

EXPLORATIONS IN THE MATHEMATICS OF
INVISCID INCOMPRESSIBLE FLUIDS

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Abstract

The main subject of this dissertation is smooth incompressible fluids. The emphasis is on the incompressible Euler equations in all of \mathbb{R}^2 or \mathbb{R}^3 , but many of the ideas and results can also be adapted to other hydrodynamic systems, such as the Navier-Stokes or surface quasi-geostrophic (SQG) equations. A second subject is the modeling of moving contact lines and dynamic contact angles in inviscid liquid-vapor-solid systems under surface tension.

The dissertation is divided into three independent parts:

First, we introduce notation and prove useful identities for studying incompressible fluids in a pointwise Lagrangian sense. The main purpose is to provide a unified treatment of results scattered across the literature. Furthermore, we prove several analogs of Constantin's local pressure formula for other nonlocal operators, such as the Biot-Savart law and Leray projection. Also, we define and study properties of a Lagrangian locally compact Abelian group in terms of which some nonlocal formulas encountered in fluid dynamics may be interpreted as convolutions.

Second, we apply the algebraic theory of scalar polynomial orthogonal invariants to the incompressible Euler equations in two and three dimensions. Using this framework, we give simplified proofs of results of Chae and Vieillefosse. We also investigate other uses of orthogonal transformations, such as diagonalizing the deformation tensor along a particle trajectory, and comment on relative advantages and disadvantages. These techniques are likely to be useful in other orthogonally invariant PDE systems as well.

Third, we propose an idealized inviscid liquid-vapor-solid model for the macroscopic study of moving contact lines and dynamic contact angles. Previous work mostly addresses viscous systems and frequently ignores a singular stress present when the contact angle is not at its equilibrium value. We also examine and clarify the role that disjoining pressure plays and outline a program for further research.

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Dedicated to my wife Kunhee,
my parents Mary and Reinhold,
and my brother Michael

Preface

This is perhaps a somewhat unusual dissertation: The topics are fairly wide-ranging and there are no major new theorems. Nevertheless, I believe there is value.

What happened is this:

I set myself the goal of finding new ways of understanding inviscid incompressible fluids with the hope of shedding new light on the question of global regularity in three dimensions. The study of the incompressible Euler equations in \mathbb{R}^3 and \mathbb{T}^3 is a very mature field by now, and it is clear that major progress requires deep new insight. One after another, however, my ideas either turned out to have already been studied before or simply failed to produce new insights beyond what was known already.

Now it is frequently preached, but seldom practiced, that scientists ought to document their negative as well as their positive results. In mathematics, I view the purpose of this as follows:

1. *It deters other minds from making the same dead-end investigations.*
2. *It invites other minds to try to complete the investigation or at least draw inspiration for their own work.*
3. *Most importantly, it encourages work on more interesting problems.* When only publication of positive results is rewarded, people naturally work on more “safe” problems such as minor technical improvements of known results or contrived problems easily seen to be solvable by current methods. Such work seldom leads to great new insight or innovation.

With the first two points in mind, I have tried to document the more substantial of my “explorations” in Chapters 2 and 3. They also provide a unified exposition of some ideas otherwise found in rather disparate segments of the literature, and I hope this juxtaposition may also be of value.

Chapter 4, finally, represents an attempt to move into a less mature field. However, even just formulating a concrete system to study, and a concrete research question to address, turned out to be a far more complex task than I originally imagined. Nonetheless, and with especially the second point in mind, I have tried to document what I in the end think could be an interesting research program.

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Chapter 1

Introduction

1.1 Structure of this dissertation

The main body of this dissertation is divided into three chapters that can be read independently. In Chapters 2 and 3, we explore properties of smooth incompressible fluids, especially smooth solutions to the incompressible Euler equations in \mathbb{R}^2 and \mathbb{R}^3 . In Chapter 4, we turn our attention to modeling inviscid liquid-vapor-solid systems under surface tension. Finally, we provide an Appendix A that lists some identities used throughout the dissertation.

The remainder of this chapter is organized as follows: In §1.2, we summarize the main points of Chapters 2–4. In §1.3, we explain our reasons for focusing on the incompressible Euler equations. In §1.4, we explain our notation and establish some conventions.

1.2 Overview of the main chapters

In Chapter 2, we begin by introducing notation and proving a number of identities that are useful for studying incompressible fluids pointwise along Lagrangian particle paths. Although most of these ideas may already be found in the literature, the reader

may find our unified exposition helpful.

Next, we prove several analogs of the local pressure formula of Constantin [22] for other nonlocal operators of interest in the study of incompressible fluids, including the Biot-Savart law and Leray projection. An example is the formula

$$u(x, t) - \int_{S_r(x)} u(y, t) \, dS(y) = -\frac{1}{4\pi} \int_{B_r(x)} \frac{(x - y) \times (\omega(y, t) - \omega(x, t))}{|x - y|^3} \, dy. \quad (1.1)$$

It is local in the sense that the right-hand side can be made to depend on an arbitrarily small neighborhood of x by choosing r sufficiently small. The trade-off is that the left-hand side is no longer just $u(x, t)$. Such formulas are useful for, e.g., proving Hölder estimates.

Finally, we observe that, upon defining

$$a \oplus b := A(X(a, t) + X(b, t), t), \quad (1.2)$$

hydrodynamic integro-differential equations of the form

$$D_t X(a, t) = \int_{\mathbb{R}^n} \mathbf{K}(X(a, t) - X(b, t)) \mathbf{F}(X(b, t), \nabla_b X(b, t), \varphi(b)) \, db \quad (1.3)$$

can be viewed as convolutions with respect to \oplus ,

$$D_t X(a, t) = \int_{\mathbb{R}^n} \mathbf{K}(a \ominus b) \mathbf{F}(X(b, t), \nabla_b X(b, t), \varphi(b)) \, db. \quad (1.4)$$

We state some properties of the LCA group (\mathbb{R}^n, \oplus) , such as the existence of an L^p convolution inequality, and of its associated Fourier transform.

Although parts of the chapter are written explicitly for the incompressible Euler equations in \mathbb{R}^3 , most of the ideas and results also apply or can be adapted to other incompressible hydrodynamic systems.

In Chapter 3, we apply the algebraic theory of scalar polynomial orthogonal invariants to the incompressible Euler equations in two and three dimensions. For three dimensions, this leads to a system of the form

$$\left\{ \begin{array}{l} D_t \eta = 3\beta - \varphi - \pi_1, \\ D_t \mu = 2\varphi, \\ D_t \beta = \frac{2}{3}\eta^2 + \frac{4}{3}\eta\mu - 2\psi + \pi_2, \\ D_t \varphi = -\frac{2}{3}\mu^2 + \frac{8}{3}\eta\mu - 2\psi + \pi_3, \\ D_t \psi = \frac{4}{3}\eta\varphi - \frac{1}{3}\mu\varphi + 3\mu\beta + \pi_4, \end{array} \right. \quad (1.5)$$

where $\eta, \mu, \beta, \varphi, \psi$ are scalar invariants related to $\nabla_x u$, while the π_i invariants also depend on the pressure Hessian.

To illustrate the usefulness of this framework, we give a simpler proof of the following a priori bound of Chae [17]:

$$\sup_{0 < t < T} \|\omega\|_{L_x^2} \leq \exp\left(\int_0^T \|\lambda_2^+\|_{L_x^\infty} dt\right) \|\omega_0\|_{L_x^2}. \quad (1.6)$$

(Here λ_2 denotes the intermediate eigenvalue of the deformation tensor \mathcal{D} .) We also give a simpler discussion of a model of Vieillefosse [113, 114].

Finally, we investigate other uses of orthogonal transformations, such as rotating the reference frame in order to diagonalize the deformation tensor along a particle trajectory, and comment on relative advantages and disadvantages of this approach over the use of the scalar polynomial invariants.

The techniques in this chapter are likely to be useful in other orthogonally invariant PDE systems as well.

In Chapter 4, we discuss some issues related to modeling inviscid liquid-vapor-solid systems that allow for moving contact lines and dynamic contact angles. After

reviewing the static case, we give two derivations of an idealized augmented Young-Laplace law,

$$[[p]] = \gamma H + \gamma \frac{\cos \theta_s - \cos \theta}{\sin \theta} \delta_\Sigma. \quad (1.7)$$

(In the literature, mostly the viscous case is discussed and the term with the Dirac measure is frequently ignored.) Drawing on the free boundary variational calculus literature, we discuss how to interpret the Dirac measure, especially in the static case.

Furthermore, we examine how to incorporate disjoining pressure in the model and clarify its role. In particular, we dispel the notion found in some literature that the Dirac mass should be physically interpreted as the macroscopic limit of a disjoining pressure term.

Many open questions remain, and we end by outlining a program for further research, both mathematical and physical.

1.3 Reasons for studying the Euler rather than the Navier-Stokes equations

Substantially more research is directed at the Navier-Stokes than the Euler equations. For physicists and engineers, this makes sense, as viscosity is frequently important in applications, especially close to boundaries. However, for mathematicians interested in questions of global regularity, especially in boundaryless settings like the torus \mathbb{T}^3 or all of \mathbb{R}^3 , it may make sense to first focus on the Euler equations. This is true regardless of whether one believes in finite-time blowup or not.

If one expects finite-time blowup, it should be easier to prove this for the Euler equations first, since viscosity usually has a regularizing effect.¹ (Indeed, Luo and Hou [78] recently provided numerical evidence for finite-time blowup in the Euler

¹Usually but not always. There is, for example, the *Turing instability* phenomenon in which adding viscosity can make an otherwise linearly stable system unstable. See, for example, §4.1.2 in Evans [51].

equations, though at a boundary.)

If, on the other hand, one expects global regularity, this is likely due to some sort of “nonlinear depletion” already present in the Euler equations rather than the regularizing effect of viscosity. It is well-known that the viscous problem remains supercritical, i.e., there is a “finite gap” between what norms we have control over and what norms we would need to control in order to prove global regularity (see, e.g., Constantin [27]). This is perhaps best exemplified by the Ladyzhenskaya-Prodi-Serrin criteria (see, e.g., Seregin [103] and references therein). Conversely, without some sort of extra depletion coming from the specific structure of the fluid equations, we would expect finite-time blowup. Tao [110] has, in a sense, formalized this, showing that there are equations, superficially similar to the Navier-Stokes equations in terms of scaling and conserved quantities, that blow up in finite time.

Two potential sources of nonlinear depletion have been identified in the literature. First, convection appears to have a regularizing effect, as first observed by Constantin [24] using his “distorted Euler equations” model, and later by Hou and C. Li [66] in a one-dimensional model of the axisymmetric Navier-Stokes equations. (See also the three-dimensional axisymmetric study by Hou and Lei [65].)

Second, in regions of high enstrophy, the vorticity tends to form vortex tubes where the direction of vorticity does not vary strongly. This parallel alignment of vorticity in turn leads to a geometric depletion of nonlinearity identified by Constantin, Fefferman, and Majda [29,30]. For some recent numerical evidence of this regularizing mechanism, we refer to the paper by Hou and R. Li [67].

A full and quantitative understanding, however, of the extent and limits of nonlinear depletion has not yet been achieved. This then is our preferred framing of the global regularity question for both the Euler and the Navier-Stokes equations:

What are the depletion mechanisms and are they always strong enough to prevent blowup? Or else can we identify conditions where they are not

strong enough and then exploit them to construct solutions that blow up in finite time?

1.4 Notation and conventions

Convention 1.4.1. For the Euler equations, we will denote the velocity by u , the vorticity by ω , the pressure by p , and occasionally write N for $\nabla_x u$ and P for $\nabla_x \nabla_x p$. Following Majda and Bertozzi [79], we write \mathcal{D} for the symmetric part of $\nabla_x u$ and Ω for the skew-symmetric part.²

If S is a tensor of rank k , and T is a tensor of rank ℓ , then $S \otimes T$ and $S \cdot T$ are tensors of rank $k + \ell$ and $k + \ell - 2$, respectively, defined by

$$(S \otimes T)_{i_1 \dots i_k j_1 \dots j_\ell} = S_{i_1 \dots i_k} T_{j_1 \dots j_\ell}, \quad (1.8)$$

$$(S \cdot T)_{i_1 \dots i_{k-1} j_2 \dots j_\ell} = S_{i_1 \dots i_{k-1} m} T_{m j_2 \dots j_\ell}. \quad (1.9)$$

Note that in the last equation and throughout, we adopt the Einstein convention of implicit summation over repeated indices (m in the above), unless explicitly stated otherwise, or an index appears non-repeated on one side of the equation. For example, in an equation like $A_{ij} = \lambda_i \delta_{ij}$, the index i is not summed over since it appears only once on the left-hand side.

We are, unfortunately, at odds with most of the fluids and continuum mechanics literature with the following convention.

Convention 1.4.2. For a tensor T of rank k , by $\nabla_x T$ we mean the tensor

$$(\nabla_x T)_{i_0 i_1 i_2 \dots i_k} = \partial_{x_{i_0}} T_{i_1 i_2 \dots i_k} \quad (1.10)$$

²In the literature one also finds the use of \mathcal{S} and \mathcal{J} , or \mathcal{S} and \mathcal{A} , instead of \mathcal{D} and Ω . Also, Ω is occasionally used for something altogether different, for example the tensor $\omega \otimes \omega - \frac{1}{3}|\omega|^2$, or a global rotation. With hindsight, we actually prefer the notation \mathcal{S} and \mathcal{A} .

of rank $k + 1$. That is, the derivative is the first index of the tensor $\nabla_x T$. By $\operatorname{div}_x T$ we mean the tensor of rank $k - 1$ obtained from $\nabla_x T$ by contracting the first two indices, that is

$$(\operatorname{div}_x T)_{i_2 \dots i_k} = (\nabla_x \cdot T)_{i_2 \dots i_k} = \partial_{x_j} T_{j i_2 \dots i_k}. \quad (1.11)$$

The advantage in our context is that $u \cdot \nabla_x T$ may naturally be interpreted as the tensor contraction defined above or the usual matrix product $u^\top (\nabla_x T)$. Also, the relation between Ω and ω is simply

$$\Omega_{ij} = \frac{1}{2} \epsilon_{ijk} \omega^k, \quad (1.12)$$

without a minus sign. In practice, results in this dissertation will look slightly different when compared to most of the literature, with transposes in different places, the order of matrix multiplications reversed, and so on. However, if aware of this, it is easy to translate back and forth.

To alleviate index clutter, we will mostly write indices for components of vectors as superscripts and indices for partial derivatives as subscripts, for example

$$(\nabla_a x)_{ij} = x_{a_i}^j, \quad \omega^k = \epsilon_{klm} u_{x_\ell}^m, \quad u_z^r = \partial_z (e_r \cdot u). \quad (1.13)$$

Finally, although there are some very interesting recent results related to weak solutions of the Euler equations due to De Lellis and Székelyhidi [37], in this dissertation we will solely be concerned with smooth solutions. For practically every incompressible hydrodynamic system, there is already a well-developed local-in-time well-posedness theory in sufficiently regular Hölder and Sobolev spaces. For the Euler and Navier-Stokes equations, we refer to, for example, the book of Majda and Bertozzi [79]. We restrict ourselves to studying properties of these smooth (and decaying or periodic) solutions already known to exist for at least a finite time interval.

Convention 1.4.3. *All functions occurring (such as velocity, flow map, pressure, vorticity) are assumed to be sufficiently smooth and sufficiently decaying (or periodic) for the various calculations to make sense.*

Chapter 2

Observations on Incompressible Fluids

This chapter is concerned with some general properties of incompressible fluids. Although we write with an emphasis on the incompressible Euler equations in \mathbb{R}^3 , most of the statements in this chapter either apply directly or can be easily adapted to any of the other commonly encountered incompressible hydrodynamic systems in two and three dimensions.

We remind the reader that throughout this dissertation, unless stated otherwise, we assume that we already have a smooth divergence-free velocity field $u \in L^2(\mathbb{R}^3)$ for at least some finite interval of time.

Let us also recall some standard notions for incompressible flows. The trajectory of a particle initially at position a is denoted by $X(a, t)$. For each “particle label” a , $X(a, \cdot)$ is determined by the ODE

$$\begin{cases} \frac{d}{dt}X(a, t) = u(X(a, t), t), \\ X(a, 0) = a. \end{cases} \quad (2.1)$$

As long as u is smooth, $X(\cdot, t)$ is smooth and has a smooth inverse, the “back-to-labels”

map $x \mapsto A(x, t)$, which satisfies

$$\partial_t A(x, t) + u \cdot \nabla_x A(x, t) = 0. \tag{2.2}$$

We refer to (x, t) as Eulerian coordinates and (a, t) as Lagrangian coordinates.

Many of our statements will involve the quantity

$$J(x, t) := (\nabla_a X)(A(x, t), t). \tag{2.3}$$

Clearly, $J(\cdot, 0) = \mathbb{I}$. Furthermore, from $\operatorname{div}_x u = 0$ and the evolution of J , it follows that $\det J = 1$ for all time.

The rest of the chapter is structured as follows. In §2.1, we introduce notation for working with expressions involving both Eulerian and Lagrangian derivatives, and prove some useful identities involving J . In §2.2, we study some properties of two types of vector field evolutions frequently encountered in incompressible flows. In §2.3, we briefly discuss reformulations of the Euler equations under two particular gauge choices. In §2.4, we give “local” versions of nonlocal formulas like the Biot-Savart formula and Leray projection that are of great relevance to the study of incompressible fluids. In §2.5, we introduce a locally compact Abelian group (\mathbb{R}^n, \oplus) in terms of which some Lagrangian expressions encountered in various fluid systems may be understood as convolutions.

Finally, some remarks on the novelty of the material in this chapter: Although we discovered much of the material in §§2.1–2.3 for ourselves, after more thorough literature review, we found that many of the observations in these sections are not new. In fact, some of them were reported more than 30 years ago. As much as possible, we have tried to include the most relevant references, but we cannot claim complete coverage. We hope the reader still finds our exposition useful, since it brings together ideas that are scattered in the literature. The computations and ideas in §§2.4–2.5

are, to the best of our knowledge, truly new.

2.1 Mixing Eulerian and Lagrangian derivatives

2.1.1 Motivation

There are tantalizing hints that the Lagrangian framework is more natural for the study of the regularity of fluid mechanical systems. In two dimensions, it is that the vorticity is conserved along Lagrangian particle trajectories. In three dimensions, there are the Cauchy invariants (for a nice history of these, see [55]). In arbitrary dimensions, Lagrangian particle trajectories are analytic as long as the velocity is $C^{1,\alpha}$. (This result is apparently due in some form to Liechtenstein in 1925 and was then rediscovered or reproved several times since the 1990's. For some more recent papers on this topic we refer to, e.g., [34, 56, 119].) Another nice example is Constantin's use of Lagrangian variables to prove uniqueness for systems like Oldroyd-B in low regularity [28]. See also [32].

Integrated conserved quantities like the energy $\frac{1}{2}\|u\|_{L^2}^2$ or the helicity $\int_{\mathbb{R}^n} u \cdot \omega \, dx$, of course, are indifferent to the use of Eulerian and Lagrangian coordinates: thanks to incompressibility, we have $|\det J| = 1$ and so changing variables does not affect the integral. However, these conserved quantities have proved not strong enough to control the global regularity of the fluid in three dimensions. (From scaling, it is clear that $u \in L^2$ is not enough, and although helicity scales critically for the Navier-Stokes equations, it does not have a definite sign. Constantin and Majda gave a decomposition of the helicity into a difference of two positive quantities [33], and Lei, Lin and Zhou used a similar decomposition to construct a class of arbitrarily large initial-data global solutions [76]. But this decomposition is still not strong enough to say anything about the general case.) The time seems ripe to focus on pointwise Lagrangian statements.

2.1.2 Notation

As is common, we will want to work in Eulerian coordinates, but will frequently need Lagrangian derivatives. We will also want to freely mix all four derivatives $\partial_t, \nabla_x, D_t, \nabla_a$ in expressions.

To accomplish this, we define (abusing notation slightly) operators D_t and ∇_a acting on functions of Eulerian coordinates as

$$D_t f := (D_t(f \circ X)) \circ A = (\partial_t + u \cdot \nabla_x) f, \quad (2.4)$$

$$\nabla_a f := (\nabla_a(f \circ X)) \circ A = J \nabla_x f, \quad (2.5)$$

where $J := (\nabla_a X) \circ A = \nabla_a x = (\nabla_x A)^{-1}$. Note also $J^{-1} = \nabla_x A$ and so we have $\nabla_x = J^{-1} \nabla_a$. By $f \circ X$ we mean composition in the following sense:

$$(f \circ X)(a, t) := f(X(a, t), t), \quad (2.6)$$

$$(g \circ A)(x, t) := g(A(x, t), t). \quad (2.7)$$

Of course, we can similarly define operators ∂_t and ∇_x acting on functions of Lagrangian coordinates via

$$\nabla_x = K \nabla_a = (\nabla_x a) \nabla_a, \quad (2.8)$$

$$\partial_t = D_t - u \cdot \nabla_x = D_t - (J^\top \dot{X}) \nabla_a, \quad (2.9)$$

where $K := (\nabla_x A) \circ X = \nabla_x a = (\nabla_a X)^{-1}$.

Whether to write everything in terms of Eulerian or Lagrangian coordinates is an arbitrary choice. But since in the literature it is most common to define quantities like the vorticity ω as functions of Eulerian coordinates, we will adhere to the following convention in all of the following except in §2.5.

Convention 2.1.1. *Unless stated otherwise, all our functions are assumed to be functions of Eulerian coordinates. For example, when we write u , we mean $u(x, t)$ and not $u(X(a, t), t)$.*

There are at least two quantities, however, that are most naturally expressed in terms of Lagrangian coordinates. These are the initial velocity and vorticity transported by the fluid. The latter is needed to express the Cauchy invariants. Rather than writing $u_0 \circ A$ or $\omega_0 \circ A$, we will instead introduce new symbols ψ and φ to represent these quantities as functions of Eulerian coordinates:

$$\psi(x, t) = u_0(A(x, t)), \quad (2.10)$$

$$\varphi(x, t) = \omega_0(A(x, t)), \quad (2.11)$$

$$D_t \varphi = D_t \psi = 0. \quad (2.12)$$

We provide Table 2.1 for translation between functions of Eulerian coordinates and functions of Lagrangian coordinates.

Remark 2.1.2. When working in Lagrangian variables, D_t is really just the partial time derivative $\frac{\partial}{\partial t}$. To make translating between Eulerian and Lagrangian expressions easier, however, we will keep the notation D_t for this partial time derivative and, by abuse of notation, define $\partial_t := D_t - (K^\top \dot{X}) \cdot \nabla_a$ to be the Eulerian time derivative.

The “proper” thing to do would be to call the Lagrangian time variable something different, say τ . Then we could write ∂_τ instead of D_t and less confusion would arise. However, use of t in both settings is ubiquitous in the literature, and we will not deviate from this custom here.

Eulerian	Lagrangian
f	$f \circ X$
$g \circ A$	g
∇_x	$\nabla_x := K \nabla_a$
∂_t	$\partial_t := D_t - (K^\top \dot{X}) \cdot \nabla_a$
$\nabla_a := J \nabla_x$	∇_a
$D_t := \partial_t + u \cdot \nabla_x$	D_t
x	X
A	a
u	$\dot{X} = D_t X$
φ	ω_0
ψ	u_0
$J = \nabla_a x$	$K^{-1} = \nabla_a X$
$J^{-1} = \nabla_x A$	$K = \nabla_x a$

Table 2.1: Translating between functions of Eulerian coordinates and functions of Lagrangian coordinates

2.1.3 Commutators of the Eulerian and Lagrangian derivative operators

The operators ∂_t, ∇_x do not commute with the operators D_t, ∇_a . We summarize some ways of expressing the commutators in Table 2.2. We present here only the computation of the Lagrangian versions of the last two commutators listed in the table, as the others are trivial to derive. First, we compute

$$[\partial_t, D_t] = \partial_t u \cdot \nabla_x = \partial_t u \cdot (J^{-1} \nabla_a) = (J^{-\top} \partial_t u) \cdot \nabla_a. \quad (2.13)$$

Observing that

$$D_t(J^{-\top} u) = J^{-\top} D_t u - J^{-\top} (\nabla_x u)^\top u = J^{-\top} (D_t u - u \cdot \nabla_x u) = J^{-\top} \partial_t u, \quad (2.14)$$

we arrive at

$$[\partial_t, D_t] = (D_t(J^{-\top} u)) \cdot \nabla_a. \quad (2.15)$$

Next, we compute

$$[\partial_t, \nabla_a] = (\partial_t J) \nabla_x = (D_t J - u \cdot \nabla_x J) \quad (2.16)$$

$$= (D_t J - u \cdot J^{-1} \nabla_a J) J^{-1} \nabla_a \quad (2.17)$$

$$= ((\nabla_a u) J^{-1} + u (\nabla_a J^{-1})) \nabla_a \quad (2.18)$$

$$= (\nabla_a (J^{-\top} u)) \nabla_a. \quad (2.19)$$

Commutator	Eulerian derivatives	Lagrangian derivatives
$[\nabla_x, \nabla_a]$	$(\nabla_x J) \nabla_x$	$-(\nabla_a J^{-1}) \nabla_a$
$[\nabla_x, D_t]$	$(\nabla_x u) \nabla_x$	$-(D_t J^{-1}) \nabla_a$
$[\partial_t, D_t]$	$(\partial_t u) \cdot \nabla_x$	$-(D_t (-J^{-\top} u)) \cdot \nabla_a$
$[\partial_t, \nabla_a]$	$(\partial_t J) \nabla_x$	$-(\nabla_a (-J^{-\top} u)) \nabla_a$

Table 2.2: Commutators of the Eulerian and Lagrangian derivative operators

Remark 2.1.3. This suggests thinking of $-J^{-\top} u$ as a sort of Lagrangian transport velocity. We discuss this idea a little more in §2.1.5.

2.1.4 Differential identities related to J

Lemma 2.1.4. *We have*

$$D_t J = J(\nabla_x u), \quad (2.20)$$

$$D_t J^\top = (\nabla_x u)^\top J^\top, \quad (2.21)$$

$$D_t J^{-1} = -(\nabla_x u) J^{-1}, \quad (2.22)$$

$$D_t J^{-\top} = -J^{-\top} (\nabla_x u)^\top. \quad (2.23)$$

Proof. Taking ∇_a of $D_t x = u$, we find $D_t J = \nabla_a u = J \nabla_x u$. The other equations follow from the differential matrix identity $D_t M^{-1} = -M^{-1} (D_t M) M^{-1}$ and taking transposes. ▮

Proposition 2.1.5. *We have*

$$\operatorname{div}_x J^\top = 0, \quad (2.24)$$

$$\operatorname{div}_a J^{-\top} = 0, \quad (2.25)$$

or, written out explicitly,

$$x_{a_i a_m}^j A_{x_j}^m = 0, \quad (2.26)$$

$$A_{x_p x_\ell}^m x_{a_m}^\ell = 0. \quad (2.27)$$

Proof. From $D_t J = J(\nabla_x u)$, we have

$$D_t J_{x_m}^{ij} + u_{x_m}^k J_{x_k}^{ij} = J_{x_m}^{i\ell} u_{x_\ell}^j + J^{i\ell} u_{x_\ell x_m}^j. \quad (2.28)$$

Summing over $m = j$, the right-most term vanishes thanks to $\operatorname{div}_x u = 0$, and the other two terms cancel. So we are left with just $D_t J_{x_j}^{ij} = 0$, that is,

$$D_t(\operatorname{div}_x J^\top) = 0. \quad (2.29)$$

Since $J^\top(x, 0) = \mathbb{I}$, it follows that $\operatorname{div}_x J^\top = 0$. Written out explicitly, this says

$$\partial_{x_j} x_{a_i}^j = A_{x_j}^m x_{a_i a_m}^j = 0. \quad (2.30)$$

Noting that $\mathbb{I} = J J^{-1}$, i.e.,

$$\delta_{im} = x_{a_i}^j A_{x_j}^m, \quad (2.31)$$

and taking ∂_{a_m} , we find (using (2.30)),

$$0 = x_{a_i}^j A_{x_j x_\ell}^m x_{a_m}^\ell. \quad (2.32)$$

Multiplying by $A_{x_p}^i$, this simplifies to

$$A_{x_p x_\ell}^m x_{a_m}^\ell = 0. \quad (2.33)$$

■

Proposition 2.1.6. *For a differentiable tensor field $T(x)$, we have*

$$\nabla_x T = \operatorname{div}_a (J^{-\top} \otimes T), \quad (2.34)$$

$$\nabla_a T = \operatorname{div}_x (J^\top \otimes T), \quad (2.35)$$

and

$$\operatorname{div}_x T = \operatorname{div}_a (J^{-\top} T), \quad (2.36)$$

$$\operatorname{div}_a T = \operatorname{div}_x (J^\top T). \quad (2.37)$$

Proof. By Proposition 2.1.5, we have $\operatorname{div}_a J^{-\top} = 0$. Thus,

$$\operatorname{div}_a (J^{-\top} \otimes T) = (\operatorname{div}_a J^{-\top}) \otimes T + J^{-1} \nabla_a T = 0 + \nabla_x T. \quad (2.38)$$

Contraction over the first two indices gives $\operatorname{div}_a (J^{-\top} T) = \operatorname{div}_x T$. The identities for $\nabla_a T$ and $\operatorname{div}_a T$ are proved similarly. ■

Proposition 2.1.7. *In three dimensions, for a differentiable vector field $v(x)$, we have*

$$\operatorname{curl}_a (Jv) = J^{-\top} \operatorname{curl}_x v, \quad (2.39)$$

$$\operatorname{curl}_x (J^{-1}v) = J^\top \operatorname{curl}_a v. \quad (2.40)$$

Proof. We compute

$$[\operatorname{curl}_a(Jv)]^i = \epsilon_{ijk} \partial_{a_j} (x_{a_k}^\ell v^\ell) = (\epsilon_{ijk} x_{a_j a_k}^\ell) v^\ell + \epsilon_{ijk} x_{a_k}^\ell (x_{a_j}^m \partial_{x_m}) v^\ell. \quad (2.41)$$

The first term on the right-hand side vanishes since ϵ_{ijk} is skew-symmetric under $j \leftrightarrow k$, while $x_{a_j a_k}^\ell$ is symmetric under $j \leftrightarrow k$. For the second term, we need the identity

$$\epsilon_{pml} M_{pi}^{-1} = \epsilon_{ijk} M_{jm} M_{kl}, \quad (2.42)$$

valid for all 3×3 unit-determinant matrices M (see §A.3). Taking $M = \nabla_a x = J$, we get

$$[\operatorname{curl}_a(Jv)]^i = J_{ip}^{-\top} \epsilon_{pml} v_{x_m}^\ell = [J^{-\top} \operatorname{curl}_x v]^i. \quad (2.43)$$

The proof of the second identity is similar. ▮

Remark 2.1.8. A similar formula to Proposition 2.1.7 is proved in the appendix of a 1989 paper by Vishik [115]. See also Friedlander and Vishik [54].

Lemma 2.1.9. *For a matrix M , we have*

$$D_t(JMJ^\top) = J(D_t M + (\nabla_x u)M + M(\nabla_x u)^\top)J^\top, \quad (2.44)$$

$$D_t(JMJ^{-1}) = J(D_t M + [\nabla_x u, M])J^{-1}. \quad (2.45)$$

Proof. Apply the Leibniz rule to the left-hand sides and use Lemma 2.1.4. ▮

Corollary 2.1.10. *The right¹ Cauchy-Green tensor JJ^\top evolves according to*

$$D_t(JJ^\top) = 2J\mathcal{D}J^\top. \quad (2.46)$$

Proof. Take $M = \mathbb{I}$ in Lemma 2.1.9. ▮

¹Recall our unusual index ordering, $J_{ij} = x_{a_i}^j$. In the continuum mechanics literature, this tensor is usually written as $J^\top J$.

Application to the Euler equations

Corollary 2.1.11. *We have*

$$D_t(J\mathcal{D}J^\top) = J(NN^\top - P)J^\top, \quad (2.47)$$

$$D_t(J\Omega J^\top) = 0. \quad (2.48)$$

Proof. For the Euler equations, $D_t N = -N^2 - P$. Taking $M = N$ in Lemma 2.1.9, we thus find

$$D_t(JNJ^\top) = J(-N^2 - P + N^2 + NN^\top)J^\top = J(NN^\top - P)J^\top. \quad (2.49)$$

Since the operation $A \mapsto JAJ^\top$ preserves (skew-)symmetry, decomposing this equation into symmetric and skew-symmetric parts gives the statement of the corollary. \blacksquare

Remark 2.1.12. From this corollary, it follows by integrating along particle trajectories that $(J\Omega J^\top)(X(a, t), t) = \Omega_0(a)$. This is an analog of the Cauchy formula in arbitrary dimension.

Remark 2.1.13. In view of Corollaries 2.1.10 and 2.1.11, it is natural to consider the quantity $\tilde{P} = P - NN^\top$. Note that \tilde{P} is still symmetric, but is no longer the Hessian of a scalar function. In terms of \tilde{P} , we have

$$D_t(J\mathcal{D}J^\top) = -J\tilde{P}J^\top, \quad (2.50)$$

and

$$D_t\mathcal{D} = -2\mathcal{D}^2 - \tilde{P} - [\Omega, \mathcal{D}]. \quad (2.51)$$

See also Remarks 3.4.4 and 3.5.5 for more formulas that become nicer when using \tilde{P} .

Remark 2.1.14. Another straightforward application of Lemma 2.1.9 is the identity

$$D_t(JNJ^{-1}) = J(D_tN)J^{-1}. \quad (2.52)$$

2.1.5 A sort of Lagrangian transport velocity

Let us define

$$w := -J^\top u = -u \cdot \nabla_x A. \quad (2.53)$$

Then we have

$$\partial_t x = 0, \quad (2.54)$$

$$\partial_t A = w, \quad (2.55)$$

$$\operatorname{div}_a w = 0, \quad (2.56)$$

$$\partial_t = D_t + w \cdot \nabla_a. \quad (2.57)$$

This is completely analogous to

$$D_t A = 0, \quad (2.58)$$

$$D_t x = u, \quad (2.59)$$

$$\operatorname{div}_x u = 0, \quad (2.60)$$

$$D_t = \partial_t + u \cdot \nabla_x. \quad (2.61)$$

So if we interchange the roles of x and A , and of the derivatives (∂_t, ∇_x) and (D_t, ∇_a) , then w takes the role of u .

It seems worthwhile to investigate this analogy more in the future. For now, let us conclude with the following observation.

Proposition 2.1.15. *If $-\zeta$ is an Eulerian vector potential for $\partial_t u$, then $J\zeta$ is a*

Lagrangian vector potential for $D_t w$.

Proof. As shown in §2.1.3, we have

$$D_t w = -J^{-\top} \partial_t u. \quad (2.62)$$

It follows from Proposition 2.1.7 that if ζ is such that

$$\partial_t u = \operatorname{curl}_x(-\zeta), \quad (2.63)$$

then

$$D_t w = \operatorname{curl}_a(J\zeta). \quad (2.64)$$

■

2.2 Two special types of vector fields

We consider two special types of vector fields with respect to incompressible fluids.

The first type satisfies

$$D_t w - (\nabla_x u)^\top w = 0. \quad (2.65)$$

The streamlines of such vector fields are transported by the fluid. Remarkably, the vorticity $\omega = \operatorname{curl}_x u$ is such a vector field. In fact, many of the properties attributed to the vorticity hold for any such vector field.

The second type satisfies

$$D_t v + (\nabla_x u)v = 0. \quad (2.66)$$

A typical example would be the gradient $\nabla_x f$ of a scalar f transported by the fluid, $D_t f = 0$. But there are many more. For example, for the incompressible Euler

equations, if we define a scalar q by $D_t q = p - \frac{1}{2}|u|^2$ with arbitrary smooth initial data, then $v = u + \nabla_x q$ is a vector field of the second type. See §2.3.2.

After writing this chapter, we discovered some more relevant prior literature on these ideas. The singling out of these two special types of vector fields occurs in the English literature at least as early as 1983 in Kuz'min [73]. Kuz'min in turn credits a 1982 paper (in Russian) by Moiseev, Sagdeev, Tur, and Yanovsky [82].

Beyond our exposition, we recommend in particular Tur and Yanovsky [112]. They give a nice geometric characterization, showing for \mathbb{R}^3 that vector fields of the first type correspond to “frozen-in” 2-forms; vector fields of the second type correspond to “frozen-in” 1-forms; and scalars transported by the fluid correspond to “frozen-in” 0- or 3-forms. (For compressible fluids, there is a distinction between the 0- and 3-form cases.) Using this unified differential form description, they straight-forwardly show that if α, β are “frozen-in” forms, then so are $d\alpha$ and $\alpha \wedge \beta$. This generalizes, for example, Propositions 2.2.6 and 2.2.4 below.

2.2.1 Basic properties

The following equivalent definitions of vector fields of the first type are fairly standard—see for example §1.6 in Majda and Bertozzi [79]. For some geometric observations related to such vector fields that we will not discuss here, see also Chae, Constantin, and Wu [19].

Proposition 2.2.1 (Equivalent definitions of vector fields of the first type). *The following are equivalent:*

$$(i) \quad D_t w - (\nabla_x u)^\top w = 0,$$

$$(ii) \quad D_t (J^{-\top} w) = 0,$$

$$(iii) \quad w(x, t) = J^\top(x, t)(w_0 \circ A) \text{ where } w_0(a) := w(a, 0),$$

(iv) $[D_t, w \cdot \nabla_x] = 0$.

Proof. For (i) \Rightarrow (ii), use $D_t J^{-\top} = -J^{-\top}(\nabla_x u)^\top$ to compute

$$D_t(J^{-\top} w) = (D_t J^{-\top})w + J^{-\top}(D_t w) = -J^{-\top}(\nabla_x u)^\top w + J^{-\top}(\nabla_x u)^\top w = 0. \quad (2.67)$$

For (ii) \Rightarrow (i), use $D_t J^\top = (\nabla_x u)^\top J^\top$ to compute

$$D_t w = D_t(J^\top J^{-\top} w) = (D_t J^\top)(J^{-\top} w) = (\nabla_x u)^\top w. \quad (2.68)$$

For (ii) \Rightarrow (iii), integrate along particle trajectories to get

$$J^{-\top}(X(a, t), t)w(X(a, t), t) = w_0(X(a, t)), \quad (2.69)$$

and multiply by $J^{-\top}(X(a, t), t)$. For (iii) \Rightarrow (ii), multiply by $J^{-\top}(X(a, t), t)$ and take D_t . For (iv) \Rightarrow (ii), we compute

$$D_t(J^{-\top} w) = D_t(w \cdot \nabla_x A) = (w \cdot \nabla_x)(D_t A) = 0. \quad (2.70)$$

Finally, for (ii) \Rightarrow (iv), we compute

$$D_t(w \cdot \nabla_x) = D_t(J^{-\top} w \cdot \nabla_a) = D_t(J^{-\top} w) \cdot \nabla_a + J^{-\top} w \cdot \nabla_a D_t = 0 + (w \cdot \nabla_x) D_t. \quad (2.71)$$

■

Remark 2.2.2. Definition (iv) is another way of saying the stream lines of w move with the fluid.

Similar calculations establish the following equivalent definitions of vector fields of the second type.

Proposition 2.2.3 (Equivalent definitions of vector fields of the second type). *The following are equivalent:*

$$(i) \quad D_t v + (\nabla_x u)v = 0,$$

$$(ii) \quad D_t(Jv) = 0,$$

$$(iii) \quad v(x, t) = J^{-1}(x, t)(v_0 \circ A) \text{ where } v_0(a) := v(a, 0).$$

The two types of vector field interact in the following interesting way.

Proposition 2.2.4. *If w is a vector field of the first type, and v is a vector field of the second type, then*

$$D_t(v \cdot w) = 0. \tag{2.72}$$

Proof. We compute

$$D_t(v \cdot w) = (D_t v) \cdot w + v \cdot (D_t w) = -(\nabla_x u)v \cdot w + v \cdot (\nabla_x u)^\top w \tag{2.73}$$

$$= -v \cdot (\nabla_x u)^\top w + v \cdot (\nabla_x u)^\top w = 0. \tag{2.74}$$

■

Remark 2.2.5. Unfortunately, we are not aware of any interesting statement about $v \times w$ in three dimensions when v and w are of different type. However, if v and w are both vector fields of the first (resp. second) type, then $v \times w$ is a vector field of the second (resp. first) type—see Kuz'min [73] or Tur and Yanovsky [112].

Proposition 2.2.6. *In three dimensions, let v be a vector field of the second type. Then $w = \text{curl}_x v$ is a vector field of the first type.*

Proof. By Proposition 2.2.3, $v = J^{-1}(v_0 \circ A)$. By Proposition 2.1.7,

$$w = \text{curl}_x v = \text{curl}_x(J^{-1}(v_0 \circ A)) = J^{-\top} \text{curl}_a(v_0 \circ A) = J^{-\top}(w_0 \circ A). \tag{2.75}$$

By Proposition 2.2.1, w is thus a vector field of the first type. ▮

Proposition 2.2.7 (Generalized Cauchy invariants formula). *Suppose $w = \text{curl}_x v$ is a vector field of the first type. Then*

$$\sum_{k=1}^3 \nabla_a v^k \times \nabla_a x^k = w_0 \circ A. \quad (2.76)$$

Proof. Using Proposition 2.1.7, we have

$$w_0 \circ A = J^{-\top} \text{curl}_x v = \text{curl}_a(Jv). \quad (2.77)$$

Switching to indices, we compute

$$[\text{curl}_a(Jv)]^i = \epsilon_{ilj} \partial_{a_\ell} (Jv)^j = \epsilon_{ilj} \partial_{a_\ell} (x_{a_j}^k v^k) \quad (2.78)$$

$$= (\epsilon_{ilj} x_{a_j a_\ell}^k) v^k + \epsilon_{ilj} v_{a_\ell}^k x_{a_j}^k \quad (2.79)$$

$$= 0 + [\nabla_a v^k \times \nabla_a x^k]^i, \quad (2.80)$$

where we used $\epsilon_{ilj} x_{a_j a_\ell}^k = 0$ due to symmetry considerations under $j \leftrightarrow \ell$. ▮

Taking $w = \omega$ and $v = u = D_t x$ in Proposition 2.2.7, we recover the usual statement of the Cauchy invariants [55].

Corollary 2.2.8 (Cauchy invariants). *For the Euler equations, we have*

$$\sum_{k=1}^3 \nabla_a u^k \times \nabla_a x^k = \varphi. \quad (2.81)$$

For vector fields of the first type (in arbitrary dimension), the divergence is preserved along particle trajectories.

Proposition 2.2.9. *For w a vector field of the first type, we have $D_t(\text{div}_x w) = 0$.*

Proof. Using Proposition 2.1.6, we compute

$$D_t(\operatorname{div}_x w) = D_t(\operatorname{div}_a(J^{-\top} w)) = \operatorname{div}_a(D_t(J^{-\top} w)) = 0. \quad (2.82)$$

■

2.2.2 The two-dimensional case

In two dimensions, it turns out a vector field of the second type is simply a $\frac{\pi}{2}$ rotation of a vector field of the first type, and vice versa.

Proposition 2.2.10. *Relative to a two-dimensional incompressible fluid, v is a vector field of the first type if and only if v^\perp is a vector field of the second type.*

Proof. Let us write

$$v = \begin{pmatrix} g \\ h \end{pmatrix}, \quad J = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad (2.83)$$

Then

$$Jv = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} g \\ h \end{pmatrix} = \begin{pmatrix} ag + bh \\ cg + dh \end{pmatrix}, \quad (2.84)$$

while

$$J^{-\top} v^\perp = \frac{1}{\det J} \begin{pmatrix} d & -c \\ -b & a \end{pmatrix} \begin{pmatrix} -h \\ g \end{pmatrix} = \begin{pmatrix} -(cg + dh) \\ ag + bh \end{pmatrix} = \frac{1}{\det J} (Jv)^\perp. \quad (2.85)$$

For an incompressible fluid, $D_t \det J = 0$, and so we have $D_t(J^{-\top} v^\perp) = 0$ if and only if $D_t(Jv) = 0$. ■

The simplest examples of vector fields of the first and second type, respectively, are ∇_x^\perp and ∇_x of a scalar carried by the fluid.

Proposition 2.2.11. *Suppose θ is a scalar carried by the fluid,*

$$D_t\theta = 0. \quad (2.86)$$

Then $\nabla_x^\perp\theta$ is a vector field of the first type and $\nabla_x\theta$ is a vector field of the second type.

Proof. Recalling the commutator $[\nabla_x, D_t] = (\nabla_x u)\nabla_x$, we have

$$D_t(\nabla_x\theta) + (\nabla_x u)(\nabla_x\theta) = 0. \quad (2.87)$$

So $\nabla_x\theta$ is a vector field of the second type. By Proposition 2.2.10, it follows that $\nabla_x^\perp\theta$ is a vector field of the first type. ■

2.2.3 Evolution of determinants

Lemma 2.2.12. *Let $u, v, w \in \mathbb{R}^3$ and $A \in \mathbb{R}^{3 \times 3}$. Then*

$$\det(Au, v, w) + \det(u, Av, w) + \det(u, v, Aw) = (\text{Tr } A) \det(u, v, w). \quad (2.88)$$

Proof. We compute

$$\det(Au, v, w) + \det(u, Av, w) + \det(u, v, Aw) \quad (2.89)$$

$$\begin{aligned} &= \epsilon_{ijk} A_{i\ell} (u^\ell v^j w^k + v^\ell w^j u^k + w^\ell u^j v^k) \\ &= \frac{1}{2} A_{i\ell} \epsilon_{ijk} (u^\ell v^j w^k + v^\ell w^j u^k + w^\ell u^j v^k \\ &\quad - u^\ell v^k w^j - v^\ell w^k u^j - w^\ell u^k v^j) \end{aligned} \quad (2.90)$$

$$= \frac{1}{2} A_{i\ell} \epsilon_{ijk} \epsilon_{\ell jk} \det(u, v, w) \quad (2.91)$$

$$= \frac{1}{2} A_{i\ell} (2\delta_{i\ell}) \det(u, v, w) \quad (2.92)$$

$$= (\text{Tr } A) \det(u, v, w), \quad (2.93)$$

where for the second line we used the skew-symmetry in $j \leftrightarrow k$. ▮

Remark 2.2.13. More generally, let v_1, \dots, v_n be n -dimensional vectors and A an $n \times n$ matrix over any field. Then

$$\sum_{i=1}^n \det(v_1, \dots, Av_i, \dots, v_n) = (\operatorname{Tr} A) \det(v_1, \dots, v_n). \quad (2.94)$$

One can prove this in basically the same manner as above, but it is cumbersome to do so without introducing additional notation. We were unable to find a published reference for this lemma, but found an alternate and much more elegant proof in an online forum [83]. This proof employs the uniqueness (up to a scalar multiple) of multilinear alternating tensors—see, e.g., Theorem 2 in §5.3 of Hoffman and Kunze [64]. Define $D_A(v_1, \dots, v_n)$ to be the left-hand side in (2.94). Clearly, D_A is a multilinear alternating tensor and hence

$$D_A(V) = (\det V) D_A(\mathbb{I}) = (\det V) (\operatorname{Tr} A). \quad (2.95)$$

Corollary 2.2.14. *Let v, ω be vectors and N a matrix such that*

$$D_t \omega - N^\top \omega = 0, \quad (2.96)$$

$$D_t v + Nv = 0, \quad (2.97)$$

$$\operatorname{Tr} N = 0. \quad (2.98)$$

Then

$$D_t \det(\omega, \alpha, \beta) = \det(\omega, D_t \alpha - N^\top \alpha, \beta) + \det(\omega, \alpha, D_t \beta - N^\top \beta), \quad (2.99)$$

$$D_t \det(v, \alpha, \beta) = \det(v, D_t \alpha + N\alpha, \beta) + \det(v, \alpha, D_t \beta + N\beta). \quad (2.100)$$

Proof. With the help of Lemma 2.2.12, we compute

$$D_t \det(\omega, \alpha, \beta) = \det(N^\top \omega, \alpha, \beta) + \det(\omega, D_t \alpha, \beta) + \det(\omega, \alpha, D_t \beta) \quad (2.101)$$

$$\begin{aligned} &= - \left(\det(\omega, N^\top \alpha, \beta) + \det(\omega, \alpha, N^\top \beta) \right) \\ &\quad + \det(\omega, D_t \alpha, \beta) + \det(\omega, \alpha, D_t \beta) \end{aligned} \quad (2.102)$$

$$= \det(\omega, D_t \alpha - N^\top \alpha, \beta) + \det(\omega, \alpha, D_t \beta - N^\top \beta). \quad (2.103)$$

A similar calculation holds for v . ▮

Remark 2.2.15. In particular, if α, β, γ are either all vectors of the first type or all vectors of the second type, then we have

$$D_t \det(\alpha, \beta, \gamma) = 0. \quad (2.104)$$

2.2.4 On some determinants in the Euler and Navier-Stokes equations in \mathbb{R}^3

Via a simple change of gauge, we can rewrite the Navier-Stokes equations in \mathbb{R}^3 in the form

$$\partial_t u - \nu \Delta_x u + \nabla_x p_+ = u \times \omega, \quad (2.105)$$

where

$$p_+ := p + \frac{1}{2}|u|^2. \quad (2.106)$$

Written in this form, it is easy to see that determinants of the form $\det(u, \omega, v)$ for some vector field v are of interest.

Proposition 2.2.16. *Solutions of the Navier-Stokes equations satisfy*

$$\|\nabla_x p_+\|_{L^2}^2 = \int_{\mathbb{R}^3} \det(u, \omega, \nabla_x p_+) \, dx, \quad (2.107)$$

$$\frac{\nu}{2} \frac{d}{dt} \|\nabla u\|_{L^2}^2 + \|\partial_t u\|_{L^2}^2 = \int_{\mathbb{R}^3} \det(u, \omega, \partial_t u) \, dx, \quad (2.108)$$

$$\frac{1}{2} \frac{d}{dt} \|\nabla u\|_{L^2}^2 + \nu \|\Delta u\|_{L^2}^2 = \int_{\mathbb{R}^3} \det(u, \omega, -\Delta u) \, dx. \quad (2.109)$$

Proof. Since $\operatorname{div}_x u = 0$, it follows from (2.105) that

$$\partial_t u - \nu \Delta_x u = \mathbb{P}_x(u \times \omega), \quad (2.110)$$

$$\nabla_x p_+ = \mathbb{P}_x^\perp(u \times \omega), \quad (2.111)$$

where \mathbb{P}_x and \mathbb{P}_x^\perp denote the Leray projectors onto divergence-free and curl-free vector fields, respectively. Taking the L^2 inner product of (2.111) with $\nabla_x p_+$ gives

$$\|\nabla_x p_+\|_{L^2}^2 = \langle \nabla_x p_+, \mathbb{P}_x^\perp(u \times \omega) \rangle = \langle \mathbb{P}_x^\perp \nabla_x p_+, u \times \omega \rangle \quad (2.112)$$

$$= \langle \nabla_x p_+, u \times \omega \rangle = \int_{\mathbb{R}^3} \det(u, \omega, \nabla_x p_+) \, dx. \quad (2.113)$$

The other two equations are similarly obtained by taking the inner product of (2.110) with $\partial_t u$ and $-\Delta u$, respectively. ▮

Simply setting $\nu = 0$ in the above, we get the following analog for the Euler equations.

Proposition 2.2.17. *Solutions of the Euler equations satisfy*

$$\|\nabla_x p_+\|_{L^2}^2 = \int_{\mathbb{R}^3} \det(u, \omega, \nabla_x p_+) \, dx, \quad (2.114)$$

$$\|\partial_t u\|_{L^2}^2 = \int_{\mathbb{R}^3} \det(u, \omega, \partial_t u) \, dx, \quad (2.115)$$

$$\frac{1}{2} \frac{d}{dt} \|\nabla u\|_{L^2}^2 = \int_{\mathbb{R}^3} \det(u, \omega, -\Delta u) \, dx. \quad (2.116)$$

In particular, we point out that the integrals of $\det(u, \omega, \nabla_x p_+)$ and $\det(u, \omega, \partial_t u)$ are nonnegative.

2.3 Two special gauge choices

The basic idea here is to look at the quantity $v = u + \nabla_x q$ for some scalar q of our choosing. (Buttke [11] calls any such quantity v a *velocity*.) Since u is divergence-free, we can recover u from v via Leray projection, $u = \mathbb{P}_x v$. Since \mathbb{P}_x is a singular integral operator, all the usual norms of u are controlled by the corresponding norms of v . Depending on the choice of q , it is possible to give many other self-contained formulations of incompressible fluid flow. In this section, we will talk a little about two particular choices of q that have interesting properties.

It should be noted that these ideas are far from new—we include this material here primarily as an application of the material in §2.2. Both gauge choices can be termed folklore. Furthermore, all of the results in §2.3.2 already appear in Buttke [11]. See also Buttke and Chorin [10], where the name “magnetization variable” is introduced, and §1.4 in Chorin [21]. Earlier, Kuz’min [73] and Oseledets [89] already used this gauge to give a Hamiltonian formulation of the Euler equation. Somewhat related is also Constantin’s Eulerian-Lagrangian approach for the Euler and Navier-Stokes equations [25, 26]. Finally, another special choice of gauge, not discussed here, is found in the works of E and Liu [46, 47]. It consists in taking $(\partial_t - \nu \Delta)q = p$, and is shown to be useful in overcoming difficulties of specifying boundary conditions in numerical simulations. For a more extensive literature survey we refer to Russo and Smereka [102], who refer to the gauge choices as *impulse formulations* of the Euler equations.

2.3.1 Eulerian variable v_+

If we define q_+ by

$$\begin{cases} \partial_t q_+ = p + \frac{1}{2}|u|^2, \\ q_+(x, 0) = 0, \end{cases} \quad (2.117)$$

and define v_+ by

$$v_+ = u + \nabla_x q_+, \quad (2.118)$$

then we have

$$\partial_t v_+ + \omega \times u = 0. \quad (2.119)$$

Thus, we may rewrite the incompressible Euler equations as

$$\begin{cases} \partial_t v_+ = \mathbb{P}_x v_+ \times \operatorname{curl}_x v_+, \\ v_+(x, 0) = u_0(x), \\ u = \mathbb{P}_x v_+. \end{cases} \quad (2.120)$$

This formulation makes it particularly easy to prove a sort of Fourier version of the Beale-Kato-Majda criterion [8].

Proposition 2.3.1. *Solutions to the 3d Euler equations with smooth initial data are smooth on $[0, T]$ if*

$$\int_0^T \|\hat{\omega}(\cdot, t)\|_{L^1_\xi} dt < \infty. \quad (2.121)$$

Sketch of proof. Note that, in Fourier space,

$$|\hat{u}(\xi, t)| \leq |(u + \widehat{\nabla_x q})(\xi, t)| \quad (2.122)$$

for any q . Thus, from

$$\partial_t v_+ = u \times \omega, \quad (2.123)$$

we easily derive by a convolution inequality in Fourier space and Gronwall's inequality that

$$\|v_+(\cdot, t)\| \leq e^{C \int_0^t \|\omega(\xi, t)\|_{L_\xi^1} dt} \|v_+(\cdot, 0)\|, \quad (2.124)$$

where $\|\cdot\|$ is, for example, any Besov norm of v_+ . Since $\|u\| \leq \|v_+\|$, it follows that $\|u(\cdot, t)\|$ remains finite as long as (2.121) holds. \blacksquare

Remark 2.3.2. Of course, $\|f\|_{L_x^\infty} \leq C \|\hat{f}\|_{L_\xi^1}$ holds, so the Beale-Kato-Majda criterion is better than this. As observed by Kozono and Taniuchi [71], it even suffices to just control $\|\omega\|_{L_t^1(\text{BMO}_x)}$. For a very nice explanation of this observation using the Fefferman-Stein decomposition of BMO, we recommend Ohkitani [85].

2.3.2 Magnetization variable v_-

If we define q_- by

$$\begin{cases} D_t q_- = p - \frac{1}{2}|u|^2, \\ q_-(x, 0) = 0, \end{cases} \quad (2.125)$$

and set

$$v_- = u + \nabla_x q_-, \quad (2.126)$$

then we have

$$D_t v_- + (\nabla_x u) v_- = 0. \quad (2.127)$$

So v_- is a vector field of the second type and so satisfies the many properties described in §2.2. For example, we have

$$D_t(v_- \cdot \omega) = 0, \quad (2.128)$$

and

$$v_- = J^{-1}\psi, \quad u = \mathbb{P}_x(J^{-1}\psi), \quad (2.129)$$

where ψ is the initial velocity field transported by the fluid,

$$\psi(x, t) = u_0(A(x, t), t). \quad (2.130)$$

The formula $u = \mathbb{P}_x(J^{-1}\psi)$ can be viewed as a nonlocal velocity analog of the Cauchy vorticity formula $\omega = J^\top \varphi$, or as a generalization of the Clebsch variable representation for the velocity—see Constantin [25].

Finally, we mention that if the vorticity is initially compactly supported, then it is possible to choose initial data $q_0(x, 0)$ such that v_- is compactly supported for all time—see Buttke [11].

2.4 On “local” versions of some nonlocal formulas

In incompressible fluids, a number of nonlocal relations exist between quantities of interest. For example, in \mathbb{R}^3 , the velocity is determined by the vorticity through the Biot-Savart law:

$$u(x, t) = -\frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{(x - y) \times \omega(y, t)}{|x - y|^3} dy. \quad (2.131)$$

Another example is that, for the Euler equations, $\partial_t u = -\mathbb{P}(u \cdot \nabla u)$ is the Leray projection of $-u \cdot \nabla u$ onto the space of divergence-free vector fields. (We review the derivation of formulas like (2.131) in §§2.4.1–2.4.4.)

In \mathbb{R}^n and \mathbb{T}^n , these nonlocal relations are most easily analyzed in Fourier space. For example, the Biot-Savart law (2.131) is simply

$$\hat{u}(\xi, t) = \frac{i\xi \times \hat{\omega}(\xi, t)}{|\xi|^2}. \quad (\xi \neq 0) \quad (2.132)$$

(For $\xi = 0$, note that one usually restricts to studying mean-zero vorticity and velocity: $\hat{u}(0, t) = \hat{\omega}(0, t) = 0$.) However, the physical-space representation is better suited to, for example, proving bounds in Hölder spaces or maximum principles.

In bounded domains, as a substitute for the Fourier basis, one may use the eigenfunctions of the Stokes operator—see Constantin and Foias [31]—but this is less explicit. Similarly, physical-space formulas like (2.131) are not readily available, since the Green’s function for the bounded domain may be far more complicated or not known explicitly.

As an alternative, inspired by Constantin’s local pressure formula [22] (see Proposition 2.4.9 below), we prove in §§2.4.5–2.4.9 a number of “local” formulas like the following (see Proposition 2.4.6 below):

$$u(x, t) - \int_{S_r(x)} u(y, t) \, dS(y) = -\frac{1}{4\pi} \int_{B_r(x)} \frac{(x - y) \times (\omega(y, t) - \omega_c)}{|x - y|^3} \, dy, \quad (2.133)$$

where r must be less than the distance of x to the boundary of the domain. We are free to choose $\omega_c = \omega_c(x, t)$, and choices like $\omega_c = 0$, $\omega_c = \omega(x, t)$, and $\omega_c = \int_{B_r(x)} \omega(z, t) \, dz$ could all be useful, depending on the sort of estimates being proved. (For an example applying a “local” pressure formula, see the proof in Constantin [22] that if the velocity is C^α , then the pressure is $C^{2\alpha}$ or Lipschitz.)

The formula is local in the sense that only knowledge of ω in an arbitrarily small neighborhood of x is required to determine the left-hand side of (2.133). However, we put “local” in quotes since the left-hand side is not $u(x, t)$, but rather the difference between $u(x, t)$ and a spherical average of u around x . We remark, however, that this is not a huge disadvantage for many purposes: The spherical average is easily replaced by a volume average over $B_r(x)$, and the volume average is bounded if $u \in L^p$ for some $p \in [1, \infty]$. Alternatively, we could simply prove estimates in terms of Campanato seminorms for a domain $\Omega \subset \mathbb{R}^n$:

$$[u]_{p,\lambda} := \sup_{x \in \Omega, 0 < r < \text{diam}(\Omega)} \left(\frac{1}{r^\lambda} \int_{B_r(x) \cap \Omega} |u(y) - u_{x,r}|^p \, dy \right)^{1/p}, \quad (2.134)$$

where

$$u_{x,r} := \int_{B_r(x) \cap \Omega} u(y) \, dy, \quad (2.135)$$

and $1 \leq p \leq \infty$, $0 \leq \lambda \leq n + p$. These seminorms are equivalent to the BMO seminorm for $\lambda = n$ and to the $C^{0,\alpha}$ Hölder seminorms, with $\alpha = (\lambda - n)/p$, for $n < \lambda \leq n + p$. For more on Morrey-Campanato theory, see for example Chapter III in Giaquinta [58].

2.4.1 The Newton potential for \mathbb{R}^3 and its distributional derivatives

Recall that the Newton potential for \mathbb{R}^3 is

$$\Phi(x) = \frac{1}{4\pi|x|}. \quad (2.136)$$

That is, Φ satisfies $-\Delta\Phi(x) = \delta(x)$ in the sense of distributions. The following computations are standard (see, e.g., §2.4.2 in Majda and Bertozzi [79] or the classic books of Stein [108, 109] for the general theory of singular integral operators):

$$\nabla\Phi(x) = -\frac{1}{4\pi} \frac{x}{|x|^3}, \quad (2.137)$$

and

$$\partial_{x_i x_j}^2 \Phi(x) = \frac{1}{4\pi} \text{p. v.} \frac{\sigma_{ij}(x)}{|x|^3} - \frac{1}{3} \delta_{ij} \delta(x), \quad (2.138)$$

where

$$\sigma(x) = 3\hat{x} \otimes \hat{x} - \mathbb{I}, \quad (2.139)$$

or, written out explicitly,

$$\sigma_{ij}(x) = 3 \frac{x_i x_j}{|x|^2} - \delta_{ij}. \quad (2.140)$$

As a sanity check, note that since $\text{Tr } \sigma = 0$, we indeed recover $-\Delta\Phi = \delta(x)$ from the formula for $\partial_{x_i x_j}^2 \Phi(x)$.

2.4.2 u as a singular integral operator of $\omega \otimes x$

Recalling the identity $-\Delta = \text{curl curl}$ for divergence-free vector fields, we see that there is a differential relation

$$u = \nabla \times (-\Delta)^{-1} \omega \tag{2.141}$$

between the velocity u and the vorticity $\omega = \text{curl } u$. Since $(-\Delta)^{-1} \omega = \Phi * \omega$, we obtain the formula

$$u = \nabla \times (\Phi * \omega) = \nabla \Phi \overset{\times}{*} \omega. \tag{2.142}$$

Written out explicitly, this says

$$u(x, t) = -\frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{(x - y) \times \omega(y, t)}{|x - y|^3} dy, \tag{2.143}$$

and is commonly referred to as the Biot-Savart law in the fluid mechanics literature. So far this is all standard material. See, for example, §2.4 in the book of Majda and Bertozzi [79], but beware of sign errors. (Our sign in (2.143) is correct. Consider, for example, $\omega(x_1, x_2, x_3) = \delta(x_1)\delta(x_2)e_3$, i.e., an infinite constant-strength vortex line in the $+e_3$ direction. By the right-hand rule, this should generate a velocity field in the e_θ direction. Indeed, equation (2.143) yields $u(x, t) = \frac{1}{2\pi\sqrt{x_1^2+x_2^2}}e_\theta$, as expected.)

Note that ω and u are at different levels of regularity, ω being a derivative of u . To get quantities at a comparable level, we can look at u and $\omega \otimes x$. Indeed, u may be written as a singular integral operator of $\omega \otimes x$, as we now show.

Proposition 2.4.1. *We have*

$$u(x, t) + \frac{1}{3}\omega(x, t) \times x = \frac{1}{4\pi} \text{p. v.} \int_{\mathbb{R}^3} y \cdot \frac{\sigma(x-y)}{|x-y|^3} \times \omega(y, t) \, dy, \quad (2.144)$$

$$u(x, t) = \frac{1}{4\pi} \text{p. v.} \int_{\mathbb{R}^3} (y-x) \cdot \frac{\sigma(x-y)}{|x-y|^3} \times (\omega(y, t) - \omega(x, t)) \, dy. \quad (2.145)$$

Proof. First, we remark that since $\int_{\mathbb{R}^3} \nabla \Phi \, dx = 0$, we may insert a vector ω_c independent of y in the above:

$$u = \nabla \times (\Phi * \omega) = \nabla \Phi \overset{\times}{*} (\omega - \omega_c). \quad (2.146)$$

Taking for example $\omega_c = \omega(x, t)$, we get the formula:

$$u(x, t) = -\frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{(x-y) \times (\omega(y, t) - \omega(x, t))}{|x-y|^3} \, dy. \quad (2.147)$$

Furthermore, since $\text{div } \omega = 0$, we have

$$\omega - \omega_c = \text{div}((\omega - \omega_c) \otimes (x - x_c)) \quad (2.148)$$

for any vectors ω_c, x_c independent of y . Thus, we may compute

$$u = \nabla \Phi \overset{\times}{*} \text{div}((\omega - \omega_c) \otimes (x - x_c)) \quad (2.149)$$

$$= \nabla \nabla \Phi \overset{\bullet \times}{*} ((\omega - \omega_c) \otimes (x - x_c)) \quad (2.150)$$

$$= \frac{1}{4\pi} \text{p. v.} \frac{\sigma(x)}{|x|^3} \overset{\bullet \times}{*} ((\omega - \omega_c) \otimes (x - x_c)) - \frac{1}{3}(\omega - \omega_c) \times (x - x_c). \quad (2.151)$$

Taking $\omega_c = x_c = 0$ and $\omega_c = \omega(x, t), x_c = x$, respectively, gives the two equations in the statement of the proposition. █

2.4.3 Pressure formula

Proposition 2.4.2. *We have*

$$p(x, t) + \frac{1}{3}|u(x, t)|^2 = \frac{1}{4\pi} \text{p. v.} \int_{\mathbb{R}^3} \frac{\sigma(x-y)}{|x-y|^3} : u(y) \otimes u(y) \, dy, \quad (2.152)$$

$$p(x, t) = \frac{1}{4\pi} \text{p. v.} \int_{\mathbb{R}^3} \frac{\sigma(x-y)}{|x-y|^3} : (u(y) - u(x)) \otimes (u(y) - u(x)) \, dy. \quad (2.153)$$

Proof. From $-\Delta p = \text{div div}(u \otimes u) = \text{div div}((u - u_c) \otimes (u - u_c))$, we have

$$p = \Phi * \text{div div}((u - u_c) \otimes (u - u_c)) \quad (2.154)$$

$$= \nabla \nabla \Phi \ddot{*} ((u - u_c) \otimes (u - u_c)) \quad (2.155)$$

$$= \frac{1}{4\pi} \text{p. v.} \frac{\sigma(x)}{|x|^3} \ddot{*} ((u - u_c) \otimes (u - u_c)) - \frac{1}{3}|u - u_c|^2. \quad (2.156)$$

Now take $u_c = 0$ and $u_c = u(x, t)$, respectively, to get the two equations in the statement of the proposition. ▮

2.4.4 Formulas for Leray projectors

Proposition 2.4.3. *Suppose $v = u + \nabla q$ with u divergence-free. Then*

$$\nabla q(x) = \mathbb{P}^\perp v(x) = \frac{1}{3}v(x) - \frac{1}{4\pi} \text{p. v.} \int_{\mathbb{R}^3} \frac{\sigma(x-y)}{|x-y|^3} \cdot v(y) \, dy, \quad (2.157)$$

$$u(x) = \mathbb{P}v(x) = \frac{2}{3}v(x) + \frac{1}{4\pi} \text{p. v.} \int_{\mathbb{R}^3} \frac{\sigma(x-y)}{|x-y|^3} \cdot v(y) \, dy. \quad (2.158)$$

Alternatively,

$$\nabla q(x) = \mathbb{P}^\perp v(x) = -\frac{1}{4\pi} \text{p. v.} \int_{\mathbb{R}^3} \frac{\sigma(x-y)}{|x-y|^3} \cdot (v(y) - v(x)) \, dy, \quad (2.159)$$

$$u(x) = \mathbb{P}v(x) = \frac{1}{4\pi} \text{p. v.} \int_{\mathbb{R}^3} \frac{\sigma(x-y)}{|x-y|^3} \cdot (v(y) - v(x)) \, dy. \quad (2.160)$$

Proof. From $\operatorname{div} v = \operatorname{div} u + \Delta q = \Delta q$, we get

$$q = -(-\Delta)^{-1} \operatorname{div} v = -(-\Delta)^{-1} \operatorname{div}(v - v_c), \quad (2.161)$$

and hence

$$\nabla q = -\nabla \Phi * \operatorname{div}(v - v_c) = -\nabla \nabla \Phi \dot{*} (v - v_c) \quad (2.162)$$

$$= -\frac{1}{4\pi} \text{p. v.} \frac{\sigma(x)}{|x|^3} \dot{*} (v - v_c) + \frac{1}{3}(v - v_c). \quad (2.163)$$

The formula for u follows from this using $u = v - \nabla q$. The two variants are obtained by choosing $v_c = 0$ and $v_c = v(x)$, respectively. ▮

Corollary 2.4.4. *For the Euler equations, we have*

$$\partial_t u(x) + \frac{2}{3}(u \cdot \nabla u)(x) = \frac{1}{4\pi} \text{p. v.} \int_{\mathbb{R}^3} \frac{\sigma(x-y)}{|x-y|^3} \cdot (u \cdot \nabla u)(y) \, dy, \quad (2.164)$$

$$\partial_t u(x) = \frac{1}{4\pi} \text{p. v.} \int_{\mathbb{R}^3} \frac{\sigma(x-y)}{|x-y|^3} \cdot ((u \cdot \nabla u)(y) - (u \cdot \nabla u)(x)) \, dy, \quad (2.165)$$

$$\partial_t u(x) + \frac{2}{3}(\omega \times u)(x) = \frac{1}{4\pi} \text{p. v.} \int_{\mathbb{R}^3} \frac{\sigma(x-y)}{|x-y|^3} \cdot (\omega \times u)(y) \, dy, \quad (2.166)$$

$$\partial_t u(x) = \frac{1}{4\pi} \text{p. v.} \int_{\mathbb{R}^3} \frac{\sigma(x-y)}{|x-y|^3} \cdot ((\omega \times u)(y) - (\omega \times u)(x)) \, dy. \quad (2.167)$$

Proof. Apply Proposition 2.4.3 to the formulas

$$-u \cdot \nabla u = \partial_t u + \nabla p, \quad (2.168)$$

$$-\omega \times u = \partial_t u + \nabla(p + \frac{1}{2}|u|^2). \quad (2.169)$$

Remark 2.4.5. Of course, we can write down similar formulas for ∇p . ▮

2.4.5 Nonlocal formulas over a bounded domain

Let Φ denote the Newton potential in \mathbb{R}^3 , and let $U \subset \mathbb{R}^3$ be a bounded domain containing a point x . Then by Green's formula we have

$$u(x) = \int_U \Phi(x-y)(-\Delta u)(y) \, dy + \int_{\partial U} [\Phi(x-y)\partial_n u(y) + u(y)\partial_n \Phi(x-y)] \, dS(y). \quad (2.170)$$

It is common at this point to eliminate one of the two boundary terms by replacing $\Phi(y-x)$ by a Dirichlet or Neumann Green function $G_D(x,y)$ or $G_N(x,y)$ —see, for example, §2.2.4 in Evans [51] and §3.7 in DiBenedetto [41]. However, we will just keep Φ as is for the moment. For the choice $U = B_r(x)$ that we will focus on here, the calculations turn out simpler this way. For other choices, however, the calculations should be redone using the appropriate G_D or G_N .

In the following, we will need these integration-by-parts formulas for vectors v and tensors T :

$$\int_U \Phi(x-y) \operatorname{div} T(y) \, dy = \int_U T(y) \cdot \nabla \Phi(x-y) \, dy + \int_{\partial U} \Phi(x-y)n(y) \cdot T(y) \, dS(y), \quad (2.171)$$

$$\int_U \Phi(x-y) \operatorname{curl} v(y) \, dy = \int_U \nabla \Phi(x-y) \times v(y) \, dy + \int_{\partial U} \Phi(x-y)n(y) \times v(y) \, dS(y), \quad (2.172)$$

$$\begin{aligned} \int_U \Phi(x-y) \nabla T(y) \, dy &= \int_U (\nabla \Phi(x-y)) \otimes T(y) \, dy \\ &\quad + \int_{\partial U} \Phi(x-y)n(y) \otimes T(y) \, dS(y). \end{aligned} \quad (2.173)$$

To make calculations more legible, we will frequently write formulas like the above in

abbreviated notation as

$$\Phi *_U \operatorname{div} T = \nabla \Phi \overset{\bullet}{*_U} T + \Phi *_\partial U (n \cdot T), \quad (2.174)$$

$$\Phi *_U \operatorname{curl} v = \nabla \Phi \overset{\times}{*_U} v + \Phi *_\partial U (n \times v), \quad (2.175)$$

$$\Phi *_U \nabla T = \nabla \Phi \overset{\otimes}{*_U} T + \Phi *_\partial U (n \otimes T). \quad (2.176)$$

2.4.6 Local Biot-Savart formula

Plugging $-\Delta u = \operatorname{curl}(\omega - \omega_c)$ into (2.170) and using (2.172), we find

$$\begin{aligned} u(x) &= \int_U \Phi(x-y) \operatorname{curl}(\omega(y) - \omega_c) \, dy \\ &\quad + \int_{\partial U} [\Phi(x-y) \partial_n u(y) + u(y) \partial_n \Phi(x-y)] \, dS(y) \end{aligned} \quad (2.177)$$

$$\begin{aligned} &= \int_U \nabla \Phi(x-y) \times (\omega(y) - \omega_c) \, dy + \int_{\partial U} u(y) \partial_n \Phi(x-y) \, dS(y) \\ &\quad + \int_{\partial U} [\Phi(x-y) (\partial_n u(y) + n(y) \times (\omega(y) - \omega_c))] \, dS(y). \end{aligned} \quad (2.178)$$

Let's specialize now to $U = B_r(x)$. Then $\Phi(x-y)$ is constant on $\partial U = S_r(x)$, giving rise to a nice cancellation of boundary terms:

$$\int_{S_r} \partial_n u \, dS(y) = \int_{B_r} \Delta u \, dy = - \int_{B_r} \operatorname{curl}(\omega - \omega_c) \, dy = - \int_{S_r} n \times (\omega - \omega_c) \, dS(y). \quad (2.179)$$

Since $\partial_n \Phi(x-y) = \frac{1}{4\pi r^2} = \frac{1}{|S_r|}$ for $y \in S_r(x)$, the remaining boundary term is just the average of u over the boundary,

$$\int_{S_r} u(y) \partial_n \Phi(x-y) \, dS(y) = \int_{S_r} u(y) \, dS(y). \quad (2.180)$$

Putting this all together, we have the following proposition.

Proposition 2.4.6. *We have*

$$u(x, t) - \int_{S_r(x)} u(y, t) dS(y) = -\frac{1}{4\pi} \int_{B_r(x)} \frac{(x-y) \times (\omega(y, t) - \omega_c)}{|x-y|^3} dy. \quad (2.181)$$

Remark 2.4.7. As in Proposition 2.4.1, we could also again use $\omega = \text{div}(\omega \otimes x)$ to get a formula for u as a singular integral operator of $\omega \otimes x$.

Remark 2.4.8. Using the formula (see §A.4)

$$\int_{B_r(x)} u(y) dy = dr^{1-d} \int_0^r \rho^{d-1} \int_{S_\rho(x)} u(y) dS(y) d\rho, \quad (B_r(x) \subset \mathbb{R}^d) \quad (2.182)$$

we can get the following volume-averaged version of Proposition 2.4.6:

$$u(x, t) - \int_{B_r(x)} u(y, t) dy = -\frac{3}{4\pi r^2} \int_0^r \rho^2 \int_{B_\rho(x)} \frac{(x-y) \times (\omega(y, t) - \omega_c)}{|x-y|^3} dy d\rho \quad (2.183)$$

$$= -\frac{1}{4\pi} \int_{B_r(x)} \int_{B_{|z|}(x)} \frac{(x-y) \times (\omega(y, t) - \omega_c)}{|x-y|^3} dy dz. \quad (2.184)$$

2.4.7 Local pressure formula

Proposition 2.4.9 (Constantin (2014) [22]). *We have*

$$p(x, t) + \frac{1}{3}|u(x, t) - u_c|^2 = \frac{1}{4\pi} \text{p. v.} \int_{B_r(x)} \frac{\sigma(x-y)}{|x-y|^3} : (u(y, t) - u_c)^{\otimes 2} dy \quad (2.185)$$

$$+ \int_{S_r(x)} (p(y, t) + |n(y) \cdot (u(y, t) - u_c)|^2) dS(y). \quad (2.186)$$

In particular, taking $u_c = u(x, t)$, we have

$$p(x, t) - \int_{S_r(x)} p(y, t) dS(y) = \frac{1}{4\pi} \text{p. v.} \int_{B_r(x)} \frac{\sigma(x-y)}{|x-y|^3} : (u(y, t) - u(x, t))^{\otimes 2} dy. \quad (2.187)$$

Proof. Let us set $M = (u - u_c) \otimes (u - u_c)$, and recall that we have $-\Delta p = \text{div div } M$. Using Green's formula (2.170) and integrating by parts twice according to (2.171), we

find

$$p = \nabla \nabla \Phi \ddot{*}_U M + \Phi \dot{*}_{\partial U} (\partial_n p + n \cdot \operatorname{div} M) + \partial_n \Phi \dot{*}_{\partial U} p + \nabla \Phi \dot{*}_{\partial U} (n \cdot M). \quad (2.188)$$

Observe that

$$\partial_n p + n \cdot \operatorname{div} M = n \cdot \operatorname{div}(p\mathbb{I} + u \otimes u) = -n \cdot \partial_t u. \quad (2.189)$$

Let us fix now $U = B_r(x)$. Then $\Phi(x - y) = \frac{1}{4\pi r}$ is constant on $S_r(x)$, and so we have

$$\Phi \dot{*}_{S_r(x)} (\partial_n p + n \cdot \operatorname{div} M) = -\frac{1}{4\pi r} \int_{S_r(x)} (n \cdot \partial_t u) \, dS(y) = -\frac{1}{4\pi r} \int_{B_r(x)} \operatorname{div}(\partial_t u) \, dy = 0. \quad (2.190)$$

Similarly, since $\partial_n \Phi(x - y) = \frac{1}{|S_r|}$ on $S_r(x)$, we have

$$(\partial_n \Phi \dot{*}_{S_r(x)} p)(x) = \int_{S_r(x)} p(y) \, dS(y). \quad (2.191)$$

Finally, we compute (noting that $n(y) = \frac{y-x}{|y-x|}$ and $|y-x| = r$)

$$\left(\nabla \Phi \dot{*}_{S_r(x)} (n \cdot M) \right) (x) = - \int_{S_r(x)} \frac{x-y}{4\pi|x-y|^3} \cdot (n \cdot M) \, dS(y) \quad (2.192)$$

$$= \int_{S_r(x)} n \cdot M \cdot n \, dS(y) \quad (2.193)$$

$$= \int_{S_r(x)} |n \cdot (u - u_c)|^2 \, dS(y). \quad (2.194)$$

Putting this all together, we get

$$p + \frac{1}{3}|u - u_c|^2 = \frac{1}{4\pi} \text{p.v.} \frac{\sigma(x)}{|x|^3} \ddot{*}_{B_r} (u - u_c) \otimes (u - u_c) + \int_{S_r} (p + |n \cdot (u - u_c)|^2). \quad (2.195)$$

■

It turns out the formula becomes nicer if we use volume averages over B_r instead of surface averages over S_r , as we will show in the remainder of this section.

Lemma 2.4.10. *If $\operatorname{div} v = 0$, then*

$$\int_{B_r(x)} (y - x) \cdot v(y) \, dy = 0. \quad (2.196)$$

Proof. First observe that

$$\int_{S_\rho(x)} (y - x) \cdot v(y) \, dS(y) = \rho \int_{S_\rho(x)} n(y) \cdot v(y) \, dS(y) = \rho \int_{B_\rho(x)} \operatorname{div} v(y) \, dy = 0 \quad (2.197)$$

for any $\rho > 0$. Using the spherical coarea formula, we thus have

$$\int_{B_r(x)} (y - x) \cdot v(y) \, dy = \int_0^r \int_{S_\rho(x)} (y - x) \cdot v(y) \, dS(y) \, d\rho = 0. \quad (2.198)$$

■

Remark 2.4.11. In fact, if $\operatorname{div} v = 0$, we have

$$\int_{B_r(x)} F(|y - x|) (y - x) \cdot v(y) \, dy = 0 \quad (2.199)$$

for any nice enough $F : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}$. But we will not need this more general formula here.

Corollary 2.4.12. *For the Euler equations, we have*

$$\int_{B_r(x)} p - \int_{S_r(x)} p = \int_{S_r(x)} |n(y) \cdot (u(y, t) - u_c)|^2 - \frac{1}{3} \int_{B_r(x)} |u(y, t) - u_c|^2 \, dy. \quad (2.200)$$

Proof. Taking $F(\rho) = 1$ and $v = \partial_t u = -\operatorname{div}(p\mathbb{I} + (u - u_c)^{\otimes 2})$ in Lemma 2.4.10, we

find

$$0 = - \int_{B_r(x)} (y - x) \cdot \operatorname{div}(p\mathbb{I} + (u - u_c)^{\otimes 2})(y) \, dy \quad (2.201)$$

$$= \int_{B_r(x)} \mathbb{I} : (p\mathbb{I} + (u - u_c)^{\otimes 2}) \, dy - \int_{S_r(x)} n(y) \otimes (y - x) : (p\mathbb{I} + (u - u_c)^{\otimes 2}) \, dS(y) \quad (2.202)$$

$$= \int_{B_r(x)} (3p + |u - u_c|^2) \, dy - r \int_{S_r(x)} (p + |n \cdot (u - u_c)|^2) \, dS(y), \quad (2.203)$$

where we integrated by parts to obtain the second equality, and we used $y - x = rn(y)$ and $|n(y)|^2 = 1$ to obtain the third equality. Dividing by $|S_r|r$ and rearranging gives the statement of the corollary. \blacksquare

Combining Proposition 2.4.9 and Corollary 2.4.12, we get the following volume-averaged version of the local pressure formula.

Corollary 2.4.13. *We have*

$$\begin{aligned} p(x, t) + \frac{1}{3}|u(x, t) - u_c|^2 - \oint_{B_r(x)} \left(p(y, t) - \frac{1}{3}|u(y, t) - u_c|^2 \right) dy \\ = \frac{1}{4\pi} \text{p. v.} \int_{B_r(x)} \frac{\sigma(x - y)}{|x - y|^3} : (u(y, t) - u_c)^{\otimes 2} \, dy. \end{aligned} \quad (2.204)$$

Remark 2.4.14. The Euler equation can be written as

$$\partial_t u + \operatorname{div} S + \nabla q = 0, \quad (2.205)$$

where

$$S = (u - u_c) \otimes (u - u_c) - \frac{1}{3}|u - u_c|^2 \mathbb{I}, \quad (2.206)$$

$$q = p + \frac{1}{3}|u - u_c|^2. \quad (2.207)$$

This is not, in fact, an unusual way to write the Euler equations. The advantage is

that S is now a traceless, symmetric matrix. With $u_c = 0$, this is also the form used by De Lellis and Székelyhidi in their seminal paper [37].

Since $\text{Tr } \sigma = 0$, we have $\sigma : (u - u_c)^{\otimes 2} = \sigma : S$, and so Corollary 2.4.13 allows us to write the relation between q and S as simply

$$q(x, t) - \int_{B_r(x)} q(y, t) \, dy = \frac{1}{4\pi} \text{p. v.} \int_{B_r(x)} \frac{\sigma(x - y)}{|x - y|^3} : S(y, t) \, dy. \quad (2.208)$$

Remark 2.4.15. Everything in this section holds for the Navier-Stokes equations as well, since we used only that u and $\nabla p + u \cdot \nabla u$ are divergence-free (and hence that $-\Delta p = \text{div div}(u \otimes u)$).

2.4.8 Local formulas for Leray projectors

Proposition 2.4.16. *Suppose $v = u + \nabla q$ with u divergence-free. Then*

$$\begin{aligned} \nabla q(x) = \mathbb{P}^\perp v(x) &= \frac{1}{3}(v(x) - v_c) - \frac{1}{4\pi} \text{p. v.} \int_{B_r(x)} \frac{\sigma(x - y)}{|x - y|^3} \cdot (v(y) - v_c) \, dy \\ &+ \int_{S_r(x)} (\nabla q(y) - n(y) (n(y) \cdot (v(y) - v_c))) \, dS(y). \end{aligned} \quad (2.209)$$

Proof. Since $-\Delta \nabla q = \nabla(-\Delta)q = -\nabla \text{div}(v - v_c)$, Green's formula (2.170) gives

$$\nabla q(x) = -\Phi *_{\mathcal{U}} \nabla \text{div}(v - v_c) + \Phi *_{\partial \mathcal{U}} \partial_n \nabla q + \partial_n \Phi *_{\partial \mathcal{U}} \nabla q. \quad (2.210)$$

Integrating by parts twice using (2.173) and (2.171), we get

$$\begin{aligned} \nabla q(x) &= -\nabla \nabla \Phi \dot{*}_{\mathcal{U}} (v - v_c) + \Phi *_{\partial \mathcal{U}} (\partial_n \nabla q - n \text{div}(v - v_c)) \\ &+ \partial_n \Phi *_{\partial \mathcal{U}} \nabla q - \nabla \Phi *_{\partial \mathcal{U}} (n \cdot (v - v_c)). \end{aligned} \quad (2.211)$$

Specializing to $U = B_r$ and using $\operatorname{div}(v - v_c) = \Delta q$, the first boundary term is

$$\frac{1}{4\pi r} \int_{S_r} (n \cdot \nabla \nabla q - n \operatorname{div} \nabla q) \, dS(y) = \frac{1}{4\pi r} \int_{B_r} ([\operatorname{div}, \nabla] \nabla q) \, dy = 0, \quad (2.212)$$

where we used that $[\operatorname{div}, \nabla] = -\operatorname{curl} \operatorname{curl}$ annihilates gradients. For the second and third boundary terms, we use $\nabla \Phi(x - y) = \frac{1}{|S_r|} n(y)$ for $y \in S_r(x)$ to see that they equal

$$\int_{S_r(x)} (\nabla q - n(n \cdot (v - v_c))) \, dS(y). \quad (2.213)$$

Putting these observations together and expanding $\nabla \nabla \Phi$ gives the desired formula. \blacksquare

Remark 2.4.17. As in the case of \mathbb{R}^3 , we can obtain a formula for $u = \mathbb{P}v$ from the above formula by using $u = v - \nabla q$. We write this out for the nicer volume-average expression in Corollary 2.4.18 below.

As with the local pressure formula, it turns out that replacing surface averages by volume averages yields a nicer expression. From $\operatorname{div} u = \operatorname{div}(v - v_c - \nabla q) = 0$, we get $\operatorname{div}(\nabla u)^\top = \operatorname{div}(\nabla(v - v_c - \nabla q))^\top = 0$. Using Lemma 2.4.10, we thus have

$$\int_{B_r(x)} \nabla \nabla q(y) \cdot (y - x) \, dy = \int_{B_r(x)} \nabla(v(y) - v_c) \cdot (y - x) \, dy. \quad (2.214)$$

Integrating by parts both sides of the equation, we find

$$\begin{aligned} 3 \int_{B_r(x)} \nabla q(y) \, dy - r \int_{S_r(x)} \nabla q(y) \, dS(y) = \\ 3 \int_{B_r(x)} (v(y) - v_c) \, dy - r \int_{S_r(x)} n(y) (n(y) \cdot (v(y) - v_c)) \, dS(y). \end{aligned} \quad (2.215)$$

Dividing by $|S_r|r$ and combining the resulting equation with Proposition 2.4.16, we finally arrive at the following formulas:

Corollary 2.4.18. *Suppose $v = u + \nabla q$ with u divergence-free. Then*

$$\begin{aligned} \nabla q(x) - \frac{1}{3}(v(x) - v_c) - \int_{B_r(x)} \left(\nabla q(y) - \frac{1}{3}(v(y) - v_c) \right) dy \\ = -\frac{1}{4\pi} \text{p. v.} \int_{B_r(x)} \frac{\sigma(x-y)}{|x-y|^3} \cdot (v(y) - v_c) dy, \end{aligned} \quad (2.216)$$

$$\begin{aligned} u(x) - \frac{2}{3}(v(x) - v_c) - \int_{B_r(x)} \left(u(y) - \frac{2}{3}(v(y) - v_c) \right) dy \\ = \frac{1}{4\pi} \text{p. v.} \int_{B_r(x)} \frac{\sigma(x-y)}{|x-y|^3} \cdot (v(y) - v_c) dy. \end{aligned} \quad (2.217)$$

2.4.9 Local ∇u from ω formula

Proposition 2.4.19. *We have*

$$\begin{aligned} \nabla u(x) - \frac{2}{3}(\Omega(x) - \Omega_c) - \int_{S_r(x)} (\nabla u(y) + n(y) \otimes (n(y) \times (\omega(y) - \omega_c))) dS(y) \\ = \frac{1}{4\pi} \text{p. v.} \int_{B_r(x)} \frac{\sigma(x-y)}{|x-y|^3} \times (\omega(y) - \omega_c) dy. \end{aligned} \quad (2.218)$$

Here we defined $(\Omega_c)_{ij} = \frac{1}{2}\epsilon_{ijk}\omega_c^k$ analogously to the formula relating Ω and ω .

Proof. Using $-\Delta \nabla u = \nabla \text{curl}(\omega - \omega_c)$, we get by Green's formula (2.170),

$$\nabla u = \Phi *_U \nabla \text{curl}(\omega - \omega_c) + \Phi *_\partial U (\partial_n \nabla u) + \partial_n \Phi *_\partial U \nabla u. \quad (2.219)$$

Integrating by parts twice using (2.173) and (2.172), this becomes

$$\begin{aligned} \nabla u = \nabla \nabla \Phi \overset{\times}{*_U} (\omega - \omega_c) + \Phi *_\partial U (\partial_n \nabla u + n \otimes \text{curl}(\omega - \omega_c)) \\ + \partial_n \Phi *_\partial U \nabla u + \nabla \Phi \overset{\otimes}{*_\partial U} (n \times (\omega - \omega_c)). \end{aligned} \quad (2.220)$$

As before, we specialize to $U = B_r$ and use that $\Phi(y-x)$ is constant on $S_r(x)$ to show

that the first boundary term vanishes:

$$\int_{S_r} \partial_n \nabla u \, dS(y) = \int_{B_r} \nabla \Delta u \, dy = - \int_{B_r} \nabla \operatorname{curl}(\omega - \omega_c) \, dy \quad (2.221)$$

$$= - \int_{S_r} n(y) \otimes \operatorname{curl}(\omega - \omega_c) \, dS(y). \quad (2.222)$$

For the second and third boundary terms, we use $\nabla \Phi(y - x) = \frac{1}{|S_r|} n(y)$ on $S_r(x)$ to compute:

$$\partial_n \Phi *_{\partial U} \nabla u = \int_{S_r(x)} \nabla u(y) \, dS(y), \quad (2.223)$$

$$\nabla \Phi \overset{\otimes}{*}_{\partial U} (n \times (\omega - \omega_c)) = \int_{S_r(x)} n(y) \otimes (n(y) \times (\omega(y) - \omega_c)) \, dS(y). \quad (2.224)$$

Finally, we note that

$$\left[-\frac{1}{3} \mathbb{I} \times (\omega - \omega_c) \right]_{ij} = -\frac{1}{3} \delta_{ik} \epsilon_{jkl} (\omega - \omega_c)^\ell = -\frac{1}{3} \epsilon_{jil} (\omega - \omega_c)^\ell = \frac{2}{3} (\Omega - \Omega_c)_{ij}. \quad (2.225)$$

■

Remark 2.4.20. More generally, we have

$$[A \times \omega]_{ij} = A_{ik} \epsilon_{jkl} \omega^\ell = 2A_{ik} \Omega_{jk} = -2[A\Omega]_{ij}. \quad (2.226)$$

Written purely in terms of Ω and Ω_c , the formula in the proposition is thus

$$\begin{aligned} \nabla u(x) - \frac{2}{3} (\Omega(x) - \Omega_c) &= \int_{S_r(x)} (\nabla u(y) - 2(n(y) \otimes n(y))(\Omega(y) - \Omega_c)) \, dS(y) \\ &= -\frac{1}{4\pi} \text{p.v.} \int_{B_r(x)} \frac{2\sigma(x-y)(\Omega(y) - \Omega_c)}{|x-y|^3} \, dy. \end{aligned} \quad (2.227)$$

2.5 A “Lagrangian” locally compact Abelian group

2.5.1 Motivation

For several fluid-mechanical systems, we can obtain a self-contained Lagrangian evolution equation of the form²

$$D_t X(a, t) = \int_{\mathbb{R}^n} \mathbf{K}(X(a, t) - X(b, t)) \mathbf{F}(X(b, t), \nabla_b X(b, t), \varphi(b)) db, \quad (2.228)$$

where $\varphi(b)$ depends only on initial data. For example, thanks to the Biot-Savart law and $D_t \omega = 0$, the 2d Euler equation may be written as

$$D_t X(a, t) = \frac{1}{2\pi} \int_{\mathbb{R}^2} \frac{(X(a, t) - X(b, t))^\perp}{|X(a, t) - X(b, t)|^2} \omega_0(b) db. \quad (2.229)$$

Similarly, using the Biot-Savart law and the Cauchy formula,

$$\omega(X(a, t), t) = (\nabla_a X(a, t))^\top \omega_0(a), \quad (2.230)$$

the 3d Euler equation may be written as

$$D_t X(a, t) = -\frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{X(a, t) - X(b, t)}{|X(a, t) - X(b, t)|^3} \times \left[(\nabla_b X(b, t))^\top \omega_0(b) \right] db. \quad (2.231)$$

(For the Euler equations, this is discussed extensively in §4 of Majda and Bertozzi [79].

Similar formulas hold for the 2d surface quasi-geostrophic, 2d incompressible porous medium, and 2d Boussinesq equations—see §2 of Constantin, Vicol, and Wu [34].)

The point is that (2.228) looks almost like a convolution. In fact, if we define a

²For this section, we will for obvious reasons write expressions as functions of Lagrangian rather than Eulerian variables. Recall that we write D_t for the partial time derivative even when working in Lagrangian variables. See Remark 2.1.2.

new group operation \oplus on \mathbb{R}^n by³

$$a \oplus b := A(X(a, t) + X(b, t), t), \quad (2.232)$$

then it is exactly a convolution in the locally compact Abelian (LCA) group (\mathbb{R}^n, \oplus) ,

$$D_t X(a, t) = \int_{\mathbb{R}^n} \mathbf{K}(X(a \ominus b, t)) \mathbf{F}(X(b, t), \nabla_b X(b, t), \varphi(b)) db. \quad (2.233)$$

In this section, we will discuss some properties of the LCA group (\mathbb{R}^n, \oplus) , including a Fourier transform and an L^p convolution inequality.

Good references on locally compact groups are the books by Folland [53], Hewitt and Ross [61, 62], Reiter and Stegeman [96], and Rudin [101].

2.5.2 Haar measure and convolution inequality

Thanks to incompressibility, it turns out the Haar measure for (\mathbb{R}^n, \oplus) is simply Lebesgue measure.

Proposition 2.5.1. *The Haar measure of (\mathbb{R}^n, \oplus) is (up to a constant scalar multiple) just Lebesgue measure da . That is, for any $b \in \mathbb{R}^n$ and any integrable f , we have*

$$\int_{\mathbb{R}^n} f(a \oplus b) da = \int_{\mathbb{R}^n} f(a) da. \quad (2.234)$$

Proof. For fixed b , set

$$c(a) = a \oplus b = A(X(a, t) + X(b, t), t). \quad (2.235)$$

Then

$$\nabla_a c = (\nabla_a X(a, t)) \nabla_x A(X(a, t) + X(b, t), t). \quad (2.236)$$

³Note that \oplus depends on t , but for aesthetic reasons we prefer to keep this implicit rather than writing something like \oplus_t .

Since $\det \nabla_x A = \det \nabla_a X = 1$ everywhere, it follows that

$$dc = |\det \nabla_a c| da = da. \quad (2.237)$$

So the Lebesgue measure da is translation-invariant under \oplus . ▮

As a consequence, we have the following convolution inequality (see, for example, §20 in Hewitt and Ross [61] or §2.5 in Folland [53]).

Proposition 2.5.2 (Young's convolution inequality for (\mathbb{R}^n, \oplus)). *Let $1 \leq p, q, r \leq \infty$ such that $1 + \frac{1}{r} = \frac{1}{p} + \frac{1}{q}$ and let $f \in L^p(\mathbb{R}^n), g \in L^q(\mathbb{R}^n)$. Then h defined by*

$$h(a) = \int_{\mathbb{R}^n} f(a \ominus b)g(b) db \quad (2.238)$$

is in $L^r(\mathbb{R}^n)$ and the following estimate holds:

$$\|h\|_{L^r(\mathbb{R}^n)} \leq \|f\|_{L^p(\mathbb{R}^n)} \|g\|_{L^q(\mathbb{R}^n)}. \quad (2.239)$$

2.5.3 Fourier transform

Lemma 2.5.3. *The characters of (\mathbb{R}^n, \oplus) , i.e., the continuous group homomorphisms $(\mathbb{R}^n, \oplus) \rightarrow (\mathbb{T}, \cdot)$, are*

$$\chi_\xi(a) = e^{i\xi \cdot X(a,t)}. \quad (\xi \in \mathbb{R}^n) \quad (2.240)$$

Proof. Clearly, these are continuous. To see they are group homomorphisms, we compute

$$\chi_\xi(a \oplus b) = e^{i\xi \cdot X(a \oplus b, t)} = e^{i\xi \cdot (X(a,t) + X(b,t))} = e^{i\xi \cdot X(a,t)} e^{i\xi \cdot X(b,t)} = \chi_\xi(a) \chi_\xi(b). \quad (2.241)$$

Conversely, if χ is a continuous group homomorphism $(\mathbb{R}^n, \oplus) \rightarrow (\mathbb{T}, \cdot)$, then $\chi \circ A(\cdot, t)$ is a continuous group homomorphism $(\mathbb{R}^n, +) \rightarrow (\mathbb{T}, \cdot)$ and hence of the form $x \mapsto e^{i\xi \cdot x}$

for some ξ . Thus, $\chi = (\chi \circ A) \circ X$ is of the form $a \mapsto e^{i\xi \cdot X(a,t)} = \chi_\xi(a)$ for some ξ . \blacksquare

Thus, we have the following Fourier transform for (\mathbb{R}^n, \oplus) . Much like the usual Fourier transform for $(\mathbb{R}^n, +)$, it comes with an inversion (i.e., Pontryagin duality) theorem, Plancherel identity, and Hausdorff-Young inequality. Instead of additive convolutions, it sends \oplus -convolutions to multiplication. We refer to, e.g., §§4.2–4.3 in Folland [53] for detailed statements.

Definition 2.5.4. The \oplus -Fourier transform of a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is

$$(\mathcal{F}_\oplus f)(\xi) := \int_{\mathbb{R}^n} e^{-i\xi \cdot X(a,t)} f(a) \, da. \quad (2.242)$$

Remark 2.5.5. The relation to the usual Fourier transform is as follows:

$$(\mathcal{F}_\oplus f)(\xi) = \int_{\mathbb{R}^n} e^{-i\xi \cdot X(a,t)} f(a) \, da = \int_{\mathbb{R}^n} e^{-i\xi \cdot x} f(A(x,t)) \, dx \quad (2.243)$$

$$= (\mathcal{F}(f \circ A(\cdot, t)))(\xi). \quad (2.244)$$

In words, the \oplus -Fourier transform with respect to \oplus of a function f of Lagrangian variables is the usual Fourier transform of f as a function of Eulerian coordinates.

Since \oplus is time-dependent, \mathcal{F}_\oplus does not commute with D_t . In fact, the commutator is the Fourier transform of the advection term.

Proposition 2.5.6. For a tensor $f(a, t)$, we have

$$[D_t, \mathcal{F}_\oplus]f(\xi, t) = -i\xi \cdot \mathcal{F}_\oplus[D_t X \otimes f](\xi, t) = -\mathcal{F}[u \cdot \nabla_x(f \circ A)](\xi, t). \quad (2.245)$$

Proof. We compute

$$D_t(\mathcal{F}_\oplus f)(\xi, t) = \int_{\mathbb{R}^n} e^{-i\xi \cdot X(a,t)} \{D_t f(a, t) - (i\xi \cdot D_t X(a, t))f(a, t)\} \, da \quad (2.246)$$

$$= [\mathcal{F}_\oplus(D_t f)](\xi, t) - i\xi \cdot \mathcal{F}_\oplus[D_t X \otimes f](\xi, t). \quad (2.247)$$

Using Remark 2.5.5 and recalling that $u = (D_t X) \circ A$ and $\operatorname{div}_x u = 0$, we find

$$[D_t, \mathcal{F}_\oplus]f(\xi, t) = -i\xi \cdot \mathcal{F}[(D_t X \circ A) \otimes (f \circ A)](\xi, t) \quad (2.248)$$

$$= -\mathcal{F}[\operatorname{div}_x(u \otimes (f \circ A))](\xi, t) \quad (2.249)$$

$$= -\mathcal{F}[u \cdot \nabla_x(f \circ A)](\xi, t). \quad (2.250)$$

■

The interaction with spatial derivatives ∇_a is also not as straightforward as for the usual Fourier transform.

Proposition 2.5.7. *For a tensor $f(a, t)$, we have*

$$\mathcal{F}_\oplus(\nabla_a f)(\xi, t) = i\xi \cdot \mathcal{F}_\oplus[K^{-\top} \otimes f](\xi, t). \quad (2.251)$$

Proof. Integrating by parts, we find

$$\mathcal{F}_\oplus(\nabla_a f)(\xi, t) = \int_{\mathbb{R}^n} e^{-i\xi \cdot X(a, t)} \nabla_a f(a, t) \, da \quad (2.252)$$

$$= \int_{\mathbb{R}^n} e^{-i\xi \cdot X(a, t)} i\xi \cdot (\nabla_a X(a, t))^\top \otimes f(a, t) \, da \quad (2.253)$$

$$= i\xi \cdot \mathcal{F}_\oplus[(\nabla_a X)^\top \otimes f](\xi, t). \quad (2.254)$$

(We introduced the notation $K = \nabla_x a$ and $K^{-1} = \nabla_a X$ in §2.1.2.)

■

Remark 2.5.8. It is clear from Remark 2.5.5 that \mathcal{F}_\oplus satisfies the usual relationships with respect to ∇_x and ∂_t . That is, for a tensor $f(a, t)$, we have

$$[\partial_t, \mathcal{F}_\oplus]f = 0, \quad (2.255)$$

$$\mathcal{F}_\oplus(\nabla_x f)(\xi, t) = i\xi \otimes (\mathcal{F}_\oplus f)(\xi, t). \quad (2.256)$$

By ∂_t and ∇_x we mean the operators on functions of Lagrangian variables, as defined in §2.1.2. That is, $\nabla_x f(a, t) := (\nabla_x(f \circ A)) \circ X$ and $\partial_t f(a, t) := (\partial_t(f \circ A)) \circ X$.

Remark 2.5.9. In the other direction, we can also use Remark 2.5.5 to translate Proposition 2.5.7 into the setting of functions of Eulerian variables. For this, recall first from §2.1.2 that we define ∇_a as an operator on functions of Eulerian variables via $\nabla_a f = (\nabla_a(f \circ X)) \circ A$. Thus, for an Eulerian tensor $f(x, t)$, Proposition 2.5.7 says

$$\mathcal{F}[\nabla_a f](\xi, t) = i\xi \cdot \mathcal{F}[J^\top \otimes f](\xi, t). \quad (2.257)$$

Another way to see this is by means of Proposition 2.1.6. Taking the Fourier transform of the identity

$$\nabla_a f = \operatorname{div}_x(J^\top \otimes f) \quad (2.258)$$

leads directly to (2.257).

2.5.4 Discussion

The availability of an L^p convolution inequality makes it easy to prove a priori bounds like the following.

Proposition 2.5.10. *For the 2d Euler equations, we have*

$$\|u\|_{L^\infty} \leq \frac{1}{\sqrt{2\pi}} \|\omega_0\|_{L^1}^{\frac{1}{2}} \|\omega_0\|_{L^\infty}^{\frac{1}{2}}. \quad (2.259)$$

Proof. By (2.229), we have

$$|u(X(a, t), t)| = |D_t X(a, t)| = \left| \frac{1}{2\pi} \int_{\mathbb{R}^2} \frac{X(b, t)^\perp}{|X(b, t)|^2} \omega_0(a \ominus b) \, db \right| \quad (2.260)$$

$$\leq \int_{|X(\cdot, t)| < R} \frac{1}{2\pi |X(b, t)|} |\omega_0(a \ominus b)| \, db + \int_{|X(\cdot, t)| \geq R} \frac{1}{2\pi |X(b, t)|} |\omega_0(a \ominus b)| \, db. \quad (2.261)$$

Using the convolution inequality, Proposition 2.5.2, it follows that

$$\|u\|_{L^\infty} \leq \|\omega_0\|_{L^\infty} R + \frac{1}{2\pi R} \|\omega_0\|_{L^1}. \quad (2.262)$$

Taking $R = \frac{\|\omega_0\|_{L^1}^{1/2}}{\sqrt{2\pi}\|\omega_0\|_{L^\infty}^{1/2}}$ completes the proof. ▀

To be fair, however, we should point out that this inequality may also be obtained easily by conventional means. Namely, we could have also started from the Eulerian convolution

$$u(x, t) = \frac{1}{2\pi} \int_{\mathbb{R}^2} \frac{y^\perp}{|y|^2} \omega(x - y, t) \, dy, \quad (2.263)$$

and obtained

$$\|u(\cdot, t)\|_{L^\infty} \leq \frac{1}{\sqrt{2\pi}} \|\omega(\cdot, t)\|_{L^1}^{\frac{1}{2}} \|\omega(\cdot, t)\|_{L^\infty}^{\frac{1}{2}} \quad (2.264)$$

by a similar calculation to the above. Finally, since $D_t \omega = 0$ in two dimensions and consequently $\|\omega(\cdot, t)\|_{L^p} = \|\omega_0\|_{L^p}$ for $1 \leq p \leq \infty$, we would have arrived at the same inequality without any need for a \oplus -convolution inequality.

A naive hope when first thinking about this idea was that some methods related to Hilbert's fifth problem could be useful. Any merely continuous LCA group is in fact isomorphic to an analytic LCA group, and there are fascinating tricks used in step-by-step proving this upgrade in regularity—we recommend the exposition by Tao [111]. Unfortunately, trying to apply these ideas in our setting ends up merely telling us what we already know: That the map $X(\cdot, t) : (\mathbb{R}^n, \oplus) \rightarrow (\mathbb{R}^n, +)$ gives an isomorphism of (\mathbb{R}^n, \oplus) with the analytic group $(\mathbb{R}^n, +)$.

Chapter 3

Orthogonal Invariants

Physically meaningful quantities should be independent of the choice of coordinates. The incompressible Euler equations are invariant under orthogonal changes of coordinates, and so it might be worthwhile to look at orthogonal invariants of $\nabla_x u$. Equivalently, we may look for orthogonal invariants of the tuple (\mathcal{D}, Ω) , since the traceless symmetric matrices and the skew-symmetric matrices are both irreducible representations of the orthogonal group (as are the isotropic matrices—but for traceless matrices like $\nabla_x u$ they are not needed). This chapter is devoted to the study of such orthogonal invariants.

Mostly, we will be concerned with the algebraic approach of scalar polynomial orthogonal invariants. We briefly review this theory in §3.1, and we illustrate how to apply it to the incompressible Euler equations in §§3.2–3.4. In the final section, §3.5, we discuss an alternate approach based on rotating the reference frame along a particle trajectory. This allows us to obtain, for example, Lagrangian evolution equations for the eigenvalues of \mathcal{D} and for the vorticity components in the eigenvector basis of \mathcal{D} .

When applying these ideas to the incompressible Euler equations (or other incompressible hydrodynamic systems), the key obstacle is the nonlocality of the pressure

Hessian. Without any pointwise bounds available for pressure-related invariants, pointwise Lagrangian analysis of the invariants of $\nabla_x u$ is ultimately fruitless. In §3.4.5, this obstacle is overcome by looking instead at spatial integrals of invariants; and in §3.4.6, it is overcome by working with Vieillefosse’s model of the Euler equations obtained by simply setting the non-isotropic part of the pressure Hessian to zero. For turbulent fluids, more sophisticated local models for the pressure Hessian have been proposed (see, e.g., Chevillard et al. [20]). Conceivably, these techniques could be fruitfully applied to some such model in the future.

Apart from the Euler equations, we also believe these techniques could be more useful for the study of other physical systems of partial differential equations, especially *local* ones. Working with scalars has the frequent benefit of making cancellations easier to see. Also, bounds are commonly easier to prove, since some invariants have a definite sign. This is best illustrated in §3.4.6.

Finally, a brief comment on the novelty of this material: In the literature, various orthogonal invariants of the Euler equations have been studied on an ad hoc basis, but to our knowledge there has not been an as systematic attempt as this one to identify all of them and their evolutions. The applications we give in §§3.4.5 and 3.4.6 are not new (see Chae [17] and Vieillefosse [113], respectively). However, the proofs are, in our opinion, improved by using our invariants framework.

3.1 Scalar polynomial orthogonal invariants

For scalar polynomial invariants of m -tuples of matrices under the simultaneous action of the orthogonal group, there is a well-developed algebraic theory. We will describe it only in a simple form, with a view towards applications. For more details, we refer to Procesi [91] and §§1, 2, and 10 in Kraft and Procesi [72].

The basic idea is this. Given an m -tuple of $n \times n$ matrices $A = (A_1, \dots, A_m)$, one

considers the subring of the ring of polynomials in the components of A_1, \dots, A_m (let us denote it $\mathbb{R}[A]$) that is invariant under the diagonal action of the orthogonal group:

$$R = \{p \in \mathbb{R}[A] \mid p(A_1, \dots, A_m) = p(\mathcal{O}A_1\mathcal{O}^\top, \dots, \mathcal{O}A_m\mathcal{O}^\top) \text{ for all } \mathcal{O} \in O(n)\}. \quad (3.1)$$

The First Fundamental Theorem of Invariant Theory for the orthogonal group states that R is generated by polynomials of the form

$$\text{Tr } U_1 \cdots U_p, \quad (3.2)$$

where each U_i is equal to A_j or A_j^\top for some j . That is, every scalar (polynomial) orthogonal invariant of the tuple A can be expressed as a polynomial in traces of products of the A_i 's and their transposes.

There are a few partial results for how large we need to take p to get a complete set of generators ($p \leq 2^n - 1$ suffices) and for the relations satisfied by the generators, but really it depends a lot on the specific choices of dimension n and number of matrices m . Indeed, this is still an active area of research—see, e.g., Lopatin [77], Đoković [87], and references therein. Most importantly, as proved by Procesi [91], it turns out that all relations between generators follow from the Cayley-Hamilton Theorem. This is how in practice we may find a set of generators for any particular system of interest. We will illustrate this for the 2d and 3d Euler equations in the following sections.

Before doing this, however, let us recall without proof some basic properties of the trace operator and state the Cayley-Hamilton theorem. (This is, of course, standard linear algebra material. For more details and proofs see, e.g., §§9–10 in Axler [6] or §§7–8 in Roman [100]).

Definition 3.1.1. The *trace* $\text{Tr } A$ of an $n \times n$ matrix A with entries A_{ij} is

$$\text{Tr } A = \sum_{i=1}^n A_{ii}. \quad (3.3)$$

Proposition 3.1.2. *The trace operator satisfies*

$$\text{Tr}(cA + B) = c \text{Tr } A + \text{Tr } B, \quad (\text{linearity}) \quad (3.4)$$

$$\text{Tr } A = \text{Tr } A^\top, \quad (\text{invariance under transpose}) \quad (3.5)$$

$$\text{Tr } A_1 A_2 \cdots A_n = \text{Tr } A_2 \cdots A_n A_1. \quad (\text{invariance under cyclic permutation}) \quad (3.6)$$

Corollary 3.1.3. *The trace is independent of the choice of basis: If B is an invertible matrix, then*

$$\text{Tr } A_1 \cdots A_n = \text{Tr} [(BA_1 B^{-1}) \cdots (BA_n B^{-1})]. \quad (3.7)$$

In particular, the trace is orthogonally invariant: If \mathcal{O} is an orthogonal matrix, then

$$\text{Tr } A_1 \cdots A_n = \text{Tr} [(\mathcal{O}A_1 \mathcal{O}^\top) \cdots (\mathcal{O}A_n \mathcal{O}^\top)]. \quad (3.8)$$

Corollary 3.1.4. *If A is symmetric and B is skew-symmetric, then*

$$\text{Tr } AB = \text{Tr } BA = 0. \quad (3.9)$$

Proof. Using invariance under transpose and cyclic invariance:

$$\text{Tr } AB = \text{Tr}(AB)^\top = \text{Tr } B^\top A^\top = -\text{Tr } BA = -\text{Tr } AB. \quad (3.10)$$

■

Definition 3.1.5. The *characteristic polynomial* p_A of an $n \times n$ matrix A is

$$p_A(\lambda) = \det(\lambda \mathbb{I}_n - A), \quad (3.11)$$

where \mathbb{I}_n denotes the $n \times n$ identity matrix.

Theorem 3.1.6 (Cayley-Hamilton). *If A is an $n \times n$ matrix over a commutative ring, then $p_A(A) = 0$. More explicitly, for $n = 2$ and $n = 3$, we have*

$$A^2 - (\operatorname{Tr} A)A + (\det A)\mathbb{I} = 0, \quad (n = 2) \quad (3.12)$$

$$A^3 - (\operatorname{Tr} A)A^2 + \frac{1}{2}((\operatorname{Tr} A)^2 - \operatorname{Tr} A^2)A - (\det A)\mathbb{I} = 0. \quad (n = 3) \quad (3.13)$$

In practice, it is usually easier to work with the following special case.

Corollary 3.1.7 (Cayley-Hamilton for traceless matrices). *For traceless $n \times n$ matrices A , we have*

$$A^2 = \frac{1}{2}(\operatorname{Tr} A^2)\mathbb{I}, \quad (n = 2) \quad (3.14)$$

$$A^3 = \frac{1}{2}(\operatorname{Tr} A^2)A + \frac{1}{3}(\operatorname{Tr} A^3)\mathbb{I}. \quad (n = 3) \quad (3.15)$$

Proof. The equations in Theorem 3.1.6 simplify in the case $\operatorname{Tr} A = 0$ to

$$A^2 + (\det A)\mathbb{I} = 0, \quad (n = 2) \quad (3.16)$$

$$A^3 - \frac{1}{2}(\operatorname{Tr} A^2)A - (\det A)\mathbb{I} = 0. \quad (n = 3) \quad (3.17)$$

Taking the trace of these equations, we find

$$\det A = -\frac{1}{2} \operatorname{Tr} A^2, \quad (n = 2) \quad (3.18)$$

$$\det A = \frac{1}{3} \operatorname{Tr} A^3. \quad (n = 3) \quad (3.19)$$

Combining the last two sets of equations yields the corollary. █

3.2 Invariants of the incompressible Euler equations

In this section, we will look at orthogonal invariants of the incompressible Euler system

$$\begin{cases} D_t u + \nabla_x p = 0, \\ \operatorname{div}_x u = 0. \end{cases} \quad (3.20)$$

Writing $N = \nabla_x u$ and $P = \nabla_x \nabla_x p$, we have

$$\begin{cases} D_t N + N^2 + P = 0, \\ \operatorname{Tr} N = 0, \\ \operatorname{Tr} P = -\operatorname{Tr} N^2, \\ P = P^\top. \end{cases} \quad (3.21)$$

The first equation is obtained by taking ∇_x of $D_t u + \nabla_x p = 0$, while the second equation is just a restatement of the incompressibility constraint $\operatorname{div}_x u = 0$. The third equation is obtained by taking the trace of the first equation, and the fourth equation is clear since P is a Hessian matrix (assuming $p \in C^2$).

Remark 3.2.1. Unfortunately, there is no evolution equation for P , but this is still a closed system, since P is determined nonlocally by the orthogonal invariant $\operatorname{Tr} N^2$ via

$$P = \nabla_x \nabla_x (-\Delta_x)^{-1} \operatorname{Tr} N^2 = (\mathcal{R}_x \otimes \mathcal{R}_x) \operatorname{Tr} N^2, \quad (3.22)$$

where \mathcal{R}_x denotes the Riesz transform in x . This follows from $P = \nabla_x \nabla_x p$ and $-\Delta_x p = -\operatorname{Tr} P = -\operatorname{Tr} N^2$.

As a first simplification, let us define Q to be the traceless part of P , that is,

$$Q = P - \frac{1}{n}(\text{Tr } P)\mathbb{I} = P + \frac{1}{n}(\text{Tr } N^2)\mathbb{I}. \quad (3.23)$$

This allows us to use the traceless version of the Cayley-Hamilton theorem, Corollary 3.1.7, and will greatly simplify later calculations. Since $\text{Tr } P = -\text{Tr } N^2$, we can recover P from N and Q , so there is no loss of information in doing this substitution.

The new system is

$$\begin{cases} D_t N = \frac{1}{n}(\text{Tr } N^2)\mathbb{I} - N^2 - Q, \\ \text{Tr } N = \text{Tr } Q = 0, \\ Q = Q^\top. \end{cases} \quad (3.24)$$

Next, let us decompose N into symmetric and skew-symmetric parts \mathcal{D} and Ω , respectively. That is,

$$N = \mathcal{D} + \Omega, \quad \mathcal{D} = \frac{1}{2}(N + N^\top), \quad \Omega = \frac{1}{2}(N - N^\top). \quad (3.25)$$

Since $\text{Tr } N = 0$ and Ω vanishes on the diagonal, we have $\text{Tr } \mathcal{D} = \text{Tr } \Omega = 0$. Taking the symmetric and skew-symmetric parts of the equation for $D_t N$ yields

$$\begin{cases} D_t \mathcal{D} = \frac{1}{n} \text{Tr}(\mathcal{D} + \Omega)^2 \mathbb{I} - \mathcal{D}^2 - \Omega^2 - Q, \\ D_t \Omega = -\mathcal{D}\Omega - \Omega\mathcal{D}. \end{cases} \quad (3.26)$$

In the following, then, we shall study triplets of $n \times n$ matrices (\mathcal{D}, Ω, Q) satisfying (3.26) as well as

$$\text{Tr } \mathcal{D} = \text{Tr } \Omega = \text{Tr } Q = 0, \quad \mathcal{D} = \mathcal{D}^\top, \quad Q = Q^\top, \quad \Omega = -\Omega^\top. \quad (3.27)$$

3.3 The two-dimensional case

For the Euler equations in two dimensions, the invariants approach is somewhat overkill. However, it is useful for illustrating the sorts of calculations involved, as these become much more complex even for the case of three dimensions.

In two space dimensions, for arbitrary $a, b \in \mathbb{R}$, we have by the Cayley-Hamilton formula (3.14),

$$(\mathcal{D} + a\Omega + bQ)^2 = \frac{1}{2} \text{Tr}(\mathcal{D} + a\Omega + bQ)^2 \mathbb{I}. \quad (3.28)$$

Expanding both sides gives

$$\begin{aligned} & \mathcal{D}^2 + a^2\Omega^2 + b^2Q^2 + a(\mathcal{D}\Omega + \Omega\mathcal{D}) + b(\mathcal{D}Q + Q\mathcal{D}) + ab(\Omega Q + Q\Omega) \\ &= \left(\frac{1}{2} \text{Tr} \mathcal{D}^2 + \frac{1}{2} a^2 \text{Tr} \Omega^2 + \frac{1}{2} b^2 \text{Tr} Q^2 + b \text{Tr} \mathcal{D}Q \right) \mathbb{I}. \end{aligned} \quad (3.29)$$

Equating the coefficients of the various monomials in a, b , we find

$$\begin{aligned} \mathcal{D}^2 &= \frac{1}{2}(\text{Tr} \mathcal{D}^2)\mathbb{I}, & \Omega^2 &= \frac{1}{2}(\text{Tr} \Omega^2)\mathbb{I}, & Q^2 &= \frac{1}{2}(\text{Tr} Q^2)\mathbb{I}, \\ \mathcal{D}Q + Q\mathcal{D} &= (\text{Tr} \mathcal{D}Q)\mathbb{I}, & \mathcal{D}\Omega + \Omega\mathcal{D} &= \Omega Q + Q\Omega = 0. \end{aligned} \quad (3.30)$$

Using these matrix-level relations, we can find a minimal set of generators for the ring of orthogonal invariants.

Theorem 3.3.1. *The ring of orthogonal invariants for triplets (\mathcal{D}, Ω, Q) of traceless 2×2 matrices, with \mathcal{D}, Q symmetric and Ω skew-symmetric, is generated by the*

following five invariants:

$$\eta = \frac{1}{2} \operatorname{Tr} \mathcal{D}^2 = \frac{1}{2} |\mathcal{D}|^2, \quad (3.31)$$

$$\mu = -\frac{1}{2} \operatorname{Tr} \Omega^2 = \frac{1}{2} |\Omega|^2 = \frac{1}{4} \omega^2, \quad (3.32)$$

$$\pi_1 = \operatorname{Tr} \mathcal{D}Q = \operatorname{Tr} Q\mathcal{D}, \quad (3.33)$$

$$\pi_2 = \frac{1}{2} \operatorname{Tr} Q^2 = \frac{1}{2} |Q|^2, \quad (3.34)$$

$$\pi_3 = \operatorname{Tr} \mathcal{D}\Omega Q. \quad (3.35)$$

These satisfy the relation

$$\pi_3^2 = 4\eta\mu\pi_2 - \mu\pi_1^2. \quad (3.36)$$

Proof. First let us prove that these five invariants are indeed a complete set of generators. By the First Fundamental Theorem (see §3.1 above), it suffices to show that each invariant of the form $T = \operatorname{Tr} A_1 \cdots A_p$, where each A_i is one of \mathcal{D}, Ω , or Q , can be expressed in terms of η, μ, π_1 , and π_2 . So let some such invariant T be given. The proof is by induction on p .

1. If $p = 1$, then T vanishes since \mathcal{D}, Ω, Q are all traceless.
2. If $p = 2$, then T is one of η, μ, π_1, π_2 or else vanishes. For if T is not one of η, μ, π_1, π_2 , then it must be one of $\operatorname{Tr} \mathcal{D}\Omega = \operatorname{Tr} \Omega\mathcal{D}$ or $\operatorname{Tr} Q\Omega = \operatorname{Tr} \Omega Q$. These vanish by symmetry considerations—see Corollary 3.1.4.
3. If $p \geq 3$, then T either vanishes or can be written in terms of π_3 and invariants of the form $S = \operatorname{Tr} B_1 \cdots B_q$ with each B_i equal to one of \mathcal{D}, Ω, Q and $q < p$.

First note that, with the help of the anticommutation relations in (3.30), we can freely reorder the factors A_i at the expense of possibly changing sign and adding terms like $\pi_1 S$ with S as just described.

If $A_i = A_j$ for some $i \neq j$, then we can reorder such that $j = i + 1$ and then use

the first line of equations in (3.30) to reduce this remaining term to one of ηS , μS , or $\pi_2 S$, with S as described.

The only remaining possibility is that $p = 3$ and A_1, A_2, A_3 is some permutation of \mathcal{D}, Ω, Q . Then we can reorder to the case $T = \pm \text{Tr } \mathcal{D}\Omega Q = \pm \pi_3$.

The relation (3.36) can be proved by applying the Cayley-Hamilton theorem 3.1.6 to the matrix $\mathcal{D}\Omega Q$ and using reorderings and reductions as in the induction step above. The two-dimensional case is simple enough, however, that it is more instructive to just write out the invariants explicitly. Without loss of generality, thanks to orthogonal conjugation, we may assume \mathcal{D} is diagonal. Then the matrices have the explicit form

$$\mathcal{D} = \begin{pmatrix} \lambda & 0 \\ 0 & -\lambda \end{pmatrix}, \quad \Omega = \frac{1}{2} \begin{pmatrix} 0 & \omega \\ -\omega & 0 \end{pmatrix}, \quad Q = \begin{pmatrix} p & q \\ q & -p \end{pmatrix} \quad (3.37)$$

for some real numbers λ, ω, p, q . The invariants are then found to be

$$\eta = \lambda^2, \quad \mu = \frac{1}{4}\omega^2, \quad \pi_1 = 2\lambda p, \quad \pi_2 = p^2 + q^2, \quad \pi_3 = \lambda\omega q. \quad (3.38)$$

Using these expressions, it is straightforward to verify relation (3.36). Furthermore, it is clear that no lower-order relations hold. ▮

Remark 3.3.2. Owing to the relation (3.36), in practice we do not need π_3 .

Remark 3.3.3. Note that η, μ, π_2 are nonnegative, but the signs of π_1 and π_3 are indeterminate.

Remark 3.3.4. With the help of (3.30), the evolution equations (3.26) for \mathcal{D} and Ω simplify to

$$D_t \mathcal{D} = -Q, \quad D_t \Omega = 0. \quad (3.39)$$

This gives straight-forwardly

$$D_t \eta = -\pi_1, \quad D_t \mu = 0. \quad (3.40)$$

So looking at orthogonal invariants has naturally led us to the observation that vorticity is conserved along Lagrangian particle trajectories. Beyond this, however, the two-dimensional case is really geometrically too simple for the invariants approach to be useful. The three-dimensional case discussed next is far more interesting.

Remark 3.3.5. The statement $D_t \Omega = 0$ is fully equivalent to the usual statement $D_t \omega = 0$, but the scalar $\mu = \frac{1}{4} \omega^2$ loses sign information about ω . To recover ω , we should really look at *special orthogonal* and not just orthogonal invariants. In even dimensions, the Pfaffian of skew-symmetric matrices is a special orthogonal invariant. In our case,

$$(\text{Pf } \Omega)^2 = \det \Omega = \frac{1}{4} \omega^2, \quad (3.41)$$

so we find that $\frac{1}{2} \omega$ is a special orthogonal invariant. In odd dimensions, the special orthogonal invariants coincide with the orthogonal ones—see Aslaksen [5].

3.4 The three-dimensional case

As in the two-dimensional case, we begin by using Cayley-Hamilton to derive some matrix-level identities for \mathcal{D}, Ω, Q .

Lemma 3.4.1. *For \mathcal{D}, Ω, Q traceless 3×3 matrices with \mathcal{D}, Q symmetric and Ω*

skew-symmetric, we have

$$\mathcal{D}^3 = \frac{1}{2} \text{Tr}(\mathcal{D}^2)\mathcal{D} + \frac{1}{3}(\text{Tr } \mathcal{D}^3)\mathbb{I}, \quad (3.42)$$

$$\Omega^3 = \frac{1}{2} \text{Tr}(\Omega^2)\Omega, \quad (3.43)$$

$$Q^3 = \frac{1}{2} \text{Tr}(Q^2)Q + \frac{1}{3}(\text{Tr } Q^3)\mathbb{I}, \quad (3.44)$$

and

$$\mathcal{D}^2\Omega + \mathcal{D}\Omega\mathcal{D} + \Omega\mathcal{D}^2 = \frac{1}{2}(\text{Tr } \mathcal{D}^2)\Omega, \quad (3.45)$$

$$\mathcal{D}^2Q + \mathcal{D}Q\mathcal{D} + Q\mathcal{D}^2 = \frac{1}{2}(\text{Tr } \mathcal{D}^2)Q + (\text{Tr } \mathcal{D}Q)\mathcal{D} + (\text{Tr } \mathcal{D}^2Q)\mathbb{I}, \quad (3.46)$$

$$\Omega^2\mathcal{D} + \Omega\mathcal{D}\Omega + \mathcal{D}\Omega^2 = \frac{1}{2}(\text{Tr } \Omega^2)\mathcal{D} + (\text{Tr } \mathcal{D}\Omega^2)\mathbb{I}, \quad (3.47)$$

$$\Omega^2Q + \Omega Q\Omega + Q\Omega^2 = \frac{1}{2}(\text{Tr } \Omega^2)Q + (\text{Tr } \Omega^2Q)\mathbb{I}, \quad (3.48)$$

$$Q^2\mathcal{D} + Q\mathcal{D}Q + \mathcal{D}Q^2 = \frac{1}{2}(\text{Tr } Q^2)\mathcal{D} + (\text{Tr } \mathcal{D}Q)Q + (\text{Tr } \mathcal{D}Q^2)\mathbb{I}, \quad (3.49)$$

$$Q^2\Omega + Q\Omega Q + \Omega Q^2 = \frac{1}{2}(\text{Tr } Q^2)\Omega, \quad (3.50)$$

and

$$\mathcal{D}\Omega Q + \Omega Q\mathcal{D} + Q\mathcal{D}\Omega + \mathcal{D}Q\Omega + Q\Omega\mathcal{D} + \Omega\mathcal{D}Q = (\text{Tr } \mathcal{D}Q)\Omega. \quad (3.51)$$

Proof. For arbitrary $a, b \in \mathbb{R}$, we have by the Cayley-Hamilton formula (3.15),

$$\begin{aligned} (\mathcal{D} + a\Omega + bQ)^3 &= \frac{1}{2} [\text{Tr}(\mathcal{D} + a\Omega + bQ)^2] (\mathcal{D} + a\Omega + bQ) \\ &\quad + \frac{1}{3} [\text{Tr}(\mathcal{D} + a\Omega + bQ)^3] \mathbb{I}. \end{aligned} \quad (3.52)$$

Expanding both sides and equating the coefficients of the various monomials in a, b leads to the stated identities. ▮

Finding and proving a full analog of Theorem 3.3.1 in three dimensions is much

harder. Already for a single traceless 3×3 matrix N , six generators are required:

$$\mathrm{Tr} N^2, \mathrm{Tr} NN^\top, \mathrm{Tr} N^3, \mathrm{Tr} N^2N^\top, \mathrm{Tr} N^2(N^\top)^2, \mathrm{Tr} NN^\top N^2(N^\top)^2. \quad (3.53)$$

We refer to, e.g., Theorem 2 in Đoković [87], who credits Sibirskii [104] (in Russian). According to the proof of Theorem 3 in Đoković [87], the first five of the generators are independent, while the sixth may be determined from the first five via a (very complicated!) quadratic equation. In practice, this means the sixth invariant is redundant (much like π_3 was redundant in the two-dimensional case), and so we will not further consider it. Furthermore, we will use generators expressed in terms of \mathcal{D} and Ω rather than N and N^\top . It is easy to go back and forth between the two, and we omit spelling this out in detail. Without further ado, we introduce the five invariants of (\mathcal{D}, Ω) that will occupy us for the remainder of this section:

$$\eta = \frac{1}{2} \mathrm{Tr} \mathcal{D}^2, \quad (3.54)$$

$$\mu = -\frac{1}{2} \mathrm{Tr} \Omega^2, \quad (3.55)$$

$$\beta = -\frac{1}{3} \mathrm{Tr} \mathcal{D}^3, \quad (3.56)$$

$$\varphi = \mathrm{Tr} \mathcal{D}\Omega^2, \quad (3.57)$$

$$\psi = -\frac{1}{2} \mathrm{Tr} \mathcal{D}^2\Omega^2. \quad (3.58)$$

For the full triplet (\mathcal{D}, Ω, Q) , there are many more invariants. Fortunately, having restricted to the above invariants for (\mathcal{D}, Ω) , we will need only four of them in the

following:

$$\pi_1 = \text{Tr } \mathcal{D}Q, \quad (3.59)$$

$$\pi_2 = \text{Tr } \mathcal{D}^2Q, \quad (3.60)$$

$$\pi_3 = -\text{Tr } \Omega^2Q, \quad (3.61)$$

$$\pi_4 = \text{Tr } \mathcal{D}\Omega^2Q. \quad (3.62)$$

3.4.1 Evolution equations

Proposition 3.4.2. *We have*

$$D_t\eta = 3\beta - \varphi - \pi_1, \quad (3.63)$$

$$D_t\mu = 2\varphi, \quad (3.64)$$

$$D_t\beta = \frac{2}{3}\eta^2 + \frac{4}{3}\eta\mu - 2\psi + \pi_2, \quad (3.65)$$

$$D_t\varphi = -\frac{2}{3}\mu^2 + \frac{8}{3}\eta\mu - 2\psi + \pi_3, \quad (3.66)$$

$$D_t\psi = \frac{4}{3}\eta\varphi - \frac{1}{3}\mu\varphi + 3\mu\beta + \pi_4. \quad (3.67)$$

Remark 3.4.3. Instead of ψ , it may be preferable to work with the quantity $\zeta = 2\eta\mu - 2\psi$ (see Proposition 3.4.11). In terms of ζ , we have

$$D_t\beta = \frac{2}{3}\eta(\eta - \mu) + \zeta + \pi_2, \quad (3.68)$$

$$D_t\varphi = \frac{2}{3}\mu(\eta - \mu) + \zeta + \pi_3, \quad (3.69)$$

$$D_t\zeta = \frac{4}{3}(\eta - \mu)\varphi - 2\mu\pi_1 - 2\pi_4. \quad (3.70)$$

See also the *ab*-system (3.165) below.

Remark 3.4.4. In Remark 2.1.13, we observed that

$$\tilde{P} = P - NN^\top \quad (3.71)$$

may be an interesting quantity to study instead of P or its traceless part Q . If instead of the π -invariants, we use the $\tilde{\pi}$ -invariants defined by

$$\tilde{\pi}_1 = \text{Tr } \mathcal{D}\tilde{P}, \quad \tilde{\pi}_3 = -\text{Tr } \Omega^2 \tilde{P}, \quad (3.72)$$

$$\tilde{\pi}_2 = \text{Tr } \mathcal{D}^2 \tilde{P}, \quad \tilde{\pi}_4 = \text{Tr } \mathcal{D}\Omega^2 \tilde{P}, \quad (3.73)$$

then the evolution equations simplify to

$$D_t \eta = 6\beta - \tilde{\pi}_1, \quad (3.74)$$

$$D_t \mu = 2\varphi, \quad (3.75)$$

$$D_t \beta = 4\eta^2 + \tilde{\pi}_2, \quad (3.76)$$

$$D_t \varphi = 4\eta\mu + \tilde{\pi}_3, \quad (3.77)$$

$$D_t \psi = 3\eta\varphi + 5\mu\beta + \tilde{\pi}_4. \quad (3.78)$$

In particular, note that if we treat $\tilde{\pi}_1, \tilde{\pi}_2$ as known, the evolutions for η, β form a closed system. Treating also $\tilde{\pi}_3$ as known, the evolutions for $\eta, \mu, \beta, \varphi$ form a closed system. See also Remark 3.5.5 below for the evolution equations of the eigenvalues of \mathcal{D} and of the vorticity components in the eigenvector basis of \mathcal{D} .

Remark 3.4.5. Similarly, if we set

$$\bar{P} = P + NN^\top, \quad (3.79)$$

and define corresponding $\bar{\pi}_i$ invariants, the evolution equations take the form

$$D_t \eta = -2\varphi - \bar{\pi}_1, \quad (3.80)$$

$$D_t \mu = 2\varphi, \quad (3.81)$$

$$D_t \beta = -4\psi + \bar{\pi}_2, \quad (3.82)$$

$$D_t \varphi = -4\psi + 4(\eta - \mu)\mu + \bar{\pi}_3, \quad (3.83)$$

$$D_t \psi = (\eta - \mu)\varphi + \mu(\beta - \varphi) + \bar{\pi}_4. \quad (3.84)$$

Replacing η by $a = \eta - \mu$ and β by $b = \beta - \varphi$ (see also (3.165) below), this simplifies to

$$D_t a = -4\varphi - \bar{\pi}_1, \quad (3.85)$$

$$D_t b = 4a\mu + \bar{\pi}_2 - \bar{\pi}_3, \quad (3.86)$$

$$D_t \mu = 2\varphi, \quad (3.87)$$

$$D_t \varphi = -4\psi + 4a\mu + \bar{\pi}_3, \quad (3.88)$$

$$D_t \psi = a\varphi + \mu b + \bar{\pi}_4. \quad (3.89)$$

Proof of Proposition 3.4.2. According to (3.26), the evolutions equations for \mathcal{D} and Ω in three dimensions are:

$$D_t \mathcal{D} = \frac{2}{3}(\eta - \mu)\mathbb{I} - \mathcal{D}^2 - \Omega^2 - Q, \quad (3.90)$$

$$D_t \Omega = -\mathcal{D}\Omega - \Omega\mathcal{D}. \quad (3.91)$$

With help of Lemma 3.4.1, we compute

$$D_t \mathcal{D}^2 = \frac{4}{3}(\eta - \mu)\mathcal{D} - 2(\eta\mathcal{D} - \beta\mathbb{I}) - \mathcal{D}(\Omega^2 + Q) - (\Omega^2 + Q)\mathcal{D}, \quad (3.92)$$

and

$$D_t \Omega^2 = -\mathcal{D}\Omega^2 - \Omega^2 \mathcal{D} - 2\Omega \mathcal{D}\Omega \quad (3.93)$$

$$= -2(\Omega^2 \mathcal{D} + \Omega \mathcal{D}\Omega + \mathcal{D}\Omega^2) + \Omega^2 \mathcal{D} + \mathcal{D}\Omega^2 \quad (3.94)$$

$$= -2(\varphi \mathbb{I} - \mu \mathcal{D}) + \Omega^2 \mathcal{D} + \mathcal{D}\Omega^2. \quad (3.95)$$

Furthermore,

$$D_t \mathcal{D}^3 = 2(\eta - \mu) \mathcal{D}^2 - 3(\eta \mathcal{D}^2 - \beta \mathcal{D}) \quad (3.96)$$

$$- [\mathcal{D}^2(\Omega^2 + Q) + \mathcal{D}(\Omega^2 + Q)\mathcal{D} + (\Omega^2 + Q)\mathcal{D}^2],$$

and

$$D_t(\mathcal{D}\Omega^2) = \frac{2}{3}(\eta - \mu)\Omega^2 - \mathcal{D}^2\Omega^2 + \mu\Omega^2 - Q\Omega^2 - 2\varphi\mathcal{D} + 2\mu\mathcal{D}^2 \quad (3.97)$$

$$+ \mathcal{D}\Omega^2\mathcal{D} + \mathcal{D}^2\Omega^2$$

$$= -2\varphi\mathcal{D} + \frac{2}{3}\eta\Omega^2 - \frac{1}{3}\mu\Omega^2 + 2\mu\mathcal{D}^2 + \mathcal{D}\Omega^2\mathcal{D} - Q\Omega^2, \quad (3.98)$$

and finally

$$D_t(\mathcal{D}^2\Omega^2) = \frac{4}{3}(\eta - \mu)\mathcal{D}\Omega^2 - 2(\eta\mathcal{D}\Omega^2 - \beta\Omega^2) - \mathcal{D}(\Omega^2 + Q)\Omega^2 \quad (3.99)$$

$$- (\Omega^2 + Q)\mathcal{D}\Omega^2 - 2(\varphi\mathcal{D}^2 - \mu\mathcal{D}^3) + \mathcal{D}^2\Omega^2\mathcal{D} + \mathcal{D}^3\Omega^2$$

$$= -\frac{2}{3}\eta\mathcal{D}\Omega^2 - \frac{4}{3}\mu\mathcal{D}\Omega^2 + 2\beta\Omega^2 - 2\varphi\mathcal{D}^2 + 2\mu\mathcal{D}^3 \quad (3.100)$$

$$+ (\mathcal{D}^2\Omega^2\mathcal{D} + \mathcal{D}^3\Omega^2) - (Q\mathcal{D}\Omega^2 + \mathcal{D}Q\Omega^2) - (\mathcal{D}\Omega^4 + \Omega^2\mathcal{D}\Omega^2).$$

Observe now that

$$\mathcal{D}^3\Omega^2 = (\eta\mathcal{D} - \beta\mathbb{I})\Omega^2, \quad (3.101)$$

and hence

$$\text{Tr}(\mathcal{D}^3\Omega^2) = \eta\varphi + 2\mu\beta. \quad (3.102)$$

Similarly,

$$\Omega^4 = -\mu\Omega^2, \quad (3.103)$$

and hence

$$\text{Tr}(\mathcal{D}\Omega^4) = -\mu\varphi. \quad (3.104)$$

Taking traces of the above evolution equations, we thus find

$$D_t\eta = 3\beta - \varphi - \pi_1, \quad (3.105)$$

$$D_t\mu = 2\varphi, \quad (3.106)$$

$$D_t\beta = -\frac{4}{3}(\eta - \mu)\eta + 2\eta^2 - 2\psi + \pi_2 = \frac{2}{3}\eta^2 + \frac{4}{3}\eta\mu - 2\psi + \pi_2, \quad (3.107)$$

$$D_t\varphi = -\frac{4}{3}(\eta - \mu)\mu - 2\mu^2 + 4\eta\mu - 2\psi + \pi_3 = -\frac{2}{3}\mu^2 + \frac{8}{3}\eta\mu - 2\psi + \pi_3, \quad (3.108)$$

$$D_t\psi = -\frac{2}{3}(\eta - \mu)\varphi + (\eta\varphi + 2\mu\beta) - \mu\varphi + \pi_4 + (2\eta\varphi + 3\mu\beta) - (\eta\varphi + 2\mu\beta) \quad (3.109)$$

$$= -\frac{2}{3}(\eta - \mu)\varphi + 2\eta\varphi + 3\mu\beta - \mu\varphi + \pi_4 \quad (3.110)$$

$$= \frac{4}{3}\eta\varphi - \frac{1}{3}\mu\varphi + 3\mu\beta + \pi_4. \quad (3.111)$$

■

3.4.2 Related invariants

Aside from the scalar polynomial orthogonal invariants, there are of course many other orthogonal invariants that are non-scalar (like the vorticity vector ω) or non-polynomial (like the eigenvalues λ_i of \mathcal{D}). We will list some of these other orthogonal invariants and their basic properties in this section, and prove more detailed statements and bounds relating them to the scalar polynomial orthogonal invariants in §3.4.3.

Invariants related to \mathcal{D}

\mathcal{D} is real symmetric and hence orthogonally diagonalizable. We call its three real eigenvalues

$$\lambda_1 \geq \lambda_2 \geq \lambda_3. \quad (3.112)$$

Let us record some elementary observations about the eigenvalues. Since \mathcal{D} is traceless, we have

$$\lambda_1 + \lambda_2 + \lambda_3 = 0. \quad (3.113)$$

From this it follows immediately that

$$\lambda_1 \geq 0 \geq \lambda_3. \quad (3.114)$$

Furthermore, we will be interested in the spectral radius ρ of \mathcal{D} ,

$$\rho = \max\{\lambda_1, -\lambda_3\}, \quad (3.115)$$

and the quantity

$$\rho_- = \min\{\lambda_1, -\lambda_3\}. \quad (3.116)$$

Then we have

$$|\lambda_2| + \rho_- = \rho, \quad (3.117)$$

and since $|\lambda_2| \leq \rho_- \leq \rho$, this implies

$$0 \leq |\lambda_2| \leq \frac{1}{2}\rho \leq \rho_- \leq \rho. \quad (3.118)$$

Invariants related to Ω

Recall that Ω is related to the vorticity ω via $\Omega_{ij} = \frac{1}{2}\epsilon_{ijk}\omega^k$. That is,

$$\Omega = \frac{1}{2} \begin{pmatrix} 0 & \omega_3 & -\omega_2 \\ -\omega_3 & 0 & \omega_1 \\ \omega_2 & -\omega_1 & 0 \end{pmatrix}. \quad (3.119)$$

We find by direct computation that

$$\mu = -\frac{1}{2} \text{Tr} \Omega^2 = \frac{1}{4} |\omega|^2. \quad (3.120)$$

The direction of vorticity is

$$\xi = \frac{\omega}{|\omega|} = \frac{\omega}{2\sqrt{\mu}}. \quad (3.121)$$

Invariants involving both \mathcal{D} and Ω

An alternative to ψ is

$$\zeta = \frac{1}{4} |\mathcal{D}\omega|^2 = \mu |\mathcal{D}\xi|^2. \quad (3.122)$$

(See also Remark 3.4.3 above and Proposition 3.4.11 below.)

The vorticity stretching factor is

$$\alpha = \frac{\varphi}{\mu} = \xi \cdot \mathcal{D}\xi. \quad (3.123)$$

It is called *vorticity stretching factor* because of the identity $D_t \log |\omega| = \alpha$ for the Euler equations. The invariants α and ξ play an important role in the Constantin-Fefferman-Majda regularity criterion for the Euler equations [30].

Galanti, Gibbon, and Heritage [57] introduced the vector

$$\chi = \xi \times \mathcal{D}\xi \quad (3.124)$$

in their study of vorticity alignment. The vector χ (along with the scalar α) also plays a prominent role in the elegant quaternion-based formulation of the Euler equations of Gibbon et al. [59]. Note that, if we let θ denote the angle between ξ and $\mathcal{D}\xi$, then

$$\alpha^2 = \frac{\zeta}{\mu} \cos^2 \theta, \quad (3.125)$$

$$|\chi|^2 = \frac{\zeta}{\mu} \sin^2 \theta, \quad (3.126)$$

Thus, we have

$$\frac{\zeta}{\mu} = \alpha^2 + |\chi|^2. \quad (3.127)$$

Also, plugging $\alpha = \frac{\varphi}{\mu}$ into the equation for α^2 , we find

$$\frac{\varphi^2}{\mu\zeta} = \cos^2 \theta. \quad (3.128)$$

3.4.3 Algebraic relations and constraints

First, we observe that η is approximately the spectral radius of \mathcal{D} , while $\frac{\beta}{\eta}$ is approximately the middle eigenvalue λ_2 of \mathcal{D} .

Proposition 3.4.6 (Properties of η and β).

$$(i) \quad \eta = \lambda_i^2 + \lambda_i \lambda_j + \lambda_j^2 \text{ for } i \neq j,$$

$$(ii) \quad \eta \leq \rho^2 \leq \frac{4}{3}\eta,$$

$$(iii) \quad \beta = -\det(\mathcal{D}) = -\lambda_1 \lambda_2 \lambda_3,$$

$$(iv) \quad 0 \leq \beta^2 \leq \frac{4}{27}\eta^3,$$

$$(v) \quad \frac{2}{3} \leq \frac{\beta}{\lambda_2 \eta} \leq 1.$$

Proof. For (i), we use $\sum_{i=1}^3 \lambda_i = 0$ and the definition of η to compute

$$\eta = \frac{1}{2} \left(\lambda_i^2 + \lambda_j^2 + (\lambda_i + \lambda_j)^2 \right) = \lambda_i^2 + \lambda_i \lambda_j + \lambda_j^2. \quad (3.129)$$

In particular, we have

$$\eta = \rho^2 - \rho\rho_- + \rho_-^2. \quad (3.130)$$

Holding ρ fixed, this expression is maximized when $\rho_- = \rho$ (i.e., $\lambda_2 = 0$) and minimized when $\rho_- = \frac{1}{2}\rho$ (i.e., $|\lambda_2| = \rho_-$). Evaluating at these extreme cases gives (ii).

For (iii), we compute

$$-3\beta = \lambda_1^3 + \lambda_2^3 + \lambda_3^3 \quad (3.131)$$

$$= \lambda_1^2(-\lambda_2 - \lambda_3) + \lambda_2^2(-\lambda_1 - \lambda_3) + \lambda_3(\lambda_1 + \lambda_2)^2 \quad (3.132)$$

$$= \lambda_1\lambda_2(-\lambda_1 - \lambda_2) + 2\lambda_1\lambda_2\lambda_3 \quad (3.133)$$

$$= 3\lambda_1\lambda_2\lambda_3. \quad (3.134)$$

Using this, we find that

$$\beta^2 = \lambda_1^2\lambda_2^2\lambda_3^2 = \rho^2\rho_-^2(\rho - \rho_-)^2 \quad (3.135)$$

is maximized for $\rho_- = \frac{1}{2}\rho$. In combination with (ii), we find

$$\beta^2 \leq \frac{1}{16}\rho^6 \leq \frac{4}{27}\eta^3, \quad (3.136)$$

as desired. (v) is similarly obtained by observing that

$$\frac{\beta}{\lambda_2\eta} = \frac{\rho\rho_-}{\rho^2 - \rho\rho_- + \rho_-^2} \quad (3.137)$$

is maximized when $\rho_- = \rho$ and minimized when $\rho_- = \frac{1}{2}\rho$ for fixed ρ and subject to the constraint $\rho_- \in [\frac{1}{2}\rho, \rho]$. ▮

Remark 3.4.7. Recall that there is nothing specifically fluid-dynamic about \mathcal{D} here. Proposition 3.4.6 is valid for any 3×3 traceless real symmetric matrix \mathcal{D} . The same

remark applies to all of this section: Ω likewise stands in for any real skew-symmetric matrix.

Remark 3.4.8. All the inequalities are sharp, as they are attained in the extreme cases $\lambda_2 = 0$ or $\lambda_2 = \pm\frac{1}{2}\rho$. Furthermore, if $|\lambda_2|$ can be bounded away from 0 or $\frac{1}{2}\rho$, then there is room for improvement in the inequalities. This is perhaps most easily seen when writing η as

$$\eta = \rho^2 \left(1 + \frac{\lambda_2}{\rho} + \left(\frac{\lambda_2}{\rho} \right)^2 \right). \quad (3.138)$$

Proposition 3.4.9 (Properties of μ and φ).

$$(i) \quad \frac{\varphi}{\mu} = \sum_{i=1}^3 \lambda_i \xi_i^2,$$

$$(ii) \quad 0 \leq \varphi^2 \leq \rho^2 \mu^2 \leq \frac{4}{3} \eta \mu^2.$$

Proof. We compute in a basis where \mathcal{D} is diagonal, i.e., $\mathcal{D} = \text{diag}(\lambda_1, \lambda_2, \lambda_3)$. By direct computation, we have

$$\Omega^2 = \mu(\xi \otimes \xi - \mathbb{I}). \quad (3.139)$$

Recalling that $\sum_{i=1}^3 \lambda_i = 0$, this gives

$$\frac{\varphi}{\mu} = \frac{\text{Tr}(\mathcal{D}\Omega^2)}{\mu} = \sum_{i=1}^3 \lambda_i \xi_i^2. \quad (3.140)$$

Using $\lambda_i^2 \leq \rho^2 \leq \frac{4}{3}\eta$ (see the previous Proposition), (ii) follows immediately from (i). \blacksquare

Proposition 3.4.10 (Determinant of $N = \mathcal{D} + \Omega$). *We have*

$$\det N = \varphi - \beta. \quad (3.141)$$

Proof. Since N is a 3×3 traceless matrix, we have (see the proof of Corollary 3.1.7)

$$\det N = \frac{1}{3} \operatorname{Tr} N^3 = \frac{1}{3} \operatorname{Tr}(\mathcal{D}^3 + \mathcal{D}\Omega^2 + \Omega\mathcal{D}\Omega + \Omega^2\mathcal{D}) \quad (3.142)$$

$$= \frac{1}{3} \operatorname{Tr} \mathcal{D}^3 + \operatorname{Tr} \mathcal{D}\Omega^2 = -\beta + \varphi. \quad (3.143)$$

Here we used that

$$\operatorname{Tr}(\Omega^3 + \Omega\mathcal{D}^2 + \mathcal{D}\Omega\mathcal{D} + \mathcal{D}^2\Omega) = \operatorname{Tr} \Omega^3 + 3 \operatorname{Tr} \mathcal{D}^2\Omega = 0 \quad (3.144)$$

by symmetry considerations (see Corollary 3.1.4). ▮

Proposition 3.4.11 (Properties of ψ and ζ).

$$(i) \quad \frac{\zeta}{\mu} = \sum_{i=1}^3 \lambda_i^2 \xi_i^2 = |\mathcal{D}\xi|^2,$$

$$(ii) \quad \zeta + 2\psi = 2\eta\mu,$$

$$(iii) \quad \lambda_2^2 \mu \leq \zeta \leq \rho^2 \mu \text{ (hence } 0 \leq \zeta \leq \frac{4}{3}\eta\mu),$$

$$(iv) \quad (\eta - \frac{1}{2}\rho^2)\mu \leq \psi \leq (\eta - \frac{1}{2}\lambda_2^2)\mu \text{ (hence } \frac{1}{3}\eta\mu \leq \psi \leq \eta\mu).$$

Proof. (i) is immediate from the definition of ζ upon recalling $4\mu = |\omega|^2$, and (iii) follows immediately from (i). For (ii), we compute in a basis where \mathcal{D} is diagonal. Then using $\mathcal{D}^2 = \operatorname{diag}(\lambda_1^2, \lambda_2^2, \lambda_3^2)$ and (3.139), we may compute

$$-2\psi = \operatorname{Tr}(\mathcal{D}^2\Omega^2) = \mu \sum_{i=1}^3 \lambda_i^2 \xi_i^2 - \mu \sum_{i=1}^3 \lambda_i^2 = \zeta - 2\eta\mu. \quad (3.145)$$

(iv) now follows from combining (ii) and (iii). For the ‘‘hence’’ statements, recall that $\rho^2 \leq \frac{4}{3}\eta$. ▮

Proposition 3.4.12. *We have*

$$\varphi^2 \leq \mu\zeta. \quad (3.146)$$

Proof. Since $\sum_{i=1}^3 \xi_i^2 = 1$, Jensen's inequality gives

$$\left(\frac{\varphi}{\mu}\right)^2 = \left(\sum_{i=1}^3 \lambda_i \xi_i^2\right)^2 \leq \sum_{i=1}^3 \lambda_i^2 \xi_i^2 = \frac{\zeta}{\mu}. \quad (3.147)$$

Alternatively, this follows immediately from the geometric equation (3.128):

$$\frac{\varphi^2}{\mu\zeta} = \cos^2 \theta. \quad (3.148)$$

■

3.4.4 Spatial integrals of some of the invariants

Proposition 3.4.13. *For sufficiently smooth and decaying (or periodic) solutions of the 3d incompressible Euler equations, we have*

$$(i) \int (\eta - \mu) dx = 0,$$

$$(ii) \int \pi_1 dx = 0,$$

$$(iii) \int (\beta - \varphi) dx = 0,$$

$$(iv) \int (\pi_2 - \pi_3) dx = -\frac{2}{3} \int (\eta - \mu)^2 dx,$$

$$(v) \int \eta dx = \int \mu dx = \frac{1}{4} \|\omega\|_{L_x^2}^2 = \frac{1}{4} \|\nabla_x u\|_{L_x^2}^2.$$

Proof. (i) is immediate from $-\Delta_x p = \text{Tr}(N^2) = 2(\eta - \mu)$. Next, since $\text{Tr } N = 0$ by $\text{div } u = 0$, and $\text{Tr } \Omega Q = 0$ by symmetry considerations, we have

$$\pi_1 = \text{Tr } \mathcal{D}Q = \text{Tr } NQ = \text{Tr } NP, \quad (3.149)$$

and hence

$$\int \pi_1 dx = \int \nabla_x \nabla_x p : \nabla_x u dx = - \int \nabla_x p \cdot \nabla_x (\text{div}_x u) dx = 0. \quad (3.150)$$

(iii) follows from (i) and (ii) by integrating

$$D_t(\eta - \mu) = 3(\beta - \varphi) - \pi_1, \quad (3.151)$$

and (iv) in turn follows from (iii) by integrating

$$D_t(\beta - \varphi) = \frac{2}{3}(\eta - \mu)^2 + (\pi_2 - \pi_3). \quad (3.152)$$

Since $\mu = \frac{1}{4}|\omega|^2$, (v) follows from (i) and the calculation

$$\begin{aligned} \int |\nabla_x u|^2 dx &= \int u \cdot (-\Delta_x u) dx = \int u \cdot \operatorname{curl}_x \operatorname{curl}_x u dx \\ &= \int \operatorname{curl}_x u \cdot \operatorname{curl}_x u dx = \int |\omega|^2 dx, \end{aligned} \quad (3.153)$$

which is valid for any divergence-free u , thanks to the differential identity

$$-\Delta v = \operatorname{curl} \operatorname{curl} v - \nabla \operatorname{div} v. \quad (3.154)$$

■

Corollary 3.4.14. *We have*

$$\frac{d}{dt} \|\omega\|_{L^2}^2 = 8 \int \varphi dx = 8 \int \beta dx. \quad (3.155)$$

Proof. This follows from the previous proposition by integrating $D_t \mu = 2\varphi$. ■

Remark 3.4.15. In terms of the (non-isotropic) pressure Hessian P , the integrals (ii) and (iv) in Proposition 3.4.13 take the form

$$\int \operatorname{Tr} NP dx = 0, \quad (3.156)$$

$$\int \operatorname{Tr} N^2 P dx = -2 \int (\eta - \mu)^2 dx. \quad (3.157)$$

Another interesting integral is

$$\int \operatorname{Tr}(NN^\top P) \, dx = \int u_{x_i}^j u_{x_k}^j p_{x_i x_k} \, dx = \int u^j u_{x_k}^j (-\Delta_x p)_{x_k} \, dx \quad (3.158)$$

$$= \int \nabla_x \frac{1}{2} |u|^2 \cdot \nabla_x (\operatorname{Tr} N^2) \, dx = \int (-\Delta_x |u|^2) (\eta - \mu) \, dx. \quad (3.159)$$

Remark 3.4.16. In different notation, some of these integrals occur already in various places in the literature (e.g., Chae [17]), however on a somewhat ad hoc basis. We hope the reader appreciates our more systematic approach.

3.4.5 Controlling the enstrophy by the second eigenvalue of the deformation tensor

As an application of the invariants framework, we give an easy proof of the following estimate.

Theorem 3.4.17 (Chae (2006) [17]). *Sufficiently smooth and decaying (or periodic) solutions of the incompressible 3d Euler equations satisfy*

$$\sup_{0 < t < T} \|\omega\|_{L_x^2} \leq \exp\left(\int_0^T \|\lambda_2^+\|_{L_x^\infty} \, dt\right) \|\omega_0\|_{L_x^2}. \quad (3.160)$$

Proof. From Corollary 3.4.14, we have

$$\frac{d}{dt} \|\omega\|_{L_x^2}^2 = 8 \int \beta \, dx = 8 \int \left(\frac{\beta}{\eta}\right) \eta \, dx \leq 8 \left\| \left(\frac{\beta}{\eta}\right)^+ \right\|_{L_x^\infty} \int \eta \, dx. \quad (3.161)$$

From Proposition 3.4.13, we have

$$\int \eta \, dx = \frac{1}{4} \|\omega\|_{L_x^2}^2, \quad (3.162)$$

and from Proposition 3.4.6, we have $\frac{\beta}{\eta} \leq \lambda_2$. Putting this all together, we get

$$\frac{d}{dt} \|\omega\|_{L_x^2}^2 \leq 2 \|\lambda_2^+\|_{L^\infty} \|\omega\|_{L_x^2}^2, \quad (3.163)$$

or in slightly simpler form,

$$\frac{d}{dt} \|\omega\|_{L_x^2} \leq \|\lambda_2^+\|_{L^\infty} \|\omega\|_{L_x^2}. \quad (3.164)$$

The theorem now follows from Gronwall's inequality. ■

Remark 3.4.18. Finiteness of $\|\omega\|_{L_x^2}$ for all time is sufficient to guarantee a global smooth solution in the case of the Navier-Stokes equations, but it is not enough for the Euler equations.

3.4.6 On a model of Vieillefosse

In 1982, Vieillefosse proposed to study a purely local model of the incompressible Euler equations obtained by simply neglecting the anisotropic part of the pressure Hessian [113]. (In our notation, this means setting $Q = 0$. In particular, all the π_i invariants vanish then.) Vieillefosse showed that in this model there is generic blowup with $\lambda_2 \rightarrow +\infty$, and the vorticity ω aligning asymptotically with the eigenvector of \mathcal{D} corresponding to λ_2 . (See also Vieillefosse [114] and Cantwell [15].)

The model received some interest, since such vorticity alignment with the second eigenvector of \mathcal{D} was observed numerically in Navier-Stokes turbulence simulations by Ashurst et al. [4] and confirmed by many others later on. (For numerical evidence on the alignment of various vectors in the Euler rather than Navier-Stokes equations, we refer to Ohkitani and Kishiba [86].)

However, the nature of the blowup it predicts as well as its explanation for the observed alignment are highly questionable. A more convincing heuristic argument

for the vorticity alignment was provided by Jiménez [70]: Starting from the empirical observation that thin vortex tubes (where vorticity is roughly parallel) tend to form in turbulence, the vorticity alignment with the second eigenvector of \mathcal{D} is a consequence of incompressibility and the Biot-Savart law. This gives a kinematic and nonlocal explanation for the vorticity alignment, in stark contrast to the dynamic and local explanation offered by the Vieillefosse model.

Given these critiques, the Vieillefosse model now probably resides more in the category of historical curiosities. The purpose of this section is not to revive interest in the model, but primarily to illustrate the usefulness of the invariants approach to *local* systems of PDE. If in the future a sufficiently simple¹ random model for the π_i invariants becomes available (instead of just setting them to zero), we hope this method of analysis could be helpful.

To study Vieillefosse's model in our framework, let us first set² $a = \eta - \mu$ and $b = \beta - \varphi$, and $\pi_i = 0$ for all i . Then Proposition 3.4.2 yields

$$\left\{ \begin{array}{l} D_t a = 3b, \\ D_t b = \frac{2}{3}a^2, \\ D_t \mu = 2\varphi, \\ D_t \varphi = \frac{2}{3}\mu a + \zeta, \\ D_t \zeta = \frac{4}{3}a\varphi. \end{array} \right. \quad (3.165)$$

¹Some more sophisticated pressure Hessian closures than Vieillefosse's are discussed in Chevillard et al. [20].

²In the literature, Q and R (or q and r) are occasionally used instead of a and b , and signs may differ.

Conserved quantities

Two conserved quantities along particle trajectories may now easily be identified:

$$D_t(4a^3 - 27b^2) = 0, \quad (3.166)$$

$$D_t(\mu\zeta - \varphi^2) = 0. \quad (3.167)$$

Solutions to the a - b -couplet

The evolutions for a and b may be combined to form

$$D_t D_t a = 2a^2. \quad (3.168)$$

This equation possesses solutions of the form

$$a(t) = 3^{1/3} \wp \left(\frac{T-t}{3^{1/3}}; 0, C \right), \quad (3.169)$$

where C, T are constants depending on the initial data, and $\wp(z; g_2, g_3)$ denotes a Weierstrass elliptic function. (For other solutions, see Cantwell [15].) We found these solutions with the help of Mathematica, but they can be easily verified using the differential equation satisfied by \wp ,

$$\wp''(z) = 6\wp(z)^2 - \frac{1}{2}g_2. \quad (3.170)$$

In the special case $C = 0$, the solution is exactly

$$a(t) = \frac{3}{(T-t)^2}, \quad (3.171)$$

and for general C , the same form holds asymptotically:

$$a(t) = \frac{3}{(T-t)^2} + O((T-t)^4). \quad (3.172)$$

So there are many solutions where $\sqrt{a(t)}$ blows up to $+\infty$ like $O(T-t)^{-1}$.

For the above facts and much more on the Weierstrass elliptic functions, see Reinhardt and Walker [95] or Southard [106].

Blowup rate for vorticity

From here on out, we will just give an informal asymptotic discussion. For exact calculations, we refer to Cantwell [15]. Neglecting the $O(T-t)^4$ term in (3.172), which should not matter asymptotically, we have $a(t) \sim \frac{3}{(T-t)^2}$. But then

$$D_t D_t \sqrt{\mu} = \frac{2}{3} a \sqrt{\mu} + \frac{\mu \zeta - \varphi^2}{\mu^{3/2}} \sim \frac{2}{(T-t)^2} \sqrt{\mu} + \frac{C_0}{\mu^{3/2}}, \quad (3.173)$$

where we used that $\mu \zeta - \varphi^2 = C_0$ is conserved along particle trajectories. Neglecting the term $C_0/\mu^{3/2}$, which we expect to be small along a trajectory where μ blows up, we conclude that, generically,

$$\sqrt{\mu}(X(a, t), t) \approx C_1(T-t)^2 + \frac{C_2}{T-t} \sim \frac{C_2}{T-t}, \quad (3.174)$$

with $C_2 > 0$. Thus, we expect a blowup rate for $|\omega| = 2\sqrt{\mu}$ of $O(T-t)^{-1}$.

Blowup of $\lambda_2 \rightarrow +\infty$

Since μ blows up to $+\infty$, so does $\varphi = \frac{1}{2} D_t \mu$. In particular, φ is asymptotically positive.

Using

$$D_t \eta = D_t(a + \mu) = 3\beta - \varphi \quad (3.175)$$

and Proposition 3.4.6, we thus have

$$\lambda_2 \geq \frac{\beta}{\eta} \geq \frac{\beta - \frac{1}{3}\varphi}{\eta} = \frac{1}{3} \frac{D_t \eta}{\eta} = \frac{1}{3} D_t \log \eta \xrightarrow{t \rightarrow T} +\infty. \quad (3.176)$$

Vorticity alignment with the second eigenvector of \mathcal{D}

Recall that θ denotes the angle between ω and $\mathcal{D}\omega$. According to (3.128), we have

$$\sin^2 \theta = \frac{\mu\zeta - \varphi^2}{\mu\zeta} = \frac{C_0}{\mu\zeta} \leq \frac{C_0}{\lambda_2^2 \mu^2} \xrightarrow{t \rightarrow T} 0, \quad (3.177)$$

where we used the bound $\zeta \geq \lambda_2^2 \mu$ from Proposition 3.4.11, and $\lambda_2, \mu \rightarrow +\infty$. This implies that asymptotically ω becomes parallel to $\mathcal{D}\omega$ (i.e., becomes aligned with an eigenvector of \mathcal{D}).

The harder part is showing which of the eigenvectors ω becomes aligned with. Using $\frac{\varphi}{\mu} = \sum_i \lambda_i \xi_i^2$ (see Proposition 3.4.9) and (3.177), we have $\frac{\varphi}{\mu} \sim \lambda_i$, where λ_i is the eigenvalue corresponding to the eigenvector that ω asymptotically aligns with. Since φ is positive, so must be λ_i . Thus $i = 1$ or $i = 2$. Assume towards contradiction that $i = 1$. Then using $\varphi = \frac{1}{2} D_t \mu$ and $\mu = O(T - t)^{-2}$, we find

$$\lambda_1 \sim \frac{\varphi}{\mu} = \frac{1}{2} D_t \log \mu \sim \frac{1}{T - t}. \quad (3.178)$$

But then, using Proposition 3.4.6,

$$a = \eta - \mu = \lambda_1^2 + \lambda_1 \lambda_2 + \lambda_2^2 - \mu \leq 3\lambda_1^2 - \mu \sim \frac{3 - C_2^2}{(T - t)^2}. \quad (3.179)$$

This contradicts $a(t) \sim \frac{3}{(T-t)^2}$ (see (3.172)) and leaves only the possibility $i = 2$.

3.5 Rotating the reference frame along a particle trajectory

The reader may wonder:

1. Why bother with the invariants η and β when we could just use any two of the eigenvalues of \mathcal{D} to capture these degrees of freedom instead?³
2. On a similar note, instead of indirectly measuring vorticity magnitude and alignment with eigenvectors of \mathcal{D} through the invariants μ , φ and ζ , why not directly work with the three components of the vorticity ω with respect to the eigenvector basis of \mathcal{D} ?

We explore these two ideas in §3.5.1 and §3.5.2, respectively. The key idea is to introduce an orthogonal matrix $\mathcal{O}(X(a, t), t)$ along a particle trajectory such that $\overline{\mathcal{D}} = \mathcal{O}\mathcal{D}\mathcal{O}^\top$ is diagonal. In §§3.5.3–3.5.5, we show some other interesting choices for \mathcal{O} . Finally, we make some remarks on the advantages and disadvantages of this approach in §3.5.6.

3.5.1 Evolution equations for the eigenvalues of \mathcal{D}

Let us fix a particle label a . Since $\mathcal{D}(X(a, t), t)$ is real-symmetric, it can be diagonalized by an orthogonal matrix. That is, we can find a matrix $\mathcal{O}(X(a, t), t)$ such that

$$\text{diag}(\lambda_1, \lambda_2, \lambda_3) = \mathcal{O}\mathcal{D}\mathcal{O}^\top. \quad (3.180)$$

If we fix some choice of \mathcal{O} that diagonalizes \mathcal{D} at time $t = 0$ and require \mathcal{O} to vary continuously in time, then $\mathcal{O}(X(a, t), t)$ is unique—provided all the eigenvalues are distinct. To simplify exposition, we will implicitly assume that throughout this section.

³There are only two degrees of freedom since we have $\lambda_1 + \lambda_2 + \lambda_3 = 0$ by incompressibility.

Remark 3.5.1. Unfortunately, needing to take special care of situations where the eigenvalues may not be distinct is a fundamental technical downside to the eigenvalue approach, and is an argument in favor of using the scalar polynomial orthogonal invariants η and β .

Using such a diagonalization, we can derive the evolution equations for the eigenvalues of \mathcal{D} . But first we need a lemma about interchanging orthogonal conjugation and differentiation. For this, it will be convenient to introduce the notation

$$\bar{A} := \mathcal{O}A\mathcal{O}^\top. \quad (3.181)$$

Lemma 3.5.2. *If \mathcal{O} is orthogonal, then*

$$D_t\bar{A} = \overline{D_tA} + [(D_t\mathcal{O})\mathcal{O}^\top, \bar{A}], \quad (3.182)$$

where $[A, B] := AB - BA$.

Proof. By the Leibniz rule,

$$\begin{aligned} D_t\bar{A} &= \overline{D_tA} + (D_t\mathcal{O})A\mathcal{O}^\top + \mathcal{O}A(D_t\mathcal{O})^\top \\ &= \overline{D_tA} + \left((D_t\mathcal{O})\mathcal{O}^\top\right)\bar{A} + \bar{A}\left((D_t\mathcal{O})\mathcal{O}^\top\right)^\top. \end{aligned} \quad (3.183)$$

(3.183) is equivalent to (3.182) because $(D_t\mathcal{O})\mathcal{O}^\top$ is skew-symmetric:

$$0 = D_tI = D_t(\mathcal{O}\mathcal{O}^\top) = (D_t\mathcal{O})\mathcal{O}^\top + \mathcal{O}(D_t\mathcal{O}^\top) = (D_t\mathcal{O})\mathcal{O}^\top + \left((D_t\mathcal{O})\mathcal{O}^\top\right)^\top. \quad (3.184)$$

(This is related to the fact that the skew-symmetric matrices make up the Lie algebra of the orthogonal group.) █

Proposition 3.5.3. *The eigenvalues of \mathcal{D} evolve according to*

$$D_t \lambda_i = -\lambda_i^2 + \mu(1 - \xi_i^2) - \bar{P}_{ii}. \quad (3.185)$$

Proof. Take $A = \mathcal{D}$ and \mathcal{O} as in (3.180). Then by Lemma 3.5.2,

$$D_t \bar{\mathcal{D}} = -\bar{\mathcal{D}}^2 - \bar{\Omega}^2 - \bar{P} + [\bar{\mathcal{D}}, (D_t \mathcal{O}) \mathcal{O}^\top]. \quad (3.186)$$

But the commutator has zeroes on the diagonal since $\bar{\mathcal{D}}$ is diagonal and $(D_t \mathcal{O}) \mathcal{O}^\top$ is skew-symmetric (and hence has zeroes on its diagonal). Recalling the formula (3.139) for Ω^2 , we obtain (3.185) by looking at the diagonal components of the evolution. \blacksquare

Remark 3.5.4. We can find a similar result for the Navier-Stokes equations, provided a diagonalizing orthogonal matrix field $\mathcal{O}(x, t)$ is defined and differentiable for x in a neighborhood of $X(a, t)$. We must check that the diagonalization commutes with the Laplacian on the diagonal. Letting ∂_x denote one of the partial derivatives $\frac{\partial}{\partial x_i}$ for $i = 1, 2, 3$, and writing $R = (\partial_x \mathcal{O}) \mathcal{O}^\top$, we find

$$\partial_x \bar{A} = \overline{\partial_x A} + [R, A], \quad (3.187)$$

just as in Lemma 3.5.2. Applying this three times, we have

$$\partial_x \partial_x \bar{\mathcal{D}} = \partial_x \overline{\partial_x \mathcal{D}} + \partial_x [R, \bar{\mathcal{D}}] \quad (3.188)$$

$$= \overline{\partial_x \partial_x \mathcal{D}} + [R, \overline{\partial_x \mathcal{D}}] + \partial_x [R, \bar{\mathcal{D}}] \quad (3.189)$$

$$= \overline{\partial_x \partial_x \mathcal{D}} + [R, \partial_x \bar{\mathcal{D}}] - [R, [R, \bar{\mathcal{D}}]] + \partial_x [R, \bar{\mathcal{D}}]. \quad (3.190)$$

The claim now is that all the commutators vanish on the diagonal. We compute:

$$[R, \bar{\mathcal{D}}]_{ij} = R_{ik} (\lambda_k \delta_{kj}) - (\lambda_i \delta_{ik}) R_{kj} = (\lambda_j - \lambda_i) R_{ij}, \quad (3.191)$$

and similarly for $[R, \partial_x \bar{\mathcal{D}}]$ —just replace λ_k by $\partial_x \lambda_k$. Furthermore,

$$[R, [R, \bar{\mathcal{D}}]]_{ij} = R_{ik}(\lambda_j - \lambda_k)R_{kj} - (\lambda_k - \lambda_i)R_{ik}R_{kj} = (\lambda_j - \lambda_i)R_{ik}R_{kj}. \quad (3.192)$$

Clearly, these expressions all vanish for $i = j$. Thus, for the Navier-Stokes equations, the eigenvalue evolution (3.185) becomes simply

$$(D_t - \nu \Delta)\lambda_i = -\lambda_i^2 + \mu(1 - \xi_i^2) - \bar{P}_{ii}. \quad (3.193)$$

3.5.2 Evolution of the vorticity in the eigenvector basis of \mathcal{D}

Let us write $R = (D_t \mathcal{O})\mathcal{O}^\top$ where $\mathcal{O}(X(a, t), t)$ is an orthogonal matrix diagonalizing \mathcal{D} as in the previous section. It is convenient to further introduce the notation

$$\bar{\Omega}_{ij} = \frac{1}{2}\epsilon_{ijk}\bar{\omega}_k, \quad (3.194)$$

$$R_{ij} = \frac{1}{2}\epsilon_{ijk}r_k, \quad (3.195)$$

$$\bar{P}_{ij} = \delta_{ij}p_i + |\epsilon_{ijk}q_k|. \quad (3.196)$$

As we have seen, R is skew-symmetric and satisfies

$$D_t \bar{\mathcal{D}} = -\bar{\mathcal{D}}^2 - \bar{\Omega}^2 - \bar{P} + [\bar{\mathcal{D}}, R]. \quad (3.197)$$

The diagonal part of this equation gives the eigenvalue evolutions, as seen above. For the off-diagonal part, the left-hand side vanishes. This allows us to solve explicitly for R . The result is

$$r_i = \epsilon_{ijk} \frac{q_i + \frac{1}{4}\bar{\omega}_j\bar{\omega}_k}{\lambda_k - \lambda_j}. \quad (3.198)$$

Observe, once again, the breakdown of this approach when the eigenvalues are not distinct. Using (3.198), we can go further and compute the evolution of $\bar{\omega} = \mathcal{O}\omega$:

$$D_t \bar{\omega} = (\bar{\mathcal{D}} + R)\bar{\omega} = \text{diag}(\lambda_1, \lambda_2, \lambda_3)\bar{\omega} + \frac{1}{2}\bar{\omega} \times r. \quad (3.199)$$

The components of this equation are the desired evolution equations for the components of ω with respect to the eigenvector basis of \mathcal{D} .

Remark 3.5.5. Using $\tilde{P} = P - NN^\top$ (see Remark 2.1.13), we have

$$D_t \bar{\mathcal{D}} = -2\bar{\mathcal{D}}^2 - \bar{\tilde{P}} + [R - \bar{\Omega}, \bar{\mathcal{D}}]. \quad (3.200)$$

This leads to the nicer equations

$$D_t \lambda_i = -2\lambda_i^2 + \tilde{p}_i, \quad (3.201)$$

and

$$D_t \bar{\omega}_i = \lambda_i \bar{\omega}_i + |\epsilon_{ijk}| \frac{\bar{\omega}_j \tilde{q}_k}{\lambda_j - \lambda_i}. \quad (3.202)$$

3.5.3 Choosing $R = \bar{\Omega}$

Instead of diagonalizing \mathcal{D} , equation (3.200) suggests that along with using $\tilde{P} = P - NN^\top$ instead of P , it could be interesting to simply take $R = \bar{\Omega}$, with $\mathcal{O} = \mathbb{I}$ at time 0, say. In terms of \mathcal{O} , this means $(D_t \mathcal{O})\mathcal{O}^\top = \mathcal{O}\Omega\mathcal{O}^\top$, i.e., $D_t \mathcal{O} = \mathcal{O}\Omega$. We have

$$D_t(\mathcal{O}\mathcal{O}^\top) = (\mathcal{O}\Omega)\mathcal{O}^\top + \mathcal{O}(-\Omega\mathcal{O}^\top) = 0, \quad (3.203)$$

so this evolution indeed preserves orthogonality of the matrix \mathcal{O} . We find

$$D_t \bar{D} = -2\bar{D}^2 - \bar{P}, \quad (3.204)$$

$$D_t \bar{\omega} = (\bar{D} + R)\bar{\omega} = \bar{D}\bar{\omega}, \quad (3.205)$$

$$D_t \bar{v}_- = (R - \bar{D} - \bar{\Omega})\bar{v}_- = -\bar{D}\bar{v}_-, \quad (3.206)$$

where for the $\bar{\omega}$ evolution we used

$$R\bar{\omega} = \bar{\Omega}\bar{\omega} = -\frac{1}{2}\bar{\omega} \times \bar{\omega} = 0. \quad (3.207)$$

For the definition of $v_- = u + \nabla_x q_-$, see §2.3.2.

3.5.4 Fixing the direction of $\bar{\omega}$

If the vorticity is nonzero for some particle label a at time 0, then it is nonzero for all time (at least as long as the solution is regular). For such a particle label a , it is thus possible to find an orthogonal matrix $\mathcal{O}(X(a, t), t)$ that keeps the direction of the vorticity $\bar{\omega}$ fixed along the particle trajectory (in the $+e_3$ direction, say). Let us write, in this basis,

$$\bar{\omega} = \begin{pmatrix} 0 \\ 0 \\ \bar{\omega}_3 \end{pmatrix}, \quad (3.208)$$

$$R_{ij} = \frac{1}{2}\epsilon_{ijk}r_k, \quad (3.209)$$

$$\bar{D}_{ij} = \begin{pmatrix} a_1 & b_3 & -b_2 \\ b_3 & a_2 & b_1 \\ -b_2 & b_3 & a_3 \end{pmatrix}. \quad (3.210)$$

The initial data $\mathcal{O}(a, 0)$ must obviously be chosen so as to make $\bar{\omega}$ point in the $+e_3$ direction. From the equation $D_t\bar{\omega} = (\bar{\mathcal{D}} + R)\bar{\omega}$, i.e.,

$$\begin{pmatrix} 0 \\ 0 \\ D_t\bar{\omega}_3 \end{pmatrix} = \begin{pmatrix} -(b_2 + \frac{1}{2}r_2) \\ b_1 + \frac{1}{2}r_1 \\ a_3 \end{pmatrix} \bar{\omega}_3, \quad (3.211)$$

it then follows that we must take $r_1 = -2b_1, r_2 = -2b_2$. Note that we may freely choose r_3 . This is because rotating in the plane perpendicular to the vorticity leaves the vorticity unchanged. (This extra degree of freedom also applies to our choice of initial data $\mathcal{O}(a, 0)$, of course.) For the special choice of $r_3 = -2b_3 + \omega$, the evolution of \bar{v}_- involves an upper-triangular matrix:

$$D_t\bar{\omega}_3 = a_3\bar{\omega}_3, \quad (3.212)$$

$$D_t\bar{v}_- = - \begin{pmatrix} a_1 & 2b_3 & -2b_2 \\ 0 & a_2 & 2b_1 \\ 0 & 0 & a_3 \end{pmatrix} \bar{v}_-. \quad (3.213)$$

3.5.5 Diagonalizing the left Cauchy-Green tensor

The tensor $\mathcal{C} = J^\top J$ is another symmetric tensor of interest. In the continuum mechanics literature, it is referred to as the *left Cauchy-Green deformation tensor*.⁴

With the help of Lemma 2.1.4, we find

$$D_t\mathcal{C} = \mathcal{D}\mathcal{C} + \mathcal{C}\mathcal{D} - [\Omega, \mathcal{C}]. \quad (3.214)$$

Since \mathcal{C} is symmetric, we may orthogonally diagonalize it, just as we did with \mathcal{D} in §3.5.1. Since \mathcal{C} is positive-definite ($x \cdot J^\top J \cdot x = |Jx|^2 \geq 0$ for arbitrary x), its

⁴Recall our unusual index ordering $J_{ij} = x_{a_i}^j$. In the literature, the left Cauchy-Green tensor is usually written as JJ^\top , and $J^\top J$ usually denotes the *right* Cauchy-Green tensor.

eigenvalues are nonnegative, and since $\det J^\top J = 1$, they must in fact all be positive. So let us denote its eigenvalues by μ_i^2 and write

$$\bar{\mathcal{C}}_{ij} = \mu_i^2 \delta_{ij}, \quad (3.215)$$

$$R_{ij} = \frac{1}{2} \epsilon_{ijk} r^k, \quad (3.216)$$

$$\bar{\mathcal{D}}_{ij} = a_i \delta_{ij} + |\epsilon_{ijk} b_k|. \quad (3.217)$$

From the diagonal and off-diagonal parts of

$$D_t \bar{\mathcal{C}} = \bar{\mathcal{D}} \bar{\mathcal{C}} + \bar{\mathcal{C}} \bar{\mathcal{D}} + [R - \bar{\Omega}, \bar{\mathcal{C}}], \quad (3.218)$$

we then find

$$D_t \mu_i = a_i \mu_i, \quad (3.219)$$

and

$$r_i = \omega_i + \epsilon_{ijk} b_i \frac{\mu_j^2 + \mu_k^2}{\mu_j^2 - \mu_k^2}. \quad (3.220)$$

As with \mathcal{D} , trouble arises when the eigenvalues are not distinct.

Remark 3.5.6. The relationship between the eigenvalues of the *right* Cauchy-Green tensor JJ^\top and the eigenvalues of \mathcal{D} is studied in Chae, Constantin, and Wu [19].

3.5.6 Discussion

As we have seen, the evolution equations (3.185) (and especially (3.201)) for the eigenvalues of \mathcal{D} are simpler than the corresponding equations for η and β . However, this approach suffers from technical hurdles when the eigenvalues of \mathcal{D} are not distinct. So in general we think working with η and β is more advantageous. Recall also from

Proposition 3.4.6 that

$$\sqrt{\eta} \leq \rho \leq \sqrt{\frac{4}{3}\eta}, \quad \frac{|\beta|}{\eta} \leq |\lambda_2| \leq \frac{3|\beta|}{2\eta}, \quad \text{sgn } \lambda_2 = \text{sgn } \beta, \quad (3.221)$$

so the eigenvalues may be easily approximated using η and β .

There are, however, some situations where it is advantageous to work directly with the eigenvalues: In symmetric scenarios, such as on the axis of symmetry of an axisymmetric flow, at least some of the directions of the eigenvectors of \mathcal{D} are usually fixed by the symmetry, and then no issues with distinctness of eigenvalues arise. For some examples of such scenarios, we refer to §4 of Chae, Constantin, and Wu [19] and Chae [18].

Chapter 4

An Idealized Inviscid Model for Liquid-Vapor-Solid Systems

4.1 Introduction

We consider systems with two immiscible fluids in contact with a nondeformable solid. Typical examples, cross-sections of which are shown in Figure 4.1, are a glass of water, a droplet spreading on a horizontal solid surface, or a solid object floating on water. With these examples in mind, we will call one of the fluid phases *liquid* and the other

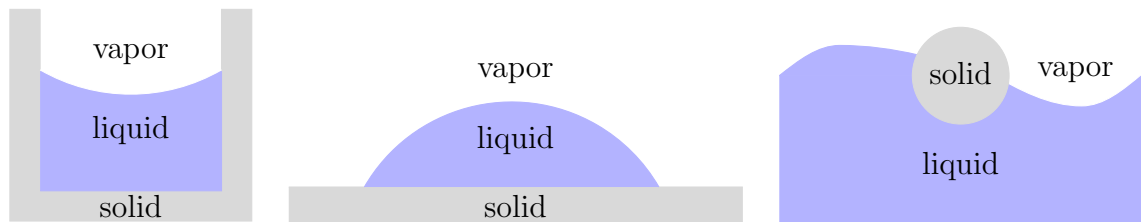


Figure 4.1: Two-dimensional cross-sections of examples of the types of systems under consideration.

vapor, but really either could be any fluid well-modeled by the incompressible Euler equations. Some of the discussion will allow for viscosity, but the main point of this chapter is to “derive” an idealized augmented Young-Laplace law (4.62) for modeling

dynamic inviscid liquid-vapor-solid systems. Ultimately, we propose to study the system (4.63) for a fixed and non-rotating solid and a partially wetting liquid:

$$\left\{ \begin{array}{ll} \rho(\partial_t u + u \cdot \nabla u) = -\nabla p, & \text{in } \Omega, \\ \operatorname{div} u = 0, & \text{in } \Omega, \\ u \cdot n = 0, & \text{on } \Gamma_{SL} \text{ and } \Gamma_{SV}, \\ \llbracket u \rrbracket \cdot n = 0, & \text{on } \Gamma, \\ \llbracket p \rrbracket = \gamma H + \gamma \frac{\cos \theta_s - \cos \theta}{\sin \theta} \delta_\Sigma, & \text{on } \Gamma. \end{array} \right. \quad (4.1)$$

(For an explanation of the notation, see §4.1.1; for the meaning of the partially wetting hypothesis, see §4.2.1.) The last equation is the idealized augmented Young-Laplace law, and it contains a singular Dirac measure δ_Σ that will eventually require a substantive interpretation.

We emphasize once more that the above system is an idealized mathematical model. Examples of simplifying assumptions we made are:

1. The fluids are inviscid.
2. The solid is nondeformable and its surface is smooth.
3. The solid is completely fixed in space and does not rotate.
4. The model is purely macroscopic: There are no conjoining/disjoining pressures like van der Waals or electrostatic interactions.

For many applications, viscosity of the liquid plays an important role, and the solid boundaries should be treated as elastic and rough (see, e.g., §3 in de Gennes et al. [36]). Also, an original motivation for this research was to better understand the curvature-driven assembly of nanoparticles reported by Cavallaro et al. [16], and for that it does not make sense to assume the solids are fixed. Furthermore, for thin films

and in the microscopic vicinity of the triple junction, van der Waals interactions and the like cannot be ignored. We discuss this last issue more in §4.5.

Despite these practical limitations, we believe this model is a useful stepping stone for clarifying the specification of boundary conditions for macroscopic dynamic models that allow for moving contact lines and dynamic contact angles. The correct specification of these boundary conditions is a long-standing source of controversy, and at least two issues are of importance here:

1. *Dynamic contact angle and surface tension:* When there is surface tension, and the contact angle differs from its equilibrium value, then there are additional stresses at the triple junction that must be incorporated into the model.
2. *Moving contact line and no-slip:* In the viscous case, the widely used no-slip boundary conditions are incompatible with motion of the triple junction and so must be modified in its vicinity.

In the literature, the second issue has received much more attention and the first is frequently ignored completely.¹ By studying inviscid models, where the second issue does not arise, we hope to shed light on the first issue. (Note also that viscous stresses are a result of the motion of particles, whereas the stresses at the triple junction due to surface tension depend purely on the instantaneous geometric configuration of the liquid, vapor, and solid.)

The rest of the chapter is structured as follows. In the remainder of this section, we explain our notation, review some geometric concepts and formulas, and discuss related literature. In §4.2, we briefly review the static problem and give a variational derivation of a static analog of the idealized augmented Young-Laplace law. In §4.3, we explain the derivation of the dynamic system (4.63). As a compatibility check, we

¹Perhaps this is why, in much of the literature, the contact angle is prescribed as its equilibrium value as a boundary condition. However, experimental evidence for moving contact lines as well as plain everyday experience suggest there should be a macroscopic model in which the contact angle can vary dynamically.

show in §4.4 that the system (4.63) gives rise to the correct equilibrium solutions, at least for the problem of a half-plane solid and irrotational flow. In §4.5, we make some remarks on modeling long-range interactions near the triple junction. Finally, in §4.6, we discuss ideas and directions for further research.

4.1.1 Setup and notation

The liquid occupies region Ω_L and the vapor occupies region Ω_V . Fluid i has velocity u_i , pressure p_i , constant density ρ_i , and constant kinematic viscosity μ_i . We will denote the solid-liquid, liquid-vapor, and vapor-solid interfaces by $\Gamma_{SL}, \Gamma_{LV}, \Gamma_{SV}$, respectively. The interface Γ_i has outer unit conormal ν_i and constant surface tension γ_i . The intersection of the three interfaces is called the *triple junction*² (or *contact line* in three dimensions) and we will denote it by Σ . The contact angle θ is defined for points on Σ by

$$\cos \theta = \nu_{LV} \cdot \nu_{SL}. \quad (4.2)$$

We assume the solid boundary is at least C^1 , and so $\nu_{SL} = -\nu_{SV}$. The normal vector on the interfaces is oriented as pointing outwards from the liquid on Γ_{SL} and Γ_{LV} , and as pointing outwards from the vapor on Γ_{SV} . Since we will mostly be concerned with the liquid-vapor surface, we frequently write just Γ for Γ_{LV} , and γ for γ_{LV} . All of this is summarized in Figure 4.2.

We write $\Omega = \Omega_L \cup \Omega_V$ and define unsubscripted versions of u, p, ρ, μ by $\rho = \rho_L \chi_{\Omega_L} + \rho_V \chi_{\Omega_V}$ and so on. On the interfaces, we use a double bracket and an over

²In general, the interfaces are hypersurfaces in \mathbb{R}^n and the triple junction is a codimension-2 manifold. We occasionally write “interface” instead of “surface” and “triple junction” instead of “contact line” to avoid dimensional connotations, following the terminology of, e.g., Depner, Garcke, and Kohsaka [39].

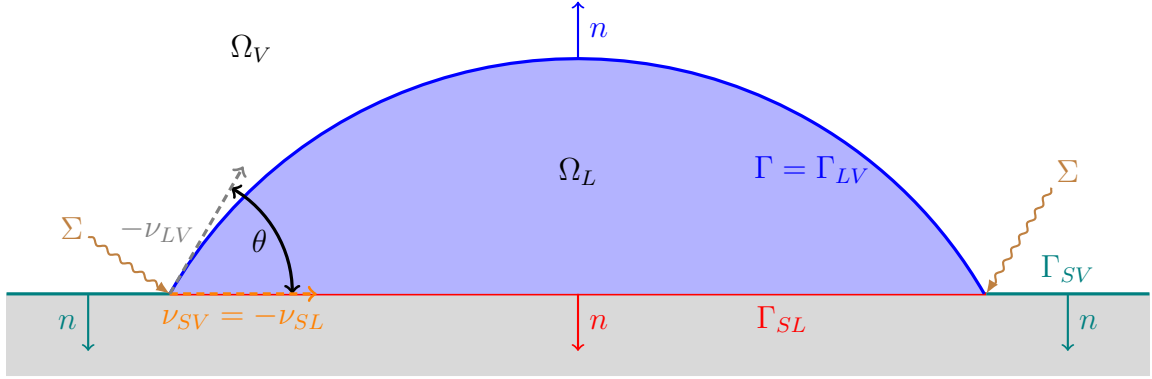


Figure 4.2: Notation

bar to denote the jump and the average of a quantity, respectively. That is,

$$\llbracket f \rrbracket = f_V - f_L, \quad (4.3)$$

$$\bar{f} = \frac{1}{2}(f_L + f_V). \quad (4.4)$$

Finally, we denote the outer normal velocity component of Γ by V and the velocity component of the triple junction in the direction ν_{SL} by v .³ It is related to V on $\Sigma = \partial\Gamma$ via

$$v = V n_{LV} \cdot \nu_{SL} = V \sin \theta. \quad (4.5)$$

4.1.2 Geometric concepts

We state here without proof and without regularity assumptions only the bare minimum necessary for this chapter, as calculations in this chapter are mostly formal. For more details and a well-developed formalism for studying evolving hypersurfaces and triple junctions, we recommend §2 of Depner's dissertation [38], where also pointers to more traditional references may be found. See also Depner, Garcke and Kohsaka [39] and references therein.

³In dimensions $n \geq 3$, the triple junction is a manifold of dimension $n - 2 \geq 1$, and so, depending on the parametrization, the velocity of the triple junction could have tangential components as well. However, the component of the velocity in the direction ν_{SL} is independent of the choice of parametrization.

Definition 4.1.1. \mathcal{H}^k denotes k -dimensional Hausdorff measure.

Definition 4.1.2. H denotes the mean curvature of a hypersurface.

For a hypersurface in \mathbb{R}^n , parametrizable as a graph $\{(x, \eta(x)) \mid x \in \mathbb{R}^{n-1}\}$, the mean curvature is given by

$$H = \operatorname{div}_x \frac{\nabla_x \eta}{\sqrt{1 + |\nabla_x \eta|^2}}. \quad (4.6)$$

Convention 4.1.3. *Following Depner [38], we use the normalization of mean curvature such that $H = -n$ for a unit sphere in \mathbb{R}^{n+1} oriented with outwards pointing normal. The sign choice varies in the literature. Traditionally, the normalization $H = \pm 1$ is more common (and is necessary to justify the “mean” in “mean curvature”). The justification of using $\pm n$ is that many formulas (like the transport identity below) are more naturally stated using this normalization.*

Proposition 4.1.4. *For a bounded evolving region $\Omega(t) \subset \mathbb{R}^n$, we have*

$$\frac{d}{dt} \int_{\Omega(t)} f \, d\mathcal{H}^n = \int_{\Omega(t)} \partial_t f \, d\mathcal{H}^n + \int_{\partial\Omega(t)} f V \, d\mathcal{H}^{n-1} \quad (4.7)$$

where V is the normal velocity of $\partial\Omega$.

Proposition 4.1.5. *For an evolving hypersurface $\Gamma(t) \subset \mathbb{R}^n$, we have*

$$\frac{d}{dt} \int_{\Gamma(t)} 1 \, d\mathcal{H}^{n-1} = - \int_{\Gamma(t)} V H \, d\mathcal{H}^{n-1} + \int_{\partial\Gamma(t)} v \, d\mathcal{H}^{n-2} \quad (4.8)$$

where V is the normal velocity of Γ , and v is the outer conormal velocity of $\partial\Gamma$.

4.1.3 Sign conventions

A number of sign choices were made and these, unfortunately, vary widely in the literature. As much as possible, we try to follow the choices of the survey paper of

Bardos and Lannes [7]. To summarize, our sign conventions are:

- The mean curvature H is negative for spheres with outwards-pointing normal.
- $(x, y)^\perp = (-y, x)$ and $\nabla^\perp f = (-\partial_y f, \partial_x f)$.
- The normal n on Γ points from Ω_L to Ω_V .
- The bracket is $[[f]] = f_V - f_L$.
- The unit tangent vector τ along Γ is chosen such that (τ, n) is a positively oriented basis of \mathbb{R}^2 . (This means $\tau = -n^\perp$.)
- Arc length s increases in the direction of τ along Γ .

4.1.4 Related literature

For the physics of surface tension and wetting, we used as our primary reference the book by de Gennes, Brochard-Wyart, and Quéré [36]. For the issue of disjoining/conjoining pressure in thin films and in the vicinity of contact lines, we also found helpful the books by Israelachvili [69], Starov, Velarde, and Radke [107], and Derjaguin, Churaev, and Muller [40].

The literature on equilibrium capillary surfaces and the related Plateau problem of area-minimizing surfaces is classical and vast. We refer to, e.g., the books of Finn [52] and Giusti [60].

Recognition of the incompatibility of moving contact lines and no-slip boundary conditions for the Navier-Stokes equations dates back several decades. For early work, we refer the reader to, e.g., Huh and Scriven [68], Dussan V. and Davis [45], Dussan V. [43, 44] and references therein. A nice exposition of these early results is given in §2.2 of Snoeijer and Andreotti [105]. For a survey of more recent results, we recommend Lauga, Brenner, and Stone [75].

For macroscopic models of liquid-vapor-solid systems in the case of viscous fluids, the mathematical state of the art appears to be the sharp interface models of Ren and E [97–99] and the diffuse interface model (with what they call *generalized Navier boundary conditions*) of Qian, Wang, and Sheng [92–94]. Roughly speaking, both prescribe the velocity at the triple junction as a function of the contact angle. In the simplest case, in [97], the authors propose

$$v = -\frac{1}{k}(\cos \theta - \cos \theta_s) \quad (4.9)$$

for a suitable constant k . This guarantees dissipation of energy. However, this approach seems unsuited for inviscid models for two reasons. First, we expect conservation of energy and, second, we may not prescribe the contact line velocity in any case. Furthermore, for inviscid fluids, there is no reason to believe the contact angle should depend only locally on the velocity in the general case. For a specific geometry, a (complicated!) local relation holds approximately in the case of Stokes flow (the high Reynolds number limit) and low Capillary number, as derived by Cox using matched asymptotic expansion [35]. For more recent work on this subject, we refer to, e.g., Eggers [48, 49] and Eggers and Stone [50]. However, we are not aware of any such work for the inviscid (i.e., low Reynolds number) limit.

Many of the ideas in this chapter were inspired by a paper of Mellet [80] studying dynamic solutions to thin film equations with constant-in-time but nonzero contact angle. Mellet uses a singular perturbation approach to studying the Dirac measure.

We are not aware of any prior studies of liquid-vapor-solid systems using the full incompressible Euler equations. Everything we could find assumed either that the contact line does not move or prescribed the contact angle to be the equilibrium value. As we shall see later on, these are precisely the cases in which no additional stresses arise at the contact line.

4.2 The static problem

To motivate the derivation of the augmented Young-Laplace equation in §4.3, and to better understand its meaning, it helps to first look at the static problem. We briefly review some physical concepts and laws related to this problem in §4.2.1, and then elaborate on a variational approach to deriving those laws in §§4.2.2–4.2.3.

4.2.1 Review of concepts

We review here some standard concepts related to the static problem, based on Chapter 1 of de Gennes et al. [36].

We consider here systems where the fluids and the solid are entirely at rest. In this case, the energy of the system consists of only the surface energies,

$$E = \sum_i \int_{\Gamma_i} \gamma_i d\mathcal{H}^{n-1}. \quad (4.10)$$

It is useful to introduce the *spreading parameter* S , defined by

$$S = \gamma_{SV} - (\gamma_{SL} + \gamma). \quad (4.11)$$

The interpretation is as follows: The surface energy per unit area of the solid-vapor interface is γ_{SV} . If a unit area of this interface is covered by an infinitesimal layer of liquid, then the change in surface energy of the system is given by $-S$. As de Gennes et al. put it:

$$S = [E_{\text{substrate}}]_{\text{dry}} - [E_{\text{substrate}}]_{\text{wet}}. \quad (4.12)$$

The point is that if $S > 0$, the *totally wetting* case, then it is energetically favorable for the liquid to cover as much of the solid as it can. (In practice, a finite-volume liquid can of course not become infinitesimally thin. At latest on molecular length scales, other effects (such as gravity or disjoining pressure) will counterbalance the

spreading and lead to some finite equilibrium height.)

In the opposite case $S < 0$, the *partially wetting* case, it is energetically favorable for a thin layer of liquid to minimize its contact with the solid surface. It will form a droplet, stopping its retreat from the solid surface only once doing so increases by too much the energy of its curved interface with the vapor.

Two laws characterize the liquid's equilibrium shape: First, the *Young-Laplace law* specifying that the mean curvature H of the liquid-vapor interface Γ is proportional the pressure difference between vapor and liquid at the interface,

$$\gamma H = \llbracket p \rrbracket, \quad (4.13)$$

and second, the *Young-Dupré law* stating that the static contact angle θ_s is given by

$$\cos \theta_s = \frac{\gamma_{SV} - \gamma_{SL}}{\gamma}. \quad (4.14)$$

These laws can be derived via energy considerations or force balances—we refer to the aforementioned references. We will give a slightly different derivation in §4.2.3.

Remark 4.2.1. In the following, even when working in the dynamic setting, we will typically write expressions involving $\gamma_{SL} - \gamma_{SV}$ in terms of γ and $\cos \theta_s$ using (4.14). Instead of $\cos \theta_s$, it is also common in the literature to use S . The relation between $S < 0$ and $\cos \theta_s$ is simply

$$S = \gamma(\cos \theta_s - 1). \quad (4.15)$$

Convention 4.2.2. *For the rest of this chapter, we work in the partially wetting regime. That is, we assume $S < 0$. Then θ_s is a well-defined angle, $0 < \theta_s < \pi$. (Some of the calculations remain valid if we eliminate θ_s in favor of S using (4.15). See Remark 4.3.4 for an example.)*

4.2.2 Variational approach for the small-angle approximation

Let us demonstrate now a neat variational calculus technique for deriving PDE's and boundary conditions in free-boundary problems. We first encountered a version of this idea in Mellet [80], but similar calculations occur in a number of earlier papers as well, and we are not sure of the exact origin. In any case, we refer to Mellet's paper for a more rigorous discussion of these toy calculations using a singular perturbation approach.

Let us work for simplicity with one-dimensional "surfaces," and consider the problem of minimizing the energy of a droplet on a plane $y = 0$ subject to a volume constraint. Let us further assume $\gamma_{SV} = \gamma_{SL} = 0$, $\gamma = 1$, and that the surface of the droplet can be represented by a graph $(x, \eta(x))$ where $|\eta_x|^2 \ll 1$. (We will drop some of these assumptions in the next section §4.2.3, but it is instructive to look at this simplified case first, as the calculations are easier to follow.)

The surface energy of the system is simply the surface area of the liquid-vapor interface. We write it as

$$E(\eta) = \int_{-\infty}^{\infty} \sqrt{1 + |\eta_x|^2} \Theta(\eta(x)) \, dx, \quad (4.16)$$

where Θ denotes the Heaviside step function,

$$\Theta(y) = \begin{cases} 1, & y > 0, \\ 0, & y \leq 0, \end{cases} \quad (4.17)$$

whose distributional derivative is the Dirac distribution,

$$\frac{d}{dy} \Theta(y) = \delta(y). \quad (4.18)$$

The use of $\Theta(\eta)$ here serves as a way of expressing the indicator function for the

wetted region. Under the small-angle approximation $|\eta_x|^2 \ll 1$, we have

$$\sqrt{1 + |\eta_x|^2} \approx 1 + \frac{1}{2}|\eta_x|^2. \quad (4.19)$$

As an aside, note also that the mean curvature operator is then approximately just the Laplacian of η ,

$$H(\eta) = \partial_x \left(\frac{\eta_x}{\sqrt{1 + \eta_x^2}} \right) \approx \eta_{xx}. \quad (4.20)$$

Oversimplifying a bit, the approximate variational problem we consider, then, is to minimize the following functional,

$$J(\eta) = \int_{-\infty}^{\infty} \left(1 + \frac{1}{2}|\eta_x|^2\right) \Theta(\eta) \, dx - \lambda \int_{-\infty}^{\infty} \eta \, dx, \quad (4.21)$$

among nonnegative functions $\eta \in \dot{H}^1(\mathbb{R})$. The Lagrange multiplier λ was introduced to enforce the volume constraint. Since $\eta_x = 0$ a.e. on $\{\eta = 0\}$, we can rewrite the functional as

$$J(\eta) = \int_{-\infty}^{\infty} \Theta(\eta) \, dx + \int_{-\infty}^{\infty} \frac{1}{2}|\eta_x|^2 \, dx - \lambda \int_{-\infty}^{\infty} \eta \, dx. \quad (4.22)$$

Now it is easy to compute that minimizers must formally satisfy

$$0 = \frac{\delta J}{\delta \eta} = \delta(\eta) - \eta_{xx} - \lambda. \quad (4.23)$$

In particular, this tells us that on the free surface $\{\eta > 0\}$, we have $\eta_{xx} = \lambda$. But what does the Dirac measure signify? It turns out it tell us something about boundary conditions on the set $\partial\{\eta > 0\}$. To see this, let us suppose $\eta(x) = 0$ on some interval $(-\kappa, 0]$ (with $\kappa > 0$) and $\eta(x) > 0$ on some interval $(0, \kappa)$. Then multiplying (4.23) by

$\eta'(x)$ and integrating over $[-\epsilon, \epsilon]$ with $0 < \epsilon < \kappa$, we find

$$0 = \int_{-\epsilon}^{\epsilon} (\eta_x \delta(\eta) - \eta_x \eta_{xx} - \lambda \eta_x) dx \quad (4.24)$$

$$= \int_{-\epsilon}^{\epsilon} \left(\partial_x [\Theta(\eta)] - \frac{1}{2} \partial_x \eta_x^2 \right) dx - \lambda \eta(\epsilon) \quad (4.25)$$

$$= \Theta(\eta(\epsilon)) - \Theta(\eta(-\epsilon)) - \frac{1}{2} (|\eta_x(\epsilon)|^2 - |\eta_x(-\epsilon)|^2) - \lambda \eta(\epsilon). \quad (4.26)$$

By our assumptions on η , $\Theta(\eta(\epsilon)) = 1$ while $\Theta(\eta(-\epsilon)) = 0$ and $\eta_x(-\epsilon) = 0$. It follows that

$$0 = 1 - \frac{1}{2} |\eta_x(\epsilon)|^2 - \lambda \eta(\epsilon). \quad (4.27)$$

Taking the limit $\epsilon \rightarrow 0$, the rightmost term vanishes and we obtain the boundary condition

$$\frac{1}{2} |\eta_x(0+)|^2 = 1. \quad (4.28)$$

Thus, at least formally, equation (4.23) really encodes both a PDE satisfied by the free surface as well as boundary conditions on the contact points with the solid,

$$\begin{cases} \eta_{xx} = \lambda, & \text{on } \{\eta > 0\}, \\ \frac{1}{2} |\eta_x|^2 = 1, & \text{on } \partial\{\eta > 0\}. \end{cases} \quad (4.29)$$

Remark 4.2.3. Our calculations here served only to illustrate the derivation of boundary conditions through variational means. In fact, the variational approach is also well-suited to studying the regularity of minimizers, especially in two and three dimensions. Alt and Caffarelli [2] proved bounds on how large the set of singularities of the free surfaces can be. In particular, they were able to prove full regularity for two-dimensional surfaces. For the three-dimensional case and a survey of other more recent results, we refer to Caffarelli, Jerison and Kenig [14]. For a related, more general two-phase problem, we refer to Alt, Caffarelli and Friedman [3] and a different paper

by Caffarelli, Jerison and Kenig [13].

4.2.3 Variational approach for the capillary problem

In this section, we repeat the calculations of the previous section, but without the small-angle approximation and for general $\gamma, \gamma_{SL}, \gamma_{SV}$ in the partially wetting regime. This will give rise to both the Young-Laplace law on the liquid-vapor interface and Young's contact angle condition. (Similar but less detailed calculations appear in Caffarelli and Friedman [12].)

Let us consider a capillary droplet on a plane with partially wetting contact angle⁴ $0 < \theta_s < \frac{\pi}{2}$. We parametrize the height of the droplet by $\eta(x)$. By (4.14), we have $\gamma \cos \theta_s = \gamma_{SV} - \gamma_{SL}$. Thus, the capillary energy relative to the absence of the droplet may be written as

$$E(\eta) - E_0 = \int_{-\infty}^{\infty} \left(\left(\gamma \sqrt{1 + \eta_x^2} + \gamma_{SL} \right) - \gamma_{SV} \right) \Theta(\eta) \, dx \quad (4.30)$$

$$= \int_{-\infty}^{\infty} \left(\gamma \sqrt{1 + \eta_x^2} - \gamma \cos \theta_s \right) \Theta(\eta) \, dx. \quad (4.31)$$

Now minimize among $\{\eta \geq 0\}$ subject to a volume constraint $\int \eta \, dx = V$. That is, minimize

$$J(\eta) = \int_{-\infty}^{\infty} \left(\gamma \sqrt{1 + \eta_x^2} \Theta(\eta) - \gamma \cos \theta_s \Theta(\eta) - \lambda \eta \right) \, dx \quad (4.32)$$

$$= \int_{-\infty}^{\infty} \left(\gamma (\sqrt{1 + \eta_x^2} - 1) + \gamma (1 - \cos \theta_s) \Theta(\eta) - \lambda \eta \right) \, dx, \quad (4.33)$$

where we introduced a Lagrange multiplier λ . Formally, this gives⁵

$$0 = \frac{\delta J}{\delta \eta} = -\gamma H + \gamma (1 - \cos \theta_s) \delta(\eta) - \lambda. \quad (4.34)$$

⁴Really, all of this applies to contact angles $\frac{\pi}{2} \leq \theta_s < \pi$ as well, but then we need to parametrize the interface in a different way. For the sake of exposition, we restrict to a suboptimal angle range.

⁵Instead of $\gamma(1 - \cos \theta_s)$, we could also write $-S$ where S is the spreading parameter. See (4.15).

Note that $\gamma H = -\lambda$ is the Young-Laplace law as expected, but also there appears a singular measure $\delta(\eta)$ that (as we will see in a moment) encodes the contact angle constraint. We will encounter this again in our augmented Young-Laplace law (4.62) for the dynamic case.

Let us show now how (4.34) gives rise to the static boundary condition $\cos \theta = \cos \theta_s$. Suppose, without loss of generality, that our solution touches the surface at $x = 0$. That is, $\eta(x) = 0$ for $x \in (-\epsilon, 0]$ and $\eta(x) > 0$ for $x \in (0, \epsilon)$ for some $\epsilon > 0$. Using the formula for the mean curvature of a graph (4.6), we have

$$\gamma H = \gamma \partial_x(A'(\eta_x)) = \gamma(1 - \cos \theta_s) \delta(\eta) - \lambda, \quad (4.35)$$

where

$$A(z) = \sqrt{1 + z^2} - 1, \quad (4.36)$$

$$A'(z) = \frac{z}{\sqrt{1 + z^2}}. \quad (4.37)$$

Multiplying by η_x and integrating from $-\delta$ to δ (with $0 < \delta < \epsilon$), we find

$$\gamma \int_{-\delta}^{\delta} \eta_x \partial_x(A'(\eta_x)) dx = \gamma(1 - \cos \theta_s) \int_{-\delta}^{\delta} \eta_x \delta(\eta) dx - 2\lambda\delta \quad (4.38)$$

$$= \gamma(1 - \cos \theta_s) \Theta(\eta)|_{-\delta}^{\delta} - 2\lambda\delta \quad (4.39)$$

$$= \gamma(1 - \cos \theta_s) - 2\lambda\delta \quad (4.40)$$

$$\xrightarrow{\delta \rightarrow 0} \gamma(1 - \cos \theta_s). \quad (4.41)$$

Since $\eta_{xx}A'(\eta_x) = \partial_x[A(\eta_x)]$, integrating by parts the left-hand side, we obtain

$$\int_{-\delta}^{\delta} \eta_x \partial_x (A'(\eta_x)) \, dx = \gamma [\eta_x A'(\eta_x) - A(\eta_x)]_{-\delta}^{\delta} \quad (4.42)$$

$$= \gamma \left(\frac{\eta_x^2}{\sqrt{1 + \eta_x^2}} - (\sqrt{1 + \eta_x^2} - 1) \right) \Big|_{-\delta}^{\delta} \quad (4.43)$$

$$= \gamma \left(1 - \frac{1}{\sqrt{1 + \eta_x^2}} \Big|_{-\delta}^{\delta} \right) \quad (4.44)$$

$$\xrightarrow{\delta \rightarrow 0} \gamma (1 - \cos \theta) . \quad (4.45)$$

Thus $\cos \theta = \cos \theta_s$. To summarize, the single equation (4.34) formally gives rise to

$$\begin{cases} \gamma H = -\lambda, & \text{on } \{\eta > 0\}, \\ \cos \theta = \cos \theta_s, & \text{on } \partial\{\eta > 0\}. \end{cases} \quad (4.46)$$

That is, it encodes both the Young-Laplace law of constant mean curvature and the contact angle boundary condition.

4.3 The dynamic problem

Now we turn our attention to the dynamic problem. For inviscid fluids, we propose an analog of the static equation (4.34) for the dynamic problem, namely the following augmented Young-Laplace law (4.62),

$$[[p]] = \gamma H + \gamma \frac{\cos \theta_s - \cos \theta}{\sin \theta} \delta_{\Sigma}, \quad \text{on } \Gamma . \quad (4.47)$$

We give two “derivations” of this equation:

First, as described in §§4.3.1–4.3.3, if we start from the incompressible Euler equations and standard boundary conditions, then demanding energy conservation

leads naturally to the augmented Young-Laplace law as the remaining boundary condition for the pressure difference across the interface Γ .

Second, we show in §4.3.4 that introducing a half-plane solid into Zakharov's Hamiltonian formulation of the water waves problem also leads to the augmented Young-Laplace law. This is less general than the first approach, but perhaps a little closer to the variational spirit of §4.2.3.

4.3.1 Standard PDE and kinematic boundary conditions

Away from the interfaces, we assume the fluids satisfy the incompressible Euler or Navier-Stokes equations for all time,

$$\begin{cases} \rho(\partial_t u + u \cdot \nabla u) = \operatorname{div} \mathcal{T}, & \text{in } \Omega, \\ \operatorname{div} u = 0, & \text{in } \Omega, \end{cases} \quad (4.48)$$

where the stress tensor \mathcal{T} is given by

$$\mathcal{T} = -p\mathbb{I} + 2\mu\mathcal{D}, \quad \mathcal{D} = \frac{1}{2}((\nabla u) + (\nabla u)^\top). \quad (4.49)$$

We will also assume throughout that the solid is impermeable,

$$u \cdot n = 0, \quad \text{on } \Gamma_{SL} \text{ and } \Gamma_{SV}, \quad (4.50)$$

and that the interface Γ_{LV} does not separate,

$$[[u]] \cdot n = 0, \quad \text{on } \Gamma_{LV}. \quad (4.51)$$

The normal velocity of Γ_{LV} is thus

$$V = u_L \cdot n = u_V \cdot n = \bar{u} \cdot n, \quad (4.52)$$

and the nontangential velocity of the triple junction is $v \nu_{SL}$.

So far none of our assumptions are controversial. However, they are not complete. For the Euler equations, one more boundary condition must be specified on Γ_{LV} , and for the Navier-Stokes equations several more are required. To fill in the missing boundary condition for the inviscid case, we look to energy conservation.

4.3.2 Time derivative of energy

Ren and E [98] use thermodynamic principles to derive boundary conditions for moving contact lines in the case of viscous fluids. We will follow a similar approach here, but for inviscid fluids. This means we will look for the “simplest” boundary condition that leads to conservation of energy. Bear in mind that the inviscid case differs from the viscous case in two essential ways:

1. As there is no friction in the inviscid model, we seek exact conservation of energy, not just dissipation of energy.
2. In the inviscid case, there are fewer degrees of freedom in prescribing boundary conditions.

Let us assume that the orientation and center of mass of the solid are fixed. Then the total energy of the system consists of the kinetic energy of the fluids plus the surface energies,

$$E = \int_{\Omega} \frac{1}{2} \rho |u|^2 d\mathcal{H}^n + \sum_i \int_{\Gamma_i} \gamma_i d\mathcal{H}^{n-1} =: T + U. \quad (4.53)$$

Let us formally compute $\frac{dE}{dt}$ subject to (4.48), (4.50), (4.51), and see what constraints this imposes on the remaining choice of boundary conditions.

Using the transport identities (4.7) and (4.8), we find

$$\frac{d}{dt} T = \int_{\Omega} \partial_t \left(\frac{1}{2} \rho |u|^2 \right) d\mathcal{H}^n - \int_{\Gamma} \left[\left[\frac{1}{2} \rho |u|^2 \right] \right] V d\mathcal{H}^{n-1}, \quad (4.54)$$

and

$$\frac{d}{dt}U = - \int_{\Gamma} \gamma HV \, d\mathcal{H}^{n-1} + \int_{\Sigma} \sum_i \gamma_i ((v \nu_{SL}) \cdot \nu_i) \, d\mathcal{H}^{n-2}. \quad (4.55)$$

Multiplying (4.48) by u and integrating over Ω , we find

$$\int_{\Omega} \partial_t \left(\frac{1}{2} \rho |u|^2 \right) \, d\mathcal{H}^n = - \int_{\Omega} \frac{1}{2} \rho u \cdot \nabla |u|^2 \, d\mathcal{H}^n + \int_{\Omega} u \cdot \operatorname{div} \mathcal{T} \, d\mathcal{H}^n \quad (4.56)$$

$$= \int_{\Gamma} \left[\left[\frac{1}{2} \rho |u|^2 \right] \right] V \, d\mathcal{H}^{n-1} - \int_{\Gamma} \llbracket u \cdot \mathcal{T} \rrbracket \cdot n \, d\mathcal{H}^{n-1} - \int_{\Omega} \mu |\nabla u|^2 \, d\mathcal{H}^n, \quad (4.57)$$

where we integrated by parts both integrals and used $\operatorname{div} u = 0$. Next we observe, using $\nu_{SV} = -\nu_{SL}$, $\nu_{SL} \cdot \nu_{LV} = \cos \theta$, and $\gamma_{SV} - \gamma_{SL} = \gamma \cos \theta_s$, that

$$\sum_i \gamma_i (v \nu_{SL}) \cdot \nu_i = v(\gamma_{SL} - \gamma_{SV} + \gamma \cos \theta) = \gamma v(\cos \theta - \cos \theta_s). \quad (4.58)$$

Putting this all together, we have

$$\begin{aligned} \frac{d}{dt}E &= - \int_{\Omega} \mu |\nabla u|^2 \, d\mathcal{H}^n - \int_{\Gamma} (\llbracket u \cdot T \rrbracket \cdot n + \gamma HV) \, d\mathcal{H}^{n-1} \\ &\quad + \int_{\Sigma} \gamma v(\cos \theta - \cos \theta_s) \, d\mathcal{H}^{n-2}. \end{aligned} \quad (4.59)$$

4.3.3 Energy conservation in the inviscid case and the augmented Young-Laplace law

Convention 4.3.1. *From here on out we assume our fluids are inviscid, i.e., $\mu \equiv 0$.*

If $\mu_L = \mu_V = 0$, then $T = -p\mathbb{I}$ and so $\llbracket u \cdot T \rrbracket \cdot n = -\llbracket p \rrbracket V$. A first look at (4.59) suggests that we should take $\llbracket p \rrbracket = \gamma H$ as the final boundary condition on Γ , in order to eliminate the integral over Γ . This is the Young-Laplace equation. However, if we

do this, then there is still the integral over Σ left,

$$\frac{d}{dt}E = \int_{\Sigma} \gamma v (\cos \theta - \cos \theta_s) d\mathcal{H}^{n-2}, \quad (4.60)$$

and so we cannot expect energy to be conserved unless $v = 0$ (the triple junction does not move) or $\theta = \theta_s$ (the contact angle is fixed at its equilibrium value).

The problem with using the plain Young-Laplace law as the boundary condition is that it only accounts for the stresses due to change in the surface energy of Γ_{LV} , and not for the stresses due to change of the surface energy of Γ_{SL} and Γ_{SV} .

To see how to incorporate these missing stresses, we recall that $V = v \sin \theta$ on Σ (see (4.5)), and use this to rewrite (4.59) for $\mu \equiv 0$ as

$$\frac{d}{dt}E = \int_{\Gamma} V \left(\llbracket p \rrbracket - \gamma H + \gamma \frac{\cos \theta - \cos \theta_s}{\sin \theta} \delta_{\Sigma} \right) d\mathcal{H}^{n-1}, \quad (4.61)$$

where δ_{Σ} denotes a Dirac measure on Γ concentrated on Σ . Written in this way, it is clear that energy will be conserved if we take the following augmented Young-Laplace law as our boundary condition:

$$\llbracket p \rrbracket = \gamma H + \gamma \frac{\cos \theta_s - \cos \theta}{\sin \theta} \delta_{\Sigma}, \quad \text{on } \Gamma. \quad (4.62)$$

We propose this as the natural dynamic analog of the equation (4.34) that we found in the static case using the variational approach. There is a singular measure δ_{Σ} in the boundary condition, but that should not frighten us. We have already seen in the static case that this innocuously encodes information about the contact line.

To summarize, the full system we propose for the case of inviscid fluids and a fixed

and non-rotating solid is:

$$\left\{ \begin{array}{ll} \rho(\partial_t u + u \cdot \nabla u) = -\nabla p, & \text{in } \Omega, \\ \operatorname{div} u = 0, & \text{in } \Omega, \\ u \cdot n = 0, & \text{on } \Gamma_{SL} \text{ and } \Gamma_{SV}, \\ \llbracket u \rrbracket \cdot n = 0, & \text{on } \Gamma, \\ \llbracket p \rrbracket = \gamma H + \gamma \frac{\cos \theta_s - \cos \theta}{\sin \theta} \delta_\Sigma, & \text{on } \Gamma. \end{array} \right. \quad (4.63)$$

Remark 4.3.2. We wish we could go further and split (4.62) into the Young-Laplace law and a statement about the contact points, as we did for the static case in §4.2.3. Unfortunately, we cannot directly follow the same procedure, since $\llbracket p \rrbracket$ is not defined off of Γ . We discuss the issue of making sense of the Dirac measure more in §4.6.

Remark 4.3.3. Using

$$\cos \theta_s = \cos((\theta - \theta_s) - \theta) = \cos \theta \cos(\theta - \theta_s) + \sin \theta \sin(\theta - \theta_s), \quad (4.64)$$

we find

$$\frac{\cos \theta_s - \cos \theta}{\sin \theta} = \cot \theta (\cos(\theta - \theta_s) - 1) + \sin(\theta - \theta_s) \quad (4.65)$$

$$= (\theta - \theta_s) - \frac{1}{2}(\cot \theta)(\theta - \theta_s)^2 + O((\theta - \theta_s)^3). \quad (4.66)$$

Remark 4.3.4. For the case of total wetting, the calculations above are still valid, but we need to write them in terms of S instead of $\cos \theta_s$. In that case, (4.62) becomes

$$\llbracket p \rrbracket = \gamma H + \frac{S + \gamma(1 - \cos \theta)}{\sin \theta} \delta_\Sigma, \quad \text{on } \Gamma. \quad (4.67)$$

Then there is no $\theta \in (0, \pi)$ that makes the coefficient of the Dirac measure vanish.

The coefficient only vanishes in the limits $\theta \rightarrow 0$ and $\theta \rightarrow \pi$.

4.3.4 Hamiltonian formulation of water waves problem

In further support of our augmented Young-Laplace law (4.62), we show in this section how it arises in a simple modification of a classical problem that is known to have a Hamiltonian structure. Namely, due to Zakharov in 1968 [118], there is a Hamiltonian formulation for the *water waves problem*. This problem concerns inviscid irrotational flow in an infinitely deep ocean of unbounded extent, subject to gravity, and with a free surface, subject to surface tension, that is representable as a graph. To keep notation simple, we will do the calculations here only for the two-dimensional case, i.e., one-dimensional interfaces, but they are easy to generalize to higher dimensions.

The idea is this: We start from the setup of the water waves problem, but replace the $x < 0$ half-plane by an infinite solid. The liquid is now merely a “half-ocean” residing in the $x > 0$ half-plane, with the vapor filling the space above it. See Figure 4.3.

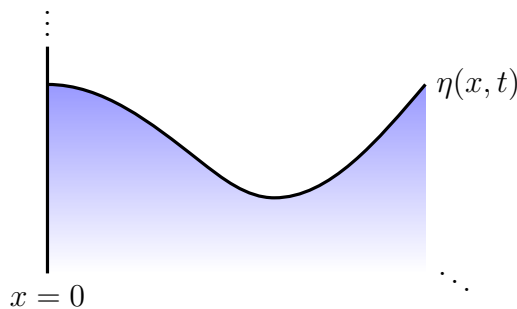


Figure 4.3: Water-waves problem for half-ocean

We write $\eta(x, t)$ for the height of the free surface and $\varphi(x, y, t)$ for the velocity potential. The trace of φ on the free surface is

$$\phi(x, t) = \varphi(x, \eta(x, t), t). \quad (4.68)$$

Since we are considering potential flow, φ is determined uniquely from ϕ via

$$\begin{cases} -\Delta\varphi = 0, & (y < \eta(x), x > 0) \\ \varphi = \phi, & (y = \eta(x), x > 0) \\ \partial_n\varphi = 0. & (x = 0) \end{cases} \quad (4.69)$$

The condition $\partial_n\varphi = u \cdot n = 0$ on $x = 0$ is just the impenetrability of the solid half-plane.

We take as our Hamiltonian $\mathcal{H} = T + U$ where

$$T = \int_0^\infty \int_{-\infty}^\eta \frac{1}{2} |\nabla\varphi|^2 dy dx, \quad (4.70)$$

$$U = \int_0^\infty \left(\frac{1}{2} g\eta^2 + \gamma(\sqrt{1 + \eta_x^2} - 1) - (\gamma \cos \theta_s)\eta(x, t)\delta(x) \right) dx. \quad (4.71)$$

The only new term compared to Zakharov's system is the rightmost one in the potential energy. This term comes from observing that $\gamma \cos \theta_s = \gamma_{SV} - \gamma_{SL}$ is the surface energy per unit length associated with decline in height of the water at $x = 0$.

Zakharov showed that the water waves problem is Hamiltonian with canonical variables η and ϕ . That is, the evolution equations for η and ϕ may be obtained from variations of \mathcal{H} ,

$$\partial_t\eta = \frac{\delta\mathcal{H}}{\delta\phi}, \quad \partial_t\phi = -\frac{\delta\mathcal{H}}{\delta\eta}. \quad (4.72)$$

Repeating Zakharov's computations for the half-ocean problem, the augmented Young-Laplace law makes another appearance, as we now show.

Proposition 4.3.5. *For the half-ocean problem, equations (4.72) are on $y = \eta(x)$,*

$$\partial_t\varphi + \frac{1}{2} |\nabla\varphi|^2 + g\eta = \gamma H + \gamma(\cos \theta_s - \cos \theta)\delta(x), \quad (4.73)$$

$$\partial_t\eta = (\varphi_y - \eta_x\varphi_x)|_{y=\eta} = \partial_n\varphi|_{y=\eta} \sqrt{1 + \eta_x^2}. \quad (4.74)$$

Proof. First, let us compute $\frac{\delta \mathcal{H}}{\delta \phi}$. Since U is independent of ϕ , we need only look at T . Given a variation $\delta \phi$, we can obtain $\delta \varphi$ from $\delta \phi$ via (4.69), just as φ is obtained from its trace ϕ . Using $\delta \varphi$, we compute:

$$\delta T = \int_0^\infty \int_{-\infty}^\eta \nabla \varphi \cdot \nabla(\delta \varphi) \, dy \, dx \quad (4.75)$$

$$\begin{aligned} &= - \int_0^\infty \int_{-\infty}^\eta (-\Delta \varphi) \delta \varphi \, dy \, dx + \int_{\{x=0, y < \eta\}} (\partial_n \varphi) \delta \varphi \, dy \\ &\quad + \int_{\{x > 0, y = \eta(x)\}} (\partial_n \varphi) \delta \varphi \, ds. \end{aligned} \quad (4.76)$$

The first two terms vanish since $-\Delta \varphi = 0$ and $\partial_n \varphi = 0$ on $x = 0$ by (4.69). For the third term, we observe that $ds = \sqrt{1 + \eta_x^2} \, dx$ to conclude

$$\delta T = \int_0^\infty \partial_n \varphi|_{y=\eta(x)} \delta \phi(x) \sqrt{1 + \eta_x^2} \, dx, \quad (4.77)$$

and hence

$$\frac{\delta \mathcal{H}}{\delta \phi} = \frac{\delta T}{\delta \phi} = \partial_n \varphi|_{y=\eta} \sqrt{1 + \eta_x^2}. \quad (4.78)$$

Since

$$\partial_n \varphi = n \cdot \nabla \varphi = \frac{(-\eta_x, 1) \cdot (\varphi_x, \varphi_y)}{\sqrt{1 + \eta_x^2}} = \frac{\varphi_y - \eta_x \varphi_x}{\sqrt{1 + \eta_x^2}}, \quad (4.79)$$

this may also be written as

$$\frac{\delta \mathcal{H}}{\delta \phi} = (\varphi_y - \eta_x \varphi_x)|_{y=\eta(x)}. \quad (4.80)$$

This establishes the second equation in the proposition.

Now let us look at the variations with respect to η . For the variation of the

potential energy, we compute, (assuming $\delta\eta \rightarrow 0$ as $x \rightarrow \infty$)

$$\delta U = \int_0^\infty (g\eta - (\gamma \cos \theta_s)\delta(x)) \delta\eta \, dx + \gamma \int_0^\infty \frac{\eta_x}{\sqrt{1 + \eta_x^2}} (\delta\eta)_x \, dx \quad (4.81)$$

$$= \int_0^\infty \left(g\eta - (\gamma \cos \theta_s)\delta(x) - \gamma \frac{\eta_x}{\sqrt{1 + \eta_x^2}} \delta(x) - \gamma \frac{\partial}{\partial x} \left(\frac{\eta_x}{\sqrt{1 + \eta_x^2}} \right) \right) \delta\eta \, dx. \quad (4.82)$$

Observing that

$$- \frac{\eta_x}{\sqrt{1 + \eta_x^2}} = \cos \theta \quad (\text{at } x = 0) \quad \text{and} \quad \frac{\partial}{\partial x} \left(\frac{\eta_x}{\sqrt{1 + \eta_x^2}} \right) = H, \quad (4.83)$$

we arrive at

$$\frac{\delta U}{\delta\eta} = g\eta + \gamma(\cos \theta - \cos \theta_s)\delta(x) - \gamma H. \quad (4.84)$$

The variation of the kinetic energy is a little more complicated since it involves also φ , and a variation $\delta\eta$ also induces a variation $\delta\varphi$ via (4.69), even when ϕ is not changed. With this in mind, we compute

$$\delta T = \int_0^\infty \frac{1}{2} |\nabla\varphi|^2 \delta\eta \, dx + \int_0^\infty \int_{-\infty}^\eta \nabla\varphi \cdot \nabla(\delta\varphi) \, dy \, dx. \quad (4.85)$$

Using $\Delta\varphi = 0$ and $\partial_n\varphi = 0$ on $x = 0$, we may integrate the second integral by parts to get

$$\delta T = \int_0^\infty \frac{1}{2} |\nabla\varphi|^2 \delta\eta \, dx + \int_0^\infty [(\partial_n\varphi)\delta\varphi]_{y=\eta} \sqrt{1 + \eta_x^2} \, dx. \quad (4.86)$$

Thanks to (4.69), we have⁶ $\delta\varphi = -(\partial_y\varphi)\delta\eta$ on $y = \eta$. To see this, note that varying η but holding ϕ fixed, we have

$$(\varphi + \delta\varphi)(x, \eta(x) + \delta\eta(x)) = \varphi(x, \eta(x)) = \phi(x); \quad (4.87)$$

⁶This is stated with an incorrect sign in Zakharov's paper.

hence, by formal infinitesimal calculation,

$$\delta\varphi(x, \eta(x)) = \delta\varphi(x, \eta(x) + \delta\eta(x)) = \varphi(x, \eta(x)) - \varphi(x, \eta(x) + \delta\eta(x)) \quad (4.88)$$

$$= -\delta\eta(x)\varphi_y(x, \eta(x)). \quad (4.89)$$

Furthermore, we have shown

$$\partial_t\eta = \frac{\delta\mathcal{H}}{\delta\phi} = \sqrt{1 + \eta_x^2} \partial_n\varphi|_{y=\eta}. \quad (4.90)$$

Thus,

$$\delta T = \int_0^\infty \left[\frac{1}{2} |\nabla\varphi|^2 - (\partial_t\eta)\varphi_y \right] \delta\eta \, dx, \quad (4.91)$$

and so

$$\frac{\delta T}{\delta\eta} = \frac{1}{2} |\nabla\varphi|^2 - (\partial_t\eta)\varphi_y. \quad (4.92)$$

Combining (4.84) and (4.92), we thus find that

$$\frac{\partial\phi}{\partial t} = -\frac{\delta\mathcal{H}}{\delta\eta} = (\partial_t\eta)\varphi_y - \frac{1}{2} |\nabla\varphi|^2 - g\eta + \gamma H + \gamma(\cos\theta_s - \cos\theta)\delta(x). \quad (4.93)$$

Finally, since $\partial_t\phi = \partial_t\varphi + (\partial_t\eta)\varphi_y$, we may rewrite this in terms of φ , as stated in the proposition. ▮

Remark 4.3.6. For comparison, the Euler equation for $u = \nabla\varphi$ (and $\rho_L = 1$, $\rho_V = 0$) reads

$$0 = \partial_t\nabla\varphi + \nabla\varphi \cdot \nabla\nabla\varphi + \nabla p + g\hat{y} = \nabla\left(\partial_t\varphi + \frac{1}{2} |\nabla\varphi|^2 + gy + p\right), \quad (4.94)$$

and hence on $y = \eta(x)$,

$$p = -\left(\partial_t\varphi + \frac{1}{2} |\nabla\varphi|^2 + g\eta\right) + C(t). \quad (4.95)$$

As usual, we view the spatially constant term $C(t)$ as the atmospheric pressure p_{atm} at the water surface, and thus we may interpret the $\partial_t \varphi$ equation in Proposition 4.3.5 as specifying the pressure difference at the free surface,

$$\llbracket p \rrbracket = p_{atm} - p = \gamma H + \gamma(\cos \theta_s - \cos \theta) \delta(x). \quad (4.96)$$

Remark 4.3.7. Equation (4.96) is almost the same as the augmented Young-Laplace equation (4.62) we found earlier. To reconcile, note that δ_Σ is a Dirac mass relative to the hypersurface measure $d\mathcal{H}^{n-1}$ on Γ . Thus, in (4.96) we should change variables from horizontal distance x to arc length s . Since

$$\delta(x) = \delta(s) \frac{ds}{dx} = \delta(s) \sqrt{1 + \eta_x^2} = \frac{\delta(s)}{\sin \theta}, \quad (4.97)$$

we then recover (4.62) exactly.

4.4 Compatibility with the static case

As a compatibility check for the augmented Young-Laplace law (4.62) with known results, we show in this section that static solutions to the dynamic inviscid system (4.63) indeed satisfy the Young-Laplace law and the correct contact angle condition, at least in the irrotational case.

4.4.1 On irrotational equilibrium solutions

Let us consider the inviscid system (4.63), and look for steady irrotational solutions. Under the irrotational assumption, we have $u = \nabla \varphi$ for some velocity potential φ ,

and the system may be rewritten as (see Remark 4.3.6)

$$\left\{ \begin{array}{ll} \rho(\partial_t \varphi + \frac{1}{2} |\nabla \varphi|^2) = \gamma H + \gamma \frac{\cos \theta_s - \cos \theta}{\sin \theta} \delta_\Sigma & \text{on } \Gamma, \\ -\Delta \varphi = 0, & \text{in } \Omega, \\ \nabla \varphi \cdot n = 0, & \text{on } \Gamma_{SL} \text{ and } \Gamma_{SV}, \\ \llbracket \nabla \varphi \rrbracket \cdot n = 0, & \text{on } \Gamma. \end{array} \right. \quad (4.98)$$

Under the steadiness assumption, the interface does not move, and so we in fact have $u \cdot n = \nabla \varphi \cdot n = 0$ on Γ , and not just $\llbracket \nabla \varphi \rrbracket \cdot n = 0$. But then φ satisfies

$$\left\{ \begin{array}{ll} -\Delta \varphi = 0, & \text{in } \Omega, \\ \partial_n \varphi = 0, & \text{on } \partial \Omega. \end{array} \right. \quad (4.99)$$

It follows that

$$\varphi(x, t) = C_L(t) \chi_{\Omega_L}(x) + C_V(t) \chi_{\Omega_V}(x) \quad (4.100)$$

for some spatially constant functions C_L and C_V . (We restrict ourselves here to looking for solutions where both Ω_L and Ω_V are connected. For other solutions (such as multiple droplets), a separate spatially constant function may be required for each connected component.) From the first equation in (4.98), we then have

$$\rho_L C'_L(t) = \rho_V C'_V(t) = \gamma H + \gamma \frac{\cos \theta_s - \cos \theta}{\sin \theta} \delta_\Sigma. \quad (4.101)$$

Since the right-hand side is independent of time, we must have $C_L''(t) = C_V''(t) = 0$, and hence

$$C_L(t) = A_L t + B_L, \quad C_V(t) = A_V t + B_V, \quad (4.102)$$

for some constants A_L, B_L, A_V, B_V . Since $\rho_L C'_L(t) = \rho_V C'_V(t)$, we further know that A_L and A_V are related to each other via

$$\rho_L A_L = \rho_V A_V = \gamma H + \gamma \frac{\cos \theta_s - \cos \theta}{\sin \theta} \delta_\Sigma. \quad (4.103)$$

Since the left-hand sides are constant along Γ , the coefficient of δ_Σ must vanish, i.e., the expected contact angle condition holds,

$$\cos \theta_s = \cos \theta. \quad (4.104)$$

What remains is the Young-Laplace law of constant mean curvature,

$$\gamma H = \rho_L A_L = \rho_V A_V. \quad (4.105)$$

4.4.2 Example: half-plane solid in two dimensions

To get a little sense of the meaning of the constants A_L and A_V , let us specialize now to the two-dimensional case where the solid occupies the half plane $y < 0$.

When $A_L = A_V = 0$, the mean curvature vanishes and so the liquid-vapor interface is a straight line. Thanks to the contact angle condition, the line must meet the solid at angle θ_s . See Figure 4.4.

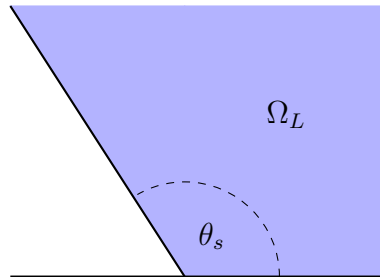


Figure 4.4: Wedge solution for half-plane solid in two dimensions.

Otherwise, the interface must be a spherical cap meeting the solid at angle θ_s and

of radius

$$R = \frac{1}{|H|} = \frac{\gamma}{\rho_L |A_L|} = \frac{\gamma}{\rho_V |A_V|}. \quad (4.106)$$

The sign of A_L and A_V then determines whether the liquid is in the interior of the spherical cap (negative sign) or exterior to the spherical cap (positive sign). See Figure 4.5.

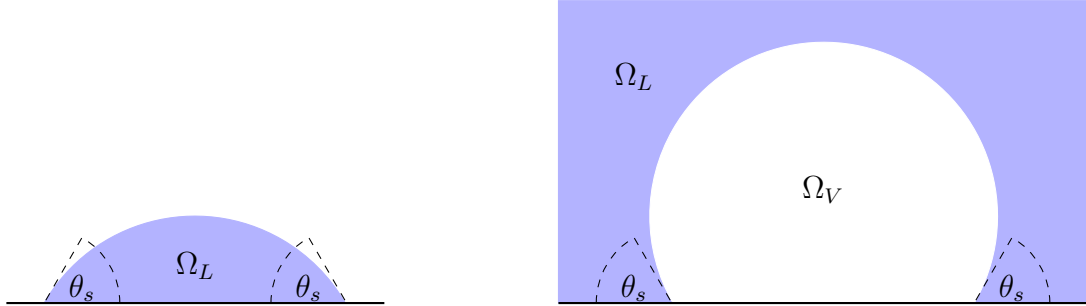


Figure 4.5: Liquid and vapor droplet solutions for half-plane solid in two dimensions.

4.5 On modeling long-range interactions

As pointed out in §4 of de Gennes et al. [36] (and also emphatically in §1 of Starov, Velarde and Radke [107]), using macroscopic quantities like pressure and surface tension is really only justified if the length scales of interest are significantly larger than the length scale of the molecular long-range interactions. For example, if the long-range interactions decay over a length scale r_0 , then the separation δ between the interfaces should really be of order $\delta \gg r_0$. However, the assumption $\delta \gg r_0$ is clearly violated in two common scenarios: (1) in thin films, especially totally wetting films; and (2) in the vicinity of triple junctions.

Since we are particularly interested in triple junctions and contact angles, it seems worthwhile to think about how to add long-range effects into our inviscid model. Again, we find it conceptually useful to study the inviscid rather than the viscous case. Viscosity introduces the further complication of somehow needing to violate non-slip

boundary conditions at distances close to the boundary (usually done by introducing another “slip” length scale).

4.5.1 Disjoining pressure for thin films of uniform thickness

In the thin film literature, it is common to add an ad hoc *disjoining pressure* $\Pi(h)$ into the augmented Young-Laplace equation. To illustrate this, let us consider the following example, adapted with modifications from §10.2 in Israelachvili [69]. A thin film of liquid in vacuum covers a solid that fills the infinite half-space $z < 0$, and we would like to incorporate interactions between liquid and solid molecules into our model. Let us assume an attractive, additive interaction potential between liquid and solid molecules of the form

$$W(r) = -\frac{C}{r^6}, \quad (4.107)$$

where r denotes the distance between the molecules; C is a physiochemically determined constant; and the exponent 6 is for van der Waals interactions. (For more sophisticated models and for explanations of the *Hamaker* constant C , we refer to §§10–11 in Israelachvili [69].) Then the net interaction energy of a liquid molecule at height $z = h$ with the solid is

$$U(h) = -\int_{-\infty}^0 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{C\rho_N^S}{|x^2 + y^2 + (h+z)^2|^3} dx dy dz = -\frac{\pi C\rho_N^S}{6h^3}, \quad (4.108)$$

where ρ_N^S denotes the number of molecules per unit volume of the solid. Multiplying by the corresponding liquid number density ρ_N^L gives us then the energy per unit volume in the liquid due to the long-range interactions,

$$e(h) = -\frac{\pi C\rho_N^S\rho_N^L}{6h^3}. \quad (4.109)$$

If we parametrize the liquid-vacuum interface by $(x, \eta(x))$, then there is an extra energy term of the form

$$E_W = \int_{-\infty}^{\infty} \int_0^{\eta(x)} e(h) dh dx, \quad (4.110)$$

where we ignore for a moment the singularity in e as $h \rightarrow 0$. If we now redo the derivation of the static augmented Young-Laplace equation in §4.2.3, then there is an extra term $-\Pi := \frac{\delta E_W}{\delta \eta} = e(\eta)$ in the equation:

$$0 = -\gamma H + \gamma(1 - \cos \theta_s) \delta(\eta) - \lambda - \Pi(\eta). \quad (4.111)$$

Away from the interface, this simplifies to

$$\gamma H + \Pi(\eta) = -\lambda, \quad (\eta > 0) \quad (4.112)$$

and such an equation is what is usually referred to as an augmented Young-Laplace law in the literature. The function $\Pi(h)$ is for historical reasons called a *disjoining pressure*. Depending on its sign, the term *conjoining pressure* may also be used.

However, we cannot incorporate $\Pi = -e$ as specified in (4.109) into our continuous model, since $\Pi(h)$ diverges to $-\infty$ as $h \rightarrow 0$. Using, say, a Lennard-Jones potential instead of just van der Waals interactions does not help either because then the pressure diverges to $+\infty$ as $h \rightarrow 0$. The problem is that the derivation of e above was done using molecular potentials. However, in our continuous, sharp interface model we have essentially already taken the limit to zero of the molecular length scale, summarizing everything that happens at and beneath that length scale by surface tension.

A resolution is given in §4 in de Gennes et al. [36] for the simple scenario of a thin liquid film of height h covering the solid. In this case the energy per unit area of

wetted surface is

$$E(h) = \gamma_{SL} + \gamma_{LV} + P_W(h), \quad (4.113)$$

where $\frac{dP_W}{dh} = -\Pi_W$. In the limit $h \rightarrow 0$, we should recover the dry energy per unit area of the solid, i.e., $E(0) = \gamma_{SV}$. Hence P_W should satisfy

$$P_W(0) = \gamma_{SV} - (\gamma_{SL} + \gamma_{LV}) = S. \quad (4.114)$$

(We discussed the spreading parameter S in §4.2.1.) In the other direction, we demand $P_W(+\infty) = 0$, since for large h we should recover the pure surface tension model, since the long-range interactions become negligible. These limits for $P_W(0)$ and $P_W(+\infty)$ tell us how to sensibly modify the original diverging $e(h)$ in favor of one that is compatible with our macroscopic model. For example, if the signs of C and S are the same, we could take⁷

$$P_W(h) = \frac{S}{1 + \left(\frac{h}{h_0}\right)^2}. \quad (4.115)$$

This satisfies the correct boundary conditions, $P_W(0) = S$ and $P_W(+\infty) = 0$. Furthermore, we have

$$-\frac{d}{dh}P_W \approx \frac{2h_0^2 S}{h^3}, \quad \text{for } h \gg h_0. \quad (4.116)$$

So for h_0 suitably chosen, we can match this for large h with the formula (4.109) for $\Pi(h) = -e(h)$.

This provides an acceptable resolution for, say, the study of thin films in equilibrium, and a variety of specific forms of $\Pi(h)$ have been proposed in the literature, depending on the nature of the molecules involved.

⁷The functional form given here is just an example chosen to simplify exposition.

4.5.2 Disjoining pressure near triple junctions

The form $\Pi(h)$ for the disjoining pressure was derived under the simplified assumption of a thin film of uniform thickness. In general, Π depends nonlocally on the geometry of the problem and cannot accurately be approximated by a local function of the form $\Pi(h)$ near the triple junction.

The most advanced work to address this problem appears to be that of Wu and Wong [116]. (They build upon earlier work by Hocking [63] and Miller and Ruckenstein [81]. See also Yi and Wong [117] for an extension of these ideas to Lennard-Jones potentials.) They compute the van der Waals potential due to all possible molecular interactions between solid, liquid, and vapor molecules inside an infinite wedge of liquid on a planar solid, and arrive at a slope-dependent disjoining pressure $\Pi(h, h_x)$. All of this is derived for thin films and under a small-angle approximation.

Unfortunately, parts of their argument do not easily generalize. We would propose instead to study this issue along the following lines: Let us assume the molecular length scale has already been dealt with somehow, leaving us with bounded, decaying, additive interaction potentials $\Phi_{ij}(r)$, where r denotes distance and Φ_{ij} specifies energy per unit volume of material i and per unit volume of material j . Replacing for simplicity the vapor by a vacuum, the potential energy of the system is

$$E - E_0 = \int_{\Omega_L} \left(\int_{\Omega_S} \Phi_{SL}(|x - y|) dy + \int_{\Omega_L} \Phi_{LL}(|x - y|) dy \right) dx, \quad (4.117)$$

where we subtracted off the dry energy E_0 . With the help of the transport identity (4.7), we find that variation of the interface Γ by normal displacement $\delta\Gamma$ leads to

$$\delta E = \int_{\Gamma} \delta\Gamma(x) \left(\int_{\Omega_S} \Phi_{SL}(|x - y|) dy + 2 \int_{\Omega_L} \Phi_{LL}(|x - y|) dy \right) d\mathcal{H}^{n-1}(x), \quad (4.118)$$

and hence a nonlocal pressure term at the interface,

$$\frac{\delta E}{\delta \Gamma}(x) = \int_{\Omega_S} \Phi_{SL}(|x - y|) dy + 2 \int_{\Omega_L} \Phi_{LL}(|x - y|) dy. \quad (x \in \Gamma) \quad (4.119)$$

Simplified local models of disjoining pressure could then be derived from this expression using assumptions on the nature of Φ .

If we replace $\Phi_{ij}(r)$ by the rescaled version $\frac{1}{r_0^n} \Phi_{ij}(\frac{r}{r_0})$ and take the macroscopic limit $r_0 \rightarrow 0$, then (4.119) becomes (assuming sufficient decay of Φ_{ij})

$$\frac{\delta E}{\delta \Gamma}(x) = \begin{cases} \lambda_{LL}, & (x \in \Gamma \setminus \Sigma) \\ \frac{1}{2} \lambda_{SL} + \frac{\theta}{\pi} \lambda_{LL}, & (x \in \Sigma) \end{cases} \quad (4.120)$$

where

$$\lambda_{LL} = \int_{\mathbb{R}^n} \Phi_{LL}(|y|) dy, \quad \lambda_{SL} = \int_{\mathbb{R}^n} \Phi_{SL}(|y|) dy. \quad (4.121)$$

This indicates that the effect of disjoining pressure far away from the solid is just to modify the constant λ in (4.111), whereas close to the solid (and, in particular, near the triple junction), there is a dependence on the contact angle θ . For a planar solid, this suggests taking a disjoining potential of the form $\Pi(h, \theta)$ that interpolates continuously between these two limit cases.

4.5.3 Can disjoining pressure explain the Dirac measure?

We can now clarify a misconception found in some of the mathematics literature. Mellet [80] uses a singular perturbation approach of replacing the Heaviside function $\Theta(h)$ (see §4.2.2) by a diffuse approximation $Q(\frac{h}{h_0})$ and studying the limit $h_0 \rightarrow 0$. This then leads to a (small-angle) augmented Young-Laplace law of the form

$$\eta_{xx}(x) = \lambda + P(\eta(x)), \quad P(h) = \frac{1}{h_0} Q'\left(\frac{h}{h_0}\right). \quad (4.122)$$

As $h_0 \rightarrow 0$, we have $P(h) \rightarrow \delta(h)$, and so we recover the version (4.23) we derived earlier. Mathematically, this is a productive way of making sense of the Dirac mass and is in widespread use for variational free-boundary problems.

Citing earlier work of Bertsch, Giacomelli and Karali [9], however, Mellet then proceeds to vaguely claim that $P(h)$ may be identified with disjoining pressure. This is conceptually incorrect. The Dirac mass is a consequence of the surface tension model. As defined in the physics literature, disjoining pressure adds *additional* long-range interactions into the surface tension model. It does not modify the existing surface tension terms, and, in particular, it does not replace the Dirac mass. See the full augmented Young-Laplace law with disjoining pressure (4.111) above.

The correct physical interpretation of this mathematical technique is more akin to a sharp interface limit of a diffuse interface model. Understanding this in detail could be a fruitful research question.

4.6 Ideas and directions for future research

On the mathematics side, our understanding of the idealized model (4.63) is still extremely limited and all the usual PDE questions remain open. Examples are:

Question 4.6.1. *Are the equilibrium solutions stable? In particular, what happens when the contact angle and contact line are perturbed slightly?*

Question 4.6.2. *Do there exist solutions with moving contact lines and dynamic contact angles different from their equilibrium value?*

Question 4.6.3. *Do there always exist weak solutions? Are they unique?*

Question 4.6.4. *Is there a function space for which the Cauchy problem is locally well-posed in time?*

There are several difficulties to overcome before addressing these questions:

First, we need to decide how to deal with the Dirac mass. Our critique of the physical interpretation aside (see §4.5.3), we think some variant of Mellet’s singular perturbation approach is likely to be a good way to mathematically make sense of the Dirac measure in the idealized augmented Young-Laplace law (4.62). To decide which variant to employ, it may be helpful to first further study the physics literature and determine a suitable diffuse interface approximation whose sharp interface limit gives rise to (4.62). (In the literature, diffuse interface models have, in particular, been proposed for removing the viscous stress singularity. See, e.g., Pismen and Pomeau [90], Qian, Wang, and Sheng [92–94], and references therein.)

Second, given the complicated geometry of the problem, it is nontrivial to even come up with a good parametrization of the free interface and triple junction. For two-fluid interfaces, a number of methods have been proposed, though most deal only with irrotational fluids. We refer to Bardos and Lannes [7] for an overview. To handle also triple junctions, perhaps a more geometric approach like that of Depner, Garcke, and Kohsaka [39] would be more suitable. Their methods, however, would need to be adjusted from mean curvature flow and prescribed contact angle to fluid equations and dynamic contact angle.

Third, there is the question of what function spaces to consider. Presumably, we may expect classical regularity away from the triple junction. However, the regularity near the triple junction will necessarily be lower and could depend on the contact angle. (We refer to, e.g., Lacave, Miot, and Wang [74] and references therein for some discussion of fluids in fixed domains with corners.) A suitable notion of weak solution would need to be devised.

Finally, we remark that the question of uniqueness of solutions is particularly important. This could tell us how concerned we need to be about the exact choice of singular perturbation approach adopted. In other words, to what extent do the details of the molecular modeling affect the macroscopic limit?

On the physics side, we already mentioned some current limitations of the model in §4.1. Adding viscosity and allowing for freely moving solids, in particular, would make the model far more useful for real-world applications. Viscous models already are available in the literature (see §4.1.4 for references), but may not incorporate the Young stresses due to non-equilibrium contact angles correctly. Integrating the insights gained from the inviscid problem could lead to new and improved viscous models.

In closing, we think a research program as sketched in this section could be fruitful for both physics and mathematics. On the physics side, there is potential for new insight and conceptual clarification that could help settle controversies surrounding the modeling of liquid-vapor-solid systems. On the mathematics side, the system poses many interesting challenges, whose resolution is likely going to require techniques spanning several fields, such as mathematical fluid dynamics, geometric PDE's, PDE's in singular domains, and variational calculus.

Appendix A

Identities

For ease of reference, we collect here some definitions, conventions, and identities used throughout the dissertation. With the exception of §A.3, all of this is standard and may be found in many textbooks. We omit giving proofs or detailed references for those sections.

A.1 Differential identities

A.1.1 Vectors

For v, w differentiable vector fields and f, g differentiable scalar functions, we have

$$-\Delta v = \operatorname{curl} \operatorname{curl} v - \nabla \operatorname{div} v, \quad (\text{A.1})$$

$$\operatorname{div}(fv) = f \operatorname{div} v + v \cdot \nabla f, \quad (\text{A.2})$$

$$\operatorname{curl}(fv) = f \operatorname{curl} v + \nabla f \times v, \quad (\text{A.3})$$

$$\operatorname{div}(v \times w) = (\operatorname{curl} v) \cdot w - v \cdot (\operatorname{curl} w), \quad (\text{A.4})$$

$$\operatorname{curl}(v \times w) = \operatorname{div}(w \otimes v - v \otimes w), \quad (\text{A.5})$$

$$(\operatorname{curl} v) \times w = w \cdot \nabla v - (\nabla v)w = -((\nabla v) - (\nabla v)^\top)w, \quad (\text{A.6})$$

$$\operatorname{div}(v \otimes w) = \partial_{x_j}(v^j w) = v \cdot \nabla w + (\operatorname{div} v)w. \quad (\text{A.7})$$

A.1.2 Matrices

Given a differentiable one-parameter family of invertible matrices $A(t)$, we have

$$D_t \log |\det A| = \operatorname{Tr}(A^{-1} D_t A), \quad (\text{A.8})$$

$$D_t A^{-1} = -A^{-1} (D_t A) A^{-1}. \quad (\text{A.9})$$

Remark A.1.1. If $A(t)$ is not necessarily invertible, we still have

$$D_t(\det A) = \operatorname{Tr}(C^\top D_t A), \quad (\text{A.10})$$

where C is the cofactor matrix of A . (C^\top is also known as the adjugate matrix of A .)

For invertible $A(t)$ this reduces to (A.8) thanks to the formula $(\det A)A^{-1} = C^\top$.

A.1.3 Gauss-Green identities

Let $\Omega \subset \mathbb{R}^n$ be a sufficiently regular domain and ν the outwards pointing normal on $\partial\Omega$. Then for sufficiently regular u, v , we have (from Appendix C in Evans [51]),

$$\int_{\Omega} u_{x_i} dx = \int_{\partial\Omega} u\nu^i dS, \quad (\text{A.11})$$

$$\int_{\Omega} u_{x_i} v dx = - \int_{\Omega} uv_{x_i} dx + \int_{\partial\Omega} uv\nu^i dS, \quad (\text{A.12})$$

$$\int_{\Omega} \Delta u dx = \int_{\partial\Omega} \frac{\partial u}{\partial \nu} dS, \quad (\text{A.13})$$

$$\int_{\Omega} \nabla u \cdot \nabla v dx = - \int_{\Omega} u\Delta v dx + \int_{\partial\Omega} u \frac{\partial v}{\partial \nu} dS, \quad (\text{A.14})$$

$$\int_{\Omega} u\Delta v - v\Delta u dx = \int_{\partial\Omega} \left(u \frac{\partial v}{\partial \nu} - v \frac{\partial u}{\partial \nu} \right) dS, \quad (\text{A.15})$$

$$\int_{\Omega} \operatorname{div} u dx = \int_{\partial\Omega} u \cdot \nu dS. \quad (\text{A.16})$$

A.2 Fourier transform

We use the following normalization of the Fourier transform,

$$\mathcal{F}[f](\xi) = \hat{f}(\xi) = \int_{\mathbb{R}^n} e^{-ix \cdot \xi} f(x) dx. \quad (\text{A.17})$$

Under this convention, the following identities hold:

$$f(x) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} e^{ix \cdot \xi} \hat{f}(\xi) \, d\xi, \quad (\text{A.18})$$

$$\mathcal{F}[fg](\xi) = \frac{1}{(2\pi)^n} (\hat{f} * \hat{g})(\xi), \quad (\text{A.19})$$

$$\mathcal{F}[f * g](\xi) = \hat{f}(\xi) \hat{g}(\xi), \quad (\text{A.20})$$

$$\mathcal{F}[\partial_{x_i} f](\xi) = i\xi_i \hat{f}(\xi), \quad (\text{A.21})$$

$$\mathcal{F}[x_i f] = i\partial_{\xi_i} \hat{f}(\xi), \quad (\text{A.22})$$

$$\mathcal{F}[\hat{f}](\xi) = (2\pi)^n f(-\xi), \quad (\text{A.23})$$

$$\mathcal{F}[f(Ax)](\xi) = \frac{1}{|\det A|} \hat{f}(A^{-\top} \xi), \quad (\text{A.24})$$

$$\mathcal{F}[f(\lambda x)](\xi) = \lambda^{-n} \hat{f}(\lambda^{-1} \xi), \quad (\text{A.25})$$

$$\mathcal{F}[f(x + y)](\xi) = e^{i\xi \cdot y} \hat{f}(\xi). \quad (\text{A.26})$$

The Parseval and Plancherel identities are:

$$\int_{\mathbb{R}^n} |f(x)|^2 \, dx = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} |\hat{f}(\xi)|^2 \, d\xi, \quad (\text{A.27})$$

$$\int_{\mathbb{R}^n} f(x) \overline{g(x)} \, dx = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \hat{f}(\xi) \overline{\hat{g}(\xi)} \, d\xi. \quad (\text{A.28})$$

A.3 Inverse of matrix using Levi-Civita symbol

We first learned of Corollary A.3.4 below from unpublished lecture notes of Constantin [23], who aptly terms such calculations “index orgy.” Unfortunately, we were unable to find a published proof and so orchestrating the dirty deed seems to have fallen to us. The proof given here is a much expanded version of a sketch we found in an online forum [84].

Lemma A.3.1. *The determinant of an $n \times n$ matrix A may be written as*

$$\det A = \frac{1}{n!} \epsilon_{i_1 \dots i_n} \epsilon_{j_1 \dots j_n} A_{i_1 j_1} \cdots A_{i_n j_n}. \quad (\text{A.29})$$

Proof. We start from the well-known formula,

$$\det A = \epsilon_{j_1 \dots j_n} A_{1 j_1} \cdots A_{n j_n}. \quad (\text{A.30})$$

Since permuting the rows of a matrix just changes its determinant by the sign of the permutation, we may, for an arbitrary permutation $\sigma \in S_n$, rewrite (A.30) as

$$\det A = (\text{sgn } \sigma) \epsilon_{j_1 \dots j_n} A_{\sigma(1) j_1} \cdots A_{\sigma(n) j_n}. \quad (\text{A.31})$$

Since $\text{sgn } \sigma = \epsilon_{\sigma(1) \dots \sigma(n)}$, writing i_k for $\sigma(k)$ and averaging over all $\sigma \in S_n$ gives (A.29). ▮

Lemma A.3.2. *The cofactor matrix C of an $n \times n$ matrix A may be written as*

$$C_{ij} = \frac{1}{(n-1)!} \epsilon_{i i_2 \dots i_n} \epsilon_{j j_2 \dots j_n} A_{i_2 j_2} \cdots A_{i_n j_n}. \quad (\text{A.32})$$

Proof. With the help of Lemma A.3.1, we may write C_{11} as

$$C_{11} = \frac{1}{(n-1)!} \epsilon_{1 i_2 \dots i_n} \epsilon_{1 j_2 \dots j_n} A_{i_2 j_2} \cdots A_{i_n j_n}. \quad (\text{A.33})$$

For general i and j , let \tilde{A} be the matrix obtained from A by cyclically permuting the first i rows and the first j columns. Let us call the permutations σ^{-1} and τ^{-1} , respectively. Then the (i, j) -minor of A is equal to the $(1, 1)$ -minor of \tilde{A} and so by the definition of the cofactor matrix,

$$C_{ij} = (-1)^{i+j} \tilde{C}_{11} = \frac{1}{(n-1)!} \epsilon_{1 i'_2 \dots i'_n} \epsilon_{1 j'_2 \dots j'_n} \tilde{A}_{i'_2 j'_2} \cdots \tilde{A}_{i'_n j'_n}. \quad (\text{A.34})$$

Let us now apply σ to the indices $1, i'_2, \dots, i'_n$ and τ to the indices $1, j'_2, \dots, j'_n$. Since we have $i = \sigma(1)$ and $j = \tau(1)$, this gives, upon writing i_k for $\sigma(i'_k)$ and j_k for $\tau(j'_k)$,

$$C_{ij} = (\text{sgn } \sigma)(\text{sgn } \tau) \frac{(-1)^{i+j}}{(n-1)!} \epsilon_{ii_2 \dots i_n} \epsilon_{jj_2 \dots j_n} A_{i_2 j_2} \cdots A_{i_n j_n}. \quad (\text{A.35})$$

Since $\text{sgn } \sigma = (-1)^{i-1}$ and $\text{sgn } \tau = (-1)^{j-1}$, this simplifies to (A.32). ▮

Proposition A.3.3. *If A is an $n \times n$ invertible matrix, then*

$$A_{ij}^{-1} = \frac{1}{(n-1)! (\det A)} \epsilon_{jj_2 \dots j_n} \epsilon_{ii_2 \dots i_n} A_{j_2 i_2} \cdots A_{j_n i_n}. \quad (\text{A.36})$$

Proof. We start from the standard linear algebra identity for the inverse of a matrix A in terms of its cofactor matrix C ,

$$A_{ij}^{-1} = \frac{C_{ji}}{\det A}. \quad (\text{A.37})$$

Expanding C_{ji} using Lemma A.3.2 gives (A.36). ▮

Corollary A.3.4. *For an invertible 3×3 matrix A , we have*

$$A_{ij}^{-1} = \frac{1}{2(\det A)} \epsilon_{ikl} \epsilon_{j pq} A_{pk} A_{ql}. \quad (\text{A.38})$$

If $\det A = 1$, then

$$\epsilon_{irs} A_{ij}^{-1} = \epsilon_{j pq} A_{pr} A_{qs}, \quad (\text{A.39})$$

$$\epsilon_{jrs} A_{ij}^{-1} = \epsilon_{ikl} A_{rk} A_{sl}. \quad (\text{A.40})$$

Proof. Equation (A.38) is just a special case of Proposition (A.3.3). To obtain (A.39), set $\det A = 1$ and multiply by ϵ_{irs} . Using the identity

$$\epsilon_{irs} \epsilon_{ikl} = \delta_{rk} \delta_{sl} - \delta_{r\ell} \delta_{sk}, \quad (\text{A.41})$$

we find

$$\epsilon_{irs} A_{ij}^{-1} = \frac{1}{2} \epsilon_{j pq} (A_{pr} A_{qs} - A_{ps} A_{qr}). \quad (\text{A.42})$$

The final expression is obtained by observing that the second term is equal to the first:

$$- \epsilon_{j pq} A_{ps} A_{qr} = \epsilon_{j qp} A_{ps} A_{qr} = \epsilon_{j pq} A_{qs} A_{pr}. \quad (\text{A.43})$$

Here we first used $\epsilon_{j pq} = -\epsilon_{j qp}$ and then switched the roles of the summation variables p and q . The proof of (A.40) is similar. ▮

A.4 Spherical averages

Following Appendix A in Evans [51], let us introduce the notation

$$\alpha(n) = \frac{\pi^{n/2}}{\Gamma\left(\frac{n}{2} + 1\right)}, \quad (\text{volume of unit ball in } \mathbb{R}^n) \quad (\text{A.44})$$

$$n\alpha(n) = \frac{n\pi^{n/2}}{\Gamma\left(\frac{n}{2} + 1\right)}. \quad (\text{surface area of unit ball in } \mathbb{R}^n) \quad (\text{A.45})$$

For a function $u \in L^1_{\text{loc}}(\mathbb{R}^n)$, we denote spherical averages by

$$\bar{u}(x, r) = \int_{S_r(x)} u(y) \, dS(y). \quad (\text{A.46})$$

Using the spherical coarea formula

$$\int_{B_r(x)} u(y) \, dy = \int_0^r \int_{S_\rho(x)} u(y) \, dS(y) \, d\rho, \quad (\text{A.47})$$

we find the following relation between averages over balls and spheres,

$$\int_{B_r(x)} u(y) \, dy = n\alpha(n) \int_0^r \rho^{n-1} \bar{u}(x, \rho) \, d\rho, \quad (\text{A.48})$$

$$\int_{B_r(x)} u(y) \, dy = nr^{1-n} \int_0^r \rho^{n-1} \bar{u}(x, \rho) \, d\rho. \quad (\text{A.49})$$

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