Conservation and Transport: From the Microscopic to the Macroscopic

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(Dated: March 13, 2018)

In these lecture notes, we will examine the Navier-Stokes equations for classical hydrodynamics from two physical viewpoints. The first is from the perspective of a general conservation principle. Quantities such as mass, momentum, and energy are macroscopically conserved, giving rise in a natural manner to equations that govern the transport of associated local quantities when the medium is subjected to external influences. Classically, the most well-known example of such equations are the Navier-Stokes equations for viscous fluid flow. The transport equations that are derived this way must be closed with phenomenological relations that model the behavior of an experimental medium, which have prefactors that should be interpreted in terms of microscopic processes. The second viewpoint is that of microscopic conservation laws of the same quantities during inter-molecular collisions. The Navier-Stokes equations can be derived from the Hamiltonian dynamics of the system, giving rise to the same hydrodynamic transport equations on length and time scales much larger than those associated with the molecular processes. This route is more challenging to follow—it posed a major challenge to 19th century physics—but also more rewarding. For starters, the derivation provides insights into the microscopic origin of the imposed closure and expressions for the phenomenological prefactors in the Navier-Stokes equations. In addition, it allows us to engage with a variety of concepts that reappear throughout physics: the Liouville theorem, the BBGKY hierarchy, the Boltzmann transport equation, and the Chapman-Enskog expansion. Furthermore, exploring this route builds appreciation for the historical unification of the molecular and continuum ways of thinking about (conservative) transport phenomena in the world around us, as was first successfully achieved by Ludwig Boltzmann. Finally, the insight that hydrodynamic equations can be recovered from the mesoscale Boltzmann transport equation forms the basis of the lattice-Boltzmann method. This is a highly successful class of efficient numerical fluid dynamics solvers and we will touch upon the basics in these notes. This lecture series will be round out by considering the various regimes of fluid flow described by the Navier-Stokes equations. We solve these equations in the nonlinear regime numerically using a simple LB algorithm and place an emphasis in the linear regime on the way microorganisms achieve self-propulsion.

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CONTENTS

I.   INTRODUCTION

Most undergraduate courses in physics will contain some treatment of the classical hydrodynamic equations, which describe the flow of fluids and gasses. The set of equations governing such flows are referred to as the Navier-Stokes equations, in honor of Claude-Louis Navier and Sir George Gabriel Stokes. These equations are based on general conservation principles. Mass, momentum, and energy are macroscopically conserved quantities. Therefore, they behave in a certain way, when a medium is put into motion under the action of an external force or some boundary stress. This conservation property leads to a set of associated transport equations for the density, fluid velocity, and energy density, which together comprise the classic Navier-Stokes equations.

The Navier-Stokes equations are the cumulation of centuries of experimental and theoretical work aimed at solving the problem of describing fluid flows. One of the oldest works stems from the first century AD, when Sextus Julius Frontinus commented on the flow of water in aqueducts and fountains [1]. Many of the finest minds in science have worked on solving the hydrodynamic problem since the time of Frontinus, including: Torricelli, Pascal, Newton, Bernoulli, D'Alembert, Cauchy, Poisson, and Euler. Euler was the first to obtain set of differential equations to describe fluid flow in the mid-18th century [2]. His work was based on the transformation between quantities observed in a co-moving and laboratory frame; proving instrumental in advancing the field of calculus. However, Euler's equations have one major drawback. They describe ideal fluids, which do not possess internal friction (viscosity). As pointed out by D'Alembert [3], this means that a falling ball does not experience friction. That being said, Euler's equations have always had their application, as the behavior of rarefied gasses subjected to adiabatic flow can be well approximated by solutions to Euler's equations. More recently, the ideal-fluid description has seen a resurgence with the realization of superfluids [4].

It took until 1821, before Euler's equations could be extended to describe viscous fluid flow; a challenge that was completed by Navier [5]. Navier's work was subsequently improved upon throughout the middle of the 19th century by Stokes. The resulting Navier-Stokes equations allowed for a revolution in the physical description of flow phenomena, despite them not being easy to solve. They have been successfully applied in a wide range of settings, from understanding the fluid flow though tiny tubes in our body driven ion gradients, to analyzing the motion of fish, optimizing the design of boats and airplanes, predicting the weather, studying oceanic currents, computing the motion of the earth's mantle, and understanding the evolution of galaxies. In addition, many generalized versions have been formulated by incorporating additional conservation laws. For example, magnetohydrodynamics combines the Navier-Stokes equations with Maxwell's laws, which is relevant to the description of plasma and stellar dynamics.

The discipline of hydrodynamics has had a tremendous impact on the way we describe and are able to manipulate our world. It is therefore well worth having a closer look at the classic hydrodynamic equations. The connection between hydrodynamics and statistical mechanics is often not exposed in undergraduate or even graduate programs, and this set of lecture notes aims to rectify this omission. We first introduce the hydrodynamic equations, before deriving them via the molecular route. Starting from the Hamiltonian of the molecular system, we will encounter in succession: the Liouville theorem, the BBGKY hierarchy, the Boltzmann transport equation, and the Chapman-Enskog expansion. This derivation provides us with expressions for the closure relation for the deviatoric stress in the case of a simple fluid, as well as insights into the microscopic origin of the prefactors that appear in the Navier-Stokes equations.

Next, we show how the Boltzmann transport equation can be discretized into one of the most sophisticated numerical methods available to study fluid flow today, namely the lattice-Boltzmann algorithm. A simple variant of this algorithm is presented, based on the Bhatnagar-Gross-Krook approximation[1]. This will be useful to understand what is going on in the Python-based lattice-Boltzmann scripts that accompany these notes. These scripts will be used to visualize flow fields in exercises that pertain to the last part of these notes.

Finally, we return to the Navier-Stokes equations and briefly discuss the various regimes of flow that can occur, under which conditions these regimes are found, and how this ties into the Reynolds number. In the nonlinear regime, we examine the onset of the Kármán vortex street, which is a particularly pretty example of the impact of interia on the evolution of fluid flow. We conclude by discussing the consequences of being in the laminar-flow regime. We introduce E.M. Purcell's *Scallop Theorem* [6] and its implications for the way microorganisms can achieve self-propulsion. In addition, we briefly touch upon a far-field description of the hydrodynamic interactions between microorganisms and their surrounds. These are based on the well-known Greens-functions for laminar hydrodynamic flow: the Stokeslet and Stresslet.

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[1] They are **not** the BGK in the B**BGK**Y hierarchy.

Acknowledgements and the Use of these Notes

These notes were written with an undergraduate background in physics in mind and require basic knowledge of statistical mechanics, as well as a limited background in hydrodynamics. It might help to consult relevant textbooks, should some of the concepts here appear unfamiliar—references will be provided where it is deemed necessary. You will find exercises sprinkled throughout the text, rather than grouped at the end of chapters. The idea behind this is that you can go through the notes in a linear fashion, solving problems as you go along, to improve understanding of certain details of the calculations involved and to explore the material in greater depth. A star-label convention is used to give some indication of the difficulty of these exercises: $*$ implies relatively trivial, but sometimes lengthy algebra; $**$ implies non-trivial algebra or requires careful physical argumentation, and finally $***$ is a challenging exercise that will probably require literature reading to solve. As the lecture series does not assume familiarity with the Python programming language, any exercise involving the use of Python will be labelled $***$, even if the algebra is trivial. You will only be expected to perform some limited parameter variation.

II.   THE CLASSICAL ROUTE TO HYDRODYNAMIC EQUATIONS

In this section, we follow the standard approach to obtaining the classic hydrodynamic transport equations in three-dimensional (3D) space, closely following the approach outlined in Ref. [7]. For further reading, we suggest Refs. [8, 9].

A.   Transforming between Lagrangian and Eulerian Coordinates

The first thing to do in thinking about transport phenomena, is to connect the two standard ways of tracking observables in classical fluid dynamics. The goal is to transform frames that do not deform due to fluid flow to ones that do. This will enable us to change coordinates in integrating over domains, which is necessary in formulating conservation laws, because it facilitates the exchange of integration and differentiation. This is the route first taken by Euler [2], but it is presented here in modern notation.

Consider an infinitesimal volume of fluid, labeled by the coordinate of its center $\boldsymbol{a}$ at time $t = 0$. One way to think about this parcel of fluid is in the *co-moving* or *Lagrangian* description, also referred to as *material coordinates*. An observer moving along with the parcel sees a quantity Q—this could be pressure, energy, etc.—on this parcel change with time. Another observer can monitor the same parcel of fluid in an external or laboratory frame, and report on the evolution of the same quantity on this parcel, which we denote as q to distinguish the two frames. The second frame is most commonly referred to as the *Eulerian* frame, but it is not an absolute frame of reference, as any non-co-moving frame is equally valid, and one can readily Galilei transform from one Eulerian frame into another. The key is that the parcel of fluid maintains the shape it had at time $t = 0$ throughout in the Lagrangian frame, while in the Eulerian frame it may become significantly distorted, *e.g.*, in the case of swirl or turbulent flow.

The question now arises: "How can these two observers relate their measurements to each other?" More precisely, how is a change in $Q(\boldsymbol{a}, t)$, as measured by the Lagrangian observer, mapped to a change in $q(\boldsymbol{r}, t)$, which is what the Eulerian observer is tracking, accounting for the deformations of the fluid parcel that this observer also notices. We are interested in the time evolution of quantities after all, when we are talking about transport processes. Clearly, the parcel coordinate $\boldsymbol{a}$ must be transformed to map to the Eulerian frame. We write the position of the Lagrangian observer in the Eulerian coordinate frame as $\boldsymbol{r}(\boldsymbol{a}, t)$, which has the property $\boldsymbol{r}(\boldsymbol{a}, 0) = \boldsymbol{a}$. The rate of change in the quantity Q on this volume labeled $\boldsymbol{a}$ is now given by

$$\frac{d}{dt}Q(\boldsymbol{a}, t) = \frac{d}{dt}q(\boldsymbol{r}(\boldsymbol{a}, t), t)\bigg|_{\boldsymbol{a}} = \frac{\partial}{\partial t}q(\boldsymbol{r}(\boldsymbol{a}, t), t) + \sum_{i=1}^{3} \left(\frac{\partial}{\partial R_i}q(\boldsymbol{R}, t)\bigg|_{\boldsymbol{R}=\boldsymbol{r}(\boldsymbol{a}, t)}\right)\left(\frac{\partial}{\partial t}r_i(\boldsymbol{a}, t)\right), \tag{1}$$

where in the first identity, we insist that the derivative with respect to time is applied to the specific point $\boldsymbol{r}$ which maps back to $\boldsymbol{a}$ at time $t = 0$, as indicated by the evaluation condition. The chain rule leads to the partial derivatives with respect to time in the second identity, for which we can recognize

$$u_i \equiv \frac{\partial}{\partial t}r_i(\boldsymbol{a}, t) \tag{2}$$

as the i-th component of the velocity $\boldsymbol{u}$ of the material, which is naturally taken at the point $\boldsymbol{r}(\boldsymbol{a}, t)$ at time t, as it is observed in the Eulerian coordinate frame. Combining Eqs. (1) and (2) we arrive at a definition of the material derivative

$$\frac{D}{Dt}q(\boldsymbol{r}, t) \equiv \left(\frac{\partial}{\partial t} + \boldsymbol{u}(\boldsymbol{r}, t) \cdot \boldsymbol{\nabla}_{\boldsymbol{r}}\right) q(\boldsymbol{r}, t), \tag{3}$$

which is a time derivative that follows the material as it deforms (Lagrangian frame), with '$\cdot$' the inner product and $\boldsymbol{\nabla}_{\boldsymbol{r}}$ the gradient with respect to position in the Eulerian frame. Here, we have dropped the notation $(\boldsymbol{a}, t)$ for the position coordinate $\boldsymbol{r}$, since Eq. (3) holds for all choices of $\boldsymbol{a}$.

This seems a rather convoluted way to write down, what is nothing more than a total derivative with a physical interpretation for one of the terms in the chain rule. However, the strength of Eq. (3) lies in the physical interpretation of the mapping back to a frame where the volume and boundary are not varying. This will allow us to swap derivatives and integrals, as we will do in Section II B 1. When we change coordinates in an integral, we also need to deal with the determinant of the Jacobian. As a final step, we therefore examine the determinant of the coordinate transformation

$$J(\boldsymbol{r}(\boldsymbol{a}, t), t) \equiv \det\left(\frac{D}{D\boldsymbol{p}}\boldsymbol{r}(\boldsymbol{p}, t)\bigg|_{\boldsymbol{p}=\boldsymbol{a}}\right), \tag{4}$$

where we take a total derivative of a vector valued function. We have that $J(\boldsymbol{a}, 0) = \det(\mathbb{I}_3) = 1$, with $\mathbb{I}_3$ the 3D identity matrix, and one readily finds

$$\frac{d}{dt} J(\boldsymbol{r}, t) = \left(\boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \boldsymbol{u}(\boldsymbol{r}, t) \right) J(\boldsymbol{r}, t), \tag{5}$$

which makes sense, since the divergence of the speed is related to the rate of change in volume. Physically, a material is volume preserving when $J(\boldsymbol{r}, t) = 1$, for all $\boldsymbol{r}$ and t, such that $\boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \boldsymbol{u}(\boldsymbol{r}, t) = 0$ in that case, a condition referred to as *incompressibility*.

> **Exercise 1***: Show that Eq. (5) holds from the definition of the determinant in Eq. (4). It may help to rewrite the expressions using the Einstein summation convention and the Levi-Civita symbol. Alternatively, one can think of the determinant in terms of a cross and dot product of the columns comprising the total derivative and use vector identities to arrive at the above result.

B. Conservation of Mass, Momentum, and Energy

Using the definitions in Section II A, we can now write down the basic conservation equations in the Eulerian frame, which give rise to transport equations in a natural way. We will consider mass and momentum here and leave derivation of the energy transport equation as an exercise for the reader.

1. Mass Conservation

The mass $M(t)$ of a volume $\Omega(t)$ is determined by integrating the mass density $\rho(\boldsymbol{r}, t)$ over this volume. When no mass is created or destroyed—a sensible condition in classical systems—we have

$$0 = \frac{d}{dt} M(t) = \frac{d}{dt} \int_{\Omega(t)} \mathrm{d}\boldsymbol{r} \, \rho(\boldsymbol{r}, t) = \frac{d}{dt} \int_{\Omega(0)} \mathrm{d}\boldsymbol{a} \, \rho(\boldsymbol{r}(\boldsymbol{a}, t), t) J(\boldsymbol{r}(\boldsymbol{a}, t), t), \tag{6}$$

where in the last equality we transformed to the Lagrangian description to eliminate the time dependence of the volume of the control volume. Note that we have sneakily omitted the absolute bars that are necessary to perform integration by substitution. This is permissible, since physical deformations of a fluid parcel cannot invert the sign of the volume, which is what the determinant of the Jacobian indicates and why the absolute value is taken in general. Now pulling the time derivative into the integral, we find

$$\begin{aligned} \frac{d}{dt} M(t) &= \int_{\Omega(0)} \mathrm{d}\boldsymbol{a} \, \left(\frac{D}{Dt} \rho(\boldsymbol{r}(\boldsymbol{a}, t), t) + \rho(\boldsymbol{r}(\boldsymbol{a}, t), t) \boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \boldsymbol{u}(\boldsymbol{r}(\boldsymbol{a}, t), t) \right) J(\boldsymbol{r}(\boldsymbol{a}, t), t) \\ &= \int_{\Omega(t)} \mathrm{d}\boldsymbol{r} \, \left(\frac{D}{Dt} \rho(\boldsymbol{r}, t) + \rho(\boldsymbol{r}, t) \boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \boldsymbol{u}(\boldsymbol{r}, t) \right) = 0. \end{aligned} \tag{7}$$

Since this holds for all volumes $\Omega(t)$, we may write

$$\frac{D}{Dt} \rho(\boldsymbol{r}, t) + \rho(\boldsymbol{r}, t) \boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \boldsymbol{u}(\boldsymbol{r}, t) = 0, \tag{8}$$

for the conservation of mass. This can be rewritten in the (more common) form

$$\frac{\partial}{\partial t} \rho(\boldsymbol{r}, t) = -\boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \left(\rho(\boldsymbol{r}, t) \boldsymbol{u}(\boldsymbol{r}, t) \right). \tag{9}$$

Equation (9) implies that the density on a fluid parcel can only change through convective transport from adjacent parcels, which takes the form of a mass density flux. Here, we have seen the consequences of conservation in action: a conservation law leads to an associated transport equation when things move around.

2. Momentum Conservation

Similarly, we may obtain the well-known Navier-Stokes equations for the fluid velocity by considering the conservation of momentum. The momentum contained in the volume $\Omega(t)$ is given by

$$\boldsymbol{p}(t) = \int_{\Omega(t)} \mathrm{d}\boldsymbol{r}\, \rho(\boldsymbol{r},t)\boldsymbol{u}(\boldsymbol{r},t), \tag{10}$$

which leads to

$$\frac{d}{dt}\boldsymbol{p}(t) = \int_{\Omega(t)} \mathrm{d}\boldsymbol{r}\, \left(\boldsymbol{u}(\boldsymbol{r},t)\frac{D}{Dt}\rho(\boldsymbol{r},t) + \rho(\boldsymbol{r},t)\frac{D}{Dt}\boldsymbol{u}(\boldsymbol{r},t) + \rho(\boldsymbol{r},t)\boldsymbol{u}(\boldsymbol{r},t)\left(\boldsymbol{\nabla_r} \cdot \boldsymbol{u}(\boldsymbol{r},t)\right) \right). \tag{11}$$

This expression can be rewritten using Eq. (8) to read

$$\frac{d}{dt}\boldsymbol{p}(t) = \int_{\Omega(t)} \mathrm{d}\boldsymbol{r}\, \rho(\boldsymbol{r},t)\frac{D}{Dt}\boldsymbol{u}(\boldsymbol{r},t). \tag{12}$$

The momentum in the control volume may change through the application of external body forces $\boldsymbol{f}(\boldsymbol{r},t)$ acting on the fluid and surface forces, such as viscous and elastic stresses, which can typically be written as $\hat{\boldsymbol{n}}(\boldsymbol{r},t)\cdot\underline{\boldsymbol{\sigma}}(\boldsymbol{r},t)$, where $\hat{\boldsymbol{n}}(\boldsymbol{r},t)$ is the outward-pointing normal vector to the surface $\partial\Omega(t)$ of $\Omega(t)$ and $\underline{\boldsymbol{\sigma}}(\boldsymbol{r},t)$ is the Cauchy stress tensor; $\boldsymbol{b}\cdot\underline{\boldsymbol{A}}$ may be written as $\sum_i b_i A_{ij}$. The Cauchy stress tensor indicates how different surfaces (three orthogonal ones in 3D) experience surface forces (three 3-vectors). This leads to a 9-component matrix $\underline{\boldsymbol{\sigma}}$ with symmetry conditions to account for Newton's third law; these symmetries are referred to as Cauchy's fundamental lemma. Applying Newton's second law and balancing the various force contributions we obtain

$$\frac{d}{dt}\boldsymbol{p}(t) = \int_{\Omega(t)} \mathrm{d}\boldsymbol{r}\, \rho(\boldsymbol{r},t)\frac{D}{Dt}\boldsymbol{u}(\boldsymbol{r},t) = \int_{\Omega(t)} \mathrm{d}\boldsymbol{r}\, \boldsymbol{f}(\boldsymbol{r},t) + \int_{\partial\Omega(t)} \mathrm{d}\boldsymbol{s}\, \hat{\boldsymbol{n}}(\boldsymbol{s},t) \cdot \underline{\boldsymbol{\sigma}}(\boldsymbol{s},t), \tag{13}$$

where the last integral is a surface integral, as indicated by the use of the integration variable $\boldsymbol{s}$. Using the divergence theorem, we may write

$$\int_{\Omega(t)} \mathrm{d}\boldsymbol{r}\, \rho(\boldsymbol{r},t)\frac{D}{Dt}\boldsymbol{u}(\boldsymbol{r},t) = \int_{\Omega(t)} \mathrm{d}\boldsymbol{r}\, \left(\boldsymbol{f}(\boldsymbol{r},t) + \boldsymbol{\nabla_r} \cdot \underline{\boldsymbol{\sigma}}(\boldsymbol{r},t)\right), \tag{14}$$

with $\boldsymbol{\nabla_r} \cdot \underline{\boldsymbol{\sigma}}(\boldsymbol{r},t)$ the three vector that has components $\sum_{i=1}^{3} \partial\sigma_{ij}/\partial r_i$, such that the momentum transport equation becomes

$$\rho(\boldsymbol{r},t)\left(\frac{\partial}{\partial t} + \boldsymbol{u}(\boldsymbol{r},t)\cdot\boldsymbol{\nabla_r}\right)\boldsymbol{u}(\boldsymbol{r},t) = \boldsymbol{\nabla_r} \cdot \underline{\boldsymbol{\sigma}}(\boldsymbol{r},t) + \boldsymbol{f}(\boldsymbol{r},t), \tag{15}$$

which is the general form of the Navier-Stokes equation for the velocity of a fluid. Note that it is nonlinear in the fluid velocity (second term on the left-hand side), which we will come back to in Section V A.

3. The Closure Relation for a Newtonian Fluid

Equation (15) is not particularly useful in and of itself, as we now have a form for momentum transport that requires knowledge of the Cauchy stress tensor $\underline{\boldsymbol{\sigma}}(\boldsymbol{r},t)$, which is prescribed by a material's properties. This should not come as a huge surprise, as general conservation principles do not have this level of molecular detail baked into them. We therefore need to specify how a fluid behaves under the application of forces and shear. Macroscopically, one would characterize the fluid in this way by putting it in a rheometer.

By specifying the Cauchy stress tensor's form, or more commonly an evolution equation for $\underline{\boldsymbol{\sigma}}(\boldsymbol{r},t)$, we can prescribe phenomenological laws for the behavior of a fluid. A host of fluids can be modeled in this way: water, polymer suspensions, blood, corn starch, etc. Before we get to this, we rewrite $\underline{\boldsymbol{\sigma}}(\boldsymbol{r},t) = -p(\boldsymbol{r},t)\mathbb{I}_3 + \underline{\boldsymbol{\tau}}(\boldsymbol{r},t)$, with $p(\boldsymbol{r},t)$ the pressure and $\underline{\boldsymbol{\tau}}(\boldsymbol{r},t)$ the deviatoric stress tensor, which contains viscous and other stresses. This rewrite does nothing more than to isolate the normal stresses from the shear stresses. The normal stresses on the diagonal are equal in the case of fluids—fluids cannot bear heterogeneous loads in the same way solids can—and are therefore grouped in a term that is identified as the pressure.

Now we need to impose an expression for $\underline{\tau}(\boldsymbol{r}, t)$ that captures the behavior of the fluid we are interested in. It will turn out that for most intents and purposes the pressure, *i.e.*, the equation of state, will not be of huge importance. Let us turn to the simplest case of a fluid, also referred to as a *simple fluid*. This is a Newtonian fluid defined on phenomenological grounds to be isotropic and to have a stress that is linear in the applied strain. Such a fluid models the behavior of monoatomic media with short-ranged interactions, such as inert gases, but also water, ethanol, and many others. Let us discuss what is meant by the strain and how, in the case of an imposed linear relation, this leads to a closure for $\underline{\tau}(\boldsymbol{r}, t)$.

If we consider a fluid velocity field $\boldsymbol{u}(\boldsymbol{r}, t)$, the Taylor series of the velocity around the point $\boldsymbol{r}$ is given by

$$\boldsymbol{u}(\boldsymbol{r} + \mathrm{d}\boldsymbol{r}) = \boldsymbol{u}(\boldsymbol{r}, t) + \left(\frac{D}{D\boldsymbol{r}} \boldsymbol{u}(\boldsymbol{r}, t) \right) \mathrm{d}\boldsymbol{r} + \text{h.o.t.}, \tag{16}$$

where we taken the total derivative of the velocity, which is a rank-two tensor, which acts on the infinitesimal line segment $\mathrm{d}\boldsymbol{r}$. We now decompose the total derivative of the velocity into symmetric and antisymmetric parts

$$\frac{D}{D\boldsymbol{r}} \boldsymbol{u}(\boldsymbol{r}, t) \equiv \frac{1}{2} \left(\underline{\dot{\gamma}}(\boldsymbol{r}, t) + \underline{\omega}(\boldsymbol{r}, t) \right); \tag{17}$$

$$\underline{\dot{\gamma}}(\boldsymbol{r}, t) \equiv \left(\frac{D}{D\boldsymbol{r}} \boldsymbol{u}(\boldsymbol{r}, t) \right) + \left(\frac{D}{D\boldsymbol{r}} \boldsymbol{u}(\boldsymbol{r}, t) \right)^T; \tag{18}$$

$$\underline{\omega}(\boldsymbol{r}, t) \equiv \left(\frac{D}{D\boldsymbol{r}} \boldsymbol{u}(\boldsymbol{r}, t) \right) - \left(\frac{D}{D\boldsymbol{r}} \boldsymbol{u}(\boldsymbol{r}, t) \right)^T, \tag{19}$$

with $\underline{\dot{\gamma}}(\boldsymbol{r}, t)$ the strain-rate tensor and $\underline{\omega}(\boldsymbol{r}, t)$ the vorticity tensor and T denoting transposition. This way of expanding the fluid field locally gives insight into the action of the two quantities that we have introduced. The strain-rate tensor indicates how a control volume is deformed. For instance, the application of a nonzero $\underline{\dot{\gamma}}(\boldsymbol{r}, t)$ will transform a spherical control volume into an ellipsoid. The dot in the notation for the strain-rate tensor indicates that the variation of deformation over time is being considered. The vorticity tensor gives rise to rigid body rotations of a control volume, about the axis $\boldsymbol{\omega}(\boldsymbol{r}, t) = \boldsymbol{\nabla}_{\boldsymbol{r}} \times \boldsymbol{u}(\boldsymbol{r}, t)$, where we have used the cross product. This quantity is called the *vorticity* of the fluid and the rotation rate is equal to $\omega(\boldsymbol{r}, t) = |\boldsymbol{\omega}(\boldsymbol{r}, t)|$.

> **Exercise 2***: Prove using linear algebra that the strain-rate tensor indeed gives rise to such deformations and that the vorticity tensor leads to rotations about the axis defined by the vorticity at a rate equal to the norm of this vector.

In a rheometer, a shear stress may be applied and this may be related to the stress in the fluid, based on the amount of force or torque required to maintain a certain shear rate. Water was found to have a linear stress-strain relation, hence the definition of a classical Newtonian fluid. Returning to the closure relation, we have that $\underline{\tau}(\boldsymbol{r}, t)$ is symmetric and we know that $\underline{\dot{\gamma}}(\boldsymbol{r}, t)$ is symmetric. There is, however, one additional symmetric tensor that can be constructed in terms of the deformation of the fluid, namely $(\boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \boldsymbol{u}(\boldsymbol{r}, t))\mathbb{I}_3$. Therefore, the most general form of a *linear* stress-strain relation for an isotropic fluid, must be given by a linear combination of these two, which is commonly written as

$$\underline{\tau}(\boldsymbol{r}, t) = \mu \left(\underline{\dot{\gamma}}(\boldsymbol{r}, t) - \frac{2}{3} \left(\boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \boldsymbol{u}(\boldsymbol{r}, t) \right) \mathbb{I}_3 \right) + \mu' \left(\boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \boldsymbol{u}(\boldsymbol{r}, t) \right) \mathbb{I}_3. \tag{20}$$

Here, the prefactor μ in front of the traceless part of $\underline{\tau}(\boldsymbol{r}, t)$ is called the dynamic fluid viscosity, and is a measure for internal friction or equivalently momentum diffusion, because the combination μ/ρ has the dimensionality of a diffusion constant. The prefactor μ' is called the dilatational viscosity and is related to the level of compressibility that the medium exhibits.

The most interesting thing about Eq. (20) is that the prefactors μ and μ' do not depend on the density of the gas and therefore do not vary in time and space—this is, of course, subject to some constraints. We will get back to this in Section III E, when we have followed the kinetic route to obtaining these expressions. Maxwell was the first to derive this property of μ (and μ') using kinetic theory and was himself highly surprised by the result, writing [10]: "*Such a consequence of the mathematical theory is very startling and the only experiment I have met with on the subject does not seem to confirm it.*" He therefore took matters into his own hands, building a device capable of measuring the viscosity and performing the experiment that confirmed his own prediction [11]. Historically, this provided evidence for the existence of molecules. At that time, the molecular nature of matter had met with considerable skepticism. Unfortunately, despite Maxwell's efforts, it continued to be called into question well into the early 20th century, when

the work of Perrin [12], and Geiger, Marsden, and Rutherford [13] managed to silence the last remaining protagonists of the microscopic continuum picture of matter.

Exercise 3[***]: Use similar arguments to the ones provided in Section II B 2 to construct the form of the energy conservation equation for the internal energy per unit mass $\tilde{U}(\boldsymbol{r}, t)$. We use the "tilde" to distinguish this quantity form the notation that we will use throughout for the interaction potential between particles. Here, you may assume the simple form of the Newtonian closure obtained in Section II B 3 as well as incompressibility of the medium. The expression you should arrive at reads

$$\rho(\boldsymbol{r}, t)\frac{D}{Dt}\tilde{U}(\boldsymbol{r}, t) = \mu\underline{\dot{\gamma}}(\boldsymbol{r}, t) : \underline{\dot{\gamma}}(\boldsymbol{r}, t) + \boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \left(k(\boldsymbol{r}, t)\boldsymbol{\nabla}_{\boldsymbol{r}}T(\boldsymbol{r}, t)\right),\tag{21}$$

where ':' denotes the commutative double dot product, which is defined as $\underline{\boldsymbol{A}} : \underline{\boldsymbol{B}} \equiv \sum_{i=1}^{3} A_{ii}B_{ii}$, using the Einstein summation convention. Obtaining the left-hand side is straightforward, but for the right-hand side you will need to argue how changes in the internal energy can come about, we refer to Ref. [8] for an in-depth discussion. You will also need to use Eq. (15) to eliminate the pressure and force terms and recognize Fick's law of heat conduction $\boldsymbol{q}(\boldsymbol{r}, t) = -k(\boldsymbol{r}, t)\boldsymbol{\nabla}_{\boldsymbol{r}}T(\boldsymbol{r}, t)$ in your result, with $k(\boldsymbol{r}, t)$ the thermal conductivity and $T(\boldsymbol{r}, t)$ the temperature.

C. The Hydrodynamic Transport Equations

If we assume that we are working with a Newtonian medium that is essentially incompressible, we can summarize the result of the above discussion in the following set of transport equations

$$\boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \boldsymbol{u}(\boldsymbol{r}, t) = 0;\tag{22}$$

$$\frac{D}{Dt}\rho(\boldsymbol{r}, t) = 0;\tag{23}$$

$$\rho(\boldsymbol{r}, t)\frac{D}{Dt}\boldsymbol{u}(\boldsymbol{r}, t) = -\boldsymbol{\nabla}_{\boldsymbol{r}}p(\boldsymbol{r}, t) + \mu\underline{\boldsymbol{\Delta}}_{\boldsymbol{r}}\boldsymbol{u}(\boldsymbol{r}, t) + \boldsymbol{f}(\boldsymbol{r}, t);\tag{24}$$

$$\rho(\boldsymbol{r}, t)\frac{D}{Dt}\tilde{U}(\boldsymbol{r}, t) = \mu\underline{\dot{\gamma}}(\boldsymbol{r}, t) : \underline{\dot{\gamma}}(\boldsymbol{r}, t) + \boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \left(k(\boldsymbol{r}, t)\boldsymbol{\nabla}_{\boldsymbol{r}}T(\boldsymbol{r}, t)\right).\tag{25}$$

Here Eq. (22) is an expression of incompressibility, Eq. (23) of mass conservation[2], Eq. (24) of momentum conservation, and Eq. (25) of energy conservation. Note that we have introduced the vector Laplacian $\underline{\boldsymbol{\Delta}}_{\boldsymbol{r}} \equiv \mathbb{I}_3\nabla_{\boldsymbol{r}}^2$ in Eq. (24). For a compressible system, the equations are slightly more convoluted, but not tremendously so.

Exercise 4[*]: Write down the system of conservation equations that governs the behavior of a compressible Newtonian medium. Note that we have already provided two of the necessary equations and you should have obtained the third in deriving Eq. (21).

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[2] Be careful, an incompressible medium is not the same as a homogeneous incompressible medium. The mass density need not be spatially constant. Think, for instance, about the situation wherein sea water with different salinities meet. Clearly, both media behave essentially incompressible, but their mass density may differ substantially due to the presence of the salt.

III. OBTAINING HYDRODYNAMIC TRANSPORT EQUATIONS VIA KINETIC THEORY

In this section, we will derive the hydrodynamic transport equations from the ground up, starting out with the Hamiltonian describing the system and the associated microscopically conserved quantities. We largely follow the route outlined in lecture notes "Kinetic Theory" by David Tong [14], but will deviate from this towards the end of the derivation. Historically speaking, the route described in this chapter is the one followed by Ludwig Boltzmann and his work brought about the development of the field of statistical physics.

A. From Liouville to the BBGKY Hierarchy

We start our derivation from the Hamiltonian that describes a system of N identical, isotropic particles, where $N \gg 1$ is of sufficient size to allow us to use the tools of statistical mechanics. Let the Hamiltonian be of the form

$$H_N(\{\boldsymbol{r}\}, \{\boldsymbol{p}\}, t) = \frac{1}{2m} \sum_{i=1}^{N} \boldsymbol{p}_i^2 + \sum_{i=1}^{N} V(\boldsymbol{r}_i) + \sum_{i=1}^{N} \sum_{j<i} U(\boldsymbol{r}_i - \boldsymbol{r}_j), \tag{26}$$

where m is the particle mass, $\boldsymbol{p}_i$ is the momentum of the i-th particle, there is a conservative external force acting on the particles $\boldsymbol{F}(\boldsymbol{r}) = -\boldsymbol{\nabla}_{\boldsymbol{r}} V(\boldsymbol{r})$, and the particles interact via a pair potential $U(\boldsymbol{r})$. Note that we write the Hamiltonian as a function of the two $3N$-dimensional sets of vectors $\{\boldsymbol{r}\}$ and $\{\boldsymbol{p}\}$, respectively, and the time t; we used the subscript N to emphasize this, which will become convenient later. We have dropped the time dependence of the positions and momenta for notational convenience.

Now let $f_N(\{\boldsymbol{r}\}, \{\boldsymbol{p}\}, t)$ be the (continuous) probability density function (PDF) that gives us the chance of finding the system around the $6N$-dimensional point specified by $\{\boldsymbol{r}\}$ and $\{\boldsymbol{p}\}$ at a time t. This PDF is normalized to

$$\int \left(\prod_{i=1}^{N} \mathrm{d}\boldsymbol{r}_i \mathrm{d}\boldsymbol{p}_i \right) f_N(\{\boldsymbol{r}\}, \{\boldsymbol{p}\}, t) = 1, \tag{27}$$

when integrating over the entire phase-space volume. We will encounter examples of f in the following that are differently normalized, but we will maintain the label PDF in referring to these for convenience. Henceforth, except when it is absolutely necessary for understanding the notation, we will drop the dependence on $\{\boldsymbol{r}\}$, $\{\boldsymbol{p}\}$, and t from the Hamiltonian and the PDFs, to lighten the notation substantially.

Recall from classical mechanics, that the evolution of a phase-space PDF is governed by the action of the Hamiltonian under the Poisson bracket

$$\frac{\partial f_N}{\partial t} = \{H_N, f_N\}. \tag{28}$$

Equation (28) is better known as the Liouville equation and it is an expression of Liouville's theorem, which states that probability is conserved in a closed region of phase space under the action of the Hamiltonian.

Exercise 5*: If you have forgotten the action of the Poisson bracket and the way this governs the evolution of phase-space PDFs in relation to the Hamiltonian of the system, then derive Eq. (28). Start with Hamilton's equations $\partial \boldsymbol{p}_i/\partial t = -\boldsymbol{\nabla}_{\boldsymbol{r}_i} H_N$ and $\partial \boldsymbol{r}_i/\partial t = \boldsymbol{\nabla}_{\boldsymbol{p}_i} H_N$, wherein the symplectic form of the Hamilton formalism can be recognized. Next, write down the continuity equation (over phase space) of the PDF to arrive at:

$$\left(\frac{\partial}{\partial t} + \sum_{i=1}^{N} \boldsymbol{\nabla}_{\boldsymbol{r}_i} \cdot \frac{\partial \boldsymbol{r}_i}{\partial t} + \sum_{i=1}^{N} \boldsymbol{\nabla}_{\boldsymbol{p}_i} \cdot \frac{\partial \boldsymbol{p}_i}{\partial t} \right) f_N = 0, \tag{29}$$

since probability is a conserved quantity and one can straightforwardly apply the chain rule. Next rewrite Eq. (29) in terms of the Hamiltonian, using Hamilton's equations, and regroup this using the definition of the Poisson bracket

$$\{A, B\} = \sum_{i=1}^{N} \left(\boldsymbol{\nabla}_{\boldsymbol{r}_i} A \cdot \boldsymbol{\nabla}_{\boldsymbol{p}_i} B - \boldsymbol{\nabla}_{\boldsymbol{p}_i} A \cdot \boldsymbol{\nabla}_{\boldsymbol{r}_i} B \right), \tag{30}$$

with A and B two functions depending on $3N$-dimensional vectors $\{\boldsymbol{r}\}$ and $\{\boldsymbol{p}\}$.

If we have some function on phase space Q, which may depend on some or all of the particle positions and momenta, then the expectation value of this function is given by

$$\langle Q \rangle(t) = \int \left(\prod_{i=1}^{N} \mathrm{d}\boldsymbol{r}_i \mathrm{d}\boldsymbol{p}_i \right) Q f_N, \tag{31}$$

and by natural extension of the Liouville equation, its time evolution is given by

$$\frac{d\langle Q \rangle}{dt}(t) = \langle \{Q, H_N\} \rangle. \tag{32}$$

Note that this implies that quantities which Poisson commute with the Hamiltonian are conserved. Therefore, any equilibrium PDF, for which the time derivative is zero, must commute with the Hamiltonian, implying that it is likely a function of H_N. However, extracting that it has the shape of the Boltzmann distribution does not follow trivially from this observation.

> **Exercise 6***: If the result in Eq. (32) is not obvious, go through the derivation to obtain this expression. Recall that the Poisson bracket anti-commutes: the order of Q and f_N does not matter in Eq. (31), but the order of Q and H_N in Eq. (32) does.

Moving to phase-space PDFs has not made things any easier. Instead of $6N$ particle coordinates that we do not know a great deal about, we now have a single function of those coordinates, of which we know equally little. That is somewhat comforting, though, as we at least have conservation of complexity. However, we now need to start making reductions in order to progress and the first thing is to perform another rewrite which will enable us to do so. We are, of course, thinking of the BBGKY hierarchy, named after Bogoliubov, Born, Green, Kirkwood, and Yvon, who all contributed significantly to the development of our understanding of kinetic transport phenomena.

Let us start by defining the one-particle PDF, f_1, which indicates the likelihood of finding a particle around a phase-space point $(\boldsymbol{r}_1, \boldsymbol{p}_1)$

$$f_1(\boldsymbol{r}_1, \boldsymbol{p}_1, t) = N \int \left(\prod_{i=2}^{N} \mathrm{d}\boldsymbol{r}_i \mathrm{d}\boldsymbol{p}_i \right) f_N, \tag{33}$$

where we singled out the first position and momentum coordinates, since all particles are identical, which is also reflected in the combinatorial prefactor N. Note that this implies that f_1 is normalized to N upon integration over $\boldsymbol{r}_1$ and $\boldsymbol{p}_1$, which means that it is not a PDF in a strict sense, but we will use the label nonetheless for notational convenience and because N is only a multiplicative constant. The PDF f_1 gives us sufficient information on the system to determine all our quantities of interest

$$n(\boldsymbol{r}_1, t) = \int \mathrm{d}\boldsymbol{p}_1 \, f_1; \tag{34}$$

$$\boldsymbol{u}(\boldsymbol{r}_1, t) = \frac{1}{m} \int \mathrm{d}\boldsymbol{p}_1 \, \boldsymbol{p}_1 f_1; \tag{35}$$

$$\boldsymbol{\mathcal{E}}(\boldsymbol{r}_1, t) = \frac{1}{m} \int \mathrm{d}\boldsymbol{p}_1 \, \boldsymbol{p}_1 E(\boldsymbol{p}_1) f_1, \tag{36}$$

for the position-dependent average density, velocity, and energy flux, respectively, where the functional form $E(\boldsymbol{p}) = \boldsymbol{p}^2/(2m)$ for the kinetic energy is assumed.

Determining the evolution of f_1 is the next step in obtaining equations that govern the transport of the above quantities

$$\frac{\partial f_1}{\partial t} = N \int \left(\prod_{i=2}^{N} \mathrm{d}\boldsymbol{r}_i \mathrm{d}\boldsymbol{p}_i \right) \frac{\partial}{\partial t} f_N = N \int \left(\prod_{i=2}^{N} \mathrm{d}\boldsymbol{r}_i \mathrm{d}\boldsymbol{p}_i \right) \{H_N, f_N\}. \tag{37}$$

By writing out the Hamiltonian of the system, as given by Eq. (26), and defining the one-particle Hamiltonian as

$$H_1(\boldsymbol{r}_1, \boldsymbol{p}_1, t) = \frac{1}{2m} \boldsymbol{p}_1^2 + V(\boldsymbol{r}_1, t), \tag{38}$$

one readily obtains

$$\frac{\partial f_1}{\partial t} = \{H_1, f_1\} + N \int \left(\prod_{i=2}^{N} \mathrm{d}\boldsymbol{r}_i \mathrm{d}\boldsymbol{p}_i \right) \sum_{j=2}^{N} \boldsymbol{\nabla}_{\boldsymbol{r}_1} U(\boldsymbol{r}_1 - \boldsymbol{r}_j) \cdot \boldsymbol{\nabla}_{\boldsymbol{p}_1} f_N. \tag{39}$$

Exercise 7*: Perform the trivial, but rather lengthy calculations necessary to arrive at Eq. (39). Make use of partial integration to move the derivatives around. The boundary terms naturally do not contribute, if we wish our integrations to be well defined to begin with.

Equation (39) represents a Liouville-like equation for the evolution of the one-particle PDF, consisting of term that governs motion through phase space under the action of the one-particle Hamiltonian, and another term that describes interactions with other particles. This form is leading up to what will, under the application of appropriate reductions, become the Boltzmann transport equation. In the nomenclature of the Boltzmann transport equation, the first term on the right-hand side is called a streaming term, while the second is called the collision term, which we can define and rewrite as

$$\left(\frac{\partial f_1}{\partial t} \right)_{\mathrm{coll}} \equiv N(N-1) \int \mathrm{d}\boldsymbol{r}_2 \mathrm{d}\boldsymbol{p}_2 \, \boldsymbol{\nabla}_{\boldsymbol{r}_1} U(\boldsymbol{r}_1 - \boldsymbol{r}_2) \cdot \boldsymbol{\nabla}_{\boldsymbol{p}_1} \int \left(\prod_{i=3}^{N} \mathrm{d}\boldsymbol{r}_i \mathrm{d}\boldsymbol{p}_i \right) f_N, \tag{40}$$

where we have used that all particles are identical to pull out a combinatorial factor and to isolate the $\boldsymbol{r}_2$ and $\boldsymbol{p}_2$ coordinates. The reason for referring to this term as a *collision*, is because it accounts for interactions between two particles, as will become much clearer in Section III B. Recognizing the two-particle PDF

$$f_2(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{p}_1, \boldsymbol{p}_2, t) = N(N-1) \int \left(\prod_{i=3}^{N} \mathrm{d}\boldsymbol{r}_i \mathrm{d}\boldsymbol{p}_i \right) f_N, \tag{41}$$

the collision term reduces to

$$\left(\frac{\partial f_1}{\partial t} \right)_{\mathrm{coll}} = \int \mathrm{d}\boldsymbol{r}_2 \mathrm{d}\boldsymbol{p}_2 \, \boldsymbol{\nabla}_{\boldsymbol{r}_1} U(\boldsymbol{r}_1 - \boldsymbol{r}_2) \cdot \boldsymbol{\nabla}_{\boldsymbol{p}_1} f_2, \tag{42}$$

which allows us to write

$$\frac{\partial f_1}{\partial t} = \{H_1, f_1\} + \int \mathrm{d}\boldsymbol{r}_2 \mathrm{d}\boldsymbol{p}_2 \, \boldsymbol{\nabla}_{\boldsymbol{r}_1} U(\boldsymbol{r}_1 - \boldsymbol{r}_2) \cdot \boldsymbol{\nabla}_{\boldsymbol{p}_1} f_2; \tag{43}$$

one step closer to the Boltzmann transport equation. Note that Eq. (43) implies that, if we want to know how our one-particle PDF evolves, we still need information about the two-particle PDF. That was to be expected, since we have only rewritten the equations a bit and no information has been lost in the process.

One can now examine the evolution equation for the two-particle PDF. This, it turns out, depends on the three-particle PDF; unsurprisingly. In fact, playing this trick *ad nauseam* one arrives at a hierarchical form of the equations, namely the BBGKY hierarchy, that obeys the following structure

$$f_n(\{\boldsymbol{r}\}_n, \{\boldsymbol{p}\}_n, t) = \frac{N!}{(N-n)!} \int \left(\prod_{i=n+1}^{N} \mathrm{d}\boldsymbol{r}_i \mathrm{d}\boldsymbol{p}_i \right) f_N(\{\boldsymbol{r}\}_N, \{\boldsymbol{p}\}_N, t); \tag{44}$$

$$H_n(\{\boldsymbol{r}\}_n, \{\boldsymbol{p}\}_n, t) = \frac{1}{2m} \sum_{i=1}^{n} \boldsymbol{p}_i^2 + \sum_{i=1}^{n} V(\boldsymbol{r}_i, t) + \sum_{i=1}^{n} \sum_{j<i} U(\boldsymbol{r}_i - \boldsymbol{r}_j); \tag{45}$$

$$\frac{\partial}{\partial t} f_n(\{\boldsymbol{r}\}_n, \{\boldsymbol{p}\}_n, t) = \{H_n(\{\boldsymbol{r}\}_n, \{\boldsymbol{p}\}_n, t), f_n(\{\boldsymbol{r}\}_n, \{\boldsymbol{p}\}_n, t)\}$$

$$+ \sum_{i=1}^{n} \int \mathrm{d}\boldsymbol{r}_{n+1} \mathrm{d}\boldsymbol{p}_{n+1} \, \boldsymbol{\nabla}_{\boldsymbol{r}_i} U(\boldsymbol{r}_i - \boldsymbol{r}_{n+1}) \cdot \boldsymbol{\nabla}_{\boldsymbol{p}_i} f_{n+1}(\{\boldsymbol{r}\}_{n+1}, \{\boldsymbol{p}\}_{n+1}, t), \tag{46}$$

where we have maintained the full form of the expressions for the purposes of clarity and we have resorted to subscript notation to emphasize that there are "sets of vectors" $\{\boldsymbol{r}\}$ and $\{\boldsymbol{p}\}$ of different length.

> **Exercise 8**∗∗**:** Derive the BBGKY hierarchy from the definitions provided above and convince yourself that it has the structure given by Eqs. (44) - (46).

It seems that we have not accomplished much, since we now have a hierarchical set of equations that is no easier to solve than the evolution equation for the Hamiltonian itself. However, there are a few things worth noting that will help us reduce the set of BBGKY hierarchy drastically.

- The one-particle PDF, see Eq. (43), is special. It only has an interaction-energy related term in the collision operator. This is obvious, since a single particle does not interact with itself, which eliminates the interaction term from the streaming operator. However, it also implies that the rate of change in $f_1(\boldsymbol{r}_1, \boldsymbol{p}_1, t)$, is typically dominated by the collision term, as we will argue next. Note that $\boldsymbol{\nabla}_{\boldsymbol{r}_1} U(\boldsymbol{r}_1 - \boldsymbol{r}_2) \cdot \boldsymbol{\nabla}_{\boldsymbol{p}_1}$ has the dimensions of an inverse time—the other terms in the equation following from the application of the Poisson bracket naturally also have this dimensionality. This time we can identify as the typical time for an interaction to take place, τ_{coll}. To be more precise, when two particles with *short*-ranged interactions collide, the particles will interact over a length comparable to their diameter σ. The interaction time is given by $\tau_{\mathrm{coll}} \approx \sigma/\bar{v}_{\mathrm{rel}}$, with $\bar{v}_{\mathrm{rel}}$ the average speed between atoms. In a dilute gas at room temperature, say nitrogen, we have that $\sigma \approx 1.5 \times 10^{-10}$ m, while invoking equipartition, we further have $\bar{v}_{\mathrm{rel}} = \sqrt{3k_{\mathrm{B}}T/m} \approx 5 \times 10^2$ m/s, with k_{B} the Boltzmann constant and T the temperature, so that $\tau_{\mathrm{coll}} \approx 3 \times 10^{-13}$ s. By contrast, the time scale for non-collisional processes is controlled by the mean-free path length, $l \propto 1/(n\sigma^2)$, with n the particle density. In a typical gas at atmospheric pressure one finds $l \approx 10^{-7}$ m, implying that the time for these processes is a factor of 10^3 longer. Hence, we can safely state that the change in the one-particle PDF is dominated by collision processes.

- In writing the equations in a hierarchical form, one can more readily see that each subsequent level $(n + 1)$ of the hierarchy contributes less to the evolution of the n-particle PDF. Let us examine specifically the relation between the two- and three-particle PDFs, which one can readily obtain from Eqs. (44) - (46). Note that

$$\int \mathrm{d}\boldsymbol{r}_3 \mathrm{d}\boldsymbol{p}_3 f_3(\{\boldsymbol{r}\}_3, \{\boldsymbol{p}\}_3, t) = (N - 2) f_2(\{\boldsymbol{r}\}_2, \{\boldsymbol{p}\}_2, t) \approx N f_2(\{\boldsymbol{r}\}_2, \{\boldsymbol{p}\}_2, t) \tag{47}$$

where we integrate over all of phase space available to $\boldsymbol{r}_3$ and $\boldsymbol{p}_3$ and we use $N \gg 1$. Examining the right-hand side of Eq. (46) reveals that there is only a nonzero contribution to the integral in the collision term, whenever the particles interact. Assuming again that this interaction is short ranged—contributing only in a region in space, where the particles are separated by roughly their diameter σ—the total positional integral picks up a nonzero contribution over a region with volume $\approx \sigma^3$. This means that the collision term contributes by a factor of $\approx N\sigma^3/V$, where V is the volume of space, compared to the terms on the left-hand side. In this expression we recognize the particle volume fraction ϕ, which for realistic gases $\phi \approx 10^{-3}$.

These two points mean that one can truncate the hierarchy at first order to make progress, without losing too much detail, which is exactly what Boltzmann did. You might think that the two statements above contradict each other. That is, for the one-particle PDF, the two-particle PDF greatly affects the evolution through the collision term—it is, in fact, dominant—while for the relation between the two- and three-particle PDFs, the collision term is sub-dominant. The resolution to this apparent conflict is that the streaming term in the one-particle PDF does not contain interactions, while the two-particle PDF has interaction terms in the streaming Hamiltonian as well.

> **Exercise 9**∗**:** Write down the explicit forms of the first two terms in the BBGKY hierarchy and convince yourself that the above arguments hold. You can check your result against Eqs. (48) and (49), which provide these terms without the interaction-potential term included.

B. The Boltzmann Transport Equation

The idea to recover the Boltzmann transport equation is to rewrite Eq. (39) in terms of the one-particle PDFs alone. That is, to truncate the BBGKY hierarchy to first order and to close it using an approximate expression for the collision operator dependent on f_1 alone. One can see that this idea has merit: outside of the region where the particles interact, it is natural to write $f_2(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{p}_1, \boldsymbol{p}_2, t) = f_1(\boldsymbol{r}_1, \boldsymbol{p}_1, t) f_1(\boldsymbol{r}_2, \boldsymbol{p}_2, t)$ provided the positions and momenta are uncorrelated. Unfortunately, as we have just argued, it is exactly those bits of phase space where two particles interact, that contribute significantly to the collision term. We therefore have our work cut out for us.

We proceed by rewriting the first two terms in the BBGKY hierarchy, ignoring the external potential for simplicity. The first may be written as

$$\left(\frac{\partial}{\partial t} + \frac{1}{m}\boldsymbol{p}_1 \cdot \boldsymbol{\nabla}_{\boldsymbol{r}_1}\right) f_1 = \int \mathrm{d}\boldsymbol{r}_2 \mathrm{d}\boldsymbol{p}_2 \, \boldsymbol{\nabla}_{\boldsymbol{r}_1} U(\boldsymbol{r}_1 - \boldsymbol{r}_2) \cdot \boldsymbol{\nabla}_{\boldsymbol{p}_1} f_2 \tag{48}$$

Using our second argument concerning the weighting by volume fraction, we can neglect the collision term stemming from the three-particle PDF and write the second term in the hierarchy as

$$\left(\frac{\partial}{\partial t} + \frac{1}{m}\boldsymbol{p}_1 \cdot \boldsymbol{\nabla}_{\boldsymbol{r}_1} + \frac{1}{m}\boldsymbol{p}_2 \cdot \boldsymbol{\nabla}_{\boldsymbol{r}_2} - \boldsymbol{\nabla}_{\boldsymbol{r}_1} U(\boldsymbol{r}_1 - \boldsymbol{r}_2) \cdot \left(\boldsymbol{\nabla}_{\boldsymbol{p}_1} - \boldsymbol{\nabla}_{\boldsymbol{p}_2}\right)\right) f_2 \approx 0, \tag{49}$$

where we have manipulated the gradient of the potential to group the two gradients with respect to the momentum, introducing a minus sign and assuming a symmetric potential. Next, we substitute the center-of-mass and relative positions $\boldsymbol{R} \equiv (\boldsymbol{r}_1 + \boldsymbol{r}_2)/2$ and $\boldsymbol{r} \equiv \boldsymbol{r}_1 - \boldsymbol{r}_2$, respectively, as well as similar expressions for the momentum: $\boldsymbol{P} \equiv \boldsymbol{p}_1 + \boldsymbol{p}_2$ and $\boldsymbol{p} \equiv (\boldsymbol{p}_1 - \boldsymbol{p}_2)/2$. We can then write

$$f_2(\boldsymbol{R}, \boldsymbol{r}, \boldsymbol{P}, \boldsymbol{p}, t) \equiv f_2(\boldsymbol{R} + \boldsymbol{r}/2, \boldsymbol{R} - \boldsymbol{r}/2, \boldsymbol{P}/2 + \boldsymbol{p}, \boldsymbol{P}/2 - \boldsymbol{p}, t), \tag{50}$$

and for the gradient of the interaction potential $\boldsymbol{\nabla}_{\boldsymbol{r}_1} U(\boldsymbol{r}_1 - \boldsymbol{r}_2) = \boldsymbol{\nabla}_{\boldsymbol{r}} U(\boldsymbol{r})$. In addition, we have for the gradients of the momenta and position

$$\boldsymbol{\nabla}_{\boldsymbol{p}_1} - \boldsymbol{\nabla}_{\boldsymbol{p}_2} = \boldsymbol{\nabla}_{\boldsymbol{p}}; \tag{51}$$

$$\boldsymbol{p}_1 \cdot \boldsymbol{\nabla}_{\boldsymbol{r}_1} + \boldsymbol{p}_2 \cdot \boldsymbol{\nabla}_{\boldsymbol{r}_2} = \frac{1}{2}\boldsymbol{P} \cdot \boldsymbol{\nabla}_{\boldsymbol{R}} + 2\boldsymbol{p} \cdot \boldsymbol{\nabla}_{\boldsymbol{r}}, \tag{52}$$

so that Eq. (49) may be recast into the form

$$\left(\frac{\partial}{\partial t} + \frac{1}{2m}\boldsymbol{P} \cdot \boldsymbol{\nabla}_{\boldsymbol{R}} + \frac{2}{m}\boldsymbol{p} \cdot \boldsymbol{\nabla}_{\boldsymbol{r}} - \boldsymbol{\nabla}_{\boldsymbol{r}} U(\boldsymbol{r}) \cdot \boldsymbol{\nabla}_{\boldsymbol{p}}\right) f_2(\boldsymbol{R}, \boldsymbol{r}, \boldsymbol{P}, \boldsymbol{p}, t) = 0. \tag{53}$$

We now recognize that the interaction term only affects the relative coordinates, as expected on the basis of momentum and energy conservation. Note that in light of our first argument, which we can also apply to this situation, the rapid changes in $f_2(\boldsymbol{R}, \boldsymbol{r}, \boldsymbol{P}, \boldsymbol{p}, t)$ stem from the interaction terms. Therefore, the evolution of the center-of-mass coordinates in this PDF can be considered slow compared to the relative ones, *i.e.*, they are slave to the external force, which we ignored here.

Since the relative distributions in $f_2(\boldsymbol{R}, \boldsymbol{r}, \boldsymbol{P}, \boldsymbol{p}, t)$ vary more quickly than $f_1(\boldsymbol{r}_1, \boldsymbol{p}_1, t)$ itself, we may assume that on time scales relevant to the one-particle PDF, the two-particle PDF reaches an approximate equilibrium. This allows us to write

$$\left(\frac{2}{m}\boldsymbol{p} \cdot \boldsymbol{\nabla}_{\boldsymbol{r}} - \boldsymbol{\nabla}_{\boldsymbol{r}} U(\boldsymbol{r}) \cdot \boldsymbol{\nabla}_{\boldsymbol{p}}\right) f_2(\boldsymbol{R}, \boldsymbol{r}, \boldsymbol{P}, \boldsymbol{p}) \approx 0, \tag{54}$$

neglecting the slow variations in $\boldsymbol{R}$ and $\boldsymbol{P}$ and dropping the time dependence, because of the equilibrium assumption. Equation (54) is nothing more a streaming process that satisfies conservation of momentum and energy. This form now puts us in a position to rewrite the collision term in Eq. (42) as follows

$$\left(\frac{\partial f_1}{\partial t}\right)_{\mathrm{coll}} = \int \mathrm{d}\boldsymbol{r}_2 \mathrm{d}\boldsymbol{p}_2 \, \boldsymbol{\nabla}_{\boldsymbol{r}} U(\boldsymbol{r}) \cdot \left(\boldsymbol{\nabla}_{\boldsymbol{P}} + \frac{1}{2}\boldsymbol{\nabla}_{\boldsymbol{p}}\right) f_2(\boldsymbol{R}, \boldsymbol{r}, \boldsymbol{P}, \boldsymbol{p});$$

$$\approx \frac{1}{2} \int \mathrm{d}\boldsymbol{r}_2 \mathrm{d}\boldsymbol{p}_2 \, \boldsymbol{\nabla}_{\boldsymbol{r}} U(\boldsymbol{r}) \cdot \boldsymbol{\nabla}_{\boldsymbol{p}} f_2(\boldsymbol{R}, \boldsymbol{r}, \boldsymbol{P}, \boldsymbol{p});$$

$$\approx \frac{1}{m} \int \mathrm{d}\boldsymbol{r}_2 \mathrm{d}\boldsymbol{p}_2 \, \boldsymbol{p} \cdot \boldsymbol{\nabla}_{\boldsymbol{r}} f_2(\boldsymbol{R}, \boldsymbol{r}, \boldsymbol{P}, \boldsymbol{p}), \tag{55}$$

where in the first line we have substituted the relative coordinate notation, without transforming the integration, so that we avoid terms coming from the Jacobian of a coordinate transformation. In the second line, we have neglected the slow variations in the center-of-mass variables, and finally in the third line, we have employed our approximate expression (54). Note that while we have maintained our integration domain, it is clear that we only need to evaluate the $\boldsymbol{r}_2$ integral in Eq. (55) over a region $|\boldsymbol{r}_1 - \boldsymbol{r}_2| \lesssim \sigma$, where the gradient of the potential is nonzero, again employing the assumption that the interaction is short ranged.

We may now transition to a more convenient coordinate system to perform the necessary integrations. A rather obvious choice is cylindrical polar coordinates about the axis aligned with the direction specified by $\boldsymbol{p}$, as given by the unit vector $\hat{\boldsymbol{p}}$. Let $x \equiv \hat{\boldsymbol{p}} \cdot \boldsymbol{r}$ be the axial coordinate and let $\boldsymbol{b}$ map out the coordinates of planes perpendicular to this axis. Writing $p = \boldsymbol{p} \cdot \hat{\boldsymbol{p}}$, Eq. (55) reduces to

$$
\begin{aligned}
\left(\frac{\partial f_1}{\partial t}\right)_{\text{coll}} &\approx \frac{1}{m} \int \mathrm{d}\boldsymbol{p}_2 \, p \int_{-\infty}^{\infty} \mathrm{d}x \int \mathrm{d}\boldsymbol{b} \, \frac{\partial}{\partial x} f_2(\boldsymbol{R}, \boldsymbol{r}, \boldsymbol{P}, \boldsymbol{p}) \\
&= \frac{1}{m} \int \mathrm{d}\boldsymbol{p}_2 \, p \int \mathrm{d}\boldsymbol{b} \, \left(f_2(\boldsymbol{R}, \boldsymbol{r}_+, \boldsymbol{P}, \boldsymbol{p}) - f_2(\boldsymbol{R}, \boldsymbol{r}_-, \boldsymbol{P}, \boldsymbol{p})\right),
\end{aligned}
\tag{56}
$$

where we have kept the approximate sign in the first line to indicate that in obtaining this result, we have already made use of several approximations. In the second line, we integrate over the derivative to arrive at a difference between two-particle PDFs in the relative coordinates. These are the $\boldsymbol{r}$s just before the particles come into the interaction range, $\boldsymbol{r}_-$, and the ones that they have just after $\boldsymbol{r}_+$ exiting this range, respectively.

To rewrite Eq. (56) further, we use that Eq. (54) can be used to relate the PDF at different points in phase space and that interactions preserve the total momentum and center-of-mass coordinates. This means that there is a relative momentum, say $\boldsymbol{p}'$, at $\boldsymbol{r}_-$, for which $f_2(\boldsymbol{R}, \boldsymbol{r}_-, \boldsymbol{P}, \boldsymbol{p}') = f_2(\boldsymbol{R}, \boldsymbol{r}_+, \boldsymbol{P}, \boldsymbol{p})$. The relation between $\boldsymbol{p}$ and $\boldsymbol{p}'$ can be made explicit by integrating over the equations of motion, which is difficult in general, but will not turn out to be necessary. Using this equivalence leads to

$$
\left(\frac{\partial f_1}{\partial t}\right)_{\text{coll}} \approx \frac{1}{m} \int \mathrm{d}\boldsymbol{p}_2 \, p \int \mathrm{d}\boldsymbol{b} \, \left(f_2(\boldsymbol{R}, \boldsymbol{r}_-, \boldsymbol{P}, \boldsymbol{p}') - f_2(\boldsymbol{R}, \boldsymbol{r}_-, \boldsymbol{P}, \boldsymbol{p})\right),
\tag{57}
$$

where we now evaluate both f_2s at the same value of $\boldsymbol{r} = \boldsymbol{r}_-$, allowing us to rewrite the remaining bit of the positional integral (over $\boldsymbol{b}$).

Invoking conservation laws, which Eq. (53) obeys, the impact of two particles can only lead to a reorientation of $\boldsymbol{p}'$ to $\boldsymbol{p}$, since the magnitude of the relative momentum remains unaffected. That is $\boldsymbol{p}$, which is aligned along the axis of our coordinate system, is reoriented to a direction $\boldsymbol{p}'$ given by a solid angle $\hat{\boldsymbol{\Omega}}$ in spherical polars. This $\hat{\boldsymbol{\Omega}}$ has a one-to-one correspondence to $\boldsymbol{b}$, which enables us to perform another coordinate transformation, of which the exact shape is not known to us, but we know it exists, because of the one-to-one relation. This transformation gives rise to the following form of the collision term

$$
\left(\frac{\partial f_1}{\partial t}\right)_{\text{coll}} \approx \int \mathrm{d}\boldsymbol{p}_2 \int \mathrm{d}\hat{\boldsymbol{\Omega}} \, \frac{p}{m} \left|\det\left(\frac{D\boldsymbol{b}}{D\hat{\boldsymbol{\Omega}}}\right)\right| \left(f_2(\boldsymbol{R}, \boldsymbol{r}_-, \boldsymbol{P}, \boldsymbol{p}') - f_2(\boldsymbol{R}, \boldsymbol{r}_-, \boldsymbol{P}, \boldsymbol{p})\right).
\tag{58}
$$

So, what has this really solved? We have gone through several transformations of frame and are seemingly no closer to obtaining a sensible form of the collision term. However, we are actually almost done, the grouping

$$
\frac{p}{m} \left|\det\left(\frac{D\boldsymbol{b}}{D\hat{\boldsymbol{\Omega}}}\right)\right| \mathrm{d}\hat{\boldsymbol{\Omega}}
\tag{59}
$$

has a physical interpretation, namely that of the differential cross section weighted with the incoming particle flux. If we consider the frame in which particle 1 is stationary, then it is clear that the combination $(p/m)\mathrm{d}\boldsymbol{b}$ is nothing more than the flux of particles coming into the area element $\mathrm{d}\boldsymbol{b}$ around $\boldsymbol{b}$, which itself indicates how off center two particles impact. The coordinate transformation (59) indicates to where ($\hat{\boldsymbol{\Omega}}$) these incoming particles are scattered. The coordinate transformation thereby implicitly contains all the information on the nature of our interaction potential.

Exercise 10*: In this exercise we aim to gain additional insight into the concept of the differential cross section. Draw the picture that corresponds to the scattering of one particle off of a stationary second particle and use it to gain intuition for the meaning of the transformation from $\boldsymbol{b}$ to $\hat{\boldsymbol{\Omega}}$. It is useful to write d$\boldsymbol{b}$ in cylindrical polar coordinates as $\mathrm{d}\boldsymbol{\sigma} = b\,\mathrm{d}b\,\mathrm{d}\phi$ with ϕ the azimuthal angle, and $\mathrm{d}\hat{\boldsymbol{\Omega}}$ in spherical polar coordinates as $\mathrm{d}\hat{\boldsymbol{\Omega}} = \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$, with θ the polar angle. The use of the symbol $\boldsymbol{\sigma}$ is a historic convention in the field and is not, in any way, related to the Cauchy stress tensor or the typical notation for the diameter of a hard sphere σ. The differential cross section may now be cast in the traditional form as

$$\left| \det\left(\frac{D\boldsymbol{b}}{D\hat{\boldsymbol{\Omega}}} \right) \right| \equiv \left| \frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}\hat{\boldsymbol{\Omega}}} \right| = \frac{b}{\sin\theta} \left| \frac{\mathrm{d}b}{\mathrm{d}\theta} \right| = \frac{1}{2} \left| \frac{\mathrm{d}b^2}{\mathrm{d}\cos\theta} \right|, \tag{60}$$

Compute the differential cross section for hard spheres with diameter σ and show that it is given by $\sigma^2/16$, which leads to a total cross section of

$$\int \mathrm{d}\hat{\boldsymbol{\Omega}} \left| \frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}\hat{\boldsymbol{\Omega}}} \right| = \frac{\pi\sigma^2}{4}; \tag{61}$$

exactly the projected area of the sphere stationary sphere onto a plane. Equation (61) thus gives information on what the interaction with the stationary object looks like on average to incoming particles. In the case of a hard sphere, it is a disk and the differential cross section is independent of θ and the speed of impact p/m. This is a rather unusual situation. Next, compute the differential cross section for Coulombic scattering of unit charges in vacuum, where you can use $U(\boldsymbol{r}) = \kappa/r$ for the interaction potential, with $\kappa = e^2/(4\pi\epsilon_0)$, e the elementary charge, and ϵ_0 the vacuum permittivity. Then the differential cross section becomes

$$\left| \frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}\hat{\boldsymbol{\Omega}}} \right| = \left(\frac{\kappa}{4E_\infty} \frac{1}{\sin^2(\theta/2)} \right)^2, \tag{62}$$

with $E_\infty = p_\infty^2/(2m)$ the kinetic energy of the incoming particle at infinity. You may want to consult Ref. [15] before embarking on this calculation, since scattering theory is a subject unto itself. Historically, this form was used by Rutherford to characterize the scattering experiments by Geiger and Marsden of alpha particles on a thin gold film [13], which revealed that the nucleus of an atom is less than 2.7×10^{-14} m in diameter.

The combination of the two, as given by Eq. (59), is the rate with which two particles with $\boldsymbol{r}$ and $\boldsymbol{p}$ transition through a collision to a state with the same $\boldsymbol{r}$, but $\boldsymbol{p}'$. Let this transition rate be given by $\omega(\boldsymbol{p}, \boldsymbol{p}')$, then one obtains

$$\left(\frac{\partial f_1}{\partial t} \right)_{\mathrm{coll}} \approx \int \mathrm{d}\boldsymbol{p}_2 \int \mathrm{d}\boldsymbol{p}' \, \omega(\boldsymbol{p}, \boldsymbol{p}') \left(f_2(\boldsymbol{R}, \boldsymbol{r}_-, \boldsymbol{P}, \boldsymbol{p}') - f_2(\boldsymbol{R}, \boldsymbol{r}_-, \boldsymbol{P}, \boldsymbol{p}) \right);$$

$$\approx \int \mathrm{d}\boldsymbol{p}_2 \int \mathrm{d}\boldsymbol{p}' \, \omega(\boldsymbol{p}, \boldsymbol{p}') \left(f_2(\boldsymbol{R}, \boldsymbol{r}, \boldsymbol{P}, \boldsymbol{p}') - f_2(\boldsymbol{R}, \boldsymbol{r}, \boldsymbol{P}, \boldsymbol{p}) \right), \tag{63}$$

where in going to the second line, we have used the point-particle approximation $\boldsymbol{r} \approx \boldsymbol{r}_-$, *i.e.*, that the range over which the scattering events takes place is very limited in terms of the variations of f_1.

One more step remains, which is known as *molecular chaos*, which traces its origins back to the early work of Maxwell on the kinetic theory of gasses [16]. Molecular chaos implies that just before particles enter a collision, they are uncorrelated. This seems reasonable, since it these two particles are unlikely to come from a previous scattering event, during which they became correlated. Moreover, between subsequent collision events the motion of the particles can become decorrelated again. Invoking molecular chaos allows us to write

$$f_2(\boldsymbol{R}, \boldsymbol{r}, \boldsymbol{P}, \boldsymbol{p}) = f_1(\boldsymbol{r}_1, \boldsymbol{p}_1) f_1(\boldsymbol{r}_2, \boldsymbol{p}_2); \tag{64}$$

$$f_2(\boldsymbol{R}, \boldsymbol{r}, \boldsymbol{P}, \boldsymbol{p}') = f_1(\boldsymbol{r}_1, \boldsymbol{p}_1') f_1(\boldsymbol{r}_2, \boldsymbol{p}_2'), \tag{65}$$

where the coordinates are such that $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$, $\boldsymbol{p} = (\boldsymbol{p}_1 - \boldsymbol{p}_2)/2$, $\boldsymbol{p}' = (\boldsymbol{p}_1' - \boldsymbol{p}_2')/2$, $\boldsymbol{R} \equiv (\boldsymbol{r}_1 + \boldsymbol{r}_2)/2$, and $\boldsymbol{P} \equiv \boldsymbol{p}_1 + \boldsymbol{p}_2 = \boldsymbol{p}_1' + \boldsymbol{p}_2'$. Introducing these expressions into Eq. (63) gives us the collision term in the famous

Boltzmann equation

$$\frac{\partial f_1}{\partial t}(\boldsymbol{r},\boldsymbol{p},t) = \{H_1(\boldsymbol{r},\boldsymbol{p},t), f_1(\boldsymbol{r},\boldsymbol{p},t)\} + \left(\frac{\partial f_1}{\partial t}\right)_{\text{coll}}; \tag{66}$$

$$\left(\frac{\partial f_1}{\partial t}\right)_{\text{coll}} \approx \int\!\mathrm{d}\boldsymbol{p}_2 \int\!\mathrm{d}\boldsymbol{p}' \int\!\mathrm{d}\boldsymbol{p}_2'\, \omega(\boldsymbol{p}-\boldsymbol{p}_2,\boldsymbol{p}'-\boldsymbol{p}_2') \left(f_1(\boldsymbol{r},\boldsymbol{p}')f_1(\boldsymbol{r},\boldsymbol{p}_2') - f_1(\boldsymbol{r},\boldsymbol{p})f_1(\boldsymbol{r},\boldsymbol{p}_2)\right), \tag{67}$$

where we have slightly abused notation. That is, in the streaming operation, we only have a single position and momentum coordinate, hence we may use $\boldsymbol{r}$ and $\boldsymbol{p}$ without any indices, with $\boldsymbol{r}$ indicating a regular coordinate here, not a relative one. In the collision operator, we have two position and momentum coordinates. However, we have already seen that only those parts where $|\boldsymbol{r}_1 - \boldsymbol{r}_2| \lesssim \sigma$ contribute to the collision, so that we can write $\boldsymbol{r}_1 \approx \boldsymbol{r}_2 \equiv \boldsymbol{r}$. A final note on the rewrites that have taken place above, is that in introducing the transition rate $\omega(\boldsymbol{p}-\boldsymbol{p}_2,\boldsymbol{p}'-\boldsymbol{p}_2')$ and changing the integrations, we have—by writing a double integral over $\boldsymbol{p}'$ and $\boldsymbol{p}_2'$—obscured the explicit conditions of conservation of momentum and energy, which originally led to a two-dimensional integral over $\hat{\boldsymbol{\Omega}}$. However, this is not an issue, as it is taken care of by the four constraints that these two conservation principles impose on the form of the transition rate ω. It can be helpful to use the definition with integration over $\boldsymbol{p}$ and $\hat{\boldsymbol{\Omega}}$ interchangeably, suiting the needs of a specific calculation.

Equations (66) and (67) are very useful, even if the derivation of this closed form makes use of a long series of truncations and estimates. Full rigor in deriving the Boltzmann transport equation with appropriate estimates for all errors that are incurred in making approximations along the way is possible, *e.g.*, see Ref. [17] for a slightly more mathematically inclined derivation, but much of this serves only to convolute an already difficult to follow set of physical arguments. This is something that at least some of the followers of Boltzmann's work realized: Einstein has ascribed the quote "*Eleganz sei die Sache der Schuster und Schneider*" to Boltzmann [18], which translates to English as "*Elegance should be left to shoemakers and tailors*"; although no record exists of him having uttered these words.

C. The H-Theorem

Regardless of your views on the rigor of the derivation of the Boltzmann transport equation presented in Section III B, and we will come back to this, there is something worth noting that sneaked in the back door. We know there is no arrow of time in the Hamiltonian formalism. Classical mechanics allows you to turn back the clock to return to an initial condition, without loss of information. Yet, as we will see, that is not the case with the Boltzmann transport equation, which reflected in the second law of thermodynamics. How does this come about?

Let us first consider the condition for equilibrium, which may be expressed as $\partial f_1^{\text{eq}}/\partial t = 0$. From the form of the Liouville equation (28), a sufficient criterion for getting rid of the streaming term in the Boltzmann equation (66) is to make f_1^{eq} a function of the Hamiltonian H_1 or some function that Poisson commutes with this Hamiltonian. That leaves us the collision term (67), which we worked so hard towards deriving. An obvious way to make this term disappear is to write the condition for detailed balance

$$f_1^{\text{eq}}(\boldsymbol{r},\boldsymbol{p}')f_1^{\text{eq}}(\boldsymbol{r},\boldsymbol{p}_2') = f_1^{\text{eq}}(\boldsymbol{r},\boldsymbol{p})f_1^{\text{eq}}(\boldsymbol{r},\boldsymbol{p}_2), \tag{68}$$

which can be recast in a logarithmic form as

$$\log\left(f_1^{\text{eq}}(\boldsymbol{r},\boldsymbol{p}')\right) + \log\left(f_1^{\text{eq}}(\boldsymbol{r},\boldsymbol{p}_2')\right) = \log\left(f_1^{\text{eq}}(\boldsymbol{r},\boldsymbol{p})\right) + \log\left(f_1^{\text{eq}}(\boldsymbol{r},\boldsymbol{p}_2)\right). \tag{69}$$

The challenge now lies in finding a form for $\log f_1^{\text{eq}}$, such that the equality in Eq. (69) holds for all momenta. Thinking in terms of collisions helps again, because we know the momentum and energy are conserved during such processes. Therefore, the general form of the distribution should take the form

$$\log\left(f_1^{\text{eq}}(\boldsymbol{r},\boldsymbol{p})\right) = \beta\left(\mu - E(\boldsymbol{p}) + \boldsymbol{u}\cdot\boldsymbol{p}\right), \tag{70}$$

where β is a prefactor with dimension of inverse energy, μ is sets the base energy level and is related to the normalization of f_1^{eq}, $E(\boldsymbol{p})$ is the kinetic energy, as before, and $\boldsymbol{u}$ a constant vector with the dimension of velocity, which will turn out to be related to the average velocity. Writing $\boldsymbol{p} = m\boldsymbol{v}$ and setting μ based on the normalization of f_1^{eq} gives us

$$f_1^{\text{eq}}(\boldsymbol{p}) = n\left(\frac{\beta}{2\pi m}\right)^{3/2} \exp\left(-\beta m\left(\boldsymbol{v}-\boldsymbol{u}\right)\right) \tag{71}$$

with $\rho \equiv N/V$ the particle density, after integrating over $\boldsymbol{r}$. This is simply the Maxwell-Boltzmann distribution, when we identify $\beta = 1/(k_{\text{B}}T)$ and $\boldsymbol{u}$ as a drift velocity.

Exercise 11**: Convince yourself of the accuracy of the above result (71) and generalize it by dropping the requirement of f_1 Poisson commuting with the Hamiltonian. The result you should obtain may be written

$$f_1^{\mathrm{loc}}(\boldsymbol{r}, \boldsymbol{p}) = n(\boldsymbol{r}, t) \left(\frac{\beta(\boldsymbol{r}, t)}{2\pi m} \right)^{3/2} \exp\left(-\beta(\boldsymbol{r}, t) m \left(\boldsymbol{v} - \boldsymbol{u}(\boldsymbol{r}, t) \right) \right) \tag{72}$$

This form satisfies detailed balance, but is no longer in global equilibrium, since it has a non-zero streaming term. Verify this as well. The solution turns out to describe local equilibrium, for which transport of density, momentum, and energy is possible.

Exercise 12*: For quantum-mechanical systems the collision operator in the integrand of Eq. (67) may be written as

$$\omega(\boldsymbol{p} - \boldsymbol{p}_2, \boldsymbol{p}' - \boldsymbol{p}_2') \bigg(\left(1 \pm f_1(\boldsymbol{r}, \boldsymbol{p}) \right) \left(1 \pm f_1(\boldsymbol{r}, \boldsymbol{p}_2) \right) f_1(\boldsymbol{r}, \boldsymbol{p}_2') f_1(\boldsymbol{r}, \boldsymbol{p}')$$

$$- \left(1 \pm f_1(\boldsymbol{r}, \boldsymbol{p}') \right) \left(1 \pm f_1(\boldsymbol{r}, \boldsymbol{p}_2') \right) f_1(\boldsymbol{r}, \boldsymbol{p}_2) f_1(\boldsymbol{r}, \boldsymbol{p}) \bigg), \tag{73}$$

where the "+" variant accounts for bosons and the "−" one for fermions, see also Ref. [19]. Provide physical arguments why the collision kernel should have this form. Next use the form of Eq. (73) and the condition of detailed balance to derive the Bose-Einstein and Fermi-Dirac distributions

$$f_1^{\mathrm{eq}}(\boldsymbol{p}) = \left(\exp\left(-\beta \left(\mu - E(\boldsymbol{p}) + \boldsymbol{u} \cdot \boldsymbol{p} \right) \right) \mp 1 \right)^{-1}, \tag{74}$$

which may also be generalized into a local equilibrium form.

Now that we have seen the equilibrium distribution, let us turn to the question: "How do things brought out of equilibrium settle back into equilibrium?" Provided we are not actively driving the system, thereby maintaining an out-of-equilibrium state, it is intuitively clear that the system should reach a state of equilibrium. But this is where the issues with an arrow of time come into play. Reversing time, we find that the system that has reached equilibrium, remains in equilibrium.

In our discussion of equilibrium, we have seen that $\log f_1$ is a measure for kinetic energy in the system, so that the combination

$$\mathcal{H}(t) = \int \mathrm{d}\boldsymbol{r} \mathrm{d}\boldsymbol{p} \, f_1 \log f_1, \tag{75}$$

can be seen as the expectation value of this energy. It should also look very familiar, since this is, in fact, the definition of entropy S, barring a prefactor $-k_{\mathrm{B}}$. We want to examine the quantity $\mathcal{H}$, because—as we will see—it is a constant in (local) equilibrium and when the system is taken out of equilibrium, its value is indicative of how great the deviation from the Maxwell-Boltzmann distribution is. Thus, examining the time dependence of $\mathcal{H}$ will give us information on how the non-equilibrium distribution relaxes towards equilibrium. A pleasant feature of this way of charting the deviation from the Maxwell-Boltzmann distribution, it turns out, is that any deviation from (local) equilibrium leads to a strictly positive difference, which means that $\mathcal{H}$ decreases when the system relaxes towards equilibrium.

Taking the time derivative of the quantity $\mathcal{H}$ we find

$$\frac{d\mathcal{H}}{dt}(t) = \int \mathrm{d}\boldsymbol{r} \mathrm{d}\boldsymbol{p} \, (\log f_1 + 1) \frac{\partial f_1}{\partial t}$$

$$= \int \mathrm{d}\boldsymbol{r} \mathrm{d}\boldsymbol{p} \, \log f_1 \left(\{H_1, f_1\} + \left(\frac{\partial f_1}{\partial t} \right)_{\mathrm{coll}} \right), \tag{76}$$

where we can drop the addition by 1 in the first line, since the time derivative of the integral over f_1 is zero, and in the second line we have used the Boltzmann equation.

Exercise 13*: Show that the integration of $\log f_1$ multiplied with the Poisson bracket in Eq. (76) vanishes.

Rewriting Eq. (76) a bit using the definition of the collision operator, gives us the following expression

$$\frac{d\mathcal{H}}{dt}(t) = \int d\boldsymbol{r} d\boldsymbol{p} d\boldsymbol{p}_2 d\boldsymbol{p}' d\boldsymbol{p}_2' \, \omega(\boldsymbol{p} - \boldsymbol{p}_2, \boldsymbol{p}' - \boldsymbol{p}_2') \log\left(f_1(\boldsymbol{r}, \boldsymbol{p})\right) \left(f_1(\boldsymbol{r}, \boldsymbol{p}') f_1(\boldsymbol{r}, \boldsymbol{p}_2') - f_1(\boldsymbol{r}, \boldsymbol{p}) f_1(\boldsymbol{r}, \boldsymbol{p}_2)\right), \tag{77}$$

All momenta are integrated over, so that when we perform the exchange $\boldsymbol{p} \leftrightarrow \boldsymbol{p}_2$, we obtain the exact same result. Summing these expressions and dividing by two gives

$$\frac{d\mathcal{H}}{dt}(t) = \frac{1}{2} \int d\boldsymbol{r} d\boldsymbol{p} d\boldsymbol{p}_2 d\boldsymbol{p}' d\boldsymbol{p}_2' \, \omega(\boldsymbol{p} - \boldsymbol{p}_2, \boldsymbol{p}' - \boldsymbol{p}_2') \log\left(f_1(\boldsymbol{r}, \boldsymbol{p}) f_1(\boldsymbol{r}, \boldsymbol{p}_2)\right)$$
$$\times \left(f_1(\boldsymbol{r}, \boldsymbol{p}') f_1(\boldsymbol{r}, \boldsymbol{p}_2') - f_1(\boldsymbol{r}, \boldsymbol{p}) f_1(\boldsymbol{r}, \boldsymbol{p}_2)\right). \tag{78}$$

Repeating the process of exchange with the primed and unprimed indices yields again the same result—there is a minus sign introduced by the term depending on the products of f_1; ω is symmetric under the exchange—and this leads the following symmetrized expression

$$\frac{d\mathcal{H}}{dt}(t) = -\frac{1}{4} \int d\boldsymbol{r} d\boldsymbol{p} d\boldsymbol{p}_2 d\boldsymbol{p}' d\boldsymbol{p}_2' \, \omega(\boldsymbol{p} - \boldsymbol{p}_2, \boldsymbol{p}' - \boldsymbol{p}_2')$$
$$\times \left(\log\left(f_1(\boldsymbol{r}, \boldsymbol{p}') f_1(\boldsymbol{r}, \boldsymbol{p}_2')\right) - \log\left(f_1(\boldsymbol{r}, \boldsymbol{p}) f_1(\boldsymbol{r}, \boldsymbol{p}_2)\right)\right)$$
$$\times \left(f_1(\boldsymbol{r}, \boldsymbol{p}') f_1(\boldsymbol{r}, \boldsymbol{p}_2') - f_1(\boldsymbol{r}, \boldsymbol{p}) f_1(\boldsymbol{r}, \boldsymbol{p}_2)\right). \tag{79}$$

Realizing that a function of the form $(\log x - \log y)(x - y)$ is always positive for x and $y \geq 0$[3] and that the scattering rate is positive (or zero), we find that

$$\frac{d\mathcal{H}}{dt}(t) \leq 0, \tag{80}$$

which translates into the well-known condition $dS/dt \geq 0$, *i.e.*, the second law of thermodynamics. Note further that by definition, any equilibrium distribution, or in fact any distribution, for which $(\partial f_1/\partial t)_{\text{coll}} = 0$ (local equilibrium), has the property that $d\mathcal{H}/dt = 0$. This means that the equilibrium state minimizes the $\mathcal{H}$ function or, equivalently, maximizes the entropy. That is, $\mathcal{H}$ decreases steadily from a non-equilibrium value until it reaches equilibrium.

Now that we have the $\mathcal{H}$ function and its properties, it is possible to revisit our derivation of the Boltzmann equation and pinpoint the location where irreversibility enters. It turns out (unsurprisingly) that imposing condition molecular chaos, namely that the momenta of colliding particles are uncorrelated and independent of position, eventually leads to Eq. (80). If, instead, one had imposed that particles exiting a collision are decorrelated, then one would have obtained an increasing $\mathcal{H}$. Indeed, this issue led to Boltzmann's work receiving a healthy and not undeserved dose of criticism, with the most well-known counterarguments given by Loschmidt (Loschmidt's Paradox) and Zemelo through application of Poincaré recurrence. In any finite system, the value of $\mathcal{H}$ can and will go up, as there are fluctuations from the mean, so that the statements concerning an ever-decreasing value of $\mathcal{H}$ only hold in the thermodynamic limit. In finite systems, the extreme fluctuations necessary to return to a highly localized initial state become increasingly less likely with increasing N. Ultimately, these issues were more elegantly addressed by Josiah Gibbs [20] and Edwin Jaynes [21], leading to the modern formulation of (equilibrium) statistical mechanics that is based on state-counting arguments.

Boltzmann's efforts, although not perfect, were instrumental to proving the second law of thermodynamics. In addition, his approach includes out-of-equilibrium properties in a natural way, and clearly shows how these give rise to limiting equilibrium behaviors. Moreover, the condition of detailed balance, which lies at the heart of statistical-mechanics inspired phase-space integrators, such as Metropolis Monte Carlo [22], appear along the way. Finally, the Boltzmann transport equation bridges the microscopic theory of molecular motion and macroscopic transport descriptions, as we will explore further in Section III D. This has greatly benefited the development of fast means to describe transport phenomena in a wide range of applications, from quantum, to classical, and to relativistic systems.

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[3] For a fixed value of one of the variables, this function assumes its minimum in $x = y$, for which it is zero. Evaluating the function in any other point $x \geq 0$ (if y is fixed and vice versa) leads to a positive value, hence the function is strictly positive on the quadrant of interest.

D.   From The Boltzmann Transport Equation to Hydrodynamics

The idea behind recovering hydrodynamics from the Boltzmann transport equation has been hinted at several times. Thus far, we have successively thrown away faster modes of decay in our system, favoring on larger length and longer time scales those quantities that are weakly affected by higher-order collisions. The same holds for recovering the hydrodynamic equations. We are interested in quantities that vary slowly over space and time, at least compared to the collision processes. This implies that we are interested in the average of quantities with respect to the momentum.

Let Q be a function of $\boldsymbol{r}$ and $\boldsymbol{p}$, then its average with respect to momentum is given by

$$\langle Q \rangle_{\boldsymbol{p}}(\boldsymbol{r}, t) = \frac{\int \mathrm{d}\boldsymbol{p}\, Q f_1}{\int \mathrm{d}\boldsymbol{p}\, f_1} = \frac{1}{n(\boldsymbol{r}, t)} \int \mathrm{d}\boldsymbol{p}\, Q f_1, \tag{81}$$

where we have dropped the subscript 1 from the position and momentum notation, since we are working with a single f_1 for now. Also, we have introduced the subscript $\boldsymbol{p}$ for our averaging bracket notation to distinguish this momentum average from the phase-space average introduced in Eq. (31). Because, the density $n(\boldsymbol{r}, t)$ is independent of the momentum, we can pull it into the integral and write

$$\langle nQ \rangle_{\boldsymbol{p}}(\boldsymbol{r}, t) = \int \mathrm{d}\boldsymbol{p}\, Q f_1. \tag{82}$$

Taking the time derivative leads to

$$\begin{aligned}
\frac{\partial \langle nQ \rangle_{\boldsymbol{p}}}{\partial t}(\boldsymbol{r}, t) &= \int \mathrm{d}\boldsymbol{p}\, \frac{\partial}{\partial t}(Q f_1) = \int \mathrm{d}\boldsymbol{p}\, Q \left(\frac{\partial f_1}{\partial t} \right) = \int \mathrm{d}\boldsymbol{p}\, Q \left(\{H_1, f_1\} + \left(\frac{\partial f_1}{\partial t} \right)_{\mathrm{coll}} \right) \\
&= -\int \mathrm{d}\boldsymbol{p}\, Q \left(\frac{\boldsymbol{p}}{m} \cdot \boldsymbol{\nabla_r} + \boldsymbol{F} \cdot \boldsymbol{\nabla_p} \right) f_1 + \int \mathrm{d}\boldsymbol{p}\, Q \left(\frac{\partial f_1}{\partial t} \right)_{\mathrm{coll}} \\
&= -\boldsymbol{\nabla_r} \cdot \langle n\boldsymbol{v}Q \rangle_{\boldsymbol{p}} + \langle n\boldsymbol{v} \cdot \boldsymbol{\nabla_r} Q \rangle_{\boldsymbol{p}} + \langle n\boldsymbol{F} \cdot \boldsymbol{\nabla_p} Q \rangle_{\boldsymbol{p}} + \int \mathrm{d}\boldsymbol{p}\, Q \left(\frac{\partial f_1}{\partial t} \right)_{\mathrm{coll}}
\end{aligned} \tag{83}$$

where we have reintroduced $\boldsymbol{F} = -\boldsymbol{\nabla_r} \Phi$ the force coming from the external potential in the second line, the velocity $\boldsymbol{v} \equiv \boldsymbol{p}/m$ in the third, and we have use integration by parts and a rewrite of the divergence of f_1 to arrive the final expression. This implies the following equality

$$\frac{\partial \langle nQ \rangle_{\boldsymbol{p}}}{\partial t} + \boldsymbol{\nabla_r} \cdot \langle n\boldsymbol{v}Q \rangle_{\boldsymbol{p}} - \langle n\boldsymbol{v} \cdot \boldsymbol{\nabla_r} Q \rangle_{\boldsymbol{p}} - \langle n\boldsymbol{F} \cdot \boldsymbol{\nabla_p} Q \rangle_{\boldsymbol{p}} = \int \mathrm{d}\boldsymbol{p}\, Q \left(\frac{\partial f_1}{\partial t} \right)_{\mathrm{coll}}. \tag{84}$$

If we now focus only on those quantities that are left invariant under the collision: the identity, momentum, and energy, we will obtain the desired hydrodynamic transport equations. As we have argued before, in these cases the right-hand side of Eq. (84) is zero.

> **Exercise 14*:** Perform the algebraic manipulations necessary to show that collisional invariants, *i.e.*, those quantities that result in a vanishing right-hand side in Eq. (84), satisfy the equation
>
> $$Q(\boldsymbol{r}, \boldsymbol{p}) + Q(\boldsymbol{r}, \boldsymbol{p}_2) = Q(\boldsymbol{r}, \boldsymbol{p}') + Q(\boldsymbol{r}, \boldsymbol{p}_2') \tag{85}$$
>
> which is unsurprisingly similar to the form which we obtained in deriving the equilibrium Maxwell-Boltzmann distribution.

Now we go through the list of conserved quantities. Setting $Q = m$[4] we obtain

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla_r} \cdot (\rho \boldsymbol{u}) = 0, \tag{86}$$

with $\boldsymbol{u} \equiv \langle \boldsymbol{v} \rangle_{\boldsymbol{p}}$ the average velocity of the particles at $(\boldsymbol{r}, t)$ and ρ the particle mass density. This is the same result as Eq. (9). The definition of $\boldsymbol{u}$ and is consistent with the definition of the local-equilibrium distribution that can be derived from the collision term, see Eq. (72).

---

[4] If unity is conserved, then unity times the particle mass is too.

Next, we consider the momentum, so that $Q = \boldsymbol{p}$. Note that we have thus far not considered the average of vector quantities and implicitly used this assumption in deriving the form of Eq. (84). We therefore work with component notation here, make use of moving a m from a $\boldsymbol{p}$ onto an n to obtain a mass density ρ, and that ρ. Doing so, we arrive at

$$\frac{\partial \langle \rho v_i \rangle_{\boldsymbol{p}}}{\partial t} + \sum_{j=1}^{3} \frac{\partial}{\partial r_j} \langle \rho v_j v_i \rangle_{\boldsymbol{p}} - \left\langle \frac{\rho}{m} F_i \right\rangle_{\boldsymbol{p}} = 0, \tag{87}$$

where one can rewrite the term $\rho \langle v_j v_i \rangle_{\boldsymbol{p}} = \rho \langle (v_j - u_j)(v_i - u_i) \rangle_{\boldsymbol{p}} + \rho u_j u_i \equiv -\sigma_{ji} + \rho u_j u_i$, by recognizing the Cauchy stress tenor[5]. Note that $\sigma_{ij} = \sigma_{ji}$ per definition and we now find

$$\frac{\partial \rho u_i}{\partial t} + \sum_{j=1}^{3} \frac{\partial}{\partial r_j} \left(-\sigma_{ji} + \rho u_j u_i \right) - \frac{\rho}{m} F_i = 0 \Rightarrow \tag{88}$$

$$\rho \left(\frac{\partial}{\partial t} + \sum_{j=1}^{3} u_j \frac{\partial}{\partial r_j} \right) u_i = \sum_{j=1}^{3} \frac{\partial}{\partial r_j} \sigma_{ij} + \frac{\rho}{m} F_i \Rightarrow \tag{89}$$

$$\rho \left(\frac{\partial}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla_r} \right) \boldsymbol{u} = \boldsymbol{\nabla_r} \underline{\boldsymbol{\sigma}} + \boldsymbol{f}, \tag{90}$$

where we have made use of Eq (86) to cross off terms that resulted from applying the product rule to arrive at the second line, and we transition to vector notation in the third, identifying the body force on the fluid $\boldsymbol{f} \equiv (\rho/m)\boldsymbol{F}$.

Exercise 15*: Derive the form of the energy transport equation. Start from the kinetic energy $Q = E = (m/2)|\boldsymbol{v}|^2$ and introduce the following equivalences

$$\frac{3}{2} m k_B T = \frac{1}{2} \left\langle |\boldsymbol{v} - \boldsymbol{u}|^2 \right\rangle_{\boldsymbol{p}}; \tag{91}$$

$$\boldsymbol{q} = \frac{1}{2} \rho \left\langle |\boldsymbol{v} - \boldsymbol{u}|^2 (\boldsymbol{v} - \boldsymbol{u}) \right\rangle_{\boldsymbol{p}}, \tag{92}$$

where the first is the local temperature (inspired by equipartition) and the second is the heat flux. It is highly recommended to use index notation in going through the algebraic manipulations, as these are pretty strenuous. You will also need to recognize the definition of (half) a strain-rate tensor, and use both Eq. (86) and Eq. (90) to arrive at the following expression

$$\rho \left(\frac{\partial}{\partial t} + \sum_{i=1}^{3} u_i \frac{\partial}{\partial r_i} \right) k_B T = -\frac{2}{3} \sum_{i=1}^{3} \frac{\partial}{\partial r_i} q_i - \frac{2}{3m} \sum_{i=1}^{3} \sum_{j=1}^{3} \sigma_{ij} \dot{\gamma}_{ij}. \tag{93}$$

where we used index notation to indicate the order in which the elements of the two tensors need to be summed to form a scalar.

E. Fixing the Prefactors through the Chapman-Enskog Expansion

Now that we have written down the three transport equations for the mass, momentum, and energy, we already recognize the form of the continuum-level Navier-Stokes equations. We will need to justify the identification of the Cauchy stress tensor, temperature, and heat flux, as well as compute what these quantities are to close our system of equations. That is, if we identify $\sigma_{ij} = -\rho \langle (v_j - u_j)(v_i - u_i) \rangle_{\boldsymbol{p}}$, then we should compute this average. However, that requires knowledge of the solution to the Boltzmann equation, namely what f_1 is, which depends on the nature of the collision term.

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[5] Technically one recognises the pressure tensor, but these are related. That this is the form of the pressure tensor should be intuitively clear. In a gas the pressure (diagonal terms) will be related to the average of the velocity squared, while shear terms will be an average of cross-terms in the velocity.

There is a general recipe for approximating solutions to the Boltzmann equation, which will help in determining these coefficients. This recipe was developed independently by Sydney Chapman and David Enskog, and is named the Chapman-Enskog expansion in their honor. We will have another look at a specific form of the collision term in Section IV A, for which progress in computing the prefactors in the Navier-Stokes equations can be made, albeit with considerable effort.

The idea of Chapman and Enskog was to linearize the Boltzmann equation using a perturbation expansion of the form

$$f_1 = \sum_{n=0}^{\infty} \epsilon^n f_1^{(n)}, \tag{94}$$

where ϵ is the expansion parameter and $f_1^{(0)}$ is typically chosen to be the local equilibrium solution, *i.e.*, $f_1^{(0)} = f_1^{\text{loc}}$ as defined in Eq. (72). In their original work the expansion parameter they considered was the Knudsen number, $\mathsf{Kn} = \lambda/\mathsf{L}$, which is the ratio of the mean-free path λ to a physically relevant length scale L, such as the vessel size. The Knudsen number defined in this manner is small when the fluid (gas) is hydrodynamic on the length scale L, while it behaves more like a rarefied gas in the case that $\mathsf{Kn} \gg 1$. Moreover, de-dimensionalizing the collision term in such a way that the Knudsen number appears naturally leads to naturally to a factor $1/\mathsf{Kn}$ appearing in front of the dimensionfree collision operator. This makes sense, since the collision operator accounts for molecular interactions, which are the dominant term when the gas is dilute, as we argued earlier. However, any small expansion parameter ϵ around the local Maxwell-Boltzmann distribution will work, provided the collision term is weighted with ϵ^{-1} for consistency. A full derivation of the expansion and how this leads to the coefficients in terms of the collisional cross section is given in, *e.g.*, Refs. [23, 24]; we will only sketch the first steps here.

Taking the expansion (94) and putting it into the Boltzmann equation, we obtain after grouping the terms with equal order in ϵ

$$\left(\frac{\partial}{\partial t} + \frac{\boldsymbol{p}}{m} \cdot \boldsymbol{\nabla_r} + \boldsymbol{F} \cdot \boldsymbol{\nabla_p} \right) f_1^{(n)} = \sum_{k=0}^{n+1} \int \mathrm{d}\boldsymbol{p}_2 \int \mathrm{d}\boldsymbol{p}' \int \mathrm{d}\boldsymbol{p}_2' \, \omega(\boldsymbol{p} - \boldsymbol{p}_2, \boldsymbol{p}' - \boldsymbol{p}_2')$$
$$\times \left(f_1^{(k)}(\boldsymbol{r}, \boldsymbol{p}') f_1^{(n+1-k)}(\boldsymbol{r}, \boldsymbol{p}_2') - f_1^{(n+1-k)}(\boldsymbol{r}, \boldsymbol{p}) f_1^{(k)}(\boldsymbol{r}, \boldsymbol{p}_2) \right). \tag{95}$$

Here, it is implied that the $n = 0$ term only has a streaming contribution, which is sensible if one expands around local equilibrium. Truncating the expansion to first order we obtain

$$\left(\frac{\partial}{\partial t} + \frac{\boldsymbol{p}}{m} \cdot \boldsymbol{\nabla_r} + \boldsymbol{F} \cdot \boldsymbol{\nabla_p} \right) f_1^{\text{loc}}(\boldsymbol{r}, \boldsymbol{p}) = \int \mathrm{d}\boldsymbol{p}_2 \int \mathrm{d}\boldsymbol{p}' \int \mathrm{d}\boldsymbol{p}_2' \, \omega(\boldsymbol{p} - \boldsymbol{p}_2, \boldsymbol{p}' - \boldsymbol{p}_2')$$
$$\times \left(f_1^{\text{loc}}(\boldsymbol{r}, \boldsymbol{p}_2') f_1^{(1)}(\boldsymbol{r}, \boldsymbol{p}') + f_1^{\text{loc}}(\boldsymbol{r}, \boldsymbol{p}') f_1^{(1)}(\boldsymbol{r}, \boldsymbol{p}_2') \right.$$
$$\left. - f_1^{\text{loc}}(\boldsymbol{r}, \boldsymbol{p}_2) f_1^{(1)}(\boldsymbol{r}, \boldsymbol{p}) - f_1^{\text{loc}}(\boldsymbol{r}, \boldsymbol{p}) f_1^{(1)}(\boldsymbol{r}, \boldsymbol{p}_2) \right). \tag{96}$$

which is still rather intractable. However, note that we now have an equation for the perturbation in terms of f_1^{loc} only, which is linear in $f_1^{(1)}$. This gives some hope that there is a solution to be had.

The left-hand side of Eq. (96) can be evaluated using the definition of f_1^{loc} and reads

$$\left(\frac{\partial}{\partial t} + \frac{\boldsymbol{p}}{m} \cdot \boldsymbol{\nabla_r} + \boldsymbol{F} \cdot \boldsymbol{\nabla_p} \right) f_1^{\text{loc}}(\boldsymbol{r}, \boldsymbol{p}) =$$

$$\left(\frac{1}{T} \left(\frac{m}{2k_{\text{B}}T} |\boldsymbol{v} - \boldsymbol{u}|^2 - \frac{5}{2} \right) (\boldsymbol{v} - \boldsymbol{u}) \cdot \boldsymbol{\nabla_r} T + \frac{m}{k_{\text{B}}T} \sum_{i=1}^{3} \sum_{j=1}^{3} \left((v_i - u_i)(v_j - u_j) - \frac{1}{3} |\boldsymbol{v} - \boldsymbol{u}|^2 \delta_{ij} \right) \dot{\gamma}_{ij} \right) f_1^{\text{loc}}(\boldsymbol{r}, \boldsymbol{p}), \tag{97}$$

with δ_{ij} the Kronecker delta. You may have encountered this expression in showing that the f_1^{loc} as defined in Eq. (72) does not have a zero streaming term. Next, we write $f_1^{(1)} \equiv f_1^{\text{loc}}(1 + \Phi)$, with Φ some function, and we regroup the terms on the right-hand side of Eq. (96). Using properties of the exchange rate and collision acting on f_1^{loc}, we arrive at

$$\int \mathrm{d}\boldsymbol{p}_2 \int \mathrm{d}\boldsymbol{p}' \int \mathrm{d}\boldsymbol{p}_2' \, \omega(\boldsymbol{p} - \boldsymbol{p}_2, \boldsymbol{p}' - \boldsymbol{p}_2') f_1^{\text{loc}}(\boldsymbol{r}, \boldsymbol{p}) f_1^{\text{loc}}(\boldsymbol{r}, \boldsymbol{p}_2) \left(\Phi(\boldsymbol{r}, \boldsymbol{p}_2') + \Phi(\boldsymbol{r}, \boldsymbol{p}') - \Phi(\boldsymbol{r}, \boldsymbol{p}_2) - \Phi(\boldsymbol{r}, \boldsymbol{p}) \right), \tag{98}$$

for the collision term.

To find a solution for Φ, we need to equate Eqs (97) and (98), which gives rise to a rather horrifying looking expression; even more so than the one we started out with. However, to deal with this, one can make use of insights gained in deriving the Boltzmann equation. Equation (98) has a similar property as the regular collision operator, namely that a sum of a constant, drift, and energy term for Φ will lead to a zero value of the collision term. This forms the basis for constructing a homogenous solution to the Chapman-Enskog problem. Next, we recognize in Eq. (97) a linear combination of gradients of the temperature and velocity. This tells us that on the right-hand side, we also require a linear combination of these quantities to obtain a particular solution. Hence, the particular solution for Φ is expanded in terms of these quantities, giving rise, ultimately, to a linear equation system for the coefficients.

Following this rather lengthy and arduous route, it can be shown that the full solution may be written in an integral form over the collision operator [23, 24]. The solution can then be used to construct the moments of the distribution functions, leading to expressions for the viscosity and thermal conductivity in terms of integrals over the collision operator. We will not reproduce all these steps here and we refer to Refs. [23, 24] for the obtained expressions.

IV. A SIMPLE LATTICE-BOLTZMANN ALGORITHM

In this section, we have a quick look at a class of numerical methods that is used to solve hydrodynamic equations, based on the Boltzmann transport equation. We are, of course, referring to the lattice-Boltzmann (LB) algorithm, which traces its roots in the derivation we provided above. As we have shown in Section III, one can arrive at equations for viscous hydrodynamic flow from microscopic kinetics, by passing through the mesoscopic Boltzmann transport equation. The Boltzmann transport equation has one major advantage over the Navier-Stokes equations from an algorithmic perspective: it has an inherent locality to it. The Navier-Stokes equations are boundary-value differential equations—both in their nonlinear and linear form, to which we will come back in Section V. These specific equations are in general difficult to solve using local (and therefore parallelizable) numerical methods. It turns out that it is numerically favorable to solve a seemingly more complicated equation, the Boltzmann transport equation, and recover hydrodynamics at sufficiently long length and time scales, rather tackle the Navier-Stokes equations directly. In this section, we will make it clearer what we mean by the inherent locality of the Boltzmann transport equation and how this, using suitable approximations, may be exploited to obtain a fast numerical solver.

A. The Bhatnagar-Gross-Krook Approximation for the Collision Term

Although many flavors of lattice-Boltzmann exist with various ranges of application and properties, we shall restrict ourselves to the simplest form here. This will give sufficient insight into the workings of LB to grasp the concepts that underlie the more sophisticated variants. We will first make a few observations in continuous phase space, before moving onto a discretized form that will form the basis of the algorithm. Many of the physical properties of the LB algorithms can be equally well understood in their continuous and discretized forms, with the latter often only convoluting the argument due to the additional constraints imposed by the discretization itself. (Un)fortunately, a discussion of these discretization artefacts goes beyond the scope of these notes.

As we have seen in Section III E, recovering the prefactors of the hydrodynamic transport equations in general is not a pleasant experience, since it requires an expansion in terms of the deviation from local equilibrium f_1^{loc}, see Section III E. There is, however, a short cut that was introduced by Bhatnagar, Gross, and Krook [25]. Taking this short cut makes things a lot easier but comes at the price of throwing away some physical effects. The approximation is that there is a single time scale that dominates the collision processes, which we will refer to as the *relaxation time* τ. Generally, τ can be a function of the momentum, but in a drastic reduction, we will assume it is just a constant. In this case, we may approximate

$$\left(\frac{\partial f_1}{\partial t}\right)_{\mathrm{coll}} \approx -\frac{1}{\tau}\left(f_1 - f_1^{\mathrm{loc}}\right), \tag{99}$$

where we have made use of the fact that the collision operator is inversely proportional to this characteristic time and that non-equilibrium PDFs relax towards equilibrium. When we ignore any external force acting on the system $\boldsymbol{F}(\boldsymbol{r}) = 0^6$, we obtain

$$\frac{\partial}{\partial t}f_1 + \boldsymbol{v}\cdot\boldsymbol{\nabla}_{\boldsymbol{r}}f_1 \approx -\frac{1}{\tau}\left(f_1 - f_1^{\mathrm{loc}}\right). \tag{100}$$

for the Boltzmann transport equation in the Bhatnagar-Gross-Krook (BGK) approximation.

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[6] At this point, we should remark that in most LB implementations external forces are grouped in the collision term, rather than in the streaming term, by modifying the local equilibrium towards which the PDFs relax. This is why we have dropped it here.

Exercise 16*: Consider the Chapman-Enskog-like approximation that there are only small deviations from equilibrium, *i.e.*, $f_1 = f_1^{\text{loc}} + \delta f_1$, with δf_1 the non-equilibrium perturbation and f_1^{loc} given by the form in Eq. (72). Use Eq. (97) to arrive at

$$\delta f_1 = -\tau \left(\frac{1}{T} \left(\frac{m}{2k_{\text{B}}T}|\boldsymbol{v} - \boldsymbol{u}|^2 - \frac{5}{2} \right)(\boldsymbol{v} - \boldsymbol{u}) \cdot \boldsymbol{\nabla}_{\boldsymbol{r}}T \right.$$

$$\left. + \frac{m}{k_{\text{B}}T} \sum_{i=1}^{3} \sum_{j=1}^{3} \left((v_i - u_i)(v_j - u_j) - \frac{1}{3}|\boldsymbol{v} - \boldsymbol{u}|^2 \delta_{ij} \right) \dot{\gamma}_{ij} \right) f_1^{\text{loc}}, \tag{101}$$

Now use this expression to compute the viscosity and thermal conductivity, from the definitions given above and find that $\mu = nk_{\text{B}}T\tau$ and $\kappa = (5/2)\tau nk_{\text{B}}^2 T$, respectively, in the BGK approximation. The calculation is pretty lengthy; we recommend that you read Ref. [14] should you become stuck at any point. The obtained results give an indication that the BGK approximation is a bit drastic, since now the viscosity is density dependent. Remember, density independence was exactly the surprising result that Maxwell arrived at by studying kinetic theory and subsequently verified using experiments designed by him. However, when the density remains relatively homogeneous, reasonable results may be obtained for realistic viscous flow.

B. Discretizing Momentum Space to obtain Lattice Boltzmann

The two terms on the left-hand side of Eq. (100) constitute streaming, while the term on the right-hand side accounts for collisions. To make this more explicit, we can discretize the Boltzmann transport equation, by partitioning time t and momentum $\boldsymbol{p}$ (equivalently $\boldsymbol{v}$) in a clever way. Let $\boldsymbol{v}_i$ be a discrete velocity vector belonging to a set of velocity vectors. This set is chosen such that when start in the origin and move in discrete time intervals Δt along the vectors $\boldsymbol{v}_i$, *i.e.*, along distance vectors of length $\boldsymbol{v}_i\Delta t$, we span a regular space-filling lattice. The convention is that if a vector $\boldsymbol{v}_i$ is in the set, then $-\boldsymbol{v}_i$ is also in the set to guarantee an isotropic propagation along the spatial grid. The most convenient choice for the velocity vectors is one that spans a regular cubic grid in 3D, while in 2D the most common choices lead to a square and triangular grid pattern, however, any space-filling tessellation may be used. Our velocity vector set does not have to be an orthogonal basis, in fact, it is desirable to have many non-orthogonal components to approximate a spherically symmetric distribution in $\boldsymbol{p}$.

Now that we have introduced these velocity vectors, we can discretize our PDF $f_1(t, \boldsymbol{r}, \boldsymbol{p})$ into a set of associated *population densities*. These population densities $f_i(t_n, \boldsymbol{r}_m)$ are proportional to the probability to have a velocity $\boldsymbol{v}_i$ at a grid point $\boldsymbol{r}_m$ at a time $t_n = n\Delta t$. Like the regular f_1 the set is normalized to give the density, rather than to unity, to which we will come back shortly. Going through the procedure to properly discretize Eq. (100) based on this information requires a bit of finesse and knowledge of Hermite polynomials, and therefore goes beyond the scope of these notes. We refer any interested reader to Refs. [26, 27] for the full derivation using Hermite polynomials. The end-result of the derivation is that one obtains the discrete Boltzmann transport equation

$$f_i(t_{n+1}, \boldsymbol{r}_m + \boldsymbol{v}_i) = f_i(t_n, \boldsymbol{r}_m) - \frac{1}{\tau}\left(f_i(t_n, \boldsymbol{r}_m) - f^{\text{loc}}(t_n, \boldsymbol{r}_m) \right), \tag{102}$$

where we have rescaled time, such that $\Delta t = 1$ and the local equilibrium distribution in the collision term is given by

$$f^{\text{loc}}(t_n, \boldsymbol{r}_m) = w_i n \left(1 + \frac{\boldsymbol{u} \cdot \boldsymbol{v}_i}{c_s^2} + \frac{(\boldsymbol{u} \cdot \boldsymbol{v}_i)^2}{2c_s^4} - \frac{\boldsymbol{u} \cdot \boldsymbol{u}}{2c_s^2} \right), \tag{103}$$

with c_s the speed of sound, w_i a set of weights for the velocities deriving from the discretization, and n the density. The speed of sound is found to be given by $c_s^2 = (1/3)\Delta x/\Delta t$, *i.e.*, it is a function of the lattice spacing and time step. Choosing these two to be 1, we obtain the oddly geometric identity $c_s = \sqrt{1/3}$. In analogy to the continuous form of f_1, we have that

$$n = \sum_i f_i, \tag{104}$$

gives the density on a specific lattice node. Finally, the weights w_i follow from the Hermite expansion and satisfy $\sum_i w_i = 1$. However, they may be physically interpreted, since they depend on the distance from the central node.

That is, the velocity distribution is not homogeneous, vectors with a large velocity, necessary to bridge large distances on the grid for a given time step, are less likely to occur.

As we have seen, the f_i behave similar to the continuous PDF, in the sense that moments of the distribution give rise to physical quantities, like the density (104) and momentum

$$n\boldsymbol{u} = \sum_i \boldsymbol{v}_i f_i, \tag{105}$$

with even higher order modes giving rise to the stress tensor, etc. Returning to the lattice-Boltzmann equation, it is now clear why it can be straightforwardly parallelized. We rewrite it as two operations executed in succession

$$f_i^*(t_n, \boldsymbol{r}_m) = f_i(t_n, \boldsymbol{r}_m) - \frac{1}{\tau}\left(f_i(t_n, \boldsymbol{r}_m) - f^{\mathrm{loc}}(t_n, \boldsymbol{r}_m)\right); \tag{106}$$

$$f_i(t_{n+1}, \boldsymbol{r}_m + \boldsymbol{v}_i) = f_i^*(t_n, \boldsymbol{r}_m), \tag{107}$$

where we have isolated the collision and streaming steps, respectively. This is permitted, since the collision step needs no information on the neighboring lattice points in the BGK approximation and streaming merely moves around post-collision populations. So, the LB algorithm consists of iterating over the nodes and performing the collisions, followed by an iteration that transports the post-collision populations along their respective velocity vectors to a neighboring node. It is elegant and simple to implement, as you will see in the Python scripts that complement these notes, as well as highly parallelizable. The latter makes it perfectly suited for implementation on graphics-card (GPU) architectures.

Finally, we would like to mention boundary conditions and the implementation of forces onto the LB fluid. These are the last two items that we require to understand the provided Python scripts. (i) Forces on the LB fluid can be straightforwardly implemented by realizing that $\Delta\boldsymbol{p} = \boldsymbol{F}\Delta T$ in the continuum picture. In terms of the BGK discretization this results in the following: it suffices to modify the local equilibrium distribution (103) and relaxing towards $\boldsymbol{u} + \tau \boldsymbol{F} n$ in each time step [28]. (ii) The most common boundary condition for LB is that of zero fluid velocity on a boundary. This can be accomplished by tagging all the nodes belonging to a boundary and during each collision step, replacing the population that comes out of the boundary along a direction $\boldsymbol{v}_i$, by the one going into the boundary along this direction. This method is called *bounce back* as it literally bounces the populations back off the boundary. Intuitively, it is clear why this works. Consider a planar wall in the LB simulation and realize that the populations times the velocity vectors represent the momentum of the fluid via Eq. (105). Then the fact that we bounce back, can be thought of as there being a second fluid on the other side of the wall, with exactly the same properties, except that it flows in the opposite direction. Between the flow being in one direction on the set of nodes not comprising the wall, and the imaginary counter-flow on the wall nodes, there must logically be a zero-momentum plane. This is exactly what happens in an LB simulation: the effective zero-velocity boundary implemented via bounce back is found to be located half-way between the boundary and fluid nodes.

V. PROPERTIES OF THE HYDRODYNAMIC EQUATIONS

After our excursion to the numerical methods to solve the Boltzmann transport equation, let us return to the Navier-Stokes equations for incompressible simple media. We have repeated them here, further imposing homogeneity, *i.e.*, the mass density ρ is spatially constant, and dropping explicit time and position dependencies

$$\boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \boldsymbol{u} = 0; \tag{108}$$

$$\rho \left(\frac{\partial}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla}_{\boldsymbol{r}} \right) \boldsymbol{u} = -\boldsymbol{\nabla}_{\boldsymbol{r}} p + \mu \underline{\boldsymbol{\Delta}}_{\boldsymbol{r}} \boldsymbol{u} + \boldsymbol{f}; \tag{109}$$

$$\rho \left(\frac{\partial}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla}_{\boldsymbol{r}} \right) \tilde{U} = \mu \underline{\dot{\boldsymbol{\gamma}}} : \underline{\dot{\boldsymbol{\gamma}}} + \boldsymbol{\nabla}_{\boldsymbol{r}} \cdot (k \boldsymbol{\nabla}_{\boldsymbol{r}} T), \tag{110}$$

rewriting the material derivatives using the incompressibility criterion. Please refer back to Section II B for a discussion of the use of the symbols, should these be unclear to you. We can now analyze these equations further and explore the different regimes of fluid flow that can occur.

A. Characterizing Flow via the Reynolds Number

Singling out Eq. (109), we note that there are nonlinear terms in the fluid velocity $\boldsymbol{u}$, due to the second term on the left-hand side. One can estimate the importance of these nonlinearities by means of a dimensional analysis. We write $t = \mathsf{T} t^*$, $\boldsymbol{r} = \mathsf{L} \boldsymbol{r}^*$, $\boldsymbol{u} = \mathsf{U} \boldsymbol{u}^*$, $p = \mu \mathsf{U} p^* / \mathsf{L}$, and $\boldsymbol{f} = \mu \mathsf{U} \boldsymbol{f}^* / \mathsf{L}^2$, where we have introduced dimensionless (starred) quantities and the following representative properties of the system: a characteristic time T, length L, and speed U. Expressing the momentum transport equation in terms of these parameters results in

$$\mathsf{Re} \left(\mathsf{St} \frac{\partial}{\partial t^*} + \boldsymbol{u}^* \cdot \boldsymbol{\nabla}_{\boldsymbol{r}^*} \right) \boldsymbol{u}^* = -\boldsymbol{\nabla}_{\boldsymbol{r}^*} p^* + \underline{\boldsymbol{\Delta}}_{\boldsymbol{r}^*} \boldsymbol{u}^* + \boldsymbol{f}^*, \tag{111}$$

where we have introduced the Reynolds number

$$\mathsf{Re} = \frac{\rho \mathsf{U} \mathsf{L}}{\mu}, \tag{112}$$

and the Strouhal number

$$\mathsf{St} = \frac{\mathsf{L}}{\mathsf{U} \mathsf{T}}. \tag{113}$$

The Reynolds number is a measure for the importance of inertia in the system, compared to viscous dissipation. For a high Reynolds number inertia dominates, as represented by the time derivatives and convective transport on the left-hand side of Eq. (111), while for low Reynolds numbers, the right-hand side of the equation dominates, which represents viscous effects. The Strouhal number is a measure for the relative importance of convective transport to temporal perturbations of the flow field. For example, in systems wherein the fluid is subjected to oscillatory drive, like in a rheometer, the driving frequency may such that velocity perturbations are produced on a time scale that is shorter or comparable to that of the viscous transport. When $\mathsf{Re} \ll 1$, but the combination $\mathsf{Re}\mathsf{St} \gtrsim 1$, the nonlinear term drops out of the Navier-Stokes equations, but the time derivative remains important. This form of the Navier-Stokes equations is sometimes referred to as the *unsteady Stokes equations*.

When both $\mathsf{Re} \ll 1$ and $\mathsf{St} \ll 1$ viscous dissipation dominates over inertia and Eq. (111) can be approximated by the linear Stokes form

$$\mu \underline{\boldsymbol{\Delta}}_{\boldsymbol{r}} \boldsymbol{u} = \boldsymbol{\nabla}_{\boldsymbol{r}} p - \boldsymbol{f}, \tag{114}$$

which describes fluid flows that are referred to as *laminar* and for which we have reinstated the dimensionful notation. Laminarity refers to a tendency of the fluid to flow in parallel layers. This can be readily observed in a setup where fluid flows through a tube and dies are injected at various distances from the center. The streams of dies flow along with the fluid, without significant lateral mixing due to the fluid motion; they mix only due to diffusion. Such experiments were famously carried out by Osborne Reynolds, who considered the transition from laminar to turbulent flow in a smooth pipe [29]. The turbulent regime is characterized by chaotic changes in pressure and flow velocity, resulting in significant convective mixing.

Exercise 17[*]**:** Look up the characteristic quantities that describe: the motion of microscopic bacteria, human swimmers, weather patterns like a cyclone, oceanic currents, and flow in the earth's mantle, and compute their Reynolds number to determine whether the Stokes equations may be used to describe such flow or if the full Navier-Stokes equations need to be solved.

B. From Laminar to Turbulent Flow

As you have seen by completing the exercise on the Reynolds numbers, there are a few ways to obtain laminar flow. Low values of Re may be obtained by reducing the length scale and/or speed, whilst keeping the medium's properties ρ and μ constant. At very large length scales, low Re are obtained through very small speeds, incredibly high viscosities, or ultra-low densities. In our daily experience, we are typically confronted with turbulent flow, as is visualized by smoke billowing out of a chimney. The enhanced mixing that turbulence can bring about in these settings is quite desirable, as it makes the surroundings of factories relatively habitable. Interestingly, this observation has all kinds of consequences for the way microscopic structures in our body and microorganisms have to deal with their waste management. Laminarity imposes that mixing is diffusion dominated on these length scales, but there are some clever ways to move around this condition: either by outrunning diffusion oneself, or by generating recirculating flow patterns that draw in fresh "food" and flush away waste. We will come back to this in Section V C 2.

The most striking aspect of the Reynolds number, compared to other dimensionfree control parameters that you have encountered in physics thus far, is the location where the transition between turbulence and laminarity takes place. A control parameter typically assumes the value 1 roughly in the middle of the transition region between the two limiting behaviors. Through significant experimental effort in a wide range of hydrodynamic settings, it has become very clear that Re $\ll$ 1 is a sufficient condition for obtaining laminar flow[7]. The issues with the Reynolds number as a control parameter come in when considering the onset of turbulence from a situation that is laminar by, *e.g.*, increasing the flow speed. It turns out that for flow in a smooth tube with circular cross section, laminarity may be preserved up to Re $\approx$ 2300 [32, 33], with L chosen as the diameter of the tube in this case and U the flow speed in the center. Turbulence sets in above Re $\approx$ 2600 [32, 33]. In boundary-layer flows, this number can be even higher, with turbulence setting in above Re $\approx 5 \times 10^5$ [34]. This oddly high crossover in terms of the Reynolds number is found everywhere, with the so-called critical Reynolds number having different values for every geometry considered. It should be noted that numerical solutions display similar transition trends, with the caveat that in certain cases the laminar flow profile may be numerically maintained if no perturbations are imposed, *i.e.*, this flow can be metastable state. This makes it difficult to predict whether a flow is laminar or turbulent based on dimensional analysis alone.

The onset of turbulence is not yet well understood and continues to be a topic of intense fundamental study. The nonlinearities in the Navier-Stokes equations hinder progress via analytic routes, which has led to the development of numerical methods to study flow, such as the LB algorithm discussed in Section IV. From a practical standpoint, these numerical methods have contributed significantly to industrial developments, such as hull design for ships and modeling of flow around airplanes. However, here too there are still many open questions. Perhaps surprisingly, it is still not fully understood how airplanes manage to achieve lift, although we know that boundary-layer flows play an important role in this process, rather than simple Bernoulli-type pressure-difference arguments based on relative flow speed above and below the wing [35].

Before we move onto the laminar flow regime associated with microhydrodynamics, with which we will finish out these lecture notes, we will make a quick stop in the transition region between fully turbulent and laminar flow. One of the prettiest examples of a crossover between the two types of flow can be found in the Kármán vortex street. When fluid flows past a spherical object in 3D the flow profile adjusts to the presence of the object[8]. Deep into the laminar regime, Re $\ll$ 1, the profile can be computed by solving Stokes' equation (114) using a stream-function approach. For sufficiently high Re $\leq$ 49 two symmetrically placed vortices develop behind the cylinder, which comprise the wake of the flow. When the flow speed is increased further, $49 <$ Re $\lesssim$ 140 to 190 [36], the recirculation region develops instabilities leading to vortices being shed behind the obstacle in a regular pattern. This is what Theodore von Kármán observed experimentally [37], after whom the effect is named, although it had been observed earlier, see Refs. [38, 39]. The vortices are attributed to the thin boundary layer of fast fluid flow around the object being shed off the wake due to the instabilities. Increasing the Reynolds number further leads to an irregular pattern of vortices and eventually the onset of turbulence.

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[7] As an aside, the term bacterial turbulence that has cropped up recently is only an apparent low-Re instance of turbulence and not actual turbulence [30], though there are striking similarities to actual turbulence [31].

[8] The 2D variant in bulk fluid is problematic due to Stokes' paradox.

Exercise 18*****: Study the Python-based LB solver for the Kármán vortex street problem that has been provided to you. The setup simulates the motion of a fluid over an object with a circular cross section, for which the velocity of the fluid is zero at the boundary. Tune the parameters to go from laminar flow to vortex shedding. You will note that technically the LB solver is 2D, however, we do not encounter the Stokes' paradox, since the hydrodynamic breakdown only occurs in an infinite system with infinitely fast momentum diffusion. In addition, a sinusoidal fluid velocity perturbation is added to the flow over the cylinder to aid the development of the vortex street. Bear in mind that the LB solver provided is not unconditionally stable and it may be necessary to check the quality of a solution or modify the parameters to achieve convergence. Finally, it should be noted that it is difficult to observe turbulence in this 2D setup, as in the experiment the first indication of irregular flow is the appearance of 3D instabilities.

C.   The Microhydrodynamics of Self-Propelled Organisms

We now turn to the Stokes equations for a homogeneous fluid medium, for which the time-dependence of processes is such that the Strouhal number is negligible. In this section, we are interested in the motion of microorganisms and what the consequences are of the low-Re flow regime in which they find themselves. We repeat the two relevant equations here

$$\mu \underline{\boldsymbol{\Delta}}_{\boldsymbol{r}} \boldsymbol{u} = \boldsymbol{\nabla}_{\boldsymbol{r}} p - \boldsymbol{f}; \tag{115}$$

$$\boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \boldsymbol{u} = 0. \tag{116}$$

Provided we do not impose significant external temperature gradients, it is permitted to ignore the energy transport equation, which is why we say "two relevant equations." This reduction is justifiable for laminar flows, since low-Re viscous dissipation does not result in significant local heating of the fluid and the system may therefore be assumed to be isothermal. This is one of the reasons why the energy transport equation has been relegated to the exercises in this set of lecture notes, the other being that it is the most involved from the perspective of algebraic manipulation.

Exercise 19*: Perform the dimensional analysis on Eq. (110) that is required to show that viscous dissipation results in local temperature increases that scale as $\mu \mathsf{U}^2/\mathsf{K}$, with U the typical velocity as before, and K the characteristic thermal conductivity, *i.e.*, $k = \mathsf{K}k^*$. Find the relevant numbers for microscale motion in water and argue that low-Re systems are effectively isothermal provided there is no external heating.

Under the above conditions, we see that there are no derivatives with respect to time left in the system of equations that governs laminar flow. Time-dependent flow can be introduced into the system either via the body force $\boldsymbol{f}$ or via the boundary conditions. Despite the linearity of Eqs. (115) and (116), it is difficult to obtain analytic solutions in all but a few simple geometries. The most well-known example of an analytically solvable system is that of pressure driven flow between two parallel plates, which is called Hagen-Poiseuille flow. Here, the fluid velocity is zero on the walls and forms a parabola in the direction normal to the walls. The zero-velocity boundary condition is commonly imposed to model the interaction of a fluid with a hard wall and it manages to capture many experimental observations.

Exercise 20*****: Compute the velocity profile in a Hagen-Poiseuille geometry and show that the peak fluid velocity is given by $V = H^2 \Delta P/(8\mu L)$, where H is the plate separation and Δp the pressure drop over a channel of length L. Use symmetry arguments to reduce Eqs. (115) and (116) to a suitable form. Verify that your solution is correct using the Python script that has been provided. Note that in this Python script we have imposed an external force density, rather than a pressure difference; the relation between these two is trivial. The reason for doing so, is that imposing pressure boundaries is less trivial than imposing body forces, also see Section IV A.

1.   Achieving Motion by Irreversible Shape Changes

The elimination of explicit time dependence from the Navier-Stokes equations in the laminar flow regime has very interesting consequences for the way self-propelled microorganisms can effect motion. Typically, Re $\ll 10^{-4}$ for microswimmers and they are therefore deep in the laminar regime of fluid flow. A microswimmer and its surrounding

comprise a force-free system, provided we ignore the effects of gravity. The microswimmer also does not apply a body force on the fluid ($\boldsymbol{f} = \boldsymbol{0}$). Therefore, such an organism can only propel by changing its body shape, in much the same way that we do when we go swimming. There is a major difference, however: we swim in the inertia dominated regime, while microorganisms cannot coast on their own momentum. Any momentum that is generated in the laminar-flow regime is instantaneously dissipated away to infinity and thus a delta-like application of force leads to negligible motion. On human length scales an analogy with swimming in honey is often made, but if you run the numbers (assuming one somehow manages to maintain the same swim speed), you would find that viscosities more in the range of pitch. Particles *can* move with a constant speed in the laminar regime, but this requires the constant application of a force, *e.g.*, gravitational sedimentation. But, there is no external force acting on the organism to move it like that.

The dominance of viscous dissipation implies that if one reverses the arrow of time, the path followed by a microswimmer is retraced. Crucially, the speed with which you do this time reversal does not impact the retracing, provided the system maintains a low Reynolds number, because of the linearity of the underlying equations. It is like playing back a movie at half or quarter speed, the retraced path is not affected by doing so. A further consequence is that there is no net motion when a change in boundary conditions is reciprocal in time. That is, a cyclic configurational motion that does not enclose an area in configuration space leads to zero net displacement. This was first realized by Edward Purcell, who considered the motion of an organism with a single hinge: a scallop. Purcell realized that the only kind of motion a scallop can achieve is reciprocal in time: it can open and close its hinge, but the speed at which it does so is irrelevant in the linear flow regime. In other words, a scallop can move just fine on the basis of inertia on our length scales, but a microscallop cannot swim. He published this observation in the lecture "Life at Low Reynolds Number" [6] and the observation has since gone under the name *Scallop Theorem*. Purcell went further to suggest a model microswimmer that had two hinges and is therefore capable of non-reciprocal motion, which formed the basis for more recent modelling efforts on microswimmers[9].

It should come as no surprise then, that actual microorganisms—by necessity—employ non-reciprocal shape changes to achieve propulsion. These break the time-reversal symmetry and allow for directed motion. *Escherichia coli* bacteria, for instance, can have long, thin tail-like appendages, so-called flagella, which they spin around at a high rate. These bundle together to form a cork-screw-like flagellar bundle. Because a cork screw has a chirality that breaks time-reversal symmetry, the *E. coli* can use rotation of this helical bundle to move forward. Sperm employ a similar strategy to *E. coli*, albeit typically using only a single flagellum, while *Chlamydomonas* algae have two "antennae" at their front, which they move in a breast-stroke like manner to self-propel.

2. Long-Ranged Interactions through the Fluid

As a final consequence of being immersed in a fluid medium, we will discuss hydrodynamic interactions. These are the long-ranged interactions mediated by the fluid medium. To get a feeling for this, let us consider a stream. A leaf that falls in the stream, is carried along by the flow. An object moving around in a fluid, either under the action of an external force or via self-propulsion, creates a fluid flow field around itself. Other objects in the medium are affected by this flow field, similar to the leaf in the stream. In addition, the flow field generated by a moving object can influence the motion of the object itself, when there are "obstacles" present in the system. The flow field that would be produced by the swimmer in bulk, is modified to account for the obstacles, which couples back to the motion of the swimmer itself.

We will now consider a simple model for the hydrodynamic interactions due to a swimming microorganism, to show how these differ from those of driven particles, by virtue of the force-free condition on their motion. We will use fundamental solutions to the Stokes equations (Green's functions) in the following, which we will derive from Eqs. (115) and (116) first. Then, we will construct a simple flow field description for a swimming microorganism from the so-called Stokeslet solutions that describe a situation where a point-force is applied to the fluid.

Without loss of generality we assume that the body force is given by a point force $\tilde{\boldsymbol{f}}$ located at the origin ($\boldsymbol{f}(\boldsymbol{r}) = \tilde{\boldsymbol{f}}\delta(\boldsymbol{r})$), with $\delta(\boldsymbol{r})$ the Dirac delta distribution. In that case, $\boldsymbol{r}$ is the point in the fluid where we want to determine the velocity. We take the divergence of Eq. (115) and use incompressibility to obtain

$$\boldsymbol{\nabla} \cdot \left(-\boldsymbol{\nabla} p(\boldsymbol{r}) + \mu \underline{\boldsymbol{\Delta}} \boldsymbol{u}(\boldsymbol{r})\right) = -\boldsymbol{\nabla} \cdot \tilde{\boldsymbol{f}}\delta(\boldsymbol{r}) \Rightarrow \nabla^2 p(\boldsymbol{r}) = \tilde{\boldsymbol{f}} \cdot \boldsymbol{\nabla}\delta(\boldsymbol{r}). \tag{117}$$

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[9] The most famous variant is the three-bead swimmer by Ali Najafi and Ramin Golestanian, which uses non-reciprocal actuation to achieve forward motion at low Reynolds numbers [40].

Next, we define the Fourier transform of a function ϕ and its inverse as

$$\check{\phi}(\boldsymbol{k}) \equiv \int_{\mathbb{R}^3} \mathrm{d}\boldsymbol{r}e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\phi(\boldsymbol{r}), \qquad\qquad \phi(\boldsymbol{r}) \equiv \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\mathrm{d}\boldsymbol{k}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\check{\phi}(\boldsymbol{k}), \qquad (118)$$

respectively, with i the imaginary unit. Here, we use the "check" symbol for the Fourier transform to avoid confusion with the standard "hat" notation for normalized vectors. Applying the Fourier transform (118) we obtain

$$-k^2\check{p}(\boldsymbol{k}) = i\boldsymbol{k}\cdot\tilde{\boldsymbol{f}} \Rightarrow \check{p}(\boldsymbol{k}) = -i\frac{\hat{\boldsymbol{k}}}{k}\cdot\tilde{\boldsymbol{f}}. \qquad (119)$$

Note that $\check{p}$ is parallel to the $\hat{\boldsymbol{k}}$ vector[10]. The next step is to Fourier transform the Stokes equation (115) to obtain

$$-i\boldsymbol{k}\check{p}(\boldsymbol{k}) - \mu k^2\tilde{\boldsymbol{u}}(\boldsymbol{k}) = -\tilde{\boldsymbol{f}} \overset{(119)}{\Rightarrow} \tilde{\boldsymbol{u}}(\boldsymbol{k}) = \frac{1}{\mu k^2}\left(\mathbb{I} - \hat{\boldsymbol{k}}\otimes\hat{\boldsymbol{k}}\right)\tilde{\boldsymbol{f}}, \qquad (120)$$

where $\otimes$ denotes the dyadic product $(\boldsymbol{a}\otimes\boldsymbol{b})_{ij} \equiv a_ib_j$. This results in the following expression for the velocity field and pressure using the inverse Fourier transform

$$\boldsymbol{u}(\boldsymbol{r}) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\mathrm{d}\boldsymbol{k}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\frac{1}{\mu k^2}\left(\mathbb{I} - \hat{\boldsymbol{k}}\otimes\hat{\boldsymbol{k}}\right)\tilde{\boldsymbol{f}}; \qquad (121)$$

$$p(\boldsymbol{r}) = -i\frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\mathrm{d}\boldsymbol{k}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\frac{\hat{\boldsymbol{k}}\cdot\tilde{\boldsymbol{f}}}{k}. \qquad (122)$$

Using the properties of the harmonic and biharmonic fundamental solutions, see, *e.g.*, Ref. [41] for additional details, one recovers

$$p(\boldsymbol{r}) = \frac{\hat{\boldsymbol{r}}}{4\pi r^2}\cdot\tilde{\boldsymbol{f}}, \qquad (123)$$

and

$$\boldsymbol{u}(\boldsymbol{r}) = \frac{1}{8\pi\mu r}\left(\mathbb{I} + \hat{\boldsymbol{r}}\otimes\hat{\boldsymbol{r}}\right)\tilde{\boldsymbol{f}} \equiv \frac{1}{8\pi\mu}\underline{\boldsymbol{S}}(\boldsymbol{r})\tilde{\boldsymbol{f}}, \qquad (124)$$

with

$$\underline{\boldsymbol{S}}(\boldsymbol{r}) = \frac{1}{r}\left(\mathbb{I} + \hat{\boldsymbol{r}}\otimes\hat{\boldsymbol{r}}\right), \qquad (125)$$

where Eqs. (124) and (125) introduce the fundamental solution known as the Stokeslet $\underline{\boldsymbol{S}}(\boldsymbol{r})$. Flow induced by a point-force is characterized by a pinching of the fluid around the point where the force acts.

> **Exercise 21***: Plot the velocity profile given by the Stokeslet solution. Use the associated Python script to visualize the flow field as well. Note that we have distributed the force acting on the fluid over several nodes to obtain a smoother solution. In addition, due to the periodicity of the simulation domain, we have added a counter-force density to ensure that there is no momentum added to the system. Explain why the bulk Stokeslet is so different from the one obtained in the periodic simulation domain. Argue on the basis of the decay of Stokes flow, why it is problematic to reach the bulk solution in the periodic domain; an analogy may be drawn to electrostatics and the use of the Ewald sum.

Now that we have a solution for the application of a point force onto the fluid, we can consider the leading order decay of the flow field around a microswimmer. Recall that swimming itself is force free. In the case of an *E. coli* bacterium, one can envision this as the body of the *E. coli* exerting a drag on the fluid, while the flagellar bundle exerts a driving force on the fluid. This is obviously a bit of an oversimplified view, since both the head and the

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[10] This is an expression of the fact that the pressure acts as a Lagrange multiplier to impose incompressibility on the (Navier-)Stokes equations, accounting for there being four equations with only three parameters in terms of the velocity vector components. In other words, in Fourier space $\check{p}$ lies along $\hat{\boldsymbol{k}}$, so that the relevant velocities lie orthogonal to this vector, in the subspace that is the kernel of the divergence operator. This may be exploited to write a simple grid-based Fourier solver for determining the flow field due to a force distribution in a system with periodic boundary conditions.

bundle experience drag from the fluid and, similarly, they both exert a force onto the fluid, but this model will suffice for now.

Starting from the Stokeslet $\underline{\boldsymbol{S}}$, we now consider two point forces $\pm\tilde{\boldsymbol{f}}$ of equal magnitude and opposite directions, separated by a distance l. This construction ensures that the system is force free. Without any loss of generality we place the origin between the two forces, so that they are placed at $\frac{l}{2}\hat{\boldsymbol{p}}$ and $-\frac{l}{2}\hat{\boldsymbol{p}}$, with $\tilde{\boldsymbol{f}} = \pm F\hat{\boldsymbol{p}}$, such that the system is force free. Summing up the two Stokeslets, the velocity field at a point $\boldsymbol{r}$ in the fluid is thus given by

$$\boldsymbol{u}(\boldsymbol{r}) = \frac{F}{8\pi\mu}\left[\underline{\boldsymbol{S}}\left(\boldsymbol{r} - \frac{l}{2}\hat{\boldsymbol{p}}\right) - \underline{\boldsymbol{S}}\left(\boldsymbol{r} + \frac{l}{2}\hat{\boldsymbol{p}}\right)\right]\hat{\boldsymbol{p}}. \tag{126}$$

We now obtain the corresponding expression for the (point) Stresslet by taking the limit $l \to 0$. By first multiplying with $1 = l/l$ and defining the (constant) dipole strength $\kappa = Fl$ we now recognize the (negative of) the directional derivative in the limit of $l \to 0$:

$$(\hat{\boldsymbol{p}} \cdot \boldsymbol{\nabla})\,\underline{\boldsymbol{S}}(\boldsymbol{r}) \equiv \lim_{l \to 0} \frac{1}{l}\left[\underline{\boldsymbol{S}}\left(\boldsymbol{r} + \frac{l}{2}\hat{\boldsymbol{p}}\right) - \underline{\boldsymbol{S}}\left(\boldsymbol{r} - \frac{l}{2}\hat{\boldsymbol{p}}\right)\right]. \tag{127}$$

Using Eq. (127) we can thus write for the Stresslet velocity field:

$$\boldsymbol{u}(\boldsymbol{r}) = -\frac{\kappa}{8\pi\mu}\left[(\hat{\boldsymbol{p}} \cdot \boldsymbol{\nabla})\,\underline{\boldsymbol{S}}(\boldsymbol{r})\right]\hat{\boldsymbol{p}}. \tag{128}$$

The expression for $\left[(\hat{\boldsymbol{p}} \cdot \boldsymbol{\nabla})\,\underline{\boldsymbol{S}}(\boldsymbol{r})\right]\hat{\boldsymbol{p}}$ can be derived using the standard tensor index notation, and leads to the well-known expression for the velocity field induced by a point Stresslet:

$$\boldsymbol{u}(\boldsymbol{r}) = \frac{\kappa}{8\pi\mu r^2}\left(3(\hat{\boldsymbol{p}} \cdot \hat{\boldsymbol{r}})^2 - 1\right)\hat{\boldsymbol{r}}. \tag{129}$$

In our construction, positive values of κ correspond to pusher (extensile) swimmers and negative values to puller (contractile) swimmers. A well-known pusher is the *E. coli* bacterium, while *Chlamydomonas* algae are archetypical pullers. Note that the flow field around a swimmer decays more quickly r^{-2} than around a point force r^{-1}, as was to be expected. In addition, from this derivation you can start to appreciate that may of the principles you learned in electrostatics carry over to Stokesian hydrodynamics. The Stresslet is simply the second term in a multipole expansion describing the far-away flow field around a general force distribution.

> **Exercise 22**[***]**:** Visualize the velocity profile given by the Stresslet. Use the associated Python script to visualize the flow field of an extended dipolar flow field.

Returning to our analogy of a leaf being carried along by the stream, we have one last observation to make regarding the way a microorganism can interact with its surroundings using its flow field. Let us assume that this swimmer is moving along the z-axis and starts off at $z = -L/2$ at time $t = 0$ and we track it until it has reached $z = L/2$ at time $t = L/v_s$ with v_s its swim speed. The swim speed can be related to the dipole strength according to $v_s = |\kappa|/(6\pi\mu)$, assuming that the swimmer is a sphere with radius a and experiences an "effective" propulsion force F that is related to a dipole which has a length comparable to a. The exact relation is not particularly relevant and will depend on the properties of the swimmer; what is important to acknowledge, is that there should be a linear proportionality between the dipole strength of a swimmer's flow field and the speed of self-propulsion. Note that the sign of the dipole does not impose the direction of swimming. A small molecule that is at a radial coordinate r_m with respect to the z-axis and at height $z = 0$ at time $t = 0$ will move along in the flow field produced by the moving swimmer. Let the time-dependent positions of the swimmer and the molecule be given by $\boldsymbol{r}_s$ and $\boldsymbol{r}_m$, respectively. Then the equations of motion describing this problem are given by

$$\frac{\partial \boldsymbol{r}_m}{\partial t}(t) = \boldsymbol{u}(\boldsymbol{r}_m(t) - \boldsymbol{r}_s(t)), \qquad\qquad \frac{\partial \boldsymbol{r}_s}{\partial t}(t) = v_s\hat{\boldsymbol{z}}, \tag{130}$$

with $\boldsymbol{u}$ the velocity field generated by the swimmer, as given by Eq. (129). One can numerically integrate these equations of motion to obtain the trajectory of the small molecule in the flow field of the swimmer. The molecule will follow part of what is a triangular trajectory, which depends on the ratio r_m/L, as well as the sign of κ. What this means is, that when a swimmer passes by, it moves around molecules in its surroundings over trajectories that are not (typically) closed. This is quite different from the situation that is found for driven particles, where the trajectories are closed, as we will explore in the last exercise of these notes. Note that this implies that bacteria can effectively mix

their surroundings, leading to and enhanced (effective) diffusion of materials in their surroundings. This phenomenon was first reported by Wu *et al.* [42] and later theoretically explained by Underhill *et al.* [43]. Since then, many more have worked on this topic, due to the exciting possibilities for microfluidic mixing.

Exercise 23***:** Numerically solve the equation system (130) and recover the typical trajectories of a small molecule in the flow field of a microorganism. Analyze the separation between the begin point and end point of the molecule's trajectory as a function of the parameters the govern the system. Repeat the calculation and show that when you do the same with a driven particle, there is no such separation, as can be easily argued on the basis of symmetry.

VI.   SUGGESTIONS FOR FURTHER STUDY

We hope that this lecture series has wet your appetite for transport phenomena. Beyond the relatively well-understood work that was described here, there is a wealth of new physics, mathematics, and numerics to be explored. There are many open (even fundamental) problems in the field of hydrodynamics that require the attention of talented researchers.

For instance, there remains the Millennium problem on the existence of solutions to the Navier-Stokes equations [44]. Although there are few physicists who would doubt the existence of such solutions, the problem remains open and offers opportunities for the development of new mathematics. We also encountered the issue of understanding the onset of turbulence in these lecture notes, which is of fundamental interest, but has obvious interest from the perspective of applications that operate in the transition regime. From a more practical viewpoint, there are also issues with a description of the flow of granular matter. Materials like sand, grains, and rocks can flow under certain conditions, but behave more like a solid under others. Can their flow be described in terms of the hydrodynamic conservation equation formalism? If so, under what conditions, and how is the transition between the solid-like and liquid-like behavior captured. Tackling this issue will require detailed experimental work, as well as a strong theoretical effort, although some progress has been made in both regards. In addition, we touched upon the locomotion of self-propelled organisms in these notes. Much of the current work in this direction has been performed for Newtonian media. However, we know that polymer solutions can be highly non-Newtonian—think along the lines of the nonlinear response encountered in corn starch—which begs the question: "How accurate are our current predictions, when we want to apply them to situations encountered in the human body?" The simple answer is: not very, and this has been realized by a large group of physicists who are currently working towards finding answers to the problems encountered in analytically and numerically solving the much harder equations that describe non-Newtonian flow in a microbiological setting. On a vastly different scale, it has proven difficult to solve the full set of electrohydrodynamic equations efficiently in order to describe the behavior of our sun, even disregarding the nuclear reactions that are going on. Such equations also need to be solved on a smaller scale for the development of nuclear fusion plants.

These examples are but a few of the problems where hydrodynamic equations are involved and many questions on the specifics of the formalism remain. In fact, for quite a few of these, the solution may require making the connection between the microscopic description of a material and the way this leads to transport equations, using strategies like the ones outlined in these lecture notes.

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