\, v^\ell = \sum_i \sigma_{ij} \partial_{v^i} h.\end{aligned}$$

So we get $\mathrm{d}h(x_t, v_t) = 0$, that is to say $|v|_g^2$ is a constant. So we have that if the initial condition is such that $|v_0|_g = 1$, then, up to explosion time, we have $|v|_g = 1$, and then this is a solution of (2.5). The pathwise uniqueness is then obvious, since a solution of (2.5) is also solution of (A.17). Since $\mathrm{d}x^i = v^i\, \mathrm{d}t$, the explosion time is greater than T if the geodesic ball of radius T and centered at x_0 is included in the local chart.

For the second part of the proposition, we use the correspondence with Itō formula, see for example [44], section 4.3.6. The Fokker–Planck equation for the law $\widetilde{f}$ of a system satisfying (A.17) is given by

$$\partial_t \widetilde{f} + \sum_i \partial_{x^i}(v^i \widetilde{f}) + \partial_{v^i}((\widetilde{\eta}^i(x, \widetilde{\omega}) - \sum_{j,k} \Gamma^i_{jk}\, v^j\, v^k) \widetilde{f}) = d \sum_{i,j,k} \partial_{v^i}[b_{ik} \partial_{v^j}(b_{jk} \widetilde{f})],$$

where $b_{ij} = \sigma_{ij} - \widetilde{\omega}^i \sum_{k,\ell} \widetilde{\omega}^\ell\, g_{\ell k}\, \sigma_{kj}$.

Actually, this equation must be understood in the weak sense for $\widetilde{f}$ as a measure on $\mathcal{U} \times \mathbb{R}^n$, that is to say that for any function $\widetilde{h} : \mathcal{U} \times \mathbb{R}^n \to \mathbb{R}$, smooth with compact support, we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} \int_{U \times \mathbb{R}^n} \widetilde{h}\, \mathrm{d}\widetilde{f} = \int_{U \times \mathbb{R}^n} \sum_i \left(v^i \partial_{x^i} \widetilde{h} + (\widetilde{\eta}^i(x, \widetilde{\omega}) - \sum_{j,k} \Gamma^i_{jk}\, v^j\, v^k) \partial_{v^i} \widetilde{h} \right) \mathrm{d}\widetilde{f} \\ + \int_{U \times \mathbb{R}^n} d \sum_{i,j,k} b_{jk} \partial_{v^j}(b_{ik} \partial_{v^i} \widetilde{h})\, \mathrm{d}\widetilde{f}.\end{aligned} \tag{A.18}$$

Now the previous point shows that if the initial condition is a random variable taking values on UM, then the measure $\widetilde{f}$ is supported on UM. We denote by f its density probability function with respect to the natural measure of UM,

so for any function h such that $h(x,\omega) = \widetilde{h}(x,\omega)$ for all ω such that $|\omega|_g = 1$, we have $\int_{U\times\mathbb{R}^n} \widetilde{h}\,\mathrm{d}\widetilde{f} = \int_{UM} h\,f\,\mathrm{d}\mu = \int_M (\int_{\mathbb{S}_g^x} h(x,\omega) f(x,\omega)\mathrm{d}^x\omega)\mathrm{d}m(x)$.

If we take a smooth function $h : UM \to \mathbb{R}$, we define $\widetilde{h}(x,v)$ to be $h(x,\widetilde{\omega})$. By definition since η is orthogonal to ω (with respect to the metric $g(x)$), then it can be viewed as a vector field on $\mathbb{S}_g^x$, written $\sum_i \eta^i \partial_{v^i}$ in local coordinates, and then $g_x(\nabla_\omega h, \eta)$ is written $\sum_i \eta^i \partial_{v^i} h$. So we get, by Stokes' theorem, that

$$\begin{aligned}\int_{U\times\mathbb{R}^n} \textstyle\sum_i \widetilde{\eta}^i(x,\widetilde{\omega})\,\partial_{v^i}\widetilde{h}\,\mathrm{d}\widetilde{f} &= \int_M (\int_{\mathbb{S}_g^x} g_x(\nabla_\omega h, \eta) f(x,\omega)\mathrm{d}^x\omega)\mathrm{d}m(x)\\ &= \int_M (\int_{\mathbb{S}_g^x} g_x(\nabla_\omega h, \eta f)\mathrm{d}^x\omega)\mathrm{d}m(x)\\ &= -\int_M (\int_{\mathbb{S}_g^x} h\nabla_\omega\cdot(\eta f)\,\mathrm{d}^x\omega)\mathrm{d}m(x) = -\int_{UM} h\,\nabla_\omega\cdot(\eta f)\,\mathrm{d}\mu.\end{aligned}$$

Similarly, the horizontal vector field Ξ (the geodesic flow) is given, in local coordinates, by $\sum_i \omega^i \partial_{x_i} - \sum_{j,k} \Gamma^i_{jk}\, v^j\, v^k \partial_{v^i}$, hence we have (with g^s the Sasaki metric):

$$\begin{aligned}\int_{U\times\mathbb{R}^n} (\textstyle\sum_i \omega^i \partial_{x_i}\widetilde{h} - \sum_{j,k} \Gamma^i_{jk}\, v^j\, v^k \partial_{v^i}\widetilde{h})\,\mathrm{d}\widetilde{f} &= \int_{UM} g^s(\nabla_{UM} h, \Xi f)\,\mathrm{d}\mu\\ &= -\int_{UM} h\nabla_{UM}\cdot(\Xi f)\,\mathrm{d}\mu\\ &= -\int_{UM} h\,f\,\nabla_{UM}\cdot\Xi\,\mathrm{d}\mu - \int_{UM} h\,g^s(\nabla_{UM} f, \Xi)\,\mathrm{d}\mu\\ &= -\int_{UM} h\,g_x(\nabla^h_x f, \omega)\,\mathrm{d}\mu\end{aligned}$$

by the definition of the Sasaki metric on horizontal vector fields, where $\nabla^h_x f$ is the projection on T_xM of the horizontal part of $\nabla_{UM} f$. In the last line of the previous computation, we have used the fact that the geodesic flow is incompressible, hence $\nabla_{UM}\cdot\Xi = 0$ (see [69] for more details).

It remains to show that $\sum_{i,j,k} b_{jk}\partial_{v^j}(b_{ik}\partial_{v^i}\varphi) = \Delta^g_\omega\varphi$ on $\mathbb{S}_g^x$ for a function $\varphi(\widetilde{\omega})$, in order to get, by a double integration by parts,

$$\int_{U\times\mathbb{R}^n} \sum_{i,j,k} b_{jk}\partial_{v^j}(b_{ik}\partial_{v^i}\widetilde{h})\,\mathrm{d}\widetilde{f} = \int_{UM} h\,\Delta^g_\omega f\,\mathrm{d}\mu.$$

The above claim is very similar to Theorem 3.1.4 of [48]. We will use the isometry defined in the proof of Lemma (3.1). We work in the tangent space T_xM identified to $\mathbb{R}^n$ with local coordinates (v^i). For φ a function of $\widetilde{\omega}$ (being itself a function of v), with $\widetilde{\omega} = \frac{v}{|v|_g}$ for $\frac{1}{2} \leqslant |v|_g \leqslant 2$, we write $\bar{\varphi}$ the function such that $\varphi(v) = \bar{\varphi}(\bar{v})$, with $\sigma\bar{v} = v$, and $\sigma\bar{\omega} = \widetilde{\omega}$, where σ is the positive symmetric square root of g. We write $\langle\cdot,\cdot\rangle$ for the canonical inner product, $\langle\cdot,\cdot\rangle_g$ for the inner product induced by g. We have $\langle u, v\rangle = \langle\sigma u, \sigma v\rangle_g$ so the linear map $\omega \mapsto \sigma\omega$ is an isometry from the manifold $\mathbb{S}_{n-1}$ to $\mathbb{S}_g$. Therefore we have $\Delta^g_\omega\varphi(\widetilde{\omega}) = (\Delta_{\bar{\omega}}\bar{\varphi})(\bar{\omega}))$. If we denote by $\beta_{ij} = (Id - \bar{\omega}\otimes\bar{\omega})_{ij} = \delta_{ij} - \bar{\omega}^i\bar{\omega}^j$, and we define $\bar{P}_k = \sum_i \beta_{ik}\partial_{v^i}$ (this is the orthogonal projection of the vector e_k on the standard unit sphere at the point ω, seen as a vector field on the unit sphere), we have that $\Delta_{\bar{\omega}} = \sum_k \bar{P}_k^2$ by Theorem 3.1.4 of [48]. So since

$$(\bar{P}_k\bar{\varphi})(\bar{\omega}) = \sum_i \beta_{ik}\partial_{v^i}(\varphi(\sigma\bar{\omega})) = \sum_{i,j} \beta_{ik}\sigma_{ij}(\partial_{v^j}\varphi)(\widetilde{\omega}) = (P_k\varphi)(\widetilde{\omega}),$$

which gives then that $\Delta_\omega^g = \sum_k P_k^2$, with

$$\begin{aligned} P_k &= \sum_{i,j} \beta_{ik}\sigma_{ij}\partial_{v^j} = \sigma_{kj}\partial_{v^j} - \sum_{i,j} \bar{\omega}^i\bar{\omega}^k\sigma_{ij} \\ &= \sigma_{kj}\partial_{v^j} - \sum_{i,j,\ell,m} \widetilde{\omega}^\ell\sigma^{i\ell}\widetilde{\omega}^m\sigma^{km}\sigma_{ij}\partial_{v^j} = \sigma_{kj}\partial_{v^j} - \sum_{j,m} \widetilde{\omega}^j\widetilde{\omega}^m\sigma^{km}\partial_{v^j} \end{aligned}$$

where (σ^{ij}) is the inverse matrix of σ. We get $\sigma^{km} = \sum_\ell g_{k\ell}\sigma_{\ell m}$, and the terms b_{jk} appear. We have $P_k = \sum_i b_{jk}\partial_{v^j}$, and this gives the claim.

So we finally have, using (A.18):

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{UM} h\, f + \int_{UM} h\,[\nabla_\omega \cdot (\eta f) + g_x(\nabla_x^h f, \omega) - d\,\Delta_\omega^g f]\,\mathrm{d}\mu = 0,$$

which gives that the law f is a weak solution of the partial differential equation (A.16), and this ends the proof. □

Part II

Dynamics of convergence in Doi equation

Chapter 4

Dynamics in a kinetic model of oriented particles with phase transition

This chapter has been done in collaboration with Jian-Guo Liu, when visiting him in Duke University, and later on at the Mathematical Sciences Center of Tsinghua University, Beijing. It has given an article [42] submitted in SIAM Journal on Mathematical Analysis.

Abstract

Motivated by a phenomenon of phase transition in a model of alignment of self-propelled particles, we obtain a kinetic mean-field equation which is nothing else than the Doi equation (also called Smoluchowski equation) with dipolar potential.

In a self-contained presentation, using only basic tools, we analyze the dynamics of this equation in any dimension. We first prove global well-posedness of this equation, starting with an initial condition in any Sobolev space. We then compute all possible steady-states. There is a threshold for the noise parameter: over this threshold, the only equilibrium is the uniform distribution, and under this threshold, there is also a family of non-isotropic equilibria.

We give a rigorous prove of convergence of the solution to a steady-state as time goes to infinity. In particular we show that in the supercritical case, the only initial conditions leading to the uniform distribution in large time are those with vanishing momentum. For any positive value of the noise parameter, and any initial condition, we give rates of convergence towards equilibrium, exponentially for both supercritical and subcritical cases and algebraically for the critical case.

Key words: Doi–Onsager equation, Smoluchowski equation, nonlinear Fokker–Planck equation, dipolar potential, phase transition, LaSalle invariance principle, convergence to steady-states.

AMS subject classification: 35K55, 35Q84, 35R01, 82B26, 82C26.

1 Introduction

Phase transition and large time behavior of large interacting oriented/rod-like particle systems and their mean field limits have shown to be interesting in many physical and biological complex systems. Examples are: paramagnetism to ferromagnetism phase transition near Curie temperature, nematic phase transition in liquid crystal or rod-shaped polymers, emerging of flocking dynamics near critical mass of self-propelled particles, etc.

The dynamics on orientation for self-propelled particles proposed by Vicsek *et al* [74] to describe, for instance, fish schooling or bird flocking, present such a behavior in numerical simulations. As the density increases (or as the noise decreases) and reaches a threshold one can observe strong correlations between the orientations of particles. The model is discrete in time and particles move at constant speed following their orientation. At each time step, the orientation of each particle is updated, replaced by the mean orientation of its neighbors, plus a noise term.

A way to provide a time-continuous version of this dynamical system, which allows to take a mean-field limit (and even a macroscopic limit), has been proposed by Degond and Motsch [28]. Instead of replacing the orientation at the next time step, they introduce a parameter playing the role of a rate of relaxation towards this mean orientation. Unfortunately the mean-field limit of this model does not present phase transition. In Chapter 1, we proved the robustness of the behavior of this model when this rate of relaxation depends on a local density. In particular, phase transition is still absent. However, when this parameter is set to be proportional to the local momentum of the neighboring particles, we will see that the model present a phenomenon of phase transition. This phenomenon occurs on the orientation dynamics, so we will only consider here the spatial homogeneous dynamics. The study of this model when we take in account the space variable is the object of Chapter 2, in collaboration with J.-G. Liu and P. Degond.

The particular model is described as follows: we have N oriented particles, described by vectors $\omega_1, \dots, \omega_N$ belonging to $\mathbb{S}$, the unit sphere of $\mathbb{R}^n$, and satisfying the following system of coupled stochastic differential equations (which must be understood in the Stratonovich sense), for $k \in [\![1, N]\!]$:

$$\mathrm{d}\omega_k = (\mathrm{Id} - \omega_k \otimes \omega_k) J_k \,\mathrm{d}t + \sqrt{2\tau}\,(\mathrm{Id} - \omega_k \otimes \omega_k) \circ \mathrm{d}B_t^k, \tag{1.1}$$

$$J_k = \frac{1}{N} \sum_{j=1}^{N} \omega_j. \tag{1.2}$$

The term $(\mathrm{Id} - \omega_k \otimes \omega_k)$ denotes the projection on the hyperplane orthogonal to ω_k, and constrains the norm of ω_k to be constant. The terms B_t^k stand for N independent standard Brownian motions on $\mathbb{R}^n$, and then the stochastic term $(\mathrm{Id} - \omega_k \otimes \omega_k) \circ \mathrm{d}B_t^k$ represents the contribution of a Brownian motion on the sphere $\mathbb{S}$ to the model. For more details on how to define Brownian motion on a Riemannian manifold, see [48].

Without this stochastic term, equation (1.1) can be written

$$\dot{\omega_k} = \nabla_\omega (\omega \cdot J_k)|_{\omega = \omega_k},$$

where ∇_ω is the tangential gradient on the sphere (see the beginning of Section 2.1 for some useful formulas on the unit sphere). So the model can be understood as

a relaxation towards a unit vector in the direction of J_k, subjected to a Brownian motion on the sphere with intensity $\sqrt{2\tau}$. The only difference with the model proposed in [28] (in the spatial homogeneous case) is that J_k is there replaced by $\nu\Omega_k$, where Ω_k is the unit vector in the direction of J_k and the frequency of relaxation ν is constant (or dependent on the local density in Chapter 1). One point to emphasize is that, in that model, the interaction cannot be seen as a sum of binary interactions, contrary to the model presented here. Here the mean momentum J_k does not depend on the index k (but this is not true in the inhomogeneous case, where the mean is taken among the neighboring particles).

To simplify notations, we work with the uniform measure of total mass 1 on the sphere $\mathbb{S}$. We denote by $f^N : \mathbb{R}_+ \times \mathbb{S} \to \mathbb{R}_+$ the probability density function (depending on time) associated to the position of one particle. Then, as the number N of particles tends to infinity, f^N tends to a probability density function f satisfying

$$\partial_t f = Q(f), \tag{1.3}$$

with

$$Q(f) = -\nabla_\omega \cdot ((\mathrm{Id} - \omega \otimes \omega) J[f] f) + \tau \Delta_\omega f, \tag{1.4}$$

$$J[f] = \int_{\mathbb{S}} \omega\, f(.,\omega)\, \mathrm{d}\omega. \tag{1.5}$$

In the model of [28], $J[f]$ is just replaced in (1.4) by $\nu\, \Omega[f]$, where $\Omega[f]$ is the unit vector in the direction of $J[f]$.

The first term of $Q(f)$ can be formally derived using a direct computation with the empirical distribution of particles. And the diffusion part comes from Itō's formula. In a recent work [13], a rigorous derivation of this mean-field limit has been provided, even in the inhomogeneous case. This derivation is linked with the so-called "propagation of chaos" property. We refer to [73] for an introduction to this notion. The laboratory example given in this reference is the original model of McKean [59] which is a more general version of our system in $\mathbb{R}^n$ instead of $\mathbb{S}$ (in that case, equation (1.3) is called McKean-Vlasov equation). The main point is to adapt the theory in the framework of stochastic analysis on Riemannian manifolds.

Notice that equation (1.3) can be written in the form

$$\partial_t f = \nabla \cdot (f \nabla \Psi) + \tau \Delta f,$$

with

$$\Psi(\omega, t) = -\omega \cdot J(t) = \int_{\mathbb{S}} K(\omega, \bar{\omega})\, f(t, \bar{\omega})\, \mathrm{d}\bar{\omega}.$$

This equation is known as Doi equation (or Doi–Onsager, Smoluchowski, or even nonlinear Fokker–Planck equation) and was introduced by Doi [32] as a gradient flow equation for the Onsager free energy functional:

$$\mathcal{F}(f) = \tau \int_{\mathbb{S}} f(.,\omega) \ln f(.,\omega) \mathrm{d}\omega + \tfrac{1}{2} \int_{\mathbb{S}\times\mathbb{S}} K(\omega,\bar{\omega}) f(.,\omega)\, f(.,\bar{\omega})\, \mathrm{d}\omega \mathrm{d}\bar{\omega}. \tag{1.6}$$

This functional was proposed by Onsager [65] to describe the equilibrium states of suspensions of rod-like polymers. They are given by the critical points of this functional.

Defining the chemical potential μ as the first order variation of $\mathcal{F}(f)$ under the constraint $\int_{\mathbb{S}} f = 1$, we get $\mu = \tau \ln f + \Psi$, and the Doi equation becomes

$$\partial_t f = \nabla \cdot (f \nabla \mu).$$

In the original work of Onsager, the kernel has the form $K(\omega, \bar{\omega}) = |\omega \times \bar{\omega}|$, but there is another form, introduced later by Maier and Saupe [58], which leads to similar quantitative results: $K(\omega, \bar{\omega}) = -(\omega \cdot \bar{\omega})^2$. In our case, the potential given by $K(\omega, \bar{\omega}) = -\omega \cdot \bar{\omega}$ is called the dipolar potential. This is a case where the arrow of the orientational direction has to be taken in account.

One of the interesting behavior of the Doi–Onsager equation is the phase transition bifurcation. This is indeed easy to see (here with the dipolar potential) from the following linearization around the uniform distribution: if f is a probability density function, solution of (1.3), we write $f = 1 + g$, so $\int_{\mathbb{S}} g \, \mathrm{d}\omega = 0$ and we can get the equation for g. We multiply the equation by ω and integrate, using the formula $\int_{\mathbb{S}} \omega \otimes \omega \, \mathrm{d}\omega = \frac{1}{n} \mathrm{Id}$ (this is a matrix with trace one and commuting with any rotation) and the tools in the beginning of Section 2.1. We get the linearized equation for g and $J[g]$:

$$\begin{aligned} \partial_t g &= \tau \Delta_\omega g + (n-1)\, \omega \cdot J[g] + O(g^2), \\ \frac{\mathrm{d}}{\mathrm{d}t} J[g] &= (n-1)(\tfrac{1}{n} - \tau) J[g] + O(g^2). \end{aligned}$$

Therefore if we take the linear part of this system, we can solve the second equation directly, and the first one becomes the heat equation with a known source term. Finally, around the constant state, the linearized Doi equation is stable if $\tau \geqslant \frac{1}{n}$, and unstable if $\tau < \frac{1}{n}$. We expect to find another kind of equilibrium in this regime. The work has been done in [37] for the dimension $n = 3$, the distribution obtained is called Fisher-Von Mises distribution [82]. As far as we know, this is the only work dealing with the dipolar potential alone.

A lot of work has been done to study the equilibrium states for the Maier–Saupe potential, and in particular to show the axial symmetry of these steady states. A complete classification has been achieved for the two and three-dimensional cases in [55] (see also [85], including the analysis of stability under a weak external shear flow). The interesting behavior, besides the phase transition, is the hysteresis phenomenon: before a first threshold, only the anisotropic equilibrium is stable, then both anisotropic and uniform equilibria are stable, and after a second threshold, the only equilibrium is the uniform distribution. In the case of a coupling between the Maier–Saupe and the dipolar, it is shown in [89] that the only stable equilibrium states are axially symmetric. To our knowledge, less work has been done to study the dynamics of the Doi–Onsager equation, in particular the rate at which the solution converges to a steady-state.

The purpose of this chapter is to give a rigorous proof of the phase transition in any dimension for the dipolar potential, and study the large time dynamics and the convergence rates towards equilibrium states.

In Section 2, we give some general results concerning equation (1.3). We provide a self-contained proof for existence and uniqueness of a solution with initial nonnegative condition in any Sobolev space. We show that the solution is instantaneously

positive and in any Sobolev space (and actually analytic in the space variable), and we obtain uniform bounds in time for each Sobolev norm.

In Section 3, we use the Onsager free energy (decreasing in time) to analyze the general behavior of the solution as time goes to infinity. We prove a kind of LaSalle principle, implying that the solution converges, in the ω-limit sense, to a given set of equilibria. We determine all the steady states, and see that the value $\frac{1}{n}$ is indeed a threshold for the noise parameter τ. Over this threshold, the only equilibrium is the uniform distribution. When $\tau < \frac{1}{n}$, two kinds of equilibria exist: the uniform distribution, and a family of non-isotropic distributions (called Fischer-Von Mises distributions), with a concentration parameter κ depending on τ.

Finally, in Section 4, we show that the solution converges strongly to a given equilibrium. We first obtain a new conservation relation, which plays the role of an entropy when $\tau \geqslant \frac{1}{n}$, and shows a global convergence to the uniform distribution with rate proportional to $\tau - \frac{1}{n}$. Then we prove that, in the supercritical case $\tau < \frac{1}{n}$, the solution converges to a non-isotropic equilibrium if and only if the initial drift velocity $|J[f_0]|$ is non-zero (if it is zero, the equation reduces to the heat equation, and the solution converges exponentially fast to the uniform distribution). We prove in that case that the convergence to this steady-state is exponential in time, and we give the asymptotic rate of convergence. Finally, in the critical case $\tau = \frac{1}{n}$, we show that the speed of convergence to the uniform distribution is algebraic (more precisely the decay in any Sobolev norm is at least $\frac{C}{\sqrt{t}}$).

2 General results

2.1 Preliminaries: some results on the unit sphere

This subsection consists essentially in a main lemma, allowing to perform some estimates on the norm of integrals of the form $\int_{\mathbb{S}} g \nabla_\omega h$, where h and g are real functions with mean zero.

But let us start by some useful formulas.

For V a constant vector in $\mathbb{R}^n$, we have:

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

where ∇_ω (resp. $\nabla_\omega \cdot$) stands for the tangential gradient (resp. the divergence) on the unit sphere. When no confusion is possible, we will just use the notation ∇.

Then, taking the dot product with a given tangent vector field A or multiplying by a regular function f and integrating by parts, we get

$$\int_{\mathbb{S}} \omega\, \nabla_\omega \cdot A(\omega) \mathrm{d}\omega = -\int_{\mathbb{S}} A(\omega) \mathrm{d}\omega$$
$$\int_{\mathbb{S}} \nabla_\omega f \mathrm{d}\omega = (n-1) \int_{\mathbb{S}} \omega f \mathrm{d}\omega.$$

We then introduce some notations. We denote by $\dot{H}^s(\mathbb{S})$ the subspace composed of mean zero functions of the Sobolev space $H^s(\mathbb{S})$. This is a Hilbert space, associated to the inner product $\langle g, h \rangle_{\dot{H}^s}^2 = \langle (-\Delta)^s g, h \rangle$, where Δ is the Laplace–Beltrami

operator on the sphere. This has also a sense for any $s \in \mathbb{R}$ by spectral decomposition of this operator. We will denote by $\|\cdot\|_{\dot{H}^s}$ the norm on this Hilbert space.

We then define the so-called conformal Laplacian $\widetilde{\Delta}_{n-1}$ on the sphere (see [9]) which plays a role in some Sobolev inequalities. This is a positive definite operator (pseudodifferential operator of degree $n-1$, mapping continuously $\dot{H}^s(\mathbb{S})$ into $\dot{H}^{s-n+1}(\mathbb{S})$, which is a differential operator when n is odd) given by

$$\widetilde{\Delta}_{n-1} = \begin{cases} \displaystyle\prod_{0\leqslant j\leqslant \frac{n-3}{2}} (-\Delta + j(n-j-2)) & \text{for } n \text{ odd,} \\ \displaystyle\left(-\Delta + (\tfrac{n}{2}-1)^2\right)^{\frac{1}{2}} \prod_{0\leqslant j\leqslant \frac{n}{2}-2} (-\Delta + j(n-j-2)) & \text{for } n \text{ even.} \end{cases} \tag{2.7}$$

Equivalently, it can be also defined by

$$\widetilde{\Delta}_{n-1}\, Y_\ell = \ell(\ell+1)\dots(\ell+n-2) Y_\ell \text{ for any spherical harmonic } Y_\ell \text{ of degree } \ell. \tag{2.8}$$

Here is the main lemma.

Lemma 4.1. *Estimates on the sphere.*

1. *If h in $\dot{H}^{-s+1}(\mathbb{S})$ and g in $\dot{H}^s(\mathbb{S})$, the following integral is well defined and we have*
$$\left|\int_{\mathbb{S}} g \nabla h\right| \leqslant C \|g\|_{\dot{H}^s} \|h\|_{\dot{H}^{-s+1}} \tag{2.9}$$
where the constant C depends only on s and n.

2. *We have the following estimation, for any $g \in \dot{H}^{s+1}(\mathbb{S})$:*
$$\left|\int_{\mathbb{S}} g \nabla (-\Delta)^s g\right| \leqslant C \|g\|_{\dot{H}^s}^2, \tag{2.10}$$
where the constant C depends only on s and n.

3. *We have the following identity, for any $g \in \dot{H}^{-\frac{n-3}{2}}$:*
$$\int_{\mathbb{S}} g \nabla \widetilde{\Delta}_{n-1}^{-1} g = 0 \tag{2.11}$$

Let us make some remarks on these statements. The first one is just expressing the fact that the gradient operator (or more precisely any of its component $e \cdot \nabla$ for a given unit vector e) is well defined as an operator sending $\dot{H}^{-s+1}(\mathbb{S})$ continuously into $\dot{H}^{-s}(\mathbb{S})$ for any s.

The second one is actually a commutator estimate. It is equivalent to the fact that for any given unit vector e, and for any $g, h \in \dot{H}^{s+1}$ we have

$$\left|\int_{\mathbb{S}} ge \cdot \nabla(-\Delta)^s h + he \cdot \nabla(-\Delta)^s g\right| \leqslant \widetilde{C} \|g\|_{\dot{H}^s} \|h\|_{\dot{H}^s}.$$

Defining the operator F by

$$Fg = e \cdot \nabla(-\Delta)^s g - (-\Delta)^s \nabla \cdot ((\mathrm{Id} - \omega \otimes \omega) e g)$$

and integrating by parts, this inequality becomes $|\int_{\mathbb{S}} h\, Fg| \leqslant \widetilde{C}\|g\|_{\dot{H}^s}\|h\|_{\dot{H}^s}$. In other words, F sends $\dot{H}^s(\mathbb{S})$ continuously into $\dot{H}^{-s}(\mathbb{S})$ for any s.

So since $F = [e\cdot\nabla, (-\Delta)^s] + (n-1)(-\Delta)^s e\cdot\omega$, this second statement (2.10) expresses that the commutator $[\nabla, (-\Delta)^s]$ is an operator of degree $2s$.

With the same point of view, the last equality (2.11) gives an exact computation of the commutator of the gradient and the inverse of conformal Laplacian.

This is just saying that $[\nabla, \widetilde{\Delta}_{n-1}^{-1}] = -(n-1)\widetilde{\Delta}_{n-1}^{-1}\omega$, or, multiplying left and right by $\widetilde{\Delta}_{n-1}$, that $[\nabla, \widetilde{\Delta}_{n-1}] = (n-1)\omega\widetilde{\Delta}_{n-1}$.

The proof of this lemma relies on some computations on spherical harmonics, and is given in Appendix A.

2.2 Existence, uniqueness, positivity, regularity.

We present here a self-contained proof of well-posedness of the problem (1.3), working in any Sobolev space for the initial condition. Some analogous claims are given in [21], without proof, starting for a continuous nonnegative function. They are based on arguments of [15], stating that the Galerkin method based on spherical harmonics converges (exponentially fast) to the unique solution. They are weaker with respect to the initial conditions and the positivity, but stronger for the regularity of the solution (analytic in space). As a remark we will give the same regularity results, and prove it in Appendix A.2.

Definition 2.1. *Weak solution.*

For $T > 0$, the function $f \in L^2((0,T), H^{s+1}(\mathbb{S})) \cap H^1((0,T), H^{s-1}(\mathbb{S}))$ is said to be a weak solution of (1.3) if for almost all $t \in [0,T]$, we have for all $h \in H^{-s+1}(\mathbb{S})$

$$\langle \partial_t f, h\rangle = -\tau\langle \nabla_\omega f, \nabla_\omega h\rangle + \langle f, J[f]\cdot\nabla_\omega h\rangle, \tag{2.12}$$

where $\langle\cdot,\cdot\rangle$ is the usual duality product for distributions on the sphere $\mathbb{S}$.

Since it is sometimes more convenient to work with mean zero functions (in order to use the main lemma of the previous subsection), we reformulate this problem in another framework. We set $f = 1 + g$ so that f is a weak solution if and only if $g \in L^2((0,T), \dot{H}^{s+1}(\mathbb{S})) \cap H^1((0,T), \dot{H}^{s-1}(\mathbb{S}))$ with, for almost all $t \in [0,T]$, and for all $h \in \dot{H}^{-s+1}(\mathbb{S})$,

$$\langle \partial_t g, h\rangle = -\tau\langle \nabla_\omega g, \nabla_\omega h\rangle + (n-1)J[g]\cdot J[h] + \langle g, J[g]\cdot\nabla_\omega h\rangle. \tag{2.13}$$

That makes sense to look for a weak solution with prescribed initial condition in H^s, since it always belongs to $C([0,T], H^s(\mathbb{S}))$, as stated by the following proposition.

Proposition 2.1. *If $g \in L^2((0,T), \dot{H}^{s+1}(\mathbb{S})) \cap H^1((0,T), \dot{H}^{s-1}(\mathbb{S}))$, then, up to redefining it on a set of measure zero, it belongs to $C([0,T], \dot{H}^s(\mathbb{S}))$, and we have*

$$\max_{[0,T]} \|u(t)\|_{\dot{H}^s}^2 \leqslant C\int_0^T \|u\|_{\dot{H}^{s+1}}^2 + \|\partial_t u\|_{\dot{H}^{s-1}}^2,$$

where the constant C depends only on T.

The proof in the case $s = 0$ is the same as in [35], Thm 3, §5.9.2. To do the general case, we apply the result to $(-\Delta)^{\frac{s}{2}} g$.

Theorem 4.1. *Given an initial probability measure f_0 in $H^s(\mathbb{S})$, there exists a unique weak solution f of (1.3) such that $f(0) = f_0$. This solution is global in time (the definition above is valid for any time $T > 0$). Moreover, $f \in C^\infty((0, +\infty) \times \mathbb{S})$, with $f(t, \omega) > 0$ for all positive t.*

We also have the following instantaneous regularity and uniform boundedness estimates (for $m \in \mathbb{N}$, the constant C depending only on τ, m, s), for all $t > 0$:

$$\|f(t)\|^2_{H^{s+m}} \leqslant C \left(1 + \frac{1}{t^m}\right) \|f_0\|^2_{H^s}.$$

The proof consists in several steps, which we will treat as propositions. We first use a Galerkin method to prove existence on a small interval. We then show the continuity with respect to initial conditions on this interval (and so the uniqueness). Next, we prove the positivity of $1 + g$ for regular solutions. This gives us a better estimate of $J[g]$. Repeating the procedure on the following small interval, and so on, we can show that this extends to any $t > 0$. Regularizing the initial condition give then global existence in any case.

We finally obtain the instantaneous regularity and boundary estimates by decomposing the solution between low and high modes.

For the proof of all propositions, we will denote by $C_0, C_1, \dots$ some positive constants which depends only on s and τ. We will also fix one parameter $K > 0$ (which will be a bound on the norm of initial condition), and denote by $M_0, M_1, \dots$ some positive constants which depends only on s and τ, and K.

Proposition 2.2. *Existence: Galerkin method.*

We set

$$T = \frac{1}{C_1} \ln \left(1 + \frac{1}{1 + 2C_2 K}\right), \tag{2.14}$$

where the constant C_1 and C_2 will be defined later.

If $\|g_0\|_{\dot{H}^s} \leqslant K$, then we have existence of a weak solution on $[0, T]$ satisfying (2.13), uniformly bounded in $L^2((0, T), \dot{H}^{s+1}(\mathbb{S})) \cap H^1((0, T), \dot{H}^{s-1}(\mathbb{S}))$ by a constant M_1.

Proof. We denote by P_N the space spanned by the first N (non-constant) eigenvectors of the Laplace–Beltrami operator. This is a finite dimensional vector space, included in $\dot{H}^p(\mathbb{S})$ for all p, and containing the functions of the form $\omega \mapsto V \cdot \omega$ (see Appendix A for more details).

Let $g^N \in C^1(I, P_N)$ be the unique solution of the following Cauchy problem, defined on a maximal interval $I \subset \mathbb{R}_+$ ("non-linear" ODE on a finite dimensional space):

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t} g^N = \Pi_N(\tau \Delta_\omega g^N + (n-1)(1 + g^N)\, \omega \cdot J[g^N] - J[g^N] \cdot \nabla_\omega g^N), \\ g^N(0) = \Pi_N(g_0), \end{cases}$$

where Π_N is the orthogonal projection on P_N. The first equation is equivalent to the fact that for any $h \in P_N$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle g^N, h\rangle = -\tau\langle \nabla_\omega g^N, \nabla_\omega h\rangle + (n-1)J[g^N]\cdot J[h] + \langle g^N, J[g^N]\cdot\nabla_\omega h\rangle. \tag{2.15}$$

The goal is to prove that $[0,T] \subset I$ and that there exists an extracted sequence N_k such that, as $k \to \infty$,

- g^{N_k} converges weakly in $L^2((0,T), \dot{H}^{s+1}(\mathbb{S}))$ to a function g,
- $\partial_t g^{N_k}$ converges weakly to $\partial_t g$ in $L^2((0,T), \dot{H}^s(\mathbb{S}))$,
- $J[g^{N_k}] \to J[g]$ uniformly.

We have that $(-\Delta)^s g^N \in P_N$, so we can take it for h, put it in (2.15) and use the second part of Lemma 4.1 to get:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g^N\|^2_{\dot{H}^s} + \tau\|g^N\|^2_{\dot{H}^{s+1}} \leqslant C_0|J[g^N]|\|g^N\|^2_{\dot{H}^s} + (n-1)^s|J[g^N]|^2 \tag{2.16}$$

$$\leqslant C_1\|g^N\|^2_{\dot{H}^s}(1 + C_2\|g^N\|_{\dot{H}^s}). \tag{2.17}$$

Indeed, any component of ω belongs to any $\dot{H}^{-s}$, then $J[g^N] = \langle \omega, g^N\rangle$ is controlled by any $\dot{H}^s$ norm of g^N.

Solving this inequality, we obtain for $0 \leqslant t < C_1^{-1}\ln(1 + (C_2\|\Pi^N(g_0)\|_{\dot{H}^s})^{-1})$,

$$\|g^N\|_{\dot{H}^s} \leqslant \frac{\|\Pi^N(g_0)\|_{\dot{H}^s}}{e^{-C_1 t} - C_2\|\Pi^N(g_0)\|_{\dot{H}^s}(1 - e^{-C_1 t})}. \tag{2.18}$$

Then we have $\|g^N(t)\|_{\dot{H}^s} \leqslant 2\|g_0\|_{\dot{H}^s}$ for all t in $[0,T]$. There is no finite-time blow up in $[0,T]$, then the ODE (2.15) has a solution on $[0,T]$, for any $N \in \mathbb{N}$.

Now we denote by M_0 a bound for $|J[g^N]|$ on $[0,T]$. The inequality (2.16) gives

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g^N\|^2_{\dot{H}^s} + \tau\|g^N\|^2_{\dot{H}^{s+1}} \leqslant (1 + M_0)C_3\|g\|^2_{\dot{H}^s}.$$

Solving this inequality, we get for $t \in [0,T]$

$$\|g^N\|^2_{\dot{H}^s} + \tau\int_0^T \|g^N\|^2_{\dot{H}^{s+1}} \leqslant \|g_0\|^2_{\dot{H}^s} e^{(1+M_0)C_3 T}.$$

We then use the ODE (2.15) and this estimate to control the derivative of g.

Taking $h \in L^2((0,T), \dot{H}^{-s+1}(\mathbb{S}))$, and integrating the equation in time, we get

$$\int_0^T \|\partial_t g^N\|^2_{\dot{H}^{s-1}} \leqslant (C_4 + M_0)\|g_0\|^2_{\dot{H}^s} e^{(1+M_0)C_3 T}$$

Then we can take $M_1^2 = K^2 e^{(1+M_0)C_3 T}\max(\tau^{-1}, C_4 + M_0)$, and we get that g^N is bounded by M_1 in $L^2((0,T), \dot{H}^{s+1}(\mathbb{S})) \cap H^1((0,T), \dot{H}^{s-1}(\mathbb{S}))$.

Now, we just need estimates for $\frac{\mathrm{d}}{\mathrm{d}t}J[g^N]$. We can take $h = \omega\cdot V$ in the ODE (2.15) and use the tools given in the beginning of this section. We get

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}J[g^N]\right| = \left|\frac{n-1}{n}(1-\tau n)J[g^N] - \int_{\mathbb{S}}(\mathrm{Id}-\omega\otimes\omega)J[g^N]g^N\,\mathrm{d}\omega,\right|$$
$$\leqslant (C_5 + M_0C_6)\|g_0\|_{\dot{H}^s}e^{\frac{1}{2}(1+M_0)C_3T}.$$

Indeed, again, since any component of $\mathrm{Id}-\omega\otimes\omega$ is in $\dot{H}^{-s}$, we can control the term $\int_{\mathbb{S}}(\mathrm{Id}-\omega\otimes\omega)g^N\,\mathrm{d}\omega$ by any $\dot{H}^s$ norm of g^N, uniformly in N and in $t\in[0,T]$.

In summary if we suppose that g_0 is in $\dot{H}^s(\mathbb{S})$, for some $s\in\mathbb{R}$, we have that g^N is bounded in $L^2((0,T),\dot{H}^{s+1}(\mathbb{S}))\cap H^1((0,T),\dot{H}^{s-1}(\mathbb{S}))$, and that $J[g^N]$ and $\frac{\mathrm{d}}{\mathrm{d}t}J[g^N]$ are uniformly bounded in N and $t\in[0,T]$.

Then, using weak compactness and the Ascoli-Arzela theorem, we can find an increasing sequence N_k, a function $g\in L^2((0,T),\dot{H}^{s+1}(\mathbb{S}))\cap H^1((0,T),\dot{H}^{s-1}(\mathbb{S}))$, and a continuous function $J:[0,T]\to\mathbb{R}^n$ such that, as $k\to\infty$,

- $J[g^{N_k}]$ converges uniformly to J on $[0,T]$,
- g^{N_k} converges weakly to g in $L^2((0,T),\dot{H}^{s+1}(\mathbb{S}))$ and in $H^1((0,T),\dot{H}^{s-1}(\mathbb{S}))$.

The limit g is also bounded by M_1 in $L^2((0,T),\dot{H}^{s+1}(\mathbb{S}))\cap H^1((0,T),\dot{H}^{s-1}(\mathbb{S}))$.

Then, since we have $\int_0^T\int_{\mathbb{S}}\varphi(t)\omega(g^{N_k}-g)\,\mathrm{d}\omega\,\mathrm{d}t\to 0$ for any smooth function φ, we get $\int_0^T\varphi(t)(J[g]-J)\,\mathrm{d}t=0$ and so $J=J[g]$.

For a fixed $h\in P_M$ passing the weak limit in (2.15) (for $N_k\geqslant M$), we get for almost every $t\in[0,T]$ that

$$\forall h\in P_M,\ \langle\partial_t g,h\rangle = -\tau\langle\nabla_\omega g,\nabla_\omega h\rangle + (n-1)J[g]\cdot J[h] + \langle g, J[g]\cdot\nabla_\omega h\rangle.$$

And this is valid for any M (except on a countable union of subsets of $[0,T]$ of zero measure). By density (and using the first part of Lemma 4.1), we have that g is a weak solution of our problem.

Now for any $h\in\dot{H}^{-s+1}(\mathbb{S})$, we have that $\langle g^N(t)-\Pi_N(g_0),h\rangle = \int_0^t\langle\partial_t g^N,h\rangle$ is controlled by $M_1\sqrt{t}\|h\|_{\dot{H}^{-s+1}}$, uniformly in N. So, passing the limit, we get that $g(t)\to g_0$ in $\dot{H}^{-s+1}(\mathbb{S})$ as $t\to 0$. But since we know that $g\in C([0,T],H^s(\mathbb{S}))$, by uniqueness, we get $g(0)=g_0$. □

Proposition 2.3. *Continuity with respect to the initial condition.*

Set $T=\frac{1}{C_1}\ln(1+\frac{1}{1+2C_2K})$, as in (2.14). Suppose we have two solutions g and $\widetilde{g}$, with $\|g(0)\|_{\dot{H}^s}\leqslant K$ and $\|\widetilde{g}(0)\|_{\dot{H}^s}\leqslant K$.

Then there exists a constant M_3 such that $g-\widetilde{g}$ is bounded in $L^2((0,T),\dot{H}^{s+1}(\mathbb{S}))$ and in $H^1((0,T),\dot{H}^{s-1}(\mathbb{S}))$ by $M_3\|g(0)-\widetilde{g}(0)\|_{\dot{H}^s}$.

This automatically gives uniqueness of a weak solution on $(0,T)$ with initial condition g_0.

Proof. Putting $h=(-\Delta)^s g\in\dot{H}^{-s+1}$ in (2.13), we do the same estimations as in the previous proposition. We have the same estimate as (2.16)-(2.17):

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g\|_{\dot{H}^s}^2 + \tau\|g\|_{\dot{H}^{s+1}}^2 \leqslant C_0|J[g]|\|g\|_{\dot{H}^s}^2 + (n-1)^s|J[g]|^2 \tag{2.19}$$
$$\leqslant C_1\|g\|_{\dot{H}^s}^2(1+C_2\|g\|_{\dot{H}^s}). \tag{2.20}$$

So if we set $T = C_1^{-1}\ln(1+(1+2C_2K)^{-1})$, we can solve this inequality on $[0,T]$, exactly as in (2.18). These solutions are then uniformly bounded in $L^2((0,T),\dot{H}^{s+1}(\mathbb{S}))$ and in $H^1((0,T),\dot{H}^{s-1}(\mathbb{S}))$ (by the constant M_1).

Taking $u = g-\widetilde{g}$, and using (2.13) gives an equation for u: for almost all $t\in[0,T]$, for all $h\in\dot{H}^{-s}(\mathbb{S})$,

$$\langle\partial_t u,h\rangle = -\tau\langle\nabla_\omega u,\nabla_\omega h\rangle+(n-1)J[u]\cdot J[h]+\langle u,J[g]\cdot\nabla_\omega h\rangle+\langle\widetilde{g},J[u]\cdot\nabla_\omega h\rangle. \quad (2.21)$$

Now we take $h=(-\Delta)^s u$ and use the first and second parts of Lemma 4.1 to get

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|_{\dot{H}^s}^2+\tau\|u\|_{\dot{H}^{s+1}}^2 &\leqslant (1+M_1)C_3\|u\|_{\dot{H}^s}^2+C_7\|u\|_{\dot{H}^s}\|\widetilde{g}\|_{\dot{H}^{s+1}}\|(-\Delta)^s u\|_{\dot{H}^{-s}}\\ &\leqslant M_2(1+\|\widetilde{g}\|_{\dot{H}^{s+1}})\|u\|_{\dot{H}^s}^2. \quad (2.22)\end{aligned}$$

Grönwall's lemma gives then the following estimate:

$$\begin{aligned}\|u\|_{\dot{H}^s}^2+\tau\int_0^T\|u\|_{\dot{H}^{s+1}}^2 &\leqslant \|u_0\|_{\dot{H}^s}^2\exp\left(M_2\int_0^T(1+\|\widetilde{g}\|_{\dot{H}^{s+1}})\right)\\ &\leqslant \|u_0\|_{\dot{H}^s}^2 e^{M_2(T+M_1^2)}.\end{aligned}$$

Using (2.21), we get that u is bounded in $L^2((0,T),\dot{H}^{s+1}(\mathbb{S}))\cap H^1((0,T),\dot{H}^{s-1}(\mathbb{S}))$ by a constant M_3 times $\|u(0)\|_{\dot{H}^s}$. □

Proposition 2.4. *Positivity for regular solutions (maximum principle). Suppose that g_0 is in $\dot{H}^s(\mathbb{S})$, with s sufficiently large (according to the Sobolev embeddings, so $s>\frac{n+3}{2}$ is enough) so that the (unique) solution belongs to $C^0([0,T],C^2(\mathbb{S}))$. Here T is defined as in* (2.14)*, with $K=\|g_0\|_{\dot{H}^s}$. We go back to the original formulation $f=1+g$. Then f is a classical solution of* (1.3)*.*

If f_0 is nonnegative, then f is positive for any positive time, and more precisely we have the following estimates, for all $t\in(0,T]$ and $\omega\in\mathbb{S}$ (if f_0 is not equal to the constant function 1*):*

$$e^{-(n-1)\int_0^t|J[f]|}\min_{\mathbb{S}} f_0 < f(t,\omega) < e^{(n-1)\int_0^t|J[f]|}\max_{\mathbb{S}} f_0. \quad (2.23)$$

Proof. Since the solution is in $C^0([0,T],C^2(\mathbb{S}))$, we can do the reverse integration by parts in the weak formulation (2.12). We get that the function $\partial_t f$, as an element of $L^2((0,T),H^{s-1}(\mathbb{S}))$, is equal to $\tau\Delta_\omega f-\nabla_\omega\cdot((\mathrm{Id}-\omega\otimes\omega)J[f]f)$ (almost everywhere), which is an element of $C^0([0,T]\times\mathbb{S})$. So up to redefining it on a set of measure zero, the function f belongs to $C^1([0,T],C(\mathbb{S}))\cap C^0([0,T],C^2(\mathbb{S}))$, and satisfies the partial differential equation.

Applying the chain rule and using the tools given in the beginning of this section, we get another formulation of the PDE (1.3):

$$\partial_t f=\tau\Delta_\omega f-J[f]\cdot\nabla_\omega f+(n-1)J[f]\cdot\omega\, f. \quad (2.24)$$

The next part of the proposition is just a classical strong maximum principle. We only prove here the left part of the inequality, the other part is very similar, once we have that f is positive.

Suppose first that f_0 is positive. We denote by $\widetilde{T} > 0$ the first time such that the minimum on the unit sphere of f is zero (or $\widetilde{T} = T$ if f is always positive).

Then we have for $t \in [0, \widetilde{T}]$, that $\partial_t f \geqslant \tau \Delta_\omega f - J[f] \cdot \nabla_\omega f - (n-1)|J[f]|f$. If we write $\widetilde{f} = f\, e^{-(n-1)\int_0^t |J[f]|}$, we get

$$\partial_t \widetilde{f} \geqslant \tau \Delta_\omega \widetilde{f} - J[f] \cdot \nabla_\omega \widetilde{f}. \tag{2.25}$$

Then the weak maximum principle (see [35], Thm 8, §7.1.4, which is also valid on the sphere) gives us that the minimum of $\widetilde{f}$ on $[0, \widetilde{T}] \times \mathbb{S}$ is reached on $\{0\} \times \mathbb{S}$. That means that we have a non-strict version of the left part of the inequality (2.23):

$$\forall t \in [0, \widetilde{T}], \forall \omega \in \mathbb{S}, f(\omega, t) \geqslant e^{-(n-1)\int_0^t |J[f]|} \min_{\mathbb{S}} f_0. \tag{2.26}$$

Consequently, we have that $\min_{\mathbb{S}} f(\widetilde{T}) > 0$ and so $\widetilde{T} = T$. If now f_0 is only nonnegative, take $f_0^\varepsilon = \frac{f+\varepsilon}{1+\varepsilon}$, and by continuity with respect to initial condition, inequality (2.26) is still valid. That gives that f is nonnegative on $[0, T]$, and consequently we have that inequality (2.25) is valid on $[0, \widetilde{T}]$.

Now we can use the strong maximum principle (see [35], Thm 11, §7.1.4), which gives that if the inequality (2.26) is an equality for some $t > 0$ and $\omega \in \mathbb{S}$, then $\widetilde{f}$ is constant on $[0, t] \times \mathbb{S}$. So f_0 is the constant function 1. □

Proposition 2.5. *Global existence, positivity. Suppose f_0 is a probability measure belonging to $H^s(\mathbb{S})$ (this is always the case for $s < -\frac{n-1}{2}$, according to Sobolev embeddings). Then there exists a global weak solution of* (1.3)*, which remains a probability measure for any time.*

We remark that the uniqueness of the solution on any time interval remains by Proposition 2.3.

Proof. We first prove this proposition in the case $s > \frac{n+3}{2}$.

We define a solution by constructing it on a sequence of intervals.

We set $T_1 = \frac{1}{C_1} \ln(1 + \frac{1}{1+2C_2\|g_0\|_{\dot{H}^s}})$, as in (2.14). This gives existence to a solution g in $C([0, T_1], \dot{H}^s(\mathbb{S}))$. By induction we define $T_{k+1} = T_k + \frac{1}{C_1} \ln(1 + \frac{1}{1+2C_2\|g(T_k)\|_{\dot{H}^s}})$, which gives existence to a solution $g \in C([T_k, T_{k+1}], \dot{H}^s(\mathbb{S}))$.

So we have a solution on $[0, T]$, provided that $T \leqslant T_k$ for some integer k.

Now by the previous proposition, this solution $f = 1 + g$ is nonnegative. We obviously have $|J[g]| = |J[f]| \leqslant \int_{\mathbb{S}} |\omega| f = 1$. Then we can do better estimates, starting from (2.19):

$$\begin{aligned} \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g\|_{\dot{H}^s}^2 + \tau\|g\|_{\dot{H}^{s+1}}^2 &\leqslant C_0|J[g]|\|g\|_{\dot{H}^s}^2 + (n-1)^s|J[g]|^2 \\ &\leqslant C_8\|g\|_{\dot{H}^s}^2. \end{aligned} \tag{2.27}$$

Then, Grönwall's lemma gives us that $\|g(T_k)\|_{\dot{H}^s} \leqslant \|g_0\|_{\dot{H}^s} e^{C_8 T_k}$. Suppose now that the sequence (T_k) is bounded, then $\|g(T_k)\|_{\dot{H}^s}$ is also bounded. By the definition of T_{k+1}, the difference $T_{k+1} - T_k$ does not tend to zero, which implies that the increasing sequence (T_k) is unbounded, and this is a contradiction. So we have that $T_k \overset{k\to\infty}{\to} \infty$, and the solution is global in time.

Now we do the general case for any s. Take g_0^k a sequence of elements of $\dot{H}^{\frac{n}{2}+2}$ converging to g_0 in $\dot{H}^s$, and such that $f_0^k = 1 + g_0^k$ are positive functions. Let g^k be the solutions associated to these initial conditions.

Then we have the same estimates as before, since we still have $|J[g]| \leqslant 1$, solving (2.27) gives

$$\|g^k(t)\|_{\dot{H}^s}^2 + \tau \int_0^t \|g^k(t)\|_{\dot{H}^{s+1}}^2 \leqslant \|g_0^k\|_{\dot{H}^s} e^{C_8 t}.$$

So we can now study the difference $u = g^k - g^j$, as in (2.21),(2.22), which satisfies, for any $h \in \dot{H}^{-s}(\mathbb{S})$,

$$\langle \partial_t u, h\rangle = -\tau\langle \nabla_\omega u, \nabla_\omega h\rangle + (n-1)J[u]\cdot J[h] + \langle u, J[g^k]\cdot\nabla_\omega h\rangle + \langle g^j, J[u]\cdot\nabla_\omega h\rangle. \quad (2.28)$$

We take $h = (-\Delta)^s u$ and use the first and second part of Lemma 4.1 to get

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|_{\dot{H}^s}^2 + \tau\|u\|_{\dot{H}^{s+1}}^2 &\leqslant C_9\|u\|_{\dot{H}^s}^2 + C_7\|u\|_{\dot{H}^s}\|g^k\|_{\dot{H}^{s+1}}\|(-\Delta)^s u\|_{\dot{H}^{-s}} \\ &\leqslant C_{10}(1 + \|\tilde{g}\|_{\dot{H}^{s+1}})\|u\|_{\dot{H}^s}^2. \end{aligned} \quad (2.29)$$

If we fix $T > 0$, Grönwall's lemma gives then the following estimate:

$$\begin{aligned}\|u\|_{\dot{H}^s}^2 + \tau\int_0^T \|u\|_{\dot{H}^{s+1}}^2 &\leqslant \|u_0\|_{\dot{H}^s}^2 \exp\left(C_{10}\int_0^T (1 + \|g^j\|_{\dot{H}^{s+1}})\right) \\ &\leqslant \|u_0\|_{\dot{H}^s}^2 \exp\left(C_{10}(T + \tau^{-1}\sqrt{T}\|g_0^k\|_{\dot{H}^s} e^{C_8 T})\right).\end{aligned}$$

Since $\|g_0^k\|_{\dot{H}^s}$ is bounded (because g_0^k converges in $\dot{H}^s$), together with (2.21), we finally get that u is bounded in $L^2((0,T),\dot{H}^{s+1}(\mathbb{S})) \cap H^1((0,T),\dot{H}^{s-1}(\mathbb{S}))$ by a constant C_T times $\|u(0)\|_{\dot{H}^s}$. This gives that g^k is a Cauchy sequence in that space, and then it converges to a function g, which is a weak solution of our problem (by Proposition 2.1, we have that $g(0) = g_0$). This is valid for any $T > 0$, so this solution is global.

If we take φ in $C^\infty(\mathbb{S})$, since $f^k(t) = 1 + g^k(t)$ is a positive function with mean 1, we have that

$$-\|\varphi\|_\infty = \langle f^k(t), -\|\varphi\|_\infty\rangle \leqslant \langle f^k(t), \varphi\rangle \leqslant \langle f^k(t), \|\varphi\|_\infty\rangle = \|\varphi\|_\infty.$$

Then passing the limit gives $|\langle g(t), \varphi\rangle| \leqslant \|\varphi\|_\infty$. Furthermore we have $\langle f^k(t), 1\rangle = 1$ so $\langle f(t), 1\rangle = 1$, and if φ is a nonnegative function, then $\langle f^k(t), \varphi\rangle \geqslant 0$ and we get $\langle f(t), \varphi\rangle \geqslant 0$. This gives that $f(t)$ is a positive radon measure with mass 1, which is a probability measure. □

Proposition 2.6. *Instantaneous regularity and boundedness estimates. If f_0 is a probability measure, then the solution f belongs to $C^\infty((0,+\infty)\times\mathbb{S})$, is positive for any time $t > 0$, and we have the following estimates, for all $s \in \mathbb{R}$ and $m \geqslant 0$:*

$$\|f(t)\|_{H^{s+m}}^2 \leqslant C\left(1 + \frac{1}{t^m}\right)\|f_0\|_{H^s}^2,$$

where the constant C depends only on τ, s, and m.

In particular we have that for $t_0 > 0$, f is uniformly bounded on $[t_0, +\infty)$ in any H^s norm.

Proof. Suppose $f_0 \in H^s(\mathbb{S})$, and fix $t > 0$. The solution f is in $C([0,+\infty), H^s(\mathbb{S}))$, and in $L^2((0,t), H^{s+1}(\mathbb{S}))$. Then there exists $s < t$ such that $f(s) \in H^{s+1}(\mathbb{S})$. So we can construct a solution belonging to $C([s,+\infty), H^{s+1}(\mathbb{S}))$. But this solution is also a weak solution in $L^2((s,T), H^{s+1}(\mathbb{S})) \cap H^{-1}((s,T), H^{s-1}(\mathbb{S}))$, for all $T > s$ so by uniqueness it is equal to f. Then f belongs to $C([t,+\infty), H^{s+1}(\mathbb{S}))$. Since this is true for all $t > 0$, then f belongs to $C((0,+\infty), H^{s+1}(\mathbb{S}))$. We can repeat this argument and have that f belongs to $C((0,+\infty), H^p(\mathbb{S}))$ for any p, and is a positive classical solution, by Proposition 2.4. Using the equation, differentiating in time gives that it is also in $C^k((0,+\infty), H^p(\mathbb{S}))$ for any p and any k, so, by Sobolev embeddings, it is a C^∞ function of $(0,+\infty) \times \mathbb{S}$.

Since we have positivity, we can have estimates for any of the modes of $f = 1+g$. Let us denote f^N the orthogonal projection of f on the N first eigenspaces of the Laplacian, and $g^N = f - f^N$ the projection on the other ones (high modes).

We have a Poincaré inequality on this space: $\|g^N\|^2_{\dot{H}^s} \leqslant \frac{1}{(N+1)(N+n-1)} \|g^N\|^2_{\dot{H}^{s+1}}$ (we recall that the eigenvalues of $-\Delta$ are given by $\ell(\ell+n-2)$ for $\ell \in \mathbb{N}$). We use the estimate (2.19):

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g\|^2_{\dot{H}^s} + \tau\|g\|^2_{\dot{H}^{s+1}} &\leqslant C_0|J[g]|\|g\|^2_{\dot{H}^s} + (n-1)^s|J[g]|^2 \\ &\leqslant \tfrac{C_0}{(N+1)(N+n-1)}\|g\|^2_{\dot{H}^{s+1}} + (n-1)^s|J[g]|^2 + C_0\|f^N - 1\|^2_{\dot{H}^s}. \quad (2.30)\end{aligned}$$

Now we have, since f is a probability measure, that

$$\|f^N - 1\|^2_{\dot{H}^s} = \int_{\mathbb{S}} (-\Delta)^s f^N f \mathrm{d}\omega \leqslant \|(-\Delta)^s f^N\|_{L^\infty} \leqslant K_N \|f^N - 1\|_{\dot{H}^s},$$

the last inequality being the equivalence between norms in finite dimension. Dividing by this last norm, this gives that the low modes of f are uniformly bounded in time by a constant K_N. Then we have, taking N sufficiently large,

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g\|^2_{\dot{H}^s} + \frac{\tau}{2}\|g\|^2_{\dot{H}^{s+1}} \leqslant C_{11},$$

Now multiplying by t this formula at order $s+1$, we get

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}(t\|g\|^2_{\dot{H}^{s+1}}) + \frac{\tau}{2}t\|g\|^2_{\dot{H}^{s+2}} \leqslant C_{12}t + \frac{1}{2}\|g\|^2_{\dot{H}^{s+1}},$$

and finally

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}(\|g\|^2_{\dot{H}^s} + \tfrac{\tau}{2}t\|g\|^2_{\dot{H}^{s+1}}) + \tfrac{\tau}{4}(\|g\|^2_{\dot{H}^{s+1}} + \tfrac{\tau}{2}t\|g\|^2_{\dot{H}^{s+2}}) \leqslant C_{11} + C_{12}\tfrac{\tau}{2}t.$$

Together with Poincaré inequality, solving this inequality gives us

$$\|g\|^2_{\dot{H}^s} + \frac{\tau}{2}t\|g\|^2_{\dot{H}^{s+1}} \leqslant \|g_0\|^2_{\dot{H}^s} e^{-(n-1)\frac{\tau}{4}t} + C_{13}(1+t).$$

So we have the result for $\|f\|^2_{H^s} = 1 + \|g\|^2_{\dot{H}^s}$, and $m = 1$:

$$\|f(t)\|^2_{H^{s+1}} \leqslant C\left(1 + \frac{1}{t}\right)\|f_0\|^2_{H^s}.$$

Then we apply this inequality between 0 and $\frac{t}{2}$, and the inequality at order m between $\frac{t}{2}$ and t to get the result at order $m+1$. The case where m is any nonnegative real also works, by interpolation. □

This last proposition ends the proof of Theorem 4.1. Let us do here two small comments concerning the analyticity of the solution and the limit case with no noise: $\tau = 0$.

Remark 2.1. *Analyticity of the solution. We can show, as claimed in [19], [21] that at any time $t > 0$ the solution is analytic in the space variable. The idea is to show, following [21] (based on [15], [40]), that the solution is in some Gevrey class of functions, defined by a parameter depending on time. This class is a subset of the set of real analytic functions on the sphere. More details and a complete proof are given in Appendix A.2. We could have directly dealt with this classes of functions instead of working in the Sobolev spaces, but we will not need these properties of analyticity in the following. In any case, to prove analyticity we need the initial condition to be in $H^{-\frac{n-1}{2}}(\mathbb{S})$, so this study of instantaneous regularization was necessary.*

Remark 2.2. *Case where $\tau = 0$: no noise. The proof is also valid, except that the solution belongs to $L^\infty((0,T), H^s(\mathbb{S})) \cap H^1((0,T), H^{s-1}(\mathbb{S}))$ if the initial condition is in $H^s(\mathbb{S})$. By an optimal regularity argument, we can get that a solution is in fact in $C([0,T], H^s(\mathbb{S}))$. The non-negativity argument is then also valid, and so the solution is global. Obviously, we do not have the instantaneous regularity and boundedness estimates.*

3 Using the free energy

In this section, we derive the Onsager free energy (1.6) for Doi equation (1.3), and use it to get general results on the steady states.

3.1 Free energy and steady states

We rewrite the equation (1.3):

$$\partial_t f = Q(f) = \nabla_\omega \cdot (\tau \nabla_\omega f - \nabla_\omega(\omega \cdot J[f]) f) = \nabla_\omega \cdot (f \nabla_\omega (\tau \ln f - \omega \cdot J[f])).$$

Since any solution is in $C^\infty((0,+\infty) \times \mathbb{S})$, and positive for any $t > 0$, there is no problem with using $\ln f$, and doing any integration by parts. We multiply the equation by $\tau \ln f - \omega \cdot J[f]$ and integrate by parts, we get

$$\int_{\mathbb{S}} \partial_t f (\tau \ln f - \omega \cdot J[f]) \, \mathrm{d}\omega = - \int_{\mathbb{S}} f |\nabla_\omega (\tau \ln f - \omega \cdot J[f])|^2 \, \mathrm{d}\omega.$$

Since the left part can be recast as a time derivative, this is a conservation relation. We define the free energy $\mathcal{F}(f)$ and the dissipation term $\mathcal{D}(f)$ by

$$\mathcal{F}(f) = \tau \int_{\mathbb{S}} f \ln f - \tfrac{1}{2} |J[f]|^2, \tag{3.31}$$

$$\mathcal{D}(f) = \int_{\mathbb{S}} f |\nabla_\omega (\tau \ln f - \omega \cdot J[f])|^2, \tag{3.32}$$

and we have the following conservation relation:

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{F} + \mathcal{D} = 0. \tag{3.33}$$

We define a steady state as a (weak) solution which does not depend on time. Here are some characterizations of the steady states.

Proposition 3.1. *Steady states.*
The steady states of Doi equation (1.3) *are the probability measures f on $\mathbb{S}$ which satisfy one of the following equivalent conditions.*

1. *Equilibrium: $f \in C^2(\mathbb{S})$ and $Q(f) = 0$*
2. *No dissipation: $f \in C^1(\mathbb{S})$ and $\mathcal{D}(f) = 0$*
3. *The probability density $f \in C^0(\mathbb{S})$ is positive and a critical point of $\mathcal{F}$ (under the constraint of mean 1).*
4. *There exists $C \in \mathbb{R}$ such that $\tau \ln f - J[f] \cdot \omega = C$.*

Proof. By definition, a steady state f is a solution independent of t. Since it is a solution, it is positive and C^∞, and we get that $Q(f) = 0$. By the conservation relation (3.33), we get that $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F} = 0$, so $\mathcal{D}(f) = 0$. Since it is positive, we get that $\nabla_\omega(\tau \ln f - \omega \cdot J[f]) = 0$, so there exists $C \in \mathbb{R}$ such that $\tau \ln f - J[f] \cdot \omega = C$.

Now we do a variational study of $\mathcal{F}$ around f. We take a small perturbation $f+h$ of f which remains a probability density function (which means that $\int_{\mathbb{S}} h = 0$).

We can expand the function $x \mapsto x \ln x$ around f, since $f \geqslant \varepsilon > 0$, and we have

$$\begin{aligned}\mathcal{F}(f+h) &= \tau \int_{\mathbb{S}} (f \ln f + h \ln f + h) - \frac{1}{2}|J[f]|^2 - J[f] \cdot \int_{\mathbb{S}} \omega h + O(\|h\|_\infty^2) \\ &= \mathcal{F}(f) + \int_{\mathbb{S}} h(\tau \ln f - J[f] \cdot \omega) + O(\|h\|_\infty^2), \\ &= \mathcal{F}(f) + O(\|h\|_\infty^2),\end{aligned}$$

which means that f is a critical point of $\mathcal{F}$. So f satisfies the four conditions.

Conversely if $f \in C^2(\mathbb{S})$ and $Q(f) = 0$, then f is obviously a steady-state.

If $\tau \ln f - J[f] \cdot \omega = C$, then $f \in C^2(\mathbb{S})$ and $Q(f) = 0$. We will show that the second and third conditions reduce to this fourth condition.

Doing the above computation around a positive $f \in C^0(\mathbb{S})$ gives that if f is a critical point for the free energy, then $\int_{\mathbb{S}} h(\tau \ln f - J[f] \cdot \omega)$ is zero for any h with mean zero. This is exactly saying that $\tau \ln f - J[f] \cdot \omega$ is constant.

Finally if we suppose $f \in C^1(\mathbb{S})$ and $\mathcal{D}(f) = 0$, at any point $\omega_0 \in \mathbb{S}$ such that $f(\omega_0) > 0$ we have that $\nabla(\tau \ln f - J[f] \cdot \omega) = 0$ on a neighborhood of ω_0.

The function φ defined by $\varphi(\omega) = \tau \ln f - J[f] \cdot \omega$ is then locally constant at any point where it is finite, so $\varphi^{-1}(\{C\})$ is open in $\mathbb{S}$ for any $C \in \mathbb{R}$.

Now if $\varphi(\omega_k) = C$, with ω_k converging to ω_∞, then $f(\omega_k) = \exp(\frac{C + J[f]\cdot\omega_k}{\tau})$. Passing to the limit, we get that $f(\omega_\infty) = \exp(\frac{C + J[f]\cdot\omega_\infty}{\tau})$, which gives $\varphi(\omega_\infty) = C$. So $\varphi^{-1}(\{C\})$ is closed.

Since f is not identically zero, there exists $C \in \mathbb{R}$ such that $\varphi^{-1}(\{C\}) \neq \emptyset$, and by connectedness of the sphere, we get $\varphi^{-1}(\{C\}) = \mathbb{S}$, so $\tau \ln f - J[f] \cdot \omega = C$. □

3.2 LaSalle principle

We give here an adaptation of LaSalle's invariance principle to our PDE framework.

Proposition 3.2. *LaSalle's invariance principle.*

Let f_0 be a probability measure on the sphere $\mathbb{S}$. We denote by $\mathcal{F}_\infty$ the limit of $\mathcal{F}(f(t))$ as $t \to \infty$, where f is the solution to Doi equation (1.3) with initial condition f_0.

Then the set $\mathcal{E}_\infty = \{f \in C^\infty(\mathbb{S}) \text{ s.t. } \mathcal{D}(f) = 0 \text{ and } \mathcal{F}(f) = \mathcal{F}_\infty\}$ is not empty.

Furthermore $f(t)$ converges in any H^s norm to this set of equilibria (in the following sense):

$$\lim_{t\to\infty} \inf_{g\in\mathcal{E}_\infty} \|f(t) - g\|_{H^s} = 0.$$

Proof. First of all $\mathcal{F}(f(t))$ is decreasing in time, and bounded below by $-\frac{1}{2}$, so $\mathcal{F}_\infty$ is well defined.

Let (t_n) be an unbounded increasing sequence, and suppose that $f(t_n)$ converges in $H^s(\mathbb{S})$ to f_∞ for some $s \in \mathbb{R}$. We first remark that $f(t_n)$ is uniformly bounded in $H^{s+2p}(\mathbb{S})$ (using Theorem 4.1), and then by a simple interpolation estimate we get that $\|f(t_n) - f(t_m)\|^2_{\dot{H}^{s+p}} \leqslant \|f(t_n) - f(t_m)\|_{\dot{H}^s} \|f(t_n) - f(t_m)\|_{\dot{H}^{s+2p}}$, and $f(t_n)$ also converges in $H^{s+p}(\mathbb{S})$. So f_∞ is in any $H^s(\mathbb{S})$.

We want to prove that $\mathcal{D}(f_\infty) = 0$. Supposing this is not the case, we write

$$\begin{aligned}\mathcal{D}(f) &= \tau^2 \int_{\mathbb{S}} \frac{|\nabla_\omega f|^2}{f} + J[f] \cdot \int_{\mathbb{S}} (\mathrm{Id} - \omega \otimes \omega) f \, J[f] - 2\tau J[f] \cdot \int_{\mathbb{S}} \nabla_\omega f \\ &= \tau^2 \int_{\mathbb{S}} \frac{|\nabla_\omega f|^2}{f} + (1 - 2(n-1)\tau)|J[f]|^2 - \int_{\mathbb{S}} (\omega \cdot J[f])^2 f. \end{aligned} \tag{3.34}$$

Now we take s sufficiently large such that $H^s(\mathbb{S}) \subset L_\infty(\mathbb{S}) \cap H^1(\mathbb{S})$. If f_∞ is positive, then $\mathcal{D}$, as a function from the nonnegative elements of $H^s(\mathbb{S})$ to $[0, +\infty]$, is continuous at the point f_∞. In particular since $\mathcal{D}(f_\infty) > 0$, there exist $\delta > 0$ and $M > 0$ such that if $\|f - f_\infty\|_{H^s} \leqslant \delta$, then we have $\mathcal{D}(f) \geqslant M$. We want to show the same result in the case where f_∞ is only nonnegative. We define

$$\mathcal{D}_\varepsilon(f) = \tau^2 \int_{\mathbb{S}} \frac{|\nabla_\omega f|^2}{f + \varepsilon} + (1 - 2(n-1)\tau)|J[f]|^2 - \int_{\mathbb{S}} (\omega \cdot J[f])^2 f.$$

We have that by monotone convergence that $\mathcal{D}_\varepsilon(f_\infty)$ converges to $\mathcal{D}(f_\infty)$ as $\varepsilon \to 0$. So there exists $\varepsilon > 0$ such that $\mathcal{D}_\varepsilon(f_\infty) > 0$. Now by continuity of $\mathcal{D}_\varepsilon$ at the point f_∞, we get that there exists $\delta > 0$ and $M > 0$ such that if $\|f - f_\infty\|_{H^s} \leqslant \delta$, then $\mathcal{D}_\varepsilon(f) \geqslant M$. And the fact that $\mathcal{D}(f) \geqslant \mathcal{D}_\varepsilon(f)$ gives the same result as before.

Now since $\partial_t f$ is uniformly bounded in H^s (for $t \geqslant t_1 > 0$), there exists $\eta > 0$ such that if $|t - t'| \leqslant \eta$, then $\|f(t) - f(t')\|_{H^s} \leqslant \frac{\delta}{2}$. We take then N sufficiently large such that $\|f(t_n) - f_\infty\|_{H^s} \leqslant \frac{\delta}{2}$ for all $n \geqslant N$.

Then we have that for $n \geqslant N$, $\mathcal{D}(f) \geqslant M$ on $[t_n, t_n + \eta]$. Up to extracting, we can assume that $t_{n+1} \geqslant t_n + \eta$, so we have

$$\mathcal{F}(f(t_N)) - \mathcal{F}(f(t_{N+p})) = \int_{t_N}^{t_{N+p}} \mathcal{D}(f) \geqslant p\eta M.$$

Since the left term is bounded by $\mathcal{F}(f(t_N)) - \mathcal{F}_\infty$, taking p sufficiently large gives the contradiction.

Now if we suppose that for a given s the distance (in H^s norm) between $f(t)$ and $\mathcal{E}_\infty$ does not tend to 0, we get $\varepsilon > 0$ and a sequence t_n such that for all $g \in \mathcal{E}_\infty$, we have $\|f(t_n) - g\|_{H^s} \geqslant \varepsilon$. Since $f(t_n)$ is bounded in $H^{s+1}(\mathbb{S})$, by a compact Sobolev embedding, up to extracting we can assume that $f(t_n)$ is converging in $H^s(\mathbb{S})$ to f_∞. By the previous argument $f \in C^\infty(\mathbb{S})$ and we have $\mathcal{D}(f_\infty) = 0$. Obviously since $\mathcal{F}(f)$ is decreasing in time we have that $\mathcal{F}(f_\infty) = \mathcal{F}_\infty$. So f_∞ belongs to $\mathcal{E}_\infty$, and then $\|f(t_n) - f_\infty\|_{H^s} \geqslant \varepsilon$ for all n. This is a contradiction.

Since the distance between $f(t)$ and $\mathcal{E}_\infty$ tends to 0, obviously this set is not empty. □

3.3 Computation of equilibria

Define, for a unit vector $\Omega \in \mathbb{S}$, and $\kappa \geqslant 0$ the Fisher-Von Mises distribution with concentration parameter κ and orientation Ω by

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

Note that the denominator depends only on κ. We have that the density of $M_{\kappa\Omega}$ is 1, and the flux is

$$J[M_{\kappa\Omega}] = \frac{\int_{\mathbb{S}} \omega \exp(\kappa\,\omega \cdot \Omega)\mathrm{d}\omega}{\int_{\mathbb{S}} \exp(\kappa\,\omega \cdot \Omega)\mathrm{d}\omega} = c(\kappa)\Omega, \tag{3.35}$$

where

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

If f is an equilibrium, $\tau \ln f - J[f] \cdot \omega$ is constant, and then $f = C\exp(\tau^{-1}J[f] \cdot \omega)$. Since f is a probability density function, we get $f = M_{\kappa\Omega}$ with $\kappa\Omega = \tau^{-1}J[f]$ (in the case where $|J[f]| = 0$, then $\kappa = 0$ and we can take any Ω, this is just the uniform distribution). Finally with (3.35) we get $J[f] = c(\kappa)\Omega$, which gives the following compatibility condition

$$c(\kappa) = \tau\kappa.$$

We give the solutions of this equation in a proposition.

Proposition 3.3. *Compatibility condition*

- *If $\tau \geqslant \frac{1}{n}$, there is only one solution to the compatibility condition: $\kappa = 0$. The only equilibrium is the constant function $f = 1$.*
- *If $\tau < \frac{1}{n}$, the compatibility condition has exactly two solutions: $\kappa = 0$ and one unique positive solution, that we will denote $\kappa(\tau)$. Apart from the constant function $f = 1$ (the case $\kappa = 0$), the equilibria form a manifold of dimension $n-1$: the functions of the form $f = M_{\kappa(\tau)\Omega}$, where $\Omega \in \mathbb{S}$ is an arbitrary unit vector.*

Proof. Let us denote $\widetilde{\tau}(\kappa) = \frac{c(\kappa)}{\kappa}$. A simple Taylor expansion gives $\widetilde{\tau}(\kappa) \underset{\kappa\to 0}{\to} \frac{1}{n}$. Since the function $\widetilde{\tau}$ tends to 0 as $\kappa \to +\infty$ (because $c(\kappa) \leqslant 1$), it is sufficient to prove that it is decreasing. Indeed the function is then a one-to-one correspondence from $\mathbb{R}_+^*$ to $(0, \frac{1}{n})$, and the compatibility condition for $\kappa > 0$ is exactly solving $\tau = \widetilde{\tau}(\kappa)$.

But we have (after one integration by parts) that $\widetilde{\tau}'(\kappa) = \frac{1}{\kappa}(1 - n\widetilde{\tau}(\kappa) - c(\kappa)^2)$, which, by the following lemma is negative for $\kappa > 0$. □

Lemma 4.2. *Define $\beta = c(\kappa)^2 + n\widetilde{\tau}(\kappa) - 1$. Then for any $\kappa > 0$, we have $\beta > 0$.*

Proof. Define $[\gamma(\cos\theta)]_\kappa = \int_0^\pi \gamma(\cos\theta)\, e^{\kappa\cos\theta} \sin^{n-2}\theta \,\mathrm{d}\theta$.

Then we have by definition $\kappa[1]_\kappa^2\beta = \kappa[\cos\theta]_\kappa^2 + n[\cos\theta]_\kappa[1]_\kappa - \kappa[1]_\kappa^2$. So we only have to show that this term is positive. We will prove in fact that the Taylor expansion of this term in κ has only positive terms.

We have, if we denote $a_p = \frac{1}{(2p)!}\int_0^\pi \cos^{2p}\theta \sin^{n-2}\theta \,\mathrm{d}\theta \geqslant 0$,

$$[1]_\kappa = \sum_{p=0}^{\infty} a_p \kappa^{2p} \quad \text{and} \quad [\cos\theta]_\kappa = \sum_{p=0}^{\infty} (2p+2)\, a_{p+1}\kappa^{2p+1}.$$

Now doing an integration by part in the definition of a_{p+1}, we get

$$a_{p+1} = \tfrac{2p+1}{n-1}\big(\tfrac{1}{(2p+1)(2p+2)}a_p - a_{p+1}\big), \text{ which gives } (2p+2)\, a_{p+1} = \frac{a_p}{2p+n}. \tag{3.36}$$

We have, for $\kappa > 0$,

$$\begin{aligned}
\beta\kappa[1]_\kappa^2 &= \sum_{k=0}^{\infty}\left(\sum_{p+q=k-1}(2p+2)\, a_{p+1}(2q+2)\, a_{q+1} + \sum_{p+q=k} n(2p+2)\, a_{p+1}a_q - a_p a_q\right)\kappa^{2k+1} \\
&= \sum_{k=0}^{\infty}\left(\sum_{p+q=k,p\geqslant 1} 2p\, a_p \tfrac{1}{2q+n} a_q + \sum_{p+q=k}\big(\tfrac{n}{2p+n} - 1\big)\, a_p a_q\right)\kappa^{2k+1} \\
&= \sum_{k=0}^{\infty}\left(\sum_{p+q=k} 2p\left(\tfrac{1}{2q+n} - \tfrac{1}{2p+n}\right)\, a_p a_q\right)\kappa^{2k+1} \\
&= \sum_{k=0}^{\infty}\left(\sum_{p+q=k}\Big(p\big(\tfrac{1}{2q+n} - \tfrac{1}{2p+n}\big) + q\big(\tfrac{1}{2p+n} - \tfrac{1}{2q+n}\big)\Big)\, a_p a_q\right)\kappa^{2k+1} \\
&= \sum_{k=0}^{\infty}\left(\sum_{p+q=k} \tfrac{2(p-q)^2}{(2p+n)(2q+n)}\, a_p a_q\right)\kappa^{2k+1}
\end{aligned}$$

So we finally get

$$\beta = \left(\sum_{p=0}^{\infty} a_p\kappa^{2p}\right)^{-1} \sum_{k=0}^{\infty}\left(\sum_{p+q=k} \tfrac{2(p-q)^2}{(2p+n)(2q+n)}\, a_p a_q\right)\kappa^{2k},$$

which gives that $\beta > 0$ when $\kappa > 0$. □

Remark 3.1. *We can do another proof, following an argument of [88], which does not need to compute explicitly β.*

The idea is that we compute $\widetilde{\tau}'' = (n-1)\frac{\beta}{\kappa^2} - 2\widetilde{\tau}(\widetilde{\tau} - \beta)$*, so we see (except in the case* $\kappa = 0$*) that if* $\widetilde{\tau}' = -\frac{\beta}{\kappa} = 0$*, then* $\widetilde{\tau}'' < 0$ *(indeed, we will easily see in* (4.42) *that* $\widetilde{\tau} - \beta$ *is positive). For the case* $\kappa = 0$*, we can compute the Taylor expansion of* $\widetilde{\tau}$ *up to order 2:* $\widetilde{\tau}(\kappa) = \frac{1}{n} - \frac{1}{n^2(n+2)}\kappa^2 + O(\kappa^4)$*. So we have that any critical point of* $\widetilde{\tau}$ *is a maximum. Since there is a local maximum at* $\kappa = 0$ *then the function is decreasing.*

We can have an asymptotic expansion of the order parameter $c(\kappa(\tau))$ as τ reaches the critical value $\frac{1}{n}$. Indeed we have that $\tau - \frac{1}{n} \sim -\frac{1}{n^2(n+2)}\kappa(\tau)^2$ by the expansion of $\widetilde{\tau}$ in the previous remark. So

$$c(\kappa(\tau)) \sim \tfrac{1}{n}\kappa(\tau) \sim \sqrt{(n+2)(\tfrac{1}{n} - \tau)} \text{ as } \tau \to \tfrac{1}{n}. \tag{3.37}$$

Proposition 3.4. *Minimum of the free energy*

- *If* $\tau \geqslant \frac{1}{n}$*, the minimum of the free energy is* 0*, only reached by the uniform distribution. Any solution converges to the uniform distribution in any* H^s *norm.*
- *If* $\tau < \frac{1}{n}$*, the minimum of the free energy is negative, only reached by any non-isotropic equilibrium* $M_{\kappa(\tau)\Omega}$*.*

Proof. By LaSalle principle (Proposition 3.2), we have that

$$\min_{f \in C^\infty(\mathbb{S}),\, f>0} \mathcal{F}(f) = \min_{f \in C^\infty(\mathbb{S}),\, f>0,\, \mathcal{D}(f)=0} \mathcal{F}(f).$$

Indeed for any positive initial condition f in $C^\infty(\mathbb{S})$, there exists an equilibrium f_∞ such that $\mathcal{F}(f_\infty) = \mathcal{F}_\infty \leqslant \mathcal{F}(f)$. This gives

$$\inf_{f \in C^\infty(\mathbb{S}),\, f>0} \mathcal{F}(f) = \inf_{f \in C^\infty(\mathbb{S}),\, f>0,\, \mathcal{D}(f)=0} \mathcal{F}(f).$$

Since the set of equilibria is compact (either a single point or one point and a manifold homeomorphic to $\mathbb{S}$), this infimum is a minimum.

Furthermore, if f_0 is not an equilibrium, then $\mathcal{D}(f_0) > 0$, and then $\mathcal{F}(f(t))$ is decreasing in the neighborhood of $t = 0$. So the minimum of $\mathcal{F}$ cannot be reached for f_0.

In the case $\tau \geqslant \frac{1}{n}$, this gives the result since the only equilibrium is the constant function 1. By LaSalle principle, we also get that the solution is converging to in any H^s norm.

In the case $\tau < \frac{1}{n}$, we have that $\mathcal{F}(1 + \varepsilon\omega \cdot \Omega) \sim \frac{1}{n}(\tau - \frac{1}{n})\varepsilon^2$ for a fixed unit vector $\Omega \in \mathbb{S}$, so there exists f_0 such that $\mathcal{F}(f_0) < 0$. Then the uniform distribution cannot be a global minimizer. Since $\mathcal{F}(M_{\kappa(\tau)\Omega})$ is independent of Ω, we get that this value is the minimum. □

4 Convergence to equilibrium

In this section, we establish and study the convergence of the solution to an equilibrium for any initial condition, in the three different regimes, depending whether τ is greater, less, or equal to $\frac{1}{n}$.

4.1 A new entropy, application to the subcritical case $\tau > \frac{1}{n}$

In this section we derive a convex entropy, which shows global decay to the uniform distribution in the case $\tau > \frac{1}{n}$.

We define on $\dot{H}^{-\frac{n-1}{2}}(\mathbb{S})$ the norm $\|\cdot\|_{\widetilde{H}^{-\frac{n-1}{2}}}$ by $\|g\|^2_{\widetilde{H}^{-\frac{n-1}{2}}} = \int_{\mathbb{S}} g\widetilde{\Delta}^{-1}_{n-1}g$, where the conformal Laplacian $\widetilde{\Delta}_{n-1}$ is defined by (2.7). This norm is equivalent to $\|\cdot\|_{\dot{H}^{-\frac{n-1}{2}}}$. We also define $\|\cdot\|_{\widetilde{H}^{-\frac{n-3}{2}}}$ by $\|g\|^2_{\widetilde{H}^{-\frac{n-3}{2}}} = \int_{\mathbb{S}} \Delta g\widetilde{\Delta}^{-1}_{n-1}g$, and this norm is equivalent to the $\|\cdot\|_{\dot{H}^{-\frac{n-3}{2}}}$ norm .

Taking $h = \widetilde{\Delta}^{-1}_{n-1}g$ in the weak formulation (2.13), and using the last part of Lemma 4.1, we obtain a conservation relation:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g\|^2_{\widetilde{H}^{-\frac{n-1}{2}}} = -\tau\|g\|^2_{\widetilde{H}^{-\frac{n-3}{2}}} + \frac{1}{(n-2)!}|J[g]|^2. \tag{4.38}$$

We remark that this is a conservation law between quadratic quantities, as it would be the case for a linear equation.

Since the component of g on the space of spherical harmonics of degree 1 is given by $n\omega \cdot J[g]$, a simple computation shows that the contribution to $\|g\|^2_{\widetilde{H}^{-\frac{n-1}{2}}}$ of this component is equal to $\frac{n}{(n-1)!}|J[g]|^2$. Then the last term of the conservation relation (4.38) is bounded by $\frac{n-1}{n}\|g\|^2_{\widetilde{H}^{-\frac{n-1}{2}}}$. Together with the Poincaré inequality $\|g\|^2_{\widetilde{H}^{-\frac{n-3}{2}}} \geqslant (n-1)\|g\|^2_{\widetilde{H}^{-\frac{n-3}{2}}}$, we get the following estimate:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g\|^2_{\widetilde{H}^{-\frac{n-1}{2}}} \leqslant (n-1)(\tfrac{1}{n}-\tau)\|g\|^2_{\widetilde{H}^{-\frac{n-1}{2}}}.$$

This gives in the case $\tau > \frac{1}{n}$ an exponential decay of rate $(n-1)(\tau - \frac{1}{n})$ for the norm $\|\cdot\|_{\widetilde{H}^{-\frac{n-1}{2}}}$:

$$\|g\|_{\widetilde{H}^{-\frac{n-1}{2}}} \leqslant \|g_0\|_{\widetilde{H}^{-\frac{n-1}{2}}} \exp(-(n-1)(\tau-\tfrac{1}{n})t).$$

In the general case, if $f_0 \in H^s(\mathbb{S})$ with $s > -\frac{n-1}{2}$, we use the estimate (2.30):

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g\|^2_{\dot{H}^s} + \tau\|g\|^2_{\dot{H}^{s+1}} \leqslant \tfrac{C_0}{(N+1)(N+n-1)}\|g\|^2_{\dot{H}^{s+1}} + (n-1)^s|J[g]|^2 + C_0\|f^N - 1\|^2_{\dot{H}^s}.$$

Now we have, since f is a probability measure,

$$(n-1)^s|J[g]|^2 + \|f^N-1\|^2_{\dot{H}^s} \leqslant K_N\|f^N-1\|^2_{\widetilde{H}^{-\frac{n-1}{2}}} \leqslant K_N\|g_0\|^2_{\widetilde{H}^{-\frac{n-1}{2}}} e^{-2(n-1)(\tau-\frac{1}{n})t},$$

the first inequality being the equivalence between norms in finite dimension. For any $\varepsilon < \frac{1}{n}$, taking N sufficiently large, together with Poincaré inequality we get

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g\|^2_{\dot{H}^s} + (n-1)(\tau-\varepsilon)\|g\|^2_{\dot{H}^s} \leqslant C\|g_0\|^2_{\widetilde{H}^{-\frac{n-1}{2}}} e^{-2(n-1)(\tau-\frac{1}{n})t},$$

where the constant C depends only on s.

Solving this equation, we get

$$\|g\|^2_{\dot{H}^s} \leqslant \|g_0\|^2_{\dot{H}^s} e^{-2(n-1)(\tau-\varepsilon)t} + \tfrac{C}{(n-1)(\frac{1}{n}-\varepsilon)}\|g_0\|^2_{\widetilde{H}^{-\frac{n-1}{2}}} e^{-2(n-1)(\tau-\frac{1}{n})t}.$$

Taking for example $\varepsilon = \frac{1}{2n}$, since $s > -\frac{n-1}{2}$, we get

$$\|g\|^2_{\dot{H}^s} \leqslant (1 + 2\widetilde{C}_{\frac{n}{n-1}})\|g_0\|^2_{\dot{H}^s} e^{-2(n-1)(\tau-\frac{1}{n})t}.$$

In summary, we have the following theorem:

Theorem 4.2. *New entropy. For a given probability density function f, we define the quantities $\mathcal{H}(f) = \|f-1\|^2_{\widetilde{H}^{-\frac{n-1}{2}}}$ and $\widetilde{\mathcal{D}}(f) = 2\tau\|f-1\|^2_{\widetilde{H}^{-\frac{n-3}{2}}} - \frac{2}{(n-2)!}|J[f]|^2$.*

We have a conservation relation, for any solution f of Doi equation (1.3)*:*

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(f) + \widetilde{\mathcal{D}}(f) = 0. \tag{4.39}$$

When $\tau \geqslant \frac{1}{n}$, the term $\widetilde{\mathcal{D}}(f)$ is nonnegative, so the new entropy $\mathcal{H}(f)$ is decreasing in time.

Furthermore, if $\tau > \frac{1}{n}$, then in any Sobolev space $H^s(\mathbb{S})$ with $s \geqslant -\frac{n-1}{2}$, we have global exponential decay of the solution to the uniform distribution, with rate given by $(n-1)(\tau - \frac{1}{n})$.

More precisely there is a constant C depending only on s such that for all initial condition $f_0 \in H^s(\mathbb{S})$, we have

$$\|f-1\|_{H^s} \leqslant C\|f_0 - 1\|_{H^s} e^{-(n-1)(\tau-\frac{1}{n})t}.$$

Let us do a small remark here. Actually this conservation relation is true for any solution, without any positivity condition. We only need the mean of f to be 1. And since we have existence and uniqueness in small time for any initial condition, with the same instantaneous regularity results (only valid for a short time existence), we get that the solution belongs to $H^{-\frac{n-1}{2}}(\mathbb{S})$ at some time. But the conservation relation gives then that we have a global solution. So we can state a stronger theorem of existence and uniqueness:

Theorem 4.3. *Given an initial condition f_0 in $H^s(\mathbb{S})$ (not necessarily nonnegative), there exists a unique weak solution f of* (1.3) *such that $f(0) = f_0$. This solution is global in time (the definition 2.1 is valid for any time $T > 0$). Moreover, f is a classical solution, belonging to $C^\infty((0,+\infty)\times\mathbb{S})$ (and even analytic in space, see Appendix A.2).*

Remark 4.1. *In this case, we do not have any uniform bound on $H^s(\mathbb{S})$, and we can derive the same existence theorem for the case $\tau = 0$ (see Remark 2.2), but only for the case $s \geqslant -\frac{n-1}{2}$ (which does not include all Radon signed-measures).*

Another remark is that if we change the sign in front of the alignment term in Doi equation (1.3) *(taking $K(\omega,\bar{\omega}) = \omega\cdot\bar{\omega}$, every particle tends to go away from the mean direction), then we can derive a conservation relation in the same way. But here the "dissipation term" is $\widetilde{\mathcal{D}}(f) = 2\tau\|f-1\|^2_{\widetilde{H}^{-\frac{n-3}{2}}} + \frac{2}{(n-2)!}|J[f]|^2 \geqslant 2\tau(n-1)\mathcal{H}(f)$, without any condition on $\tau > 0$. So in any Sobolev space $H^s(\mathbb{S})$, with $s \geqslant -\frac{n-1}{2}$ we have global exponential decay of the solution to the uniform distribution, with rate $(n-1)\tau$.*

4.2 Study of the supercritical case $\tau < \frac{1}{n}$

In this section, we fix $\tau < \frac{1}{n}$ and we study the behavior of a solution as $t \to +\infty$. We will write κ for $\kappa(\tau)$ and c for $c(\kappa(\tau))$. We first establish that the limit set of equilibria $\mathcal{E}_\infty$ given by LaSalle principle (Proposition 3.2) depends only on the fact that $J[f_0]$ is zero or not.

Proposition 4.1. *If $J[f_0] = 0$ then $\mathcal{E}_\infty$ is reduced to the uniform distribution. Equation* (1.3) *becomes the heat equation. We have exponential decay to the uniform distribution with rate $2n\tau$ in any $H^s(\mathbb{S})$.*

If $J[f_0] \neq 0$ then $J[f(t)] \neq 0$ for all $t > 0$. The limit set $\mathcal{E}_\infty = \{M_{\kappa\Omega}, \Omega \in \mathbb{S}\}$ consists in all the non-isotropic equilibria. Furthermore, we have for any $s \in \mathbb{R}$,

$$\lim_{t\to\infty} \|f(t) - M_{\kappa\Omega(t)}\|_{H^s} = 0, \tag{4.40}$$

where $\Omega(t) = \frac{J[f(t)]}{|J[f(t)]|}$ is the mean direction of $f(t)$.

Proof. First of all, we write the equation for $J[f]$, multiplying equation (1.3) and integrating on the sphere. We get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}J[f] &= -\tau(n-1)J[f] + \left(\int_{\mathbb{S}} (\mathrm{Id} - \omega\otimes\omega)\, f\, \mathrm{d}\omega\right) J[f] \\ &= \left((1-(n-1)\tau)\mathrm{Id} - \int_{\mathbb{S}} \omega\otimes\omega\, f\right) J[f],\end{aligned} \tag{4.41}$$

which can be viewed as a first order linear ODE of the form $\frac{\mathrm{d}}{\mathrm{d}t}J[f] = M(t)J[f]$. The matrix M is a smooth function of time, so we have a global unique solution. Consequently, if $J[f(t_0)] = 0$ for $t_0 \geqslant 0$, then we have $J[f(t)] = 0$, for all $t \geqslant 0$, and equation (1.3) reduces to the heat equation. The distribution f has no component on the first eigenspace of the Laplace–Beltrami operator, and the second eigenvalue is $2n$, so we have exponential decay with rate $2n\tau$ in any H^s norm.

Now we suppose that $J[f_0] \neq 0$, so by the previous argument we have $J[f(t)] \neq 0$ for all $t \geqslant 0$. There are two possibilities for the limiting set, either the uniform distribution, or the set $\{M_{\kappa\Omega}, \Omega \in \mathbb{S}\}$ (by Proposition 3.4, they do not have the same level of free energy).

In the first case, by LaSalle principle, $f(t)$ converges to the uniform distribution. Then the matrix $M(t) = (1-(n-1)\tau)\mathrm{Id} - \int_{\mathbb{S}} \omega\otimes\omega\, f$ converges to $(n-1)(\frac{1}{n} - \tau)\mathrm{Id}$. Using the ODE for $J[f]$, we get

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|J[f]|^2 = J[f]\cdot M(t)J[f] \geqslant ((n-1)(\tfrac{1}{n} - \tau) - \varepsilon)|J[f]|^2,$$

for t sufficiently large. Taking ε sufficiently small, we get that $|J[f]|$ tends to infinity, which is a contradiction.

So we have that $\mathcal{E}_\infty = \{M_{\kappa\Omega}, \Omega \in \mathbb{S}\}$. Now suppose that $\|f(t) - M_{\kappa\Omega(t)}\|_{H^s}$ does not tend to 0. We take t_n tending to infinity such that $\|f(t_n) - M_{\kappa\Omega(t_n)}\|_{H^s} \geqslant \varepsilon > 0$. By our LaSalle principle, there exists $\Omega_n \in \mathbb{S}$ such that $\|f(t_n) - M_{\kappa\Omega_n}\|_{H^s} \to 0$. Up to extracting, we can suppose that $\Omega_n \to \Omega_\infty \in \mathbb{S}$, so $f(t_n) \to M_{\kappa\Omega_\infty}$ in $H^s(\mathbb{S})$. In particular we have that $J[f(t_n)] \to c(\kappa)\Omega_\infty$, and then $\Omega(t_n) \to \Omega_\infty$. Then $M_{\kappa\Omega(t_n)}$ converges to $M_{\kappa\Omega_\infty}$, giving that $\|f(t_n) - M_{\kappa\Omega(t_n)}\|_{H^s} \to 0$, which is a contradiction. □

Now we focus on the case $J[f_0] \neq 0$. We define $\Omega(t)$ as in the previous proposition, and we will expand the solution around $M_{\kappa\Omega(t)}$. We first show the convergence in $L^2(\mathbb{S})$ to a given equilibrium, with exponential rate, assuming conditions on the initial data.

Proposition 4.2. *There exists an "asymptotic rate" $r_\infty(\tau) > 0$ satisfying the following property.*

Suppose that $\|f(t) - M_{\kappa\Omega(t)}\|_{H^s}$ is uniformly bounded on $[t_0, +\infty)$ by a constant K, with $s > \frac{3(n-1)}{2}$. Then for all $r < r_\infty(\tau)$, there exists $\Omega_\infty \in \mathbb{S}$ and $\delta, C > 0$, such that if $\|f(t_0) - M_{\kappa\Omega(t_0)}\|_{L^2} \leqslant \delta$, we have

$$\|f(t) - M_{\kappa\Omega_\infty}\|_{L^2} \leqslant C\|f(t_0) - M_{\kappa\Omega(t_0)}\|_{L^2} e^{-r(t-t_0)}.$$

The constants δ and C depend only on τ, s, K, and r. Moreover, as $\tau \to \frac{1}{n}$, we have that $r_\infty(\tau) \geqslant 2(n-1)(\frac{1}{n} - \tau) + O((\frac{1}{n} - \tau)^{\frac{3}{2}})$.

Proof. We first introduce some notations. When there is no confusion, we just write Ω for $\Omega(t)$, and we will always assume $t \geqslant t_0$. We write $\cos\theta = \omega \cdot \Omega$. We denote by $\langle\cdot\rangle_{M_{\kappa\Omega}}$ the mean of a function against the probability measure $M_{\kappa\Omega}$.

We have the following identities (we recall, by Lemma 4.2, that $\beta = c^2 + n\tau - 1$ is positive):

$$\begin{aligned} \langle\omega\rangle_{M_{\kappa\Omega}} &= \langle\cos\theta\rangle_{M_{\kappa\Omega}}\Omega = c\,\Omega, \\ \langle\cos^2\theta\rangle_{M_{\kappa\Omega}} &= 1 - (n-1)\tau, \\ \langle(\cos\theta - c)^2\rangle_{M_{\kappa\Omega}} &= 1 - (n-1)\tau - c^2 = \tau - \beta > 0. \end{aligned} \tag{4.42}$$

We can write $f = (1+h)M_{\kappa\Omega}$, then we have $\langle h\rangle_{M_{\kappa\Omega}} = 0$. Since Ω is the direction of $J[f] = \langle(1+h)\omega\rangle_{M_{\kappa\Omega}}$, we get that $\langle h\omega\rangle_{M_{\kappa\Omega}} = \langle h\cos\theta\rangle_{M_{\kappa\Omega}}\Omega$.

So we can do an expansion of the free energy and its dissipation in terms of h. Since we know that $M_{\kappa\Omega(t)}$ is a critical point of $\mathcal{F}$, we already know that the expansion of $\mathcal{F}((1+h)M_{\kappa\Omega}) - \mathcal{F}(M_{\kappa\Omega})$ will contain no term of order 0 and 1 in h. We get, using (3.31),

$$\mathcal{F}((1+h)M_{\kappa\Omega}) - \mathcal{F}(M_{\kappa\Omega}) = \tau\tfrac{1}{2}\langle h^2\rangle_{M_{\kappa\Omega}} - \tfrac{1}{2}|\langle h\omega\rangle_{M_{\kappa\Omega}}|^2 + O(\|h\|_\infty^3).$$

Using Sobolev embedding and interpolation, we have (writing C for a generic constant, depending only on τ, s, and K)

$$\|f - M_{\kappa\Omega}\|_\infty \leqslant C\|f - M_{\kappa\Omega}\|_{H^{\frac{n-1}{2}}} \leqslant C\|f - M_{\kappa\Omega}\|_{L^2}^{1-\frac{n-1}{2s}} K^{\frac{n-1}{2s}}.$$

So since $1 - \frac{n-1}{2s} > \frac{2}{3}$ and $f - M_{\kappa\Omega} = hM_{\kappa\Omega}$, with $M_{\kappa\Omega}$ uniformly bounded below and above, we get that $\|h\|_\infty^3 = o(\langle h^2\rangle_{M_{\kappa\Omega}})$ (and more precisely, for any $\varepsilon > 0$ there exists $\eta > 0$ depending only on ε, τ, s, and K such that $\|h\|_\infty^3 \leqslant \varepsilon\langle h^2\rangle_{M_{\kappa\Omega}}$ as soon as $\langle h^2\rangle_{M_{\kappa\Omega}} \leqslant \eta$). We get

$$\mathcal{F}(f) - \mathcal{F}(M_{\kappa\Omega}) = \tfrac{1}{2}[\tau\langle h^2\rangle_{M_{\kappa\Omega}} - \langle h\cos\theta\rangle_{M_{\kappa\Omega}}^2] + o(\langle h^2\rangle_{M_{\kappa\Omega}}). \tag{4.43}$$

We use the definition (3.32) of $\mathcal{D}(f)$:

$$\begin{aligned} D(f) &= \langle (1+h)|\nabla(\tau \ln(M_{\kappa\Omega}(1+h)) - \langle (1+h)\omega\rangle_{M_{\kappa\Omega}} \cdot \omega)|^2\rangle_{M_{\kappa\Omega}} \\ &= \langle (1+h)|\nabla(\tau \ln(1+h) - \langle h\cos\theta\rangle_{M_{\kappa\Omega}} \cos\theta)|^2\rangle_{M_{\kappa\Omega}} \\ &\geqslant (1-\|h\|_\infty)\langle |\nabla(\tau \ln(1+h) - \langle h\cos\theta\rangle_{M_{\kappa\Omega}} \cos\theta)|^2\rangle_{M_{\kappa\Omega}}. \end{aligned}$$

Now we can derive a Poincaré inequality of the form

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

Indeed, we use the fact that $M_{\kappa\Omega}$ is positive and bounded:

$$\begin{aligned} \langle |\nabla g|^2\rangle_{M_{\kappa\Omega}} &\geqslant \min M_{\kappa\Omega} \int_{\mathbb{S}} |\nabla g|^2 \\ &\geqslant \min M_{\kappa\Omega}(n-1) \int_{\mathbb{S}} (g - \textstyle\int_{\mathbb{S}} g)^2 \\ &\geqslant \frac{\min M_{\kappa\Omega}}{\max M_{\kappa\Omega}}(n-1)\langle (g - \textstyle\int_{\mathbb{S}} g)^2\rangle_{M_{\kappa\Omega}} \\ &\geqslant (n-1)e^{-2\kappa}\langle (g - \langle g\rangle_{M_{\kappa\Omega}})^2\rangle_{M_{\kappa\Omega}}. \end{aligned} \tag{4.44}$$

Actually this is a rough estimate, we have here $\Lambda_\kappa \geqslant (n-1)e^{-2\kappa}$, a more precise study of Λ_κ can be done using separation of variable, and is given in the appendix of Chapter 2. The problem then reduces to finding the smallest eigenvalue of a one-dimensional Sturm-Liouville problem, but even in that case, we did not manage to find a better estimate for now.

So we finally get

$$\begin{aligned} \mathcal{D}(f) &\geqslant (1-\|h\|_\infty)\Lambda_\kappa \langle [\tau \ln(1+h) - \tau\langle \ln(1+h)\rangle_{M_{\kappa\Omega}} - \langle h\cos\theta\rangle_{M_{\kappa\Omega}}(\cos\theta - c)]^2\rangle_{M_{\kappa\Omega}} \\ &\geqslant (1-\|h\|_\infty)\Lambda_\kappa \langle [\tau h - \langle h\cos\theta\rangle_{M_{\kappa\Omega}}(\cos\theta - c) + O(\|h\|_\infty^2)]^2\rangle_{M_{\kappa\Omega}} \\ &\geqslant (1-\|h\|_\infty)\Lambda_\kappa (\tau^2\langle h^2\rangle_{M_{\kappa\Omega}} - (\beta+\tau)\langle h\cos\theta\rangle^2_{M_{\kappa\Omega}}) + O(\|h\|_\infty^3). \end{aligned}$$

With the same argument as before, we get that

$$\mathcal{D}(f) \geqslant \Lambda_\kappa (\tau^2\langle h^2\rangle_{M_{\kappa\Omega}} - (\beta+\tau)\langle h\cos\theta\rangle^2_{M_{\kappa\Omega}}) + o(\langle h^2\rangle_{M_{\kappa\Omega}}). \tag{4.45}$$

The goal is now to express the bounds in (4.45) and (4.43) as the sum of positive terms. Indeed, we expect to have a Grönwall's inequality which will give a rate of convergence.

We set $\alpha = \frac{1}{\tau-\beta}\langle h\cos\theta\rangle_{M_{\kappa\Omega}}$, and we write $h = \alpha(\cos\theta - c) + g$. Using (4.42) we have that α is well defined since $\tau - \beta > 0$ and we get $\langle g\rangle_{M_{\kappa\Omega}} = 0$ and $\langle g\omega\rangle_{M_{\kappa\Omega}} = 0$.

Plugging $\langle h^2\rangle_{M_{\kappa\Omega}} = (\tau-\beta)\alpha^2 + \langle g^2\rangle_{M_{\kappa\Omega}}$ into (4.43) and (4.45) gives

$$\begin{aligned} \mathcal{F}(f) - \mathcal{F}(M_{\kappa\Omega}) &= \tfrac{1}{2}[\beta(\tau-\beta)\alpha^2 + \tau\langle g^2\rangle_{M_{\kappa\Omega}}] + o(\langle h^2\rangle_{M_{\kappa\Omega}}), \\ \mathcal{D}(f) &\geqslant \Lambda_\kappa(\beta^2(\tau-\beta)\alpha^2 + \tau^2\langle g^2\rangle_{M_{\kappa\Omega}}) + o(\langle h^2\rangle_{M_{\kappa\Omega}}) \\ &\geqslant \Lambda_\kappa\beta(\beta(\tau-\beta)\alpha^2 + \tau\langle g^2\rangle_{M_{\kappa\Omega}}) + o(\langle h^2\rangle_{M_{\kappa\Omega}}). \end{aligned} \tag{4.46}$$

So for all $r < \Lambda_\kappa\beta$, if $\langle h^2\rangle_{M_{\kappa\Omega}}$ is sufficiently small, we have $\mathcal{D}(f) \geqslant r(\mathcal{F}(f) - \mathcal{F}(M_{\kappa\Omega}))$. Using the conservation relation (4.39), there exists $\delta_0 > 0$ (depending only on τ, s, K and r) such that if $\|f(t) - M_{\kappa\Omega(t)}\|_{L^2} \leqslant \delta_0$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathcal{F}(f) - \mathcal{F}(M_{\kappa\Omega})] = -\mathcal{D}(f) \leqslant -2r[\mathcal{F}(f) - \mathcal{F}(M_{\kappa\Omega})].$$

Then we obtain, for all T, such that $\|f - M_{\kappa\Omega}\|_{L^2} \leqslant \delta_0$ on $[t_0, T]$,

$$\mathcal{F}(f(T)) - \mathcal{F}(M_{\kappa\Omega(T)}) \leqslant [\mathcal{F}(f(t_0)) - \mathcal{F}(M_{\kappa\Omega(t_0)})]e^{-2r(T-t_0)},$$

and then, using the estimate (4.46), we get that for $t \in [t_0, T]$,

$$\|f - M_{\kappa\Omega}\|_{L^2} \leqslant C_0\|f(t_0) - M_{\kappa\Omega(t_0)}\|_{L^2}e^{-r(t-t_0)}. \tag{4.47}$$

So if we take $\delta < \frac{\delta_0}{C_0} \leqslant \delta_0$, and we start with $\|f(t_0) - M_{\kappa\Omega(t_0)}\|_{L^2} \leqslant \delta$, we get that $\|f - M_{\kappa\Omega}\|_{L^2} \leqslant \delta_0$ on $[t_0, T]$ for all $T \geqslant t_0$. Otherwise, the largest of such a T would satisfy $\delta_0 = \|f(T) - M_{\kappa\Omega(T)}\|_{L^2} \leqslant C\delta e^{-r(T-t_0)} < \delta_0$. So the inequality (4.47) holds for all $t \in [t_0, +\infty)$.

It remains to prove that $\Omega(t)$ converges to some Ω_∞, if we want to have strong convergence to a given steady state. This is possible using the ODE satisfied by Ω.

Indeed, we have $J[f] = c\Omega + \langle h\omega\rangle_{M_{\kappa\Omega}} = (c + \alpha(\tau - \beta))\Omega$, and then

$$\frac{\mathrm{d}}{\mathrm{d}t}J[f] = (c + \alpha(\tau - \beta))\frac{\mathrm{d}}{\mathrm{d}t}\Omega + (\tau - \beta)\Omega\frac{\mathrm{d}}{\mathrm{d}t}\alpha.$$

So applying $\mathrm{Id} - \Omega \otimes \Omega$ to the ODE (4.41) gives an ODE for Ω, in terms of α and g. We get

$$\begin{aligned}(\mathrm{Id} - \Omega \otimes \Omega)\frac{\mathrm{d}}{\mathrm{d}t}J[f] &= -(\mathrm{Id} - \Omega \otimes \Omega)\left(\int_{\mathbb{S}} \omega \otimes \omega\, f\, \mathrm{d}\omega\right) J[f] \\ &= -(c + \alpha(\tau - \beta))(\mathrm{Id} - \Omega \otimes \Omega)[\langle h\cos\theta\,\omega\rangle_{M_{\kappa\Omega}} + \langle\cos\theta\,\omega\rangle_{M_{\kappa\Omega}}].\end{aligned}$$

Since $\langle(\cos\theta - c)\cos\theta\,\omega\rangle_{M_{\kappa\Omega}}$ and $\langle\cos\theta\,\omega\rangle_{M_{\kappa\Omega}}$ are parallel to Ω, we get that

$$(c + \alpha(\tau - \beta))\frac{\mathrm{d}\Omega}{\mathrm{d}t} = -(c + \alpha(\tau - \beta))(\mathrm{Id} - \Omega \otimes \Omega)\langle g\cos\theta\,\omega\rangle_{M_{\kappa\Omega}}.$$

Since $(c + \alpha(\tau - \beta))$ is the norm of $J[f]$, it is never zero, and we get (the notation C standing for a generic constant depending only on r, s, τ and K)

$$\left|\frac{\mathrm{d}\Omega}{\mathrm{d}t}\right| \leqslant C\sqrt{\langle g^2\rangle_{M_{\kappa\Omega}}} \leqslant C\|f - M_{\kappa\Omega}\|_{L^2}.$$

So we have exponential decay of $\frac{\mathrm{d}\Omega}{\mathrm{d}t}$ with rate r, in particular Ω is converging to some $\Omega_\infty \in \mathbb{S}$. More precisely,

$$|\Omega(t) - \Omega_\infty| \leqslant \int_t^\infty |\tfrac{\mathrm{d}\Omega}{\mathrm{d}t}|\mathrm{d}t \leqslant C\|f(t_0) - M_{\kappa\Omega(t_0)}\|_{L^2}e^{-r(t-t_0)}.$$

Now we have that $\|M_{\kappa\Omega(t)} - M_{\kappa\Omega_\infty}\|_{L^2} \leqslant C|\Omega(t) - \Omega_\infty|$ (the function $\Omega \mapsto e^{\kappa\omega\cdot\Omega}$ from $\mathbb{S}$ to $\mathbb{R}$ is globally Lipschitz with a constant independent of $\omega \in \mathbb{S}$). So we get the final estimation:

$$\|f - M_{\kappa\Omega_\infty}\|_{L^2} \leqslant \|f - M_{\kappa\Omega}\|_{L^2} + \|M_{\kappa\Omega(t)} - M_{\kappa\Omega_\infty}\|_{L^2} \leqslant C\|f(t_0) - M_{\kappa\Omega(t_0)}\|_{L^2}e^{-r(t-t_0)}.$$

So the proposition is true with $r_\infty(\tau) = \Lambda_\kappa\beta > 0$. By the estimate (4.44), we know that $\Lambda_\kappa \geqslant (n-1)e^{-2\kappa}$. And by the expansions of c and κ as $\tau \to \frac{1}{n}$ given in (3.37), we get that $r_\infty(\tau) \geqslant 2(n-1)(\frac{1}{n} - \tau) + O((\frac{1}{n} - \tau)^{\frac{3}{2}})$. □

By Proposition 4.1, we have that $f(t) - M_{\kappa\Omega(t)}$ tends to zero in any $H^s(\mathbb{S})$. So the hypotheses of Proposition 4.2, for any $r < r_\infty(\tau)$, are satisfied for some $t_0 > 0$.

Once more, by interpolation and uniform boundedness on $[t_0, +\infty)$ of the H^p norm, we have

$$\begin{aligned}\|f - M_{\kappa\Omega_\infty}\|_{H^s} &\leqslant C\|f - M_{\kappa\Omega_\infty}\|_{L^2}^{1-\frac{s}{p}}\|f - M_{\kappa\Omega_\infty}\|_{H^p}^{\frac{s}{p}} \\ &\leqslant \widetilde{C}\|f(t_0) - M_{\kappa\Omega(t_0)}\|_{L^2}^{1-\frac{s}{p}} e^{-r(1-\frac{s}{p})(t-t_0)},\end{aligned}$$

so taking p sufficiently large, we also get exponential convergence for the H^s norm, with rate $r(1-\delta)$ for any $\delta > 0$.

Finally we have that for all $r < r_\infty(\tau)$ and s, there exists some time t_0 and $C > 0$ such that $\|f - M_{\kappa\Omega_\infty}\|_{H^s} \leqslant Ce^{-rt}$ for $t \geqslant t_0$. We can even get rid of the constant C since for any $\widetilde{r} < r$ and t sufficiently large $Ce^{-rt} \leqslant e^{-\widetilde{r}t}$.

4.3 Study of the critical case $\tau = \frac{1}{n}$

For any $\tau \in (0, +\infty) \setminus \{\frac{1}{n}\}$, we have exponential convergence to some equilibrium. However the rate of convergence tends to 0 when τ is close to $\frac{1}{n}$ (in the case where $J[f_0] \neq 0$). So we do not expect to have a similar rate of convergence in the critical case.

First of all, we know by Proposition 3.4 that the solution converges (in any $H^s(\mathbb{S})$) to the uniform distribution as time goes to infinity. The goal of this section is to estimate the speed of convergence to this equilibrium.

Proposition 4.3. *Suppose that $\|f(t) - 1\|_{H^s}$ is uniformly bounded on $[t_0, +\infty)$ by a constant K, with $s > \frac{7(n-1)}{2}$.*

Then for all $C > 1$, there exists $\delta > 0$, such that if $\|f(t_0) - 1\|_{L^2} \leqslant \delta$, we have, for $t \geqslant t_0$,

$$\|f(t) - 1\|_{L^2} \leqslant \frac{C}{\sqrt{\frac{1}{\sqrt{2(n+2)}\|f(t_0)-1\|_{L^2}} + \frac{2(n-1)}{n(n+2)}(t - t_0)}}.$$

The constant δ depends only on τ, s, K, and C.

Proof. As in the previous section, we work on $[t_0, +\infty)$. We write $f = 1 + h$ and as in the previous case, we suppose that $J[f_0] \neq 0$. By the same argument used in Proposition 4.1, we have that $J[f(t)] \neq 0$ for all $t > 0$, so we define $\Omega(t)$ as the unit vector $\frac{J[f(t)]}{|J[f(t)]|}$. Similarly we denote $\langle\cdot\rangle$ for the mean of a function on the unit sphere and $\cos\theta$ for $\omega \cdot \Omega$.

We have $\langle h\rangle = 0$. Since Ω is the direction of $J[f] = \langle(1 + h)\omega\rangle = \langle h\omega\rangle$, we get that $\langle h\omega\rangle = \langle h\cos\theta\rangle\Omega$.

We perform an expansion of the free energy and its dissipation in terms of h. We get, using (3.31) and taking $\tau = \frac{1}{n}$,

$$\mathcal{F}(1 + h) = \tfrac{1}{n}(\tfrac{1}{2}\langle h^2\rangle - \tfrac{1}{6}\langle h^3\rangle + \tfrac{1}{12}\langle h^4\rangle) - \tfrac{1}{2}\langle h\cos\theta\rangle^2 + O(\|h\|_\infty^5).$$

Now we write $\alpha = n\langle h\cos\theta\rangle$ and we define

$$g = h - \alpha\cos\theta - \tfrac{1}{2}\alpha^2(\cos^2\theta - \tfrac{1}{n}) - \tfrac{1}{6}\alpha^3(\cos^3\theta - \tfrac{3}{n+2}\cos\theta). \tag{4.48}$$

We have $\langle \cos^4\theta\rangle = \frac{3}{n(n+2)}$ (we have used the formula (3.36) to compute $\frac{4!a_2}{a_0} = \langle\cos^4\theta\rangle$). Since we have $\langle\cos^3\theta\rangle = \langle\cos\theta\rangle = 0$, and $\langle\cos^2\theta\rangle = \frac{1}{n}$, we get $\langle g\rangle = \langle g\cos\theta\rangle = 0$. We will see that the terms of order 2 in g will not vanish in the expansion of the free energy and the dissipation term. But we will need to expand the free energy in α up to order 4, and the dissipation term up to order 6 in α. We have

$$\begin{aligned}
\tfrac{1}{2}\langle h^2\rangle &= \tfrac{1}{2}\langle g^2\rangle + \tfrac{1}{2n}\alpha^2 + \tfrac{n-1}{4n^2(n+2)}\alpha^4 + \tfrac{1}{2}\alpha^2\langle g\cos^2\theta\rangle + O(\alpha^3\|g\|_\infty + \alpha^5), \qquad (4.49)\\
-\tfrac{1}{6}\langle h^3\rangle &= -\tfrac{n-1}{2n^2(n+2)}\alpha^4 - \tfrac{1}{2}\alpha^2\langle g\cos^2\theta\rangle + O(\|g\|_\infty^3 + \alpha\|g\|_\infty^2 + \alpha^3\|g\|_\infty + \alpha^5),\\
\tfrac{1}{12}\langle h^4\rangle &= \tfrac{1}{4n(n+2)}\alpha^4 + O(\|g\|_\infty^4 + \alpha\|g\|_\infty^3 + \alpha^2\|g\|_\infty^2 + \alpha^3\|g\|_\infty + \alpha^5).
\end{aligned}$$

We finally get

$$\mathcal{F}(1+h) = \tfrac{1}{2n}\langle g^2\rangle + \tfrac{1}{4n^3(n+2)}\alpha^4 + O(\|g\|_\infty^3 + \alpha\|g\|_\infty^2 + \alpha^3\|g\|_\infty + \alpha^5). \qquad (4.50)$$

Using the inequality $a^p b^q \leqslant sa^{\frac{p}{s}} + (1-s)b^{\frac{q}{1-s}}$ for $s\in(0,1)$, with $a=\alpha$ and $b=\|g\|_\infty$, we get that $\alpha\|g\|_\infty^2 \leqslant \frac{1}{5}\alpha^5 + \frac{4}{5}\|g\|_\infty^{2+\frac{1}{2}}$ and $\alpha^3\|g\|_\infty \leqslant \frac{3}{5}\alpha^5 + \frac{2}{5}\|g\|_\infty^{2+\frac{1}{2}}$.

By Sobolev embedding and interpolation, as in the previous section, we have

$$\|g\|_\infty \leqslant C\|g\|_{L^2}^{1-\frac{n-1}{2s}}\|g\|_{H^s}^{\frac{n-1}{2s}}, \qquad (4.51)$$

with $1-\frac{n-1}{2s} > \frac{6}{7}$.

Since α is controlled by $\|h\|_{H^s}$, using the definition (4.48) of g, we have a bound for $\|g\|_{H^s}$ on $[t_0,+\infty)$, depending only on s and K. We finally get $\|g\|_\infty^{2+\frac{1}{2}} \leqslant C\langle g^2\rangle^\mu$, with $\mu > \frac{1}{2}(2+\frac{1}{2})\frac{6}{7} > 1$.

So using (4.49) and (4.50), we get that for any $\varepsilon>0$, there exists $\delta>0$ such if $\|h\|_{L^2}\leqslant\delta$, we have

$$\begin{aligned}
(1-\varepsilon)(\langle g^2\rangle + \tfrac{1}{n}\alpha^2) \leqslant \langle h^2\rangle &\leqslant (1+\varepsilon)(\langle g^2\rangle + \tfrac{1}{n}\alpha^2)\\
(1-\varepsilon)(\tfrac{1}{2n}\langle g^2\rangle + \tfrac{1}{4n^3(n+2)}\alpha^4) \leqslant \mathcal{F}(1+h) &\leqslant \tfrac{1+\varepsilon}{4n^3(n+2)}(2n^2(n+2)\langle g^2\rangle + \alpha^4). \qquad (4.52)
\end{aligned}$$

From that, up to take a smaller δ, we obtain

$$\tfrac{1-\varepsilon}{1+\varepsilon}\,2n\mathcal{F}(1+h) \leqslant \langle h^2\rangle \leqslant \tfrac{1+\varepsilon}{\sqrt{1-\varepsilon}}\,2\sqrt{n(n+2)\mathcal{F}(1+h)}. \qquad (4.53)$$

We now estimate the dissipation term. We use the definition (3.32) of $\mathcal{D}(f)$ and the Poincaré inequality to get:

$$\begin{aligned}
\mathcal{D}(f) &= \langle(1+h)|\nabla(\tfrac{1}{n}\ln(1+h) - \langle(1+h)\omega\rangle\cdot\omega)|^2\rangle\\
&= \langle(1+h)|\nabla(\tfrac{1}{n}\ln(1+h) - \langle h\cos\theta\rangle\cos\theta)|^2\rangle\\
&\geqslant \tfrac{n-1}{n^2}(1-\|h\|_\infty)\langle[\underbrace{\ln(1+h) - \langle\ln(1+h)\rangle - n\langle h\cos\theta\rangle\cos\theta}_{\mathcal{S}(h)}]^2\rangle. \qquad (4.54)
\end{aligned}$$

We have

$$\begin{aligned}
\mathcal{S}(h) &= \ln(1+h) - \langle\ln(1+h)\rangle - n\langle h\cos\theta\rangle\cos\theta\\
&= h - \langle h\rangle - \alpha\cos\theta - \tfrac{1}{2}(h^2 - \langle h^2\rangle) + \tfrac{1}{3}(h^3 - \langle h^3\rangle) + O(\|h\|^4).
\end{aligned}$$

We compute,

$$\begin{aligned} h - \langle h\rangle - \alpha\cos\theta &= g + \frac{1}{2}\alpha^2(\cos^2\theta - \tfrac{1}{n}) + \tfrac{1}{6}\alpha^3(\cos^3\theta - \tfrac{3}{n+2}\cos\theta) \\ -\tfrac{1}{2}(h^2 - \langle h^2\rangle) &= -\tfrac{1}{2}(\alpha^2 + \alpha^3\cos\theta)(\cos^2\theta - \tfrac{1}{n}) + O(\|g\|^2 + \alpha\|g\|_\infty + \alpha^4) \\ \tfrac{1}{3}(h^3 - \langle h^3\rangle) &= \tfrac{1}{3}\alpha^3\cos^3\theta + O(\|g\|_\infty^3 + \alpha\|g\|_\infty^2 + \alpha^2\|g\|_\infty + \alpha^4). \end{aligned}$$

So

$$\begin{aligned} \langle \mathcal{S}(h)^2\rangle &= \langle [g + \tfrac{1}{6}\alpha^3(\tfrac{3}{n} - \tfrac{3}{n+2})\cos\theta)]^2\rangle + O(\|g\|^3 + \alpha\|g\|^2 + \alpha^4\|g\|_\infty + \alpha^7) \\ &= \langle g^2\rangle + \tfrac{1}{n^3(n+2)^2}\alpha^6 + O(\|g\|_\infty^3 + \alpha\|g\|_\infty^2 + \alpha^4\|g\|_\infty + \alpha^7). \end{aligned} \tag{4.55}$$

As before, we get that $\alpha\|g\|_\infty^2 \leqslant \frac{1}{7}\alpha^7 + \frac{6}{7}\|g\|_\infty^{2+\frac{1}{3}}$ and $\alpha^4\|g\|_\infty \leqslant \frac{4}{7}\alpha^7 + \frac{3}{7}\|g\|_\infty^{2+\frac{1}{3}}$. Using (4.51), we get $\|g\|_\infty^{2+\frac{1}{3}} \leqslant C\langle g^2\rangle^\mu$, with $\mu > \frac{1}{2}(2+\frac{1}{3})\frac{6}{7} = 1$. So using (4.54) and (4.55), up to take a smaller δ, we have, for $\|h\|_{L^2} \leqslant \delta$,

$$\mathcal{D}(f) \geqslant (1-\varepsilon)\tfrac{n-1}{n^2}(\langle g^2\rangle + \tfrac{1}{n^3(n+2)^2}\alpha^6).$$

Now for any $C, C' > 0$, if we take α and g sufficiently small (so again up to take a smaller δ), we have that $C\langle g^2\rangle + \alpha^6 \geqslant (C'\langle g^2\rangle + \alpha^4)^{\frac{3}{2}}$. So we get

$$\mathcal{D}(f) \geqslant (1-\varepsilon)\tfrac{n-1}{n^5(n+2)^2}(2n^2(n+2)\langle g^2\rangle + \alpha^4)^{\frac{3}{2}}.$$

Putting this together with (4.52) and the conservation relation (4.39), we get that for any $0 < \varepsilon < 1$, there exists $\delta_0 > 0$ such, as soon as $\|h\|_{L^2} \leqslant \delta_0$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(f) = -\mathcal{D}(f) \leqslant -\frac{8(n-1)(1-\varepsilon)}{(1+\varepsilon)^{\frac{3}{2}}\sqrt{n(n+2)}}[\mathcal{F}(f)]^{\frac{3}{2}}.$$

Then we obtain, for all T such that $\|h\|_{L^2} \leqslant \delta_0$ on $[t_0, T]$,

$$\mathcal{F}(f(T))^{-\frac{1}{2}} \geqslant \mathcal{F}(f(t_0))^{-\frac{1}{2}} + \tfrac{4(n-1)(1-\varepsilon)}{(1+\varepsilon)^{\frac{3}{2}}\sqrt{n(n+2)}}(t - t_0). \tag{4.56}$$

Then, using (4.53), we get that for $t \in [t_0, T]$,

$$\|h\|_{L^2}^{-2} \geqslant \tfrac{\sqrt{1-\varepsilon}}{(1+\varepsilon)\,2\sqrt{n(n+2)}}[\sqrt{\tfrac{2n(1-\varepsilon)}{1+\varepsilon}}\|h(t_0)\|_{L^2}^{-1} + \tfrac{4(n-1)(1-\varepsilon)}{(1+\varepsilon)^{\frac{3}{2}}\sqrt{n(n+2)}}(t-t_0)].$$

We write $C = \frac{(1+\varepsilon)^{\frac{5}{4}}}{(1-\varepsilon)^{\frac{3}{4}}}$ (a one-to-one correspondence between $0 < \varepsilon < 1$ and $C > 1$) and we get

$$\|h\|_{L^2} \leqslant C\left[\tfrac{1}{\sqrt{2(n+2)}\|h(t_0)\|_{L^2}} + \tfrac{2(n-1)}{n(n+2)}(t-t_0)\right]^{-\frac{1}{2}}. \tag{4.57}$$

So if we take $\delta < \min(\delta_0, \frac{1}{C^2\sqrt{2(n+2)}}\,\delta_0^2)$, and $\|h(t_0)\|_{L^2} \leqslant \delta$, we get that $\|h\|_{L^2} \leqslant \delta_0$ on $[t_0, T]$ for all $T \geqslant t_0$. Otherwise, the largest of such a T would satisfy

$$\delta_0 = \|h(T)\|_{L^2} \leqslant C\left[\tfrac{1}{\sqrt{2(n+2)\delta}}\right]^{-\frac{1}{2}} < \delta_0.$$

So the inequality (4.57) holds for all $t \in [t_0, +\infty)$, which ends the proof. □

With this proposition, since f tends to the uniform distribution in any $H^s(\mathbb{S})$, we get that for any $r < \frac{2(n-1)}{n(n+2)}$, there exists t_0 such that we have $\|f(t)-1\|_{L^2} \leqslant \frac{1}{\sqrt{r(t-t_0)}}$, for $t \geqslant t_0$. We can even get rid of the t_0 in this inequality since for any $r < \widetilde{r} < \frac{2(n-1)}{n(n+2)}$, for t sufficiently large, we have $\frac{1}{\sqrt{\widetilde{r}(t-t_0)}} \leqslant \frac{1}{\sqrt{rt}}$.

As in the previous section, using interpolation to deal with the other Sobolev norms of the solution would lead, for any $\eta > 0$ and t sufficiently large, to an inequality of the form $\|f(t) - 1\|_{H^p} \leqslant C_\eta t^{-\frac{1}{2}+\eta}$. But we can actually do slightly better. Indeed we have, following the notations of the proof and using (4.48),

$$\|h\|_{H^s} \leqslant |\alpha| \|\cos\theta\|_{H^p} + C_2\alpha^2 + C_3|\alpha|^3 + \|g\|_{H^p}.$$

We have $\|\cos\theta\|_{H^p} = (n-1)^{\frac{p}{2}}$. We take $t_0 > 0$ satisfying the conditions of the proposition and such that $\|h\|_{L^2} \leqslant \delta$. We have that g is uniformly bounded in any $H^p(\mathbb{S})$, and so by interpolation, we have $\|g\|_{H^s} \leqslant C_\eta \|g\|_{L^2}^{1-\eta}$ for any $\eta > 0$. Now using (4.56) and (4.52), we get

$$\left(\frac{1}{2n}\langle g^2\rangle + \frac{1}{4n^3(n+2)}\alpha^4\right)^{-\frac{1}{2}} \geqslant \frac{4(n-1)(1-\varepsilon)^{\frac{3}{2}}}{(1+\varepsilon)^{\frac{3}{2}}\sqrt{n(n+2)}}(t-t_0),$$

which gives $\|g\|_{L^2} = O(t^{-1})$ and $\alpha^2 \leqslant \frac{(1+\varepsilon)^{\frac{3}{2}} n(n+2)}{2(n-1)(1-\varepsilon)^{\frac{3}{2}}(t-t_0)}$. So finally, for any $\eta > 0$, we have that $\|h\|_{H^p} \leqslant (n-1)^{\frac{p}{2}} \sqrt{\frac{(1+\varepsilon)^{\frac{3}{2}} n(n+2)}{2(n-1)(1-\varepsilon)^{\frac{3}{2}}(t-t_0)}} + O(t^{-1+\eta})$. This gives that there exists $t_1 \geqslant t_0$ such that for all $t \geqslant t_1$, we have $\|h\|_{H^p} \leqslant (1+\varepsilon)(n-1)^{\frac{p}{2}} \sqrt{\frac{(1+\varepsilon)^{\frac{3}{2}} n(n+2)}{2(n-1)(1-\varepsilon)^{\frac{3}{2}}(t-t_0)}}$.

This is true for any $\varepsilon > 0$. In conclusion, we have that for any $r < \frac{2}{n(n-1)^{p-1}(n+2)}$, there exists t_1 such that for $t \geqslant t_1$, we have $\|f(t) - 1\|_{H^p} \leqslant \frac{1}{\sqrt{rt}}$.

4.4 Summary

In summary we can state the following theorem:

Theorem 4.4. *Convergence to equilibrium.*

Suppose f_0 is a probability measure, belonging to $H^s(\mathbb{S})$ (this is always the case for some $s < -\frac{n-1}{2}$).

Then there exists a unique weak solution f to Doi equation (1.3)*, satisfying the initial condition $f(0) = f_0$.*

Furthermore, this is a classical solution, positive for all time $t > 0$, and belonging to $C^\infty((0,+\infty) \times \mathbb{S})$.

If $J[f_0] \neq 0$, then we have the three following cases, depending on τ.

- *If $\tau > \frac{1}{n}$, then f converges exponentially fast to the uniform distribution, with global rate $(n-1)(\tau - \frac{1}{n})$ in any H^p norm.*

  More precisely, for all $t_0 > 0$, there exists a constant $C > 0$ depending only on t_0, s, p, n, and τ, such that for all $t \geqslant t_0$, we have

$$\|f(t) - 1\|_{H^p} \leqslant C\|f_0\|_{H^s} e^{-(n-1)(\tau-\frac{1}{n})t}.$$

- *If $\tau < \frac{1}{n}$, then there exists $\Omega \in \mathbb{S}$ such that f converges exponentially fast to $M_{\kappa\Omega}$, with asymptotic rate $r_\infty(\tau) > 0$ in any H^p norm.*

  More precisely, for all $r < r_\infty(\tau)$, there exists $t_0 > 0$ (depending on f_0) such that for all $t > t_0$, we have

  $$\|f(t) - M_{\kappa\Omega}\|_{H^p} \leqslant e^{-rt}.$$

  When τ is close to $\frac{1}{n}$ we have that $r_\infty(\tau) \sim 2(n-1)(\frac{1}{n} - \tau)$.

- *If $\tau = \frac{1}{n}$, then f converges to the uniform distribution in any H^p norm, with asymptotic rate $\sqrt{\frac{n(n-1)^{p-1}(n+2)}{2t}}$.*

  More precisely, for all $r < \frac{2}{n(n-1)^{p-1}(n+2)}$, there exists $t_0 > 0$ (depending on f_0) such that for all $t > t_0$, we have

  $$\|f(t) - 1\|_{H^p} \leqslant \frac{1}{\sqrt{rt}}.$$

If $J[f_0] = 0$ the equation reduces to the heat equation on the sphere, so f converges to the uniform distribution, exponentially with global rate $2n\tau$ in any H^p norm.

For the subcritical case $\tau > \frac{1}{n}$, we used Theorem 4.2. In the case where $p < -\frac{n-1}{2}$, a simple embedding gives $\|f(t) - 1\|_{H^p} \leqslant \|f(t) - 1\|_{H^{-\frac{n-1}{2}}}$ so we only have to show the result for $p \geqslant -\frac{n-1}{2}$. We get

$$\|f - 1\|_{H^p}^2 \leqslant C\|f(t_0) - 1\|_{H^p} e^{-(n-1)(\tau - \frac{1}{n})(t-t_0)} \leqslant C\|f(t_0)\|_{H^p} e^{-(n-1)(\tau-\frac{1}{n})(t-t_0)}.$$

The last inequality comes from the fact that $f(t_0)$ is a probability density function, so $f(t_0) - 1$ is the orthogonal projection of $f(t_0)$ on the space of mean-zero functions. Using Proposition 2.6, we get $\|f(t_0)\|_{H^p} \leqslant C_{t_0}\|f_0\|_{H^s}$ in the case $p \geqslant s$. Otherwise we just use a simple embedding to get first $\|f(t_0)\|_{H^p} \leqslant \|f(t_0)\|_{H^s}$ and then by the same proposition $\|f(t_0)\|_{H^p} \leqslant C\|f_0\|_{H^s}$.

Then the results in the case $\tau < \frac{1}{n}$ and $\tau = \frac{1}{n}$ are a summary of the conclusions of the two previous subsections. However, although it gives a clear understanding of how fast the solution converges to the equilibrium, in some sense, this summary is not as accurate as Propositions 4.2 and 4.3, which give a kind of stability: starting close to an equilibrium, the solution stays close.

5 Conclusion

In this chapter, we have investigated all the possible dynamics in large time for the Doi–Onsager equation (1.3) with dipolar potential. We have obtained a rate of convergence towards the equilibrium given any initial condition and any noise parameter $\tau > 0$, for all dimension $n \geqslant 2$.

The rate of convergence to the anisotropic steady state, in the case $\tau < \frac{1}{n}$, depends on a Poincaré constant which does not seem easy to estimate. A better knowledge of the behavior of this constant, for example as the noise parameter τ

tends to zero, would be useful to understand the limiting case $\tau = 0$, where we have existence and uniqueness of the solution. In this limit, the steady states are given by the sum of two antipodal Dirac masses $(1-\alpha)\delta_\Omega + \alpha\delta_{-\Omega}$ with $\Omega \in \mathbb{S}$ and $0 \leqslant \alpha \leqslant \frac{1}{2}$. We conjecture that if the initial condition is continuous (and with non zero initial momentum), then the solution converges to one of these steady states, with $\alpha = 0$.

It should also be possible to get the same kind of rates for the Maier–Saupe potential, but there the classification of the initial conditions leading to a given type of equilibria is much more difficult, in particular in the case where two types of equilibria are stable.

A Using the spherical harmonics

For the following we will use the spherical harmonics, so we recall some preliminaries results. We fix $n \geqslant 2$ and work on $\mathbb{R}^n$ and its unit sphere $\mathbb{S}_{n-1}$.

Definition A.1. *A spherical harmonic of degree ℓ on $\mathbb{S}_{n-1}$ is the restriction to $\mathbb{S}_{n-1}$ of a homogeneous polynomial of degree ℓ in n variables (seen as a function $\mathbb{R}^n \to \mathbb{R}$) which is an harmonic function (a function P such that $\Delta P = 0$, where Δ is the usual Laplace operator in $\mathbb{R}^n$). We denote $\mathcal{H}_\ell^{(n)}$ the set of spherical harmonics of degree ℓ on $\mathbb{S}_{n-1}$ (including 0 so they are vector spaces).*

We know that the space of homogeneous polynomials of degree ℓ in n variables has dimension $\binom{n+\ell-1}{n-1}$ (the number of n-tuples $(i_1, \dots i_n)$ of sum ℓ). Writing an arbitrary homogeneous polynomial P of degree ℓ under the form $P = \sum_{i=0}^{\ell} Q_{\ell-i} X_n^i$, with the polynomials Q_i being homogeneous of degree i in the first $n-1$ variables, and imposing that P is an harmonic function gives the following conditions (taking the term in X_n^{i-2}), for $i \in [\![0, \ell-2]\!]$: $\Delta Q_{\ell-i} + (i+1)(i+2)Q_{\ell-i-2} = 0$. Finally the polynomial P is only determined by the polynomials Q_ℓ and $Q_{\ell-1}$ in $n-1$ variables, of respective degrees ℓ and $\ell-1$. This gives the dimension of the space of spherical harmonics.

Proposition A.1. *The dimension of $\mathcal{H}_\ell^{(n)}$ is given by*

$$k_\ell^{(n)} = \binom{n+\ell-2}{n-2} + \binom{n+\ell-3}{n-2} = \binom{n+\ell-1}{n-1} - \binom{n+\ell-3}{n-1}.$$

The second expression comes from two successive applications of Pascal's triangle rule, and will be useful in the following. It can also be seen by the following property[1]: every homogeneous polynomial P of degree ℓ can be decomposed in a

[1]This can be shown using the appropriate inner product $(P, Q) \mapsto P(\mathrm{D})Q$ on the space of homogeneous polynomials P of degree ℓ, where $P(\mathrm{D})$ is defined as $\frac{\partial^\ell}{\partial_{X_1}^{\alpha_1} \dots \partial_{X_n}^{\alpha_n}}$ if $P = X_1^{\alpha_1} \dots X_n^{\alpha_n}$, and extended by linearity (so for example, we have that $|X|^2(\mathrm{D}) = \Delta$). If we denote by E the space of polynomials of the form $P = |X|^2 Q$, with Q of degree $\ell-2$, then the orthogonal of E consists in all the polynomials P such that for all Q of degree $\ell-2$, we have $(|X|^2 Q)(\mathrm{D})P = Q(\mathrm{D})\Delta P = 0$, that is to say in all the polynomials P such that $\Delta P = 0$. So the claimed decomposition is just the orthogonal decomposition, on E and $E^\perp$.

unique way as $H + |X|^2 Q$, where H is harmonic of degree ℓ and Q is homogeneous of degree $\ell - 2$. Iterating this decomposition, we get

$$P = H_\ell + |X|^2 H_{\ell-2} + |X|^4 H_{\ell-4} + \cdots + \begin{cases} |X|^\ell H_0 & \ell \text{ even} \\ |X|^{\ell-1} H_1 & \ell \text{ odd} \end{cases},$$

where the polynomials H_i are harmonic of degree i. This shows that any restriction of a polynomial on the sphere is equal to a sum of spherical harmonics (the terms $|X|^{2i}$ are constant when restricted to the sphere). This gives, with the Stone-Weierstrass theorem, that the sum of spherical harmonics are dense in $L^2(\mathbb{S}_{n-1})$ (since they are dense in the continuous functions). Together with the radial decomposition of the Laplacian $\Delta = \frac{1}{r^{n-1}}\partial_r(r^{n-1}\partial_r) + \frac{1}{r^2}\Delta_\omega$ (where Δ_ω is the Laplace Beltrami operator on the sphere $\mathbb{S}_{n-1}$, which is self-adjoint in $L^2(\mathbb{S}_{n-1})$), we get the following result:

Proposition A.2. *The spaces $\mathcal{H}_\ell^{(n)}$, for $\ell \in \mathbb{N}$, are the eigenspaces of the Laplace Beltrami operator Δ_ω on the sphere $\mathbb{S}_{n-1}$ for the eigenvalues $-\ell(\ell + n - 2)$. They are pairwise orthogonal and complete in $L^2(\mathbb{S}_{n-1})$.*

We can construct a basis of $\mathcal{H}_\ell^{(n)}$ by induction on the dimension, using the separation of variables. We describe this construction and will use it in the following.

For a given unit vector $e_n \in \mathbb{R}^n$, we take an orthonormal basis $(e_1, \dots, e_n)$ of $\mathbb{R}^n$. Any $\omega \in \mathbb{S}_{n-1} \setminus \{e_n, -e_n\}$ can be written $\omega = \cos\theta e_n + \sin\theta v$, with $\theta \in (0, \pi)$ and $v \in \mathbb{S}_{n-2}$. We identify $\mathbb{R}^{n-1}$ with the vector space spanned by $(e_1, \dots, e_{n-1})$. The special case $n = 2$ works if we consider $S_0 = \{e_1, -e_1\}$.

By convention, the only spherical harmonics on S_0 are the constant functions (of degree 0) and the functions $e_1 \mapsto c$, $-e_1 \mapsto -c$ (of degree 1).

Now, for $n \geqslant 1$, we choose an orthonormal basis $(Z_m^1, \dots Z_m^{k_m^{(n-1)}})$ of $\mathcal{H}_m^{(n-1)}$ for any $m \in \mathbb{N}$ and we have the following result:

Proposition A.3. *There exists polynomials $Q_{\ell,m}$ of degree $\ell - m$ such that if we denote $Y_{\ell,m}^k(\omega) = Q_{\ell,m}(\cos\theta)\sin^m\theta Z_m^k(v)$, then the $Y_{\ell,m}^k$ for $m \in [\![0, \ell]\!], k \in [\![1, k_m^{(n-1)}]\!]$ form an orthonormal basis of $H_\ell^{(n)}$.*

Proof. Writing $Y_{\ell,m}^k(\omega) = Q_{\ell,m}(\cos\theta)\sin^m\theta Z_m^k(v)$ and asking it to be a spherical harmonic is equivalent to the following linear ODE for $Q_{\ell,m}$ (we recall that the Laplace–Beltrami operator is given by $\sin^{2-n}\theta\partial_\theta(\sin^{n-2}\theta\partial_\theta) + \frac{1}{\sin^2\theta}\Delta_v$ in this coordinates):

$$\begin{aligned}\sin^{2-n}\partial_\theta(&-\sin^{n+m-1}\theta Q'_{\ell,m}(\cos\theta) + m\cos\theta\sin^{n+m-3}\theta Q_{\ell,m}(\cos\theta)) \\ &- m(m+n-3)Q_{\ell,m}(\cos\theta)\sin^{m-2}\theta = -\ell(\ell+n-2)Q_{\ell,m}(\cos\theta)\sin^m\theta.\end{aligned}$$

We write $x = \cos\theta$ and this equation transforms into

$$(1-x^2)Q''_{\ell,m} - (n+2m-1)xQ'_{\ell,m} + (\ell-m)(\ell+n+m-2)Q_{\ell,m} = 0.$$

This equation is a particular form of the Jacobi differential equation, where the two parameters α and β are equal (also called Gegenbauer differential equation). One solution of this differential equation is a polynomial, called ultraspherical polynomial

(a particular case of the Jacobi Polynomials, also called Gegenbauer polynomials), and denoted $P_i^{(\lambda)}$ following the notation of Szegö in [72]. Precisely, it satisfies the differential equation

$$(1-x^2)y'' - (2\lambda+1)xy' + i(i+2\lambda)y = 0.$$

Taking $\lambda = m - 1 + \frac{n}{2}$ and $i = \ell - m$, we get a solution $Q_{\ell,m} = \alpha_{\ell,m} P_{\ell-m}^{(m-1+\frac{n}{2})}$, where $\alpha_{\ell,m}$ is a positive constant of normalization, such that $Y_{\ell,m}^k$ is of norm 1 in $L^2(\mathbb{S}_{n-1})$. We have to be careful here because $P_i^{(\lambda)}$ is not defined for $\lambda = 0$, and so the only special case is $n = 2$, $m = 0$, for which we have a solution $Q_{\ell,0} = \sqrt{2}T_\ell$, where $T_\ell(\cos\theta) = \cos\ell\theta$ (the Chebyshev polynomial of first order of degree ℓ).

So for a fixed ℓ, we have constructed a family of spherical harmonics $Y_{\ell,m}^k$ of degree ℓ for $m \in [\![0,\ell]\!], k \in [\![1, k_m^{(n-1)}]\!]$. They are pairwise orthogonal in $L^2(\mathbb{S}_{n-1})$ since the Z_m^k are pairwise orthogonal in $L^2(\mathbb{S}_{n-2})$. The size of this family is exactly

$$\sum_{m=0}^{\ell} k_m^{(n-1)} = \sum_{m=0}^{\ell} \binom{n+m-2}{n-2} - \binom{n+m-4}{n-2} = \binom{n+\ell-2}{n-2} + \binom{n+\ell-3}{n-2} = k_\ell^{(n)}, \tag{A.58}$$

which is the dimension of $H_\ell^{(n)}$, so we get that the $Y_{\ell,m}^k$ for $m \in [\![0,\ell]\!], k \in [\![1, k_m^{(n-1)}]\!]$ form an orthonormal basis of $H_\ell^{(n)}$. □

From now on, we will use the construction done in the proof. We have that, for a fixed $m \geqslant 0$, the polynomials $Q_{\ell,m}$ for $\ell \geqslant m$ are a family of orthogonal polynomials for the inner product $(P,Q) \mapsto \int_{-1}^1 P(x)Q(x)(1-x^2)^{m-1+\frac{n-1}{2}}\mathrm{d}x$.

We will use three properties on the Gegenbauer polynomials (see [72]) for the following, for $i \geqslant 0$, $\lambda \neq 0$, and $\lambda > -\frac{1}{2}$ (with the convention $P_{-1}^{(\lambda)} = 0$):

$$\int_{-1}^1 (P_i^{(\lambda)}(x))^2 (1-x^2)^{\lambda-\frac{1}{2}}\mathrm{d}x = \frac{2^{1-2\lambda}\pi\Gamma(i+2\lambda)}{(i+\lambda)\Gamma^2(\lambda)\Gamma(i+1)} \tag{A.59}$$

$$(i+1)P_{i+1}^{(\lambda)} = 2(i+\lambda)XP_i^{(\lambda)} - (i+2\lambda-1)P_{i-1}^{(\lambda)} \tag{A.60}$$

$$(1-X^2)(P_i^{(\lambda)})' = \frac{1}{2(i+\lambda)}\Big((i+2\lambda-1)(i+2\lambda)P_{i-1}^{(\lambda)} - i(i+1)P_{i+1}^{(\lambda)}\Big) \tag{A.61}$$

We have the following normalization for the $Q_{\ell,m}$:

$$\int_{-1}^1 Q_{\ell,m}^2(x)(1-x^2)^{m-1+\frac{n-1}{2}}\mathrm{d}x = \int_{-1}^1 (1-x^2)^{\frac{n-1}{2}-1}\mathrm{d}x.$$

This gives the following relation, together with (A.59):

$$\alpha_{\ell+1,m}^2 = \frac{\left(\ell+\frac{n}{2}\right)(\ell+1-m)}{\left(\ell+\frac{n}{2}-1\right)(\ell+m+n-2)}\alpha_{\ell,m}^2. \tag{A.62}$$

A.1 Estimates on the unit sphere

By the previous construction, we can do the decomposition $g = \sum_{k,\ell,m} c^k_{\ell,m} Y^k_{\ell,m}$ and we have $\int_{\mathbb{S}_{n-1}} g^2 = \sum_{k,\ell,m} |c^k_{\ell,m}|^2$. Since g is of mean zero, we have $c^1_{0,0} = 0$ (the only spherical harmonic of degree 0 is the constant function 1). So from now, the indices k, ℓ, m of the sum will mean $\ell > 0, m \in [\![0, \ell]\!], k \in [\![1, k^{(n-1)}_m]\!]$.

We decompose in the same way $h = \sum_{k,\ell,m} d^k_{\ell,m} Y^k_{\ell,m}$. We give a first formula, in the form of a lemma.

Lemma 4.3. *We have*

$$e_n \cdot \int_{\mathbb{S}_{n-1}} g \nabla h = \frac{1}{2} \sum_{k,\ell,m} b_{\ell,m} [(\ell + n - 1) c^k_{\ell,m} d^k_{\ell+1,m} - \ell c^k_{\ell+1,m} d^k_{\ell,m}], \tag{A.63}$$

where $b_{\ell,m} = \frac{\sqrt{\ell-m+1}\sqrt{\ell+m+n-2}}{\sqrt{\ell+\frac{n}{2}-1}\sqrt{\ell+\frac{n}{2}}} \leqslant 1$.

Proof. We have

$$e_n \cdot \nabla Y^k_{\ell,m} = -\sin\theta \partial_\theta Y^k_{\ell,m} = \left[(1 - X^2) Q'_{\ell,m} - mX Q_{\ell,m}\right] (\cos\theta) \sin^m \theta Z^k_m(v),$$

and using the inductions formulas (A.60), (A.61) and (A.62), we get

$$(1 - X^2) Q'_{\ell,m} - mX Q_{\ell,m} = \frac{1}{2} [b_{\ell-1,m}(\ell + n - 2) Q_{\ell-1,m} - b_{\ell,m} \ell Q_{\ell+1,m}], \tag{A.64}$$

where $b_{\ell,m}$ is given in the statement of the lemma. In the special case $n = 2$, $m = 0$, using the formula $Q_{\ell,0}(\cos\theta) = \cos \ell\theta$ gives the same formula as (A.64), with $b_{\ell,0} = 1$.

So we have that $\int_{\mathbb{S}_{n-1}} e_n \cdot \nabla Y^k_{\ell,m} Y^{k'}_{\ell',m'}$ can be non-zero only if $m = m'$, $k = k'$, and $\ell = \ell' \pm 1$. By bilinearity, together with the fact that $Y^k_{\ell,m}$ form an orthonormal basis, this gives the claimed formula. □

Now we have all the tools to prove Lemma 4.1 (we recall it here).

Lemma 4.1. *Estimates on the sphere.*

1. *If h in $\dot{H}^{-s+1}(\mathbb{S})$ and g in $\dot{H}^s(\mathbb{S})$, the following integral is well defined and we have*
$$\left| \int_{\mathbb{S}} g \nabla h \right| \leqslant C \|g\|_{\dot{H}^s} \|h\|_{\dot{H}^{-s+1}},$$
where the constant depends only on s and n.

2. *We have the following estimation, for any $g \in \dot{H}^{s+1}(\mathbb{S})$:*
$$\left| \int_{\mathbb{S}} g \nabla (-\Delta)^s g \right| \leqslant C \|g\|^2_{\dot{H}^s},$$
where the constant depends only on s and n.

3. *We have the following identity, for any $g \in \dot{H}^{-\frac{n-3}{2}}$:*
$$\int_{\mathbb{S}} g \nabla \widetilde{\Delta}^{-1}_{n-1} g = 0.$$

Proof. Using Lemma 4.3, we get

$$\begin{aligned} e_n \cdot \int_{\mathbb{S}_{n-1}} g\nabla h \leqslant & \frac{1}{2}\sum_{k,\ell,m} \sqrt{\tfrac{\ell+n-1}{\ell+1}} \left(\tfrac{\lambda_{\ell+1}}{\lambda_\ell}\right)^{\frac{s}{2}} |\lambda_\ell^{\frac{s}{2}} c^k_{\ell,m}||\lambda_{\ell+1}^{\frac{-s+1}{2}} d^k_{\ell+1,m}| \\ & + \frac{1}{2}\sum_{k,\ell,m} \sqrt{\tfrac{\ell}{\ell+n-2}} \left(\tfrac{\lambda_\ell}{\lambda_{\ell+1}}\right)^{\frac{s}{2}} |\lambda_{\ell+1}^{\frac{s}{2}} c^k_{\ell+1,m}||\lambda_\ell^{\frac{-s+1}{2}} d^k_{\ell,m}| \\ \leqslant & C\|g\|_{\dot{H}^s}\|h\|_{\dot{H}^{-s+1}} \end{aligned}$$

where $\lambda_\ell = \ell(\ell+n-2)$ (the eigenvalue of $-\Delta$ for the spherical harmonics of degree ℓ). The last line comes from the fact that the sequences $\sqrt{\frac{\ell+n-1}{\ell+1}} \left(\frac{\lambda_{\ell+1}}{\lambda_\ell}\right)^{\frac{s}{2}}$ and $\sqrt{\frac{\ell}{\ell+n-2}} \left(\frac{\lambda_\ell}{\lambda_{\ell+1}}\right)^{\frac{s}{2}}$ are bounded (they tend to 1), together with a Cauchy-Schwarz inequality. This gives the first part of the lemma, since this is true for any unit vector e_n.

Now we take $h = (-\Delta)^s g$, which is replacing $d^k_{\ell,m}$ by $\lambda^s_\ell c^k_{\ell,m}$ in Lemma 4.3. We get

$$\begin{aligned} e_n \cdot \int_{\mathbb{S}_{n-1}} g\nabla(-\Delta)^s g = & \sum_{k,\ell,m} \frac{1}{2} b_{\ell,m} c^k_{\ell+1,m} c^k_{\ell,m} [(\ell+n-1)\lambda^s_{\ell+1} - \ell\lambda^s_\ell] \\ \leqslant & \sum_{k,\ell,m} |\lambda_{\ell+1}^{\frac{s}{2}} c^k_{\ell+1,m}||\lambda_\ell^{\frac{s}{2}} c^k_{\ell,m}||(\ell+n-1)\left(\tfrac{\lambda_{\ell+1}}{\lambda_\ell}\right)^{\frac{s}{2}} - \ell\left(\tfrac{\lambda_\ell}{\lambda_{\ell+1}}\right)^{\frac{s}{2}}| \\ \leqslant & C\|g\|^2_{\dot{H}^s}. \end{aligned}$$

Indeed we have that $\frac{\lambda_{\ell+1}}{\lambda_\ell} = 1 - \frac{2}{\ell} + O(\ell^{-2})$, so $|(\ell+n-1)\left(\frac{\lambda_{\ell+1}}{\lambda_\ell}\right)^{\frac{s}{2}} - \ell\left(\frac{\lambda_\ell}{\lambda_{\ell+1}}\right)^{\frac{s}{2}}|$ is bounded (it tends to $(n-1)+2s$). Since this computation is now valid for any unit vector e_n, this gives the second part of the lemma.

The last part is straightforward by taking $h = \widetilde{\Delta}^{-1}_{n-1} g$ with Lemma 4.3. According to the definition given in (2.8), we have $d^k_{\ell,m} = \frac{1}{\ell(\ell+1)\ldots(\ell+n-2)}\, c^k_{\ell,m}$. We get

$$e_n \cdot \int_{\mathbb{S}_{n-1}} g\nabla\widetilde{\Delta}^{-1} g = \sum_{k,\ell,m} \frac{1}{2} b_{\ell,m} c^k_{\ell+1,m} c^k_{\ell,m} [\tfrac{\ell+n-1}{(\ell+1)\ldots(\ell+n-1)} - \tfrac{\ell}{\ell(\ell+1)\ldots(\ell+n-2)}] = 0,$$

which is true for any unit vector e_n. □

A.2 Analyticity of the solution

Following [21], we will show that the solution belongs to a special Gevrey class. We define the space G_r as the set of functions g (with mean zero) such that $\widetilde{\Delta}^{-\frac{1}{2}}_{n-1} e^{r(-\Delta)^{\frac{1}{2}}} g$ is in $L^2(\mathbb{S})$. Using the notations of the previous proof, this is an Hilbert space associated to the inner product

$$\langle g, h\rangle_{\dot{G}^s_r} = \sum_{k,\ell,m} \frac{e^{2r\sqrt{\ell(\ell+n-2)}}}{\ell(\ell+1)\ldots(\ell+n-2)} c^k_{\ell,m} d^k_{\ell,m}.$$

The norm on this Hilbert space will be written $\|\cdot\|_{G_r}$.

Theorem 4.5. *We define* $r(t) = \delta \min\{1, t\}$.

If $\delta > 0$ *is sufficiently small, then for any solution of Doi equation* (1.3) *of the form* $f = 1 + g$, *with* $g(0) \in \dot{H}^{-\frac{n-1}{2}}(\mathbb{S})$, *we have that* $g(t)$ *is bounded in* $G_{r(t)}$, *uniformly for* $t \geqslant 0$.

Before giving a proof, we remark that the condition $g(0) \in \dot{H}^{-\frac{n-1}{2}}(\mathbb{S})$ is not very strong, since, by instantaneous regularization (Proposition 2.6) we have it for any time $t > 0$. The shape of $r(t)$ is not optimal, and we will provide a more precise condition in the proof. Now since G_r, for $r > 0$, is a subset of the set of analytical functions on the sphere, we get that any solution becomes instantaneously analytic in space.

Proof. We take r an arbitrary function of t, we will denote its time derivative by $\dot{r}$. For a given solution $f = 1 + g$, we put $h = \widetilde{\Delta}_{n-1}^{-1} e^{2r(-\Delta)^{\frac{1}{2}}} g$ in (2.13).

The left-hand side is

$$\begin{aligned}
\langle \partial_t g, \widetilde{\Delta}_{n-1}^{-1} e^{2r(-\Delta)^{\frac{1}{2}}} g \rangle &= \sum_{k,\ell,m} \frac{e^{2r\sqrt{\ell(\ell+n-2)}}}{\ell(\ell+1)\dots(\ell+n-2)} c_{\ell,m}^k \frac{\mathrm{d}}{\mathrm{d}t} c_{\ell,m}^k \\
&= \sum_{k,\ell,m} \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\tfrac{e^{2r\sqrt{\ell(\ell+n-2)}}}{\ell(\ell+1)\dots(\ell+n-2)} |c_{\ell,m}^k|^2\right) - \dot{r}\tfrac{e^{2r\sqrt{\ell(\ell+n-2)}}}{\sqrt{\ell(\ell+1)\dots(\ell+n-1)\sqrt{\ell+n-2}}} |c_{\ell,m}^k|^2 \\
&= \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g\|_{G_r}^2 - \dot{r}\|(-\Delta)^{\frac{1}{4}} g\|_{G_r}^2.
\end{aligned}$$

Using Lemma 4.3, we get

$$\begin{aligned}
e_n \cdot \langle g, \nabla \widetilde{\Delta}_{n-1}^{-1} e^{2r(-\Delta)^{\frac{1}{2}}} g \rangle &= \frac{1}{2} \sum_{k,\ell,m} b_{\ell,m} c_{\ell+1,m}^k c_{\ell,m}^k \frac{e^{2r\sqrt{(\ell+1)(\ell+n-1)}} - e^{2r\sqrt{\ell(\ell+n-2)}}}{(\ell+1)\dots(\ell+n-2)} \\
\leqslant &\frac{1}{2} \sum_{k,\ell,m} \tfrac{\sqrt[4]{(\ell+1)(\ell+n-1)} e^{r\sqrt{(\ell+1)(\ell+n-1)}}}{\sqrt{(\ell+1)\dots(\ell+n-2)(\ell+n-1)}} |c_{\ell+1,m}^k| \tfrac{\sqrt[4]{\ell(\ell+n-2)} e^{r\sqrt{\ell(\ell+n-2)}}}{\sqrt{\ell(\ell+1)\dots(\ell+n-2)}} |c_{\ell,m}^k| \\
&\times \sqrt[4]{\tfrac{\ell(\ell+n-1)}{(\ell+1)(\ell+n-2)}} \left(e^{r\left(\sqrt{(\ell+1)(\ell+n-1)} - \sqrt{\ell(\ell+n-2)}\right)} - e^{-r\left(\sqrt{(\ell+1)(\ell+n-1)} - \sqrt{\ell(\ell+n-2)}\right)} \right) \\
\leqslant &\sinh(r(\sqrt{2n} - \sqrt{n-1}))\|(-\Delta)^{\frac{1}{4}} g\|_{G_r}^2.
\end{aligned}$$

Indeed the expression $\sqrt{(\ell+1)(\ell+n-1)} - \sqrt{\ell(\ell+n-2)}$ is a decreasing function of $\ell \geqslant 0$. Since this is valid for any unit vector e_n, we get

$$\left| J[g] \cdot \langle g, \nabla \widetilde{\Delta}_{n-1}^{-1} e^{2r(-\Delta)^{\frac{1}{2}}} g \rangle \right| \leqslant \sinh(r(\sqrt{2n} - \sqrt{n-1}))\|(-\Delta)^{\frac{1}{4}} g\|_{G_r}^2.$$

Now since $\|(-\Delta)^{\frac{1}{4}} g\|_{G_r}^2 \leqslant \frac{1}{\sqrt{n-1}} \|(-\Delta)^{\frac{1}{2}} g\|_{G_r}^2$, and $|J[h]| \leqslant \frac{e^{2r\sqrt{n-1}}}{(n-1)!} |J[g]|$, we finally get

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g\|_{G_r}^2 + \left[\tau - \tfrac{1}{\sqrt{n-1}}(\dot{r} + \sinh(r(\sqrt{2n} - \sqrt{n-1})))\right] \|(-\Delta)^{\frac{1}{2}} g\|_{G_r}^2 \leqslant \frac{e^{2r\sqrt{n-1}}}{(n-2)!}.$$

As soon as $\dot{r} + \sinh(r(\sqrt{2n} - \sqrt{n-1})) < (\tau - \varepsilon)\sqrt{n-1}$ and r is bounded in time (for example the shape given in the statement of the theorem, $r(t) = \delta \min(1, t)$,

for δ sufficiently small), using Poincaré inequality, we have that $\|g\|^2_{G_r}$ satisfies an inequality of the form $\dot{y} + ay \leqslant b$ with some positive constants a and b. Therefore this quantity is uniformly bounded, provided $g(0)$ is in $G_{r(0)}$. So if we have $r(0) = 0$, we only need $g(0)$ to be in $\dot{H}^{-\frac{n-1}{2}}(\mathbb{S})$. □

Chapter 5

A note on the dynamics in the Doi equation with Maier–Saupe potential

This chapter is an ongoing collaboration with Jian-Guo Liu, started when visiting him in Tsinghua University.

Abstract

Following the work of Chapter 4 on the dipolar potential, we study the dynamics of the Doi equation with Maier–Saupe potential.

In the special case of dimension 2, we prove convergence to a an equilibrium for any initial condition, with exponential rate except in the critical case where the rate is algebraic.

Key words: Doi–Onsager equation, Smoluchowski equation, Maier–Saupe potential, LaSalle invariance principle, convergence to steady-states.

1 Introduction

We denote by $\mathbb{S}$ the unit sphere of $\mathbb{R}^n$, and we consider the following non-local partial differential equation on $\mathbb{S}$, for a probability density function f on the sphere:

$$\begin{cases} \partial_t f = \nabla \cdot (f \nabla \Psi_f) + \tau \Delta f, \\ \Psi_f(\omega, t) = \int_{\mathbb{S}} K(\omega, \bar{\omega})\, f(t, \bar{\omega})\, \mathrm{d}\bar{\omega}. \end{cases} \tag{1.1}$$

This equation is known as Doi equation (or Doi–Onsager, Smoluchowski, or even nonlinear Fokker–Planck equation) and was introduced by Doi [32] as a gradient flow equation for the Onsager free energy functional:

$$\mathcal{F}(f) = \tau \int_{\mathbb{S}} f(.,\omega) \ln f(.,\omega) \mathrm{d}\omega + \tfrac{1}{2} \int_{\mathbb{S}\times\mathbb{S}} K(\omega,\bar{\omega}) f(.,\omega)\, f(.,\bar{\omega})\, \mathrm{d}\omega \mathrm{d}\bar{\omega}.$$

This functional was proposed by Onsager [65] to describe the equilibrium states of suspensions of rod-like polymers. They are given by the critical points of this functional.

Defining the chemical potential μ as the first order variation of $\mathcal{F}(f)$ under the constraint $\int_{\mathbb{S}} f = 1$, we get $\mu = \tau \ln f + \Psi$, and the Doi equation becomes

$$\partial_t f = \nabla \cdot (f \nabla \mu),$$

and we have, for a smooth positive solution f of (1.1),

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{F} + \mathcal{D} = 0, \tag{1.2}$$

where the (positive) dissipation term $\mathcal{D}(f)$ is given by

$$\mathcal{D}(f) = \int_{\mathbb{S}} f |\nabla_\omega (\tau \ln f + \Psi_f)|^2 = \int_{\mathbb{S}} f |\nabla_\omega \mu|^2.$$

In the original work of Onsager, the kernel has the form $K(\omega,\bar{\omega}) = |\omega \times \bar{\omega}|$, but there is another form, introduced later by Maier and Saupe [58], which leads to similar quantitative results: $K(\omega,\bar{\omega}) = \frac{1}{n} - (\omega \cdot \bar{\omega})^2$. In particular, one observes a phenomenon of hysteresis when the parameter τ, which represents a temperature, goes from large to small values, and back to large values.

The study of the case $K = -\omega \cdot \bar{\omega}$, called the dipolar potential, has been done in Chapter 4. Motivated by the results obtained in there with respect to the analysis of the dynamics of convergence towards a given equilibria, we will show that we can apply the method in the case of the Maier–Saupe potential.

Let us briefly review what have been done previously with respect to the mathematical study of this equation. A review is available on this topic [84], but it does not take into accounts some recent developments.

The characterization of equilibria started in 2004 in dimension $n = 2$ for the Maier–Saupe potential with the paper [20], with a partial result, which was then completed by three independent groups in [22, 38, 57] (moreover, a whole family of different kernels is treated in [38] including the dipolar potential, still in dimension $n = 2$). In the case where the temperature τ is greater than or equal to $\frac{1}{4}$,

the uniform distribution is the unique steady-state, and when $\tau < \frac{1}{4}$, there is also another family of equilibria, which are non-isotropic, symmetric, and differ from one to another by a simple rotation (called nematic equilibria).

The case of the dimension 3 is a little bit more elaborated, since we need first to show that any steady-state is axisymmetric. After the partial result [20], the complete characterization was provided in 2005, independently in [37, 55, 88]. One can observe a fascinating hysteresis phenomena with two thresholds for the temperatures: $\tau_c = \frac{2}{15}$ and $\tau^* > \tau_c$. When $\tau > \tau^*$, the uniform distribution is the unique steady-state, when $\frac{2}{15} < \tau < \tau^*$, two other families of prolate (concentrated around two antipodal points) nematic equilibria appear, and when $\tau < \frac{2}{15}$, one of this family transforms into oblate equilibria (concentrated around a great circle). Analyzing stability as local minimization of Onsager free energy, this last family is proved to be unstable for $\tau < \tau^*$, as well as the uniform distribution for $\tau < \frac{2}{15}$. The other are stable in this sense. Hence, starting from a large τ, the only stable equilibrium (the uniform distribution) stays stable until τ reaches $\frac{2}{15}$, and starting from a small τ, the only family of stable equilibria (the prolate nematic equilibria) stays stable until τ reaches $\tau^* > \frac{2}{15}$, which gives the hysteresis phenomenon.

In [89], a coupling between the Maier–Saupe and the dipolar potential is proposed, and the only stable equilibria are proved to be symmetric. And finally, recently, a unified characterization of these equilibria in many cases has been provided [78], including the case of the Maier–Saupe potential in any dimension. The main idea is to prove that the so-called orientational tensor order parameter is a matrix with at most two distinct eigenvalues, which allows to reduce the compatibility condition (a Euler-Lagrange equation for the potential) to a more simple equation.

Regarding the dynamics in time, a few results were given, for the Maier–Saupe potential only, in dimension 2 and 3. Existence, uniqueness, non-negativity, and spatial-analyticity of a solution are claimed for a continuous nonnegative initial condition in [19, 21]. The system is proved to be dissipative in a certain Gevrey class of functions. Recently, the existence of inertial manifolds has been established [76, 77]. But this does not provide convergence in time to a given equilibrium.

A lot of variants were proposed and studied [80, 85, 87, 90, 75, 39] including external forces such as elongational force or shear flow, or modelling more complex phenomena with space dependence. And finally, very recently, some results were provided in dimension 2 which provide a better understanding of the case of the original Onsager kernel [18, 56, 79, 81], based on the analysis of the steady states.

Our main contributions to this field concerns the dynamical description of the system as time goes to infinity, which has not been treated a lot, as far as we know.

2 General results

If the kernel K is polynomial of degree less than p in $\bar{\omega}$, we get that Ψ_f depends linearly on the (orthogonal) projection of f on the space spanned by the spherical harmonics of degree less than p. Therefore, all the machinery introduced in Chapter 4 works, and we get the following result:

Theorem 5.1. *Existence, uniqueness, positivity and regularity.*

We suppose that the kernel K is polynomial with respect to $\bar{\omega}$. Given an initial probability measure f_0 in $H^s(\mathbb{S})$, there exists a unique global weak solution f of Doi equation (1.1) *such that $f(0) = f_0$. Moreover, $f \in C^\infty((0,+\infty)\times\mathbb{S})$, with $f(t,\omega) > 0$ for all positive t.*

We also have the following instantaneous regularity and uniform boundedness estimates (for $m \in \mathbb{N}$, the constant C depending only on τ, m, s), for all $t > 0$:

$$\|f(t)\|^2_{H^{s+m}} \leqslant C\left(1 + \frac{1}{t^m}\right)\|f_0\|^2_{H^s}.$$

The proof follows closely the one of Theorem 4.1 of Chapter 4, and will be omitted here. The first step consists in proving local existence, uniqueness and regularity, then, using regular solution, we prove positivity by a maximum principle. This implies that, up to explosion time, we have uniform bounds on Ψ_f which do not depend on f, using the fact that f is a positive function of mean 1. From this bounds we then get the global existence and the estimates for instantaneous regularity and uniform boundedness.

Let us note that this result is stronger, in some sense, than what have been claimed in [19, 21] in the sense that one can start in any Sobolev space, instead of only continuous, but in another sense, it is weaker, since we do not have analyticity in space. One can expect to get this analyticity in a way similar to what we have done in Appendix A.2 of Chapter 4, showing that the solution belongs to a certain Gevrey class (the result of [21] is that this is the case for the Maier–Saupe potential in dimension 2 and 3). In [20], a similar claim is given, for a general smooth kernel, with continuous initial condition.

Once we have this results, we can then study the steady states of (1.1). The proof of the following proposition is the same as the one of Proposition 3.1 of Chapter 4.

Proposition 2.1. *Steady states.*

The steady states of Doi equation (1.1) *are the probability measures f on $\mathbb{S}$ which satisfy one of the following equivalent conditions.*

1. *Equilibrium: $f \in C^2(\mathbb{S})$ and $Q(f) = 0$*
2. *No dissipation: $f \in C^1(\mathbb{S})$ and $\mathcal{D}(f) = 0$*
3. *The probability density $f \in C^0(\mathbb{S})$ is positive and a critical point of $\mathcal{F}$ (under the constraint of mean 1).*
4. *There exists $C \in \mathbb{R}$ such that $\tau \ln f + \Psi_f = C$.*

We then get exactly the same properties of convergence to a given set of equilibria, as in Proposition 3.2 of Chapter 4:

Proposition 2.2. *LaSalle's invariance principle.*

Let f_0 be a probability measure on the sphere $\mathbb{S}$. We denote by $\mathcal{F}_\infty$ the limit of $\mathcal{F}(f(t))$ as $t \to \infty$, where f is the solution to Doi equation (1.1) *with initial condition f_0.*

Then the set $\mathcal{E}_\infty = \{f \in C^\infty(\mathbb{S})$ s.t. $\mathcal{D}(f) = 0$ and $\mathcal{F}(f) = \mathcal{F}_\infty\}$ is not empty.

Furthermore $f(t)$ converges in any H^s norm to this set of equilibria (in the following sense):

$$\lim_{t\to\infty} \inf_{g\in\mathcal{E}_\infty} \|f(t)-g\|_{H^s} = 0.$$

This principle is crucial and allows to show convergence to a given equilibrium, if we know the structure of the equilibria. In the case of the Maier–Saupe potential, recent results have provided, little by little, the complete classification of the equilibria in dimension 2 [22, 38, 57], then in dimension 3 [37, 55, 88], and finally in any dimension in [78].

3 The Maier–Saupe potential

When the kernel K is of the form $K(\omega,\bar\omega) = \frac{1}{n} - (\omega\cdot\bar\omega)^2 = (\frac{1}{n}\mathrm{Id} - \omega\otimes\omega) : \bar\omega\otimes\bar\omega$, we introduce the operator S with values in trace-free symmetric matrices by:

$$S[f] = \int_{\mathbb{S}} (\tfrac{1}{n}\mathrm{Id} - \omega\otimes\omega) f \mathrm{d}\omega. \tag{3.3}$$

It is then easy to see that Ψ_f is given by $\Psi_f(\omega) = \omega\otimes\omega : S[f] = \omega\cdot S[f]\omega$ and is a spherical harmonic of degree 2. Indeed we have, for any trace-free symmetric matrix A,

$$\begin{cases} \nabla_\omega(\omega\otimes\omega : A) = 2(\mathrm{Id}-\omega\otimes\omega)A\omega \\ \nabla_\omega\cdot((\mathrm{Id}-\omega\otimes\omega)A\omega) = -n\,\omega\otimes\omega : A \end{cases}, \tag{3.4}$$

so we get $\Delta_\omega\Psi_f = -2n\Psi_f$.

Let us first state the existence of a threshold of dynamic instability for the uniform distribution, by deriving the ordinary differential equation satisfied by $S[f]$.

Proposition 3.1. *Instability of the uniform distribution below a threshold.*

If we have $S[f_0] = 0$, then we have $S[f(t)] = 0$ for all $t \geqslant 0$, and the Doi equation (1.1) becomes the heat equation on the sphere. The solution converges exponentially fast to the uniform distribution.

If we have $S[f_0] \neq 0$, then we have $S[f(t)] \neq 0$ for all $t \geqslant 0$. Moreover, in the case where $\tau < \frac{2}{n(n+2)}$, the solution cannot converge to the uniform distribution.

Proof. For a trace-free symmetric matrix A, we have $(\frac{1}{n}\mathrm{Id}-\omega\otimes\omega) : A = -\omega\otimes\omega : A$, and then, for a solution f of Doi equation (1.1), we get

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}S[f] : A &= \int_{\mathbb{S}} -\omega\otimes\omega : A\,\nabla_\omega\cdot(f\nabla_\omega(\omega\otimes\omega : S[f]))\mathrm{d}\omega - \tau\int_{\mathbb{S}}(\omega\otimes\omega : A)\Delta_\omega f\mathrm{d}\omega \\
&= \int_{\mathbb{S}} \nabla_\omega(\omega\otimes\omega : A)\cdot\nabla_\omega(\omega\otimes\omega : S[f])\, f\mathrm{d}\omega - \tau\int_{\mathbb{S}}\Delta_\omega(\omega\otimes\omega : A)\, f\,\mathrm{d}\omega \\
&= 4\int_{\mathbb{S}} A\omega\cdot(\mathrm{Id}-\omega\otimes\omega)S[f]\omega\, f\mathrm{d}\omega + 2n\tau\int_{\mathbb{S}}\omega\otimes\omega : A\, f\,\mathrm{d}\omega \\
&= 4A : \int_{\mathbb{S}}\omega\otimes[(\mathrm{Id}-\omega\otimes\omega)S[f]\omega]\, f\mathrm{d}\omega - 2n\tau\int_{\mathbb{S}}(\tfrac{1}{n}\mathrm{Id}-\omega\otimes\omega) : A\, f\,\mathrm{d}\omega \\
&= A : L_f(S[f]) - 2n\tau A : S[f].
\end{aligned}$$

The operator L_f is a linear operator on matrices, hence, considering it as a smooth time-depending linear operator $\mathcal{L}_t$ we get that $S[f]$ satisfies the linear ordinary differential equation with variable coefficients:

$$\frac{\mathrm{d}}{\mathrm{d}t}S[f] = \mathcal{L}_t(S[f]) - 2n\tau S[f]. \tag{3.5}$$

Therefore, we have by uniqueness that if $S[f](t_1) = 0$ for some $t_1 \in \mathbb{R}_+$, then $S[f]$ is identically zero for all non-negative time (the ODE is linear, we can go backwards and forwards in time), and the equation (1.1) reduces to the heat equation on the sphere, with temperature τ.

Now we suppose that $S[f_0] \neq 0$, and then we have $S[f(t)] \neq 0$ for all $t \geqslant 0$. If we introduce the function $g = f - 1$, we have $S[f] = S[g]$. A direct computation shows that for a trace-free symmetric matrix A, we have

$$\int_{\mathbb{S}} (\omega \otimes \omega : A)\,(\omega \otimes \omega : e_i \otimes e_j)\mathrm{d}\omega = \tfrac{2}{n(n+2)} a_{ij} = \tfrac{2}{n(n+2)} A : e_i \otimes e_j. \tag{3.6}$$

Hence, using the fact that $\int_{\mathbb{S}} \omega \otimes \omega = \frac{1}{n}\mathrm{Id}$, the ODE (3.5) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}S[g] = 2n(\tfrac{2}{n(n+2)} - \tau)S[g] + 4\int_{\mathbb{S}} \omega \otimes [(\mathrm{Id} - \omega \otimes \omega)S[g]\omega]\, g\mathrm{d}\omega.$$

Writing $|S[g]|^2$ for $S[g] : S[g]$, we get

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|S[g]|^2 = 2n(\tfrac{2}{n(n+2)} - \tau)|S[g]|^2 + 4\int_{\mathbb{S}} (|S[g]\omega|^2 - (S[g] : \omega \otimes \omega)^2)\, g\mathrm{d}\omega.$$

Now, if we suppose that $\tau < \frac{2}{n(n+2)}$ and that g tends to 0 in a given Sobolev norm, then we get by the uniform bounds of Theorem 5.1 and by interpolation that g converges uniformly to 0. So for $t \geqslant t_1$ we get that the last term in the previous equation is bounded by $\varepsilon|S[g]|^2$, for $\varepsilon < \frac{2}{n(n+2)} - \tau$. Therefore we have

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|S[g]|^2 \geqslant 2n(\tfrac{2}{n(n+2)} - \tau - \varepsilon)|S[g]|^2,$$

with a non-zero initial condition, so this yields that $|S[g]|^2$ increases exponentially, which is a contradiction. □

We now define, in the spirit of Chapter 4, the distribution M_A associated to a given trace-free symmetric matrix A by

$$M_A(\omega) = \frac{e^{\omega\otimes\omega:A}}{\int_{\mathbb{S}} e^{\upsilon\otimes\upsilon:A}\mathrm{d}\upsilon} \tag{3.7}$$

By Proposition 2.1, a density probability function f on the sphere is a steady-state if and only if $\tau \ln f + \omega \otimes \omega : S[f]$ is constant, which is equivalent to say that f is of the form M_A, with $A = -\tau^{-1}S[f]$. Hence, we have the following compatibility condition for A:

$$\tau A + S[M_A] = 0, \tag{3.8}$$

and conversely any solution A to this compatibility equation give rise to a steady state of the form M_A. The first thing to remark is that since all the equilibria are even with respect to ω, that is to say $M_A(\omega) = M_A(-\omega)$, then we can use LaSalle principle to show that the odd part of f, given by $f_o(\omega) = \frac{1}{2}[f(\omega) - f(-\omega)]$ will converge to zero in any H^s norm. Indeed, since f_o is orthogonal to any even function, we get, using the notations of Proposition 2.2, and writing $f_e = f - f_o$ the even part of f, that

$$\inf_{g\in\mathcal{E}_\infty} \|f(t) - g\|_{H^s}^2 = \|f_o(t)\|_{H^s}^2 + \inf_{g\in\mathcal{E}_\infty} \|f_e(t) - g\|_{H^s}^2 \to 0 \text{ as } t \to \infty.$$

It is an easy matter to see that the even part of f also satisfies the same Doi equation (1.1), since $\Psi_f = \Psi_{f_e}$, therefore we can restrict the study to the case where the function f is even.

With the complete classification of [78], we now have the structure of the equilibria in any dimension. We can then study the dynamics of convergence, using the same tools as in Chapter 4. We know that a matrix satisfying the compatibility condition (3.8) has only two distinct eigenvalues, so the classification is done according to the smallest dimension of the two eigenspaces. For example if this dimension is 1 (this is always the case when $n = 2$ or 3), the matrix A can be put under the form $\kappa(\frac{n-1}{n}\Omega\otimes\Omega - \frac{1}{n}(\mathrm{Id} - \Omega\otimes\Omega))$ with $\kappa \in \mathbb{R}$ and $\Omega \in \mathbb{S}$, we can rewrite the function M_A as

$$\mathcal{M}_{\kappa,\Omega} = \frac{e^{\kappa(\omega\cdot\Omega)^2 - \frac{\kappa}{n}}}{\int_{\mathbb{S}} e^{\kappa(\upsilon\cdot\Omega)^2 - \frac{\kappa}{n}}\mathrm{d}\upsilon} = \frac{e^{\kappa(\omega\cdot\Omega)^2}}{\int_{\mathbb{S}} e^{\kappa(\upsilon\cdot\Omega)^2}\mathrm{d}\upsilon}, \tag{3.9}$$

and we finally get that compatibility condition (3.8) becomes

$$\tfrac{n-1}{n}\tau\kappa + \langle \tfrac{1}{n} - (\omega\cdot\Omega)^2\rangle_{\mathcal{M}_{\kappa,\Omega}} = 0, \tag{3.10}$$

where $\langle\cdot\rangle_{\mathcal{M}_{\kappa,\Omega}}$ denotes the mean against the probability density $\mathcal{M}_{\kappa,\Omega}$.

We present the results in the two-dimensional case, in which we have a complete understanding of the long-time dynamics, since it is very similar to the dipolar potential. We have also other results in higher dimensions, but not enough complete to be put in this report.

3.1 The two-dimensional case

In a two-dimensional framework the characterization of the equilibria is easy. We can compute these equilibria in the same manner as in Chapter 4, but we will use a transformation which reduces the case of Maier–Saupe potential for an even function, to the case of the dipolar potential.

We use the special conservation relation derived in Proposition A.1 (in appendix): if we denote $g = f - 1$, we have

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g\|^2_{H^{-\frac{1}{2}}(\mathbb{S}_1)} = 4S[(-\Delta)^{-\frac{1}{2}}g] : S[g] - \tau\|g\|^2_{H^{\frac{1}{2}}(\mathbb{S}_1)}, \tag{3.11}$$

where the H^s norm is given by $\|g\|^2_{H^s(\mathbb{S}_1)} = \int_{\mathbb{S}_{n-1}} g(-\Delta)^s g\,\mathrm{d}\omega$ for a function g with mean zero. This conservation relation was derived in [19] for a solution which is

symmetric and even. Here the result is general. This is important to note that this type of special cancellation of the non-linear component is very special to the dimension 2. We can use Lemma 5.1 in higher dimensions, to get precise estimates, but we have not managed to get an exact cancellation, as in this case of dimension 2, and in the general case for the dipolar potential.

We first show that we can restrict ourselves to the case where f is even. Indeed, if we write g_o and g_e the odd and even parts of g we get that they are orthogonal in any H^s norm: g_o (resp. g_e) is the component of g composed only by spherical harmonics of odd (resp. even) degree. Therefore, we have, since $S[g] = S[g_e]$,

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}(\|g_o\|^2_{H^{-\frac{1}{2}}} + \|g_e\|^2_{H^{-\frac{1}{2}}}) = 4S[(-\Delta)^{-\frac{1}{2}} g_e] : S[g_e] - \tau(\|g_o\|^2_{H^{\frac{1}{2}}} + \|g_e\|^2_{H^{\frac{1}{2}}}).$$

But we know that the even part of f is also a solution to Doi equation (1.1), and then g_e satisfies the same conservation relation as in (3.11), and we get by taking the difference:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g_o\|^2_{H^{-\frac{1}{2}}} = -\tau\|g_o\|^2_{H^{\frac{1}{2}}},$$

which gives, by a Poincaré inequality, exponential decay of g_o to zero in $H^{-\frac{1}{2}}(\mathbb{S})$, and then in any H^s norm by interpolation, using the uniform bounds of Theorem 5.1. Let us remark that this argument is valid without conditions on τ, so we always have exponential convergence of the odd part of f to zero in any H^s.

We can now focus on the case where g is even. Since we are on the circle $\mathbb{S}_1$, we can identify g with a 2π-periodic function of $\theta \in \mathbb{R}$, considering ω as the vector $\binom{\cos\theta}{\sin\theta}$. An even function in the previous framework is a function with the same value on two antipodal points, so with this identification, that means that g is actually π-periodic.

We can write Doi equation (1.1) with this identification:

$$\begin{cases} \partial_t f = \partial_\theta(f\partial_\theta \Psi_f) + \tau\partial_{\theta\theta} f, \\ \Psi_f(\theta, t) = \frac{1}{2\pi}\int_0^{2\pi} K(\theta,\bar\theta)\, f(t,\bar\theta)\,\mathrm{d}\bar\theta. \end{cases} \tag{3.12}$$

We have that

$$\begin{aligned} \Psi_f(\theta) &= \frac{1}{2\pi}\int_0^{2\pi} [\tfrac{1}{2} - (\cos\theta\cos\bar\theta + \sin\theta\sin\bar\theta)^2] f(\bar\theta)\mathrm{d}\bar\theta \\ &= \frac{1}{2\pi}\int_0^{2\pi} [\tfrac{1}{2} - \cos^2(\theta-\bar\theta)] f(\bar\theta)\mathrm{d}\bar\theta \\ &= -\frac{1}{2\pi}\int_0^{2\pi} \tfrac{1}{2}\cos(2\theta - 2\bar\theta) f(\bar\theta)\mathrm{d}\bar\theta. \end{aligned}$$

So if we consider the dipolar potential $\widetilde{K}(\theta,\bar\theta) = -\cos\theta\cos\bar\theta - \sin\theta\sin\bar\theta = -\cos(\theta - \bar\theta)$, and the function $\widetilde{f}$ such that $\widetilde{f}(2\theta) = f(\theta)$ (which is then a 2π-periodic function), we get that

$$\begin{aligned} \Psi_f(\theta) &= \frac{1}{2\pi}\int_0^{\pi} \widetilde{K}(2\theta, 2\bar\theta)\cos(2\theta - 2\bar\theta)\widetilde{f}(2\bar\theta)\mathrm{d}\bar\theta \\ &= \frac{1}{2\pi}\int_0^{2\pi} \tfrac{1}{2}\widetilde{K}(2\theta,\theta')\cos(2\theta-\theta')\widetilde{f}(\theta')\mathrm{d}\theta' \\ &= \tfrac{1}{2}\widetilde{\Psi}_{\widetilde{f}}(2\theta). \end{aligned}$$

Therefore we easily get that $\widetilde{f}$ satisfies the following equation:

$$\begin{cases} \frac{1}{2}\partial_t \widetilde{f} = \partial_\theta(\widetilde{f}\partial_\theta \widetilde{\Psi}_{\widetilde{f}}) + 2\tau\partial_{\theta\theta}\widetilde{f}, \\ \widetilde{\Psi}_{\widetilde{f}}(\theta,t) = \frac{1}{2\pi}\int_0^{2\pi} \widetilde{K}(\theta,\bar{\theta})\,\widetilde{f}(t,\bar{\theta})\,\mathrm{d}\bar{\theta}. \end{cases}$$

This is nothing else than the Doi equation with dipolar potential, up to a time scaling factor of $\frac{1}{2}$, and a temperature $\widetilde{\tau} = 2\tau$. It is also easy to get that $S[f] = 0$ if and only if $J[\widetilde{f}] = 0$.

We can directly apply Theorem 4.4 of Chapter 4 to get the results of convergence for the even part of f (the rates have to be multiplied by a factor 2, and the critical threshold is $\widetilde{\tau} = \frac{1}{2}$, that is to say $\tau = \frac{1}{4}$). Including the rate of convergence τ of the odd part of f, we get, in summary, the following theorem:

Theorem 5.2. *Convergence to equilibrium.*

Suppose f_0 is a probability measure, belonging to $H^s(\mathbb{S}_1)$ (this is always the case for some $s < -\frac{1}{2}$).

Then there exists a unique weak solution f to Doi equation (3.12)*, satisfying the initial condition $f(0) = f_0$.*

Furthermore, this is a classical solution, positive for all time $t > 0$, and belonging to $C^\infty((0,+\infty)\times\mathbb{S})$.

If $S[f_0] \neq 0$, then we have the three following cases, depending on τ.

- *If $\tau > \frac{1}{4}$, then f converges exponentially fast to the uniform distribution, with global rate $\min\{\tau, 4\tau - 1\}$ in any H^p norm.*

  More precisely, for all $t_0 > 0$, there exists a constant $C > 0$ depending only on t_0, s, p, and τ, such that for all $t \geqslant t_0$, we have

  $$\|f(t) - 1\|_{H^p} \leqslant C\|f_0\|_{H^s} e^{-\min\{\tau,4\tau-1\}t}.$$

- *If $\tau < \frac{1}{4}$, then there exists $\Omega \in \mathbb{S}_1$ such that f converges exponentially fast to $\mathcal{M}_{\kappa\Omega}$, with asymptotic rate $r_\infty(\tau) > 0$ in any H^p norm, where κ is the unique positive solution of the compatibility condition 3.10.*

  More precisely, for all $r < r_\infty(\tau)$, there exists $t_0 > 0$ (depending on f_0) such that for all $t > t_0$, we have

  $$\|f(t) - M_{\kappa\Omega}\|_{H^p} \leqslant e^{-rt}.$$

  When τ is close to $\frac{1}{4}$ we have that $r_\infty(\tau) \sim 2 - 8\tau$.

- *If $\tau = \frac{1}{4}$, there exists $r_c > 0$ such that f converges to the uniform distribution in any H^p norm, with asymptotic rate $\sqrt{\frac{1}{r_c t}}$.*

  More precisely, for all $r < r_c$, there exists $t_0 > 0$ (depending on f_0) such that for all $t > t_0$, we have

  $$\|f(t) - 1\|_{H^p} \leqslant \frac{1}{\sqrt{rt}}.$$

If $S[f_0] = 0$ the equation reduces to the heat equation on the sphere, so f converges to the uniform distribution, exponentially with global rate τ in any H^p norm.

4 Conclusion

In this chapter, we have proved that the method previously used to study the case of the dipolar potential still works in the Maier–Saupe potential, with complications due to the more complex structure of the equilibria. In particular, the theoretical results of existence for an initial condition in any Sobolev space still hold, and we can derive a LaSalle's invariance principle adapted to our problem.

In the case of dimension 2, were the structure of the equation is very similar to the case of the dipolar potential, we have been able to get the same results of convergence to an equilibrium for any initial condition.

In higher dimensions, the method for the nematic phase applies locally for the stable nematic equilibrium, and also for the case where the uniform distribution is stable. Some investigations are in progress on this topic. An interesting issue is the behavior of the odd part of a solution (with LaSalle principle, we already know that it is converging to zero, but we do not have a rate of convergence).

A Special cancellation in dimension 2

We first rewrite the equation in a weak formulation, and using $g = f-1$. We multiply by a function h with mean zero on the sphere, and we get the weak formulation for Doi equation (1.1) by integrating by parts on the unit sphere:

$$\int_{\mathbb{S}} \partial_t g h \mathrm{d}\omega = 2nS[h] : S[g] + \tau \int_{\mathbb{S}} \nabla_\omega h \cdot \nabla_\omega g \,\mathrm{d}\omega - 2S[g] : \int_{\mathbb{S}} \omega \otimes \nabla_\omega h \, g \,\mathrm{d}\omega. \quad \text{(A.13)}$$

In order to have a quadratic conservation law, as in the case of the dipolar potential, we want to cancel the last term. So we compute it in the basis of spherical harmonics.

We can decompose $g = \sum_{k,\ell,m} c^k_{\ell,m} Y^k_{\ell,m}$ with the notations of Appendix A of Chapter 4. Since g is of mean zero, we have $c^1_{0,0} = 0$ and the indices k, ℓ, m of the sum will always mean $\ell > 0, m \in [\![0, \ell]\!], k \in [\![1, k_m^{(n-1)}]\!]$. We decompose in the same way $h = \sum_{k,\ell,m} d^k_{\ell,m} Y^k_{\ell,m}$.

We give a first formula, in the form of a lemma.

Lemma 5.1. *We have*

$$\begin{aligned} e_n \otimes e_n : \int_{\mathbb{S}_{n-1}} g\, \omega \otimes \nabla h &= \frac{1}{2} \sum_{k,\ell,m} \gamma_{\ell,m} c^k_{\ell,m} d^k_{\ell,m} \\ &+ \frac{1}{2} \sum_{k,\ell,m} \beta_{\ell,m} [(\ell+n-1) c^k_{\ell-1,m} d^k_{\ell+1,m} - (\ell-1) c^k_{\ell+1,m} d^k_{\ell-1,m}], \end{aligned} \quad \text{(A.14)}$$

where the coefficients $\beta_{\ell,m}$ and $\gamma_{\ell,m}$ will be defined later on in (A.16).

Proof. We have

$$\begin{aligned} e_n \cdot \omega \, e_n \cdot \nabla Y^k_{\ell,m} &= -\cos\theta \sin\theta \partial_\theta Y^k_{\ell,m} \\ &= \left[X(1-X^2) Q'_{\ell,m} - m X^2 Q_{\ell,m} \right] (\cos\theta) \sin^m \theta Z^k_m(v), \end{aligned}$$

and using the inductions formulas (A.60), (A.61) and (A.62) of Appendix A of Chapter 4, we get (except for $n = 2$, $m = 0$)

$$\begin{cases} XQ_{\ell,m} = \frac{1}{2}[b_{\ell-1,m}Q_{\ell-1,m} + b_{\ell,m}Q_{\ell+1,m}] \\ (1-X^2)Q'_{\ell,m} - mXQ_{\ell,m} = \frac{1}{2}[b_{\ell-1,m}(\ell+n-2)Q_{\ell-1,m} - b_{\ell,m}\ell Q_{\ell+1,m}], \end{cases} \tag{A.15}$$

where $b_{\ell,m} = \frac{\sqrt{\ell-m+1}\sqrt{\ell+m+n-2}}{\sqrt{\ell+\frac{n}{2}-1}\sqrt{\ell+\frac{n}{2}}} \leqslant 1$.

In the special case $n = 2$,$m = 0$, using the formula $Q_{\ell,0}(\cos\theta) = \cos\ell\theta$ gives the same formulas as (A.15), with $b_{\ell,0} = 1$ (note that when $n = 2$ the only possibilities for m are 0 and 1, and we also have $b_{\ell,1} = 1$).

Hence we get

$$\begin{aligned} X(1-X^2)Q'_{\ell,m} - mXQ_{\ell,m} &= \tfrac{1}{2}[b_{\ell-1,m}b_{\ell-2,m}(\ell+n-2)Q_{\ell-2,m} - b_{\ell,m}b_{\ell+1,m}\ell Q_{\ell+2,m}] \\ &\quad + \tfrac{1}{2}(b_{\ell-1,m}^2(\ell+n-2) - b_{\ell,m}^2\ell)Q_{\ell,m} \\ &= \tfrac{1}{2}[\beta_{\ell-1,m}(\ell+n-2)Q_{\ell-2,m} - \beta_{\ell+1,m}\ell Q_{\ell+2,m} + \gamma_{\ell,m}Q_{\ell,m}], \end{aligned}$$

with, using the expression for $b_{\ell,m}$, when $n \geqslant 2$,

$$\begin{cases} \beta_{\ell,m} = \frac{\sqrt{\ell-m+1}\sqrt{\ell+m+n-2}\sqrt{\ell-m}\sqrt{\ell+m+n-3}}{(\ell+\frac{n}{2}-1)\sqrt{\ell+\frac{n}{2}-2}\sqrt{\ell+\frac{n}{2}}} \\ \gamma_{\ell,m} = \frac{(n-2)\ell(\ell+n-2)}{(\ell+\frac{n}{2}-2)(\ell+\frac{n}{2})} - \frac{2(n-1)m}{\ell+\frac{n}{2}-1} + \frac{nm(m(\ell+\frac{n}{2}-1)-1)}{(\ell+\frac{n}{2}-2)(\ell+\frac{n}{2}-1)(\ell+\frac{n}{2})}, \end{cases} \tag{A.16}$$

When $n = 2$ we get $\beta_{\ell,m} = 1$ and $\gamma_{\ell,m} = 0$. Finally, we have

$$e_n \cdot \omega\, e_n \cdot \nabla Y_{\ell,m}^k = \tfrac{1}{2}[\beta_{\ell-1,m}(\ell+n-2)Y_{\ell-2,m}^k - \beta_{\ell+1,m}\ell Y_{\ell+2,m}^k + \gamma_{\ell,m}Y_{\ell,m}^k],$$

so we have that $\int_{\mathbb{S}_{n-1}} e_n \cdot \omega\, e_n \cdot \nabla Y_{\ell,m}^k Y_{\ell',m'}^{k'}$ can be non-zero only if $m = m'$, $k = k'$, and $\ell = \ell'$ or $\ell' \pm 2$. By bilinearity, together with the fact that $Y_{\ell,m}^k$ form an orthonormal basis, this gives the claimed formula. □

Now, if we are in dimension 2, we chose $h = (-\Delta)^{-\frac{1}{2}}g$, that is to say $d_{\ell,m}^k = \frac{1}{\ell}c_{\ell,m}^k$, and we get, with Lemma 5.1, since $\beta_{\ell,m} = 1$ and $\gamma_{\ell,m} = 0$

$$e_n \otimes e_n : \int_{\mathbb{S}_{n-1}} g\,\omega \otimes \nabla((-\Delta)^{-\frac{1}{2}}g)) = 0.$$

Since this is true for all unit vector e_n, if A is a symmetric matrix, we can decompose it in an orthonormal basis: $A = \sum_i \lambda_i e_i \otimes e_i$, and we get that $A : \int_{\mathbb{S}_{n-1}} g\,\omega \otimes \nabla((-\Delta)^{-\frac{1}{2}}g))$ vanishes. Hence, going back to the weak formulation (A.13), we get immediately the following result:

Proposition A.1. *Special conservation relation in dimension* 2.

If f is a solution of Doi equation (1.1) *with the Maier–Saupe potential in dimension $n = 2$, then we have the following conservation relation, for $g = f - 1$:*

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|g\|_{H^{-\frac{1}{2}}(\mathbb{S}_1)}^2 = 4S[(-\Delta)^{-\frac{1}{2}}g] : S[g] - \tau\|g\|_{H^{\frac{1}{2}}(\mathbb{S}_1)}^2, \tag{A.17}$$

where the H^s norm is given by $\|g\|_{H^s(\mathbb{S}_1)}^2 = \int_{\mathbb{S}_{n-1}} g(-\Delta)^s g\,\mathrm{d}\omega$ for a function g with mean zero.

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