

## Introduction

### 1.1 Connecting Statistical Mechanics to Vortex Problems

The “unreasonable effectiveness of mathematics in the physical sciences,” a phrase coined by Eugene Wigner<sup>1</sup>, is often mentioned as an exotic property of mathematics. It is an expression of the wonder that models constructed from purely theoretical considerations and reasoned out can predict real systems with great precision. A modern instance of this wonder is found in the writings of Subrahmanyan Chandrasekhar<sup>2</sup>: “In my entire scientific life, the most shattering experience has been the realization that an exact solution of Einstein’s equations of general relativity, discovered by Roy Kerr, provides the absolutely exact representation of untold numbers of massive black holes that populate the Universe.”

The relationship between mathematics and reality was remarked on even by the Pythagoreans, but was probably not seen as noteworthy to the point of becoming cliché in the earliest era of mechanics. A prediction of the orbits of planets and comets based on Newtonian mechanics and gravitation, for example, could be excellent; but since the laws describing gravitation came from observations of planetary orbits that should be expected. If observation and theory did not agree the theory would not have been used.

It is probably in the laws of gasses that this effectiveness became distracting. The dynamics of a gas can in theory be developed by a Newtonian system, provided one knows to represent it as particle interactions – atomic theory, not generally accepted until the 19th century and still worth debate until Brownian motion was explained – and one knows the laws by which

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<sup>1</sup> Eugene Paul Wigner, 1902 - 1995, introduced “parity” to quantum mechanics and discovered the curious properties of the strong nuclear force. [288]

<sup>2</sup> Subrahmanyan Chandrasekhar, 1910 - 1995, was a master of the mechanisms of stars, and predicted the existence of black holes from 1930. [288]

they interact – quantum theory – and one can handle the staggering number of variables needed. These were formidable challenges.

Attempted instead were models based on simple theoretical constraints and few details. Assuming simply that gas was made of particles and these particles moved independently provides the ideal gas law which had been noted and publicized by Robert Boyle, 1627-1691, and Jacques-Alexandre-César Charles, 1746-1823, and others centuries earlier. For such a simple model matching the general behavior of real gases was a surprise. Adding the assumptions atoms had a minimum size and some interaction allowed Johannes Diderik van der Waals, 1837-1923, to offer in 1873 a correction to the ideal gas law and an even better match to observation [25] [64].

Erwin Schrödinger<sup>3</sup> [389], in his compelling 1944 essay “What is life?”, presented a famous argument for the apparent exactness and determinateness of macroscopic laws which are nonetheless based on physical laws of a statistical nature for the detailed components of a system. He argued the macroscopic law of bulk diffusion (which is clearly deterministic) is based on the completely and purely statistical phenomenon of random walks at the microstate level. The random walk of molecules is not only statistical in nature but it is also completely symmetrical: a molecule takes a jump to the right or left in say a one-dimensional model with equal probability. Yet its consequence at the macroscopic level is clearly asymmetric because the law of bulk diffusion has a clear direction: from high concentration to low concentration.

This is our textbook’s inspiration. A simple model of fluid flow will be made from theoretical considerations. The model will be studied through several alternative strategies and adjusted to make it more natural.

We are more concerned with statistical equilibria than with dynamical equilibria. A dynamical equilibrium requires the components of a state to be in a spatially rigid and temporally stationary relationship with each other. This is too restrictive for the problems in this book. Statistical equilibria have stationary macroscopic variables which offer vastly more degrees of freedom in the fine details of the state. A rule of thumb for the appearance of seemingly exact macroscopic laws is that the macroscopic system must have large enough number  $N$  of microscopic components in order for the fluctuations of size  $1/\sqrt{N}$  in the macroscopic variable to be small.

This book is our attempt to connect two main topics of asymptotic states in vortex flows and equilibrium statistical mechanics. While fully developed turbulence in a damped driven flow is a non-equilibrium phenomena, many powerful arguments (by Kolmogorov [223], [224], Oboukhov [330]) have been presented, asserting that for certain inertial ranges in the power spectrum of driven viscous flows, the methods of equilibrium statistical mechanics can be adopted. We will avoid such arguments and treat the phenomena of isolated

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<sup>3</sup> Erwin Rudolf Josef Alexander Schrödinger, 1887 - 1961, got the inspiration for the wave form of quantum mechanics from a student’s suggestion at a seminar Schrödinger gave on the electron theory of Louis de Broglie, 1892 - 1987. [288]

inviscid fluid turbulence within the context of equilibrium statistical mechanics.

The concept of negative temperature was introduced into vortex dynamics by Lars Onsager. Vortical systems in two dimensions and in 2.5 dimensions (which we will describe) support negative temperatures at high kinetic energies where the thermal equilibria are characterized by highly organized large-scale coherent structures. Thus, besides the standard application of Planck's theorem to thermal systems at positive temperatures, where one minimizes the free energy, we are also interested in vortex problems at negative temperatures, where one maximizes the free energy to obtain stable statistical equilibria.

In addition to the first common theme of Monte Carlo simulations of organized and of turbulent fluid flows in this book, a second theme is the relationship between dynamics and equilibrium statistical mechanics: the **extremals** (maxima and minima) of the energy determine the equilibria, but the extremals of the free energy give us the most probable states of the equilibrium statistics.

Vortex statistics has many noteworthy examples where the range of temperatures is quite large, over which extremals of the free energy are close to the corresponding extremals of the internal energy. We will explore the physical reasons for these interesting phenomena in several archetypical examples of vortex dynamics. The most important of these problems are the crystalline or polyhedral equilibria of  $N$  point vortices on the sphere, the thermal equilibria of the Onsager vortex gas on the unbounded plane with respect to dynamical equilibria of the rotating two-dimensional Euler equations, and the thermal equilibria at negative temperatures of barotropic vortex dynamics on a rotating sphere.

In the first case,  $N$  similar point vortices on a sphere, the Monte Carlo simulator running at positive temperatures achieves thermal equilibria which are very close to the polyhedral relative equilibria of the dynamical equations. These polyhedral crystalline states have extremely regular and uniform spatial separations, and thus minimize the interaction energy though without simultaneously maximizing the entropy. This situation provides one of the canonical ways in which minimizers of the free energy are close to the dynamical equilibria for a range of positive temperatures.

The second case concerns the unbounded Onsager point vortex gas, whose thermal equilibria of uniform vorticity distributions in a disk are close to the dynamic equilibria of the rotating two-dimensional Euler equations over a wide range of positive temperatures. The physical reason in this case is the same as the first, that is, the free energy minimizers are given by vortex states which minimize the internal energy.

The physical reason for the third case is that free energy maximizers corresponding to stable thermal equilibria at negative temperatures are achieved by vortex states with very low entropy. Unlike standard thermodynamic applications where entropy is maximized, the solid-body rotation flow states have

the minimum entropy and maximum kinetic energy over allowed flow states with the same relative enstrophy.

A non-extensive continuum limit is allowed for two-dimensional flows in a fixed finite domain. The canonical examples for such flow domains are the fixed bounded regions on the plane, and finite but boundary-less domains such as the surface of the sphere or of the torus. Finite boundary-less domains are computationally convenient because boundary conditions are often complex. And among finite, boundary-less domains the problem of flows on the sphere is more important than flows on more topologically complex surfaces because of their applicability to atmospheric sciences, to which we will return.

Our principal focus is the of inviscid fluids. We justify this choice – which seems to exclude most of the fluids of the real world – on several grounds. The first is that often the viscosity of a fluid is a minor effect, and these slightly viscous fluids can be modelled by inviscid fluids, where we represent the interior of the flow by a fluid without viscosity, and add boundary layers in the regions where viscosity becomes relatively significant. More, even if we want to consider viscous fluids, we can still represent an interesting aspect of them – the non-linear convective aspects of the flows – by treating this portion of the flow as an inviscid fluid.

And furthermore much of what we can study in the thermal equilibrium of inviscid two-dimensional vortex dynamics (such as the minimizers of free energy functions) can be extended naturally to the ground states of augmented energy functionals, or to the steady states of two-dimensional Euler equations. These in turn are related, by the Principle of Selective Decay, also termed the Principle of Minimum Enstrophy, to the asymptotic flows of the decaying two-dimensional Navier<sup>4</sup>-Stokes<sup>5</sup> equations. The minimizers of the Dirichlet quotient, the ratio of enstrophy to energy, corresponds to the inviscid steady states we explicitly study [26].

## 1.2 Euler’s Equation for Inviscid Fluid Flow

To write Leonhard Euler’s<sup>6</sup> equation for fluid flow, we begin with the fluid velocity. Letting  $\mathbf{u}$  stand for the velocity and  $\rho$  the density of the fluid, we

<sup>4</sup> Claude Louis Marie Henri Navier, 1785 - 1836, was in his day famous as a builder of bridges. He developed the first theory of suspension bridges, which had previously been empirical affairs. [288]

<sup>5</sup> George Gabriel Stokes, 1819 - 1903, besides the theory of fluid flow and the theorem about the integrals over surfaces, provided the first theory and the name for fluorescence. [288]

<sup>6</sup> It is almost impossible to overstate the contributions of Leonhard Euler, 1707 - 1783. The scope is suggested by the fact after his death it required fifty years to complete the publication of the backlog of his papers. He is credited with the modern uses of the symbols  $e$ ,  $i$ ,  $\pi$ ,  $\Sigma$ , the finite differences  $\Delta t$  and  $\Delta^2 t$ , and  $f(x)$  as a general symbol for a function. [288]

choose some fluid properties. We want the fluid to be incompressible, inviscid, and to experience no outside forces.

The obviously important properties of the fluid are the density at a time  $t$  and a point  $\mathbf{r}$  – call that  $\rho(t, \mathbf{r})$  – and the velocity, again a function of time and position. Call that  $\mathbf{u}(t, \mathbf{r})$ . We will build on three properties [88].

First is the conservation of mass. Suppose the fluid is incompressible, which is nearly correct for interesting fluids such as water at ordinary temperatures and pressures. Incompressibility demands a divergence of zero:

$$\nabla \cdot \mathbf{u} = 0 \quad (1.1)$$

A nonzero divergence over some region  $A$  corresponds to either a net loss or net gain of mass, so the fluid density is changing and the fluid is either expanding or compressing.

The next property is the conservation of momentum. The momentum inside region  $A$ , the total of mass times velocity, will be

$$\mathbf{p} = \int_A \rho \mathbf{u} dV \quad (1.2)$$

(with  $dV$  the differential volume within the region  $A$ ). So the rate of change of the momentum in time will be

$$\frac{\partial}{\partial t} \mathbf{p} = \int_A \frac{\partial}{\partial t} (\rho \mathbf{u}) dV \quad (1.3)$$

Without external pressure, or gravity, or viscosity or intermolecular forces the momentum over the region  $A$  cannot change on the interior. Only on the surface can momentum enter or exit  $A$ :

$$\frac{\partial}{\partial t} \mathbf{p} = \int_{\partial A} (\rho \mathbf{u}) \mathbf{u} \cdot d\mathbf{S} \quad (1.4)$$

with  $\partial A$  the surface of  $A$  and  $d\mathbf{S}$  the differential element of area for that surface. Using Green's theorem<sup>7</sup>, the integral is

$$\frac{\partial}{\partial t} \mathbf{p} = - \int_A \rho (\mathbf{u} \cdot \nabla) \mathbf{v} dV \quad (1.5)$$

If there is a force, which we will generalize by calling the pressure and denoting it as  $P(\mathbf{r}, r)$ , then momentum may enter or exit the region  $A$ , but again only through its surface. Even more particularly only the component of the force which is parallel to the outward unit normal vector  $\hat{n}$  can affect the fluid, in or out. So the change in the momentum of the fluid caused by the pressure term  $P$ , is

<sup>7</sup> George Green, 1793 - 1841, besides his theorem connecting surface integrals to volume integrals, is credited with introducing the term “potential function” in the way we use it today. [288]

$$\frac{\partial}{\partial t} \mathbf{p} = \int_{\partial A} P \hat{n} d\mathbf{S} \quad (1.6)$$

$$= - \int_A \nabla P d\mathbf{V} \quad (1.7)$$

using again Green's theorem.

As we may have momentum gained or lost through either the fluid flow or through the pressure we add the two terms:

$$\frac{\partial}{\partial t} \mathbf{p} = - \int_A \rho (\mathbf{u} \cdot \nabla) \mathbf{v} dV - \int_A \nabla P d\mathbf{V} \quad (1.8)$$

Between equations 1.3 and 1.8 we have two representations of the derivative of momentum with respect to time. Setting them equal

$$\frac{\partial}{\partial t} \mathbf{p} = \int_A \frac{\partial}{\partial t} (\rho \mathbf{u}) dV = \int_A \rho (\mathbf{u} \cdot \nabla) \mathbf{u} dV - \int_A \nabla P d\mathbf{V} \quad (1.9)$$

for all regions  $A$ . For the middle and right half of equation 1.9 to be equal independently of  $A$  requires the integrands be equal<sup>8</sup>:

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) = -\rho (\mathbf{u} \cdot \nabla) \mathbf{u} - \nabla P \quad (1.10)$$

which is Euler's equation for inviscid, incompressible, unforced fluid flow. Assuming incompressibility makes  $\rho$  constant in time, so we may divide it out.

Having introduced the pressure, we will proceed now to drop it for nearly the entirety of the book, as we will find abundant interesting material even before adding pressure to the system. In this form and confined to one spatial dimension is often known as Burgers' equation<sup>9</sup>, though we will keep a bit more freedom in space:

$$\frac{\partial}{\partial t} \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = 0 \quad (1.11)$$

Up to this point we have considered only two important physical properties. The third we will add in order to convert this equation into a form more suitable for treatment as a particle problem, which we will do in chapter 6. There we will also change our attention from the velocity of the fluid into the vorticity, that is, the curl of the velocity. This combination lets us recast the flow of an inviscid fluid as a statistical mechanics problem.

<sup>8</sup> Strictly speaking, they must be equal "almost everywhere" – the set of points that are exceptions must have measure zero. For example, finitely many exceptions are allowed.

<sup>9</sup> Johannes Martinus Burgers, 1895 - 1981. Burgers is known also for the Burgers dislocation, a method of describing the irregularities in a crystal. He was also expert on the study of polymers, and a sort of viscoelastic material is named for him.

Our roots in statistical mechanics and thermodynamics suggests a question: is there a temperature to a vortex dynamical system? Statistical mechanics defines the temperature of any system to be the derivative of energy with respect to the entropy. In the kinetic theory of gases this equals the physical heat. Although there is no physical heat in this problem, there is an energy and there is an entropy; therefore, it has a temperature.

This extension of temperature is not unique. Most physical models have an energy. The entropy of a model can be given through information-theoretical methods – as long as a system can contain information, it has an entropy. Therefore the idea of temperature can be applied to systems that have no resemblance at all to the gas particles the idea began with.

One fascinating consequence is that vortex systems can have a negative temperature. There are configurations for which adding more energy will decrease the entropy of the system. The derivative is then negative and the temperature is therefore less than zero. More remarkably these negative temperature states are extremely high-energy ones. These negative temperature states will receive considerable attention. (Vortex dynamics is not the only context in which negative temperatures arise. They can develop in systems in which a maximum possible energy exists. One noteworthy example is in describing the states of a laser.)

We will need to simplify our problem to be able to apply statistical mechanics methods to it. We want a large but finite number of particles or lattice sites which obey some interaction law. Our interests will lead us to rewrite the Euler equation from several perspectives. In one we will describe the vorticity of the fluid as a set of discrete “charged” particles which are free to move. In another we will construct a piecewise-continuous approximation to the vorticity based around a fixed set of mesh sites and allow the value of the function on these pieces to vary.

If we are interested in the “vortex gas” problem, placing a set of vortices of fixed strength and allowing them to move, then we could write it as a dynamical systems problem, with a Hamiltonian<sup>10</sup>, a representation using the form of classical mechanics. With that we can use tools such as the Monte Carlo Metropolis Rule to explore this space and study the equilibrium statistical mechanics.

Unfortunately the Monte Carlo study of the vortex gas problem does not well handle vortices of positive and negative strengths mixed together. The Metropolis-Hastings rule will tend to make vortices of opposite sign cluster together. Similarly negative temperatures cannot be meaningfully applied; trying simply causes all like-signed vortices to cluster together. But as long as

<sup>10</sup> These functions were introduced by Sir William Rowan Hamilton, 1805 - 1865, and have become a fundamental approach to dynamical systems. Hamilton also discovered quaternions, famously carving the inspired equation  $i^2 = j^2 = k^2 = ijk = -1$  into the stones of the Brougham Bridge. [288]

we are interested in a single sign and positive temperatures interesting work may be done.

In the lattice problem (our mesh sites may not be the regularly organized rows and columns of a proper lattice, but it is a fixed set of sites) we approximate the continuous vorticity field by a piecewise-continuous approximation. Changes in the fluid flow are represented by changes in the relative strengths of lattice sites. This approach resembles strongly a finite-elements study. This approach also well handles both positive and negative vorticities, and both positive and negative temperatures are meaningfully studied.

There is also a useful approach not based on points and site vorticities at all. Anyone who has studied enough differential equations has encountered Fourier decompositions of problems – supposing that the solution to a differential equation is the sum of sine and cosines of several periods, and finding the relative amplitudes of the different components. This sort of approach is called the spectral method. The analogy to identifying the components of a material by the intensities at different frequencies of the spectrum of light that has passed through the material is plain.

Through these approaches, we plan to show how analytical and computational mathematics complement one another. Analytic study of fluid flow provides a problem well-suited to numerical study. Numerical experiments will improve the understanding of old and will inspire new analysis. In combination we make both approaches stronger.

To end this introduction, we remember that the astronomical and cosmological examples alluded to above have a different scale of predictability than fluid phenomena such as flow turbulence and the weather. Astronomers have predicted solar and lunar eclipses to the second for centuries. But the weather cannot even now be predicted with anywhere near the same scale of accuracy. The accuracy in astronomical prediction is largely dependent on the exactness of the initial data at an earlier epoch. The inaccuracies in weather prediction persists in spite of greatly improved meteorological methods and instruments for measuring the state of an atmosphere. These are two very different realms of applied and computational mathematics, underscoring the theoretical and technical difficulties of the latter.