Statistical Mechanics and Hydrodynamics of Active Fluids

by

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Abstract

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In this thesis, I present work pertaining to the continuum modeling of active fluids. The main results are as follows. I derive Green-Kubo equations for the components of the viscosity in two-dimensional fluids with and without internal angular momentum. These equations illustrate the connection between the breaking of time-reversal symmetry at the microscopic level and the emergence of odd viscosity, a non-dissipative transport coefficient. They also show the potential for a new, previously unconsidered rotational viscosity in fluids in which internal spin couples to velocity. By numerically verifying the Green-Kubo equation for odd viscosity, we provide support for the use of the Onsager regression hypothesis in its derivation, where this hypothesis is applied to fluctuations about a nonequilibrium steady state. I also study the canonical active system known as Active Brownian Particles via a coarse-graining analysis. This approach indicates that in such systems, activity manifests at the continuum level in the form of a body force, rather than as an addition to the stress tensor, as has been previously assumed in the literature. It also elucidates the connection between mass currents and inter-particle alignment interactions. Taken as a whole, these results provide guidance for the project of writing down continuum descriptions of active matter, and elucidate the connections between microscopic and macroscopic behavior for nonequilibrium systems.

To the memories of my grandparents: Lois and Charles Epstein; Barbara and Henry Lewis.

Contents

Acknowledgments

The work presented in this thesis is the product of a roughly three year collaboration with my advisor, Kranthi Mandadapu. I am fortunate to have found in Kranthi a dedicated and caring mentor, an insightful scientist, and an open mind. I imagine it is extremely unusual to find in one person both the relish for scientific disagreement and the intellectual charisma that I have observed in Kranthi. It is my sincere hope that, even as I move into a different field post-graduation, we will continue to have a lively exchange of ideas.

Although it not not represented in this document, I spent an enjoyable portion of my time at Berkeley working on projects in quantum information. I am lucky to have done so in collaboration with and guided by Birgitta Whaley and Josh Combes. As I transition back into the quantum world, I hope to continue collaborating with both of them. Norm Tubman has also been a significant source of guidance from his arrival in Berkeley to the present, and indeed was the one who introduced me to Kranthi when I was unsure what I wanted to do. He has been a consistent grounding influence, helping me to keep the problems of graduate school in perspective while aiding in my search for solutions.

Carlos Mejuto Zaera and Katie Klymko have been steadfast friends throughout the last several years, and both have been inspirations to me on academic and personal levels. One of the great disappointments of the covid era has been that I will end my time in Berkeley without the weekly Tuesday lunches with Carlos at Thai House, traditional for at least three years. These lunches served as refreshing midday breaks, as much-needed grievance sessions, and as venues for discussion of whatever physics was interesting to us in the moment. Some day I will convince Carlos that "What is a quantum field?" is a good question. Katie has been an impressive role model for me from the time I met her. I am particularly inspired by how quickly and successfully she has moved between fields, and hope to follow in her footsteps. I have always been able to talk through academic and personal problems with her in a way that makes the world seem more manageable. Our Saturday coffees have been a highlight of my week.

From the beginning of the program, Sam Dixon, Jennet Dickinson, and Dragoș Potîrniche have been close friends in and out of the Physics Department. Sam and Jennet were frequent brunch partners, and I spent more evenings than I can count hanging out at their apartment. I've always been able to count on both of them to keep me from obsessing unnecessarily about my problems (or at least to tell me when that's what I'm doing). My frequent morning zoom calls with Sam during covid have been a source of comfort and connection, as were the short-lived but productive Attic Greek sessions with Jennet. I lived with Dragoș for five and a half years, and was lucky to have a roommate who became a good friend. Although neither of us remembers exactly why, we spent two years learning krav maga together. I highly recommend occasional bouts of close contact sparring for strengthening a friendship.

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Chapter 1

Introduction

I think that the mistake behind Kretschmann's argument is an excessively legalistic reading of the scientific enterprise. It is the mistake of taking certain common physicists' statements too literally. Physicists often write that a certain symmetry or a certain principle "uniquely determines" a certain theory. At a close reading, these statements are almost always much exaggerated. The uniqueness only holds under a vast number of other assumptions that are left implicit and which are facts or ideas the physicist considers natural, and does not bother detailing. The typical physicist carelessly dismisses counter-examples by saying that they would be unphysical, implausible, or completely artificial. The connection between general physical ideas, general principles, intuitions, symmetries, is a burning melt of powerful ideas, not the icy demonstration of a mathematical theorem. What is at stake is finding the most effective language for thinking the world, not writing axioms. It is language in formation, not bureaucracy. [1]

Active materials are non-equilibrium systems that consume and dissipate energy throughout their bulks at the microscopic level even in the absence of spatial inhomogeneity [2, 3, 4, 5]. This feature distinguishes them from the better-understood class of boundary-driven nonequilibrium systems, in which externally imposed gradients in temperature, pressure, chemical potential, or other thermodynamical variables drive fluxes that result in the production of entropy. This class of systems has been unified under the framework of linear irreversible thermodynamics [6]. Active systems, in contrast, produce entropy due to internal processes, generally chemical, at the level of single particles. No unifying framework yet exists for treating their phenomenology. Nonetheless, or perhaps because of this unresolved state of the field, it is widely expected that studying active systems will provide novel insights into biological processes [7], lead to potential technological applications [8], perhaps through tunable rheologies [9, 10, 11, 12], and promote the development of new fundamental tools in statistical mechanics [13, 14, 15, 16, 17, 18, 19].

Active matter has been studied in several experimental realizations, both natural and synthetic. On the natural side are colonies or suspensions of motile bacteria [20, 21, 22, 23] and actomyosin networks [24, 25]. In both cases, energy is released and converted into motion via the hydrolysis of ATP. In the bacterial case, this motion is due to the operation of a flagellum or other driving mechanism, such as those based on pili growth and retraction, while for actomyosin gels, it drives the stepping of the myosin motors along actin filaments. On the synthetic side, there are at least two major paradigms of active matter - wet and dry. Wet active matter consists of self-propelled particles in solution, and has been realized for example by the so-called Janus particles, colloids half-coated in a catalyst that drives hydrolysis of a hydrogen peroxide, generate a propulsive force [26]. Dry active matter lacks a solvent, and has been implemented by systems of asymmetric walkers on vibrating substrates [27] and particles rotated by a time-dependent magnetic field [28]. The asymmetry of the walker rectifies the random vibrations into directed motion, breaking time-reversal symmetry.

Numerous examples of active matter phenomenology have been studied in the literature. I mention here some of the most striking. Motility-induced phase separation (MIPS) is the phenomenon wherein driven particles, even in the absence of attractive interparticle forces, phase separate into dense and dilute regions [26, 29]. Odd viscosity is an emergent non-dissipative transport coefficient that has been observed in particles rotated via a time-dependent magnetic field [28]. In some active fluids, the pressure exerted on an immersed surface is curvature-dependent, so that pressure fails to be a state function [30].

In this thesis, I present the results of work towards understanding how to model various classes of active fluids at the continuum level of description. Such a compressed description of these physical systems will be crucial for studying their phenomenology and for understanding how microscopic properties of active systems manifest at the macroscale. The common thread running through this work is exactly this micro-to-macro transition. My hope is that the results presented here will contribute to the project of unifying the treatment of active materials by providing a few "design principles" for continuum equations.

In Chapter 2, I present the results of a study of active fluids with no internal structure. The main conclusion of this chapter is that odd viscosity, a non-dissipative component of the viscosity tensor that may appear in two-dimensional fluids, is a manifestation of time-reversal symmetry breaking at the level of stress fluctuations. This outcome is obtained in the concrete form of a Green-Kubo equation for the coefficient of odd viscosity. In order to obtain this result, we make use of Onsager's regression hypothesis. Roughly speaking, this is the assumption that fluctuations about a steady state decay in a manner compatible with the deterministic equations of macroscopic flows. By providing the results of numerical simulations that confirm the Green-Kubo relation for a simple model active fluid, composed of actively rotated dumbbells, we provide support for the application of this hypothesis to non-equilibrium steady states, widening its realm of validity from that originally considered by Onsager. This chapter also serves as a quick introduction to and discussion of basic approaches of continuum mechanics, linear irreversible thermodynamics, and time-reversal symmetry, including an argument that previous cases made for the connection between odd viscosity and time-reversal symmetry breaking are flawed.

In Chapter 3, I extend the analysis of chapter 2 to fluids that support an internal "spin" angular momentum, as proposed originally by Dahler and Scriven [31]. In doing so, I find a new component of rotational viscosity that may couple the internal and external angular momenta of fluids with internal structure, compared to the model used in recent work on such fluids. This new component is nonvanishing when equipartition is broken between linear and rotational velocity fluctuations, i.e. when there are unequal linear and rotational temperatures, and so is a possible macroscopic manifestation of activity-related departure from equilibrium in complex fluids. We also find that there is a possibility for the emergence of odd viscosity in systems that are time-reversal symmetric at the level of fluctuations but which violate objectivity of the stress.

In Chapter 4, I switch approaches, and begin at the microscale, studying a particular system of active matter known as Active Brownian Particles (ABPs). These feature a vector degree of freedom for each particle, the "director", along which an active force is applied, driving the system away from equilibrium. I use the method of Irving and Kirkwood [32] to coarse-grain this system, providing a set of continuum balance laws for a fluid of ABPs. In doing so, I find that the active force manifests at the continuum level via a body force applied along a director field, as opposed to as an additional component of the stress tensor, the "swim pressure", as assumed in several recent works. Because the swim pressure approach has however been successfully used to reproduce ABP phenomenology, namely motility-induced phase separation (MIPS), I also provide a reconciliation of these two approaches to incorporating activity at the continuum level. Finally, I show that mass currents are only possible in homogeneous systems of ABPs in the presence of alignment interactions.

Taken as a whole, the results in this thesis contribute to the project of formulating physically-motivated continuum equations for active fluids and to the reconciliation of macroscopic behavior with energy dissipation and entropy production at the microscale. Additionally, by demonstrating the validity of extending the Onsager regression hypothesis to non-equilibrium steady states, they contribute to the project of developing a unified non-equilibrium thermodynamics. It is my hope that this work will advance the study and classification of active matter phenomenology and lead towards a unification of these diverse systems. Future work along these lines already in progress includes a study of odd diffusivity, another nonequilibrium transport coefficient, and the Green-Kubo analysis of liquid crystals, where we hypothesize that it is possible to recover the connection between time-reversal symmetry and the Parodi relations is the same manner as we treat the odd viscosity here. This will be a crucial development for understanding the role of time-reversal symmetry breaking in bacterial colonies, in the spirit of [20].

Finally, a note on the quotation with which I opened this introduction. Taken from Carlo Rovelli's book *Quantum Gravity*, it captures how I have come to think about the process of devising equations for physical systems. At the beginning of my doctoral studies, I thought of physics in terms of derivations and proof. I now think of it in terms of argumentation and plausibility. Perhaps more importantly, I have come to see the equations as little more than starting points for the prediction of phenomena. Thus I see this thesis as merely a beginning.

The work presented in this thesis has been published in the following papers:

1. *Statistical Mechanics of Transport Processes in Active Fluids II: Equations of Hydrodynamics for Active Brownian Particles.* JME, K. Klymko, K. K. Mandadapu. 2019.

2. *Time reversal symmetry breaking in two-dimensional non-equilibrium viscous fluids.* JME, K. K. Mandadapu. 2020.

3. *Time reversal symmetry breaking and odd viscosity in active fluids: Green-Kubo and NEMD results.* C. Hargus, K. Klymko, JME, K. K. Mandadapu. 2020.

During my time at Berkeley, I have also pursued work in quantum information. This work, not discussed in this thesis, is represented in the following papers:

1. *Quantum Speed Limits for Quantum Information Processing Tasks.* JME, K. B. Whaley. 2017.

2. *Postponing the orthogonality catastrophe: efficient state preparation for electronic structure simulations on quantum devices.* N. M. Tubman, C. Mejuto Zaera, JME, *et al.*. 2018.

3. *Continuous quantum error correction for evolution under time-dependent Hamiltonians.* J. Atalaya, S. Zhang, M. Y. Niu, A. Babakhani, H. C. H. Chan, JME, K. B. Whaley. 2020.

4. *Quantum noise limits for a class of nonlinear amplifiers.* JME, K. B. Whaley, J. Combes. 2020.

Chapter 2

Green-Kubo analysis of two dimensional active fluids with no internal structure

Newtonian mechanics takes as its basic objects point particles moving under the influence of forces. Classical equilibrium thermodynamics takes as its basic objects discrete systems characterized by temperatures, chemical potentials, and other intensive properties conjugate to conserved extensive quantities. For many purposes, this is an insufficient picture of the world, and we would like to be able to describe the behavior of inhomogeneous continuum bodies. The states of such bodies are characterized by several fields, such as velocity, temperature, chemical potential, pressure, and density, and the evolution of these fields is modeled by sets of partial differential equations.

In the first two sections of this chapter, I will introduce two well-known frameworks for developing these partial differential equations in a principled manner that respects the lessons of Newtonian mechanics and equilibrium thermodynamics. These are, respectively, the framework of mechanical balance laws and of linear irreversible thermodynamics, see e.g. [33, 34, 6]. In the third section of the chapter, I will present a combination of the two frameworks that is often used to argue that the viscosity tensor of a fluid must obey a certain symmetry (Onsager symmetry) if the microscopic dynamics of the system are time-reversal invariant. I will argue that this is an improper application of the framework of linear irreversible thermodynamics. In the final section, I will recover the connection between the time-reversal and Onsager symmetries in a way that avoids the problems I discuss.

I emphasize here that in no sense will the equations modeling continuum bodies be derived. Rather, they should be seen as one particular *implementation* of a set of physical principles learned through observation and obeyed by other phyiscal theories. Instead of a derivation or a proof, the following argument should be seen as a *motivation*, and instead of a series of lemmas, it consists of a series of what the philosophers seem to call “moves”. The end result will be a “physically reasonable”, but certainly non-unique set of closed equations of motion for the fields that specify the state of a continuum body (more accurately, a family of partial differential equation models with a few parameters that must be fixed by other means). These equations must then be tested against experiments to determine their validity for any particular system. In my present opinion, it is best to think of them as playing two major roles:

1. They serve as a starting point for predictions of phenomena that may then be sought in the lab.
2. Phenomena observed in the lab may be sought in the differential equations in order to determine the suitability of the basic physical model. If there are observed (qualitative) phenomena not captured by the equations, this may be an indicator that there should be more or different elements included in the ontology of the theory.

Having allowed ourselves this short rumination, we now begin to work towards the promised continuum models.

2.1 Mechanics and the continuum

The state of a fluid with no internal structure is characterized by a vector velocity field v_i and a scalar density field ρ. The goal of this section will be to present a well-known strategy for proposing evolution equations for these fields, see e.g. [33]. This framework works by enforcing conservation laws at the level of subregions of the body under consideration.

We begin with conservation of mass. Consider a region $\mathcal{R}$ convected with the body. Such a region is considered to be defined by a boundary consisting of physical mass points moving with the fluid velocity v_i. Thus $\mathcal{R}$ consists at all times of the same set of mass points, and the mass contained in the region is constant:

$$\frac{d}{dt}\int_{\mathcal{R}(t)} \rho \, dv = 0. \tag{2.1}$$

We may rewrite the left-hand side of this equation using the Reynolds transport theorem and the divergence theorem:

$$\frac{d}{dt}\int_{\mathcal{R}(t)} \rho \, dv = \int_{\mathcal{R}(t)} \frac{\partial \rho}{\partial t} \, dv + \int_{\partial\mathcal{R}(t)} (\mathbf{v}\cdot\mathbf{n})\,\rho \, da = \int_{\mathcal{R}(t)} \left[\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{v})\right] dv. \tag{2.2}$$

This should hold for any choice of region $\mathcal{R}$, which suggests proposing the mass continuity equation

$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla}\cdot(\rho\mathbf{v}) \tag{2.3}$$

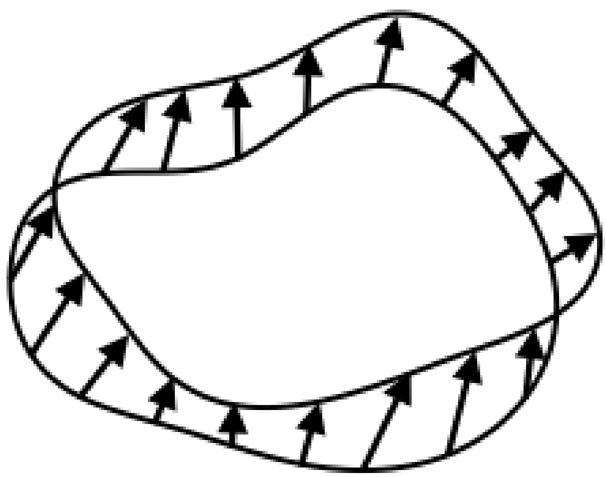

Figure 2.1: Visualization of Reynolds transport theorem.

or, equivalently

$$\frac{D\rho}{\partial t} = -\rho \boldsymbol{\nabla} \cdot \mathbf{v}, \tag{2.4}$$

where we have defined the material derivative $D/Dt = \partial/\partial t + \mathbf{v} \cdot \boldsymbol{\nabla}$. Note that (2.3) and (2.4) imply (2.2), but we have not established rigorously the other direction. Because we are taking the point of view that our equations will be an implementation of fundamental principles, rather than a consequence of them, this is sufficient for our purposes. For an incompressible fluid, i.e. one with constant density, the balance of mass is implemented by the condition $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$.

We turn now to the balance of linear momentum. Again take a region $\mathcal{R}$, convected with the body. The momentum contained by this region may be identified with the integral over the region of the product $\rho\mathbf{v}$. In a body not subject to external influence, it is often a good assumption that the region of the body under examination feels forces at its surface from the surrounding region. Suppose that a small region da of the surface feels a force density $\mathbf{t}\, da$, where $\mathbf{t}$ is known as the traction. Then we may write

$$\frac{d}{dt} \int_{\mathcal{R}(t)} \rho v_i \, dv = \int_{\partial\mathcal{R}(t)} t_i \, da. \tag{2.5}$$

Let's think about the form of the traction. The following analysis is known as the Cauchy tetrahedron argument. I will present it in two spatial dimensions, but it generalizes to any number of dimensions. In any reasonable continuum body, there should be a length scale at which the force density t_i is constant on any (fictitious) surface. Consider a triangle with sides characterized by normal vectors $\mathbf{n}_a$, $\mathbf{n}_b$, and $\mathbf{n}_c$ and side lengths $\ell_a = ax$, $\ell_b = bx$, and

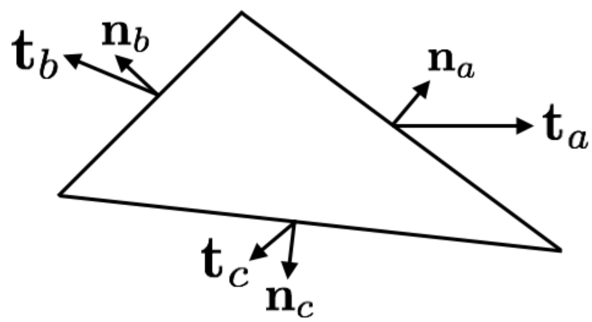

Figure 2.2: The relevant normal vectors and tractions for the Cauchy tetrahedron argument.

$\ell_c = \sqrt{a^2 + b^2 + 2ab\,\mathbf{n}_a \cdot \mathbf{n}_b}\,x$. If x is small compared to the traction homogeneity length scale, then the total force exerted on the triangle by the surrounding medium is given by

$$\mathbf{F} = \left(a\,\mathbf{t}(\mathbf{n}_a) + b\,\mathbf{t}(\mathbf{n}_b) + \sqrt{a^2 + b^2 + 2ab\,\mathbf{n}_a \cdot \mathbf{n}_b}\,\mathbf{t}(\mathbf{n}_c)\right) x. \tag{2.6}$$

We also have

$$\mathbf{F} = m\mathbf{a}, \tag{2.7}$$

where $\mathbf{a}$ is the acceleration of the triangular region of the body, and m it's mass. But m goes as area, i.e. as x^2, so that we have

$$Cx^2\mathbf{a} = \left(a\,\mathbf{t}(\mathbf{n}_a) + b\,\mathbf{t}(\mathbf{n}_b) + \sqrt{a^2 + b^2 + 2ab\,\mathbf{n}_a \cdot \mathbf{n}_b}\,\mathbf{t}(\mathbf{n}_c)\right) x. \tag{2.8}$$

for some constant C depending on the mass density and the geometry of the triangle. The acceleration $\mathbf{a}$ should be finite, and this equation should hold for $x \to 0$, i.e. as the triangle shrinks to a point, which requires

$$a\,\mathbf{t}(\mathbf{n}_a) + b\,\mathbf{t}(\mathbf{n}_b) + \sqrt{a^2 + b^2 + 2ab\,\mathbf{n}_a \cdot \mathbf{n}_b}\,\mathbf{t}(\mathbf{n}_c) \to 0. \tag{2.9}$$

Thus shrinking the triangle to a point, we have the relation

$$\mathbf{t}(\mathbf{n}_c) = -\frac{a\,\mathbf{t}(\mathbf{n}_a) + b\,\mathbf{t}(\mathbf{n}_b)}{\sqrt{a^2 + b^2 + 2ab\,\mathbf{n}_a \cdot \mathbf{n}_b}}. \tag{2.10}$$

From geometry alone, we also have

$$-\boldsymbol{n}_c = \frac{a\,\mathbf{n}_a + b\,\mathbf{n}_b}{\sqrt{a^2 + b^2 + 2ab\,\mathbf{n}_a \cdot \mathbf{n}_b}}. \tag{2.11}$$

By the equality of action and reaction, we should have $\mathbf{t}(\mathbf{n}) = -\mathbf{t}(-\mathbf{n})$. Thus we may conclude

$$\mathbf{t}\left(\frac{a\,\mathbf{n}_a + b\,\mathbf{n}_b}{\sqrt{a^2 + b^2 + 2ab\,\mathbf{n}_a \cdot \mathbf{n}_b}}\right) = \frac{a\,\mathbf{t}(\mathbf{n}_a) + b\,\mathbf{t}(\mathbf{n}_b)}{\sqrt{a^2 + b^2 + 2ab\,\mathbf{n}_a \cdot \mathbf{n}_b}}. \tag{2.12}$$

In other words, the map from surface normals to tractions is linear. The most obvious way to extend the function $\mathbf{t}$ to the whole vector space is simply to take it to be a linear function from vectors to vectors, i.e. a tensor. Then we have

$$t_i(\mathbf{n}) = T_{ij} n_j. \tag{2.13}$$

Returning to the change of momentum, we may now write

$$\frac{d}{dt}\int_{\mathcal{R}(t)} \rho\mathbf{v}\,dv = \int_{\partial\mathcal{R}(t)} \mathbf{T}\cdot\mathbf{n}\,da = \int_{\mathcal{R}(t)} \boldsymbol{\nabla}\cdot\mathbf{T}\,dv, \tag{2.14}$$

where we have used the divergence theorem to express the change in momentum in terms of a volume integral. As before, we may apply the Reynolds transport theorem and the divergence theorem to the left-hand side, obtaining

$$\frac{d}{dt}\int_{\mathcal{R}(t)} \rho\mathbf{v}\,dv = \int_{\mathcal{R}(t)} \frac{\partial}{\partial t}(\rho\mathbf{v})\,dv + \int_{\partial\mathcal{R}(t)} (\mathbf{v}\cdot\mathbf{n})\rho\mathbf{v} = \int_{\mathcal{R}(t)} \left[\frac{\partial}{\partial t}(\rho\mathbf{v}) + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}\otimes\mathbf{v})\right]. \tag{2.15}$$

As before, we may now propose

$$\frac{\partial}{\partial t}(\rho\mathbf{v}) + \boldsymbol{\nabla}\cdot(\rho\mathbf{v}\otimes\mathbf{v}) = \boldsymbol{\nabla}\cdot\mathbf{T}, \tag{2.16}$$

which, using the balance of mass (2.3) or (2.4) may be rearranged to give the momentum balance equation

$$\rho\frac{\partial\mathbf{v}}{\partial t} = -\rho\mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v} + \boldsymbol{\nabla}\cdot\mathbf{T}, \tag{2.17}$$

or, equivalently

$$\rho\frac{D\mathbf{v}}{Dt} = \boldsymbol{\nabla}\cdot\mathbf{T}. \tag{2.18}$$

At this point, we do not have a closed system of equations: it remains to determine the form of $\mathbf{T}$, which should be dependent on ρ and $\mathbf{v}$. It turns out that by enforcing the conservation of angular momentum, it is possible to constrain the form of the stress tensor $\mathbf{T}$. The angular momentum of a region $\mathcal{R}$ about the (arbitrary) origin of coordinates can be changed via the torque due to the tractions. In other words, we have

$$\frac{d}{dt}\int_{\mathcal{R}(t)} \rho\mathbf{x}\times\mathbf{v}\,dv = \int_{\partial\mathcal{R}(t)} \mathbf{x}\times(\mathbf{T}\cdot\mathbf{n})\,da. \tag{2.19}$$

Applying the Reynolds transport theorem to the left-hand side and the divergence theorem to both sides, we obtain an integral equation that may be localized to yield, in components, an equation for the antisymmetric piece of the stress tensor:

$$\epsilon^{ijk}T^{kj} = \epsilon^{ijk}\left[\frac{D}{Dt}(\rho x^j v^k) - \rho x^j v^k \boldsymbol{\nabla}\cdot\mathbf{v} - x^j\partial_l T^{kl}\right]. \tag{2.20}$$

Using the balances of mass and linear momentum, the right-hand side may be seen to vanish. Thus, the balance of angular momentum implies the symmetry of the stress tensor $T^{ij} = T^{ji}$.

We will now introduce another desideratum in our theory of fluid motion. Recall that our task, in order to close the evolution equation for the velocity field $\mathbf{v}$ is to propose a constitutive relation that defines the stress $\mathbf{T}$ in terms of $\mathbf{v}$. By Galilean invariance, the stress should not depend directly on the velocity $\mathbf{v}$. On the other hand, from experience, we know that layers of fluid moving past one another exert tractions on each other, so that $\boldsymbol{\tau}$ ought to depend on the velocity gradient $\boldsymbol{\nabla}\mathbf{v}$. We will assume in the interest of simplicity that the stress does not depend on any higher derivatives of the velocity.

As with any tensor, the velocity gradient $\boldsymbol{\nabla}\mathbf{v}$ may be split into symmetric and antisymmetric pieces. In components:

$$\partial_i v_j = \frac{1}{2}\left(\partial_i v_j + \partial_j v_i\right) + \frac{1}{2}\left(\partial_i v_j - \partial_j v_i\right) := \epsilon_{ij} + \omega_{ij}. \tag{2.21}$$

The antisymmetric component ω_{ij} is simply the vorticity of the fluid. Now imagine that an observer is looking at the fluid from a reference frame that is rotating about a fixed axis with respect to the lab frame. Denote by $\boldsymbol{\epsilon}'$ and $\boldsymbol{\omega}'$ the symmetric and antisymmetric pieces of the velocity gradient as observed by the rotating observer at the moment at which the axes of the two frames are aligned. Then we have

$$\boldsymbol{\epsilon}' = \boldsymbol{\epsilon} \tag{2.22}$$

$$\boldsymbol{\omega}' = \boldsymbol{\omega} + \boldsymbol{\Omega}, \tag{2.23}$$

where $\boldsymbol{\Omega}$ is the rate of rotation of the observer. Denote by $\mathbf{T}'$ the stress tensor observed by the rotating observer at the moment of coincidence. It is a convenient simplification to assume that $\mathbf{T} = \mathbf{T}'$. In order to enforce this, we will assume that $\mathbf{T}$ may not depend on ω.

It is convenient to divide the stress tensor into a scalar piece p, the pressure, and a remaining piece $\boldsymbol{\tau}$, known as the deviatoric stress:

$$T_{ij} = -p\delta_{ij} + \tau_{ij}. \tag{2.24}$$

We focus first on the deviatoric piece, which we assume vanishes in the absence of a velocity gradient. Then it is natural to assume that the deviatoric stress is linear in the velocity gradient. In components, we have

$$\tau^{ij} = \eta^{ijkl} v_{k,l} \tag{2.25}$$

where η^{ijkl} is a rank four tensor known as the viscosity tensor. Now, we finally have the momentum balance

$$\rho \frac{\partial v_i}{\partial t} = -\rho v_j v_{i,j} + \eta^{ijkl} v_{k,lj} - p_{,i}. \tag{2.26}$$

For an incompressible fluid, the divergence-free character of the velocity field must be preserved by time evolution. This implies the condition

$$p_{,ii} = -\rho v_{j,i} v_{i,j} + \eta^{ijkl} v_{k,lji}. \tag{2.27}$$

For a compressible fluid, pressure is generally taken to be a function of density and temperature.

2.2 Thermodynamics and the continuum

Imagine that we would like to study a continuum body at rest, but in which there are variations of thermodynamical variables such as temperature and concentrations of various chemical species. What we would like to do is to arrive, in a principled manner, at equations of motion for these fields. In the end, we will arrive at the equations

$$\frac{\partial \rho_i}{\partial t} = -\boldsymbol{\nabla} \cdot \mathbf{J}_i \tag{2.28}$$

$$\mathbf{J}_i = L_{ij} \boldsymbol{\nabla} \mu_j \tag{2.29}$$

$$\mu_j = \left.\frac{\partial s}{\partial \rho_j}\right|_{\boldsymbol{\rho}}. \tag{2.30}$$

where ρ_i are densities of extensive variables, μ_i are the corresponding thermodynamical conjugates, $s = s(\rho_1, \ldots, \rho_m)$ is a strictly concave entropy function, and L_{ij} is a symmetric, positive semidefinite matrix. Together, s and $\mathbf{L}$ parametrize a space of models for the dynamics of the fields ρ_i and μ_i. With these specified, the above equations allow us to determine the evolution of the system from arbitrary initial conditions.

As before, we proceed by a series of steps that invoke the physics of discrete thermodynamical systems as well as several plausible hypotheses. Thus the resulting equations must be considered a starting point for the study of systems described by fields of thermodynamical variables, and we shouldn't be too surprised if they fail in some regimes.

Our first step is to suppose that each small region of the body behaves like an equilibrium thermodynamical system. This supposition is known as the Local Equilibrium Hypothesis (LEH), and takes the form

$$\mu_i(x) = \left.\frac{\partial s}{\partial \rho_i}\right|_{\boldsymbol{\rho}(x)}, \tag{2.31}$$

where $\rho(x) = \{\rho_1(x), \ldots, \rho_m(x)\}$ is the thermodynamical state of the system at spatial point x, expressed in terms of extensive quantities.

We will require that the extensive quantities be conserved, and that the motion of these quantities be local in some way. We implement this by assuming that the density fields ρ_i obey continuity equations

$$\frac{\partial \rho_i}{\partial t} = -\boldsymbol{\nabla} \cdot \mathbf{J}_i, \tag{2.32}$$

where $\mathbf{J}_i$ are a set of fluxes/currents.

We recall from the thermodynamics of two equilibrium bodies in contact that evolution is driven by differences in the thermodynamical conjugate variables, which is to say by differences in the derivative of the entropies of either system with respect to exchanged quantities. Thus it is reasonable to define the thermodynamical forces

$$\mathbf{X}_i = \boldsymbol{\nabla} \mu_i \tag{2.33}$$

where μ_i is the variable conjugate to ρ_i with respect to s:

$$\mu_i(x) = \left.\frac{\partial s}{\partial \rho_i}\right|_{\rho_1(x), \ldots, \rho_m(x)}. \tag{2.34}$$

Note that the chemical potential μ differs from this conjugate variable by a sign and a factor of T.

We now suppose that the fluxes are linearly related to the forces, which should be valid at least for small forces. A first assumption might be that $\mathbf{J}_i$ depends only on $\mathbf{X}_i$. The observation of coupled transport processes indicates that this is overly restrictive. Instead we take

$$\mathbf{J}_i = L_{ij} \mathbf{X}_j, \tag{2.35}$$

where L_{ij} is a set of constants and repetition of indices is to be taken to indicate summation.

At this point, we have parametrized our system in terms of the m^2 coefficients L_{ij} and the strictly convex function $s(\rho_1, \ldots, \rho_m)$. Given a state of the system, which is to say a value of $\rho_i(x)$ for all i and all x, we may compute the conjugate variable fields $\mu_i(x)$. Taking gradients, we find the forces $\mathbf{X}_j$, which may be used to evaluate the fluxes $\mathbf{J}_i$, which then give us the continuity equations. Thus given L_{ij} and s, we have a closed set of differential equations for the state of the system. But we can do better.

We would now like to implement the second law of thermodynamics. We note that the entropy density evolves as follows:

$$\frac{\partial s}{\partial t} = \frac{\partial s}{\partial \rho_i} \frac{\partial \rho_i}{\partial t} = -\mu_i \boldsymbol{\nabla} \cdot \mathbf{J}_i. \tag{2.36}$$

In any region $\mathcal{R}$, then, we may write the rate of total entropy change as

$$\frac{dS}{dt} = \frac{d}{dt}\int_{\mathcal{R}} s\,dx \quad = \int_{\mathcal{R}} \frac{\partial s}{\partial t}\,dx = \int_{\mathcal{R}} -\mu_i \boldsymbol{\nabla}\cdot\mathbf{J}_i\,dx = -\int_{\partial\mathcal{R}} \mu_i \mathbf{J}_i \cdot da + \int_{\mathcal{R}} \boldsymbol{\nabla}\mu_i \cdot \mathbf{J}_i. \tag{2.37}$$

The first term corresponds to entropy that is carried across the boundary of the region $\mathcal{R}$. But the second term seems to correspond to entropy generated in the bulk of the region, and thus we require it to be positive. We define the entropy production rate σ and recognize

$$\sigma := \boldsymbol{\nabla}\mu_i \cdot \mathbf{J}_i = \mathbf{X}_i \cdot \mathbf{J}_i = L_{ij}\mathbf{X}_i \cdot \mathbf{X}_j \tag{2.38}$$

and our second law takes the form

$$L_{ij}\mathbf{X}_i \cdot \mathbf{X}_j \geq 0. \tag{2.39}$$

In particular, this means that $L_{ii} \geq 0$ for all i.

We now examine the relationship between the coefficients L_{ij} and L_{ji}. To begin, consider the decay of a non-uniform distribution of the thermodynamical conserved quantities on a periodic domain:

$$\partial_t \rho_i - L_{ij}\Delta\mu_j \tag{2.40}$$

$$= -L_{ij}\Delta\left(\left.\frac{\partial s}{\partial \rho_j}\right|_{\boldsymbol{\rho}}\right) \tag{2.41}$$

$$= -L_{ij}\Delta\left(\left.\frac{\partial s}{\partial \rho_j}\right|_{\boldsymbol{\rho}^0+\boldsymbol{\delta}}\right) \tag{2.42}$$

$$\approx -L_{ij}\Delta\left(\left.\frac{\partial s}{\partial \rho_j}\right|_{\boldsymbol{\rho}^0} + \left.\frac{\partial^2 s}{\partial \rho_j \partial \rho_k}\right|_{\boldsymbol{\rho}^0}\delta_k\right) \tag{2.43}$$

$$= -L_{ij}H_{jk}\Delta\delta_k, \tag{2.44}$$

where we have defined the Hessian of the entropy

$$H_{jk} = \left.\frac{\partial^2 s}{\partial \rho_j \partial \rho_k}\right|_{\boldsymbol{\rho}^0}. \tag{2.45}$$

Recall that the entropy is strictly concave, so that H_{jk} is a negative definite matrix. Moving to Fourier space, this gives the equation of motion for the Fourier components of the deviation of the density fields from uniformity:

$$\dot{\delta}_i^{(q)} = q^2 L_{ij} H_{jk} \delta_k^{(q)}. \tag{2.46}$$

At this point, we invoke Onsager's regression hypothesis. This is the proposal that fluctuations of a system at thermodynamical equilibrium are governed by the same equations of motion as a system with macroscopic inhomogeneities. Mathematically, we assume that for small t, the fluctuations of a system in the steady state obey

$$\left\langle \delta_i^{(q)}(0)\delta_j^{(q)}(t) \right\rangle \approx \left\langle \delta_i^{(q)}(0)\delta_j^{(q)}(0) \right\rangle + q^2 t L_{jk} H_{kl} \left\langle \delta_i^{(q)}(0)\delta_l^{(q)}(0) \right\rangle \tag{2.47}$$

From the theory of equilibrium fluctuations, we have

$$\left\langle \delta_i^{(q)}(0)\delta_j^{(q)}(0) \right\rangle \propto H_{ij}^{-1}, \tag{2.48}$$

so that

$$\left\langle \delta_i^{(q)}(0)\delta_j^{(q)}(t) \right\rangle \approx \left\langle \delta_i^{(q)}(0)\delta_j^{(q)}(0) \right\rangle + q^2 C t L_{ji} \tag{2.49}$$

for some constant C. Of course, we can also write

$$\left\langle \delta_j^{(q)}(0)\delta_i^{(q)}(t) \right\rangle \approx \left\langle \delta_i^{(q)}(0)\delta_j^{(q)}(0) \right\rangle + q^2 C t L_{ij}. \tag{2.50}$$

We now assume that the fluctuations obey time-reversal symmetry, so that we can subtract these two equations, obtaining $L_{ij} = L_{ji}$. We have now arrived at the model presented at the beginning of the section.

2.3 Viscous entropy production: erroneous application of Onsager symmetry

From equation 2.38, we see that the form of the entropy production is

$$\sigma = \sum_i \mathbf{J}_i \cdot \mathbf{X}_i, \tag{2.51}$$

where $\mathbf{J}_i$ is a thermodynamical flux and $\mathbf{X}_i$ the corresponding thermodynamical force, i.e. the gradient of the corresponding conjugate variable. The entropy production is, in my opinion incorrectly[1], taken as a fundamental object of study in linear irreversible thermodynamics. Part of the reason for this is that it is used as a means of identifying the conjugate pairs of forces and fluxes. This can be a useful aid to arriving at closed equations of motion for the fields that define the state of a system, see for example [35], where force-flux pairs are identified by writing down the entropy production, and then linear constitutive relations are proposed related the fluxes to the forces.

This suggests that the entropy production is a generally useful quantity to compute. Let's examine its form for an incompressible viscous fluid characterized by both a velocity

[1]Entropy is not a directly observable quantity, and therefore should always be subordinated in physical considerations to those quantities that may be measured directly in the lab. A question about entropy may appear along the way to answering a question about physics, but is not itself a question about physics.

field $\mathbf{v}$ and a temperature field T. The velocity field obeys the mass and linear momentum balance equations

$$\boldsymbol{\nabla} \cdot \mathbf{v} = 0 \tag{2.52}$$

$$\rho \frac{D\mathbf{v}}{Dt} = \boldsymbol{\nabla} \cdot \mathbf{T}, \tag{2.53}$$

as shown above. We start by performing the energy balance.

Having included the possibility of temperature variations, it now also makes sense to consider the balance of energy. In addition to a kinetic energy density $\frac{1}{2}\rho\mathbf{v}^2$, the fluid carries an internal energy density u, which depends on the temperature. A region $\mathcal{R}$ of the fluid may gain energy via two mechanisms: first, via the work done on the region by the tractions applied by the surrounding fluid; second, via heat transfer from the surrounding fluid. Thus we have

$$\frac{d}{dt} \int_{\mathcal{R}(t)} \left(\frac{1}{2}\rho\mathbf{v}^2 + \rho u \right) dv = \int_{\partial\mathcal{R}(t)} \left(\mathbf{v} \cdot \mathbf{T} \cdot \mathbf{n} - \mathbf{n} \cdot \mathbf{J}_q \right) da \tag{2.54}$$

where $\mathbf{J}_q$ is a heat flux. Applying the Reynolds transport theorem, the divergence theorem, and the symmetry of the stress, we obtain by localization

$$\frac{D}{Dt} \left(\frac{1}{2}\rho\mathbf{v}^2 + \rho u \right) = \boldsymbol{\nabla} \cdot \left(\mathbf{T} \cdot \mathbf{v} - \mathbf{J}_q \right). \tag{2.55}$$

Using the momentum balance, we find

$$\rho \frac{Du}{Dt} = -\boldsymbol{\nabla} \cdot \mathbf{J}_q + \mathbf{T} : \boldsymbol{\nabla}\mathbf{v}. \tag{2.56}$$

We now take the point of view that entropy is a physical quantity with a specific density. In contrast to the conserved quantities of mass, momentum, angular momentum, and energy, the entropy of a region may be increased, even in the absence of external influence, by both an entropy flux across the boundary and by an entropy production σ:

$$\frac{d}{dt} \int_{\mathcal{R}(t)} \rho s \, dv = \int_{\mathcal{R}(t)} \sigma \, dv - \int_{\partial\mathcal{R}(t)} \mathbf{n} \cdot \mathbf{J}_s \, da. \tag{2.57}$$

As for the prior cases, we may find a local form of this balance:

$$\rho \frac{Ds}{Dt} = \sigma - \boldsymbol{\nabla} \cdot \mathbf{J}_s. \tag{2.58}$$

From equilibrium thermodynamics, we assume that the fundamental thermodynamic relation $dS = dU/T$ holds locally, so that we may also write

$$\rho \frac{Ds}{Dt} = \frac{\rho}{T} \frac{Du}{Dt} = -\frac{1}{T} \boldsymbol{\nabla} \cdot \mathbf{J}_q + \frac{1}{T} \mathbf{T} : \boldsymbol{\nabla}\mathbf{v}, \tag{2.59}$$

obtaining the equation

$$-\frac{1}{T}\boldsymbol{\nabla}\cdot\mathbf{J}_q + \frac{1}{T}\mathbf{T} : \boldsymbol{\nabla}\mathbf{v} = \sigma - \boldsymbol{\nabla}\cdot\mathbf{J}_s. \tag{2.60}$$

We also assume $\mathbf{J}_s = \mathbf{J}_q/T$, so that

$$\sigma = \frac{1}{T}\mathbf{T} : \boldsymbol{\nabla}\mathbf{v} + \mathbf{J}_q\cdot\boldsymbol{\nabla}\frac{1}{T}. \tag{2.61}$$

Compare this form to (2.51). It is now tempting to identify two pairs of thermodynamical force-flux conjugates, and to propose linear relationships between these in the spirit of (2.35). Indeed, in their text on nonequilibrium fluids, Evans and Morriss declare at the end of their Section 2.2

> This canonical form defines what are known as thermodynamic fluxes, J_i, and their conjugate thermodynamic forces, X_i. We can see immediately that our equation takes this canonical form provided we make the identifications that: the thermodynamic fluxes are the various Cartesian elements of the heat-flux vector [...] and the viscous-pressure tensor. The thermodynamic forces conjugate to these fluxes are the *corresponding* Cartesian components of the temperature gradient divided by the square of the absolute temperature [...] and the strain-rate tensor divided by the absolute temperature [...] respectively. [...]
>
> Consistent with our use of the local thermodynamic equilibrium postulate, which is assumed to be valid sufficiently close to equilibrium, a linear relation should hold between the conjugate thermodynamic fluxes and forces. We therefore postulate the existence of a set of linear phenomenological transport coefficients $\{L_{ij}\}$ which relate the set [sic] forces $\{X_j\}$ to the set of fluxes $\{J_i\}$. [34]

Suppose we accept this interpretation of the entropy production. Then the stress should be linearly related to the velocity gradient by a set of coefficients η^{ijkl}: this is of course the viscosity tensor, which we have assumed without any appeal to entropy. But this entropic approach now allows us to say more. If the microscopic equations of motion are time-reversal symmetric, the Onsager symmetry of the coefficients implies $\eta^{ijkl} = \eta^{klij}$. Indeed, this argument has been used in the literature to justify the claim that this symmetry is required in a time-reversal symmetric system.

This interpretation is incorrect! While the term $\mathbf{J}_q\cdot\boldsymbol{\nabla}T^{-1}$ corresponds to a force-flux bilinear, the term $T^{-1}\mathbf{T} : \boldsymbol{\nabla}\mathbf{v}$ does not. There are two reasons for this. First, the force ought to be the gradient of an intensive therodynamical variable, whose conjugate extensive variable is transferred by the flux. Velocity is not a thermodynamical intensive variable, and while the stress is indeed a flux of momentum, momentum is not a thermodynamical variable either. That is, it is not an argument of the entropy function.

Second, the stress term in the entropy production is simply the stress power divided by temperature. The stress power may be seen as a body heating term at the level of fluid parcels treated as equilibrium systems: energy is injected into the thermodynamical systems from an external source, namely, the friction of the fluid against itself. Thus the stress power contribution to the entropy production rate has the same status as would the entropy source term resulting from a body heating rate, which certainly does not represent a force-flux pair.

For these reasons, the argument presented in this section is invalid, and may not be used to connect odd viscosity to time-reversal symmetry breaking. Another argument is required. This is the goal of the next section.

2.4 Simple fluids in two dimensions

Let's begin with the equations in the first section above for treating a simple incompressible fluid:

$$\rho \frac{\partial v_i}{\partial t} = T_{ij,j} \tag{2.62}$$

$$T_{ij} = -p\delta_{ij} + \eta_{ijkl} v_{k,l} \tag{2.63}$$

$$\Delta p = -\rho v_{j,i} v_{i,j} + \eta^{ijkl} v_{k,lji}, \tag{2.64}$$

where η^{ijkl} is a rank four tensor obeying $\eta^{ijkl} = \eta^{jikl} = \eta^{ijlk}$. Specializing to two dimensions and taking into account the vanishing of the trace of the velocity gradient, there are only two linearly independent components of the viscosity tensor that can contribute to the stress. The viscosity tensor may be expressed

$$\eta^{ijkl} = \eta_1 \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) + \eta_2 \left(\epsilon_{ik}\delta_{jl} + \epsilon_{jl}\delta_{ik}\right). \tag{2.65}$$

Note that the second term violates the symmetry $\eta^{ijkl} = \eta^{klij}$ discussed in the previous section. Writing everything in terms of the velocity and pressure fields:

$$\rho \frac{\partial v_i}{\partial t} = -p_{,i} + \eta_1 \Delta v_i + \eta_2 \epsilon_{ik} \Delta v_k \tag{2.66}$$

$$\Delta p = -\rho v_{i,j} v_{j,i} - \eta_2 \Delta \epsilon_{ij} v_{i,j} \tag{2.67}$$

We now consider the decay of small deviations from the $v_i = 0$, $p = \text{const}$ steady state. In this state, we have to lowest order in the fluctuations

$$\rho \frac{\partial v_i}{\partial t} = -p_{,i} + \eta_1 \Delta v_i + \eta_2 \epsilon_{ik} \Delta v_k \tag{2.68}$$

$$\Delta p = -\eta_2 \Delta \epsilon_{ij} v_{i,j} \tag{2.69}$$

Fourier transforming these to obtain

$$\rho \dot{v}_i^{(q)} = -iq^i p^{(q)} - \eta_1 q^2 v_i^{(q)} - \eta_2 \epsilon_{ik} q^2 v_k^{(q)} \tag{2.70}$$

$$-q^2 p^{(q)} = i\eta_2 q^2 \epsilon_{ij} q^j v_i^{(q)}, \tag{2.71}$$

we can eliminate the pressure to find

$$\rho \dot{v}_i^{(q)} = -iq^i \left(-i\eta_2 \epsilon_{ij} q^j v_i^{(q)} \right) - \eta_1 q^2 v_i^{(q)} - \eta_2 \epsilon_{ik} q^2 v_k^{(q)} \tag{2.72}$$

$$= -q^i q^j \eta_2 \epsilon_{ij} v_i^{(q)} - \eta_1 q^2 v_i^{(q)} - \eta_2 \epsilon_{ik} q^2 v_k^{(q)} \tag{2.73}$$

$$= -q^r q^l \delta_{rk} \delta_{jl} \eta_2 \epsilon_{ij} v_k^{(q)} - \eta_1 q^r q^l \delta_{rl} \delta_{ik} v_k^{(q)} - \eta_2 \epsilon_{ik} q^r q^l \delta_{rl} v_k^{(q)} \tag{2.74}$$

$$= - \left[\delta_{rk} \delta_{jl} \eta_2 \epsilon_{ij} + \eta_1 \delta_{rl} \delta_{ik} + \eta_2 \epsilon_{ik} \delta_{rl} \right] q^r q^l v_k^{(q)} \tag{2.75}$$

$$= - \left[\eta_1 \delta_{rl} \delta_{ik} + \eta_2 \left(\epsilon_{ik} \delta_{rl} + \epsilon_{il} \delta_{rk} \right) \right] q^r q^l v_k^{(q)}. \tag{2.76}$$

We now make the Onsager regression hypothesis, supposing that these equations hold inside of expectations, so that we may write for the fluctuating system

$$\rho \left\langle \dot{v}_i^{(q)} v_s^{(-q)} \right\rangle = - \left[\eta_1 \delta_{rl} \delta_{ik} + \eta_2 \left(\epsilon_{ik} \delta_{rl} + \epsilon_{il} \delta_{rk} \right) \right] q^r q^l \left\langle v_k^{(q)} v_s^{(-q)} \right\rangle \tag{2.77}$$

$$= - \left[\eta_1 \delta_{rl} \delta_{ik} + \eta_2 \left(\epsilon_{ik} \delta_{rl} + \epsilon_{il} \delta_{rk} \right) \right] q^r q^l \frac{\mu}{L^2} \delta_{ks} \tag{2.78}$$

$$= - \left[\eta_1 \delta_{rl} \delta_{is} + \eta_2 \left(\epsilon_{is} \delta_{rl} + \epsilon_{il} \delta_{rs} \right) \right] q^r q^l \frac{\mu}{L^2}, \tag{2.79}$$

where we have used results on the form of the correlators from Appendix C. Contracting with δ_{is}, we find

$$\eta_1 = -\frac{\rho L^2}{2\mu q^2} \delta_{is} \left\langle \dot{v}_i^{(q)} v_s^{(-q)} \right\rangle \tag{2.80}$$

Contracting with ϵ_{is} we find

$$\eta_2 = -\frac{\rho L^2}{3\mu q^2} \epsilon_{is} \left\langle \dot{v}_i^{(q)} v_s^{(-q)} \right\rangle \tag{2.81}$$

Assuming that the velocity autocorrelations vanish at large times, we may rewrite these as

$$\eta_1 = -\frac{\rho L^2}{2\mu q^2} \delta_{is} \int_{-\infty}^{0} \left\langle \dot{v}_i^{(q)}(0) \dot{v}_s^{(-q)}(t) \right\rangle dt \tag{2.82}$$

$$\eta_2 = -\frac{\rho L^2}{3\mu q^2} \epsilon_{is} \int_{-\infty}^{0} \left\langle \dot{v}_i^{(q)}(0) \dot{v}_s^{(-q)}(t) \right\rangle dt \tag{2.83}$$

We can now use the Fourier space form of the mass balance equation expressed in terms of the stress

$$\rho \dot{v}_i^{(q)} = iq^j T_{ij}^{(q)} \tag{2.84}$$

to express the viscosities in terms of stress autocorrelators:

$$\eta_1 = \frac{L^2}{2\mu\rho q^2} \delta_{ik} q^j q^l \int_{-\infty}^{0} \left\langle T_{ij}^{(q)}(0) T_{kl}^{(-q)}(t) \right\rangle dt \tag{2.85}$$

$$\eta_2 = \frac{L^2}{3\mu\rho q^2} \epsilon_{ik} q^j q^l \int_{-\infty}^{0} \left\langle T_{ij}^{(q)}(0) T_{kl}^{(-q)}(t) \right\rangle dt. \tag{2.86}$$

We can convert back to real space by using

$$\left\langle T_{ij}^{(\mathbf{q})}(0)T_{kl}^{(-\mathbf{q})}(t)\right\rangle = \frac{1}{L^4}\int d^2\mathbf{x}_1\, d^2\mathbf{x}_2 e^{-i\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{y}_1)}\left\langle T_{ij}(0,\mathbf{x}_1)T_{kl}(t,\mathbf{x}_2)\right\rangle \tag{2.87}$$

$$\approx \frac{1}{L^4}\int d^2\mathbf{x}_1\, d^2\mathbf{x}_2 \left\langle T_{ij}(0,\mathbf{x}_1)T_{kl}(t,\mathbf{x}_2)\right\rangle \tag{2.88}$$

where we've used the assumption that the stress correlations are short-range to justify keeping only the lowest order term in $\mathbf{q}$. Then we have

$$\eta_1 = \frac{1}{2\mu\rho L^2 q^2}\delta_{ik}q^j q^l \int_{-\infty}^{0} dt \int d^2\mathbf{x}_1\, d^2\mathbf{x}_2 \left\langle T_{ij}(0,\mathbf{x}_1)T_{kl}(t,\mathbf{x}_2)\right\rangle \tag{2.89}$$

$$\eta_2 = \frac{1}{3\mu\rho L^2 q^2}\epsilon_{ik}q^j q^l \int_{-\infty}^{0} dt \int d^2\mathbf{x}_1\, d^2\mathbf{x}_2 \left\langle T_{ij}(0,\mathbf{x}_1)T_{kl}(t,\mathbf{x}_2)\right\rangle . \tag{2.90}$$

Summing these equations for two orthogonal choices of $\mathbf{q}$, we find

$$\eta_1 = \frac{1}{4\mu\rho L^2}\delta_{ik}\delta_{jl} \int_{-\infty}^{0} dt \int d^2\mathbf{x}_1\, d^2\mathbf{x}_2 \left\langle T_{ij}(0,\mathbf{x}_1)T_{kl}(t,\mathbf{x}_2)\right\rangle \tag{2.91}$$

$$\eta_2 = \frac{1}{6\mu\rho L^2}\epsilon_{ik}\delta_{jl} \int_{-\infty}^{0} dt \int d^2\mathbf{x}_1\, d^2\mathbf{x}_2 \left\langle T_{ij}(0,\mathbf{x}_1)T_{kl}(t,\mathbf{x}_2)\right\rangle \tag{2.92}$$

Using translational invariance:

$$\eta_1 = \frac{1}{4\mu\rho}\delta_{ik}\delta_{jl} \int_{-\infty}^{0} dt \int d^2\mathbf{x} \left\langle T_{ij}(0,\mathbf{0})T_{kl}(t,\mathbf{x})\right\rangle \tag{2.93}$$

$$\eta_2 = \frac{1}{6\mu\rho}\epsilon_{ik}\delta_{jl} \int_{-\infty}^{0} dt \int d^2\mathbf{x} \left\langle T_{ij}(0,\mathbf{0})T_{kl}(t,\mathbf{x})\right\rangle \tag{2.94}$$

And we recall that

$$\mu = \frac{1}{2}\int d^2\mathbf{x} \left\langle \mathbf{v}(\mathbf{0})\cdot\mathbf{v}(\mathbf{x})\right\rangle \tag{2.95}$$

Now suppose that we have the time-reversal symmetry condition

$$\left\langle T_{ij}(\mathbf{x},0)T_{kl}(\mathbf{y},t)\right\rangle = \left\langle T_{ij}(\mathbf{x},t)T_{kl}(\mathbf{y},0)\right\rangle . \tag{2.96}$$

Then we have

$$\eta_2 = \frac{1}{6\mu\rho}\epsilon_{ik}\delta_{jl}\int_{-\infty}^{0} dt \int d^2\mathbf{x} \langle T_{ij}(0,\mathbf{0})T_{kl}(t,\mathbf{x})\rangle \tag{2.97}$$

$$= -\frac{1}{6\mu\rho}\epsilon_{ik}\delta_{jl}\int_{-\infty}^{0} dt \int d^2\mathbf{x} \langle T_{kl}(0,\mathbf{0})T_{ij}(t,\mathbf{x})\rangle \tag{2.98}$$

$$= -\frac{1}{6\mu\rho}\epsilon_{ik}\delta_{jl}\int_{-\infty}^{0} dt \int d^2\mathbf{x} \langle T_{ij}(t,\mathbf{x})T_{kl}(0,\mathbf{0})\rangle \tag{2.99}$$

$$= -\frac{1}{6\mu\rho}\epsilon_{ik}\delta_{jl}\int_{-\infty}^{0} dt \int d^2\mathbf{x} \langle T_{ij}(0,\mathbf{x})T_{kl}(t,\mathbf{0})\rangle \tag{2.100}$$

$$= -\frac{1}{6\mu\rho}\epsilon_{ik}\delta_{jl}\int_{-\infty}^{0} dt \int d^2\mathbf{x} \langle T_{ij}(0,\mathbf{0})T_{kl}(t,\mathbf{x})\rangle \tag{2.101}$$

$$= -\eta_2, \tag{2.102}$$

where we have also used the translational and rotational symmetries of the correlator. Thus if the stress correlator is time-reversal symmetric and Onsager's regression hypothesis holds, the odd viscosity should vanish.

2.5 Compressible Fluid in Two Dimensions

We begin with the deterministic equations

$$\frac{D\rho}{Dt} = -\rho v_{i,i} \tag{2.103}$$

$$\rho\frac{Dv_i}{Dt} = T_{ij,j} \tag{2.104}$$

$$T_{ij} = \eta_{ijkl}v_{k,l} - p\delta_{ij} \tag{2.105}$$

$$\eta_{ijkl} = \eta_1\delta_{ij}\delta_{kl} + \eta_2\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl}\right) + \eta_3\left(\epsilon_{ik}\delta_{jl} + \epsilon_{jl}\delta_{ik}\right). \tag{2.106}$$

In Fourier space and to lowest order in a perturbation about a constant-density $\rho = \rho_0$, $v_i = 0$ steady state, we have

$$\rho_0\dot{v}_i^{(q)} = -\eta^{ijkl}q^l q^j v_k^{(q)} - iq^i p^{(q)}. \tag{2.107}$$

As before, we use the regression hypothesis to write for fluctuations about the steady state

$$\rho_0\left\langle \dot{v}_i^{(q)}v_s^{(-q)}\right\rangle = -\eta^{ijkl}q^l q^j\left\langle v_k^{(q)}v_s^{(-q)}\right\rangle = -\eta^{ijkl}q^l q^j\frac{\mu}{L^2}\delta_{ks} = -\eta^{ijsl}q^l q^j\frac{\mu}{L^2} \tag{2.108}$$

$$= -\left[\eta_1\delta_{ij}\delta_{kl} + \eta_2\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl}\right) + \eta_3\left(\epsilon_{ik}\delta_{jl} + \epsilon_{jl}\delta_{ik}\right)\right]q^l q^j\frac{\mu}{L^2} \tag{2.109}$$

$$= -\left[\eta_1 q^i q^k + \eta_2\delta_{ik}q^2 + \eta_3\epsilon_{ik}q^2\right]\frac{\mu}{L^2}. \tag{2.110}$$

We have also used the fact that, to lowest order in q, the scalar pressure and the vector velocity must be uncorrelated. Contracting with δ_{ik}, we find

$$\eta_1 + 2\eta_2 = -\frac{\rho_0 L^2}{\mu q^2}\delta_{ik}\left\langle \dot{v}_i^{(q)} v_s^{(-q)} \right\rangle . \tag{2.111}$$

Contracting with ϵ_{ik}, we find

$$\eta_3 = -\frac{\rho_0 L^2}{2\mu q^2}\epsilon_{ik}\left\langle \dot{v}_i^{(q)} v_s^{(-q)} \right\rangle \tag{2.112}$$

As before, this may be rewritten in terms of the stress autocorrelation function:

$$\eta_3 = \frac{1}{4\mu\rho_0}\epsilon_{ik}\delta_{jl}\int_{-\infty}^{0} dt \int d^2\mathbf{x}\left\langle T_{ij}(0,\mathbf{0})T_{kl}(t,\mathbf{x})\right\rangle . \tag{2.113}$$

Note the difference in the numerical prefactor compared with the incompressible case.

2.6 Numerical Verification

In [36], the Green-Kubo equation (2.113) was tested against non-equilibrium molecular dynamics (NEMD) simulations for a system of actively torqued dumbbells. Over a large range of densities and activities, it gave accurate numerical values for the odd viscosity, see Fig. 2.4. In this section, I will briefly describe this result.

The microscopic model, introduced in [37], consists of dumbbells, i.e. pairs of particles interacting via harmonic potentials. Members of different dumbbells interact via a WCA potential, see Fig, 2.3. Equilibrium is broken by the application of constant equal and opposite forces f to the two particles in each dumbbell, applied perpendicular to the bond vector between them. This creates an effective "active torque" on each dumbbell. The level of activity is measured by the Péclet number $\mathrm{Pe} = 2fd/\rho_0\mu$, where d is the equilibrium bond length of the dumbbells, ρ_0 is the average density of the dumbbells, and μ is the temperature as measured by velocity fluctuations. Heuristically, Pe measures the relative importance of the active torques to the thermal fluctuations of the particles.

In order to compute the odd viscosity via the Green-Kubo equation (2.113), we require expressions for the stress tensor in terms of microscopic variables, i.e. positions and velocities of the individual particles. These are obtained in [37] via an Iriving-Kirkwood style coarse-graining analysis. A similar analysis is performed for a different model in Chapter 4.

Finally, in order to validate the Green-Kubo equation, the odd viscosity must also be computed via an independent method. In [36], the periodic Poiseuille method was used. In this approach, planar periodic Poiseuille flow is generated by the application of body forces to the fluid of dumbbells. The odd viscosity may then be extracted from the gradients of components of the stress tensor, again computed via the Irving-Kirkwood expressions of [37]. The comparison between these two methods is presented in Fig. 2.4. This may be taken as

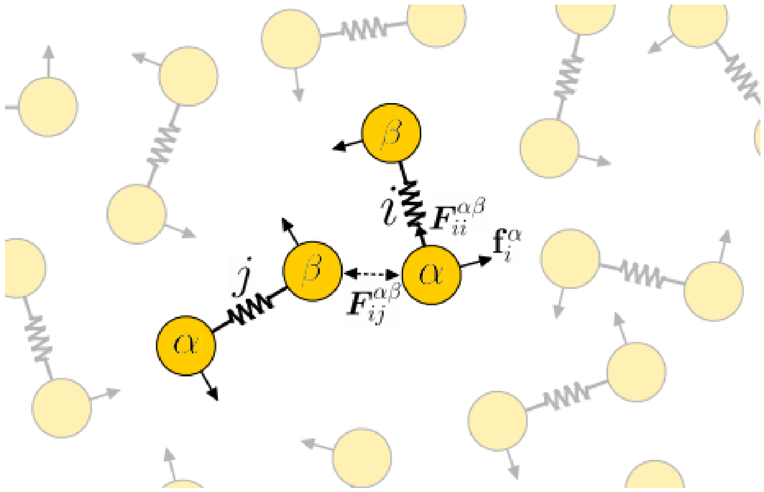

Figure 2.3: The dumbbell model studied in [36].

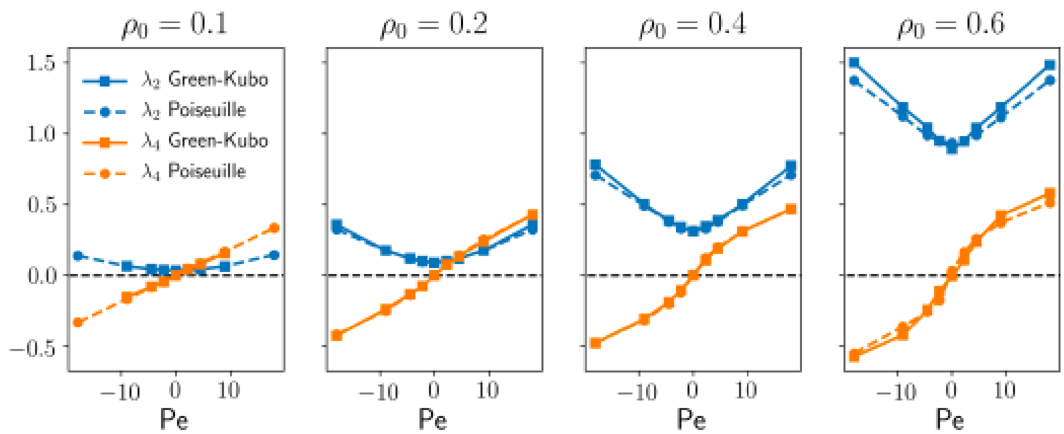

Figure 2.4: Numerical verification of the Green-Kubo equation.

a validation of the Green-Kubo equation and, on a more fundamental level, as support for the application of Onsager's regression hypothesis to fluctuations about a *non-equilibrium* steady state.

Chapter 3

Green-Kubo analysis of two dimensional active fluids with internal spin

In this chapter, we develop the continuum theory of two-dimensional fluids that carry internal angular momentum. In particular, we derive Green-Kubo relations for the components of the viscosity. As in the previous chapter, this establishes the connection between odd viscosity and time-reversal symmetry breaking. We also find a novel rotational viscosity that has not been previously included in models of fluids with spin.

3.1 Two-Dimensional Fluids with Internal Spin

To study two-dimensional fluids with internal structure, we take as fundamental dynamical fields the velocity vector v_i and a scalar internal spin m. Conservation of linear and angular momentum are guaranteed by the balance equations

$$\rho \dot{v}_i = T_{ij,j}, \tag{3.1}$$

$$\rho \dot{m} = C_{i,i} - \epsilon_{ij} T_{ij}, \tag{3.2}$$

with T_{ij} the stress tensor and C_i the couple stress or spin flux. The dot indicates the convective or material derivative $\partial_t + v_i \partial_i$, and ϵ_{ij} is the two-dimensional Levi-Civita tensor. Such a microstructural continuum theory was proposed by Dahler and Scriven [31, 38] and has been used in many contexts [39, 40, 41, 42].

The coupling term $-\epsilon_{ij} T_{ij}$ between the linear and internal angular momentum balance equations preserves conservation of total angular momentum, with density $\mathcal{J} = \rho \mathbf{x} \times \mathbf{v} + \rho m$, while permitting the existence of a nonvanishing antisymmetric component of the stress. This is forbidden by conservation of angular momentum in fluids without a microstructural field capable of absorbing angular momentum from the velocity field.

To close the equations (3.1) and (3.2) for v_i and m, we require constitutive equations relating the stress T_{ij} and couple stress C_i to the fields v_i and m. We assume these relations are linear, Galilean invariant, and contain derivatives of the fields only up to first order. The most general linear constitutive relations are then given by

$$T_{ij} = \eta_{ijkl} v_{k,l} + \gamma_{ij} m + \xi_{ijk} m_{,k}, \tag{3.3}$$
$$C_i = \beta_{ijk} v_{j,k} + \kappa_i m + \alpha_{ij} m_{,j}, \tag{3.4}$$

where repeated indices are summed, and $\boldsymbol{\eta}$, $\boldsymbol{\gamma}$, $\boldsymbol{\xi}$, $\boldsymbol{\beta}$, $\boldsymbol{\kappa}$, and $\boldsymbol{\alpha}$ are linear maps.

Imposing isotropy further restricts the couplings in (3.3) and (3.4). Isotropic tensors of any rank in dimension n may be expressed as linear combinations of terms consisting only of the rank two Kronecker tensor δ_{ij} and the rank n Levi-Civita tensor $\epsilon_{i_1 \ldots i_n}$ (see Appendix B). In two dimensions, both of these are rank two, so there are no nonzero isotropic tensors of odd rank. This forbids the existence of nontrivial isotropic linear maps between tensors with ranks differing by an odd number. For instance, the couple stress C_i, a vector, cannot depend on the spin density m, a scalar, or the velocity gradient $v_{i,j}$, a rank two tensor. Similarly, the stress tensor T_{ij}, a rank two tensor, cannot depend on the spin gradient $m_{,i}$, a vector. Therefore, the most general isotropic constitutive equations have the form

$$T_{ij} = \eta_{ijkl} v_{k,l} + \gamma_{ij} m, \tag{3.5}$$
$$C_i = \alpha_{ij} m_{,j}. \tag{3.6}$$

The maps γ_{ij} and α_{ij} may be expressed as

$$\gamma_{ij} = \gamma_1 \delta_{ij} + \gamma_2 \epsilon_{ij}, \tag{3.7}$$
$$\alpha_{ij} = \alpha_1 \delta_{ij} + \alpha_2 \epsilon_{ij}. \tag{3.8}$$

The viscosity tensor η_{ijkl} is an element of the six-dimensional space of isotropic rank four tensors in two dimensions (see Appendix I). An orthogonal basis $\mathbf{s}^{(\alpha)}$ for this space is provided in Table 3.1, along with the symmetry properties of the basis elements under various index permutations of physical significance. We can express the viscosity tensor as a linear combination of these basis elements:

$$\eta_{ijkl} = \sum_{\alpha=1}^{6} \lambda_\alpha s^{(\alpha)}_{ijkl}. \tag{3.9}$$

In Table 3.1, we also provide the components $s^{(\alpha)}_{ijkl} v_{k,l}$ of the stress tensor due to each of the basis tensors, elucidating the physical meaning of each coefficient. The bulk viscosity λ_1 and shear viscosity λ_2 resist compression and shearing as in a typical Newtonian fluid. The rotational viscosity λ_3 resists rotation, corresponding to the appearance of a torque in response to non-vanishing vorticity, breaking both symmetry and objectivity of the stress tensor. All three of these components of the viscosity are even under mirror symmetry, implying that they may arise in non-chiral systems.

Basis Tensor	Components	$i \leftrightarrow j$	$k \leftrightarrow l$	$ij \leftrightarrow kl$	P	$s^{(\alpha)}_{ijkl} v_{k,l}$
$s^{(1)}_{ijkl}$	$\delta_{ij}\delta_{kl}$	+	+	+	+	$(\boldsymbol{\nabla} \cdot \mathbf{v})\delta_{ij}$
$s^{(2)}_{ijkl}$	$\delta_{ik}\delta_{j\ell} + \delta_{i\ell}\delta_{jk} - \delta_{ij}\delta_{kl}$	+	+	+	+	$2\mathring{\mathbf{u}}$
$s^{(3)}_{ijkl}$	$\epsilon_{ij}\epsilon_{kl}$	-	-	+	+	$-2\omega\epsilon_{ij}$
$s^{(4)}_{ijkl}$	$\epsilon_{ik}\delta_{j\ell} + \epsilon_{j\ell}\delta_{ik}$	+	+	-	-	$(\boldsymbol{\sigma}_z \otimes \boldsymbol{\sigma}_x - \boldsymbol{\sigma}_x \otimes \boldsymbol{\sigma}_z) : \mathring{\mathbf{u}}$
$s^{(5)}_{ijkl}$	$\epsilon_{ik}\delta_{j\ell} - \epsilon_{j\ell}\delta_{ik} + \epsilon_{ij}\delta_{k\ell} + \epsilon_{k\ell}\delta_{ij}$	-	+	N/A	-	$(\boldsymbol{\nabla} \cdot \mathbf{v})\epsilon_{ij}$
$s^{(6)}_{ijkl}$	$\epsilon_{ik}\delta_{j\ell} - \epsilon_{j\ell}\delta_{ik} - \epsilon_{ij}\delta_{k\ell} - \epsilon_{k\ell}\delta_{ij}$	+	-	N/A	-	$4\omega\delta_{ij}$

Table 3.1: The tensors $s^{(\alpha)}_{ijkl}$ form a basis for the isotropic rank four tensors in two dimensions, and are orthogonal with respect to the inner product $A_{ijkl}B_{ijkl}$. This basis has been chosen to be an eigenbasis for the index permutations $i \leftrightarrow j$ and $k \leftrightarrow l$, corresponding to the symmetry and objectivity of the stress tensor, respectively. It is also an eigenbasis for the mirror transformation $x_1 \mapsto -x_1$, $x_2 \mapsto x_2$, also known as the parity transformation (P). Four of these basis tensors are also eigenvectors of the index permutation $i \leftrightarrow k$ and $j \leftrightarrow l$, and we also indicate the parity of the basis tensors under this transformation. In the last column, we provide the component of the stress $T_{ij} = \eta_{ijkl} v_{k,l}$ due to each basis element of the viscosity. The symmetric traceless velocity gradient is defined as $\mathring{u}_{ij} = \frac{1}{2}(v_{i,j} + v_{j,i} - v_{k,k}\delta_{ij})$, and the vorticity as $\omega = -\frac{1}{2}\epsilon_{ij}v_{i,j}$. We also use the matrices $\boldsymbol{\sigma}_z = [1,0;0,-1]$ and $\boldsymbol{\sigma}_x = [0,1;1,0]$, which are basis elements of the pure shear modes of the velocity gradient that transform into each other under rotation. The tensor $\boldsymbol{\sigma}_z \otimes \boldsymbol{\sigma}_x$ maps a pure shear mode of the velocity gradient to a rotated pure shear mode of the stress. A complete eigenbasis $\boldsymbol{e}^{(\beta)}$ for the permutation $ij \leftrightarrow kl$ is presented in Appendix B

The other three components of the viscosity are odd under mirror symmetry, and thus should be expected to vanish in non-chiral systems. The odd viscosity λ_4, corresponding to a term that violates the permutation symmetry $\eta_{ijkl} = \eta_{klij}$, responds to pure shear along one axis with pure shear stress along an axis rotated by $\pi/4$. Equivalently, it responds to simple shear along one axis with pressure or tension along the orthogonal axis, depending on the sign of the shear. An interesting feature of this component of the viscosity is that it is non-dissipative in the sense that it does not contribute to the stress power $T_{ij}v_{i,j}$. This term satisfies both objectivity and symmetry of the stress tensor, so that it is compatible with conservation of angular momentum even in the absence of internal spin.

Finally, the component λ_5 responds to compression with torque, breaking symmetry of the stress, while the component λ_6 responds to vorticity with isotropic pressure, breaking objectivity. The corresponding basis tensors $\mathbf{s}^{(5)}$ and $\mathbf{s}^{(6)}$ both violate the symmetry $\eta_{ijkl} = \eta_{klij}$. They span a two-dimensional subspace with one even and one odd direction under this index permutation, so that there are in fact two independent odd components of the viscosity.

3.2 Generalized Green-Kubo Relations

In what follows we derive Green-Kubo formulae relating the viscous coefficients introduced above to the stress-stress time correlation function in a fluctuating steady-state, starting from an assumption on the fluctuations in the spirit of Onsager's regression hypothesis. The philosophy adopted here is to suppose that the fields v_i, m, T_{ij}, and C_i are fluctuating or stochastic rather than deterministic, but that small fluctuations about a steady state behave, in expectation, in the same manner as the deterministic transport equations would predict.

The physics of matter at large scales is typically captured by theories with deterministic evolution equations. On the other hand, measurements made at small scales with high precision reveal stochastic behavior. As a consequence, a single physical system may be best described in different regimes by two different theories, one deterministic and one stochastic. Clearly, there must be some relation between these. The regression hypothesis proposed by Onsager and used in his derivation of the reciprocal relations of transport coefficients is one possible such relation [43, 44]. Informally, the content of the regression hypothesis is that the dynamical and constitutive equations that yield the transport equations obeyed by the variables in a deterministic theory are also satisfied in expectation by the stochastic theory describing fluctuations of the same system about a steady state, when conditioned on initial conditions.

We can provide a more formal account of the regression hypothesis by considering a system described by some generalized configuration variables A_i whose evolution we are interested in modeling. In a fluid, for example, these may be Fourier modes $\mathbf{v_k}$ of the velocity field. We suppose that these evolve according to some conservation laws associated with generalized flux variables B_j, obeying a relationship

$$\frac{dA_i}{dt} = M_{ij}B_j, \tag{3.10}$$

where the repeated index summation convention is used. In a fluid, the variables B_j will be Fourier modes $T^{ij}_{\mathbf{k}}$ of the stress field. We now assume that the generalized fluxes themselves depend on the configuration variables A_i via the constitutive relations

$$B_j = S_{ji}A_i, \tag{3.11}$$

where S_{ji} are transport coefficients. Together, (3.10) and (3.11) define a deterministic theory and lead to the macroscopic transport equations

$$\frac{dA_i}{dt} = M_{ij}S_{jk}A_k. \tag{3.12}$$

Let $A_i = B_j = 0$ be a fixed point for the transport equation (3.12) corresponding to some stable steady state, possibly non-equilibrium. Suppose that we are interested in spontaneous fluctuations arising in the steady state. Let $A_i(t)$ be stochastic fluctuations about the steady state $\langle A_i\rangle = \langle B_j\rangle = 0$. Any fluctuations in A_i should decay back to zero. Let $A_i(t) = a_i$ at an initial time t. There exist many trajectories of the system that are commensurate with such a choice. Let $\langle A_i(t+\Delta t)\rangle_{t,\mathbf{a}}$ be an average of the observable A_i at time $t+\Delta t$, where the subscript indicates an average of the ensemble compatible with the choice $A_i(t) = a_i$. In this case, assuming that the fluctuations are sufficiently small, one may postulate that the decay of the fluctuations towards the steady state satisfies the Onsager's regression hypothesis [43, 44, 45], i.e., the decay of the fluctuations follows the same transport equations (3.12) in a finite difference manner given by

$$\frac{\langle A_i(t+\Delta t)\rangle_{t,\mathbf{a}} - a_i}{\Delta t} = M_{ij}S_{jk}a_k. \tag{3.13}$$

Equation (3.13) is the form of the regression hypothesis implemented by Kubo-Yokota-Nakajima in their derivation of the Green-Kubo relations for responses of thermal origin [45]. Note that the conservation laws/dynamical equations (3.10) are valid for every trajectory, and it is the linear constitutive relations that are satisfied only in expectation in (3.13). In the Irving-Kirkwood framework [32, 46], for instance, the spatially coarse-grained stress field is *defined* by taking the derivative of the coarse-grained velocity field, so that the momentum balance equation is exactly satisfied for every trajectory in the ensemble. It is the constitutive relation that introduces uncertainty, as the coarse-grained velocity and density fields do not completely specify the configuration of the individual particles, which would be required for precise knowledge of the coarse-grained stress field.

We now turn to examining a consequence of the regression hypothesis, namely the general Green-Kubo relations for the transport coefficients S_{jk}, by following the procedure adopted in the original derivation of Green-Kubo relations by Kubo-Yokota-Nakajima [45]. To this end, we multiply (3.13) by a_r^* to find

$$\frac{1}{\Delta t}\Big(\langle A_i(t+\Delta t)\rangle_{t,\mathbf{a}}\, a_r^* - a_i a_r^* \Big) = M_{ij} S_{jk} a_k a_r^*. \tag{3.14}$$

where $(\cdot)^*$ indicates a complex conjugate. Taking an average over the entire ensemble on both sides of (3.14) corresponding to all possible values of a_k yields

$$\frac{1}{\Delta t}\Big[\langle A_i(t+\Delta t) A_r^*(t)\rangle - \langle A_i(t) A_r^*(t)\rangle \Big] = M_{ij} S_{jk} \left\langle A_k(t) A_r^*(t)\right\rangle,. \tag{3.15}$$

Assuming time-translation invariance, this reduces to

$$\frac{1}{\Delta t}\Big[\langle A_i(\Delta t) A_r^*(0)\rangle - \langle A_i(0) A_r^*(0)\rangle \Big] = M_{ij} S_{jk} \left\langle A_k(0) A_r^*(0)\right\rangle. \tag{3.16}$$

Consider the left hand side of (3.16):

$$\frac{1}{\Delta t}\Big[\langle A_i(\Delta t) A_r^*(0)\rangle - \langle A_i(0) A_r^*(0)\rangle \Big] = \frac{1}{\Delta t}\left[\left\langle \Big(A_i(0) + \int_0^{\Delta t} \dot{A}_i(t')dt' \Big) A_r^*(0) \right\rangle - \langle A_i(0) A_r^*(0)\rangle \right] \tag{3.17}$$

$$= \frac{1}{\Delta t}\left[\int_0^{\Delta t} dt' \left\langle \dot{A}_i(t') A_r^*(0) \right\rangle \right], \tag{3.18}$$

which reduces (3.16) to

$$\frac{1}{\Delta t}\left[\int_0^{\Delta t} dt' \left\langle \dot{A}_i(t') A_r^*(0) \right\rangle \right] = M_{ij} S_{jk} \left\langle A_k(0) A_r^*(0)\right\rangle. \tag{3.19}$$

Consider the following time derivative of the correlation function:

$$\frac{d}{d\tau}\left\langle \dot{A}_i(\tau) A_r^*(0) \right\rangle = \frac{d}{d\tau}\left\langle \dot{A}_i(0) A_r^*(-\tau) \right\rangle, \tag{3.20}$$

$$= -\left\langle \dot{A}_i(0) \dot{A}_r^*(-\tau) \right\rangle, \tag{3.21}$$

$$= -\left\langle \dot{A}_i(\tau) \dot{A}_r^*(0) \right\rangle, \tag{3.22}$$

which yields

$$\left\langle \dot{A}_i(\tau) A_r^*(0) \right\rangle = -\int_0^{\tau} dt'' \left\langle \dot{A}_i(t'') \dot{A}_r^*(0) \right\rangle + \left\langle \dot{A}_i(0) A_r^*(0) \right\rangle. \tag{3.23}$$

At this stage, we assume that the steady-state time correlation of observables $A_i(t)$ and $A_r(0)$ reaches an extremum at $t = 0$, so that

$$\left\langle \dot{A}_i(0) A_r^*(0) \right\rangle = 0. \tag{3.24}$$

This is true for equilibrium systems as it is a product of a function even in time and another function odd in time. However, we assume this to be true even for non-equilibrium steady states, and leave the general case for future work. In such a case, (3.23) reduces to

$$\left\langle \dot{A}_i(\tau) A_r^*(0) \right\rangle = -\int_0^{\tau} dt'' \left\langle \dot{A}_i(t'') \dot{A}_r^*(0) \right\rangle . \tag{3.25}$$

Using (3.25), (3.19) can be rewritten as

$$M_{ij} S_{jk} \left\langle A_k(0) A_r^*(0) \right\rangle = -\frac{1}{\Delta t} \left[\int_0^{\Delta t} dt' \int_0^{t'} d\tau \left\langle \dot{A}_i(\tau) \dot{A}_r^*(0) \right\rangle \right] \tag{3.26}$$

$$= -\int_0^{\Delta t} d\tau \Big(1 - \frac{\tau}{\Delta t}\Big) \left\langle \dot{A}_i(\tau) \dot{A}_r^*(0) \right\rangle , \tag{3.27}$$

where the second equality is obtained by exchanging the order of integration. If the time decay τ_{corr} of the auto-correlation function of $\dot{A}_i$ and $\dot{A}_r$ is small compared to the time scale Δt, then the integral in (3.27) can be rewritten to yield

$$M_{ij} S_{jk} \left\langle A_k(0) A_r^*(0) \right\rangle = -\int_0^{\infty} dt \left\langle \dot{A}_i(t) \dot{A}_r^*(0) \right\rangle , \tag{3.28}$$

which are the Green-Kubo relations relating the transport coefficients S_{jk} with the time integrals of the correlation functions of rates of the observables A_i. Since the dynamical equation or conservation law (3.10) is valid for every member of the ensemble, the Green-Kubo relations (3.28) can be rewritten in terms of the time correlation functions of the flux variables B_j as

$$M_{ij} S_{jk} \left\langle A_k(0) A_r^*(0) \right\rangle = -M_{ij} M_{rk}^* \int_0^{\infty} \left\langle B_j(t) B_k^*(0) \right\rangle dt. \tag{3.29}$$

It is this equation that will allow us to derive the Green-Kubo relations for the viscosity coefficients from the regression hypothesis on the decay of fluctuations about the steady state of the fluid described in the next section. An important component in being able to derive the Green-Kubo relations (3.28) and (3.29) is the requirement on the separation of time scales: the time scale required to observe the decay of the fluctuations about the steady state Δt is larger than the correlation time τ_{corr} measuring the molecular relaxation processes in terms of the correlation functions of flux variables, and small compared to the decay time of the external perturbation τ_{r}, i.e.,

$$\tau_{\text{corr}} \ll \Delta t \ll \tau_{\text{r}}. \tag{3.30}$$

3.3 Application to Viscous Fluid

For our fluid system, the role of the variables A_i and B_j will be played by the large wavelength components of the fluctuations of the fields v_i, m, T_{ij}, and C_i about the steady state with

$v_i = 0$ and $m = \textit{constant}$. The evolution of these components is governed by the linearized Fourier forms of the linear and angular momentum balance equations. From above, these are

$$\rho \dot{v}_i = T_{ij,j}, \tag{3.31}$$
$$\rho \dot{m} = -\epsilon_{ij} T_{ij} + C_{i,i}. \tag{3.32}$$

Let v_0^i, m_0, and so on denote the spatially-uniform values of the fields in a stable steady state. We may express the balance equations in terms of small deviations δv^i, δm, and so on from the steady state:

$$\rho \partial_t \delta v_i + \rho (v_0^j + \delta v^j) \delta v_{i,j} = \delta T_{ij,j}, \tag{3.33}$$
$$\rho \partial_t \delta m + \rho (v_0^j + \delta v^j) \delta m_{,j} = -\epsilon_{ij} (T_0^{ij} + \delta T_{ij}) + \delta C_{i,i}. \tag{3.34}$$

Now requiring $v_0 = 0$, to linear order in the deviations from the steady state, these become

$$\rho \partial_t \delta v_i = \delta T_{ij,j}, \tag{3.35}$$
$$\rho \partial_t \delta m = -\epsilon_{ij} \delta T_{ij} + \delta C_{i,i}, \tag{3.36}$$

where we have used the fact that $\epsilon_{ij} T_{ij}$ must vanish in a steady state.

Taking the fields to be defined on a square region of side length L with periodic boundary conditions, we may decompose them into Fourier components, so that

$$\delta v^i(\mathbf{x}, t) = \sum_{\mathbf{k}} v_{\mathbf{k}}^i(t) e^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}, \tag{3.37}$$
$$\delta m(\mathbf{x}, t) = \sum_{\mathbf{k}} m_{\mathbf{k}}(t) e^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}, \tag{3.38}$$
$$\delta T_{ij}(\mathbf{x}, t) = \sum_{\mathbf{k}} T_{\mathbf{k}}^{ij}(t) e^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}, \tag{3.39}$$
$$\delta C_i(\mathbf{x}, t) = \sum_{\mathbf{k}} C_{\mathbf{k}}^i(t) e^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}, \tag{3.40}$$

with $\mathbf{k}$ taking discrete values. In terms of the Fourier variables, the linearized balance equations then take the forms

$$\rho_0 \dot{v}_{\mathbf{k}}^i = \mathrm{i} k^j T_{\mathbf{k}}^{ij}, \tag{3.41}$$
$$\rho_0 \dot{m}_{\mathbf{k}} = -\epsilon_{ij} T_{\mathbf{k}}^{ij} + \mathrm{i} k^i C_{\mathbf{k}}^i. \tag{3.42}$$

As discussed above, we have the constitutive equations

$$T_{ij} = \eta_{ijkl} v_{k,l} + \gamma_{ij} m, \tag{3.43}$$
$$C_i = \alpha_{ij} m_{,j}. \tag{3.44}$$

Expressing these in the Fourier basis, we see that

$$T^{ij}_{\mathbf{k}} = \mathrm{i}\eta_{ijkl}k^l v^k_{\mathbf{k}} + \gamma_{ij} m_{\mathbf{k}}, \tag{3.45}$$

$$C^i_{\mathbf{k}} = \mathrm{i}\alpha_{ij}k^j m_{\mathbf{k}}. \tag{3.46}$$

The Fourier forms of the balance (or conservation) equations may be expressed in matrix form by

$$\frac{d}{dt}\begin{bmatrix} v^1_{\mathbf{k}} \\ v^2_{\mathbf{k}} \\ m_{\mathbf{k}} \end{bmatrix} = \frac{1}{\rho_0}\begin{bmatrix} \mathrm{i}k^1 & \mathrm{i}k^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathrm{i}k^1 & \mathrm{i}k^2 & 0 & 0 \\ 0 & -1 & 1 & 0 & \mathrm{i}k^1 & \mathrm{i}k^2 \end{bmatrix}\begin{bmatrix} T^{11}_{\mathbf{k}} \\ T^{12}_{\mathbf{k}} \\ T^{21}_{\mathbf{k}} \\ T^{22}_{\mathbf{k}} \\ C^1_{\mathbf{k}} \\ C^2_{\mathbf{k}} \end{bmatrix} \tag{3.47}$$

or more compactly by

$$\frac{d}{dt}\begin{bmatrix} v^r_{\mathbf{k}} \\ m_{\mathbf{k}} \end{bmatrix} = \frac{1}{\rho_0}\begin{bmatrix} \mathrm{i}k^\nu\delta_{\mu r} & 0 \\ -\epsilon_{\mu\nu} & \mathrm{i}k^\lambda \end{bmatrix}\begin{bmatrix} T^{\mu\nu}_{\mathbf{k}} \\ C^\lambda_{\mathbf{k}} \end{bmatrix}, \tag{3.48}$$

where, for convenience, Latin indices have been used to label components of the configuration variables $\mathbf{v}_{\mathbf{k}}$ and $m_{\mathbf{k}}$, and Greek indices to label components of the generalized fluxes $\mathbf{T}_{\mathbf{k}}$ and $\mathbf{C}_{\mathbf{k}}$.

The Fourier forms of the constitutive relations (3.45) and (3.46) may also be cast in matrix form:

$$\begin{bmatrix} T^{11}_{\mathbf{k}} \\ T^{12}_{\mathbf{k}} \\ T^{21}_{\mathbf{k}} \\ T^{22}_{\mathbf{k}} \\ C^1_{\mathbf{k}} \\ C^2_{\mathbf{k}} \end{bmatrix} = \begin{bmatrix} \mathrm{i}\eta_{111j}k^j & \mathrm{i}\eta_{112j}k^j & \gamma_{11} \\ \mathrm{i}\eta_{121j}k^j & \mathrm{i}\eta_{122j}k^j & \gamma_{12} \\ \mathrm{i}\eta_{211j}k^j & \mathrm{i}\eta_{212j}k^j & \gamma_{21} \\ \mathrm{i}\eta_{221j}k^j & \mathrm{i}\eta_{222j}k^j & \gamma_{22} \\ 0 & 0 & \mathrm{i}\alpha_{1j}k^j \\ 0 & 0 & \mathrm{i}\alpha_{2j}k^j \end{bmatrix}\begin{bmatrix} v^1_{\mathbf{k}} \\ v^2_{\mathbf{k}} \\ m_{\mathbf{k}} \end{bmatrix} \tag{3.49}$$

and more compactly using the aforementioned convention with the Latin and Greek indices (plus one Hebrew index) as

$$\begin{bmatrix} T^{\mu\nu}_{\mathbf{k}} \\ C^\lambda_{\mathbf{k}} \end{bmatrix} = \begin{bmatrix} \mathrm{i}\eta_{\mu\nu r\aleph}k^\aleph & \gamma_{\mu\nu} \\ 0 & \mathrm{i}\alpha_{\lambda\aleph}k^\aleph \end{bmatrix}\begin{bmatrix} v^r_{\mathbf{k}} \\ m_{\mathbf{k}} \end{bmatrix}. \tag{3.50}$$

Making the definitions

$$\mathbf{A} = \begin{bmatrix} v^r_{\mathbf{k}} \\ m_{\mathbf{k}} \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} T^{\mu\nu}_{\mathbf{k}} \\ C^\lambda_{\mathbf{k}} \end{bmatrix} \tag{3.51}$$

$$\mathbf{M} = \frac{1}{\rho_0}\begin{bmatrix} \mathrm{i}k^\nu\delta_{\mu r} & 0 \\ -\epsilon_{\mu\nu} & \mathrm{i}k^\lambda \end{bmatrix} \qquad \mathbf{S} = \begin{bmatrix} \mathrm{i}\eta_{\mu\nu r\aleph}k^\aleph & \gamma_{\mu\nu} \\ 0 & \mathrm{i}\alpha_{\lambda\aleph}k^\aleph \end{bmatrix}, \tag{3.52}$$

we see that the small deviations about the steady state obey the dynamical (or conservation) and constitutive equations

$$\frac{d}{dt}\mathbf{A} = \mathbf{M}\mathbf{B}, \tag{3.53}$$

$$\mathbf{B} = \mathbf{S}\mathbf{A}. \tag{3.54}$$

We now make the Onsager regression hypothesis to obtain the general Green-Kubo relations, which is expressed in matrix form as

$$\mathbf{M}\mathbf{S}\left\langle \mathbf{A}\otimes\mathbf{A}^*\right\rangle = -\mathbf{M}\left(\int_0^\infty \left\langle \mathbf{B}(t)\otimes\mathbf{B}^*(0)\right\rangle dt\right)\mathbf{M}^\dagger, \tag{3.55}$$

where the $\mathbf{M}^\dagger$ is the conjugate transpose of $\mathbf{M}$. We then evaluate the two sides of (3.55), discarding in each matrix element all but the lowest order non-vanishing terms in $\mathbf{k}$. To this end, using the results (C.5)-(C.8) of Appendix C, the left-hand side of (3.55) yields

$$\text{LHS} = \frac{1}{\rho_0}\begin{bmatrix} \mathrm{i}k^\nu\delta_{\mu i} & 0 \\ -\epsilon_{\mu\nu} & \mathrm{i}k^\lambda \end{bmatrix}\begin{bmatrix} \mathrm{i}\eta_{\mu\nu j\aleph}k^\aleph & \gamma_{\mu\nu} \\ 0 & \mathrm{i}\alpha_{\lambda\aleph}k^\aleph \end{bmatrix}\begin{bmatrix} \left\langle v^j_{\mathbf{k}}v^k_{-\mathbf{k}}\right\rangle & \left\langle v^j_{\mathbf{k}}m_{-\mathbf{k}}\right\rangle \\ \left\langle m_{\mathbf{k}}v^k_{-\mathbf{k}}\right\rangle & \left\langle m_{\mathbf{k}}m_{-\mathbf{k}}\right\rangle \end{bmatrix} \tag{3.56}$$

$$= \frac{1}{\rho_0}\begin{bmatrix} \mathrm{i}k^\nu\delta_{\mu i} & 0 \\ -\epsilon_{\mu\nu} & \mathrm{i}k^\lambda \end{bmatrix}\begin{bmatrix} \mathrm{i}\eta_{\mu\nu j\aleph}k^\aleph & \gamma_{\mu\nu} \\ 0 & \mathrm{i}\alpha_{\lambda\aleph}k^\aleph \end{bmatrix}\begin{bmatrix} \mu\delta_{jk} & \mathrm{i}k^r\Omega_{rj} \\ -\mathrm{i}k^r\Omega_{rk} & \nu \end{bmatrix} \tag{3.57}$$

$$= \frac{1}{\rho_0}\begin{bmatrix} -k^\nu k^\aleph\eta_{i\nu j\aleph} & \mathrm{i}k^\nu\gamma_{i\nu} \\ -\mathrm{i}k^\aleph\epsilon_{\mu\nu}\eta_{\mu\nu j\aleph} & -\epsilon_{\mu\nu}\gamma_{\mu\nu} \end{bmatrix}\begin{bmatrix} \mu\delta_{jk} & \mathrm{i}k^r\Omega_{rj} \\ -\mathrm{i}k^r\Omega_{rk} & \nu \end{bmatrix} \tag{3.58}$$

$$= \frac{1}{\rho_0}\begin{bmatrix} -k^\nu k^\aleph\mu\eta_{i\nu k\aleph} + k^r k^\nu\gamma_{i\nu}\Omega_{rk} & \mathrm{i}\nu k^\nu\gamma_{i\nu} \\ -\mathrm{i}\mu k^\aleph\epsilon_{\mu\nu}\eta_{\mu\nu k\aleph} + \mathrm{i}\epsilon_{\mu\nu}k^r\gamma_{\mu\nu}\Omega_{rk} & -\nu\epsilon_{\mu\nu}\gamma_{\mu\nu} \end{bmatrix}, \tag{3.59}$$

Next, the right-hand side of (3.55) to lowest order in the wave-vector $\mathbf{k}$ gives

$$\text{RHS} = -\frac{1}{\rho_0^2}\int_0^\infty \left\langle \begin{bmatrix} \mathrm{i}k^\nu\delta_{\mu i} & 0 \\ -\epsilon_{\mu\nu} & \mathrm{i}k^\lambda \end{bmatrix} \begin{bmatrix} T_{\mathbf{k}}^{\mu\nu}(t)T_{-\mathbf{k}}^{\rho\sigma}(0) & T_{\mathbf{k}}^{\mu\nu}(t)C_{-\mathbf{k}}^{\omega}(0) \\ C_{\mathbf{k}}^{\lambda}(t)T_{-\mathbf{k}}^{\rho\sigma}(0) & C_{\mathbf{k}}^{\lambda}(t)C_{-\mathbf{k}}^{\omega}(0) \end{bmatrix} \begin{bmatrix} -\mathrm{i}k^\sigma\delta_{\rho k} & -\epsilon_{\rho\sigma} \\ 0 & -\mathrm{i}k^\omega \end{bmatrix} \right\rangle dt \tag{3.60}$$

$$\equiv -\frac{1}{\rho_0^2}\begin{bmatrix} \mathrm{i}k^\nu\delta_{\mu i} & 0 \\ -\epsilon_{\mu\nu} & \mathrm{i}k^\lambda \end{bmatrix} \begin{bmatrix} \{TT\}_{\mu\nu\rho\sigma} & \{TC\}_{\mu\nu\omega} \\ \{CT\}_{\lambda\rho\sigma} & \{CC\}_{\lambda\omega} \end{bmatrix} \begin{bmatrix} -\mathrm{i}k^\sigma\delta_{\rho k} & -\epsilon_{\rho\sigma} \\ 0 & -\mathrm{i}k^\omega \end{bmatrix} \tag{3.61}$$

$$= -\frac{1}{\rho_0^2}\begin{bmatrix} \mathrm{i}k^\nu\{TT\}_{i\nu\rho\sigma} & \mathrm{i}k^\nu\{TC\}_{i\nu\omega} \\ -\epsilon_{\mu\nu}\{TT\}_{\mu\nu\rho\sigma} & -\epsilon_{\mu\nu}\{TC\}_{\mu\nu\omega} + \mathrm{i}k^\lambda\{CC\}_{\lambda\omega} \end{bmatrix} \begin{bmatrix} -\mathrm{i}k^\sigma\delta_{\rho k} & -\epsilon_{\rho\sigma} \\ 0 & -\mathrm{i}k^\omega \end{bmatrix} \tag{3.62}$$

$$= -\frac{1}{\rho_0^2}\begin{bmatrix} k^\nu k^\sigma\{TT\}_{i\nu k\sigma} & -\mathrm{i}\epsilon_{\rho\sigma}k^\nu\{TT\}_{i\nu\rho\sigma} \\ \mathrm{i}k^\sigma\epsilon_{\mu\nu}\{TT\}_{\mu\nu k\sigma} & \epsilon_{\mu\nu}\epsilon_{\rho\sigma}\{TT\}_{\mu\nu\rho\sigma} \end{bmatrix}, \tag{3.63}$$

where we have introduced the definitions

$$\{TT\}_{\mu\nu\rho\sigma} = \int_0^\infty \left\langle T_{\mathbf{k}}^{\mu\nu}(t)T_{-\mathbf{k}}^{\rho\sigma}(0)\right\rangle dt, \tag{3.64}$$

$$\{TC\}_{\mu\nu\omega} = \int_0^\infty \left\langle T_{\mathbf{k}}^{\mu\nu}(t)C_{-\mathbf{k}}^{\omega}(0)\right\rangle dt, \tag{3.65}$$

$$\{CT\}_{\lambda\rho\sigma} = \int_0^\infty \left\langle C_{\mathbf{k}}^{\lambda}(t)T_{-\mathbf{k}}^{\rho\sigma}(0)\right\rangle dt, \tag{3.66}$$

$$\{CC\}_{\lambda\omega} = \int_0^\infty \left\langle C_{\mathbf{k}}^{\lambda}(t)C_{-\mathbf{k}}^{\omega}(0)\right\rangle dt. \tag{3.67}$$

Equating the (2,2) entries of (3.59) and (3.63), we find

$$\epsilon_{ij}\gamma_{ij} = \frac{1}{\rho_0\nu}\epsilon_{ij}\epsilon_{kl}\{TT\}_{ijkl}\,. \tag{3.68}$$

Equating the (1,2) entries of (3.59) and (3.63) and contracting with k^i, we find

$$k^ik^j\gamma_{ij} = \frac{1}{\rho_0\nu}\epsilon_{kl}k^ik^j\{TT\}_{ijkl}\,. \tag{3.69}$$

This equation holds independently for $\mathbf{k} = k\hat{e}_1$ and $\mathbf{k} = k\hat{e}_2$, yields two equations. Summing these amounts to replacing k^ik^j with the tensor δ_{ij}, resulting in

$$\delta_{ij}\gamma_{ij} = \frac{1}{\rho_0\nu}\delta_{ij}\epsilon_{kl}\{TT\}_{ijkl}\,. \tag{3.70}$$

Equating the (1,1) entries of (3.59) and (3.63), we find

$$-k^j k^l \mu\eta_{ijkl} + k^j k^l \gamma_{il}\Omega_{jk} = -\frac{1}{\rho_0} k^j k^l \{TT\}_{ijkl} \,. \tag{3.71}$$

As before, this equation holds independently for $\mathbf{k} = k\hat{e}_1$ and $\mathbf{k} = k\hat{e}_2$, and therefore we may replace $k^j k^l$ by δ_{jl} to obtain

$$\delta_{jl}\eta_{ijkl} - \frac{\gamma_{ij}\Omega_{jk}}{\mu} = \frac{1}{\rho_0\mu}\delta_{jl} \{TT\}_{ijkl} \,. \tag{3.72}$$

Contracting this equation with δ_{ik} and ϵ_{ik} we find the two equations

$$\delta_{ik}\delta_{jl}\eta_{ijkl} - \frac{\delta_{ik}\gamma_{ij}\Omega_{jk}}{\mu} = \frac{1}{\rho_0\mu}\delta_{ik}\delta_{jl} \{TT\}_{ijkl} \,, \tag{3.73}$$

$$\epsilon_{ik}\delta_{jl}\eta_{ijkl} - \frac{\epsilon_{ik}\gamma_{ij}\Omega_{jk}}{\mu} = \frac{1}{\rho_0\mu}\epsilon_{ik}\delta_{jl} \{TT\}_{ijkl} \,. \tag{3.74}$$

Equating the (2,1) entries of (3.59) and (3.63), we find

$$k^l\epsilon_{ij}\eta_{ijkl} - \epsilon_{ij}k^l\frac{\gamma_{ij}\Omega_{lk}}{\mu} = \frac{1}{\rho_0\mu}k^l\epsilon_{ij} \{TT\}_{ijkl} \,. \tag{3.75}$$

Contracting (3.75) with k^k and replacing $k^k k^l$ by δ_{kl}, we find

$$\epsilon_{ij}\delta_{kl}\eta_{ijkl} - \epsilon_{ij}\delta_{kl}\frac{\gamma_{ij}\Omega_{lk}}{\mu} = \frac{1}{\rho_0\mu}\epsilon_{ij}\delta_{kl} \{TT\}_{ijkl} \,. \tag{3.76}$$

Contracting (3.75) instead with $\epsilon_{kr}k^r$ and replacing $k^r k^l$ by δ_{rl}, we find

$$\epsilon_{ij}\epsilon_{kl}\eta_{ijkl} - \epsilon_{ij}\epsilon_{kl}\frac{\gamma_{ij}\Omega_{lk}}{\mu} = \frac{1}{\rho_0\mu}\epsilon_{ij}\epsilon_{kl} \{TT\}_{ijkl} \,. \tag{3.77}$$

Using the basis expansions (3.7) and (3.9) of $\boldsymbol{\gamma}$ and $\boldsymbol{\eta}$ and the inner products provided in Table 3.2, we may compute

$$\delta_{ik}\delta_{jl}\eta_{ijkl} = 2\lambda_1 + 4\lambda_2 + 2\lambda_3 = 4\beta_3, \tag{3.78}$$

$$\epsilon_{ik}\delta_{jl}\eta_{ijkl} = 4\lambda_4 + 4\lambda_5 + 4\lambda_6 = 4\beta_4, \tag{3.79}$$

$$\epsilon_{ij}\delta_{kl}\eta_{ijkl} = 8\lambda_5 = 2\beta_4 + 4\beta_5 - 2\beta_6, \tag{3.80}$$

$$\epsilon_{ij}\epsilon_{kl}\eta_{ijkl} = 4\lambda_3 = -4\beta_1 + 2\beta_2 + 2\beta_3. \tag{3.81}$$

Now using $\gamma_{ij} = \gamma_1\delta_{ij} + \gamma_2\epsilon_{ij}$, defining $\tau = \epsilon_{ij}\Omega_{ij}$ and $\pi = \delta_{ij}\Omega_{ij}$, and using the equations (3.68), (3.70), (3.73), (3.74), (3.76), (3.77), we finally have the six Green-Kubo equations

	$\mathbf{s}_1$	$\mathbf{s}_2$	$\mathbf{s}_3$	$\mathbf{s}_4$	$\mathbf{s}_5$	$\mathbf{s}_6$	$\mathbf{e}_1$	$\mathbf{e}_2$	$\mathbf{e}_3$	$\mathbf{e}_4$	$\mathbf{e}_5$	$\mathbf{e}_6$
$\delta_{ik}\delta_{jl}$	2	4	2	0	0	0	0	0	4	0	0	0
$\epsilon_{ik}\delta_{jl}$	0	0	0	4	4	4	0	0	0	4	0	0
$\epsilon_{ij}\delta_{kl}$	0	0	0	0	8	0	0	0	0	2	4	-2
$\epsilon_{ij}\epsilon_{kl}$	0	0	4	0	0	0	-4	2	2	0	0	0

Table 3.2: Inner products of the tensors appearing in the Green-Kubo relations (3.84)-(3.87) with the (non-normalized) elements of the two orthogonal bases for the isotropic rank four tensors (in two dimensions) introduced in Appendix B.

relating the viscosity coefficients as

$$\gamma_1 = \frac{1}{2\rho_0\nu}\delta_{ij}\epsilon_{kl}\left\{TT\right\}_{ijkl}\,, \tag{3.82}$$

$$\gamma_2 = \frac{1}{2\rho_0\nu}\epsilon_{ij}\epsilon_{kl}\left\{TT\right\}_{ijkl}\,, \tag{3.83}$$

$$\lambda_1 + 2\lambda_2 + \lambda_3 - \frac{\gamma_1\pi}{2\mu} + \frac{\gamma_2\tau}{2\mu} = \frac{1}{2\rho_0\mu}\delta_{ik}\delta_{jl}\left\{TT\right\}_{ijkl}\,, \tag{3.84}$$

$$\lambda_4 + \lambda_5 + \lambda_6 - \frac{\gamma_1\tau}{4\mu} - \frac{\gamma_2\pi}{4\mu} = \frac{1}{4\rho_0\mu}\epsilon_{ik}\delta_{jl}\left\{TT\right\}_{ijkl}\,, \tag{3.85}$$

$$\lambda_5 - \frac{\gamma_2\pi}{4\mu} = \frac{1}{8\rho_0\mu}\epsilon_{ij}\delta_{kl}\left\{TT\right\}_{ijkl}\,, \tag{3.86}$$

$$\lambda_3 + \frac{\gamma_2\tau}{2\mu} = \frac{1}{4\rho_0\mu}\epsilon_{ij}\epsilon_{kl}\left\{TT\right\}_{ijkl}\,. \tag{3.87}$$

Using the expansion of correlation function in small $\mathbf{k}$, we may write to lowest-order in $\mathbf{k}$ for the stress-stress correlation function

$$\mathcal{T}_{ijkl} := \left\{TT\right\}_{ijkl} = \frac{1}{L^4}\int_0^\infty dt \int d^2\mathbf{x}\, d^2\mathbf{y}\, \langle \delta T_{ij}(\mathbf{x},t)\delta T_{kl}(\mathbf{y},0)\rangle\,, \tag{3.88}$$

where we have recalled that the $\mathbf{T_k}$ are fluctuations about the steady-state mean stress tensor.

and μ, ν, τ, and π are the steady-state correlation functions defined by

$$\mu\delta_{ij} = \frac{1}{L^4}\int \left\langle \delta v^i(\mathbf{x})\delta v^j(\mathbf{y})\right\rangle d^2\mathbf{x}\, d^2\mathbf{y} \tag{3.89}$$

$$\pi = \frac{1}{L^4}\int (y^i - x^i)\left\langle \delta v^i(\mathbf{x})\delta m(\mathbf{y})\right\rangle d^2\mathbf{x}\, d^2\mathbf{y} \tag{3.90}$$

$$\tau = \frac{1}{L^4}\int \epsilon_{kr}(y^r - x^r)\left\langle \delta m(\mathbf{x})\delta v^k(\mathbf{y})\right\rangle d^2\mathbf{x}\, d^2\mathbf{y} \tag{3.91}$$

$$\nu = \frac{1}{L^4}\int \langle \delta m(\mathbf{x})\delta m(\mathbf{y})\rangle\, d^2\mathbf{x}\, d^2\mathbf{y}. \tag{3.92}$$

In (3.89)-(3.92), δa indicates the fluctuation about the steady-state value of a.

The constants μ and ν provide an estimate of the effective kinetic temperature in the steady state and by the equipartition theorem are proportional to the Boltzmann temperature in the special case of equilibrium systems. The constant τ measures the correlation of the internal spin with the fluid vorticity, in other words the correlation between the internal and external angular momentum density fields. The constant π measures the correlation of the internal spin with the fluctuating divergence of the velocity field.

Several features of the Green-Kubo relations (3.82)-(3.87) are noteworthy. In the absence of internal spin (or the absence of a mechanism for coupling internal spin to the velocity field), $\gamma_1 = \gamma_2 = 0$ by assumption and $\lambda_3 = \lambda_5 = 0$ by conservation of angular momentum. Then we are left with the Green-Kubo relations

$$\lambda_1 + 2\lambda_2 = \frac{1}{2\rho_0\mu}\delta_{ik}\delta_{jl}\mathcal{T}^{ijkl}, \tag{3.93}$$

$$\lambda_4 + \lambda_6 = \frac{1}{4\rho_0\mu}\epsilon_{ik}\delta_{jl}\mathcal{T}^{ijkl}. \tag{3.94}$$

If we demand that the stress tensor be objective, then $\lambda_6 = 0$ and we are left with a Green-Kubo relation for the odd viscosity λ_4. Given the form (3.88) of the integrated stress-stress correlation function $\mathcal{T}^{ijkl}$, it is clear that only the component of the stress autocorrelation function that is odd under time reversal survives contraction with ϵ_{ik} as appears in (3.85). Therefore, non-vanishing odd viscosity $\lambda_4 \neq 0$ requires breaking time reversal symmetry at the level of the steady-state stress fluctuations for fluids without internal spin.

Now allowing for coupling of internal spin to the fluid velocity, we may observe from (3.83) and (3.87) that

$$2\lambda_3 = \left(\frac{\nu - \tau}{\mu}\right)\gamma_2. \tag{3.95}$$

In an equilibrium system, $\nu = \mu$ by equipartition and there exist no correlations between internal spin and vorticity, so that $\tau = 0$. Then $\gamma_2 = 2\lambda_3$, so that there is a single parameter characterizing the response of the stress to both the spin m and the vorticity ω. This feature is assumed in many previous works on out-of-equilibrium active systems [40, 47, 48, 41, 42]. It should be noted that such active systems may break equipartition in the steady state so that in general $\nu - \tau \neq \mu$, which leads to decoupling of the two rotational viscosity coefficients coupling the vorticity and internal spin, and therefore this assumption must be revisited.

Finally, we note that in a system with internal spin that obeys time reversal symmetry at the level of the stress correlations, the Green-Kubo relation (3.85) involving the odd viscosity reduces to

$$\lambda_4 + \lambda_5 + \lambda_6 = \frac{\gamma_1 \tau}{4\mu} + \frac{\gamma_2 \pi}{4\mu}. \tag{3.96}$$

Thus λ_4 need not necessarily vanish. Therefore, it is possible that there are systems that do not break time reversal symmetry at the level of stress correlations, yet do exhibit odd viscosity due to a coupling of internal spin to fluid velocity. This possibility merits future consideration.

Chapter 4

Coarse-Graining of Active Brownian Particles

In this chapter, we describe the simple model of active matter known as Active Brownian Particles (ABPs). This model includes a vectorial degree of freedom for each particle, along which a nonconservative active force is applied, driving the system out of equilibrium. By performing a coarse-graining analysis in the spirit of Irving and Kirkwood, we will argue that a continuum theory that captures the behavior of the ABP model should include the activity in the form of a body force proportional to a continuum director field, rather than as an additional term in the pressure as suggested elsewhere. By performing a second, continuum-to-continuum coarse-graining, we then reconcile these two approaches. We then show by analyzing the balance of angular momentum that the stress tensor need not be symmetric and provide a microscopic expression for the stress couple in the spirit of the microstructed continua of Dahler and Scriven. Finally, we perfor an Irving-Kirkwood style coarse-graining of the director dynamics in both the angularly over- and under-damped regimes, elucidating the connection between mass currents and alignment interactions.

4.1 The Active Brownian Particle Model

A smple model of active matter is the Active Brownian Particle (ABP) [49]. This is a pointlike particle equipped with a unit vector degree of freedom, the director, along which an active force is applied. The director is free to rotate, so that the direction of the applied force varies with time. Moreover, the directors of multiple ABPs need not be aligned; rather, each particle has its own director degree of freedom. This distinguishes a collection of ABPs from a system of particles in a varying external field, where the forces applied to distinct particles are perfectly correlated. A good picture to keep in mind is of a collection of small vessels, each with a motor fixed to the stern. As the vessels tumble around, the motors apply forces in different directions.

Several systems, both engineered and natural, may be modeled by ABPs. Systems of

ABPs have been realized with colloids selectively coated with light-sensitive catalysts [50, 51, 52] and with asymetric rods on vibrating substrates [53]. ABPs also provide a model, certainly simplified, for swarms of bacteria [54]. These systems exhibit interesting phenomenology, in particular the dynamical phase transition to the motility-induced phase separation (MIPS) regime [55], in which a collection of ABPs features regions of high and low density (a "vapor-liquid coexistence" [56]) as opposed to a uniform concentration.

A simple Newtonian model for the dynamics of the spatial degrees of freedom of ABPs in any spatial dimension are as follows:

$$\frac{d\mathbf{x}_i}{dt} = \frac{\mathbf{p}_i}{m} \tag{4.1}$$

$$\frac{d\mathbf{p}_i}{dt} = -\frac{\xi_p}{m}\mathbf{p}_i + f\mathbf{d}_i + \sum_j \mathbf{f}_{ij} \tag{4.2}$$

Here $\mathbf{x}_i$ and $\mathbf{p}_i$ are the positions and momenta of the i^{th} particle, $\mathbf{d}_i$ is its unit director vector, and m is the particle mass. We include the possibility of interparticle forces $\mathbf{f}_{ij}$. The damping term $-\xi_p\mathbf{p}_i/m$ is necessary to prevent runaway heating of the system due to the work done by the active forces. This damping may be physically implemented by friction with a substrate, as in the systems referred to as "dry active matter", or by drag due to a solvent, in "wet active matter". An important limitation of the model presented here is that it does not include any nonconservative two-particle interactions that might be caused by the presence of a solvent. Such effects are known to be important in many situations [57].

4.2 Coarse-Grained Fields and Balance Equations

The goal of this chapter is to provide guidance for a continuum description of the motion of a collection of ABPs. In order to make contact with a continuum theory, we define fields corresponding to the local densities of mass and linear momentum. These are field-valued functions of the microscopic variables $\mathbf{x}_i$ and $\mathbf{p}_i$. The evolution equations for these fields will then yield the appropriate continuum balance laws for describing the system at a coarse-grained level. This is essentially the strategy employed by Irving and Kirkwood to derive hydrodynamical equations from microscopic dynamics [32]. The difference in our approach is that Irving and Kirkwood perform an ensemble averaging, while we define the fields without averaging over the noise ensemble. Our balance laws will therefore be valid not only on average, but also for any individual system trajectory.

The continuum fields are defined as follows:

$$\rho(\mathbf{x}, t) = \sum_i m\Delta_i(\mathbf{x}) \tag{4.3}$$

$$\rho\mathbf{v}(\mathbf{x}, t) = \sum_i \mathbf{p}_i(\mathbf{x}) \tag{4.4}$$

Time-dependence is suppressed in the microscopic variables for notational compactness. Here, $\Delta_i(\mathbf{x}) = \Delta(\mathbf{x}-\mathbf{x}_i)$, where Δ is a normalized, non-negative function with finite support and assumed to be rotationally invariant. Our results will not depend on the specific choice of Δ. In future numerical work, however, the choice of Δ will be crucial. In particular, Δ should be chosen to have support large enough to contain several particles, so that the continuum fields are relatively smooth, and small enough that these fields capture variation on length scales of interest for the problem at hand. Ideally, the particular setup of the simulation will result in a separation of length scales, with the average interparticle spacing much smaller than the scale on which gradients become relevant. The support of Δ should be chosen to fall between these two scales.

The essential idea of these definitions is that the conserved quantities associated with a particle should be "smeared out", so that in the continuum model they are associated to a small region around the actual location of the (point-like) ABP. In order to avoid over-counting, the smearing function Δ is normalized. At the continuum level, the fields are interpreted as follows: ρ is the mass density and $\mathbf{v}$ the velocity of the ABP fluid. It will turn out to be convenient also to define a continuum director field, which does not correspond to any conserved quantity:

$$\rho\mathbf{d}(\mathbf{x},t) = \sum_i \mathbf{d}_i \Delta_i(\mathbf{x}) \tag{4.5}$$

$$\tag{4.6}$$

Note that $\mathbf{d}(\mathbf{x},t)$ is not in general a unit vector.

The equations of motion for the conserved fields (4.3) and (4.4) are directly dependent on the equations of motion (4.1) and (4.2) for the microscopic variables. In particular, if B is a field-valued function of the microscopic variables, we have

$$\frac{\partial B}{\partial t} = \mathcal{F}B, \tag{4.7}$$

where

$$\mathcal{F} = \sum_i \left[\frac{\mathbf{p}_i}{m} \cdot \frac{\partial}{\partial \mathbf{x}_i} + \left(-\frac{\xi_p}{m}\mathbf{p}_i + f\mathbf{d}_i + \sum_j \mathbf{f}_{ij} \right) \cdot \frac{\partial}{\partial \mathbf{p}_i} \right] + \mathcal{F}_{\text{int}}. \tag{4.8}$$

The derivatives with respect to microscopic variables are taken at fixed $(\mathbf{x}, t)$, and the unspecified part $\mathcal{F}_{\text{int}}$ of the operator contains derivatives with respect to internal degrees of freedom associated to the ABP directors, so that it vanishes on ρ and $\rho\mathbf{v}$, which do not depend on these variables. Its form will depend on the equations of motion chosen for the directors.

We are now in a position to derive continuum balance laws. The simplest balance equation is the balance of mass, obtained by taking the material time-derivative of the mass density field. We have

$$\begin{aligned}
\frac{D\rho}{Dt} &= \frac{\partial \rho}{\partial t} + \left(\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{x}}\right)\rho \\
&= \mathcal{F}\sum_i m\Delta_i(\mathbf{x}) + \left(\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{x}}\right)\rho \\
&= \sum_i \mathbf{p}_i\cdot\frac{\partial}{\partial \mathbf{x}_i}\Delta_i(\mathbf{x}) + \left(\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{x}}\right)\rho \\
&= -\frac{\partial}{\partial \mathbf{x}}\cdot\sum_i \mathbf{p}_i\Delta_i(\mathbf{x}) + \left(\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{x}}\right)\rho \\
&= -\frac{\partial}{\partial \mathbf{x}}\cdot(\rho\mathbf{v}) + \left(\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{x}}\right)\rho \\
&= -\rho\left(\frac{\partial}{\partial \mathbf{x}}\cdot\mathbf{v}\right),
\end{aligned}$$

and thus obtain the standard balance of mass:

$$\frac{D\rho}{Dt} = -\rho\left(\frac{\partial}{\partial \mathbf{x}}\cdot\mathbf{v}\right). \tag{4.9}$$

This validates the identification of $\mathbf{v}$ as a continuum velocity field at the coarse-grained level.

The balance of linear momentum is an expression for the material derivative of the velocity field. We begin by computing

$$\begin{aligned}
\frac{\partial}{\partial t}(\rho\mathbf{v}) &= \mathcal{F}\sum_i \mathbf{p}_i\Delta_i(\mathbf{x}) \\
&= \sum_i\left(-\frac{\xi_p}{m}\mathbf{p}_i + f\mathbf{d}_i + \sum_j \mathbf{f}_{ij}\right)\Delta_i(\mathbf{x}) + \sum_i\left(\frac{\mathbf{p}_i}{m}\cdot\frac{\partial}{\partial \mathbf{x}_i}\right)\mathbf{p}_i\Delta_i(\mathbf{x}) \\
&= \rho\left(-\frac{\xi_p}{m}\mathbf{v} + f\mathbf{d}\right) + \sum_{ij}\mathbf{f}_{ij}\Delta_i(\mathbf{x}) - \frac{\partial}{\partial \mathbf{x}}\cdot\sum_i\frac{\mathbf{p}_i\otimes\mathbf{p}_i}{m}\Delta_i(\mathbf{x}).
\end{aligned}$$

The second term, which accounts for interparticle forces, may be expressed as a gradient using Noll's formula [58, 59]

$$\Delta_i(\mathbf{x}) - \Delta_j(\mathbf{x}) = -\frac{\partial}{\partial \mathbf{x}}\cdot(\mathbf{x}_{ij}b_{ij}). \tag{4.10}$$

where the so-called bond function b_{ij} is defined as

$$b_{ij} = \int_0^1 \Delta(\mathbf{x} - \lambda\mathbf{x}_i + \mathbf{x}_{ij})d\lambda, \tag{4.11}$$

with $\mathbf{x}_{ij} = \mathbf{x}_i - \mathbf{x}_j$. Then:

$$\begin{aligned}\sum_{ij} \mathbf{f}_{ij}\Delta_i(\mathbf{x}) &= \frac{1}{2}\sum_{ij} \mathbf{f}_{ij}\left(\Delta_i(\mathbf{x}) - \Delta_j(\mathbf{x})\right) \\ &= -\frac{1}{2}\sum_{ij} \mathbf{f}_{ij}\frac{\partial}{\partial \mathbf{x}} \cdot (\mathbf{x}_{ij} b_{ij}) \\ &= -\frac{\partial}{\partial \mathbf{x}} \cdot \frac{1}{2}\sum_{ij} b_{ij}\mathbf{x}_{ij} \otimes \mathbf{f}_{ij}.\end{aligned} \tag{4.12}$$

The tensor quantity whose gradient is the third term may be expressed as a sum of mean and deviatoric parts:

$$\sum_i \frac{\mathbf{p}_i \otimes \mathbf{p}_i}{m}\Delta_i(\mathbf{x}) = \sum_i \frac{(\mathbf{p}_i - m\mathbf{v}) \otimes (\mathbf{p}_i - m\mathbf{v})}{m}\Delta_i(\mathbf{x}) + \rho\mathbf{v} \otimes \mathbf{v}.$$

Using the balance of mass and then plugging in the above expressions:

$$\begin{aligned}\rho\frac{D\mathbf{v}}{Dt} &= \frac{\partial}{\partial t}(\rho\mathbf{v}) + \frac{\partial}{\partial \mathbf{x}} \cdot (\rho\mathbf{v} \otimes \mathbf{v}) \\ &= \rho\left(-\frac{\xi_p}{m}\mathbf{v} + f\mathbf{d}\right) + \frac{\partial}{\partial \mathbf{x}} \cdot \left[-\sum_i \frac{(\mathbf{p}_i - m\mathbf{v}) \otimes (\mathbf{p}_i - m\mathbf{v})}{m}\Delta_i(\mathbf{x}) - \frac{1}{2}\sum_{ij} b_{ij}\mathbf{x}_{ij} \otimes \mathbf{f}_{ij}\right],\end{aligned}$$

and we have the balance of linear momentum

$$\rho\frac{D\mathbf{v}}{Dt} = \rho\mathbf{b} + \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{T}, \tag{4.13}$$

with the body force and stress tensor

$$\mathbf{b} = -\frac{\xi_p}{m}\mathbf{v} + f\mathbf{d} \tag{4.14}$$

$$\mathbf{T} = -\sum_i \frac{(\mathbf{p}_i - m\mathbf{v}) \otimes (\mathbf{p}_i - m\mathbf{v})}{m}\Delta_i(\mathbf{x}) - \frac{1}{2}\sum_{ij} b_{ij}\mathbf{x}_{ij} \otimes \mathbf{f}_{ij}. \tag{4.15}$$

As usual for a fluid of interacting particles, the stress decomposes into a kinetic piece and an interaction piece. The activity parameter f appears in the body force, coupled to the coarse-grained director field. This suggests that a continuum model of systems described adequately at the microscopic level by ABPs should include this director field as a basic quantity, and that the dynamics of this field is crucial to understanding the flow properties of these systems.

4.3 Virial Theorems and Swim Pressure

In [60], Takatori and Brady propose a continuum-level contribution to the stress, called the swim stress. They use the trace of this stress, the swim pressure, to explain simulations showing motility induced phase separation in ABPs. This proposal contrasts with our conclusion that the active force should be accounted for in the body force, rather than the stress, of a continuum theory. The purpose of this section is to resolve this discrepancy. In this section, we will first provide a derivation of the swim pressure in the atomistic setting. Then we will show that this term may also be understood as a manifestation of the body force via a continuum homogenization procedure in the spirit of [61].

Both the atomistic and continuum analyses presented in this section rely on the notion that pressure should be understood as a force per area that must be applied by an external agent in order to confine a system (which we think of either as a collection of particles or as a continuum body) to a region Ω. We therefore begin by defining representations of the quantities $\boldsymbol{\mathcal{F}}(\mathcal{A})$, the net confinement forces or surface tractions that must be applied to regions $\mathcal{A} \subset \partial\Omega$ of the boundary. Under the assumption that these surface tractions may be understood (on large enough length scales) in terms of a homogeneous pressure p, we may express p in terms of confinement forces acting on the near-boundary parts of the system. We then use virial theorems relating bulk and boundary variables in the atomistic and continuum settings to provide a bulk expression for p, and recover the expressions for swim pressure as introduced in [60].

Atomistic Representation

To confine particles to a region Ω, an external agent must apply confining forces $\mathbf{c}_i$, where i ranges over the particles. If this force is short-ranged, $\mathbf{c}_i$ is non-zero only for particles close to the boundary. Then we can define $\boldsymbol{\mathcal{F}}(\mathcal{A})$, the net confinement force applied on the region $\mathcal{A} \subset \partial\Omega$ of the boundary:

$$\boldsymbol{\mathcal{F}}(\mathcal{A}) = \sum_{i:\mathbf{x}_i \in \mathcal{A}_\Delta} \mathbf{c}_i, \tag{4.16}$$

where $\mathcal{A}_\Delta$ is the neighborhood with radius Δ around $\mathcal{A}$ for some Δ larger than the range of the confining force. Clearly this definition should only be used for $\mathcal{A}$ on a scale larger than the typical inter-particle spacing, as particles close to the boundary between any two adjacent regions $\mathcal{A}$ and $\mathcal{A}'$ will be double-counted.

One can define a uniform externally applied pressure p if it is the case that for sufficiently large regions $\mathcal{A}$ of the boundary we have

$$\boldsymbol{\mathcal{F}}(\mathcal{A}) \approx -\int_{\mathcal{A}} p\mathbf{n}\, da,$$

with $\mathbf{n}$ the unit normal. If on the other hand the characteristic length scale of $\mathcal{A}$ is much smaller than the smallest scale of boundary curvature (so that $\mathbf{n}$ is roughly constant on $\mathcal{A}$)

and letting $\mathbf{x}_0$ be the center of mass of $\mathcal{A}$, we may write

$$\boldsymbol{\mathcal{F}}(\mathcal{A}) \cdot \mathbf{x}_0 \approx -\int_{\mathcal{A}} p\mathbf{n} \cdot \mathbf{x}\, da. \tag{4.17}$$

If it is also the case that particles in $\mathcal{A}_\Delta$ experience approximately the same constraint force $\mathbf{c}_i$, we have from Eq. (4.16)

$$\boldsymbol{\mathcal{F}}(\mathcal{A}) \cdot \mathbf{x}_0 \approx \sum_{i:\mathbf{x}_i \in \mathcal{A}_\Delta} \mathbf{c}_i \cdot \mathbf{x}_i. \tag{4.18}$$

We are considering in other words the case in which there is an intermediate asymptotic length scale between the particle and continuum scales. If we decompose the entire boundary into regions $\mathcal{A}_k$ of this intermediate scale, we may equate expressions (4.17) and (4.18) and sum over k to obtain

$$-\int_{\partial\Omega} p\mathbf{n} \cdot \mathbf{x}\, da \approx \sum_i \mathbf{c}_i \cdot \mathbf{x}_i.$$

The left-hand side is simply $-pVd$, with V the volume of Ω and d the dimension of space. We thus obtain

$$p \approx -\frac{1}{Vd} \sum_i \mathbf{c}_i \cdot \mathbf{x}_i. \tag{4.19}$$

Note that the summation over i in Eq. (4.19) runs over all particles, but contributes only for near-boundary particles.

We would like to have an expression for the externally applied pressure in terms of bulk, rather than boundary, variables. In order to obtain such an expression, we appeal to the virial theorem (see Appendix A for a derivation):

$$\left\langle \sum_i \mathbf{f}_i \cdot \mathbf{x}_i + \sum_i \frac{\mathbf{p}_i \cdot \mathbf{p}_i}{m} \right\rangle = 0,$$

where brackets indicate ensemble-averaging and the system is assumed to be in a steady state. Here $\mathbf{f}_i$ is the total force, including the constraint forces $\mathbf{c}_i$ applied by the boundary. Separating out the constraint force and using Eq. (4.19), we have

$$\langle p \rangle \approx \frac{1}{Vd} \left\langle \sum_i (\mathbf{f}_i - \mathbf{c}_i) \cdot \mathbf{x}_i + \sum_i \frac{\mathbf{p}_i \cdot \mathbf{p}_i}{m} \right\rangle.$$

Defining $p_{\text{ext}} = \langle p \rangle$ and using the equation (4.2) for the force on particle i, we find

$$p_{\text{ext}} \approx -\frac{\xi_p n}{md} \langle \mathbf{p}_i \cdot \mathbf{x}_i \rangle + \frac{fn}{d} \langle \mathbf{d}_i \cdot \mathbf{x}_i \rangle + \frac{n}{md} \langle \mathbf{p}_i \cdot \mathbf{p}_i \rangle + \frac{1}{Vd} \left\langle \frac{1}{2} \sum_{ik} \mathbf{f}_{ik} \cdot \mathbf{x}_{ik} \right\rangle.$$

The second term is precisely the swim pressure as defined in [60].

Continuum Representation

In what follows, we show that the atomistic expression (4.20) derived in the previous subsection is consistent with the appearance of the active force in the body force obtained from the Irving-Kirkwood analysis presented earlier. We start by deriving an expression for pressure in a self-contained continuum model in the case of homogeneous surface traction.

To apply a similar argument as used in the atomistic case to the continuum setting, we start with the standard continuum equations of motion, i.e. the mass and momentum balances:

$$\frac{D\rho}{Dt} = -\rho \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{v} \tag{4.20}$$

$$\rho \frac{D\mathbf{v}}{Dt} = \rho \mathbf{b} + \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{T} \tag{4.21}$$

with body force $\mathbf{b}$ and stress $\mathbf{T}$. Note that these are the equations of motion that emerged from the Irving-Kirkwood theory. Now we consider a slightly unorthodox formulation of the theory of a continuum body with boundary. Rather than taking the surface traction on an area element da with normal $\mathbf{n}$ to be given by $\mathbf{t} = \mathbf{T} \cdot \mathbf{n}$, we instead view the traction as a part of the body force with support only very close to $\partial\Omega$. Analogous to the confining forces $\mathbf{c}_i$ in the atomistic setting, this component of the body force is considered to be applied by an external agent and is responsible for confining the system. We then decompose the total body force as $\mathbf{b} = \mathbf{b}_c + \mathbf{b}'$, where $\mathbf{b}_c$ is the confining term, vanishing away from $\partial\Omega$, and $\mathbf{b}'$ is the remaining part of the total body force.

Analogous to Eq. (4.16), we define the quantities $\boldsymbol{\mathcal{F}}(\mathcal{A})$, the net forces applied by the region $\mathcal{A}$ of the boundary, as

$$\boldsymbol{\mathcal{F}}(\mathcal{A}) = \int_{\mathcal{A}_\delta} \rho \mathbf{b}_c \, dv, \tag{4.22}$$

where $\mathcal{A}_\delta$ is a neighborhood of radius δ around $\mathcal{A}$, with δ large enough to account completely for the non-vanishing constraint body force.

As in Eq. (4.17), we suppose that for any sufficiently large $\mathcal{A}$, we have

$$\boldsymbol{\mathcal{F}}(\mathcal{A}) \approx -\int_{\mathcal{A}} p\mathbf{n} \, da. \tag{4.23}$$

If on the other hand the characteristic length scale of $\mathcal{A}$ is much smaller than the scale of boundary curvature and the scale at which the confinement body force varies, then as in Eqs. (4.17) and (4.18), we have

$$\boldsymbol{\mathcal{F}}(\mathcal{A}) \cdot \mathbf{x}_0 \approx \int_{\mathcal{A}_\delta} \rho \mathbf{b}_c \cdot \mathbf{x} \, dv \tag{4.24}$$

$$\boldsymbol{\mathcal{F}}(\mathcal{A}) \cdot \mathbf{x}_0 \approx -\int_{\mathcal{A}} p\mathbf{n} \cdot \mathbf{x} \, da \tag{4.25}$$

where $\mathbf{x}_0$ is the center of mass of $\mathcal{A}$. If we decompose the boundary into disjoint regions $\mathcal{A}_k$ characterized by the intermediate asymptotic length scale that satisfies the assumptions leading to Eqs. (4.23) and (4.25), then we can equate the two expressions in (4.24) and (4.25) and sum over k to obtain

$$-\int_{\partial\Omega} p\mathbf{n}\cdot\mathbf{x}\,da \approx \int_{\partial\Omega_\delta} \rho\mathbf{b}_c\cdot\mathbf{x}\,dv.$$

Again, the left-hand side is simply $-pVd$, so that we can express the pressure in terms of the confining body force:

$$p \approx -\frac{1}{dV}\int_{\partial\Omega_\delta} \rho\mathbf{b}_c\cdot\mathbf{x}\,dv. \tag{4.26}$$

Because the confining body force vanishes outside of $\partial\Omega_\delta$, we can extend the integral in Eq. (4.26) over all space $\mathbb{R}^d$ leading to

$$p \approx -\frac{1}{dV}\int_{\mathbb{R}^d} \rho\mathbf{b}_c\cdot\mathbf{x}\,dv. \tag{4.27}$$

As in the atomistic setting, we would like an expression of the homogeneous applied pressure p in terms of bulk variables. We therefore appeal now to the continuum version of the virial theorem, which makes use of the balance laws Eq. (4.21) (see Appendix A for a derivation):

$$0 = \int_{\mathbb{R}^d} \rho\mathbf{v}\cdot\mathbf{v}dv + \int_{\mathbb{R}^d} \rho\mathbf{b}\cdot\mathbf{x}\,dv - \int_{\mathbb{R}^d} \mathrm{tr}\ (\mathbf{T})\,dv,$$

where again the system is assumed to be in a steady state. Separating out the constraint part of the body force and using Eq. (4.27), we obtain

$$p = \frac{1}{Vd}\int_{\mathbb{R}^d} \left[\rho\mathbf{v}\cdot\mathbf{v} + \rho\left(\mathbf{b}-\mathbf{b}_c\right)\cdot\mathbf{x} - \mathrm{tr}\ (\mathbf{T})\right] dv.$$

Noting that the body force 4.14 derived via the Irving-Kirkwood procedure corresponds to $\mathbf{b}-\mathbf{b}_c$ and the microscopic expression for the stress tensor $\mathbf{T}$, it may be seen that Eq. (4.28) reproduces Eq. (4.20) for the ABP system assuming sufficiently small coarse-graining radius.

Note that in order to make contact with the standard picture in which the traction is given by the normal component of the stress at the boundary, we may assume that the constraint body force is a singular distribution supported on $\partial\Omega$. Then, in the event that the surface traction is homogeneous, we are free to reexpress this distribution as the divergence of an indicator function that is zero outside Ω and takes a constant value inside Ω. This constant term may then be added to the stress, and appears as an extra pressure. However, this may not be extended to scenarios with inhomogeneities, and therefore any continuum theory of ABPs that is able to deal with alignment and currents will have to incorporate activity via the body force, and not the stress tensor. Furthermore, it will be necessary to solve a coupled problem involving the momentum balance and the non-conservative director evolution equation.

4.4 Inclusion of Angular Momentum

In the analysis presented so far, we have derived balances of mass and linear momentum. In standard continuum mechanics, angular momentum appears only as the moment of linear momentum, and its balance simply imposes the symmetry of the stress tensor. Dahler and Scriven have proposed a more general paradigm of continuum mechanics in which microstructural features of a material introduce a separate, internal contribution to angular momentum, and thus the conservation of angular momentum provides a separate balance law for this internal angular momentum [62]. Moreover, the stress tensor need not in general be symmetric.

We will now restrict to two dimensions, and introduce equations of motion for the director. In two dimensions, we can exchange the unit director $\mathbf{d}_i$ for an angle θ_i relative to some fixed direction x, so that $\mathbf{d}_i = \cos\theta_i \mathbf{e}_x + \sin\theta_i \mathbf{e}_y$, where $\mathbf{e}_x$ and $\mathbf{e}_y$ are unit vectors in the x- and y-directions. Suppose that the particles have a significant moment of inertia, so that $\dot{\theta}_i$ contributes meaningfully to the angular momentum of the system. We can then model the evolution of the director with underdamped equations of motion:

$$\frac{d\theta_i}{dt} = I^{-1} L_i \tag{4.28}$$

$$\frac{dL_i}{dt} = \sum_j \tau_{ij}, \tag{4.29}$$

where I is the moment of inertia of a single ABP about its axis of rotation, L_i is the its angular momentum, and τ_{ij} is the torque applied to particle i by particle j.

Now the angular momentum density field can be written

$$\rho J(\mathbf{x}, t) = \sum_i \left(L_i + \mathbf{x}_i \times \mathbf{p}_i\right)\right) \Delta_i(\mathbf{x}) \tag{4.30}$$

where we abuse notation slightly by associating the cross-product of vectors with it's magnitude, as the cross product of two vectors in the $x - y$ plane always lies along the z-direction (equivalently we exploit the isomorphism between n-forms and $(d-n)$-forms). We will use the convention that $\mathbf{L}_i = L_i \mathbf{e}_z$.

we define the following densities:

$$\frac{I}{m} \rho \mathbf{w}(\mathbf{x}, t) = \sum_i \mathbf{L}_i \Delta_i(\mathbf{x}) \tag{4.31}$$

$$\rho \boldsymbol{\delta}(\mathbf{x}, t) = \sum_i m \boldsymbol{\delta}_i \Delta_i(\mathbf{x}) \tag{4.32}$$

$$\rho \boldsymbol{\iota}(\mathbf{x}, t) = \sum_i m \left[\boldsymbol{\delta}_i^2 \mathbb{1} - \boldsymbol{\delta}_i \otimes \boldsymbol{\delta}_i\right] \Delta_i(\mathbf{x}) \tag{4.33}$$

$$\rho \boldsymbol{\iota}(\mathbf{x}, t) \cdot \boldsymbol{\Omega}(\mathbf{x}, t) = \sum_i \boldsymbol{\delta}_i \times (\mathbf{p}_i - m\mathbf{v}) \Delta_i(\mathbf{x}), \tag{4.34}$$

where $\boldsymbol{\delta}_i = \mathbf{x}_i - \mathbf{x}$ measures the positions of particles relative to the material point $\mathbf{x}$, and $\boldsymbol{\iota}$ and $\boldsymbol{\Omega}$ are a moment of inertia and angular velocity which account for angular momentum about the axis of the continuum point. For large enough coarse-graining volume, we expect $\boldsymbol{\delta}$ to converge rapidly to zero, reflecting that the particles are distributed isotropically with respect to the center of mass.

The total angular momentum may now be decomposed as follows:

$$\rho \mathbf{J} = \rho \mathbf{x} \times \mathbf{v} + \rho \boldsymbol{\delta} \times \mathbf{v} + \rho \boldsymbol{\iota} \cdot \boldsymbol{\Omega} + \frac{I}{m} \rho \mathbf{w}. \tag{4.35}$$

Here, $\rho \mathbf{x} \times \mathbf{v}$ is simply the moment of linear momentum. The second and third terms in Eq. (4.35) account for the spatial microstructure of a continuum point, with $\rho\boldsymbol{\delta}\times\mathbf{v}$ accounting for the difference between the continuum point $\mathbf{x}$ and the center of mass of the particles in the coarse-graining region centered at $\mathbf{x}$, and $\rho\boldsymbol{\iota} \cdot \boldsymbol{\Omega}$ for the angular momentum about $\mathbf{x}$ remaining after transforming to the frame $\mathbf{v}$ defined by the continuum velocity. The final term $Im^{-1}\rho\mathbf{w}$ accounts for the internal angular momentum of the ABPs, a second kind of microstructural feature. Only the first and fourth terms should be expected to contribute significantly if the coarse-graining volume is large enough, so we only analyze the fourth term. Full balance equations may be found in [63].

The internal angular momentum evolves as follows:

$$\begin{aligned}
\frac{I}{m}\frac{\partial}{\partial t}(\rho w) &= \mathcal{F} \sum_i L_i \Delta_i(\mathbf{x}) \\
&= \sum_i \sum_j \tau_{ij} \Delta_i(\mathbf{x}) + \sum_i \left(\frac{\mathbf{p}_i}{m} \cdot \frac{\partial}{\partial \mathbf{x}_i} \right) L_i \Delta_i(\mathbf{x}) \\
&= \sum_{ij} \tau_{ij} \Delta_i(\mathbf{x}) - \frac{\partial}{\partial \mathbf{x}} \cdot \sum_i \frac{\mathbf{p}_i}{m} L_i \Delta_i(\mathbf{x}).
\end{aligned}$$

As in the case of linear momentum, we apply Noll's formula and split the final term into mean and deviatoric parts:

$$\begin{aligned}
\sum_{ij} \tau_{ij} \Delta_i(x) &= -\frac{\partial}{\partial \mathbf{x}} \cdot \frac{1}{2} \sum_{ij} b_{ij} \mathbf{x}_{ij} \tau_{ij} \\
\sum_i \frac{\mathbf{p}_i}{m} L_i \Delta_i(\mathbf{x}) &= \sum_i \left(\frac{\mathbf{p}_i - m\mathbf{v}}{m} \right) (L_i - Iw)\, \Delta_i(\mathbf{x}) + \frac{I}{m} \rho \mathbf{v} w.
\end{aligned}$$

Using balance of mass and plugging in the above expressions:

$$\begin{aligned}
\frac{I}{m} \rho \frac{Dw}{Dt} &= \frac{I}{m} \frac{\partial}{\partial t}(\rho w) + \frac{I}{m} \frac{\partial}{\partial \mathbf{x}} \cdot (\mathbf{v} \rho w) \\
&= \frac{\partial}{\partial \mathbf{x}} \cdot \left[-\frac{1}{2} \sum_{ij} b_{ij} \mathbf{x}_{ij} \tau_{ij} - \sum_i \left(\frac{\mathbf{p}_i - m\mathbf{v}}{m} \right) (L_i - Iw)\, \Delta_i(\mathbf{x}) \right],
\end{aligned}$$

and we have the partial balance equation

$$\frac{I}{m}\rho\frac{Dw}{Dt} = \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{C}_1, \tag{4.36}$$

with couple stress vector

$$\mathbf{C}_1 = -\frac{1}{2}\sum_{ij} b_{ij}\mathbf{x}_{ij}\tau_{ij} - \sum_i \left(\frac{\mathbf{p}_i - m\mathbf{v}}{m}\right)(L_i - Iw). \tag{4.37}$$

In the event that this couple stress does not vanish, the stress tensor need not be symmetric. Thus this is the microscopic expression that must be evaluated in any simulation to determine whether a particular system provides a realization of the model of Dahler and Scriven.

4.5 Director Field Evolution

If we introduce equations of motion for the director degrees of freedom, we can apply the Irving-Kirkwood procedure to examine the dynamics of the coarse-grained director field. We must introduce another coarse-grained field, the angular momentum density:

$$\frac{I}{m}\rho(\mathbf{x})\mathbf{w}(\mathbf{x}) = \sum_i \mathbf{L}_i\Delta_i(\mathbf{x}). \tag{4.38}$$

We will work in two regimes, angularly over- and under-damped.

Underdamped Case

In this case we have the microscopic dynamics

$$\frac{d\theta_i}{dt} = I^{-1}\mathbf{L}_i \cdot \mathbf{e}_z \tag{4.39}$$

$$\frac{d\mathbf{L}_i}{dt} = -\frac{\xi_r}{I}\mathbf{L}_i + \left(\tau + \sum_j \tau_{ij}\right)\mathbf{e}_z \tag{4.40}$$

where τ is an active torque applied to each particle and τ_{ij} are interparticle torques.

$$\begin{aligned}
\frac{\partial}{\partial t}(\rho\mathbf{d}) &= \mathcal{F}\sum_i \mathbf{e}_i\Delta_i(\mathbf{x}) = \sum_i \frac{\mathbf{p}_i}{m}\cdot\frac{\partial}{\partial \mathbf{x}_i}\left[\mathbf{e}_i\Delta_i(\mathbf{x})\right] + \sum_i \frac{L_i}{I}\frac{\partial}{\partial\theta_i}\mathbf{e}_i\Delta_i(\mathbf{x}) \\
&= -\frac{\partial}{\partial \mathbf{x}}\cdot\sum_i \frac{\mathbf{p}_i}{m}\otimes\mathbf{e}_i\Delta_i(\mathbf{x}) + \sum_i \frac{L_i}{I}\tilde{\mathbf{e}}_i\Delta_i(\mathbf{x}) \\
&= -\frac{\partial}{\partial \mathbf{x}}\cdot\sum_i\left(\frac{\mathbf{p}_i}{m}-\mathbf{v}\right)\otimes\mathbf{e}_i\Delta_i(\mathbf{x}) - \frac{\partial}{\partial \mathbf{x}}\cdot\sum_i \mathbf{v}\otimes\mathbf{e}_i\Delta_i(\mathbf{x}) \\
&\quad + \sum_i\left(\frac{L_i}{I}-w\right)\tilde{\mathbf{e}}_i\Delta_i(\mathbf{x}) + \sum_i w\tilde{\mathbf{e}}_i\Delta_i(\mathbf{x}) \\
&= -\frac{\partial}{\partial \mathbf{x}}\cdot\sum_i\left(\frac{\mathbf{p}_i}{m}-\mathbf{v}\right)\otimes\mathbf{e}_i\Delta_i(\mathbf{x}) - \frac{\partial}{\partial \mathbf{x}}\cdot(\rho\mathbf{v}\otimes\mathbf{d}) + \sum_i\left(\frac{L_i}{I}-w\right)\tilde{\mathbf{e}}_i\Delta_i(\mathbf{x}) + \rho w\tilde{\mathbf{d}}
\end{aligned} \tag{4.41}$$

where we have used a tilde to denote a vector rotated by $\pi/2$ counterclockwise. Then we can evaluate the total time derivative:

$$\begin{aligned}
\rho\frac{D\mathbf{d}}{Dt} &= \frac{\partial}{\partial t}(\rho\mathbf{d}) + \frac{\partial}{\partial \mathbf{x}}\cdot(\rho\mathbf{v}\otimes\mathbf{d}) \\
&= -\frac{\partial}{\partial \mathbf{x}}\cdot\sum_i\left(\frac{\mathbf{p}_i}{m}-\mathbf{v}\right)\otimes\mathbf{e}_i\Delta_i(\mathbf{x}) + \sum_i\left(\frac{L_i}{I}-w\right)\tilde{\mathbf{e}}_i\Delta_i(\mathbf{x}) + \rho w\tilde{\mathbf{d}} \\
&= -\frac{\partial}{\partial \mathbf{x}}\cdot\sum_i\left(\frac{\mathbf{p}_i}{m}-\mathbf{v}\right)\otimes\mathbf{e}_i\Delta_i(\mathbf{x}) + \sum_i\left(\frac{L_i}{I}-w\right)\left(\tilde{\mathbf{e}}_i-\tilde{\mathbf{d}}\right)\Delta_i(\mathbf{x}) + \rho w\tilde{\mathbf{d}}.
\end{aligned} \tag{4.42}$$

Overdamped and Averaged Case

In this case, we have the angular dynamics

$$\frac{d\theta_i}{dt} = \mu\tau + \mu\sum_j \tau_{ij} + \mu\alpha_r Z_i(t), \tag{4.43}$$

where μ is an angular mobility and Z_i are independent delta-correlated Gaussian processes. We also define fields in terms of noise averages:

$$\rho = \left\langle \sum_i m\Delta_i(\mathbf{x})\right\rangle \qquad \rho\mathbf{v} = \left\langle \sum_i m\frac{d\mathbf{x}_i}{dt}\Delta_i(\mathbf{x})\right\rangle \qquad \rho\mathbf{d} = \left\langle \sum_i \mathbf{e}_i\Delta_i(\mathbf{x})\right\rangle, \tag{4.44}$$

where we use $\dfrac{d\mathbf{x}_i}{dt}$ in place of $\mathbf{p}_i$ in order to allow for either over- or under-damped linear dynamics. The director density dynamics is then

$$\begin{aligned}\frac{\partial}{\partial t}(\rho\mathbf{d}) &= \left\langle \sum_i \frac{d\mathbf{x}_i}{dt}\cdot\frac{\partial}{\partial \mathbf{x}_i}\left[\mathbf{e}_i\Delta_i(\mathbf{x})\right]\right\rangle + \left\langle \sum_i \frac{d\theta_i}{dt}\frac{\partial}{\partial\theta_i}\left[\mathbf{e}_i\Delta_i(\mathbf{x})\right]\right\rangle \\ &= -\frac{\partial}{\partial\mathbf{x}}\cdot\left\langle\sum_i \frac{d\mathbf{x}_i}{dt}\otimes\mathbf{e}_i\Delta_i(\mathbf{x})\right\rangle + \left\langle \sum_i\left(\mu\tau + \mu\sum_j \tau_{ij} + \mu\alpha_r Z_i\right)\tilde{\mathbf{e}}_i\Delta_i(\mathbf{x})\right\rangle \\ &= -\frac{\partial}{\partial\mathbf{x}}\cdot\left\langle\sum_i \frac{d\mathbf{x}_i}{dt}\otimes\mathbf{e}_i\Delta_i(\mathbf{x})\right\rangle + \mu\tau\rho\tilde{\mathbf{d}} + \mu\left\langle\sum_{ij}\tau_{ij}\tilde{\mathbf{e}}_i\Delta_i(\mathbf{x})\right\rangle + \mu\alpha_r\left\langle\sum_i Z_i\tilde{\mathbf{e}}_i\Delta_i(\mathbf{x})\right\rangle.\end{aligned} \tag{4.45}$$

We need the mass balance in this form as well:

$$\frac{D\rho}{Dt} = \frac{\partial\rho}{\partial t} + \mathbf{v}\cdot\frac{\partial\rho}{\partial\mathbf{x}} = \left\langle\sum_i m\frac{d\mathbf{x}_i}{dt}\cdot\frac{\partial}{\partial\mathbf{x}_i}\Delta_i(\mathbf{x})\right\rangle + \mathbf{v}\cdot\frac{\partial\rho}{\partial\mathbf{x}} = -\frac{\partial}{\partial\mathbf{x}}\cdot(\rho\mathbf{v}) + \mathbf{v}\cdot\frac{\partial\rho}{\partial\mathbf{x}} = -\rho\left(\frac{\partial}{\partial\mathbf{x}}\cdot\mathbf{v}\right), \tag{4.46}$$

as in the non-averaged case. Now the total time derivative of the director field is

$$\rho\frac{D\mathbf{d}}{Dt} = -\frac{\partial}{\partial\mathbf{x}}\cdot\left\langle\sum_i\left(\frac{d\mathbf{x}_i}{dt} - \mathbf{v}\right)\otimes\mathbf{e}_i\Delta_i(\mathbf{x})\right\rangle + \mu\tau\rho\tilde{\mathbf{d}} + \mu\left\langle\sum_{ij}\tau_{ij}\tilde{\mathbf{e}}_i\Delta_i(\mathbf{x})\right\rangle + \mu\alpha_r\left\langle\sum_i Z_i\tilde{\mathbf{e}}_i\Delta_i(\mathbf{x})\right\rangle. \tag{4.47}$$

Picking some initial time $t = 0$ far in the past, we can write

$$\begin{aligned}\mathbf{e}_i(t) &= \mathbf{e}_i(0) + \int_0^t \frac{d\mathbf{e}_i}{dt'}dt' = \mathbf{e}_i(0) + \int_0^t \frac{d\mathbf{e}_i}{d\theta_i}\frac{d\theta_i}{dt'}dt' \\ &= \mathbf{e}_i(0) + \mu\tau\int_0^t\tilde{\mathbf{e}}_i dt' + \mu\sum_j\int_0^t\tilde{\mathbf{e}}_i\tau_{ij}dt' + \mu\alpha_r\int_0^t\tilde{\mathbf{e}}_i Z_i(t')dt'.\end{aligned} \tag{4.48}$$

Then:

$$\begin{aligned}\left\langle\mu\alpha_r\sum_i Z_i\tilde{\mathbf{e}}_i\Delta_i(\mathbf{x})\right\rangle &= \left\langle\mu\alpha_r\sum_i Z_i(t)\left[-\mu\alpha_r\int_0^t\mathbf{e}_i Z_i(t')dt'\right]\Delta_i(\mathbf{x})\right\rangle \\ &= -\mu^2\alpha_r^2\rho\mathbf{d},\end{aligned} \tag{4.49}$$

where we have exploited the fact that $Z_i(t)$ is uncorrelated with any variable at an earlier time and used the delta-correlation property. Now we finally have

$$\rho\frac{D\mathbf{d}}{Dt} = -\mu^2\alpha_r^2\rho\mathbf{d} + \mu\tau\rho\tilde{\mathbf{d}} + \boldsymbol{\mathcal{A}} - \frac{\partial}{\partial\mathbf{x}}\cdot\mathbf{J}_d, \tag{4.50}$$

where

$$\mathbf{J}_d = \left\langle\sum_i\left(\frac{d\mathbf{x}_i}{dt} - \mathbf{v}\right)\otimes\mathbf{e}_i\Delta_i(\mathbf{x})\right\rangle \tag{4.51}$$

$$\boldsymbol{\mathcal{A}} = \mu \left\langle \sum_{ij} \tau_{ij} \tilde{\mathbf{e}}_i \Delta_i(\mathbf{x}) \right\rangle . \tag{4.52}$$

Suppose that the system of ABPs is homogeneous and in a steady state. Then the director evolution equation (4.50) reduces to

$$0 = -\mu^2 \alpha_r^2 \rho \mathbf{d} + \mu \tau \rho \tilde{\mathbf{d}} + \boldsymbol{\mathcal{A}}. \tag{4.53}$$

In the absence of inter-particle aligning interactions, $\tau_{ij} = 0$ and therefore $\boldsymbol{\mathcal{A}}$ is identically zero. Using $\mathbf{d} \cdot \tilde{\mathbf{d}} = 0$, we see that the only solution is $\mathbf{d} = \mathbf{0}$. Homogeneity and time-independence also imply that $\mathbf{b} = \mathbf{0}$ via the linear momentum balance equation. For large enough coarse-graining volume, $\boldsymbol{\mathcal{W}}$ vanishes, so this in turn implies $\mathbf{v} = \mathbf{0}$, demonstrating that nonzero steady-state currents are impossible in homogeneous systems of ABPs without aligning interactions.

In the presence of inter-particle aligning interactions, suppose that $\mathbf{d} \neq \mathbf{0}$. The angular noise is symmetric with respect to $\mathbf{d}$, i.e., the distribution of particle directors about $\mathbf{d}$ is symmetric with respect to reflection over $\mathbf{d}$. The particles whose directors point to the left of $\mathbf{d}$ will have a torque with negative component in the z direction, while those pointing to the right a positive torque. Thus, in the sum that defines $\boldsymbol{\mathcal{A}}$, the components of the various $\tilde{\mathbf{e}}_i$ in the direction orthogonal to $\mathbf{d}$ will tend to cancel, while the components in the direction of $\mathbf{d}$ will tend to add constructively, giving rise to a nonzero $\boldsymbol{\mathcal{A}}$ in the direction of $\mathbf{d}$, i.e. in opposition to the diffusion-induced decay. Thus, the existence of nonzero steady currents with $\mathbf{v} = \mathbf{0}$ in homogeneous systems of ABPs is possible.

It is also possible to study systems with boundaries that apply torques to the particles, and in such systems, currents could be expected to appear close to the boundary even in the absence of interparticle aligning interactions. However, our analysis suggests that this effect will persist only in the near-boundary region, and will be negligible deep in the bulk of sufficiently large systems. Noninteracting ABPs in boundary-less regions will not display bulk currents. On the other hand, we expect that in the presence of interparticle alignment, ABPs may display bulk currents that spontaneously break rotational symmetry, even in the absence of boundaries. Addition of boundaries with aligning interactions could then be used to select the direction of bulk currents in arbitrarily large systems.

Chapter 5

Conclusion

The main results of this thesis are as follows. I have derived Green-Kubo equations for the components of the viscosity in two-dimensional fluids with and without internal angular momentum, demonstrating the connection between time-reversal symmetry breaking and the emergence of odd viscosity. Numerical verification of the Green-Kubo equation for odd viscosity supports the case for applying the Onsager regression hypothesis to fluctuations about a nonequilibrium steady states. I have also demonstrated the potential for a new rotational viscosity coefficient in fluids in which equipartition is broken. I also performed a coarse-graining analysis of Active Brownian Particles in the spirit of Irving and Kirkwood. This established that in such systems, activity manifests at the continuum level in the form of a body force, rather than in the stress tensor, previously assumed. Together, these results guide the program of devising continuum equations to describe the behavior of systems of active matter, and elucidate the consequences of time-reversal symmetry breaking on the rheological properties of macroscopic systems.

This thesis represents a series of analyses of increasingly complex fluids, beginning with a simple fluid without internal structure, and moving on to include internal spin and a director degree of freedom. A natural next step, which is underway but not complete, is the extension of the methods used here to study active liquid crystals. These are fluids that have a nematic degree of freedom along which an active force is applied. Such models provide simplified pictures of the dynamics of bacterial colonies, which have been fruitfully studied through an active matter lens as in [20].

In the standard Leslie-Ericksen model of liquid crystals, the viscous stress tensor has six undetermined coefficients [64, 65, 66, 67]. Applying the same reasoning as that traditionally used to connect odd viscosity to time-reversal symmetry breaking, Parodi has proposed a relation between these coefficients that is satisfied for fluids at local equilibrium, reducing the number of free parameters to five [68]. This argument suffers from the same conceptual flaw discussed in Chapter 2. We hypothesize that the Parodi relation should be recoverable via a Green-Kubo type analysis of the sort we have used to replace the erroneous application of the Onsager reciprocal relations.

Another direction for future research is to combine the viscous or mechanical phenomena explored here with other thermodynamical transport phenomena, such as diffusion, and explore the effects of time-reversal symmetry breaking in such systems. Odd diffusivity, an antisymmetric component of the diffusivity tensor, is allowed in time-reversal asymmetric systems by Onsager's reciprocal relations (applicable here because diffusion is a truly thermodynamical process to which entropy considerations apply). Combining such effects with viscous phenomena would allow the study of systems of mixed active and passive particles at the continuum level.

Appendix A

Virial Theorems

In this appendix, we provide derivations of the atomistic and continuum virial theorems. Both are well-known, and in particular the atomistic version may be found in many introductions to classical mechanics, e.g. [69].

Atomistic

For a system of particles with positions $\mathbf{x}_i$, the second moment of the mass distribution takes the form

$$\mathbf{R}_2 = \sum_i (\mathbf{x}_i - \mathbf{x}_{\mathrm{cm}}) \otimes (\mathbf{x}_i - \mathbf{x}_{\mathrm{cm}}), \tag{A.1}$$

with $\mathbf{x}_{\mathrm{cm}}$ the center of mass. Taking the second time-derivative, we find

$$\frac{d^2}{dt^2}\mathbf{R}_2 = 2\sum_i \left[\left(\frac{d^2\mathbf{x}_i}{dt^2} - \frac{d^2\mathbf{x}_{\mathrm{cm}}}{dt^2} \right) \otimes (\mathbf{x}_i - \mathbf{x}_{\mathrm{cm}}) + \left(\frac{d\mathbf{x}_i}{dt} - \frac{d\mathbf{x}_{\mathrm{cm}}}{dt} \right) \otimes \left(\frac{d\mathbf{x}_i}{dt} - \frac{d\mathbf{x}_{\mathrm{cm}}}{dt} \right) \right]^{\mathrm{sym}}, \tag{A.2}$$

where the superscript denotes taking the symmetric part of the tensor. Assuming that the system is in a steady state, then we should have $d^2\mathbf{R}_2/dt^2 = 0$, where brackets indicate time- or ensemble-averaging. Moreover, the center of mass should be approximately constant, and we may as well choose coordinates such that $\mathbf{x}_{\mathrm{cm}} = 0$. Then

$$0 = \left\langle \sum_i \left[\frac{d^2\mathbf{x}_i}{dt^2} \otimes \mathbf{x}_i + \frac{d\mathbf{x}_i}{dt} \otimes \frac{d\mathbf{x}_i}{dt} \right]^{\mathrm{sym}} \right\rangle. \tag{A.3}$$

Using the equations of motion $d\mathbf{x}_i/dt = \mathbf{p}_i/m$ and $d\mathbf{p}_i/dt = \mathbf{f}_i$ and taking the trace of Eq. (A.3), we find

$$\left\langle \sum_i \mathbf{f}_i \cdot \mathbf{x}_i + \sum_i \frac{\mathbf{p}_i \cdot \mathbf{p}_i}{m} \right\rangle = 0. \tag{A.4}$$

Continuum

Proceeding in the same manner as in the atomistic case, we define the second moment of the mass distribution:

$$\mathbf{R}_2 = \int_{\mathbb{R}^d} \rho \left(\mathbf{x} - \mathbf{x}_{\rm cm}\right) \otimes \left(\mathbf{x} - \mathbf{x}_{\rm cm}\right) dv, \tag{A.5}$$

where $\mathbf{x}_{\rm cm}$ is again the center of mass. We consider the fields to be defined on all of space $\mathbb{R}^d$, and to vanish at infinity. In steady-state, we again set $\mathbf{x}_{\rm cm} = 0$. Then, taking the second time-derivative and using the continuum equations of motion

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= -\frac{\partial}{\partial \mathbf{x}} \cdot (\rho \mathbf{v}) \\ \rho \frac{\partial \mathbf{v}}{\partial t} &= \rho \mathbf{b} + \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{T} - \rho \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}} \mathbf{v} \end{aligned} \tag{A.6}$$

we find

$$\begin{aligned} \frac{d^2}{dt^2}\mathbf{R}_2 &= \frac{d^2}{dt^2} \int_{\mathbb{R}^d} \rho \mathbf{x} \otimes \mathbf{x}\, dv \\ &= \frac{d}{dt} \int_{\mathbb{R}^d} \frac{\partial \rho}{\partial t} \mathbf{x} \otimes \mathbf{x}\, dv \\ &= -\frac{d}{dt} \int_{\mathbb{R}^d} \left[\frac{\partial}{\partial \mathbf{x}} \cdot (\rho \mathbf{v})\right] \mathbf{x} \otimes \mathbf{x}\, dv \\ &= -\int_{\mathbb{R}^d} \left[\frac{\partial}{\partial \mathbf{x}} \cdot \left(\frac{\partial \rho}{\partial t}\mathbf{v} + \rho \frac{\partial \mathbf{v}}{\partial t}\right)\right] \mathbf{x} \otimes \mathbf{x}\, dv \\ &= \int_{\mathbb{R}^d} \left(\frac{\partial \rho}{\partial t}\mathbf{v} + \rho \frac{\partial \mathbf{v}}{\partial t}\right) \cdot \frac{\partial}{\partial \mathbf{x}} (\mathbf{x} \otimes \mathbf{x})\, dv \\ &= 2 \int_{\mathbb{R}^d} \left(\frac{\partial \rho}{\partial t}\mathbf{v} + \rho \frac{\partial \mathbf{v}}{\partial t}\right) \otimes \mathbf{x}\, dv \\ &= 2 \int_{\mathbb{R}^d} \left(-\left(\frac{\partial}{\partial \mathbf{x}} \cdot (\rho \mathbf{v})\right) \mathbf{v} + \rho \mathbf{b} + \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{T} - \rho \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}} \mathbf{v}\right) \otimes \mathbf{x}\, dv \\ &= 2 \int_{\mathbb{R}^d} \left(-\frac{\partial}{\partial \mathbf{x}} \cdot (\rho \mathbf{v} \otimes \mathbf{v}) + \rho \mathbf{b} + \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{T}\right) \otimes \mathbf{x}\, dv \\ &= -2 \int_{\mathbb{R}^d} \frac{\partial}{\partial \mathbf{x}} \cdot (\rho \mathbf{v} \otimes \mathbf{v}) \otimes \mathbf{x}\, dv + d \int_{\mathbb{R}^d} \rho \mathbf{b} \otimes \mathbf{x}\, dv + 2 \int_{\mathbb{R}^d} \left(\frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{T}\right) \otimes \mathbf{x}\, dv \\ &= 2 \int_{\mathbb{R}^d} \rho \mathbf{v} \otimes \mathbf{v}\, dv + 2 \int_{\mathbb{R}^d} \rho \mathbf{b} \otimes \mathbf{x}\, dv - 2 \int_{\mathbb{R}^d} \mathbf{T}\, dv, \end{aligned} \tag{A.7}$$

where we have repeatedly integrated by parts, assuming that all fields vanish at infinity. Setting $d^2\mathbf{R}_2/dt^2 = 0$ and taking the trace, we find the continuum version of the virial theorem to be

$$\int_{\mathbb{R}^d} \rho \mathbf{v} \cdot \mathbf{v} dv + \int_{\mathbb{R}^d} \rho \mathbf{b} \cdot \mathbf{x}\, dv - \int_{\mathbb{R}^d} \text{tr } (\mathbf{T}) dv = 0. \tag{A.8}$$

Appendix B

Representation of Isotropic Tensors

It is well known that the pair $(\boldsymbol{\delta}, \boldsymbol{\epsilon})$, where $\boldsymbol{\delta}$ is the rank two Kronecker tensor and $\boldsymbol{\epsilon}$ is the rank n Levi-Civita or fully antisymmetric tensor, generate all isotropic tensors on dimension n. Recall that the components of these tensors are

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j, \end{cases} \tag{B.1}$$

and

$$\epsilon_{i_1 \ldots i_n} = \begin{cases} 1 & i_1 \ldots i_n \text{ even permutation of } 1 \ldots \text{n} \\ -1 & i_1 \ldots i_n \text{ odd permutation of } 1 \ldots \text{n} \\ 0 & \text{otherwise.} \end{cases} \tag{B.2}$$

The sense in which these are generators is made clearer by the graphical calculus frequently used for tensor manipulation in the tensor network community, see for example [70] for an introduction to this streamlined language. Briefly, rank m tensors are represented by boxes with m "legs", each representing one of the indices. Connecting two legs corresponds to identifying the corresponding indices and performing a summation over all possible values of the index, so that for example the scalar product of two rank four tensors is represented pictorially by the diagram in Fig. 1a. The absence of "free legs" indicates that this is indeed a scalar. In this graphical language, the representation theorem is simple to state: a basis for the isotropic tensors of order m in n dimensions may be obtained by contracting m indexed legs with copies of the $\boldsymbol{\delta}$ and $\boldsymbol{\epsilon}$ tensors in all possible ways, which we may visualize as in Fig. 1b. For example, in two dimensions we can construct the isotropic rank four tensors drawn in Fig. 1c, which are written in component notation as $\delta_{ij}\epsilon_{kl}$, $\delta_{il}\delta_{kj}$, and $\delta_{ik}\delta_{jl}$. We note the curious circumstance, due to the fact that viscosity is rank four and the Levi-Civita tensor is rank n, that only in dimensions two and four is there a possibility of a component of the viscosity manifesting breaking of mirror symmetry.

Proofs of the fact that $\boldsymbol{\delta}$ and $\boldsymbol{\epsilon}$ tensors generate all isotropic tensors in dimension n appear in both [71] and [72], but the former reference proves a more general theorem using

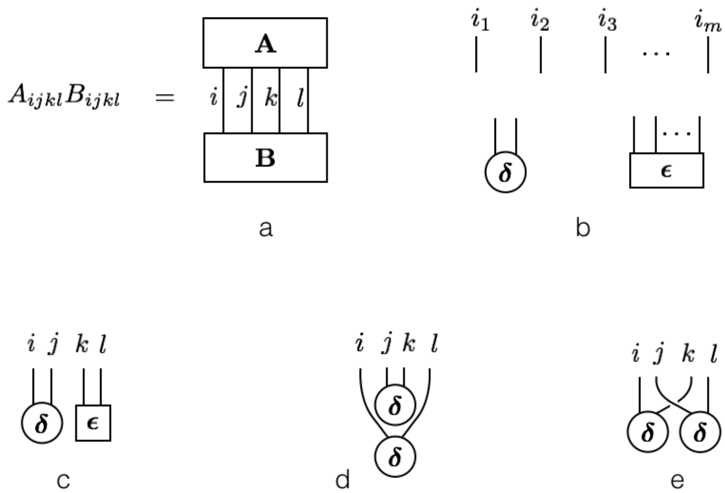

Figure B.1: In (a) the scalar product of two fourth-order tensors is represented graphically. In (b) the components for the construction of a basis for all m^{th}-order isotropic tensors in some dimension n are presented. The idea is that the indexed legs should be connected with copies of the two generator tensors $\boldsymbol{\delta}$ and $\boldsymbol{\epsilon}$. The set of all possible such diagrams spans the space of isotropic tensors. The tensor $\delta_{ij}\epsilon_{kl}$ is represented graphically in (c), $\delta_{il}\delta_{jk}$ in (d), and $\delta_{ik}\delta_{jl}$ in (e). Note that the "crossing" of the two legs in the third diagram is purely for visual convenience. There is no difference between "left over right" and "right over left".

more powerful machinery, while the latter is (for the authors) somewhat difficult to follow. We provide here for convenience a compact proof. The essential idea is simply that the two geometrical quantities that are preserved by rotations of n-dimensional Euclidean space are the inner product between pairs of vectors and the signed volume of the parallelepiped spanned by n vectors. These correspond to the tensors $\boldsymbol{\delta}$ and $\boldsymbol{\epsilon}$. The only point that must be verified is that nothing else is preserved. We approach the proof in three steps.

Let $v_1, \ldots, v_m$ and $u_1, \ldots, u_m$ be ordered m-tuples of vectors in $\mathbb{R}^n$. Let $\langle w_1, w_2 \rangle$ denote the inner product of vectors w_1 and w_2 and $[w_1, w_2, \ldots, w_n]$ denote the determinant of the matrix whose i^{th} column is w_i. Then the following hold:

1. *If $\langle v_i, v_j \rangle = \langle u_i, u_j \rangle$ for all i, j, then for some $Q \in O(n)$ we have $u_i = Qv_i$ for all i.*
2. *If moreover $[v_{i_1}, v_{i_2}, \ldots, v_{i_n}] = [u_{i_1}, u_{i_2}, \ldots, u_{i_n}]$ for all n-tuples of index assignments, then for some $Q \in SO(n)$ we have $u_i = Qv_i$ for all i.*

We can establish this result by making use of the notion of Gram-Schmidt orthogonalization. Consider forming the $n \times n$ matrix E_0 as follows:

1. Begin by setting E_0 equal to the $n \times 1$ column vector v_1.
2. For i from 2 to m, check whether v_i is in the column space of E_0, and if it is not, append v_i as the right-most column of E_0.
3. If E_0 has fewer than n columns, append columns to the right such that the column space of E_0 is $\mathbb{R}^n$.

Now we may define an orthogonal matrix $E \in O(n)$ by performing Gram-Schmidt orthogonalization on the columns of E_0. Let the columns of E be denoted by e_α, $\alpha = 1, 2, \ldots n$. The $n \times m$ matrix V with columns v_i may then be expressed as $V = EM$, where $M_{\alpha j} = \langle e_\alpha, v_j \rangle$.

We may proceed analogously with the u_i to define matrices $\tilde{E}$, $\tilde{M}$, and U such that $U = \tilde{E}\tilde{M}$. Because the inner products $\langle e_\alpha, v_j \rangle$ and $\langle \tilde{e}_\alpha, u_j \rangle$ depend only on pairwise inner products of the v_i and the u_i, respectively, we may conclude that $M = \tilde{M}$. Then $U = \tilde{E}M = \tilde{E}E^T EM = \tilde{E}E^T V \equiv QV$, so that $u_i = \tilde{E}E^T v_i$ for all i. Because E and $\tilde{E}$ (and their transposes) are orthogonal, so is $Q = \tilde{E}E^T$, establishing the first point above.

In order to establish the second point, we need to consider the determinant of $Q = \tilde{E}E^T$. Because orthogonal matrices have determinant ± 1 and the Gram-Schmidt procedure uses matrix column operations that do not change the sign of the determinant, we have

$$\det E = \operatorname{sgn} \det E_0 \tag{B.3}$$

$$\det \tilde{E} = \operatorname{sgn} \det \tilde{E}_0. \tag{B.4}$$

Then $\tilde{E}E^T \in SO(n)$ if and only if $\det E = \det \tilde{E}$.

If the v_i and u_i independently span $\mathbb{R}^n$, then all of the columns of E_0 and $\tilde{E}_0$ are members of these sets of vectors. Then the determinants are equal if and only if $[v_{i_1}, v_{i_2}, \ldots, v_{i_n}] = [u_{i_1}, u_{i_2}, \ldots, u_{i_n}]$ for all choices $i_1, \ldots, i_n$. If the v_i and u_i do not span $\mathbb{R}^n$, we are free to choose the extra basis vectors, so may arrange to have $\det(\tilde{E}E^T) = 1$. In this situation, $[v_{i_1}, v_{i_2}, \ldots, v_{i_n}] = [u_{i_1}, u_{i_2}, \ldots, u_{i_n}] = 0$. This establishes the second point above.

This fact allows us to prove the following:

Suppose that f is a function of m-tuples of vectors in $\mathbb{R}^n$ that is invariant under the orthogonal group $O(n)$ in the sense that $f(Qv_1, \ldots, Qv_n) = f(v_1, \ldots, v_n)$ for any $Q \in O(n)$. Then f can be expressed as a function of the pairwise inner products $\langle v_i, v_j \rangle$. If f is only required to be invariant under the special orthogonal group $SO(n)$, then f may be expressed as a function of the pairwise inner products $\langle v_i, v_j \rangle$ and the determinants $[v_{i_n}, \ldots, v_{i_n}]$.

Let f be invariant under $O(n)$. Suppose that $\langle v_i, v_j \rangle = \langle u_i, u_j \rangle$ for all i, j and that $f(u_1, \ldots, u_m) \neq f(v_1, \ldots v_m)$. By the result given above, the equality of pairwise inner products implies that there is some $Q \in O(n)$ such that $u_i = Qv_i$ for all i. Then $f(Qv_1, \ldots, Qv_m) \neq f(v_1, \ldots, v_m)$. But this contradicts the assumption that f is invariant under $O(n)$. Therefore, f must be completely determined by the set of pairwise inner products $\langle v_i, v_j \rangle$.

Now let f be invariant under $SO(n)$ but not necessarily under all of $O(n)$. Suppose that $\langle v_i, v_j \rangle = \langle u_i, u_j \rangle$ and $[v_{i_n}, \ldots, v_{i_n}] = [u_{i_n}, \ldots, u_{i_n}]$ for all choices of index assignments $f(u_1, \ldots, u_m) \neq f(v_1, \ldots v_m)$. By the above result, there is some $Q \in SO(n)$ such that $u_i = Qv_i$ for all i, so $f(Qv_1, \ldots, Qv_m) \neq f(v_1, \ldots, v_m)$. Again, this leads to a contradiction, so f must be determined by the set of inner products and determinants.

Now we are equipped to prove the promised representation theorem:

Theorem 1 *Let T be an order m tensor on dimension n, in other words a multilinear map*

$$T : \underbrace{\mathbb{R}^n \otimes \mathbb{R}^n \otimes \cdots \otimes \mathbb{R}^n}_{m \text{ times}} \to \mathbb{R}. \tag{B.5}$$

Suppose that T is invariant under the special orthogonal group $SO(n)$ of proper rotations in the sense that for any $Q \in SO(n)$ and any $u_1, u_2, \ldots, u_m \in \mathbb{R}^n$, we have

$$T(Qu_1 \otimes Qu_2 \otimes \cdots \otimes Qu_m) = T(u_1 \otimes u_2 \otimes \cdots \otimes u_m). \tag{B.6}$$

Then T may be expressed as a linear combination of products of order 2 Kronecker tensors δ and at most one order n alternating/Levi-Civita tensors ϵ acting on disjoint sets of tensor factors (indices). If T is invariant under the entire orthogonal group $O(n)$, then it is expressible only in terms of Kronecker tensors.

By invariance under $SO(n)$, we can conclude using the previous result that $T(u_1 \otimes u_2 \otimes \cdots \otimes u_m)$ is determined completely the pairwise inner products $\langle u_i, u_j \rangle$ and volumes $[u_{i_1}, \ldots, u_{i_n}]$. For T to be linear in each of its arguments, this function must be a linear combination of products of inner products and volume forms in which each argument u_i appears exactly once. The inner product is given by $\langle u, v \rangle = \delta(u \otimes v)$ with δ the Kronecker tensor, and the volume form is given by $[u, v, \ldots, w] = \epsilon(u \otimes v \otimes \cdots \otimes w)$ with ϵ the alternating tensor. It is easy to see that the alternating tensor itself is odd under reflections so that a product of two alternating tensors on disjoint sets of indices is even. Then such products may be expressed solely in terms of Kronecker tensors. This establishes the first part of the theorem. If T is required to be invariant under $O(n)$, it can't contain any terms with an odd number of ϵ tensors, as these are odd under parity-inverting transformations. This establishes the second, and the representation theorem is proven.

This representation theorem provides a method for generating and studying the possible isotropic viscosity tensors, as we may use it to construct orthonormal bases for the full space of isotropic rank four tensors in two dimensions that diagonalize any symmetry of interest.

Basis Tensor	Components	$j \leftrightarrow l$	$ij \leftrightarrow kl$	P
$\mathbf{e}^{(1)}$	$\delta_{ij}\delta_{kl} - \epsilon_{ij}\epsilon_{kl}$	+	+	+
$\mathbf{e}^{(2)}$	$\epsilon_{ik}\epsilon_{jl}$	-	+	+
$\mathbf{e}^{(3)}$	$\delta_{ik}\delta_{jl}$	+	+	+
$\mathbf{e}^{(4)}$	$\epsilon_{ik}\delta_{jl}$	+	-	-
$\mathbf{e}^{(5)}$	$\epsilon_{ij}\delta_{kl} + \epsilon_{kl}\delta_{ij}$	+	+	-
$\mathbf{e}^{(6)}$	$\epsilon_{jl}\delta_{ik}$	-	-	-

Table B.1: Basis for the isotropic rank four tensors in two dimensions in which the index permutations $j \leftrightarrow l$ and $i \leftrightarrow k$, $j \leftrightarrow l$ are diagonal. Components of the viscosity odd under the former do not contribute to the momentum balance, while components odd under the latter contribute to the odd viscosity. The mirror transformation $(x_1, x_2) \mapsto (-x_1, x_2)$ is also diagonal in this basis. Note that the $+(-)$ indicates that the basis tensor is even (odd) under the indicated transformation. The basis tensors are orthogonal (but not normalized) with respect to the inner product $A_{ijkl}B_{ijkl}$.

In two dimensions, the space of isotropic rank four tensors is six-dimensional. Two different orthogonal bases (eigenbases for different sets of symmetries) for this space are presented in Tables B.1 and B.2.

Basis Tensor	Components	$i \leftrightarrow j$	$k \leftrightarrow l$	$ij \leftrightarrow kl$	P
$\mathbf{s}^{(1)}$	$\delta_{ij}\delta_{kl}$	$+$	$+$	$+$	$+$
$\mathbf{s}^{(2)}$	$\delta_{ik}\delta_{j\ell} - \epsilon_{ik}\epsilon_{jl}$	$+$	$+$	$+$	$+$
$\mathbf{s}^{(3)}$	$\epsilon_{ij}\epsilon_{kl}$	-	-	$+$	$+$
$\mathbf{s}^{(4)}$	$\epsilon_{ik}\delta_{j\ell} + \epsilon_{j\ell}\delta_{ik}$	$+$	$+$	-	-
$\mathbf{s}^{(5)}$	$\epsilon_{ik}\delta_{j\ell} - \epsilon_{j\ell}\delta_{ik} + \epsilon_{ij}\delta_{k\ell} + \epsilon_{k\ell}\delta_{ij}$	-	$+$	N/A	-
$\mathbf{s}^{(6)}$	$\epsilon_{ik}\delta_{j\ell} - \epsilon_{j\ell}\delta_{ik} - \epsilon_{ij}\delta_{k\ell} - \epsilon_{k\ell}\delta_{ij}$	$+$	-	N/A	-

Table B.2: Basis for the isotropic rank four tensors in two dimensions in which the index permutation $i \leftrightarrow j$, the permutation $k \leftrightarrow l$, and again the mirror transformation are diagonal. All but two of these basis elements are also eigenvectors of the permutation $i \leftrightarrow k$, $j \leftrightarrow l$, so where possible we also indicate the eigenvalue of the basis tensors under this symmetry. It is this basis we use for discussing the Green-Kubo relations presented in the main text.

Appendix C

Tensor Correlators

In this section we derive constraints on various correlation functions resulting from the assumption of isotropy. Let $\mathbf{s}$ and $\mathbf{t}$ be zero-mean random tensor fields, possibly of different rank, defined on a square box of side length L with periodic boundary conditions. These have Fourier components

$$\mathbf{s}_{\mathbf{k}} = \frac{1}{L^2} \int e^{-i\mathbf{k}\cdot\mathbf{x}}\, \mathbf{s}(\mathbf{x})\, d^2\mathbf{x} \tag{C.1}$$

and similarly for $\mathbf{t}$. Assuming that spatial correlations decay rapidly with separation, we may expand the correlations of Fourier modes as

$$\begin{aligned}
\langle \mathbf{s}_{\mathbf{k}} \otimes \mathbf{t}_{-\mathbf{k}} \rangle &= \frac{1}{L^4} \int e^{i\mathbf{k}\cdot(\mathbf{y}-\mathbf{x})} \langle \mathbf{s}(\mathbf{x}) \otimes \mathbf{t}(\mathbf{y}) \rangle\, d^2\mathbf{x}\, d^2\mathbf{y} \\
&= \frac{1}{L^4} \int \langle \mathbf{s}(\mathbf{x}) \otimes \mathbf{t}(\mathbf{y}) \rangle\, d^2\mathbf{x}\, d^2\mathbf{y} + \frac{ik^r}{L^4} \int (y^r - x^r) \langle \mathbf{s}(\mathbf{x}) \otimes \mathbf{t}(\mathbf{y}) \rangle\, d^2\mathbf{x}\, d^2\mathbf{y} \\
&\quad - \frac{k^r k^s}{2L^4} \int (y^r - x^r)(y^s - x^s) \langle \mathbf{s}(\mathbf{x}) \otimes \mathbf{t}(\mathbf{y}) \rangle\, d^2\mathbf{x}\, d^2\mathbf{y} + \mathcal{O}(k^3).
\end{aligned} \tag{C.2}$$

Assuming isotropy, the spatial correlators must satisfy $\langle \mathbf{Q}_s \mathbf{s}(\mathbf{Q}\mathbf{x}) \otimes \mathbf{Q}_t \mathbf{t}(\mathbf{Q}\mathbf{y}) \rangle = \langle \mathbf{s}(\mathbf{x}) \otimes \mathbf{t}(\mathbf{y}) \rangle$ for any proper rotation $\mathbf{Q}$ which acts on tensors of types $\mathbf{s}$ and $\mathbf{t}$ by $\mathbf{Q}_s$ and $\mathbf{Q}_t$. Using this relation, we can note that the Fourier-space correlator is isotropic to zeroth order in $\mathbf{k}$. To see that this is the case, consider any rotation $\mathbf{Q}$. The zeroth order term in the expansion satisfies:

$$\int \langle \mathbf{s}(\mathbf{x}) \otimes \mathbf{t}(\mathbf{y}) \rangle\, d^2\mathbf{x}\, d^2\mathbf{y} = \int \langle \mathbf{Q}_s \mathbf{s}(\mathbf{Q}\mathbf{x}) \otimes \mathbf{Q}_t \mathbf{t}(\mathbf{Q}\mathbf{y}) \rangle\, d^2\mathbf{x}\, d^2\mathbf{y} \tag{C.3}$$

$$= (\mathbf{Q}_s \otimes \mathbf{Q}_t) \int \langle \mathbf{s}(\mathbf{Q}\mathbf{x}) \otimes \mathbf{t}(\mathbf{Q}\mathbf{y}) \rangle\, d^2\mathbf{x}\, d^2\mathbf{y} \tag{C.4}$$

$$= (\mathbf{Q}_s \otimes \mathbf{Q}_t) \int \langle \mathbf{s}(\mathbf{x}) \otimes \mathbf{t}(\mathbf{y}) \rangle\, d^2\mathbf{x}\, d^2\mathbf{y}$$

where the first equality uses the assumption of isotropy of the spatial correlators, and the third uses the rotational invariance of the integration measure. One consequence of this zeroth-order isotropy is that the correlators $\langle \mathbf{s_k} \otimes \mathbf{t_{-k}} \rangle$ vanish to zeroth order in $\mathbf{k}$ if the difference between the ranks of $\mathbf{s}$ and $\mathbf{t}$ is odd, as there are no isotropic odd rank tensors in two dimensions. If $\mathbf{s} = \mathbf{t}$, then the zeroth order term is also symmetric. In particular, this means that the autocorrelator of $\mathbf{v_k}$ is proportional to the Kronecker tensor.

It will be convenient for the Green-Kubo analysis in the subsequent section to give compact notation for the lowest-order non-vanishing terms of the various correlators:

$$\left\langle v^j_{\mathbf{k}} v^k_{-\mathbf{k}} \right\rangle \approx \frac{1}{L^4} \int \left\langle \delta v^j(\mathbf{x}) \delta v^k(\mathbf{y}) \right\rangle d^2\mathbf{x}\, d^2\mathbf{y} := \mu \delta_{jk}, \tag{C.5}$$

$$\left\langle v^j_{\mathbf{k}} m_{-\mathbf{k}} \right\rangle \approx \frac{ik^r}{L^4} \int (y^r - x^r) \left\langle \delta v^j(\mathbf{x}) \delta m(\mathbf{y}) \right\rangle d^2\mathbf{x}\, d^2\mathbf{y} := \mathrm{i} k^r \Omega_{rj}, \tag{C.6}$$

$$\left\langle m_{\mathbf{k}} v^k_{-\mathbf{k}} \right\rangle \approx \frac{ik^r}{L^4} \int (y^r - x^r) \left\langle \delta m(\mathbf{x}) \delta v^k(\mathbf{y}) \right\rangle d^2\mathbf{x}\, d^2\mathbf{y} := -\mathrm{i} k^r \Omega_{rk}, \tag{C.7}$$

$$\langle m_{\mathbf{k}} m_{-\mathbf{k}} \rangle \approx \frac{1}{L^4} \int \langle \delta m(\mathbf{x}) \delta m(\mathbf{y}) \rangle\, d^2\mathbf{x}\, d^2\mathbf{y} := \nu. \tag{C.8}$$

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