ON THE GEOMETRICAL AND STATISTICAL PROPERTIES OF DYNAMICAL SYSTEMS: THEORY AND APPLICATIONS

Thesis by

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In Partial Fulfillment of the Requirements

for the degree of

Doctor of Philosophy

California Institute of Technology

Pasadena, California

1994

(Submitted May 16, 1994)

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I dedicate this thesis to my family:
Ana Marija, Jadranka, Nataša and Ante

Acknowledgements

I am grateful to my advisor, professor Stephen Wiggins, for support and guidance over the last four years. His insistence on the clarity of goals helped immensely in shaping this thesis. I would also like to thank professors Anthony Leonard and John Brady for their help and encouragement. Conversations with them were crucial during the work on parts of the thesis. Professsor Jerrold Marsden listened to me explaining the material from papers consisting of the thesis, and offered his insight and encouragement. I am thankful for that.

There are many people at Caltech with whom I held lengthy conversations about parts of my work, and who helped in channeling and streamlining my ideas. I would like to thank all of them. I am specially thankful to György Haller, with whom I shared the good times in the same office for three years, and from whom I learned a lot. Professors Zoran Mrša and Luka Sopta, at the University of Rijeka, Croatia, introduced me to the wonderful world of science. I shall always be grateful.

I would like to thank my dad, Ante, for constantly overestimating my capabilities, and my mom, Nataša, for bringing me up so independent-minded. Finally, I would like to thank my wife, Jadranka, for:

- Persistently believing in me, even when I do not deserve it.
- Always seeing the sun behind the clouds.
- Giving me Ana Marija.

Abstract

We develop analytical methods for studying *particle paths* in a class of three-dimensional incompressible fluid flows. We study three-dimensional *volume preserving* vector fields that are invariant under the action of a one-parameter symmetry group whose infinitesimal generator is autonomous and volume preserving. We show that there exists a coordinate system in which the vector field assumes a simple form. In particular, the evolution of two of the coordinates is governed by a time-dependent, one-degree-of-freedom Hamiltonian system with the evolution of the remaining coordinate being governed by a first-order differential equation that depends only on the other two coordinates and time. The new coordinates depend only on the symmetry group of the vector field. Therefore they are *field independent*. The coordinate transformation is constructive. If the vector field is time independent, then it posseses an integral of motion. Moreover, we show that the system can be further reduced to *action-angle-angle* coordinates. These are analogous to the familiar action-angle variables from Hamiltonian mechanics and are quite useful for perturbative studies of the class of sytems we consider. All of the above is useful in framing a perturbative setting for analyses of chaotic, volume-preserving vector fields. In particular, explicit expressions for the transformation to action-angle-angle coordinates is given. This leads to the proof of a KAM-type theorem for volume-preserving vector fields admitting a volume-preserving group of symmetries using the KAM-type result for three-dimensional maps. The proof of the persistence of finite cylinders, relevant in fluid dynamical applications is provided. Also, a Melnikov-type theory is developed, allowing for the prediction of parameter values for which the vector field possesses chaotic behavior.We discuss the integrability of the class of flows considered, and draw an analogy with Clebsch variables in fluid mechanics.

Recently there has been a lot of numerical and experimental work on three dimensional, volume-preserving, chaotic fluid flows. The above theory can explain qualitative, geometric, features observed in these flows. But, the quantities of interest in those investigations are often of statistical nature. Furthermore, in most of these investigations, the flows considered are non-ergodic, with a rich structure of the phase space.

The theory of statistical properties of dynamical systems developed in this thesis is based on the Birkhoff's ergodic theorem, ergodic partition, and methods of probability theory. It is shown that, in the case when the system is not ergodic, the only quantities necessary to describe the limiting behavior (when the time or the number of iterations $\to \infty$) behavior of these systems are the time averages. Using this observation, necessary and sufficient condition are derived for the ubiquitous t^2 asymptotic behavior of the dispersion. A link is obtained between probability distributions of sum functions and the ergodic partition, which is used to explain the phenomenon of patchiness in fluid flows. The problem of first passage times is analyzed, and some conjectures inspired by numerical experiments proved. The theory is developed for both maps and flows, and has applications in a variety of problems related to the statistical description of chaotic motion in physical systems. Two specific applications are diffusion in two-dimensional, area-preserving maps, and shear dispersion in fluid flows. An obvious question arising from this part of the work was: how can one calculate the ergodic partition, which is an important ingredient of the statistical part of the theory. In ergodic theory, two ways of presentation of the ergodic partition exist. These two approaches can be successfully joined to provide a simple constructive algorithm for the construction of the ergodic partition. The ergodic partition of the compact metric space A, under the dynamics of a continuous automorphism T, is shown to be the *product* of measurable partitions of the space induced by the time averages of a dense, countable subset of the set of all continuous functions on A. As a consequence of this, closed ergodic components are shown to be uniquely ergodic. Also, a connection can be made between the ergodic partitions induced by the time averages of measurable, bounded functions, and the ergodic partition. Besides giving a method of constructing the ergodic partition, this work might give rise to numerical algorithms for computation of the ergodic partition.

All of the above theory is applied to the ideal, incompressible fluid flow induced by a helical vortex filament in an axisymmetric time-dependent strain field. It is shown that the helical filament stays helical for all times. Using symmetry concepts we transform the velocity field to a particularly simple form that is convenient for the use of perturbation methods. We analyze bifurcations and the structure of particle paths in the unperturbed velocity field (no strain). The underlying geometrical structures in the unperturbed problem are cylinders and two dimensional separatrices. Away from separatrices we transform the system into coordinates that enable us to use KAM theory to show the persistence of infinite cylinders in the perturbed flow. Further, we analyze the unperturbed motion on separating manifolds, and present a three-dimensional Melnikov theory for the analysis of the motion near the separatrices under perturbation. We use this analysis to propose that chaoticity of the motion provides a physical mechanism for the Ranque effect for swirling flows in pipes. Finally, we analyse the problem of *shear dispersion* of passive scalars in our flow. A natural question related to the above considerations of statistics of deterministic dynamical systems is how do they affect the statistical properties of the system when noise is added. This leads to a study of the convection-diffusion equation. We establish conditions for the *maximal*, Pe^2 behavior of the effective diffusivity in time periodic incompressible velocity fields for both the $Pe \to \infty$ and $Pe \to 0$ limits. Using ergodic theory, these conditions can be interpreted in terms of the Lagrangian time averages of the velocity. We reinterpret the maximal effective diffusivity conditions in terms of a Poincaré map of a velocity field. The connection between the Pe^2 asymptotic behavior of the effective diffusivity and t^2 asymptotic dispersion of the nondiffusive tracer is established. Several examples are analyzed: we relate the existence of the *accelerator modes* in a flow with Pe^2 effective diffusivity, and show how maximal effective diffusivity can appear as a result of a time-dependent perturbation of a steady *cellular velocity field.* Also, three-dimensional, symmetric, time-dependent *duct velocity fields* are analyzed, and the mechanism for effective diffusivity with Peclet number dependence different from Pe^2 in time-dependent flows is established, thus generalizing the Taylor-Aris dispersion theory.

Contents

Chapter 1

Introduction

Each chapter of the thesis has a specific introduction to a subject matter treated in it, with the discussion of previous work provided. In this, general, introduction we shall attempt to give a birds eye view on the thesis, with particular attention to connections between the chapters.

The work on this thesis project started off as an attempt to generalize some of the concepts developed over the years for the analysis of two-dimensional, area-preserving maps and two-dimensional, time-dependent flows to three-dimensional, volume-preserving maps and three-dimensional, volume-preserving, time-independent and time-dependent flows, with a view towards applications in fluid dynamics. In particular, two-dimensional area preserving maps and flows have a symplectic structure, which allows for the use of standard tools of Hamiltonian mechanics: action-angle coordinates, Melnikov theory and KAM theory. In a three-dimensional, volume-preserving setting, there is generally no general Hamiltonian structure (where we used general in the sense: one and the same structure for any volume-preserving flow or map that we pick). Therefore, one has to look at the specifics of volume-preserving dynamics. This has been done, for flows, in Chapter 2 of this thesis, which is based on the article which appeared in the *Journal* *of Nonlinear Science* [17]. Previous studies of volume-preserving dynamics concentrated mostly on steady fluid flows ([2], [10], and the references in Chapter 2). Notably, all of these studies deal with flows which are *not* solutions of a Navier-Stokes equation, but are Stokes flows, or solutions of linearized steady Rayleigh-Bénard convection. The nondimensionalized Navier-Stokes equation, in the vorticity formulation reads

$$\frac{\partial \omega}{\partial t} + [\mathbf{v}, \omega] = \frac{1}{Re} \Delta \omega, \tag{1.0.1}$$

where $[\mathbf{v}, \omega]$ is the Lie Bracket of the velocity $\mathbf{v}$ and vorticity ω, and $Re = Vl/\nu$, with V being the characteristic velocity and l the characteristic lengthscale. Arnold [1] proved that steady Euler flows, governed by

$$[\mathbf{v}, \omega] = 0, \tag{1.0.2}$$

are typically integrable. In this sense, chaoticity in three-dimensional flows is typically induced by the viscosity and time-dependence. Suppose $\mathbf{v}$ is steady. Then, away from the boundaries we might expand the velocity field as $\mathbf{v}^E + \frac{1}{Re}\mathbf{v}^p$, where $\mathbf{v}^E$ satisfies (1.0.2). Therefore, in the regime in which the Reynolds number is not small, the splitting of separating manifolds which causes chaos should be of the order $1/Re$ (this can be shown using Melnikov theory). An argument similar to this has been advanced, with details provided, in [11]. Therefore, in this hypothetic setting, time dependence is the only effect which can induce chaotic behavior on spatial scales larger than $\mathcal{O}(1/Re)$.

The above discussion can justify our concentration in Chapter 2 on the analysis of three-dimensional, time-dependent perturbations of steady vector fields, as our applications are mostly to fluid dynamics. Moreover, the evolution equations for magnetohydrodynamic and rotational fluid dynamic flows accept similar formulation.

Further relation to needs of specific fluid dynamical problems in Chapter 2 lies in our treatment of action-angle type variables and KAM-type theory for volume preserving vector fields. Discussions of action-angle variables nad KAM-type theories typically feature invariant tori as underlying geometrical structures. But, it is often the case in fluid dynamical problems that the underlying structures are cylinders ([6], [3]). In Chapter 2 we develop action-angle type coordinates for three-dimensional flows which are defined both in the case when the underlying geometrical structures are cylinders and tori. We also prove a result on the persistence of finite cylinders, based on the KAM theorem for the persistence of invariant tori.

All of the examples provided in Chapter 2 are fluid dynamical, and, to the best of our knowledge, new. The first two of these were obtained by searching for polynomial vector fields whose vorticity generates a symmetry group (i.e., by solving for the coefficients of a polynomial vector field in the Lie bracket equation (1.0.2)). The third example is a superposition of Hill's spherical vortex and a line vortex at the z axis.

Three-dimensional flows in which the prominent geometrical structures are invariant cylinders, the geometry of which was studied in Chapter 2, initiated studies of statistical properties of such flows leading to the results presented in Chapter 3, which is based on an article submitted to *Physica* D. The basic sources for numerical and experimental data on these flows are [3], [5] and [6]. It turned out that the mathematical framework developed in order to understand the phenomena of dispersion, particle distributions and first passage times accepts a generalization to a wide class of dynamical systems with an invariant measure. It also appeared that two-dimensional, spatially periodic flows and maps can be treated with the tools developed in Chapter 3. Two different applications of these are given in [18], [19]. These papers discuss the infinite-time asymptotics of dispersion in nonergodic flows and maps. Part of the formalism based on the methods of the probability theory, used to develop expressions for finite-time particle distributions, and finite-length first passage times developed in Chapter 3 still awaits applications. One of the important concepts used for the analysis of statistical properties of nonergodic maps and flows is that of the ergodic partition. Proofs of ergodic partition theorems existing in the literature do not provide a simple (and possibly numerically implementable) algorithm for constructing the ergodic partition. We give such a proof in Chapter 4, which is based on an article submitted to *Ergodic Theory and Dynamical Systems.* Chapter 5 contains applications of the theory developed in Chapters 2-4 to a flow induced by a helical vortex filament in an axially symmetric strain field.

Having developed the statistical theory for maps and flows, a natural question which arises is: what happens if we include some type of noise in our description of a physical system. Again motivated by fluid mechanics, the answer to this question in the context of the space and time periodic flows, and three-dimensional flows discussed in Chapter 2, is provided in Chapter 6.

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Chapter 2

On the integrability and perturbation of three-dimensional vector fields with symmetry

2.1 Introduction

For two-dimensional, incompressible time-periodic fluid flows the equations for fluid particle paths are given by

$$
\begin{aligned}
\dot{x} &= \frac{\partial \psi}{\partial y}(x, y, t), \\
\dot{y} &= -\frac{\partial \psi}{\partial x}(x, y, t),
\end{aligned}
$$

where $\psi(x, y, t)$ is the stream function periodic in t. From the dynamical systems viewpoint, these are Hamilton's equations where $\psi(x, y, t)$ is the Hamiltonian function and the phase space of this dynamical system is actually the physical space where the fluid flows. Through time periodicity the study of these equations can be reduced to the study of a two-dimensional symplectic Poincaré map and once the problem has been cast in this setting a variety of techniques and ideas from dynamical systems theory can be applied for the purpose of studying fluid transport and mixing issues. For example, KAM tori represent barriers to fluid transport and mixing, chaotic dynamics should act to enhance mixing, and invariant manifolds, such as the stable and unstable manifolds of hyperbolic periodic points, are manifested as "organized structures" in the fluid flow. See Ottino [1989] and volume 3 (1991), number 5 of the Physics of Fluids A for recent reviews.

Over the past 10 years there has been much work in the fluid mechanics community in applying these types of dynamical systems techniques to the study of fluid transport and mixing. However, most of the theoretical work has been in situations where the study of the flow kinematics is reduced to the study of a two-dimensional symplectic map.

The purpose of this chapter is to develop a framework and analytical methods for studying fluid particle paths and global structures in a class of three-dimensional, time-dependent flows. Global perturbation methods, such as KAM methods, Melnikov's method, and averaging techniques rely on a coordinate description of the underlying unperturbed phase space structure for their development. In particular, KAM theory uses action-angle variables, Melnikov's method uses "homoclinic coordinates," and averaging methods use coordinates that decompose the motion into "fast" and "slow" motions. Finding such coordinates in the two-dimensional case is particularly easy as all trajectories are given by the level sets of the Hamiltonian (streamfunction), for steady flows. However for three-dimensional flows the lack of a canonical Hamiltonian structure poses some difficulties in developing similar analytical techniques. In the past few years there has been some work dealing with Hamiltonian formulations for three-dimensional, autonomous, divergence-free vector fields by Cary and Littlejohn [1982] and Janaki and Ghosh [1987]. The work of Cary and Littlejohn is the most complete work along these lines. Starting from a variational principle for divergence-free vector fields, under the condition that the vector field does not vanish at any point, they are able to transform the system into a noncanonical Hamiltonian form where the reduced system is a one-degree-of-freedom Hamiltonian system in noncanonical coordinates. The transformation to noncanonical Hamiltonian form is dependent upon the nature of the specific vector field. Our work differs from that of Cary and Littlejohn in that our coordinate transformations depend only on the symmetry of the vector field, not its specific analytical form. Moreover, the vector field being transformed need not be autonomous.

The main purpose behind developing coordinates that reveal the global structure of the vector field is to develop analytical methods for studying transport issues. There has been recent work along these lines by MacKay [1992] who introduces the idea of *surfaces of locally minimal flux* and the *skeleton* for three dimensional volume preserving vector fields. Feingold, Kadanoff and Piro [1988] perform a numerical study of a model three-dimensional volume preserving map that highly suggests the presence of two-dimensional "KAM-like" tori. Recently there has been much theoretical work along these lines which we discuss in Section 5.

In this chapter we begin in Section 2 by developing coordinates for describing the velocity field that facilitates global analyses similar to those in the two-dimensional setting. In particular, we consider three-dimensional fluid flows that are invariant under the action of a spatial volume-preserving symmetry group. We show that the velocity field can be transformed to the form where two components have the canonical form of a one-degree-of-freedom Hamiltonian system and the third component depends only on the first two variables. Hence the velocity field is integrable in the sense that equations for the particle trajectories can be obtained by quadrature. Under certain non-degeneracy assumptions in Section 3 we show that the vector field can be further transformed to *action-angle-angle* variables. In Section 4 we discuss the relationship of our work with the work of Arnold on the topology of steady, volume-preserving vector fields as well as the relationship with a description of Euler flows in terms of Clebsch variables. In Section 5 we show how the action-angle-angle representation can be used to apply new "KAM-like" results for volume preserving maps and in Section 6 we show how our coordinates allow for the use of a generalized type of Melnikov method for three-dimensional flows. In Section 7 we give three examples that illustrate our methods.

2.2 Coordinates for three-dimensional, time-dependent vector fields with symmetry

2.2.1 General background from Lie group theory

In this section we prove the main result. First, we begin with some definitions and establish some notation. We will not state the necessary definitions and results from Lie group theory in their full generality (e.g., in multi-dimensions or for Lie groups acting on general manifolds), rather we will state them in a form that is appropriate for the fluid mechanical context that is our main interest. For more background the reader should consult Olver [1986] or Bluman and Kumei [1989].

Definition 2.2.1 (One-Parameter Lie Group) *Let $U \subset \mathbb{R}^3$ be an open set and consider the mappings*

$$(x,t) \mapsto g(x,t;\lambda), \qquad (x,t) \in U \times \mathbb{R}$$

which depend on a parameter $\lambda \in \mathcal{I} \subset \mathbb{R}$*, where* $\mathcal{I}$ *is an interval in* $\mathbb{R}$*. We assume that* $\phi(\lambda, \delta)$ *defines a law of composition for any two parameters* λ*,* $\delta \in \mathcal{I}$*. Then we say that this family of mappings forms a* one-parameter Lie group acting on $U \times \mathbb{R}$ *if the following properties hold:*

1. *For each parameter* $\lambda \in \mathcal{I}$ *the mappings are one-to-one and onto* $U \times \mathbb{R}$*. Moreover, the mappings are infinitely differentiable with respect to* $(x,t) \in U$ *and analytic in* $\lambda \in \mathcal{I}$*.*

2. $\mathcal{I}$*, with the law of composition* ϕ*, forms a group. Moreover,* $\phi(\lambda, \delta)$ *is an analytic function of* $\lambda \in \mathcal{I}$ *and* $\delta \in \mathcal{I}$*. Without loss of generality we can assume that* $\mathcal{I}$ *contains the origin and that* $\lambda = 0$ *corresponds to the identity element, e, in this group.*

3. $(x,t) = g(x,t;e)$*.*

4. *If* $(x^1,t^1) = g(x^0,t^0;\lambda^0)$ *and* $(x^2,t^2) = g(x^1,t^1;\lambda^1)$ *then* $(x^2,t^2) = g(x^0,t^0;\phi(\lambda^0,\lambda^1))$*.*

We will often denote one-parameter Lie groups generally by the symbol G*.*

The *infinitesimal generator* of the action of a one-parameter Lie group plays an important role in many computations related to symmetry issues.

Definition 2.2.2 (Infinitesimal Generator) *Let* G *be a one-parameter Lie group acting on* $U \times \mathbb{R}$*. The* infinitesimal generator *of the action of* G *is the vector field*

$$\mathbf{w} \equiv \sum_{i=1}^{3} \xi_i(x,t)\frac{\partial}{\partial x_i} + \xi_4(x,t)\frac{\partial}{\partial t}$$

where

$$\xi_i(x,t) = \frac{\partial g_i(x,t;\lambda)}{\partial \lambda}|_{\lambda=0}, \quad ,i = 1,\cdots,3, \qquad \xi_4(x,t) = \frac{\partial g_4(x,t;\lambda)}{\partial \lambda}|_{\lambda=0}.$$

Our main interest is in discussing one parameter groups of *symmetries* of first-order ordinary differential equations, henceforth referred to as "ODE's". Thus our notation (x,t) is suggestive of the dependent ("space") variable and independent ("time") variable of an ordinary differential equation. Indeed, we will want to discuss the situation where the Lie group acts only on the space variables. In this case one can easily rewrite definitions 2.2.1 and 2.2.2 with the t variable eliminated.

Now we are ready to define the notion of a symmetry of a system of ODE's.

Definition 2.2.3 (Symmetries of a System of ODE's) *Let G be a one-parameter Lie group acting on $U \times \mathbb{R}$ and let $\dot{x} = F(x,t)$, $x \in U$, $t \in \mathbb{R}$ be a system of ordinary differential equations. We say that this system admits a one-parameter group of symmetries G if and only if whenever $\varphi(t)$ is a solution then so is $g(\varphi(t),t;\lambda)$, where $g(x,t,\lambda)$ is any element of G. We will call G a* spatial *symmetry group if it acts only on the dependent variables and its infinitesimal generator is an autonomous vector field on $\mathbb{R}^3$.*

Functions that are *invariant* with respect to the group action play an important role in our analysis. We now define this notion.

Definition 2.2.4 (Functionally Independent Invariants) *Suppose we are given a one-parameter Lie group G acting on $U \times \mathbb{R}$. A scalar-valued function f is said to be an* invariant of the group action *if and only if $f(g(x,t;\lambda)) = f(x,t)$, $\forall \lambda \in \mathcal{I}, \forall (x,t) \in U \times \mathbb{R}$.*

A set of functions $f_i, i = 1,2,3$, are called functionally independent invariants *of G in some $V \subset U \times \mathbb{R}$ if and only if their (3×4) Jacobian matrix has maximal rank everywhere in V.*

Given a function $f(x,t)$ we can determine whether or not it is invariant under the group G by computing its derivative with respect to the infinitesimal generator of the group. This is known as the *Lie derivative* and is given by

$$L_{\mathbf{w}}\left(f(x,t)\right) \equiv \sum_{i=1}^{3} \xi_i \frac{\partial f}{\partial x_i}(x,t) + \xi_4 \frac{\partial f}{\partial t}(x,t) = \frac{df}{d\lambda}(g(x,t;\lambda))|_{\lambda=0}. \qquad (2.2.1)$$

If $L_{\mathbf{w}}\left(f(x,t)\right) = 0$ then $f(x,t)$ is an invariant. Moreover, it can be be proven that if $\mathbf{w}|_{(x,t)} \neq 0$, then in some neighborhood of the point (x,t) there exist three functionally independent invariants for the group G (see Olver [1986], Theorem 2.17, pg. 88).

With this background we can now state a general result from Olver [1986] that we will use in the proof of our main result in this section.

Theorem 2.2.1 *Let*

$$\frac{dx_i}{dt} = f_i(x_1, x_2, x_3, t), \quad i = 1, \cdots, 3, \qquad (2.2.2)$$

be a first-order system of ordinary differential equations. Suppose further that (2.2.2) admits a one-parameter group of symmetries, G, with the parameter λ. Then there exists a local change of variables, defined near (x,t) such that $\mathbf{w}|_{(x,t)} \neq 0$, given by

$$\begin{aligned} x_i &= \eta_i(y_1, y_2, y_3, s), \quad i = 1, \cdots, 3, \\ t &= \psi(y_1, y_2, y_3, s), \end{aligned} \qquad (2.2.3)$$

such that in coordinates (2.2.3) the system (2.2.2) becomes

$$\frac{dy_i}{ds} = g_i(y_1, y_2, s), \quad i = 1, \cdots, 3. \tag{2.2.4}$$

Furthermore, y_1, y_2, s *form a complete set of functionally independent invariants of* G *which satisfy*

$$\begin{aligned} L_{\mathbf{w}}(y_i) &= 0, \quad i = 1, 2, \\ L_{\mathbf{w}}(s) &= 0, \end{aligned} \tag{2.2.5}$$

and y_3 *satisfies*

$$L_{\mathbf{w}}(y_3) = 1. \tag{2.2.6}$$

Proof: See Olver [1986], Theorem 2.66, page 158. □

If G is a spatial symmetry group, then we have the following result.

Lemma 2.2.1 *Suppose* G *from the above proposition is a spatial symmetry group. Then we can take* $s = t$*, and* y_i, $i = 1, ..., 3$ *independent of time.*

Proof: Since we are assuming that G is a spatial symmetry group the t-component of the infinitesimal generator of the action of G is zero. Therefore the function t is an invariant for the action of the symmetry group and we can take $s = t$.

Further, the infinitesimal generator of the action of G, $\mathbf{w}$, is an autonomous vector field on $\mathbb{R}^3$. Therefore the solutions to the following equations

$$\begin{aligned} L_{\mathbf{w}}(y_i) &= 0, \ i=1,2, \\ L_{\mathbf{w}}(y_3) &= 1, \end{aligned} \tag{2.2.7}$$

are independent of time. Since the solutions to these equations give the required coordinate change, the lemma is proven. □

2.2.2 Volume-preserving vector fields and spatial, volume-preserving symmetry groups

Since our main interest is incompressible fluid mechanics we will be interested in volume-preserving vector fields. Along these lines, most applications will be concerned with spatial symmetry groups; *henceforth we will restrict ourselves to this situation.* We begin with some definitions.

Definition 2.2.5 (Volume-Preserving Systems of ODE's) *Let*

$$\frac{dx_i}{dt} = f_i(x_1, x_2, x_3, t), \quad i = 1, \cdots, 3, \tag{2.2.8}$$

be a system of ordinary differential equations on $U \times \mathbb{R}$. We call (2.2.8) a volume-preserving system *if and only if it satisfies*

$$\sum_{i=1}^{3} \frac{\partial f_i}{\partial x_i} = 0.$$

Next we define what we mean by a volume-preserving spatial symmetry group.

Definition 2.2.6 (Volume-Preserving Spatial Symmetry Group) *Let G be a one parameter spatial symmetry group acting on $U \subset \mathbb{R}^3$. We call G a volume-preserving spatial symmetry group if and only if the components of the infinitesimal generator of its action satisfy*

$$\sum_{i=1}^{3} \frac{\partial \xi_i}{\partial x_i} = 0.$$

In finding the symmetry group of a specific vector field, the following lemma is quite useful.

Lemma 2.2.2 *Neccessary and sufficient conditions for a vector field $\mathbf{w} = (\eta^1, \eta^2, \eta^3)$ to be the infinitesimal generator for the action of a volume-preserving, spatial symmetry group of a vector field $\mathbf{v} = (\xi^1, \xi^2, \xi^3)$ are*

$$\begin{aligned} \frac{\partial \mathbf{w}}{\partial t} &= 0, \\ [\mathbf{v}, \mathbf{w}] &= 0, \\ \nabla \cdot \mathbf{w} &= 0, \end{aligned} \tag{2.2.9}$$

where $[\mathbf{v}, \mathbf{w}]$ denotes the Lie bracket of vector fields $\mathbf{v}, \mathbf{w}$ defined in coordinates by

$$[\mathbf{v}, \mathbf{w}]_i = \sum_{j=1}^{3} \{\xi^j \frac{\partial \eta^i}{\partial x^j} - \eta^j \frac{\partial \xi^i}{\partial x^j}\}.$$

Proof: This is an easy calculation which stems from the general theorem on infinitesimal generators of symmetry groups for systems of differential equations and the definition of the infinitesimal generator of a spatial, volume-preserving symmetry group. The general theorem is given in e.g., Olver [1986]. □

The following theorem is the main result of this section:

Theorem 2.2.2 *Let*

$$\frac{dx_i}{dt} = f_i(x_1, x_2, x_3, t), \quad i = 1, \cdots, 3, \tag{2.2.10}$$

be a volume-preserving system of ordinary differential equations. Suppose further that (2.2.10) admits a one-parameter spatial volume-preserving symmetry group, G. Then there exists a local change of variables

$$x_i = \phi_i(z_1, z_2, z_3), \quad i = 1, \cdots, 3, \tag{2.2.11}$$

such that in variables (2.2.11) the system (2.2.10) becomes

$$\begin{aligned}
\frac{dz_1}{dt} &= \frac{\partial H(z_1, z_2, t)}{\partial z_2}, \\
\frac{dz_2}{dt} &= -\frac{\partial H(z_1, z_2, t)}{\partial z_1}, \\
\frac{dz_3}{dt} &= k_3(z_1, z_2, t).
\end{aligned} \tag{2.2.12}$$

where z_1 and z_2 are functionally independent invariants of G. Further, if (2.2.12) is autonomous, H is a first integral.

Proof: Applying Theorem 2.2.1 and Lemma 2.2.1 , there exists a transformation of coordinates in which (2.2.10) takes the form

$$\frac{dy_1}{dt} = k_1(y_1, y_2, t),$$
$$\frac{dy_2}{dt} = k_2(y_1, y_2, t),$$
$$\frac{dy_3}{dt} = k_3(y_1, y_2, t). \tag{2.2.13}$$

Next we show that

$$\frac{dy_1}{dt} = k_1(y_1, y_2, t),$$
$$\frac{dy_2}{dt} = k_2(y_1, y_2, t), \tag{2.2.14}$$

can be written in the form

$$\frac{dy_1}{dt} = \frac{1}{J}\frac{\partial K(y_1, y_2, t)}{\partial y_2},$$
$$\frac{dy_2}{dt} = -\frac{1}{J}\frac{\partial K(y_1, y_2, t)}{\partial y_1}, \tag{2.2.15}$$

for some function $K(y_1, y_2, t)$ where J is the Jacobian of the transformation $x_i = \eta_i(y_1, y_2, y_3)$.

In order for there to exist a function $K(y_1, y_2, t)$ such that

$$\frac{\partial K}{\partial y_2} = Jk_1,$$
$$\frac{\partial K}{\partial y_1} = -Jk_2,$$

it is necessary and sufficient for the second partial derivatives of $K(y_1, y_2, t)$ to be equal (provided the domain is contracible in $\mathbb{R}^2$). This condition is equivalent to

$$\frac{\partial J k_1}{\partial y_1} + \frac{\partial J k_2}{\partial y_2} = 0. \tag{2.2.16}$$

In order to show that (2.2.16) holds we will use the fact that the symmetry group is volume preserving. Since the original vector field (2.2.10) is volume preserving we have

$$\sum_{i=1}^{3} \frac{\partial f_i}{\partial x_i} = 0. \tag{2.2.17}$$

In the transformed coordinates (2.2.17) is expressed as

$$\frac{1}{J} \sum_{i=1}^{3} \frac{\partial J k_i}{\partial y_i} = 0, \tag{2.2.18}$$

where J denotes the Jacobian of the transformation $x_i = \eta_i(y_1, y_2, y_3)$. (Note: the passage from (2.2.17) to (2.2.18) is a lengthy calculation that can be found in e.g., Wrede [1963].) Thus, in order to show that (2.2.16) holds it suffices to show that

$$\frac{\partial J}{\partial y_3} = 0,$$

since k_3 does not depend on y_3 so that $\partial k_3 / \partial y_3 = 0$. In order to show this recall that by assumption the infinitesimal generator of the action of G is volume-preserving so that we have

$$\frac{1}{J} \sum_{i=1}^{3} \frac{\partial J \xi_i}{\partial y_i} = 0, \tag{2.2.19}$$

From Theorem 2.2.1 we know that $\xi_1 = \xi_2 = 0$ and $\xi_3 = 1$, so we immediately obtain

$$\frac{\partial J}{\partial y_3} = 0. \tag{2.2.20}$$

Thus (2.2.14) can be written in the form of (2.2.15).

For the final step of the proof we show that (2.2.15) can be written in the following Hamiltonian form

$$\begin{aligned} \frac{dz_1}{dt} &= \frac{\partial H(z_1, z_2, t)}{\partial z_2}, \\ \frac{dz_2}{dt} &= -\frac{\partial H(z_1, z_2, t)}{\partial z_1}. \end{aligned} \tag{2.2.21}$$

We will show that the transformation of coordinates (recall form (2.2.20) that J does not depend on y_3)

$$\begin{aligned} z_1 &= \int J(y_1, y_2) dy_1, \\ z_2 &= y_2, \\ z_3 &= y_3, \end{aligned} \tag{2.2.22}$$

takes the system

$$\begin{aligned} \frac{dy_1}{dt} &= \frac{1}{J}\frac{\partial K(y_1, y_2, t)}{\partial y_2}, \\ \frac{dy_2}{dt} &= -\frac{1}{J}\frac{\partial K(y_1, y_2, t)}{\partial y_1}, \\ \frac{dy_3}{dt} &= k_3(y_1, y_2, t) \end{aligned} \tag{2.2.23}$$

to the form (2.2.12).

This construction is an explicit implementation of Darboux's theorem (see Abraham and Marsden [1978], Arnold [1978], Olver [1986]). Let $H(z_1, z_2, t) = K(y_1(z_1, z_2), z_2, t)$, and we will calculate $\dot{z}_1$ and $\dot{z}_2$ in the new coordinates. We begin with $\dot{z}_2$, since it is easier.

Using the chain rule, we obtain

$$\dot{z}_2 = \dot{y}_2 = -\frac{1}{J}\frac{\partial K}{\partial y_1} = -\frac{1}{J}\frac{\partial H}{\partial z_1}\frac{\partial z_1}{\partial y_1} = -\frac{\partial H}{\partial z_1} \tag{2.2.24}$$

where we have used (2.2.22) from which follows $\frac{\partial z_1}{\partial y_1} = J$.

Now we calculate $\dot{z}_1$. Using the chain rule, we obtain

$$\dot{z}_1 = \frac{\partial z_1}{\partial y_1}\dot{y}_1 + \frac{\partial z_1}{\partial y_2}\dot{y}_2 = \frac{1}{J}\frac{\partial z_1}{\partial y_1}\frac{\partial K}{\partial y_2} - \frac{1}{J}\frac{\partial z_1}{\partial y_2}\frac{\partial K}{\partial y_1} = \frac{\partial K}{\partial y_2} - \frac{1}{J}\frac{\partial z_1}{\partial y_2}\frac{\partial K}{\partial y_1}. \tag{2.2.25}$$

Moreover, we have

$$\frac{\partial H}{\partial z_2} = \frac{\partial K}{\partial z_2} + \frac{\partial y_1}{\partial z_2}\frac{\partial K}{\partial y_1}. \tag{2.2.26}$$

Now from (2.2.22) we have $\frac{\partial K}{\partial z_2} = \frac{\partial K}{\partial y_2}$ so that if we show

$$-\frac{1}{J}\frac{\partial z_1}{\partial y_2} = \frac{\partial y_1}{\partial z_2}, \tag{2.2.27}$$

then it follows that

$$\dot{z}_1 = \frac{\partial H}{\partial z_2}.$$

The Jacobian of the transformation $y_i = y_i(z_1, z_2, z_3)$ defined in (2.2.22) is given by

$$\begin{pmatrix} \frac{\partial z_1}{\partial y_1} & \frac{\partial z_1}{\partial y_2} & \frac{\partial z_1}{\partial y_3} \\ \frac{\partial z_2}{\partial y_1} & \frac{\partial z_2}{\partial y_2} & \frac{\partial z_2}{\partial y_3} \\ \frac{\partial z_3}{\partial y_1} & \frac{\partial z_3}{\partial y_2} & \frac{\partial z_3}{\partial y_3} \end{pmatrix} = \begin{pmatrix} J & \frac{\partial}{\partial y_2}\int J(y_1, y_2)dy_1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad (2.2.28)$$

and the inverse of these two matrices is easily calculated to be

$$\begin{pmatrix} \frac{\partial y_1}{\partial z_1} & \frac{\partial y_1}{\partial z_2} & \frac{\partial y_1}{\partial z_3} \\ \frac{\partial y_2}{\partial z_1} & \frac{\partial y_2}{\partial z_2} & \frac{\partial y_2}{\partial z_3} \\ \frac{\partial y_3}{\partial z_1} & \frac{\partial y_3}{\partial z_2} & \frac{\partial y_3}{\partial z_3} \end{pmatrix} = \frac{1}{J}\begin{pmatrix} 1 & -\frac{\partial}{\partial y_2}\int J(y_1, y_2)dy_1 & 0 \\ 0 & J & 0 \\ 0 & 0 & 1 \end{pmatrix}. \qquad (2.2.29)$$

From (2.2.29) and (2.2.22) we have

$$\frac{\partial y_1}{\partial z_2} = -\frac{1}{J}\frac{\partial}{\partial y_2}\int J(y_1, y_2)dy_1 = -\frac{1}{J}\frac{\partial z_1}{\partial y_2}.$$

Hence the theorem is proved. □

Remarks:

1. An important point is that the coordinates in which the vector field takes the form (2.2.12) *do not* depend on the explicit form of the original vector field. Rather, they depend only on the volume-preserving spatial symmetry group.

2. An obvious question is "given a vector field, how do we know that it is invariant under a volume-preserving symmetry group"? In many cases a knowledege of the physical geometry and boundary conditions, as well as inspection of the system of ODE's, often can be used to reveal the symmetries. One can also find an infinitesimal generator of the volume preserving, spatial symmetry group by using

requirements on the infinitesimal generator spelled out in Lemma 2.2.2. In particular, an arbitrary vector field $\mathbf{w}$ can be substituted in (2.2.9) which then become equations for components of $\mathbf{w}$.

3. Transformation $x_i = \phi_i(z_1, z_2, z_3)$ is volume preserving, i.e., its Jacobian is 1.

2.3 Action-angle-angle variables

Action-Angle variables have played an important role in the development of perturbation methods for the study of near-integrable Hamiltonian systems. In particular, the KAM theorem as well as the Nekhoroshev theorem are both proven in a context where the unperturbed system is expressed in action-angle variables. Action-Angle variables have the virtue of rendering certain geometric features of the system transparent (e.g., the foliation of the phase space by invariant tori) as well as providing a natural decomposition of the dynamics into "fast" and "slow" time scales. We refer the reader to Arnold *et al.* [1988] for many examples of the analytical and geometrical virtues of action-angle variables.

The construction of action-angle variables uses the symplectic structure of the system. Nevertheless, in this section we show how one can take the volume-preserving system of the equations given in Theorem 2.2.2 and further transform the system into coordinates that have many of the virtues of standard action-angle variables.

We assume that we are dealing with autonomous vector fields so that (2.2.12) takes the following form:

$$\frac{dz_1}{dt} = \frac{\partial H(z_1, z_2)}{\partial z_2},$$

$$\frac{dz_2}{dt} = -\frac{\partial H(z_1,z_2)}{\partial z_1},$$
$$\frac{dz_3}{dt} = k_3(z_1,z_2). \tag{2.3.30}$$

Since the z_1 and z_2 components of the vector field *do not* depend on z_3 we can consider transforming this two-dimensional vector field into the standard action-angle variables.

Assumption. There is some subset of $z_1 - z_2$ plane, denoted $\mathcal{D}$, in which the level sets $H(z_1, z_2) = h$ are closed curves.

If this assumption holds, then it is well known from classical mechanics (see, e.g., Arnold [1978]) that there is a transformation

$$(z_1, z_2) \mapsto (I, \theta)$$

satisfying the following properties.

1. $I = I(h)$, i.e., I is constant on the closed orbits.
2. $\oint_{H=h} d\theta = 2\pi$.
3. $\dot{\theta} = \Omega_1(I)$

The action variable is given by (see e.g., Wiggins [1990] or Arnold [1978])

$$I = \frac{1}{2\pi}\int_{H=h} z_2 dz_1, \tag{2.3.31}$$

while the a igle variable reads

$$\theta = \frac{2\pi}{T(H)}t, \tag{2.3.32}$$

where $T(H)$ is a period on the orbit on $z_1 - z_2$ plane (which is a level set of H), and t denotes the time along the orbit measured from a certain point on the orbit.

We assume that this action-angle transformation on the $z_1 - z_2$ component of (2.3.30) has been carried out so that these equations subsequently take the form

$$\begin{aligned} \dot{I} &= 0, \\ \dot{\theta} &= \Omega_1(I), \\ \dot{z}_3 &= h_3(I,\theta), \end{aligned} \tag{2.3.33}$$

where $h_3(I,\theta) = k_3(z_1(I,\theta), z_2(I,\theta))$.

The following theorem gives the construction of action-angle-angle variables.

Theorem 2.3.1 *Suppose* $\Omega_1 \neq 0$ *in (2.3.33). The transformation of variables* $(I,\theta,z_3) \rightarrow (I,\phi_1,\phi_2)$ *defined by*

$$\begin{aligned} I &= I \\ \phi_1 &= \theta, \\ \phi_2 &= z_3 + \frac{\Delta z_3}{2\pi}\theta - \int \frac{h_3(I,\theta)}{\Omega_1(I)} d\theta, \end{aligned}$$

where

$$\Delta z_3 = \int_0^{2\pi} \frac{h_3(I,\theta)}{\Omega_1(I)} d\theta,$$

then brings the system (2.3.33) to the form

$$\dot{I} = 0,$$

$$\begin{aligned}\dot{\phi}_1 &= \Omega_1(I),\\ \dot{\phi}_2 &= \Omega_2(I),\end{aligned} \tag{2.3.34}$$

where $I \in \mathbb{R}^+$, $\phi_1 \in S^1$, *and* $\phi_2 \in S^1$ *or* $\mathbb{R}$. *Furthermore, the transformation is volume-preserving.*

Proof: Note first that the transformation is well-defined for both z_3 defined on $\mathbb{R}^1$ (when the invariant manifolds are cylinders) and z_3 defined on S^1 (when the invariant manifolds are tori), as the appropriate points are identified. The rest of the proof involves straightforward calculations. Clearly, Δz_3 is a function of I only so that

$$\begin{aligned}\dot{\phi}_1 &= \dot{\theta} = \Omega_1(I),\\ \dot{\phi}_2 &= \dot{z}_3 + \frac{\Delta z_3}{2\pi}\dot{\theta} - \frac{d}{dt}\int h_3(I,\theta)dt = \frac{\Delta z_3}{2\pi}\dot{\theta} = \frac{\Delta z_3}{2\pi}\Omega_1(I) = \Omega_2(I),\end{aligned}$$

as claimed. It follows immediately that ϕ_1 is an angular variable and that the nature of ϕ_2 depends on z_3. If z_3 is an angular variable, then so is ϕ_2; if $z_3 \in \mathbb{R}$, then so is ϕ_2. Further, a direct computation shows that the Jacobian of the transformation $(I, \theta, z_3) \to (I, \phi_1, \phi_2)$ is 1. □

This theorem shows that the phase space of a three-dimensional, volume preserving, time-independent flow that satisfies the above assumptions is naturally foliated into two-dimensional tori or cylinders. If one removes the requirement that the flow is invariant under a one-parameter spatial volume preserving symmetry group then the situation is not so simple, even if a system posseses an integral of motion, as the following theorem of Kolmogorov describes.

Theorem 2.3.2 *Consider a three-dimensional, volume-preserving autonomous vector field,* $\dot{x} = f(x)$, $x \in U \subset \mathbb{R}^3$, *having an integral* $F(x)$. *Let* $M_c \equiv \{x | F(x) = c\}$. *Further, assume that the vector field does not vanish on* M_c. *Then if* M_c *is compact and connected we have*

1. M_c *is diffeomorphic to a 2-torus.*

2. *One can find angular coordinates* ϕ_1, ϕ_2 *on* M_c *such that the vector field restricted to* M_c *can be expressed as*

$$\begin{aligned} \dot{\phi}_1 &= \frac{\mu_1}{\Phi(\phi_1, \phi_2)}, \\ \dot{\phi}_2 &= \frac{\mu_2}{\Phi(\phi_1, \phi_2)}, \end{aligned}$$

   where μ_1, μ_2 *are constants and* $\Phi(\phi_1, \phi_2)$ *is a smooth positive* 2π*-periodic function in* ϕ_1 *and* ϕ_2.

Proof: See Kolmogorov [1953], also, an outline of the proof can be found in Arnold *et al.* [1988]. □

2.4 Symmetry and integrability of three-dimensional vector fields; Euler flows

2.4.1 Symmetry and integrability of three-dimensional volume-preserving vector fields

In the previous section we showed that under certain assumptions a three-dimensional vector field which admits a spatial volume-preserving symmetry group posseses invariant manifolds which are tori or cylinders. This is analogous to the more familiar results for integrable canonical Hamiltonian systems where the fact that the vector field has invariant manifolds of certain type is a purely gemetrical fact related to commutation relations between the Hamiltonian vector field and the infinitesimal generator of its symmetry groups arising from the integrals. Along these lines for three-dimensional vector fields, Arnold [1965] proved the following fundamental result.

Theorem 2.4.1 *Consider an analytic autonomous volume-preserving vector field* $\mathbf{v}$ *in a domain* $D \subset \mathbb{R}^3$ *bounded by a compact analytic surface, that admits a spatial,volume preserving symmetry group with infinitesimal generator* $\mathbf{w}$. *Further suppose that* $\mathbf{v}$ *and* $\mathbf{w}$ *are not everywhere collinear in the given domain. Then the domain* $D \subset \mathbb{R}^3$ *is partitioned in a finite number of cells and each of the cells is fibered either into tori or into annula. On an invariant torus, trajectories are either all closed or all dense. On a cylinder, all trajectories are closed.*

Proof: See Arnold [1965]. □

2.4.2 Euler flows

Arnold used Theorem (2.4.1) to show that a steady analytic Euler velocity field (i.e., an autonomous solution of Eulers equations of motion for an inviscid incompressible fluid) which is not everywhere collinear with its associated vorticity field in a certain analytic domain of $\mathbb{R}^3$ admits invariant manifolds which are tori or annula. This result uses crucially the fact that the vorticity ω associated with a steady Euler flow $\mathbf{v}$ is an infinitesimal generator of a volume-preserving spatial symmetry group of $\mathbf{v}$. This can easily be seen by noting that

$$\begin{aligned}\frac{\partial \omega}{\partial t} &= 0, \\ [\mathbf{v}, \omega] &= 0, \\ \nabla \cdot \omega &= 0\end{aligned}$$

and recalling Lemma 2.2.2.

This observation brings up a relationship between our methods and a transformation which has been known in fluid mechanics for quite some time, the Clebsch transformation, which we briefly describe. It is well-known that since the vorticity field ω is volume-preserving we can express it locally as

$$\omega = \nabla f \times \nabla g, \tag{2.4.35}$$

where f and g are some functions on $\mathbb{R}^3$. Furthermore, it can be shown then that f and g satisfy

$$\begin{aligned}\dot{f} &= \frac{\partial \lambda(f,g,t)}{\partial g}, \\ \dot{g} &= -\frac{\partial \lambda(f,g,t)}{\partial f},\end{aligned} \tag{2.4.36}$$

for some scalar valued function λ, of f and g (see e.g., Truesdell [1954], pg. 190, Serrin [1959]).

Now we show how f and g are related to our work. Notice that from (2.4.35) f and g satisfy

$$
\begin{aligned}
L_\omega(f) &= (\nabla f \times \nabla g) \cdot \nabla f = 0, \\
L_\omega(g) &= (\nabla f \times \nabla g) \cdot \nabla g = 0.
\end{aligned}
$$

It follows from these equations that f and g are functionally independent invariants of a symmetry group of $\mathbf{v}$ generated by ω (see Section 2). Therefore, we can take f and g as the new variables, and find a third function h which satisfies

$$L_\omega(h) = (\nabla f \times \nabla g) \cdot \nabla h = 1.$$

Thus an Euler flow can be written in the form (2.2.12). We will use this procedure in two examples on Euler flows in Section 7.

The derivation of (2.4.36) uses the fact that ω is the curl of $\mathbf{v}$. In the proof of Theorem (2.2.2) we used only the relations (2.2.9) describing the relationship between a vector field and the infinitesimal generator of its volume-preserving spatial symmetry group. In particular, we did not require that the infinitesimal generator be the vorticity field.

2.5 "KAM-Like" theory for three-dimensional, volume-preserving, vector fields

For two-dimensional, time-periodic flows the KAM theorem (see e.g., Arnold [1978], [1988]) plays an important kinematical role. Namely, it provides sufficient conditions for the existence of invariant circles for the associated two-dimensional *Poincaré map* of the two-dimensional, time-periodic flow. These invariant circles are significant because they act as barriers to transport. As such, they are also a central component of the *regular regions* in flows. Hence, an understanding of how KAM tori arise is an important element in understanding mixing and transport issues in two-dimensional, time-periodic flows. Many examples of this, both theoretical and experimental, can be found in Ottino [1989].

The method of the proof of KAM theorem can not be used immediately to prove "KAM"-type theorem in "odd-dimensional" settings for important technical reasons, of which a succint description can be found in de la Llave [1992]. Nevertheless, in the past two years some important advances have been made concerning "KAM-like" theories for volume-preserving maps by Cheng and Sun [1990], de la Llave and Delshams [1990], Xia [1992], and Herman [1991]. In this section we want to show how the coordinates that we developed put us in the framework where we can use these new methods to study *perturbations* of the integrable three-dimensional vector fields that we have thus far considered. We will first consider the case of *time-dependent* perturbations.

Consider a time-periodic, volume-preserving perturbation to the vector field (2.3.34) that takes the following general form

$$\begin{aligned} \dot{I} &= \epsilon F_0(I, \phi_1, \phi_2, t) \\ \dot{\phi}_1 &= \Omega_1(I) + \epsilon F_1(I, \phi_1, \phi_2, t) \\ \dot{\phi}_2 &= \Omega_2(I) + \epsilon F_2(I, \phi_1, \phi_2, t) \end{aligned} \tag{2.5.37}$$

where we now assume that *both* ϕ_1 and ϕ_2 are angular variables, ϵ is the (small) perturbation parameter, and the functions F_i, $i = 0, 1, 2$, are periodic in t with period $T = \frac{2\pi}{\omega}$. We will derive an approximate form for a three-dimensional *Poincaré map* of this system essentially using the approach from Wiggins [1990] pp. 129-132. Using regular perturbation theory, the solutions of (2.5.37) are $\mathcal{O}(\epsilon)$ close to the unperturbed solutions on time scales of $\mathcal{O}(1)$. Hence we have the following expansions of the solutions of (2.5.37)

$$\begin{aligned} I^{\epsilon}(t) &= I^0 + \epsilon I^1(t) + \mathcal{O}(\epsilon^2) \\ \phi_1^{\epsilon}(t) &= \phi_1^0 + \Omega_1(I^0)t + \epsilon\phi_1^1(t) + \mathcal{O}(\epsilon^2) \\ \phi_2^{\epsilon}(t) &= \phi_2^0 + \Omega_2(I^0)t + \epsilon\phi_2^1(t) + \mathcal{O}(\epsilon^2) \end{aligned} \tag{2.5.38}$$

where $I^1(t)$, $\phi_1^1(t)$, and $\phi_2^1(t)$ satisfy the following *first variational equation*

$$\begin{pmatrix} \dot{I}^1 \\ \dot{\phi}_1^1 \\ \dot{\phi}_2^1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ \frac{\partial\Omega_1}{\partial I}(I^0) & 0 & 0 \\ \frac{\partial\Omega_2}{\partial I}(I^0) & 0 & 0 \end{pmatrix} \begin{pmatrix} I^1 \\ \phi_1^1 \\ \phi_2^1 \end{pmatrix} + \begin{pmatrix} F_0(I^0, \Omega_1(I^0)t + \phi_1^0, \Omega_2(I^0)t + \phi_2^0, t) \\ F_1(I^0, \Omega_1(I^0)t + \phi_1^0, \Omega_2(I^0)t + \phi_2^0, t) \\ F_2(I^0, \Omega_1(I^0)t + \phi_1^0, \Omega_2(I^0)t + \phi_2^0, t) \end{pmatrix}. \tag{2.5.39}$$

Because our coordinates put the vector field in such a simple form, this equation can be easily solved, which we postpone for the moment. Instead, recall that our goal is to construct a three-dimensional Poincaré map. More precisely, we are interested in constructing a map that takes the variables I^{ϵ}, ϕ_1^{ϵ}, and ϕ_2^{ϵ} to their value after flowing along the solution trajectories of (2.5.37) for time T. This map is simply given by

$$\begin{aligned} &P_{\epsilon} : (I^{\epsilon}(0), \phi_1^{\epsilon}(0), \phi_2^{\epsilon}(0)) \mapsto (I^{\epsilon}(T), \phi_1^{\epsilon}(T), \phi_2^{\epsilon}(T)), \\ &(I^0, \phi_1^0, \phi_2^0) \mapsto (I^0 + \epsilon I^1, \phi_1^0 + \Omega_1(I^0)T + \epsilon\phi_1^1(T), \phi_2^0 + \Omega_2(I^0)T + \epsilon\phi_2^1(T)) + \mathcal{O}(\epsilon^2), \end{aligned} \tag{2.5.40}$$

where we have used (2.5.38) and taken the following initial conditions

$$\begin{aligned} I^\epsilon(0) &= I^0, \\ \phi_1^\epsilon(0) &= \phi_1^0, \\ \phi_2^\epsilon(0) &= \phi_2^0. \end{aligned}$$

Now expressions for $I^1(T)$, $\phi_1^1(T)$, and $\phi_2^1(T)$ can readily be obtained by solving (2.5.39):

$$\begin{aligned} I^1(T) &= \int_0^T F_0(I^0, \Omega_1(I^0)t + \phi_1^0, \Omega_2(I^0)t + \phi_2^0, t)dt \equiv \tilde{F}_0(I^0, \phi_1^0, \phi_2^0), \\ \phi_1^1(T) &= \tfrac{\partial \Omega_1}{\partial I}|_{I=I^0} \int_0^T \int_0^t F_0(I^0, \Omega_1(I^0)\xi + \phi_1^0, \Omega_2(I^0)\xi + \phi_2^0, \xi)d\xi dt \\ &\quad + \int_0^T F_1(I^0, \Omega_1(I^0)t + \phi_1^0, \Omega_2(I^0)t + \phi_2^0, t)dt \equiv \tilde{F}_1(I^0, \phi_1^0, \phi_2^0), \\ \phi_2^1(T) &= \tfrac{\partial \Omega_2}{\partial I}|_{I=I^0} \int_0^T \int_0^t F_0(I^0, \Omega_1(I^0)\xi + \phi_1^0, \Omega_2(I^0)\xi + \phi_2^0, \xi)d\xi dt \\ &\quad + \int_0^T F_2(I^0, \Omega_1(I^0)t + \phi_1^0, \Omega_2(I^0)t + \phi_2^0, t)dt \equiv \tilde{F}_2(I^0, \phi_1^0, \phi_2^0). \end{aligned} \tag{2.5.41}$$

Substituting these expressions into (2.5.40) and dropping the superscripts on the variables gives the following final form for the Poincaré map:

$$\begin{aligned} I &\mapsto I + \epsilon \tilde{F}_0(I, \phi_1, \phi_2) + \mathcal{O}(\epsilon^2), \\ \phi_1 &\mapsto \phi_1 + 2\pi \frac{\Omega_1(I)}{\omega} + \epsilon \tilde{F}_1(I, \phi_1, \phi_2) + \mathcal{O}(\epsilon^2), \\ \phi_2 &\mapsto \phi_2 + 2\pi \frac{\Omega_2(I)}{\omega} + \epsilon \tilde{F}_2(I, \phi_1, \phi_2) + \mathcal{O}(\epsilon^2). \end{aligned} \tag{2.5.42}$$

where we have used $T \equiv \frac{2\pi}{\omega}$.

This map is exactly in the form where the new "KAM-like" theorems for perturbations of three-dimensional volume-preserving maps can be applied. By translation and rescaling we can take the domain of I to be the interval $\mathcal{I} = [1,2]$. We can also assume $2\pi\frac{\Omega_1(I)}{\omega} = I$ without loss of generality. Further, we require $\Omega_2''(I) \geq c_1 > 0$ on $\mathcal{I}$. The theorem requires that the vector fields be real analytic on the domain of interest with analyticity holding on the extension to the following complex domain

$$D_0(\tilde{\omega}) = \{|Im\ \phi_1| \leq r_0, \quad |Im\ \phi_2| \leq r_0, \quad |I - \tilde{\omega}| \leq s_0, \quad \tilde{\omega} \in \mathcal{I}\}.$$

Under the above assumptions we have the following theorem

Theorem 2.5.1 (Cheng and Sun, 1990) *There exists a positive* ϵ_0*, which depends on* $D_0(\tilde{\omega})$*, such that if* $0 < \epsilon \leq \epsilon_0$ *the mapping (2.5.42) admits a family of invariant tori given by*

$$\begin{aligned} I &= w(\xi, \zeta, \tilde{\omega}), \\ \phi_1 &= \xi + u(\xi, \zeta, \tilde{\omega}), \\ \phi_2 &= \xi + v(\xi, \zeta, \tilde{\omega}), \end{aligned} \qquad (2.5.43)$$

with u, v, w *real analytic functions of period* 2π *in the complex domain* $|Im\,\phi_1| \leq r_0/2,\ |Im\,\phi_2| \leq r_0/2,$

Moreover, the mapping restricted to the persisting perturbed tori (2.5.43) can be parametrically written as

$$\begin{aligned} \xi &\mapsto \xi + \tilde{\omega}, \\ \zeta &\mapsto \zeta + \frac{2\pi\Omega_2(\tilde{\omega})}{\omega} + q_1(\tilde{\omega}, \epsilon), \end{aligned} \qquad (2.5.44)$$

where $q_1(\tilde{\omega}, \epsilon)$ *is a function depending on the perturbations* $\widetilde{F}_i(I, \phi_1, \phi_2)$, $i = 0, 1, 2$, *and* $q_1(\tilde{\omega}, 0) = 0$.

In fact, there is a Cantor set $S(\epsilon) \subset [1, 2]$, *depending on the perturbations* $\widetilde{F}_i(I, \phi_1, \phi_2)$, $i = 0, 1, 2$, *such that for each* $\tilde{\omega} \in S(\epsilon)$ *there is a corresponding invariant torus of the form (2.5.43). Furthermore, the measure of the set* $S(\epsilon)$ *tends to* 1 *as* $\epsilon \to 0$.

Despite the similarities with the standard KAM theorem for area-preserving twist maps, this result is quite different and may ultimately yield fundamentally new effects for three-dimensional, time-periodic flows. For example, in standard KAM theory for area-preserving twist maps the invariant circles that survive are those that have strongly irrational (Diophantine) rotation numbers. Hence, regardless of the specific form of the perturbation, if the perturbation is sufficiently small we know which invariant circles will persist.

In three-dimensional volume-preserving maps circumstances are different. From the currently available proofs we are not able to predict whether certain torus will persist the perturbation, even if it satisfies Diophantine conditions. The only claim we can make is that there will be a set of invariant tori of positive measure for the perturbed map. In this situation generally any invariant torus disintegrates as the perturbation changes with new tori (having new frequencies) created near the locations of the disintegrated invariant tori.

For time-independent perturbations, we can take time-one Poincaré map derived in the same spirit as the one for the time-dependent case, and make the same conclusions on the issue of persisting tori. Note, though, that this conclusion is nontrivial, as opposed to the case of time-independent perturbations of one degree of freedom Hamiltonian systems.

Suppose now that the map (2.5.42) is defined on $I \times S^1 \times \mathbb{R}$, so that the invariant structures in the unperturbed problem are cylinders. We show in what follows that if we restrict our velocity field to some finite distance from the origin, and consider a perturbed system in that, restricted domain, under the same conditions as the ones in the theorem of Cheng and Sun, there is a set of a positive measure of finite invariant cylinders for the perturbed system. To show this we shall need the following Lemma:

Lemma 2.5.1 *Assume f is a C^r smooth function defined on some finite subinterval of $\mathbb{R}$, $[-l, l]$. Suppose $l_1 > l$. Then there is an extension of f to $\mathbb{R}$, denoted $\tilde{f}$ such that $\tilde{f}$ is an smooth function on $\mathbb{R}$ and periodic with period $2l_1$. Further, $\tilde{f} = f$ on $[-l, l]$.*

Proof: First consider the extension for $x \subset \mathbb{R}$, $x < 0$. As f is C^r we have its derivatives at $x = -l$, $f'(l), f''(-l), ..., f^{(r)}(-l)$. Now define $\tilde{f}$ on $[-l_1, -l]$ to be

$$\tilde{f} = f(-l) + f'(-l)x + ... + f^{(r)}(l)x^r.$$

Now we turn to the interval $[l, l_1]$. As we want to ultimately extend $\tilde{f}$ to $\mathbb{R}$, we need to match its derivatives at l_1 with those already obtained at $-l_1$. So, we define $\tilde{f}$ on $[l, l_1]$ to be

$$\tilde{f} = pol(f)_l \cdot B_l + pol(f)_{l_1} \cdot B_{l_1}.$$

Where

$$\begin{aligned} pol(f)_l &= f(l) + f'(l)x + ... + f^{(r)}(l)x^r, \\ pol(f)_{l_1} &= \tilde{f}(-l_1) + \tilde{f}'(-l_1)x + ... + \tilde{f}^{(r)}(-l_1)x^r, \end{aligned} \tag{2.5.45}$$

and B_l, B_{l_1} are smooth (all derivatives exist) functions such that

$$B_l = \begin{cases} 1 & \text{if } l \leq x \leq l + \frac{l_1 - l}{8} \\ 0 & \text{if } l + \frac{l_1 - l}{4} \leq x \end{cases}$$

and

$$B_{l_1} = \begin{cases} 1 & \text{if } l_1 \geq x \geq l_1 - \frac{l_1 - l}{8} \\ 0 & \text{if } l_1 - \frac{l_1 - l}{4} \geq x \end{cases}$$

The proof that such functions exist can be found e.g., in Guillemin-Pollack [1974]. Let further $\tilde{f} = f$ on $[-l, l]$.

It is now clear from the construction of $\tilde{f}$ that it can be smoothly periodically extended to $\mathbb{R}$ and that it satisfies all of the claims of the Lemma. □

Now consider the map (2.5.42). It is defined on $I \times S^1 \times \mathbb{R}$. We restrict its definition to $I \times S^1 \times [-l, l]$. Then, as a result of the Lemma 2.5.1 we can extend the system to $I \times S^1 \times \mathbb{R}$ by extending $\widetilde{F}_0(I, \phi_1, \phi_2), \widetilde{F}_1(I, \phi_1, \phi_2)$ and $\widetilde{F}_2(I, \phi_1, \phi_2)$ periodically to $\mathbb{R}$. As the map is now periodic both in ϕ_1 and ϕ_2, theorems on the preservation on tori in action-angle-angle setting apply (note: we need the perturbation functions to be at least C^6, see Xia [1991]). So, there is a set of positive measure of invariant tori for the perturbed system. Now restricting to our original system, defined on $I \times S^1 \times [-l, l]$, we see that each preserved torus in the extended system corresponds to a preserved cylinder in the original one. Thus we proved that there is a set of positive measure of finite cylinders persisting the perturbation for any cutoff distance in ϕ_2 from the origin. Note that for any cutoff distance l, in general we might have different tori persisting. This is the consequence of the fact that three-dimensional KAM-type theory can not predict exactly which torus will persist, independently of the perturbation. As we change the perturbation functions in our construction, the set of cylinders persisting the perturbation might be different.

The above developed theory, has an immediate application in fluid mechanics to three-dimensional, time-dependent perturbations of the so-called duct flows (see e.g., Franjione and Ottino [1991]). In a real fluid mechanical situations, the cylinders involved are always finite, so the above presented result is good enough.

2.6 Melnikov's method for perturbations of integrable, three-dimensional volume-preserving vector fields

In this section we want to give a version of Melnikov's method that applies to perturbations of *autonomous* vector fields of the form of (2.2.12), i.e.,

$$\begin{aligned}
\frac{dz_1}{dt} &= \frac{\partial H(z_1,z_2)}{\partial z_2} + \epsilon F_1(z_1,z_2,z_3,t), \\
\frac{dz_2}{dt} &= -\frac{\partial H(z_1,z_2)}{\partial z_1} + \epsilon F_2(z_1,z_2,z_3,t), \\
\frac{dz_3}{dt} &= k_3(z_1,z_2) + \epsilon F_3(z_1,z_2,z_3,t)
\end{aligned} \qquad (2.6.46)$$

where we assume that the perturbation is periodic in t with period $T = \frac{2\pi}{\omega}$. The standard Melnikov method has been applied by many authors to the study of fluid particle dynamics in time-periodic perturbations of two-dimensional steady fluid flows, see Rom-Kedar *et al.* [1990] and Camassa and Wiggins [1991] for two specific examples. This method is one of the few methods that enable one to rigorously prove the existence of chaotic dynamics in a specific system as well as obtain an estimate on the size of certain chaotic regions in the flow; it also enables one to obtain an approximate analytical form for the flux across homoclinic and heteroclinic tangles that are created by time-periodic perturbation of separatrices in the steady flow. Melnikov's method is an example of a global, geometrical perturbation method that uses explicit knowledge of the invariant manifold structure of the unperturbed vector field to develop perturbation methods to determine how these invariant manifolds "break up" under the influence of the perturbation. Thus having appropriate coordinates for describing the unperturbed system is crucial for the success of the method. It turns out that the coordinates developed in Section 2 are ideal for this purpose. In fact, in these coordinates for the case where $z_3 \in S^1$ the appropriate Melnikov method is a special case of a method previously developed in Wiggins [1988] (more precisely, in the terminology of this reference, it corresponds to system I with $n = 1$, $m = 0$, and $l = 1$). In the case where $z_3 \in \mathbb{R}^1$ one must require the perturbation to be uniformly bounded in z_3, in which case an identical derivation for the Melnikov function goes through. In this section we describe these Melnikov methods. We do not go into proofs of all the details, for this we refer the reader to Wiggins [1988].

2.6.1 Analytical and geometrical structure of the unperturbed system

The unperturbed system is obtained from (2.6.46) by setting $\epsilon = 0$

$$\begin{aligned} \frac{dz_1}{dt} &= \frac{\partial H(z_1, z_2)}{\partial z_2}, \\ \frac{dz_2}{dt} &= -\frac{\partial H(z_1, z_2)}{\partial z_1}, \\ \frac{dz_3}{dt} &= k_3(z_1, z_2). \end{aligned} \tag{2.6.47}$$

The $z_1 - z_2$ component of (2.6.47) decouples from the z_3 component and thus we can discuss the structure of the phase plane associated with the $z_1 - z_2$ component of (2.6.47), the trajectories of which are given by $H(z_1, z_2) = \text{constant}$. From this we can easily build up a picture of the global dynamics of the full three-dimensional unperturbed system.

Assumption. At $(z_1, z_2) = (z_1^h, z_2^h)$ the $z_1 - z_2$ component of (2.6.47) has a hyperbolic fixed point that is connected to itself by a homoclinic orbit $(z_1^h(t), z_2^h(t))$, i.e.,

$\lim_{t\to\pm\infty}(z_1^h(t), z_2^h(t)) = (z_1^h, z_2^h)$.

From this assumption it follows that the set

$$\mathcal{M}_0 = \left\{(z_1, z_2, z_3) \,|\, z_1 = z_1^h, z_2 = z_2^h\right\} \tag{2.6.48}$$

is a one-dimensional, *normally hyperbolic invariant manifold.* Suspending the system over $\mathbb{R}^3 \times S^1$, $\mathcal{M}_0$ becomes normally hyperbolic, invariant two-torus in the case when the symmetry group is S^1, and a cylinder when the symmetry group is $\mathbb{R}$. Normal hyperbolicity is a technical property that means that, under the linearized dynamics, expansion and contraction rates transverse to the manifold dominate those tangent to the manifold (formal definitions and examples can be found in Wiggins [1988]). The significance of this property is that normally hyperbolic invariant manifolds, along with their stable and unstable manifolds, persist under perturbation. Note that if $z_3 \in S^1$ $\mathcal{M}_0$ is topologically a circle and if $z_3 \in \mathbb{R}$, or some subinterval of $\mathbb{R}$, the $\mathcal{M}_0$ is topologically a curve. Technical problems arise in the issue of the persistence of normally hyperbolic invariant manifolds which are not contained in some compact subdomain of the set on which the vector field is defined. This is treated in Kopell [1985]. The dynamics on $\mathcal{M}_0$ are described by the following equation

$$\frac{dz_3}{dt} = k_3(z_1^h, z_2^h) \tag{2.6.49}$$

having the solution

$$z_3(t) = k_3(z_1^h, z_2^h)t + z_3^0. \tag{2.6.50}$$

If $k_3(z_1^h, z_2^h) = 0$ then $\mathcal{M}_0$ consists entirely of fixed points. In this case, even though the manifold will persist under perturbation, the dynamics *on the manifold* will almost surely be dramatically altered under the perturbation. In the case where $z_3 \in S^1$, $\mathcal{M}_0$ is a periodic orbit, or circle of fixed points if $k_3(z_1^h, z_2^h) = 0$.

It also follows from our assumption on the $z_1 - z_2$ component of (2.6.47) that $\mathcal{M}_0$ has two-dimensional stable and unstable manifolds, denoted $W^s(\mathcal{M}_0)$ and $W^u(\mathcal{M}_0)$, respectively, that coincide along a two-dimensional *homoclinic manifold*, denoted Γ^h, given as follows:

$$\Gamma^h = \left\{(z_1, z_2, z_3) \mid z_1 = z_1^h(t), z_2 = z_2^h(t), -\infty < t < +\infty\right\}. \tag{2.6.51}$$

For $\epsilon = 0$ Γ^h forms a barrier to transport of the fluid as it is an invariant manifold that separates the space into two disjoint pieces. Moreover, such integrable homoclinic structures are often the key feature in the creation of chaotic dynamics under non-integrable perturbations.

2.6.2 The perturbed system and the Melnikov function

Let us consider the system (2.6.47) suspended over $\mathbb{R}^3 \times S^1$ (i.e., include the time as a dynamical variable). $\mathcal{M}_0$ in the unperturbed problem is then a two-torus or a cylinder. As previously mentioned, $\mathcal{M}_0$ along with its stable and unstable manifolds persist under perturbation, denoted $\mathcal{M}_\epsilon$, $W^s(\mathcal{M}_\epsilon)$ and $W^u(\mathcal{M}_\epsilon)$, respectively. However, it now may be the case that $W^s(\mathcal{M}_\epsilon)$ and $W^u(\mathcal{M}_\epsilon)$ *do not* coincide as three-dimensional surfaces and thus create a barrier to the transport of fluid. Indeed, we would expect this to be the case since it is not the typical case for two three-dimensional surfaces to concide in a four-dimensional space. A generalization of Melnikov's method will provide us with an analytical tool for determining certain geometrical properties of $W^s(\mathcal{M}_\epsilon)$ and $W^u(\mathcal{M}_\epsilon)$.

The Melnikov function (up to a nonzero normalization factor) is the first-order term of an expansion in ϵ of the distance between $W^s(\mathcal{M}_\epsilon)$ and $W^u(\mathcal{M}_\epsilon)$. Following the arguments in Wiggins [1988], for systems of the type described in this section it is given by

$$\begin{aligned} M(t_0, z_{30}; \phi_0) = \int_{-\infty}^{+\infty} \Big\{ &\tfrac{\partial H}{\partial z_1}(z_1^h(t), z_2^h(t)) F_1(z_1^h(t), z_2^h(t), z_3^h(t), \omega t + \omega t_0 + \phi_0) \\ &+ \tfrac{\partial H}{\partial z_2}(z_1^h(t), z_2^h(t)) F_2(z_1^h(t), z_2^h(t), z_3^h(t), \omega t + \omega t_0 + \phi_0) \Big\} \, dt \end{aligned} \tag{2.6.52}$$

where

$$z_3^h(t) \equiv \int_0^{t+t_0} k_3(z_1^h(s), z_2^h(s)) ds + z_{30}.$$

The parameter ϕ_0 correspond to the phase of the periodic time-dependence of the perturbation and when considering the Poincaré map it can be regarded as the parameter defining the Poincaré section. In this context t_0 and z_{30} can be viewed as parameters describing points on $W^s(\mathcal{M}_\epsilon)$ and $W^u(\mathcal{M}_\epsilon)$, restricted to the three-dimensional Poincaré section. Points (t_0, z_{30}) at which $\frac{\partial M}{\partial t_0}$ and $\frac{\partial M}{\partial z_{30}}$ are not *both* zero ("simple zeros") correspond to transversal intersections of $W^s(\mathcal{M}_\epsilon)$ and $W^u(\mathcal{M}_\epsilon)$ $\mathcal{O}(\epsilon)$ close to the point $(z_1^h(-t_0), z_2^h(-t_0), z_{30})$ on Γ^h.

2.6.3 Chaos

In the familiar case of time-periodic perturbations of two-dimensional steady flows, transversal intersections of stable and unstable manifolds of an hyperbolic fixed point may give rise to chaotic dynamics. This may also be true in three-dimensions, however there are also more possibilities, depending on the nature of z_3 as well as the dynamics on

$\mathcal{M}_\epsilon$. Below, we describe some possible cases. Our discussion will be in the context of the Poincaré map of (2.6.46) which can be derived similarly to the one discussed in Section 3. We consider the three-dimensional map $(z_1(0), z_2(0), z_3(0)) \mapsto (z_1(T), z_2(T), z_3(T))$. For this three- dimensional map $\mathcal{M}_\epsilon$ is manifested as a one-dimensional invariant curve, denoted $\widehat{\mathcal{M}}_\epsilon$, having two-dimensional stable and unstable manifolds, denoted $W^s(\widehat{\mathcal{M}}_\epsilon)$ and $W^u(\widehat{\mathcal{M}}_\epsilon)$.

1. $\boxed{z_3 \in S^1.}$ In this case $\widehat{\mathcal{M}}_\epsilon$ is an invariant circle (1-torus) and simple zeros of the Melnikov function correspond to transverse homoclinic orbits to a normally hyperbolic invariant 1-torus. In this case theorems in Wiggins [1988] (Theorem 3.4.1) and Beigie *et al.* [1991a,b] imply that chaotic dynamics occurs in the sense that near the homoclinic orbits there exists an invariant Cantor set of curves on which the dynamics is topologically conjugate to a Bernoulli shift. The fluid dynamical significance of this type of chaos has not been studied. In the fluid dynamical context, this case is important for studies of e.g., three-dimensional, time-dependent perturbations of steady axisymmetric swirling vortex rings.

2. $\boxed{z_3 \in \mathbb{R},\ k_3(z_1^h, z_2^h) \neq 0.}$ This is a situation that has received very little investigation mathematically, and none fluid mechanically. Generally speaking, homoclinic orbits give rise to chaotic dynamics when the invariant set to which the orbits are homoclinic is bounded. This allows one to relate the strong stretching and contraction that occurs near the hyperbolic invariant set to the global folding process associated with the homoclinic orbits in such a way that regions can be found which stretch, fold, and map back over themselves. In such a situation the Conley-Moser conditions (Moser [1973]), or certain generalizations of these conditions (Wiggins [1988]), may be applied to prove the existence of chaotic dynamics. If the invariant

set to which the orbits are homoclinic is unbounded, then there may be no recurrence, i.e., an individual orbit may not approach itself during its evolution in time. In particular, for our example, the dynamics on $\widehat{\mathcal{M}}_\epsilon$ are described by the following 1-dimensional map

$$z_3 \mapsto z_3 + k_3(z_1^h, z_2^h)T + \mathcal{O}(\epsilon).$$

Hence orbits on $\widehat{\mathcal{M}}_\epsilon$ are unbounded. Nevertheless, one cannot rule out "infinite time" chaos without a detailed study. Moreover, transient chaos is a very likely possibility; such situations have also not been studied from the point of view of fluid mechanics. This case applies to e.g., three-dimensional, time-dependent perturbations of steady flows in helical pipes with helical symmetry.

3. $\boxed{z_3 \in \mathbb{R},\ k_3(z_1^h, z_2^h) = 0.}$ In this case it may be possible to find recurrent motions, in particular periodic orbits, on $\mathcal{M}_\epsilon$. The dynamics on $\mathcal{M}_\epsilon$ is described by the following nonautonomous ordinary differential equations

$$\begin{aligned} \dot{z}_3 &= \epsilon F_3(z_1^h, z_2^h, z_3, t) + \mathcal{O}(\epsilon^2), \\ \dot{t} &= 1, \end{aligned} \tag{2.6.53}$$

which is in the standard form for applying the *method of averaging* (see, e.g., Wiggins [1990]). We consider the associated averaged equation

$$\dot{z}_3 = \epsilon \bar{F}_3(z_1^h, z_2^h, z_3), \tag{2.6.54}$$

where

$$\bar{F}_3(z_1^h, z_2^h, z_3) \equiv \frac{1}{T}\int_0^T F_3(z_1^h, z_2^h, z_3, t)dt.$$

It follows from the averaging theorem that hyperbolic fixed points of (2.6.54), denoted $z_3 = \bar{z}_3$, correspond to periodic orbits (with period T) of (2.6.53). These, in turn, correspond to hyperbolic fixed points of the associated Poincaré map. In this case, simple zeros in t_0 of the Melnikov function (2.6.52), with z_{30} fixed at $z_{30} = \bar{z}_{30}$, correspond to orbits homoclinic to a hyperbolic fixed point. In this case the Smale-Birkhoff theorem applies so that we can conclude the existence of chaotic dynamics. If (2.6.54) has no fixed points then the disussion from case 2 applies. The fluid mechanical application in this case are clear: three-dimensional time-dependent perturbations of two-dimensional steady flows (in which case $k_3(z_1, z_2) = 0$ for all z_1, z_2) .

2.6.4 Autonomous systems

Suppose that the perturbations are autonomous, but break the volume-preserving symmetry. Then the perturbed system has the form

$$\begin{aligned}
\frac{dz_1}{dt} &= \frac{\partial H(z_1, z_2)}{\partial z_2} + \epsilon F_1(z_1, z_2, z_3),\\
\frac{dz_2}{dt} &= -\frac{\partial H(z_1, z_2)}{\partial z_1} + \epsilon F_2(z_1, z_2, z_3),\\
\frac{dz_3}{dt} &= k_3(z_1, z_2) + \epsilon F_3(z_1, z_2, z_3). \qquad (2.6.55)
\end{aligned}$$

The development of the Melnikov theory goes through identically as before, except that the Melnikov function (2.6.52) in this case *does not* depend on ϕ_0.

We next discuss how chaos arises in such systems along the lines of the discussion above. The possible fluid mechanical applications are the same as in the time-dependent case, with the exception that the perturbed flows are also steady.

1. $\boxed{z_3 \in S^1,\ k_3(z_1^h, z_2^h) \neq 0.}$ In this case $\mathcal{M}_\epsilon$ is a periodic orbit and simple zeros of the Melnikov function correspond to transverse homoclinic orbits to a hyperbolic periodic orbit. In this case the standard Smale-Birkhoff homoclinic theorem applies so that we can conclude that we have "Smale horseshoe" type chaos. That is, near the homoclinic orbits ther exists an invariant Cantor set on which the dynamics is topologically conjugate to a Bernoulli shift.

2. $\boxed{z_3 \in \mathbb{R},\ k_3(z_1^h, z_2^h) \neq 0.}$ In this case the discussion for the nonautonomous case still holds.

3. $\boxed{z_3 \in \mathbb{R} \text{ or } z_3 \in S^1,\ k_3(z_1^h, z_2^h) = 0.}$ This case requires some slight modifications. In this case the dynamics on $\mathcal{M}_\epsilon$ is described by the following one-dimensional, *autonomous* ordinary differential equation

$$\dot{z}_3 = \epsilon F_3(z_1^h, z_2^h, z_3) + \mathcal{O}(\epsilon^2). \tag{2.6.56}$$

Since (2.6.56) is autonomous, we need not apply the method of averaging. Hyperbolic fixed points of (2.6.56), denoted $z_{30} = \bar{z}_{30}$, correspond to hyperbolic fixed points of (2.6.55). In this case, a zero of the Melnikov function (2.6.52), with z_{30} fixed at $z_{30} = \bar{z}_{30}$, correspond to orbits homoclinic to a hyperbolic fixed point of an autonomous ordinary differential equation. For this situation different mechanisms for chaos are possible; in particular the "Silnikov mechanisms" and "Lorenz mechanisms" as described in Wiggins [1990]. (Note: there is a technical problem with this situation that is easily handled. Namely, once z_3 is fixed at the value corresponding to a hyperbolic fixed point on $\mathcal{M}_\epsilon$ then the Melnikov function is just a number. Recall that it is just the leading order term in the expansion of the distance between the stable and unstable manifolds of $\mathcal{M}_\epsilon$. In order to show that the leading order term dominates the expression for the distance an argument using the implicit function theorem is required. This is the reason why one needs "simple" zeros in t_0 or z_3. This problem can be remedied if there are external parameter(s) in the system; in this case one need only require that the derivative with respect to an external parameter of the Melnikov function at its zero is not zero. More background on this issue can be found in Wiggins [1988].)

2.7 Examples

In this section we illustrate the techniques with three examples.

2.7.1 Example 1. Euler flow with two-dimensional elliptic vortex lines

Consider the following velocity field, $\mathbf{v}$:

$$\begin{aligned}
\frac{dx_1}{dt} &= ax_1, \\
\frac{dx_2}{dt} &= ax_2, \\
\frac{dx_3}{dt} &= bx_1^2 + cx_2^2 - 2ax_3,
\end{aligned} \tag{2.7.57}$$

where a, b and c are arbitrary coefficients.

The vorticity field of (2.7.57) is given by

$$\omega = (2cx_2, -2bx_1, 0). \tag{2.7.58}$$

It is easy to check that $\mathbf{v}$ and ω satisfy

$$[\mathbf{v}, \omega] = 0. \tag{2.7.59}$$

Moreover, both $\mathbf{v}$ and ω are autonomous and divergence free, therefore

- $\mathbf{v}$ is an Euler flow
- ω is an infinitesimal generator of a volume-preserving, spatial symmetry group for $\mathbf{v}$.

We want to find two functionally independent invariants for ω. These invariants satisfy

$$\omega_{x_1}\frac{\partial f}{\partial x_1}+\omega_{x_2}\frac{\partial f}{\partial x_2}+\omega_{x_3}\frac{\partial f}{\partial x_3}=0, \tag{2.7.60}$$

where $(\omega_{x_1},\omega_{x_2},\omega_{x_3}) = (2cx_2,-2bx_1,0)$. The classical theory of such equations shows (e.g., Olver [1986]) that the general solution of (2.7.60) can be found by integrating the corresponding system of equations

$$\begin{aligned}\frac{dx_1}{dx_2} &= \frac{\omega_{x_1}}{\omega_{x_2}},\\ \frac{dx_3}{dx_2} &= \frac{\omega_{x_3}}{\omega_{x_2}},\end{aligned} \tag{2.7.61}$$

where we assumed $\omega_{x_2}\neq 0$.

The solutions to (2.7.60) are then given by the functions $y_1(x_1,x_2,x_3), y_2(x_1,x_2,x_3)$ which satisfy

$$\begin{aligned}y_1(x_1,x_2,x_3) &= c_1,\\ y_2(x_1,x_2,x_3) &= c_2,\end{aligned} \tag{2.7.62}$$

where c_1, c_2 are the constants of integration for (2.7.61). Note that here we use the same notation for new coordinates as in the proof of the Theorem (2.2.2). In particular, y_1,y_2,y_3 denote the coordinates in which the infinitesimal generator of the symmetry group is rectified.

For simplicity we will assume $c = 1/2, b = 1, a = 1/2$. In that case, the equations corresponding to (2.7.61) are

$$\begin{aligned} \frac{dx_1}{dx_2} &= \frac{-x_2}{2x_1}, \\ \frac{dx_3}{dx_2} &= 0. \end{aligned}$$

Integrating these gives $\sqrt{x_2^2 + 2x^2} = c1, x_3 = c2$. Therefore,

$$\begin{aligned} y_1 &= \sqrt{x_2^2 + 2x_1^2}, \\ y_2 &= x_3. \end{aligned}$$

To find y_3 we need to solve

$$\omega_{x_1}\frac{\partial f}{\partial x_1} + \omega_{x_2}\frac{\partial f}{\partial x_2} + \omega_{x_3}\frac{\partial f}{\partial x_2} = 1,$$

or, in our case

$$x_2\frac{\partial f}{\partial x_1} - 2x_1\frac{\partial f}{\partial x_2} = 1.$$

The solution to this equation is found to be $f = (1/\sqrt{2})\arctan(\frac{\sqrt{2}x_1}{x_2})$, so

$$y_3 = \frac{1}{\sqrt{2}}\arctan(\frac{\sqrt{2}x_1}{x_2}).$$

The velocity field in new coordinates is now given by

$$\begin{aligned}
\frac{dy_1}{dt} &= \frac{1}{2}y_1, \\
\frac{dy_2}{dt} &= \frac{1}{2}y_1^2 - y_2, \\
\frac{dy_3}{dt} &= 0.
\end{aligned} \tag{2.7.63}$$

We can calculate the Jacobian of the transformation $x_i = x_i(y_1, y_2, y_3), i = 1, ..., 3$ to be

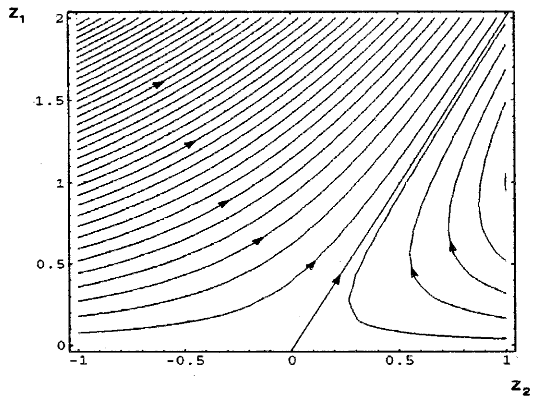

Figure 2.1: Phase portrait of the Hamiltonian part of (2.7.64).

y_1, and write (2.7.63) as

$$\begin{aligned}
\frac{dy_1}{dt} &= \frac{1}{y_1}\frac{\partial K(y_1, y_2)}{\partial y_2}, \\
\frac{dy_2}{dt} &= -\frac{1}{y_1}\frac{\partial K(y_1, y_2)}{\partial y_1}, \\
\frac{dy_3}{dt} &= 0,
\end{aligned}$$

where $K = -y_1^4/8 + y_2\ y_1^2/2$ is an integral of motion for (2.7.63). Making a further transformation $(z_1, z_2, z_3) = (y_1^2/2, y_2, y_3)$, which corresponds to (2.2.22) in the proof of the Theorem (2.2.2), our system takes the form

$$\begin{aligned} \frac{dz_1}{dt} &= \frac{1}{2}z_1 &= \frac{\partial H(z_1,z_2)}{\partial z_2}, \\ \frac{dy_2}{dt} &= z_1 - z_2 &= -\frac{\partial H(z_1,z_2)}{\partial z_2}, \\ \frac{dy_3}{dt} &= 0, \end{aligned} \tag{2.7.64}$$

where $H(z_1, z_2) = z_1 z_2 - z_1^2/2$ (see figure (2.1)). In x coordinates $H = -(x_2^2 + 2x_1^2)^2/8 + x_3(x_2^2 + 2x_1^2)/2$. It is clear from this that the velocity field (2.7.57) represents the flow of an inviscid fluid around an elliptical paraboloid given by $(x_2^2 + 2x_1^2)/4 - x_3 = 0$. We see that the transformation to symmetry coordinates simplifies the vector field significantly. In particular, in the new, symmetry coordinates the vector field is linear, two of its components form a decoupled Hamiltonian system, and one of the components is zero.

Note that y_3 in this example is defined on S^1. This is a consequence of the fact that the group acting on the flow is S^1. We now give an example where the group acting on the flow is $\mathbb{R}^1$.

2.7.2 Example 2. Euler flow with two-dimensional hyperbolic vortex lines

Consider the velocity field

$$\begin{aligned} \frac{dx_1}{dt} &= ax_1 + ax_2, \\ \frac{dx_2}{dt} &= ax_1 + ax_2, \\ \frac{dx_3}{dt} &= bx_1^2 - bx_2^2 - 2ax_3. \end{aligned}$$

The vorticity field associated with this velocity field is given by

$$\omega = (-2bx_2, -2bx_1, 0).$$

This flow is also a steady Euler flow, as can be verified by direct calculation. We assume that $b = 1/2, a = 1$. It is easy to see that the vortex lines are hyperbolas described by the equations

$$\begin{aligned} x_1^2 - x_2^2 &= c_3, \\ x_3 &= c_4. \end{aligned}$$

Hence, functionally independent invariants y_1 and y_2 are given by

$$\begin{aligned} y_1 &= x_1^2 - x_2^2, \\ y_2 &= x_3, \end{aligned}$$

(we could have obtained these through the same formal procedure as in Example 1., in particular solving the analogues of (2.7.61)). Also, using the same methods as in the Example 1. we can find y^3:

$$y_3 = -\tanh^{-1}\frac{x_1}{x_2}.$$

In the y_1, y_2, y_3 coordinates the velocity field is given by

$$\frac{dy_1}{dt} = 2y_1,$$

$$\frac{dy_2}{dt} = \frac{1}{2}y_1 - 2y_2,$$
$$\frac{dy_3}{dt} = -1. \tag{2.7.65}$$

We can immediatelly recognize that it has the following form

$$\frac{dy_1}{dt} = \frac{\partial H}{\partial y_2},$$
$$\frac{dy_2}{dt} = -\frac{\partial H}{\partial y_1},$$
$$\frac{dy_3}{dt} = -1,$$

where

$$H = -y_1^2/4 + 2y_1y_2 = -(x_1^2 - x_2^2)^2/4 + 2(x_1^2 - x_2^2)x_3.$$

The major difference between this example and Example 1. is that in this example y_3 is defined on $\mathbb{R}^1$ which is a consequence of the fact that the symmetry group is $\mathbb{R}^1$. Note that this flow describes a flow in a wedge which is three dimensional, although the wedge bounded by $\{(x_1, x_2, x_3) | x_1 = x_2,\ x_2 > 0\} \cup \{(x_1, x_2, x_3) | x_1 = -x_2,\ x_2 > 0\}$ is two-dimensional.

2.7.3 Example 3. Action-angle-angle coordinates

Consider the following flow:

$$\frac{dx_1}{dt} = x_3x_1 - 2c\frac{x_2}{x_1^2 + x_2^2},$$
$$\frac{dx_2}{dt} = x_3x_2 + 2c\frac{x_1}{x_1^2 + x_2^2},$$

$$\frac{dx_3}{dt} = 1 - 2(x_1^2 + x_2^2) - x_3^2.$$

In cylindrical coordinates the flow is given by

$$\begin{aligned}\frac{dr}{dt} &= rz,\\ \frac{dz}{dt} &= 1 - 2r^2 - z^2,\\ \frac{d\theta}{dt} &= \frac{2c}{r^2},\end{aligned} \tag{2.7.66}$$

where c is an arbitrary constant. In a fluid mechanical context, $c/2$ is the circulation. The flow (2.7.66) is a superposition of a well-known Hill's spherical vortex with a line vortex on the z axis, which induces a *swirl* velocity $\dot{\theta} = 2c/r^2$. That the superposition of these two flows is possible comes from the following argument: The vorticity equation in Cartesian components is given by

$$\frac{\partial \omega_i}{\partial t} + v_j \frac{\partial \omega_i}{\partial x_j} - \omega_j \frac{\partial v_i}{\partial x_j} = 0,$$

where v_i is the i-th component of the velocity vector $\mathbf{v}$, and ω_i is the i-th component of the vorticity $\omega = \nabla \times \mathbf{v}$. Suppose that $\mathbf{v}$ consists of the superposition of two vector fields, each of which satisfies the vorticity equation:

$$\mathbf{v} = \mathbf{v}^1 + \mathbf{v}^2.$$

Then the vorticity equation for $\mathbf{v}$ reads

$$\frac{\partial \omega_i^1}{\partial t} + \frac{\partial \omega_i^2}{\partial t} + (v_j^1 + v_j^2)\frac{\partial(\omega_i^1 + \omega_i^2)}{\partial x_j} - (\omega_j^1 + \omega_j^2)\frac{\partial(v_i^1 + v_i^2)}{\partial x_j} = 0,$$

and upon rearranging

$$\frac{\partial \omega_i^1}{\partial t} + v_j^1 \frac{\partial \omega_i^1}{\partial x_j} - \omega_j^1 \frac{\partial v_i^1}{\partial x_j} + \frac{\partial \omega_i^2}{\partial t} + v_j^2 \frac{\partial \omega_i^2}{\partial x_j} - \omega_j^2 \frac{\partial v_i^2}{\partial x_j} + v_j^1 \frac{\partial \omega_i^2}{\partial x_j} - \omega_j^2 \frac{\partial v_i^1}{\partial x_j} + v_j^2 \frac{\partial \omega_i^1}{\partial x_j} - \omega_j^1 \frac{\partial v_i^2}{\partial x_j} = 0.$$

Assuming steadyness, and using the fact that both vector fields satisfy the vorticity equation, their sum will satisfy the vorticity equation if

$$[\mathbf{v}^1, \omega^2] = [\mathbf{v}^2, \omega^1],$$

where $[\cdot,\cdot]$ denotes the Lie bracket of two vector fields. This has been already known to Truesdell [11], without a Lie bracket interpretation. Let the Hill's spherical vortex be denoted by a superscript 1, and the flow induced by a line vortex at z axis by a superscript 2. Now, the flow induced by the line vortex at the z axis is irrotational, so $\omega^2 = 0$ except at the z axis. Further, it is easy to check that $\mathbf{v}^2$ and ω^1 commute. The fact that the line vortex is singular at the z axis is largely irrelevant for the dynamics, as the z axis is invariant for both flows. The new flow can be termed "swirling Hill's vortex." So, (2.7.66) satisfies Euler's equations of motion for an inviscid incompressible fluid everywhere except on the z axis, where the swirl velocity becomes infinite. Note that we use r, z, θ instead of y_1, y_2, y_3 as notation for the "symmetry" coordinates in this example. We transform the first two components of (2.7.66) into canonical Hamiltonian form, by letting $R = r^2/2$ (this is another example of the transformation (2.2.22)). The system (2.7.66) then becomes

$$\begin{aligned} \frac{dR}{dt} &= 2Rz, \\ \frac{dz}{dt} &= 1 - 4R - z^2, \\ \frac{d\theta}{dt} &= \frac{c}{R}, \end{aligned}$$

(2.7.67)

with the $R-z$ components having the form

$$\frac{dR}{dt} = \frac{\partial H(R,z)}{\partial z},$$
$$\frac{dz}{dt} = -\frac{\partial H(R,z)}{\partial R},$$

(2.7.68)

where $H(R,z) = Rz^2 - R + 2R^2$ is the Hamiltonian. Following the procedure in section 2. we will first transform (2.7.68) to action angle variables (I,ϕ_1), and then derive the second angle variable, ϕ_2. It is easy to check that (2.7.68) satisfies the assumption from the section 2. In particular, there is an elliptic fixed point at $z = 0, R = 1/4$ surrounded by a family of periodic solutions. There are two more fixed poins for (2.7.68), at $R = 0, z = \pm 1$, which are hyperbolic. The integral H takes the values between 0 and $-1/8$ with the first value corresponds to the separatrices connecting the hyperbolic points, which are given by $\{(R,z)|R = 0, -1 < z < 1\} \cup \{(R,z)|2R+z^2 = 1\}$. $H = -1/8$ corresponds to the elliptic fixed point (see figure (2.2)). The action variable is given by (see (2.3.31))

$$I = \frac{1}{2\pi}\int_{H=const.} z dR$$
$$= \frac{2}{2\pi}\int_{R_{min}}^{R_{max}} z dR,$$

(2.7.69)

where R_{min}, R_{max} denote the values of R where a level set of H intersects R axis. These can easily be computed and found to be

$$R_{min} = \frac{1}{4}(1 - \sqrt{1+8H}),$$
$$R_{max} = \frac{1}{4}(1 + \sqrt{1+8H}).$$

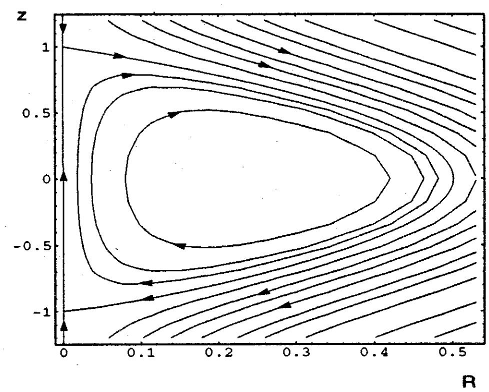

Figure 2.2: Phase portrait of (2.7.68).

(In passing from the first to the second form of the integral in (2.7.69) we used the reflectional symmetry of the level sets of H around $z = 0$. From the expression for the Hamiltonian function we have

$$z = \pm\sqrt{\frac{H + R - 2R^2}{R}}. \tag{2.7.70}$$

We also have the equation

$$H + R - 2R^2 = 2(R_{max} - R)(R - R_{min}). \tag{2.7.71}$$

Using (2.7.70) and (2.7.71), (2.7.69) becomes

$$\begin{aligned} I &= \frac{1}{\pi}\int_{R_{min}}^{R_{max}} \sqrt{\frac{H + R - 2R^2}{R}} dR, \\ &= \frac{\sqrt{2}}{\pi}\int_{R_{min}}^{R_{max}} \sqrt{\frac{(R_{max} - R)(R - R_{min})}{R}} dR. \end{aligned} \tag{2.7.72}$$

The integral in (2.7.72) can be evaluated in terms of elliptic integrals as found e.g. in

Gradshteyn/Ryzhik [1980]. So,

$$\begin{aligned} I &= \frac{2\sqrt{2}}{3\pi}\left[\frac{1}{2}E(\frac{\pi}{2},\sqrt{1-\frac{R_{min}}{R_{max}}}) - 2R_{min}F(\frac{\pi}{2},\sqrt{1-\frac{R_{min}}{R_{max}}})\right], \\ &= \frac{2\sqrt{2}}{3\pi}\left[\frac{1}{2}E(p) - 2R_{min}K(p)\right], \end{aligned} \tag{2.7.73}$$

where $F(\phi,p)$, $E(\phi,p)$ are elliptic integrals of the first and second kind, respectively, $K(p)$, $E(p)$ are the associated complete elliptic integrals, R_{min},R_{max} are as defined above, and

$$p = \sqrt{1-\frac{R_{min}}{R_{max}}}.$$

The first angle variable, ϕ_1, is given by (cf. (2.3.32))

$$\phi_1 = \frac{2\pi}{T(H)}t, \tag{2.7.74}$$

where t is the time measured from some reference point on the orbit (in our case the point $(R_{min}, 0)$), and $T(H)$ is the period of the orbit corresponding to the level set of H in the $R-z$ plane. We then must first calculate the period T on the orbits in $R-z$ plane which is given by

$$T(H) = 2\int_{R_{min}}^{R_{max}} \frac{dR}{\dot{R}}. \tag{2.7.75}$$

From (2.7.67),(2.7.70),(2.7.71), (2.7.75) we obtain

$$\begin{aligned} T(H) &= \frac{1}{\sqrt{2}}\int_{R_{min}}^{R_{max}} \frac{1}{\sqrt{R(R_{max}-R)(R-R_{min})}}dR, \\ &= \frac{\sqrt{2}}{\sqrt{R_{max}}}F(\frac{\pi}{2},\sqrt{\frac{R_{max}-R_{min}}{R_{max}}}) \\ &= \sqrt{\frac{2}{R_{max}}}K(p). \end{aligned} \tag{2.7.76}$$

To complete the calculation for ϕ_1 we need the time t. We have to distinguish between the cases $z > 0$ and $z < 0$. In particular, for $z > 0$

$$\begin{aligned} t_{z>0} &= \int_{R_{min}}^{R} \frac{dR}{\dot{R}}, \\ &= \frac{1}{2\sqrt{2}} \int_{R_{min}}^{R} \frac{dR}{\sqrt{R(R_{max}-R)(R-R_{min})}}. \end{aligned}$$

We can integrate the last expression to obtain

$$t_{z>0} = \frac{1}{\sqrt{2R_{max}}} F(\arcsin \sqrt{\frac{R_{max}(R-R_{min})}{R(R_{max}-R_{min})}}, p).$$

In the case when $z < 0$ we have

$$\begin{aligned} t_{z<0} &= \int_{R_{min}}^{R_{max}} \frac{dR}{\dot{R}} + \int_{R_{max}}^{R} \frac{dR}{\dot{R}}, \\ &= \frac{T(H)}{2} + \int_{R_{max}}^{R} \frac{dR}{\dot{R}} \\ &= \frac{T(H)}{2} + \frac{1}{2\sqrt{2}} \int_{R}^{R_{max}} \frac{dR}{\sqrt{R(R_{max}-R)(R-R_{min})}}. \end{aligned}$$

So,

$$t_{z<0} = \frac{T(H)}{2} + \frac{2\sqrt{2}}{\sqrt{R_{max}}} F(\arcsin \sqrt{\frac{R_{max}-R}{R_{max}-R_{min}}}, p).$$

Thus we have completed the calculation of all terms needed in (2.7.74). We now turn to the calculation of ϕ_2. Using Theorem (2.3.1) from section 2. ϕ_2 (in the notation of this section) is given by

$$\phi_2 = \theta + \frac{\Delta\theta}{2\pi}\phi_1 - \int_0^{\phi_1} \frac{h_3(I,\hat{\phi}_1)}{\Omega_1(I)} d\hat{\phi}_1, \tag{2.7.77}$$

where

$$\Delta\theta = \int_0^{2\pi} \frac{h_3(I,\hat{\phi}_1)}{\Omega_1(I)} d\hat{\phi}_1.$$

Fortunately, we do not have to find the inverse of the transformation $I = I(R, z), \phi_1 = \phi_1(R, z)$ in order to calculate the neccessary terms in (2.7.77), as we can replace the integration on ϕ_1 with the integration on t and, in turn, integration on R. Thus

$$\begin{aligned}\triangle\theta &= \int_{R_{min}}^{R_{max}} \frac{\dot{\theta}}{\dot{R}} dR \\ &= \frac{2c}{\sqrt{2}} \int_{R_{min}}^{R_{max}} \frac{1}{\sqrt{R^3(R_{max}-R)(R-R_{min})}} dR,\end{aligned}$$

which can be evaluated as

$$\begin{aligned}\triangle\theta &= \frac{c\sqrt{2}}{R_{min}\sqrt{R_{max}}} E\left(\frac{\pi}{2}, \sqrt{\frac{R_{max}-R_{min}}{R_{max}}}\right) \\ &= c\frac{\sqrt{2}}{R_{min}\sqrt{R_{max}}} E(p).\end{aligned}$$

Next we calculate

$$J = \int_0^{\phi_1} \frac{h_3(I,\hat{\phi}_1)}{\Omega_1(I)} d\hat{\phi}_1$$

for the cases $z > 0$ and $z < 0$. We have, for $z > 0$

$$J_{z>0} = \frac{c}{2\sqrt{2}} \int_{R_{min}}^{R} \frac{1}{\sqrt{R^3(R_{max}-R)(R-R_{min})}} dR.$$

Thus we obtain

$$J_{z>0} = \frac{c}{R_{min}\sqrt{2R_{max}}} E\left(\arcsin\sqrt{\frac{R_{max}(R-R_{min})}{R(R_{max}-R_{min})}}, p\right).$$

Similarly,

$$J_{z<0} = \frac{\triangle\theta}{2} + \frac{c}{R_{min}\sqrt{2R_{max}}}\left[E\left(\arcsin\sqrt{\frac{R_{max}-R}{R_{max}-R_{min}}}, p\right) - \sqrt{\frac{(R_{max}-R)(R-R_{min})}{R}}\right].$$

Thus we calculated all the terms neccessary for the completition of the transformation to action-angle-angle coordinates.

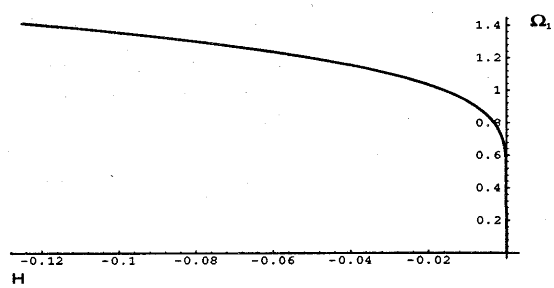

Figure 2.3: Frequency Ω_1.

The frequencies, Ω_1 and Ω_2 are given by (cf. section 2. and figures (2.3),(2.4),(2.5))

$$\begin{aligned} \Omega_1(H(I)) &= \frac{2\pi}{T(H)} = \frac{\pi\sqrt{2R_{max}}}{K(p)} \\ \Omega_2(H(I)) &= \frac{\Omega_1(H(I))\Delta\theta}{2\pi} = \frac{cE(p)}{R_{min}K(p)}. \end{aligned}$$

Now I is a monotone function of H (see figure (2.6)) so, for a particular analytic perturbation, having frequencies expressed as functions of H, we can check the nondegeneracy condition required for the validity of the KAM-type theorem stated in Section 4.

2.8 Conclusions

In this chapter we developed necessary dynamical systems tools for the analysis of three-dimensional, nonautonomous or autonomous vector fields which admit a volume-preserving spatial symmetry group. We proved that such flows admit a very simple coordinate representation. That representation allowed us to develop *action-angle-angle*

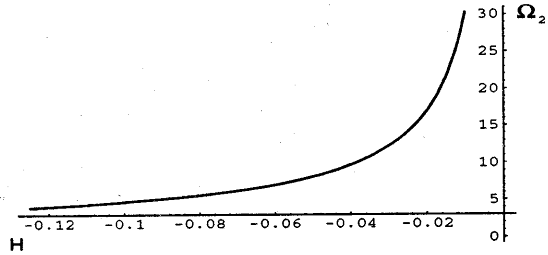

Figure 2.4: Frequency Ω_2.

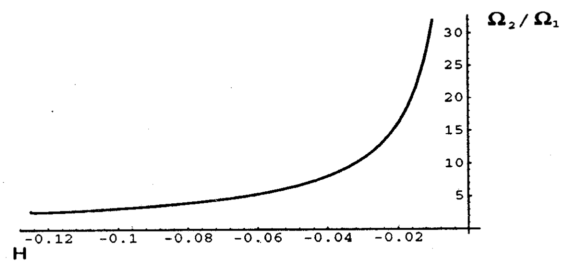

Figure 2.5: Frequency ratio.

variables and appropriate *homoclinic coordinates*, which gave rise to development of KAM-type theory and Melnikov theory, respectively. The range of applicability of these methods is quite large: it is clear from section 4 that Euler flows always possess such

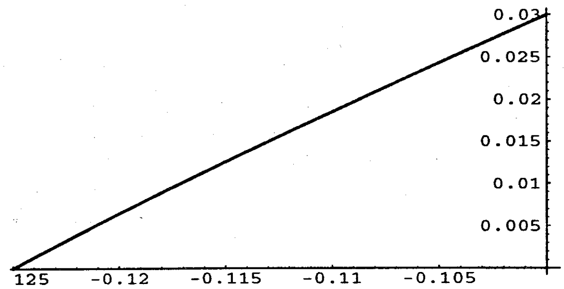

Figure 2.6: Action variable I as a function of the integral of motion, H.

a symmetry. By a direct analogy, steady magnetohydrodynamic flows in frozen-field approximation always have a magnetic field as an infinitesimal generator of a volume-preserving symmetry group. Through the geometry of the problem, it is often easy to conclude that a certain flow has a symmetry: such is the case, for example for flows in non-straight pipes, where the symmetry group is usually the translation along the axis of the pipe. That symmetry is clearly volume-preserving. In fluid mechanics, flows of the form (2.2.12) are called *regular duct flows.* Franjione and Ottino [1991] proved the linearity of stretching for such flows. There are recent experiments on chaotic three-dimensional flows performed by Kusch and Ottino [1991], in which one of the examples (the EHAM flow) is amenable to the type of the analysis we are proposing. In particular, the chaoticity of the motion is due to the time dependence of a cross-sectional flow, and it may be assumed that there is a translational symmetry in the direction of the z axis. Modifications of such flows, such as the ones shown in Figure 21 of Kusch and Ottino [1991] should also admit our analysis. The KAM-type theory developed in section 5 can be used to explain the persistence of invariant cylinders in these experiments. Melnikov method developed in section 6 can serve as a basis for the development of *lobe dynamics* in three-dimensional flows, along the same lines as for two-dimensional flows, as presented in Rom-Kedar et al. [1990]. The transport problems in chaotic three-dimensional fluid flows can thus be assesed and some of the issues of transport, raised by the previously mentioned experiments, resolved.

We also explained the geometrical meaning of so-called Clebsch variables, thus explaining why there is a Hamiltonian structure for a Euler flow when represented in those variables.

Let us mention here that the local reduction procedure developed here admits a geometrical generalization in the spirit of symplectic reduction for Hamiltonian systems (Marsden-Weinstein [1972]). Also, instead of restricting our attention to three-dimensional systems, we can consider n-dimensional flows preserving some n-form. By performing reduction (i.e., transformation of coordinates analogous to the one presented in this chapter for the three-dimensional case) we end up with an $n-1$ dimensional system preserving an $n-1$ form. Clearly, we cannot claim in general the Hamiltonian structure of the resulting $n-1$ dimensional system, as $n-1$ can be odd.

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Chapter 3

Birkhoff's ergodic theorem and statistical properties of dynamical systems

3.1 Introduction

One of the most famous results in ergodic theory is Birkhoff's ergodic theorem (B.E.T.). It plays a major role in the theory presented in this chapter. Thus we begin by stating this theorem.

Theorem 3.1.1 *Let $(A, \mathcal{A}, \mu)$ be a probability space with the and $T : A \to A$ a measure-preserving map (discrete time) , or T^t a one-parameter group of measure preserving automorphisms of A (continuous time). Then,*

1. *If f is an integrable function on A, the set $\Sigma \subset A$ on which the limit*

$$f^*(x) = \lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n-1} f \circ T^i(x) \qquad \textit{discrete time,} \tag{3.1.1}$$

or,

$$f^*(x) = \lim_{T\to\infty} \frac{1}{T} \int_0^T f \circ T^t(x)dt \qquad \textit{continuous time,} \tag{3.1.2}$$

exists is of measure 1.

2. *The function f^* is integrable and*

$$\int_A f^* d\mu = \int_A f d\mu. \tag{3.1.3}$$

3. *f^* is an invariant function under T, i.e.,*

$$f^*(Tx) = f^*(x) \qquad \textit{discrete time,}$$

or

$$f^*(T^t x) = f^*(x) \qquad \textit{continuous time.}$$

In the last 20 years vigorous research on the properties of so-called chaotic dynamical systems has taken place with the involvement of physicists, engineers and mathematicians. These investigations have usually concentrated on low-dimensional dynamical systems that exhibit both regular and chaotic behaviour. The rapid advance and availability of computing power has greatly facilitated studies of the global analysis of low dimensional dynamical systems as well as studies of the statistical properties of large ensembles of orbits. In this chapter we hope to show that Birkhoff's ergodic theorem can play a major role in proving numerically inspired conjectures about the statistical properties of dynamical systems.

Besides B.E.T., another important concept in our work is the *ergodic partition* of the phase space (for the formal definition, see section 2). From a pure mathematicians point of view, Hamiltonian systems are typically non-ergodic. This has been proved, using the KAM theory, by Markus and Meyer [M-M]. From a statistical physicists point of view (Palmer [Pal]), "broken ergodicity" (or non-ergodicity) is a general phenomenon. Numerical studies of large numbers of coupled symplectic maps and nonlinear large Hamiltonian systems show regimes in which non-ergodicity is apparent (Livi *et al.* [L-P-R-S-V], [L-P-R-V], Falcioni *et al.* [F-M-V]). Numerous studies of area preserving maps show that examples of mixed regular and stochastic behaviour are abundant. It is interesting then to ask whether the phase space can be partitioned into invariant components, such that on each of those components, the dynamical system is ergodic. This question has been answered positively in the works of von Neumann [N] and Rokhlin [R], who introduced the notion of the *ergodic partition.* In more recent work (Palmer [Pal]) on broken ergodicity in statistical mechanical systems arising in condensed matter physics, a similar idea has been put forward, and the statistical mechanical formalism for non-ergodic systems (or, those with several ergodic components) has been developed.

We will show that B.E.T., coupled with the notion of the ergodic partition of the phase space, (see Section 2), and different methods from probability theory are very useful tools for proving numerically or experimentally obtained conjectures about the statistical properties of deterministic dynamical systems. To justify this, let us mention some of the numerical and experimental works that have either motivated developments in this chapter, or can be analysed by the methods developed herein.

One statistical property often considered in numerical studies of chaotic transport is the mean square displacement $D(t)$ at time t of trajectories or orbits of a dynamical system. The dynamical system may be either a map (in which case t is discrete) or a flow. Typically, one tries to determine the positive exponent γ in the following expression such that the indicated asymptotic limit is obtained, and is nonzero:

$$\lim_{t\to\infty} \frac{D(t)}{t^\gamma}.$$

If $\gamma = 1$ then the behavior is referred to as *diffusive* and if $\gamma \neq 1$ then the term *anomalous diffusion* is used.

In early stŭdies of two-dimensional, area-preserving maps, it had been observed that the diffusion coefficient, defined as

$$D = \lim_{t\to\infty} \frac{D(t)}{t},$$

diverges in the presence of so-called "accelerator modes." In particular, Cary and Meiss [C-M] observed that D diverges for a certain regime of the "sawtooth map," but a quantity that they refer to as the "streaming coefficient," S, defined by

$$S = \lim_{t\to\infty} \frac{D(t)}{t^2}, \tag{3.1.4}$$

converges. Let us consider the issue of "diffusion" in maps more generally and describe a general mathematical framework.

Example 1.1 (Diffusion in Maps)

Let us consider a two-dimensional, area-preserving, discrete dynamical system, or map, T, defined on some domain $\mathcal{D}$ which is either the torus, the *finite* cylinder, or some compact invariant subset of $\mathbb{R}^2$, having the following form:

$$x_{i+1} \quad = x_i + f_1(x_i, y_i),$$

$$y_{i+1} = y_i + f_2(x_i, y_i). \tag{3.1.5}$$

The x_n component of the point (x_n, y_n) is written as

$$x_n = x_0 + \sum_{i=0}^{n-1} f_1(x_i, y_i) = x_0 + \sum_{i=0}^{n-1} f_1 \circ T^i(x_0, y_0).$$

Let $p(x_0, y_0)$ be some initial distribution of points such that its integral over the domain is equal to 1. Then

$$\begin{aligned} \langle x_n - x_0 \rangle &= \int_{\mathcal{D}} (x_n(x_0, y_0) - x_0) p(x_0, y_0) dx_0 dy_0 \\ &= \int_{\mathcal{D}} \left(\sum_{i=0}^{n-1} f_1 \circ T^i(x_0, y_0) \right) p(x_0, y_0)) dx_0 dy_0 \end{aligned} \tag{3.1.6}$$

denotes the mean value of x at the $n-th$ iteration. The mean square displacement associated with the x coordinate is defined as

$$\begin{aligned} D(n) &= \int_{\mathcal{D}} [x_n - x_0 - \langle x_n - x_0 \rangle]^2 p(x_0, y_0) dx_0 dy_0 \\ &= \int_{\mathcal{D}} [\sum_{i=0}^{n-1} f_1 \circ T^i(x_0, y_0) \\ &\quad - \langle \sum_{i=0}^{n-1} f_1 \circ T^i(x_0, y_0)) \rangle]^2 p(x_0, y_0) dx_0 dy_0. \end{aligned} \tag{3.1.7}$$

We want to motivate a general structure for these diffusion or dispersion problems. Define the *sum function* F^n on the domain $\mathcal{D}$ as follows

$$F^n = \sum_{i=0}^{n-1} f_1 \circ T^i.$$

It should be clear that

$$\lim_{n\to\infty} \frac{D(n)}{n^\gamma} = \lim_{n\to\infty} \frac{1}{n^\gamma} \int_{\mathcal{D}} [F^n(x_0, y_0) - \langle F^n(x_0, y_0)\rangle]^2 p(x_0, y_0) dx_0 dy_0.$$

Thus the asymptotic behavior of the diffusion of the x component of the orbits of this map is equivalent to asymptotic behavior of the diffusion of this particular *sum function.*

In section 2 we develop some general results concerning the dispersion of sum functions using the B. E. T. and the ergodic partition. Our results provide rigorous conditions under which the "streaming coefficient" S exists, with $0 < S < \infty$. We show that non-ergodicity is a fundamental characteristic involving the t^2 asymptotic behavior of $D(t)$.

The asymptotic behavior of $D(t)$ is also an important quantity in fluid mechanics. The study of this can also often be cast into the form of a study of continuous time *sum functions* as the following example shows.

Example 1.2(Dispersion in Fluids)

Consider a velocity field, a solution of the Navier-Stokes equation, having the following form

$$\dot{x} = \frac{\partial H(x,y,t)}{\partial y}, \tag{3.1.8}$$

$$\dot{y} = -\frac{\partial H(x,y,t)}{\partial x}, \tag{3.1.9}$$

$$\dot{z} = f_3(x,y,t). \tag{3.1.10}$$

There are two reasons for considering this particular mathematical form for the velocity field–one mathematical and the other physical. Mathematically, it can be shown that any divergence-free vector field on $\mathbb{R}^3$ that admits a spatial volume-preserving symmetry group can be transformed to this form (see chapter 2 or Mezić and Wiggins [M-W1]). Physically, velocity fields of this form arise when studying flows in pipes or ducts (see, e.g., Jones and Young [J-Y] and Khakar *et al.* [K-F-O]). The spatial volume-preserving symmetry arises as a result of a "preferred direction of flow" along the axial direction of the pipe or duct. In terms of our coordinates, $x-y$ denote coordinates for the cross-section of the pipe or duct and z denotes the axial coordinate. A physical problem of interest in this setting involves the axial dispersion of a passive tracer placed in the flow.

The study of this problem is facilitated by the particular form of the velocity field that we are considering. The dynamics of the x and y variables decouples from the dynamics of the z variable. In turn, the behaviour of z is dependent only on the dynamics of x and y, thus we have, from (3.1.10)

$$z(t, x_0, y_0, z_0, t_0) = \int_{t_0}^{t} f_3(x(\hat{t}, x_0, y_0, t_0), y(\hat{t}, x_0, y_0, t_0), \hat{t})d\hat{t} + z_0, \tag{3.1.11}$$

where

$$(x(t, x_0, y_0, t_0), y(t, x_0, y_0, t_0), z(t, x_0, y_0, z_0, t_0))$$

are the solutions of (3.1.8)-(3.1.10), with initial conditions

$$\begin{aligned} x(t_0, x_0, y_0, t_0) &= x_0, \\ y(t_0, x_0, y_0, t_0) &= y_0, \\ z(t_0, x_0, y_0, z_0, t_0) &= z_0. \end{aligned}$$

(3.1.12)

Suppose we are given some distribution of initial conditions $\hat{p}(x_0, y_0, z_0, t_0)$ which gives us the density of particles at (x_0, y_0, z_0) at time t_0, such that $\hat{p}(x_0, y_0, z_0, t_0)$ is integrable with a finite integral. Assume the considered particles are passive, i.e., they are advected together with the flow. The problem of shear dispersion consists of studying the statistical behaviour of such an *ensemble* of particles. Assume further that the time-dependence in (3.1.8)-(3.1.10) is such that H and f_3 are 2π-periodic in t, and (3.1.8),(3.1.9) are defined on the closure of some bounded, open subset of $\mathbb{R}^2$. We first suspend the system (3.1.8)-(3.1.10) over $A \times S^1$, by introducing the new time variable, $\tau = t$. Then we can introduce the renormalized density $p(x_0, y_0, z_0, t_0)$, by

$$p = \frac{1}{\int_{A \times \mathbb{R} \times S^1} \hat{p} dx_0 dy_0 dz_0 dt_0} \hat{p}.$$

We have

$$x' = \frac{\partial H(x, y, \tau)}{\partial y}, \tag{3.1.13}$$

$$y' = -\frac{\partial H(x, y, \tau)}{\partial x}, \tag{3.1.14}$$

$$t' = 1, \tag{3.1.15}$$

$$z' = f_3(x, y, t), \tag{3.1.16}$$

where the prime denotes the derivative with respect to τ. From (3.1.11), we obtain

$$z(\tau, x_0, y_0, z_0, t_0) = z_0 + \int_0^\tau f_3(x(\hat{\tau}, x_0, y_0, t_0), y(\hat{\tau}, x_0, y_0, t_0), \hat{\tau} + t_0)d\hat{\tau}. \qquad (3.1.17)$$

Note that $A \times S^1$ is a compact metric space, and that (3.1.13)-(3.1.15) induces a one-parameter group $T^{\bar{\tau}}$ of diffeomorphisms on it, defined by

$$T^{\bar{\tau}}(x_0, y_0, t_0) = (x(\bar{\tau}, x_0, y_0, t_0), y(\bar{\tau}, x_0, y_0, t_0), \bar{\tau} + t_0).$$

Moreover, $T^{\bar{\tau}}$ is a measure-preserving group of transformations, as the system (3.1.13)-(3.1.14) is divergence free. The dispersion in z is given by

$$D(\tau) = \int_{A\times\mathbb{R}\times S^1} \left(z(\tau, x_0, y_0, z_0, t_0) - z_0 - \langle z(\tau, x_0, y_0, z_0, t_0) - z_0\rangle\right)^2 p(x_0, y_0, z_0, t_0)d\mu,$$

where

$$\langle\cdot\rangle = \int_{A\times\mathbb{R}\times S^1} (\cdot)p(x_0, y_0, z_0, t_0)d\mu,$$

and

$$d\mu \equiv dx_0 dy_0 dz_0 dt_0.$$

However, from (3.1.17), we see that

$$\lim_{\tau\to\infty} \frac{D(\tau)}{\tau^\gamma} = \lim_{\tau\to\infty} \frac{\int_{A\times\mathbb{R}\times S^1} \left(F^\tau - \langle F^\tau\rangle\right)^2 p d\mu}{\tau^\gamma},$$

where

$$F^\tau \equiv \int_0^\tau f_3 \circ T^{\hat{\tau}} d\hat{\tau}.$$

Thus the asymptotic properties of the dispersion in z can be studied using continuous time *sum function* F^{τ}.

The work of Jones and Young [J-Y] on shear dispersion and anomalous diffusion by chaotic advection motivated much of the work in this chapter. The physical phenomenon under study in their work was the flow of a viscous fluid through twisted pipes. The flow is symmetric (in the sense of the above example), so the distance that the passive tracer particle travels along the axis of the pipe depends only on the dynamics in the cross section of the pipe. In what Jones and Young refer to as the *mixed* regime (which is the case when the motion in the cross section is non- ergodic) they find that the particle dispersion in the axial direction asymptotically (for large times t) behaves as t^2. t^2 dispersion has also been observed in other fluid dynamical studies, in a different physical contexts. Weiss and Knobloch [W-K] observe $D(t) \sim t^{1.93}$ in a study of transport by modulated traveling waves, and explain it by the fact that there is a shear in the mean flow. Pasmanter [Pas1] finds t^2 dispersion in the shallow tidal flows study, pointing out that it is due to the difference in the long time drift of particles in different regions. These physical explanations are made mathematically precise in Theorem 3.2.1. Ridderinkhof and Zimmerman [R-Z] find t^2 behaviour in the same context as Pasmanter - transport in shallow tidal seas [1]. Aranson *et al.* [A-E-R-T] in their numerical study of the impurity transport in parametrically excited capillary ripples observe that "the diffusion law ... apparently has the form $\langle r^q \rangle \sim t^q$, ... at all q", where r is the distance from some origin of coordinates, and q is an integer. Thus, it is not only that the dispersion $\langle r^2 \rangle$ asymptotically behaves like t^2, but also higher order moments show similar regularity. In connection with this observation, see the remarks after the proof

[1] t^{α}, $\alpha = 1.5$ and 1.7 behaviour for the dispersion that they get in some cases is probably due to the fact that those are really finite-time results - the time at which they stop the calculation is only 10 times bigger than the period in a cell.

of the Theorem 3.2.1. Neishtadt *et al.* [N-C-C] analyze the mean square displacement of charged particles moving at an angle to the magnetic field in the field of a wave packet. Their numerical study reveals what they call a free flight law, i.e., the mean square particle displacement increases proportionally to the square of the time. Wagenhuber *et al.* [W-G-N-O] performed a study of the motion of ballistic electrons in lateral surface superlattices, and found approximately t^2 behaviour for dispersion (note that this work is somewhat different from the rest of the above, as the motion of the single particle is considered, as opposed to the motion of an ensemble of particles).

Our results depend, through the B.E.T. on the fact that the dynamical system preserves a measure μ. The measure does not necessarily have to be smooth. Now, every continuous dynamical system preserves some measure (see Mañe [M]). The problem is that the invariant measure is not necessarily the one with respect to which we would like to calculate the dispersion. In all of the above mentioned works, the dynamical systems under consideration preserves a smooth measure. As the dispersion is usually calculated with respect to a measure which is absolutely continuous with respect to the smooth invariant measure, in those cases our results are easily applied. But, caution must be exercised when applying the results of this chapter to systems which do not preserve a smooth invariant measure. Examples where t^2 dispersion is found, but the dynamical systems do not neccessarily preserve a smooth invariant measure, are Crisanti *et al.* [C-F-P-V] , Wang *et al.* [W-B-S], [W-M-M-S], Tio *et al.* [T-G-L] (all on the passive advection of particles suspended in a fluid, with the density of the fluid different from the density of particles), Geisel *et al.* [G-N-Z] (diffusion in Josephson Junctions), Artuso *et al.* [A-C-L] (1-D maps), Aronson *et al.* [A-R-T] (passive scalar transport in the field of two orthogonal standing inertial waves in a rotating fluid, and the spiral wave motion in a nonequilibrium medium, modeled by a space-time periodic, two-dimensional, reversible velocity field). Our methods can be applied to explain their result, provided the time averages of certain functions exist almost everywhere, with respect to some appropriate measure (in other words some form of a problem-specific B.E.T. is needed).

It is interesting to mention that t^2 dispersion appears in T.J. Day's [D1], [D2] experimental measurments of the dispersion of fluid particles in natural channels.

Apart from the t^2 dispersion, here are some other numerical findings that the results in this chapter can explain: Pasmanter [Pas2] observed the "patchy" structure of the concentration of particles transported by shallow tidal flows. Khakhar *et al.* [K-F-O] in their study of chaotic mixing find that the so-called isoresidence times sets (each fluid particle in such a set spends the same time in the mixer before exiting) portrait looks similar to the phase portrait, and the more so the longer the mixer. Also, they observed multi-peaked distributions of first passage times.

We present a general theory for dealing with problems of the above sort based on the B.E.T., the concept of the ergodic partition, and the tools and analogies with the probability theory. Our methods will be centered around the analysis of either discrete or continuous time *sum functions* and general initial distributions defined by integrable functions on the phase space. It turns out that many of above presented problems can be cast in a form which requires the statistical analysis of sum functions. Moreover, the relation between sum functions and the B. E. T. should be clear. If

$$F^n = \sum_{i=0}^{n} f \circ T^i,$$

denotes a discrete time sum function, where f is some integrable function on the phase space and T is the map generating the dynamics, then the time averages of such functions e exactly the quantities considered in the B. E. T.

In section 2, we set up our framework and show that the condition under which t^2 dispersion can be expected is, loosely, that the initial distribution is not entirely contained in one of the sets on which the time average of f is constant. Through the use of the ergodic partition, we replace the time averages by the spatial averages. In section 3, we notice an analogy with probability theory and, thus, obtain results about probability distributions of sum functions and show how the ergodic partition affects their properties. In section 4, we analyse the problem of first passage times. We obtain an exact analytic expression for finite times, using a novel approach. We also analyze the problem of isoresidence set asymptotics.

In section 5, we reformulate the theory for dynamical systems with continuous time. Wiener's local ergodic theorem is used to obtain a result analogous to a known result from turbulent dispersion theory, namely, that the initial dispersion behaves like t^2.

3.2 Dispersion of sum functions

In many numerical studies of area-preserving maps, one often sees regions of phase space occupied by regular motions (periodic orbits, KAM curves) interspersed with regions in which the motions are apparently irregular (irregular regions being defined loosely as the ones in which there exist orbits that are "space-filling"). The latter regions are often called *ergodic*, although typically ergodicity is not proven. Statistical properties of the map are then studied numerically. A particular statistical property that is often investigated is the *dispersion*, $D(n)$, which measures the average square separation of points, on the n-th iteration of the map.

In this section we study the dispersion of *sum functions* for n-dimensional, measure-preserving maps with arbitrary initial distributions of points. We show that asymptotically the dispersion is proportional to n^2 for all maps that are not ergodic on the whole phase space, with certain exceptions, related to the initial distributions, to be presented in detail below. In the course of these investigations we formalize the idea of regular and irregular regions using the notion of the *ergodic partition* of the phase space. The role of the ergodic partition in this section is to allow us to calculate certain constants through spatial averages instead of time averages, resembling thus the procedure used in statistical mechanics. We will also use the ergodic partition in later sections where we analyze other statistical properties.

3.2.1 The quadratic dispersion of sum functions

We shall analyze a discrete dynamical system (A, μ, T) generated by an automorphism $T : A \to A$, defined on a compact metric space A. We assume that μ is a σ-additive, complete measure and defined on the Borel σ-algebra $\mathcal{A}$, with $\mu(A) = 1$. We denote points in A by x, and the $n-th$ iterate of T by T^n.

Consider a measurable, *bounded* function $f : A \to \mathbb{R}$. We define the function F^n on A by

$$F^n = \sum_{i=0}^{n} f \circ T^i,$$

where we put $T^0 x = x$. Clearly, F^n is measurable and bounded on A. We will refer to F^n as a *sum function.*

We shall be interested in *statistical* properties of sum functions. Consider the *ensemble* of initial conditions in A given by an *initial distribution* p, where p is a positive integrable function on A such that

$$\int_A p d\mu = 1.$$

We define the mean value of a sum function, $\langle F^n \rangle$ to be

$$\langle F^n \rangle = \int_A F^n p d\mu. \tag{3.2.18}$$

This quantity exists as p is integrable, and F^n is bounded. Also, we define the *dispersion* of a sum function as

$$D(n) = \sigma^2(n) = \int_A (F^n - \langle F^n \rangle)^2 p d\mu, \tag{3.2.19}$$

where σ is the standard deviation. The integral (3.2.19) exists by a similar argument as for (3.2.18). Our goal in this subsection is to deduce asymptotic properties (when $n \to \infty$) of $D(n)$.

We denote the *spatial average* of f over A by $\bar{f}$:

$$\bar{f} = \int_A f d\mu, \tag{3.2.20}$$

and we denote the *time average* of f on a trajectory of T passing through x by $f^*(x)$:

$$f^*(x) = \lim_{n \to \infty} \frac{1}{n} \sum_{i=0}^{n-1} f(T^i x), \quad x \in A, \quad n \in \mathbf{N}. \tag{3.2.21}$$

The subsets of A on which the time averages of a bounded, integrable function f are constant will play an important role in our theory. These will be denoted by

$$B_c = \{x \in A | f^*(x) = c, c \in \mathbb{R}\}.$$

Let us denote by Σ the set of all points in A such that f^* exists, and by Σ^c its complement. Σ^c is, by the B.E.T., of measure zero. Clearly, $A = (\cup_c B_c) \cup \Sigma^c$. Thus the sets B_c together with Σ^c form a *partition*, ξ_f, of A (for this and the following terminology, see Rokhlin [R] or Cornfeld, Sinai, and Fomin [C-S-F]). It is a *stationary partition*, as each set in ξ_f is, again by B.E.T., invariant under T. ξ_f is actually a *measurable partition*, as we will see in the next subsection. We shall use the notion of a partition heavily later, but we do not need any of its specific properties at this stage. So, we postpone a more detailed discussion for the next subsection. We can state the following theorem:

Theorem 3.2.1 *Consider a dynamical system* (A, μ, T), *a bounded, measurable function* $f : A \to \mathbb{R}$, *and an initial distribution* p, *all defined as above. Suppose that there is no* $c \in \mathbb{R}$ *such that* $\mu(supp(p) \backslash B_c) = 0$. *Then, we have*

$$\lim_{n\to\infty} \frac{D(n)}{n^2} = a < \infty,$$

where

$$a = \int_A \left[f^* - \int_A f^* p d\mu \right]^2 p d\mu, \qquad (3.2.22)$$

and $a > 0$. *Conversely, if* $0 < a < \infty$, *then* $\mu(supp(p) \backslash B_c) \neq 0, \forall c \in \mathbb{R}$.

Proof: From the definition of the dispersion of sum functions given in (3.2.19), we have

$$D(n) = \sigma^2(n) = \int_A (F^n - \langle F^n \rangle)^2 p d\mu. \qquad (3.2.23)$$

By B.E.T.

$$\lim_{n\to\infty}\frac{1}{n}\sum_{i=0}^{n}f(T^ix) = \lim_{n\to\infty}\frac{F^n(x)}{n} = f^*(x), \tag{3.2.24}$$

exists on $\Sigma \subset A$, $\mu(\Sigma) = 1$. By boundedness of f on $\Sigma \subset A$,

$$\begin{aligned}|f^*(x)| &= |\lim_{n\to\infty}\frac{1}{n}\sum_{i=0}^{n-1}f(T^ix)| \\ &\leq \lim_{n\to\infty}\frac{1}{n}\sum_{i=0}^{n-1}|f(T^ix)| \\ &\leq C,\end{aligned} \tag{3.2.25}$$

where $C \in \mathbb{R}^+$ is such that $|f(x)| \leq C$ throughout A. Now we are set up to calculate $\lim_{n\to\infty} D(n)/n^2$. We have

$$\begin{aligned}\frac{D(n)}{n^2} &= \int_A(\frac{F^n}{n} - \langle\frac{F^n}{n}\rangle)^2 p d\mu \\ &= \int_A(\frac{1}{n}\sum_{i=0}^{n} f\circ T^i - \langle\frac{1}{n}\sum_{i=0}^{n} f\circ T^i\rangle)^2 p d\mu.\end{aligned} \tag{3.2.26}$$

By boundedness of f and positiveness of p,

$$\begin{aligned}|\left(\frac{1}{n}\sum_{i=0}^{n} f\circ T^i - \langle\frac{1}{n}\sum_{i=0}^{n} f\circ T^i\rangle\right)^2 p| &\leq (|(\frac{1}{n}\sum_{i=0}^{n} f\circ T^i)| + |\langle\frac{1}{n}\sum_{i=0}^{n} f\circ T^i\rangle|)^2 p \\ &\leq (C + C\int_A p d\mu)^2 p = 4C^2 p,\end{aligned} \tag{3.2.27}$$

for every n. Now, $4C^2p$ is an integrable function on A, therefore we can use Lebesgue's bounded convergence theorem in the following computations to obtain

$$\begin{aligned}
\lim_{n\to\infty}\frac{D(n)}{n^2} &= \lim_{n\to\infty}\int_A(\frac{F^n}{n}-\langle\frac{F^n}{n}\rangle)^2 p d\mu \\
&= \int_A \lim_{n\to\infty}(\frac{F^n}{n}-\langle\frac{F^n}{n}\rangle)^2 p d\mu \\
&= \int_A (\lim_{n\to\infty}\frac{F^n}{n}-\langle\lim_{n\to\infty}\frac{F^n}{n}\rangle)^2 p d\mu \\
&= \int_A (f^*-\langle f^*\rangle)^2 p d\mu \\
&\leq \int_A 4C^2 p d\mu \\
&< \infty,
\end{aligned} \tag{3.2.28}$$

where we used (3.2.25) in the last line.

What is left to prove is $a > 0$. We summarize the necessary argument in the following lemma:

Lemma 3.2.1

$$\int_A \left[f^* - \int_A f^* p d\mu\right]^2 p d\mu = 0 \Leftrightarrow \mu(supp(p)\backslash B_c) = 0,$$

for some (unique) $c \in \mathbb{R}$.

Proof: Suppose $\mu(supp(p)\backslash B_c) = 0$ for some fixed c. Then

$$\int_A \left[f^* - \int_A f^* p d\mu\right]^2 p d\mu = \int_{supp(p)} \left[f^* - \int_{supp(p)} f^* p(x) d\mu\right]^2 p d\mu. \tag{3.2.29}$$

But, as $supp(p) \subset B_c$, except for a set of measure zero and $f^* = c$ on B_c, the right-hand side is zero.

Conversely, suppose

$$\int_A \left[f^* - \int_A f^* p d\mu \right]^2 p d\mu = 0.$$

Note that the integrand is positive. Then, for almost every $x \in A$ either

$$p(x) = 0, \tag{3.2.30}$$

so $x \notin supp(p)$, or

$$f^*(x) - \int_A f^*(x) p(x) d\mu = 0. \tag{3.2.31}$$

Let $c = \int_A f^* p d\mu$. Clearly, the set of all points for which (3.2.31) is satisfied is a subset of B_c. But, from (3.2.30) and (3.2.31) it is clear that $supp(p) \subset B_c$ except for the subset of $supp(p)$ of measure zero. Thus we are done with the proof of the lemma. □

The above lemma completes the proof, as we easily conclude that $a > 0$, and the last statement of the theorem also follows from it. □

Let us make several remarks about this theorem.

Remarks:

- Note that if T is ergodic, then, as is easily seen from (3.2.22), $a = 0$ for any initial distribution p. As far as nonergodic automorphisms on A are concerned, the above theorem gives a complete description of their asymptotic dispersive properties with respect to any bounded, measurable function f, except for the case of "biased" initial distributions, i.e., distributions whose support is almost entirely contained in one of the sets on which the time average of f is constant.

- The i-th order moment of F^n, defined by

$$M^i(n) = \int_A (F^n - \langle F^n \rangle)^i p d\mu,$$

can be calculated in the same manner as above, with

$$\lim_{n\to\infty} \frac{M^i(n)}{n^i} = a_i < \infty,$$

where

$$a_i = \int_A \left[f^* - \int_A f^* p d\mu \right]^i p d\mu.$$

Note that for all even moments we can claim $a_i \neq 0$ iff the support of p is not contained in one of B_c's (the same as for $D(n)$). For odd moments, though, it is not so. This is the consequence of the fact that we used the positivity of

$$\left[f^* - \int_A f^* p d\mu \right]^2 p,$$

in the proof of the Lemma 3.2.1.

- The converse part of the theorem allows us to check the ergodicity of T: if the initial distribution p is homogeneous, i.e., $p(x) = 1$, $\forall x \in A$, and for some measurable, bounded f, $a > 0$, then T is not ergodic on A.

3.2.2 Ergodic partition and dispersion

In this subsection we show that it is possible to compute statistical properties (like the dispersion) of sum functions F^n without calculating the time average of a function f

under the dynamics of T. Along the way, we will be able to make some precise statements about the usual intuitive notion of a partition of phase space into regular and irregular regions.

To start with the analysis of a general automorphism T, let us consider more closely the notion of a partition of the space A. We assume that A is Lebesgue space (note that every compact, metric space with the measure μ defined on a Borel σ-algebra is Lebesgue). Suppose there exists a partition of A, call it ξ (i.e., χ is a collection of disjoint sets C_β, where β is element of some index set I, such that $A = \cup_\beta C_\beta$). We shall call any union of elements of ξ a ξ-set. Consider now the space A/ξ with the projection mapping $\pi : A \rightarrow A/\xi$ which maps a point x in A to the set C_β for which $x \in C_\beta$. Suppose that the partition ξ is measurable, i.e., there exists a countable system of ξ-sets, Δ, such that for any C_{β_1}, C_{β_2} there exists $D \in \Delta$ such that $C_{\beta_1} \in D, C_{\beta_2} \in D^c$. It can be shown that if the partition ξ is measurable, A/ξ is a Lebesgue measure space, with a measure μ_ξ, defined by

$$\mu_\xi(E) = \mu(\pi^{-1}(E)), \tag{3.2.32}$$

where $E \subset A/\xi$. The notion of a measurable partition is important, as the property of measurability of a partition is necessary and sufficient for the existence of a *canonical system of measures*, $\{\mu_{C_\beta}\}$, such that

1. μ_{C_β} is a Lebesgue measure for almost every $C_\beta \in \xi$

2. If $B \subset A$ is measurable, then $B \cap C_\beta$ is measurable for almost every $C_\beta \in \xi$, $\mu_{C_\beta}(B \cap C_\beta)$ is a measurable function of C_β, and

$$\mu(B) = \int_{A/\xi} \mu_{C_\beta}(B \cap C_\beta) d\mu_\xi.$$

Getting back to our problem, we would like to find a measurable partition ξ such that it does not depend on a particular function f defined on a phase space (i.e., depends only on the dynamics of T), and still is in a certain (precise) sense a "basis" through which any partition can be obtained. A first guess on the structure of ξ is that it is a partition into orbits of T, but the resulting partition turns out not to be measurable in general. Nevertheless, Rokhlin [R] has shown that if we take the *measurable hull* of the partition into orbits, we obtain a measurable stationary partition ξ with elements C_β, which we shall call *ergodic components*, such that

- There exists a system of canonical invariant ergodic measures, $\{\mu_{C_\beta}\}$.
- T is partitioned in components T_{C_β} such that each T_{C_β} is an automorphism on C_β, for a.e. C_β.
- For a.e. $C_\beta \in \xi$, T_{C_β} is an ergodic automorphism.

This partition of A is referred to as the *ergodic partition.* Every μ_{C_β} is a probabilistic measure on C_β. It has been shown (see chapter 4 or Mezić and Wiggins [M-W2]) that the ergodic partition of automorphisms of compact, metric spaces can be obtained as the *product* of a countable number of measurable partitions of A. The product of two partitions is the collection of sets formed by the pairwise intersection of sets from two partitions (this is easily extended to $n \subset \mathbf{N}$ partitions, and to the case of a countable infinity of partitions). Each of the partitions in the product is a partition of A into sets on which the time averages of a function f in $C(A)$, the set of all continuous functions on A, are constant. We call such a partition *the partition ξ_f induced by f.* The countable number of partitions is obtained from a dense, countable subset S of the set $C(A)$. This theorem shows the connection between the ergodic partition ξ of the phase space of a particular automorphism, and the partitions ξ_f induced by the time averages of continuous functions on A. Actually, one can deduce the link between the partitions induced by the time averages of bounded, measurable functions on A, and the ergodic partition, which we shall need in later sections:

Proposition 3.2.1 *Let a set B'_c be a union of all elements C_β of ξ such that*

$$\int_{C_\beta} f_{C_\beta} d\mu_{C_\beta} = c.$$

Then $\mu\left((B_c - B'_c) \cup (B'_c - B_c)\right) = 0$, where B_c is as defined before.

Proof: See chapter 4 or Mezić and Wiggins [M-W2]. □

This proposition tells us that if we consider a partition of the phase space into sets on which the time average of a measurable, bounded function f is constant, each set in the partition ξ_f will be, up to a measure zero set, union of elements of the ergodic partition. In particular, ξ can serve as a "basis" for a partition ξ_f for arbitrary measurable, bounded f.

We shall show two applications of the ergodic partition in this subsection. The first of them is the replacement of the time averages with spatial averages on ergodic components in the expression (3.2.22). We start with the following Lemma:

Lemma 3.2.2 *Let A, T be as above and f an integrable function on A. Then*

$$\int_A f d\mu = \int_{A/\xi} \left[\int_{C_\beta} f_{C_\beta} d\mu_{C_\beta}\right] d\mu_\xi, \tag{3.2.33}$$

where f_{C_β} is a restriction of f to the ergodic component C_β, and μ_ξ is defined in (3.2.32).

Proof: Let $f = \chi_B$, where χ_B is a characteristic function of an arbitrary measurable set B. Then (3.2.33) reduces to a property 2. of a measurable partition given above. In the case of a general integrable f, we use the standard argument that any integrable function is just a limit of an infinite sequence of simple functions (i.e., those μ-measurable functions which admit only a countable number of distinct values), and each element of a sequence is a countable linear combination of characteristic functions. □

Proposition 3.2.2 *Let A, T and f be as in the Theorem 3.2.1. Then*

$$\begin{aligned} a &= \int_{A/\xi} \left[\bar{f}_{C_\beta} - \int_{M/\xi} \bar{f}_{C_\beta} \bar{p}_{C_\beta} d\mu_\xi \right]^2 \bar{p}_{C_\beta} d\mu_\xi \\ &= \int_A \left[\bar{f}_{C_\beta} - \int_M \bar{f}_{C_\beta} \bar{p}_{C_\beta} d\mu \right]^2 \bar{p}_{C_\beta} d\mu, \end{aligned} \tag{3.2.34}$$

where $\bar{f}_{C_\beta}, \bar{p}_{C_\beta}$ are the spatial averages of the restriction of f, p, respectively, to ergodic components.

Proof: As f^* is measurable and bounded, from the Lemma (3.2.2), we have

$$\int_A f^* p d\mu = \int_{A/\xi} \left[\int_{C_\beta} f^*_{C_\beta} p_{C_\beta} d\mu_{C_\beta} \right] d\mu_\xi.$$

Now, using the fact that T_{C_β} is ergodic on C_β, we have

$$f^*_{C_\beta} = \bar{f}_{C_\beta},$$

for a.e. C_β, where the spatial average is taken with respect to μ_{C_β}. So,

$$\begin{aligned} \int_A f^* p d\mu &= \int_{A/\xi} \bar{f}_{C_\beta} \left[\int_{C_\beta} p_{C_\beta} d\mu_{C_\beta} \right] d\mu_\xi \\ &= \int_{A/\xi} \bar{f}_{C_\beta} \bar{p}_{C_\beta} d\mu_\xi \\ &= \int_A \bar{f}_{C_\beta} \bar{p}_{C_\beta} d\mu, \end{aligned} \tag{3.2.35}$$

where in the last equality we used the fact that μ_{C_β} is a probabilistic measure on C_β, and Lemma 3.2.2. Now,

$$
\begin{aligned}
a &= \int_A \left[f^* - \int_A f^* p d\mu\right]^2 p d\mu \\
&= \int_A \left[f^* - \int_A \bar{f}_{C_\beta} \bar{p}_{C_\beta} d\mu\right]^2 p d\mu \\
&= \int_A \left[\bar{f}_{C_\beta} - \int_A \bar{f}_{C_\beta} \bar{p}_{C_\beta} d\mu\right]^2 p d\mu \\
&= \int_{A/\xi} \left[\bar{f}_{C_\beta} - \int_A \bar{f}_{C_\beta} \bar{p}_{C_\beta} d\mu\right]^2 \bar{p}_{C_\beta} d\mu_\xi \\
&= \int_A \left[\bar{f}_{C_\beta} - \int_A \bar{f}_{C_\beta} \bar{p}_{C_\beta} d\mu\right]^2 \bar{p}_{C_\beta} d\mu.
\end{aligned}
\tag{3.2.36}
$$

This completes the proof. □

This result allows for an economization of the procedure of calculating the coefficient a, as it is not necessary to know time averages for a specific function f: it is enough to calculate the ergodic partition and invariant measures once. Then, the coefficients a for any prescribed function are easily computable from the expression (3.2.34). Admittedly, the ergodic partition is not trivial to find, except in some simple cases (see e.g., Halmos [H]). The proof of the existence of the ergodic partition given in chapter 4 and Mezić and Wiggins [M-W2] might help in that context, as the ergodic partition is constructed through a simple algorithm. Also, an interesting consequence of the above result is that if we replaced f and p with $\bar{f}_{C_\beta}$, $\bar{p}_{C_\beta}$, the dispersion would have the same asymptotic behaviour when $n \to \infty$.

Another application of the notion of the ergodic partition is the *large ergodic component* case. In particular, we have the following

Proposition 3.2.3 *Assume that there is* $C_\beta^{large} \in \xi$ *such that* $\mu_\xi(C_\beta^{large}) = 1 - \epsilon$, *where*

$\epsilon << 1$. *Further, assume* $p = 1$. *Then we have* $a = \mathcal{O}(\epsilon)$.

Proof: First note that C_β^{large} is measurable, as every element of the ergodic partition is. For the mean value we have

$$\begin{aligned}
& \int_A \bar{f}_{C_\beta} d\mu \\
= & \int_{C_\beta^{large}} \bar{f}_{C_\beta} d\mu + \int_{A/C_\beta^{large}} \bar{f}_{C_\beta} d\mu. \\
= & \int_{C_\beta^{large}} \bar{f}_{C_\beta^{large}} d\mu + \mathcal{O}(\epsilon) \\
= & \bar{f}_{C_\beta^{large}} + \mathcal{O}(\epsilon).
\end{aligned}$$

Now,

$$\begin{aligned}
a &= \int_A \left[\bar{f}_{C_\beta} - \int_A \bar{f}_{C_\beta} d\mu\right]^2 d\mu \\
&= \int_A \left[\bar{f}_{C_\beta} - \bar{f}_{C_\beta^{large}} + \mathcal{O}(\epsilon)\right]^2 d\mu \\
&= \int_{C_\beta^{large}} \left[\bar{f}_{C_\beta} - \bar{f}_{C_\beta^{large}} + \mathcal{O}(\epsilon)\right]^2 d\mu + \mathcal{O}(\epsilon)
\end{aligned} \tag{3.2.37}$$

From the last expression, as $\mathcal{O}(1)$ terms cancel out, we have the required result. □

Note that the ergodic partition in the above proof was used essentially to precisely determine what we mean by the large ergodic component, and to assure that that set is measurable. The computational part of the proof could have been done with expressions involving time averages of f. The above proposition also clarifies the validity of the conjecture made by Jones and Young [J-Y] that the dispersion in what they call the *mixed* regime (which is the one in which ergodic components of positive measure coexist with the islands of regular motion) is proportional to the measure of the set in which the dynamics is regular. We showed that this is going to be strictly true only in the large ergodic component limit.

3.3 Asymptotics of distribution functions

In the first section we analyzed one interesting statistical property of the automorphism T, namely the dispersion of sum functions. But, much more can be said about the statistical properties of T, using the probability theory formalism combined with the notion of the ergodic partition, as it will be shown in this section. In particular, we again consider the sum functions, and we shall be interested in the function $W^n : \mathbb{R} \rightarrow \mathbb{R}$ defined by

$$W^n(y) = P\{x \in A | F^n(x) \leq y\}, \tag{3.3.38}$$

where P is a probability measure on A defined by

$$P(B) = \int_B p d\mu, \tag{3.3.39}$$

for any measurable set B.

Note that W^n is non-decreasing and continuous from the right. Further, we have

$$\lim_{y \rightarrow -\infty} W^n(y) = 0, \text{ and} \tag{3.3.40}$$

$$\lim_{y \rightarrow \infty} W^n(y) = 1. \tag{3.3.41}$$

Therefore, in the terminology of the probability theory, $W^n(y)$ is the distribution function for the random variable F^n on A (see Doob [D]). It would be useful to obtain an explicit expression for it. This can be done by pushing further the observed relationship of our problem with the probability theory formalism. Let us define a probability measure on $\mathbb{R}$, P_{W^n} by

$$P_{W^n}(I) = \int_I dW^n(y), \tag{3.3.42}$$

where the integral in (3.3.42) is a Lebesgue-Stieltjes integral.

Using Levy's inversion formula (see e.g. [Sa]), we obtain

$$\begin{aligned}
&\frac{W^n(y_2)+W^n(y_2^-)}{2}-\frac{W^n(y_1)+W^n(y_1^-)}{2}\\
&= -\lim_{v\to\infty}\int_{-v}^{v}\frac{\exp(-i\rho y_2)-\exp(-i\rho y_1)}{2\pi i\rho}\Phi(\rho)d\rho\\
&= -\lim_{v\to\infty}\int_{-v}^{v}\int_A\frac{\exp(-i\rho y_2)-\exp(-i\rho y_1)}{2\pi i\rho}\exp(i\rho F^n(x))dPd\rho, \qquad (3.3.43)
\end{aligned}$$

where

$$W^n(y^-)=\lim_{\epsilon\to 0}W^n(y-\epsilon),\quad \epsilon>0.$$

If both y_2 and y_1 are points of continuity, then

$$W^n(y_2)-W^n(y_1)=-\lim_{v\to\infty}\int_{-v}^{v}\int_A\frac{\exp(-i\rho y_2)-\exp(-i\rho y_1)}{2\pi i\rho}\exp(i\rho F^n(x))dPd\rho. \qquad (3.3.44)$$

In the case when y is a point of continuity, by (3.3.44) and (3.3.40) we have

$$W^n(y)=-\lim_{y_1\to-\infty}\lim_{v\to\infty}\int_{-v}^{v}\int_A\frac{\exp(-i\rho y)-\exp(-i\rho y_1)}{2\pi i\rho}\exp(i\rho F^n(x))dPd\rho. \qquad (3.3.45)$$

(3.3.45) is an explicit formula for the distribution function W^n.

3.3.1 The renormalized distribution function and Birkhoff's ergodic theorem

For every point $x\in\Sigma$ for which $|f^*(x)|>0$, $|F^n(x)|$ is going to become large when n is sufficiently big. For simplicity, assume $|f^*(x)|>\delta>0$, $\forall x\in\Sigma$. Then, for any $y_c\in\mathbb{R}$ there exists n_c, such that $\forall n>n_c$, $W^n(y)$ is zero for all y such that $|y|<y_c$. Moreover, it is clear from the definition of W^n, that it asymptotically approaches the distribution given by

$$W^\infty(y)=\begin{cases}0 & y<\infty\\ 1 & y=\infty.\end{cases}$$

To get a better grasp on what is happening to the distribution W^n, one can transform the origin to $\bar{f}^* \cdot n$ and rescale with the "appropriate lengthscale." We take the "appropriate lengthscale" to be the variance σ. Let us assume that the conditions for Theorem 3.2.1 are satisfied. Then we introduce the coordinate transformation on $\mathbb{R}$ by

$$z = \frac{y - \bar{f}^* \cdot n}{\sigma}.$$

Now note that

$$\begin{aligned} W^n(y) &= P\{x \in A | F^n(x) \leq y\} \\ &= P\{x \in A | F^n(x) \leq \sigma z + \bar{f}^* \cdot n\} \\ &= P\{x \in A | \frac{F^n(x) - \bar{f}^* \cdot n}{\sigma} \leq z\} \\ &\stackrel{def}{=} G^n(z). \end{aligned} \tag{3.3.46}$$

Note also that, by the B.E.T, $\bar{f}^* = \bar{f}$, so

$$G^n(z) = P\{x \in A | \frac{F^n(x) - \bar{f} \cdot n}{\sigma} \leq z\}. \tag{3.3.47}$$

We shall call the above defined distribution G^n the *renormalized distribution.* As opposed to W^n, it has very interesting asymptotic properties. To investigate the asymptotic properties of G^n when $n \to \infty$, we first observe the following:

Lemma 3.3.1 *f^* is a measurable, bounded function on Σ.*

Proof: f^* is measurable, as it is integrable by B.E.T. We already showed in Theorem 3.2.1 that f^* is bounded, so the proof is complete. □

By the Lemma 3.3.1, in the language of the probability theory, $(f^*(x) - \bar{f})/\sqrt{a}$ is a random variable on A, and $(F^n(x) - \bar{f} \cdot n)/\sigma$ is a sequence of random variables converging to it pointwise almost everywhere. The distribution function of $(f^*(x)-\bar{f})/\sqrt{a}$, denoted by G^∞, is defined as

$$G^\infty(z) = P\{x \in A | \frac{f^*(x)-\bar{f}}{\sqrt{a}} \leq z\}. \tag{3.3.48}$$

Then, we can use the following well-known theorem from the probability theory:

Theorem 3.3.1 *G^n converges to G^∞ in the sense of distributions, i.e.,*

$$\lim_{n\to\infty} G^n(z) = G^\infty(z), \quad \forall z \in C(G^\infty),$$

where $C(G^\infty)$ is the set of all points of continuity of G^∞. Also $[C(G^\infty)]^c$ is at most a countable set of points.

Proof: See e.g., Sarapa [Sa], pg 320. □

Now that we established the usefulness of studying G^∞, we state some of its properties. We can establish an explicit expression for G^∞, through the same procedure we used at the beginning of this section for W^n. We obtain

$$\begin{aligned} &\frac{G^\infty(z)+G^\infty(z^-)}{2} \\ = &-\lim_{z_1\to-\infty}\lim_{v\to\infty}\int_{-v}^{v}\int_A \frac{\exp(-i\rho z)-\exp(-i\rho z_1)}{2\pi i\rho}\exp(i\rho\frac{f^*(x)-\bar{f}}{\sqrt{a}}))dPd\rho. \end{aligned} \tag{3.3.49}$$

Note that the limiting distribution again depends only on the time averages of f. We could follow the same procedure as in the Section 1 and obtain G^∞ in terms of spatial averages. More interesting is the following theorem, in which we make a connection between G^∞ and the partition ξ_f:

Theorem 3.3.2 *There exists c_0 such that $G^\infty(z) = 0 \;\; \forall z < -c_0$ and $G^\infty = 1 \;\; \forall z > c_0$. Moreover, let $c = \sqrt{a}z + \bar{f}$. Then z is a point of discontinuity of G^∞ if and only if $P(B_c) > 0$.*

Proof: The first statement follows immediatelly from the boundedness of f^*. For the second part, note that

$$\begin{aligned} G^\infty(z) - G^\infty(z^-) &= P\{x \in A | \frac{f^*(x) - \bar{f}}{\sqrt{a}} \leq z\} - P\{x \in A | \frac{f^*(x) - \bar{f}}{\sqrt{a}} < z\} \\ &= P\{x \in A | \frac{f^*(x) - \bar{f}}{\sqrt{a}} = z\} \\ &= P(B_c). \end{aligned} \tag{3.3.50}$$

Now suppose that G^∞ has a point of discontinuity at z. As we know that G^∞ is continuous from the right, $G^\infty(z) - G^\infty(z^-) > 0 \;\Rightarrow P(B_c) > 0$. The converse proceeds in the same manner. □

The nature of G^∞ is quite clear from the above results: its support is contained in a compact set, it is a function continuous from the right, such that it has at most a countable infinity of points of discontinuity. Further, its points of discontinuity correspond to the sets of positive measure in the partition ξ_f. For initial distributions such that the measure μ is absolutely continuous with respect to P, the ergodic partition ξ plays a major role:

Proposition 3.3.1 *Suppose p is an initial distribution such that μ is absolutely continuous with respect to P, and C is an element of ξ such that $\mu(C) > 0$, and $f^*|_C = c$. Then $z = (c - \bar{f})/\sqrt{a}$ is an point of discontinuity of G^∞.*

Proof: Recall from the Proposition 3.2.1 that $\mu\left((B_c - B_c') \cup (B_c' - B_c)\right) = 0$. So, if any of the elements of ξ whose union (mod 0 set) is B_c' has the positive measure with respect to μ, then B_c has positive measure with respect to μ.

By the absolute continuity of μ with respect to P, $\mu(B_c) > 0 \Rightarrow P(B_c) > 0$, as suppose $\mu(B_c) > 0$ and $P(B_c) = 0$. By the definition of the absolute continuity, $P(B_c) = 0 \Rightarrow \mu(B_c) = 0$, so we are done by contradiction.

Now, as $P(B_c) > 0$, we can use Theorem 3.3.2 to conclude the proof. □

Proposition 3.3.1 tells us that, given any bounded, measurable function f, the points of discontinuity of the limiting renormalized distribution G^{∞} will be determined by the elements of the ergodic partition which have positive measure.

3.3.2 "Patchiness" in fluid flows and distribution functions

Pasmanter [Pas1], [Pas3] has studied mechanisms that give rise to the variability of dispersion processes in the ocean. A particularly important phenomenon to which he referred is known as "patchiness," i.e., a situation where parts of a distribution of passive tracer may disperse at different speeds compared to its surroundings. We want to show that the mathematical framework developed in this section can be useful for studying this phenomenon. We will illustrate this with an example.

Consider a (steady) convection cell whose horizontal length is much larger than its height and where the convection cells are aligned along the y-axis (figure 3.1). In this situation the flow is essentially two-dimensional and, assuming stress-free boundary conditions and single-mode convection, an explicit form of the velocity field is given by (see Chandrasekhar [C2])

$$\dot{x} = -\frac{A\pi}{k}\cos(\pi z)\sin(kx) = -\frac{\partial\psi}{\partial z}(x,z), \qquad (3.3.51)$$

$$\dot{z} = A\sin(\pi z)\cos(kx) = \frac{\partial\psi}{\partial x}(x,z), \qquad (3.3.52)$$

where $\psi(x,z) = \frac{A}{k}\sin(kx)\sin(\pi z)$, A is the maximum vertical velocity in the flow, $k = \frac{2\pi}{\lambda}$ (λ the wavelength associated with the cell pattern), and the length measures have been non-dimensionalized so that the top is $z = 1$ and the bottom $z = 0$. This flow has a countable infinity of hyperbolic fixed points on the upper boundary at $(x,z) = (\frac{j\pi}{k}, 1)$, $j = 0, \pm 1, \pm 2, \ldots$ and a countable infinity of hyperbolic fixed points on the lower boundary at $(x,z) = (\frac{j\pi}{k}, 0)$, $j = 0, \pm 1, \pm 2, \ldots$. Fixed points with the same x coordinate are connected by a heteroclinic orbit. The result is an infinite number of cells, and we will be concerned with the transport of a passive tracer (say, dye) from cell-to-cell.

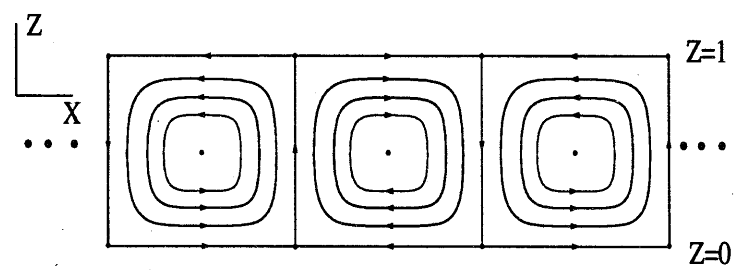

Figure 3.1: Streamlines for the steady, cellular flow.

In the absence of molecular diffusion transport between cells cannot occur. However, if the temperature difference between the top and bottom of the convection cell is increased, an additional time-periodic instability occurs, resulting in a time-periodic velocity field (Clever and Busse [C-B], Bolton *et al.* [B-B-C]). In this situation complex and chaotic fluid particle motions can occur. This has been studied in Camassa and Wiggins [C-W].

Solomon and Gollub [S-G] introduced the following model of this so called *even oscillatory roll instability*:

$$\dot{x} = -\frac{A\pi}{k}\cos(\pi z)[\sin(kx) + \epsilon k \cos\theta(t)\cos(kx)] = -\frac{\partial\psi}{\partial z}(x, z, \theta(t)), \quad (3.3.53)$$

$$\dot{z} = A\sin(\pi z)[\cos(kx) - \epsilon k \cos\theta(t)\sin(kx)] = \frac{\partial\psi}{\partial x}(x, z, \theta(t)), \quad (3.3.54)$$

$$\dot{\theta} = \omega, \quad (3.3.55)$$

where $\psi(x, z, \theta(t)) = \frac{A}{k}\sin(kx)\sin(\pi z) + \epsilon\cos\theta(t)\cos(kx)\sin(\pi z)$, $\theta(t) = \omega t$, ω is a positive number (hence the flow is time periodic), and $\epsilon \sim (R - R_c)^{\frac{1}{2}}$, where R is the Rayleigh number and R_c its critical value at which the time-periodic instability occurs. The pros and cons of this model are discussed in Solomon and Gollub [S-G] and the following discussion will be based on the fluid particle paths generated by this model.

In the cell-to-cell transport problem the time average along particle trajectories of the x-component of velocity is a useful quantity. Thus the appropriate sum function corresponds to the displacement in the x direction, and it is given by

$$x(t) - x(0) = \int_0^t \left(-\frac{A\pi}{k}\cos(\pi z(t))[\sin(kx(t)) + \epsilon k\cos(\omega t)\cos(kx(t))]\right) dt,$$

where $(x(t), z(t))$ denotes a trajectory.

In order to illustrate the "patchiness" effect we numerically determine the distribution of average x-components of velocity for fluid particle trajectories in one cell. In figure 3.2 we plot contours corresponding to initial points of trajectories that have the same average x-velocity which we obtained by numerically computing these time averages for a uniform grid of 1600 points for on a time interval of 5000 periods.

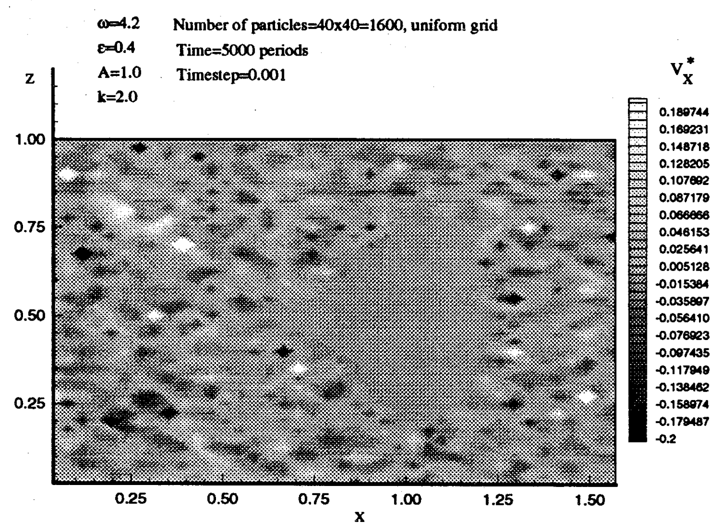

Figure 3.2: Contours corresponding to points having the same average x-component of velocity.

Regions of nonzero average x velocity correspond to "accelerator modes" and these are the points that participate in cell-to-cell transport. In figure 3.3 we plot a histogram of this data, i.e., we plot the number of points corresponding to a given "bin width" of average x velocity, where the bin width is 0.002.

R. Pasmanter in [Pas1],[Pas3] observed that the dispersion of fluid particles in laminar incompressible flows exhibits the phenomenon of "patchiness." It has been observed in those works that fluid particles in incompressible laminar flows under study tend to disperse in "patches," with different patches having different average velocities. Here

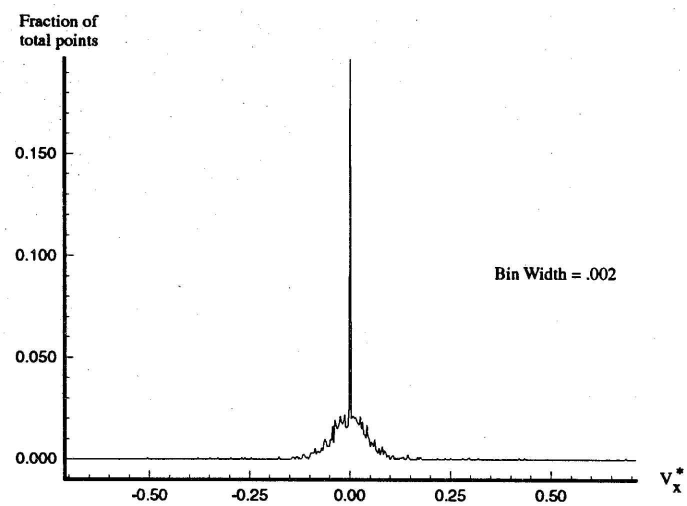

Figure 3.3: The distribution of the average x-component of velocity.

we explain this phenomenon in terms of the properties of a distribution G^∞ proved in this section. As every time-periodic flow on $\mathbb{R}^2$ can be reduced to the Poincare map, we assume that has been done with the flow (3.3.53),(3.3.54),(3.3.55). The function $f(x, y) = x(t) - x(0)$ is then a "jump" in the direction of x, defined on the finite cylinder $[0, 2] \times S^1$, and depending on the initial positions of the particle on the annulus. We can now define "patches" rigorously as sets of positive measure P in the phase space on which f has a constant time-average. Through the Theorem 3.3.2 we can then conclude that "patches" correspond to the points of discontinuity of G^∞. Also, Theorem 3.3.1 tells us that there is at most uncountably many patches. The measure of the phase space is finite. Therefore, in the case where there really are uncountably many patches, their size must go to zero if we order them with respect to their measure. So, there are either a finite number of patches, or there is an uncountable number of them, but also uncountably many of them are of smaller measure than any prescribed number. In the figure 2, the "patches" are represented by the darkest and brightest spots on the phase space. We could also define "patchines" as the regime in which more than one "patch" exists. Non-ergodicity then appears as a necessary condition for "patchiness." Namely, if the flow is ergodic, there is only one "patch," represented as one and only point of discontinuity in G^{∞}. Also, using Proposition 3.3.1 in the context of fluid flows we find that if the flow (or its Poincaré map) is such that it has an ergodic component of a positive measure, and if the initial distribution is such that the measure P of that component is also of positive measure (this is what the absolute continuity of μ with respect to P assures), then the flow will be "patchy" i.e., G^{∞} will have a point of discontinuity.

3.4 First passage times

In this section we shall analyse the following problem: we are given a set A, automorphism T and a function f on A, all defined as in previous sections. We ask: what is the measure with respect to P of a set D_n, defined by

$$D_n = \{x \in A \mid |F^i(x)| < l \ \forall i < n \text{ and } \ |F^n(x)| \geq l\}. \tag{3.4.56}$$

Let the function $E^l : \mathbf{N} \to \mathbb{R}$ be given by $E^l(n) = P(D_n)$. Determination of $E^l(n)$ is called the problem of *first passage times.* We shall first give an explicit expression for $E^l(n)$ using the connection between *Dirichlet's discontinuous integral* (see e.g., [C]), and the characteristic functions of certain sets on A. Later on we shall investigate some asymptotic properties of *renormalized first passage times.*

3.4.1 Dirichlet's discontinuous integral and characteristic functions

Consider a function δ defined by

$$\delta(\alpha, \varpi) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\sin(\alpha\rho)}{\rho} \exp(i\rho\varpi) d\rho, \tag{3.4.57}$$

where $i \equiv \sqrt{-1}$. It can be shown that

$$\delta(\alpha,\varpi)=\begin{cases}1 & -\alpha<\varpi<\alpha\\ 1/2 & \varpi=-\alpha \text{ or } \varpi=\alpha\\ 0 & \text{otherwise}\end{cases}, \tag{3.4.58}$$

see Gradshteyn-Rhyzhik [G-R], pg 414. δ is usually called Dirichlet's discontinuous integral. Define a function K_{D_n} by

$$K_{D_n}(x)=(1-\delta(l,F^n(x))\prod_{i=1}^{n-1}\delta(l,F^i(x)).$$

We have the following proposition:

Proposition 3.4.1 *Assume that P, defined in (3.3.39), is a complete measure on A. Suppose* $P(\{x||F^i(x)|=l\})=0,\ \ \forall i\in\mathbf{N}$. *Then*

$$\int_A K_{D_n}pd\mu=\int_A \chi_{D_n}pd\mu,$$

where χ_{D_n} *is the characteristic function of the set* D_n *defined in (3.4.56).*

Proof: From the definition of δ, (3.4.58), we have

$$\begin{aligned}\int_A K_{D_n}pd\mu &= \int_A(1-\delta(l,F^n(x))\prod_{i=1}^{n-1}\delta(l,F^i(x))pd\mu\\ &= P(\{x\in A\mid |F^i(x)|<l\ \forall i<n \text{ and } |F^n(x)|\geq l\})\\ +\sum_{i=1}^{n}\frac{1}{2^i}\sum_{j_1<j_2<\ldots<j_i} & P(\{x\in A\mid |F^{j_k}(x)|=l \quad\text{for}\quad 1\leq k\leq i,\\ & \text{and}\quad |F^k(x)|<l\ \forall k\neq j_1,\ldots j_i,n\ ,\\ & \text{and}\ |F^n(x)|>l\ \text{ if }\ n\neq j_1,\ldots j_i\ \}),\end{aligned} \tag{3.4.59}$$

where $j_1,j_2,\ldots,j_i\in(1,2,\ldots,n)$ for every i. Now each of the sets whose measure with respect to P appears in the sum $\sum_{j_1<j_2<\ldots<j_i}$, is a subset of of the set $\{x||F^m(x)|=l\}$ for some $m\in(1,2,\ldots,n)$. But, by assumption, these are sets of measure zero with

respect to P. As P is a complete measure, each of the summands in $\sum_{j_1<j_2<\ldots<j_i}$ is zero. Therefore,

$$\begin{aligned}\int_A K_{D_n} p d\mu &= P(\{x \in A \mid |F^i(x)| < l \; \forall i < n \text{ and } |F^n(x)| \geq l\}) \\ &= \int_A \chi_{D_n} p d\mu. \end{aligned} \tag{3.4.60}$$

□

It is easy now to obtain $E^l(n)$, if we keep the assumptions from the Proposition 3.4.1. Observe that

$$E^l(n) = P(D_n) = \int_A \chi_{D_n} p(x) d\mu = \int_A (1 - \delta(l, F^n(x)) \prod_{i=1}^{n-1} \delta(l, F^i(x)) p(x) d\mu. \tag{3.4.61}$$

Thus, we have an explicit expression for first passage times distribution, $E^l(n)$, in terms of f and T, which are known. Note that in the case of positive f, (3.4.61) reduces to

$$E^l(n) = \int_A (1 - \delta(l, F^n(x)) \delta(l, F^{n-1}(x)) p(x) d\mu, \tag{3.4.62}$$

as in that case $F^{n-1} < l \;\Rightarrow\; F^i < l \;\forall\; i < n-1$.

In the case that the condition $P(\{x \| F^i(x)| = l\}) = 0, \;\; \forall i \in \mathbf{N}$ seems too stringent to the reader, the following proposition addresses this issue:

Proposition 3.4.2 *Let* $l_p \in \mathbb{R}$. *Then,* $\forall \epsilon > 0$, $\exists l \in [l_p - \epsilon/2, l_p + \epsilon/2]$, *such that* $P(\{x \| F^i(x)| = l\}) = 0, \;\; \forall i \in \mathbf{N}$.

Proof: Fix l_p, and suppose the statement of the Proposition is false. Then there exists an ϵ such that for every $l \in [l_p - \epsilon/2, l_p + \epsilon/2]$, there exists an n such that

$$P(\{x \| F^n(x)| = l\}) > 0.$$

Assign such an $n(l)$ to each l in $[l_p - \epsilon/2, l_p + \epsilon/2]$. There must be an $m \in \mathbf{N}$ such that the set l_m of $l \in [l_p - \epsilon/2, l_p + \epsilon/2]$ such that $n(l) = m$ is not finite or countably infinite. To prove that, suppose that all such sets are either countable or finite. Then, $[l_p - \epsilon/2, l_p + \epsilon/2] = \cup_m l_m$, where $n(l_m) = m$ is a countable union of countable or finite sets, therefore it is countable (Munkres [Mu], Theorem 7.4). Thus we obtain a contradiction.

Now we know that there is an m such that the set l_m is not countable. For each $l \in l_m$, $P(\{x||F^m(x)| = l\}) > 0$. But, each such l corresponds to the point of discontinuity of W^m, and we know that the set of points of discontinuity of W^m is at most countable (Sarapa, Proposition 9.2 pg. 257). Therefore, by contradiction we are done. □

From the above proposition, we see that in every, arbitrary small neighborhood of l_p, there is an l, such that for l the first passage times distribution $E^l(n)$ is given by (3.4.61)

3.4.2 Renormalized first passage times

A physically important limit of the distribution of first passage times is that when the interval $l \to \infty$. For simplicity we shall consider the case when $|f^*(x)| > \delta > 0$, $\forall x \in \Sigma$. Now, clearly, $E^l(n)$ is (again as in the case of W^n when $n \to \infty$) rather boring when $l \to \infty$: number of iterations, for any point of Σ, needed to escape $[-l, l]$ interval goes to infinity. To get a hold on asymptotic properties of first passage times distribution, we need to do certain rescaling, just as in the case of W^n in the previous section. A natural "timescale" for n is $l/\bar{f}^* = l/\bar{f}$. Let $N(x, l)$ be the first passage time for the point x, i.e.,

$$N(x, l) = n \in \mathbf{N}|\ |F^i(x)| < l\ \forall i < n \text{ and } \ |F^n(x)| \geq l.$$

So, N is a function $N : A \times \mathbb{R} \to \mathbb{R}$. Consider the renormalized function

$$N_r(x,l) = \frac{N(x,l)\bar{f}}{l}.$$

We have the following proposition:

Proposition 3.4.3

$$\lim_{l\to\infty} N_r(x,l) = \frac{\bar{f}}{f^*(x)}$$

a.e. in Σ.

Proof: We need to show that for any sequence $\{l_i\}$, such that $l_i \to \infty$ when $i \to \infty$, for every $\epsilon > 0$ there exists I such that

$$i \geq I \Rightarrow |N_r(x,l_i) - \frac{\bar{f}}{f^*(x)}| < \epsilon.$$

So, pick such a sequence, $\{l_i\}$, and ϵ. Let $x \in \Sigma$. Note that we can always find $\zeta_2(x, N(x,l_i))$ such that

$$F^{N(x,l_i)}(x) + \zeta_2(x, N(x,l_i)) = l_i, \tag{3.4.63}$$

where $\zeta_2(x, N(x,l_i))$ is defined by the above equation. $\zeta_2(x, N(x,l_i))$ is bounded for every $i \in \mathbf{N}$, and every $x \in \Sigma$, as

$$F^{N(x,l_i)-1}(x) < l_i \leq F^{N(x,l_i)}(x),$$

so

$$\zeta_2(x, N(x,l_i)) \leq \max_{x\in A} f(x).$$

Now, by the B.E.T.,

$$F^{N(x,l_i)}(x) = N(x,l_i)f^* + \zeta_1(x, N(x,l_i)),$$

for every $x \in \Sigma$, where

$$\lim_{i\to\infty} \frac{\zeta_1(x, N(x,l_i))}{N(x,l_i)} = 0.$$

Let

$$\zeta(x, N(x,l_i)) = \zeta_1(x, N(x,l_i)) + \zeta_2(x, N(x,l_i)).$$

Now, for every $\delta > 0$, we can choose I such that

$$|\frac{\zeta(x, N(x,l_i))}{N(x,l_i)}| < \delta, \tag{3.4.64}$$

for every $i > I$. Choose

$$\delta < \min(|f^*|, \frac{\epsilon (f^*)^2}{\bar{f} + \epsilon |f^*|}). \tag{3.4.65}$$

(3.4.63), (3.4.64) and (3.4.65) now can be used to show that

$$\begin{aligned}
|N_r(x,l_i) - \frac{\bar{f}}{f^*(x)}| &= |\frac{N(x,l_i)\bar{f}}{l_i} - \frac{\bar{f}}{f^*(x)}| \\
&= |\frac{N(x,l_i)\bar{f}}{N(x,l_i)f^* + \zeta(x, N(x,l_i))} - \frac{\bar{f}}{f^*(x)}| \\
&= |\frac{\frac{\zeta(x,N(x,l_i))}{N(x,l_i)}\bar{f}}{(f^*)^2 + \frac{\zeta(x,N(x,l_i))}{N(x,l_i)} f^*}| \\
&< |\frac{\bar{f}\delta}{(f^*)^2 - \delta f^*}| \\
&< \epsilon,
\end{aligned} \tag{3.4.66}$$

for every $i > I$. The above argument is valid for every $x \in \Sigma$. As Σ^c is of measure zero, we are done. □

Note that uniform convergence in Σ can actually be proved, if Σ is closed, by taking δ in (3.4.64) to be

$$\delta < \min(\min_{x\in\Sigma} |f^*|, \min_{x\in\Sigma}(\frac{\epsilon (f^*)^2}{\bar{f} + \epsilon |f^*|})). \tag{3.4.67}$$

3.4.3 The nature of iso-residence time sets in mixing devices

Consider the following divergence free (incompressible) three-dimensional velocity field

$$\begin{aligned} \dot{x} &= u(x,y,t), \\ \dot{y} &= v(x,y,t), \\ \dot{z} &= w(x,y,t), \end{aligned} \tag{3.4.68}$$

where $z \in \mathbb{R}$ is unbounded, but $(x,y) \in A$, where A is a compact subset of $\mathbb{R}^2$. Just like in the introduction, we shall assume that the time dependence is periodic.

Recalling the discussion in the introduction, statistical properties of the motion in the direction of z can be analyzed using the sum-function formalism.

In the context of pipe or duct flows it is natural to think of an experiment where an initial distribution of points are placed in a cross section $z = z_0$ and allowed to evolve under the flow. The following question then arises. *At a fixed point $z = z_0 + L$ downstream, what is the nature of the points in the initial distribution that pass this point at the same time? Moreover, how are these points related to the particle dynamics in the cross section?* One can study fluid particle trajectories through a two-dimensional Poincaré map. The proposition (3.4.3) has an important consequence: the first passage times for big l are approximately constant on the elements of the measurable partition ξ_f. This type of behaviour has been observed in some numerical studies of the so-called exit age distributions in the types of mixing devices used in chemical engineering applications (see Khakhar *et al.* [K-F-O]. Namely, as noted in the introduction, in that work it has been found that the "isoresidence time sets" exhibited a strong resemblance to the Poincaré sections, and the more so the longer the pipe. Let $f(x, y)$ be the jump in the z direction in one step of the Poincaré map of (3.4.68) (note the abuse of a notation: x in the preceding section was a point in the phase space, while x, y here are the coordinates in the cross section of the pipe). Now the "isoresidence time sets" from that example can be precisely defined as the sets on which $N_\tau(x, y, l)$ is constant. We saw from the (3.4.3) that these sets coincide with ξ_f-sets in the limit when l goes to infinity, i.e., in the long pipe limit. As $f^*(x, y)$ is constant on the orbits, every ξ_f-set is composed of orbits. In other words, we proved that the "isoresidence time sets" in the large l limit are composed of the orbits of the Poincaré map, which explains the observation in [K-F-O].

3.5 Dynamical systems with continuous time

3.5.1 Dispersion of sum functions

In this section we extend most of our results to continuous time dynamical systems.

By a continuous time dynamical system we mean a one-parameter group of measure preserving automorphisms $\{T^t\}$, where $t \in \mathbb{R}$, of the compact, metric phase space A. We assume that A is endowed with a complete, probabilistic measure μ, as in the first section. We assume that a standard Lebesgue measure t (a slight abuse of notation, as t also denotes the parameter of a group, but hopefully understandible) is given on $\mathbb{R}$, and the measure on $A \times \mathbb{R}$ is a product measure $\nu = \mu \times t$. We shall need the following facts:

Lemma 3.5.1 *Assume that f is an bounded, measurable function on A, and $\tau > 0$. Then $\int_0^\tau f(T^t x)dt$, exists. Further, $\int_0^n f(T^t x)dt = \sum_{i=0}^{n-1} g(T^n x)$, where $g(T^n x) =$*

$\int_0^1 f(T^t x)dt$, *and* $g(x)$ *is an integrable function on* A.

Proof: This follows immediately by the boundedness and measurability of f, and compactness of A. □

Now we can define the notion of a sum function. Let f be a measurable, bounded function on $f : A \to \mathbb{R}$. The sum function, F^τ is defined by

$$F^\tau = \int_0^\tau f \circ T^t dt. \tag{3.5.69}$$

As f is bounded and measurable, F^τ is bounded and measurable a.e. for every $\tau > 0$. We require p to be integrable, and

$$\int_A p d\mu = 1.$$

We can define the mean value of a sum function,

$$\langle F^\tau \rangle = \int_A F^\tau p d\mu, \tag{3.5.70}$$

and a dispersion, $D(\tau)$

$$D(\tau) = \sigma^2(\tau) = \int_A (F^\tau - \langle F^\tau \rangle)^2 p d\mu, \tag{3.5.71}$$

(3.5.70) and (3.5.71) exist by the same argument as in the discrete case. The spatial average of f is still defined by (3.2.20). The time average is given by

$$f^*(x) = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau f(T^t(x))dt,$$

and it exists, a.e. in A by the B.E.T. for continuous-time dynamical systems (see Krengel [K]). We denote the set on which $f^*(x)$ exists by Σ. So, we can again define the partition ξ_f of the phase space A induced by the time average f^*. The elements of ξ_f are the sets $B_c = \{x \in A | f^*(x) = c, c \in \mathbb{R}\}$, and the set Σ^c. Now we state and prove the analogue of Theorem 3.2.1 for dynamical systems with continuous time:

Theorem 3.5.1 *Consider a one parameter group of measure preserving automorphisms, $\{T^t\}$ on A, a bounded, measurable function $f : A \to \mathbb{R}$, and an initial distribution p, all defined as above. Suppose that there is no $c \in \mathbb{R}$ such that $\mu(supp(p)\backslash B_c) = 0$. Then, we have*

$$\lim_{\tau\to\infty} \frac{D(\tau)}{\tau^2} = a < \infty,$$

where

$$a = \int_A \left[f^* - \int_A f^* p d\mu\right]^2 p d\mu, \tag{3.5.72}$$

and $a > 0$. Conversely, if $0 < a < \infty$, then $\mu(supp(p)\backslash B_c) \neq 0, \forall c \in \mathbb{R}$.

Proof: We only need to do the necessary steps to bring the expression $D(\tau)/\tau^2$ in the form in which Lebesgue's bounded convergence theorem is applicable. From the definition of $D(\tau)$, we have

$$\begin{aligned} \frac{D(\tau)}{\tau^2} &= \int_A (\frac{F^\tau}{\tau} - \langle\frac{F^\tau}{\tau}\rangle)^2 p d\mu \\ &= \int_A (\frac{1}{\tau}\int_0^\tau f\circ T^t dt - \langle\frac{1}{\tau}\int_0^\tau f\circ T^t dt\rangle)^2 p d\mu. \end{aligned} \tag{3.5.73}$$

Using Lemma 3.5.1, we obtain

$$\frac{D(\tau)}{\tau^2} = \int_A (\frac{1}{\tau}\sum_{i=0}^{n-1} g\circ T^i - \langle\frac{1}{\tau}\sum_{i=0}^{n-1} g\circ T^i\rangle + \frac{1}{\tau}\int_n^\tau f\circ T^t dt - \langle\frac{1}{\tau}\int_n^\tau f\circ T^t dt\rangle)^2 p d\mu, \tag{3.5.74}$$

where n is chosen such that $n \leq \tau < n+1$. Now, if for any sequence $\{\tau_n\}$ such that $\tau_n \to \infty$ when $n \to \infty$,

$$\lim_{n\to\infty} \frac{D(\tau_n)}{\tau_n^2} = a,$$

then $\lim_{\tau\to\infty} \frac{D(\tau)}{\tau^2} = a$. Choose such a sequence. We have

$$\lim_{n\to\infty} \frac{D(\tau_n)}{\tau_n^2} = \lim_{n\to\infty} \int_A (\frac{1}{\tau_n}\sum_{i=0}^{n-1} g\circ T^i - \langle\frac{1}{\tau_n}\sum_{i=0}^{n-1} g\circ T^i\rangle$$

$$+\frac{1}{\tau_n}\int_n^{\tau_n} f\circ T^t dt - \langle\frac{1}{\tau_n}\int_n^{\tau_n} f\circ T^t dt\rangle)^2 p d\mu. \tag{3.5.75}$$

Now, by the Lebesgue's bounded convergence theorem, the integral in (3.5.75) converges to

$$\int_A (\lim_{n\to\infty}\frac{1}{\tau_n}\sum_{i=0}^{n-1} g\circ T^i - \langle\lim_{n\to\infty}\frac{1}{\tau_n}\sum_{i=0}^{n-1} g\circ T^i\rangle$$
$$+\lim_{n\to\infty}\frac{1}{\tau_n}\int_n^{\tau_n} f\circ T^t dt - \langle\lim_{n\to\infty}\frac{1}{\tau_n}\int_n^{\tau_n} f\circ T^t dt\rangle)^2 p d\mu. \tag{3.5.76}$$

Noting that

$$\lim_{n\to\infty}\frac{1}{\tau_n}\sum_{i=0}^{n-1} g\circ T^i = \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^{\tau} f\circ T^t dt,$$

where they exist, we have

$$\lim_{\tau\to\infty}\frac{D(\tau)}{\tau^2} = \int_A\left[f^* - \int_A f^* p d\mu\right]^2 p d\mu.$$

The rest of the proof is exactly the same as in the discrete case. □

We now know that for all groups of automorphisms $\{T^t\}$ and initial distributions p satisfying $\mu(supp(p)\backslash B_c) = 0$, for very long times τ, $D(\tau) \sim \tau^2$, and we were able to calculate the constant a from the time averages. Sometimes it is important to know what is the behaviour of $D(\tau)$ for initial times, $\tau << 1$. It is well-known in the theory of turbulent dispersion that $D_{turb}(\tau) \sim \tau^2$ for $\tau << 1$, where $D_{turb}(\tau)$ is the mean square distance of particles at time τ in a turbulent fluid flow (see Batchelor and Townsend [B-T]). We now provide a proof of the corresponding fact in our context, using Wiener's local ergodic theorem.

Theorem 3.5.2 *Define the sets C_c as follows:*

$$C_c = \{x \in A | f(x) = c, c \in \mathbb{R}\}.$$

Consider a one parameter group of automorphisms, $\{T^t\}$ on A, a function $f : A \to \mathbb{R}$, and an initial distribution p, all defined as above. Suppose that there is no $c \in \mathbb{R}$ such that $\mu(supp(p)\backslash C_c) = 0$. Then, we have

$$\lim_{\tau \to 0} \frac{D(\tau)}{\tau^2} = a < \infty,$$

where

$$a = \int_A \left[f - \int_A f p d\mu \right]^2 p d\mu, \tag{3.5.77}$$

and $a > 0$.

Proof: The proof of this theorem essentially follows the proofs of Theorem 3.3.2, and Theorem 3.2.1. One necessary change in the line of the proof of the Theorem 3.3.2 is the replacement of the B.E.T. with the Wiener local ergodic theorem, which states

$$\lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_0^\epsilon f(T^t x) dt = f(x),$$

(see Wiener [Wi1]). □

The ergodic partition theory goes through in the continuous time setting in exactly the same manner as in the discrete time systems (see Rokhlin [R]). In particular, Lemma 3.2.2, Proposition 3.2.2, Proposition 3.2.3, and Proposition 3.2.1 all have their continuous-time analogues.

3.5.2 Other statistical properties

We can use the probability theory formalism in the analysis of dynamical systems with continuous time, too. The only difference will appear in the treatment of limits, but the type of argument used in the subsection 5.1 for the proof of Theorem 3.5.1 (arbitrary sequence argument) will serve to transfer the problem to discrete-time setting.

Let us first consider the distribution function $W^\tau : \mathbb{R} \to \mathbb{R}$ defined by

$$W^\tau(y) = P\{x \in A | F^\tau(x) \le y\}. \tag{3.5.78}$$

As we just replaced n with τ in (3.3.38), it is easy to see that all of the properties of W^n hold for W^τ. In particular, we can obtain an explicit expression for W^τ in exactly the same way as for W^n.

Assuming again, for simplicity, $|f^*(x)| > \delta > 0$, $\forall x \in \Sigma$, we can introduce the change of coordinates

$$z = \frac{y - \bar{f} \cdot \tau}{\sigma},$$

for the same reasons as in the discrete-time case. The renormalized distribution G^τ is given by

$$G^\tau(z) = P\{x \in A | \frac{F^\tau(x) - \bar{f} \cdot \tau}{\sigma} \le z\}, \tag{3.5.79}$$

and G^∞ is defined in exactly the same way as in the discrete-time case, with the definition of f^* being appropriately changed:

$$G^\infty(z) = P\{x \in A | \frac{f^*(x) - \bar{f}}{a} \le z\}. \tag{3.5.80}$$

The analogue of the Theorem 3.3.1 needs a little work.

Theorem 3.5.3 *G^τ converges to G^∞ in the sense of distributions, i.e.,*

$$\lim_{\tau \to \infty} G^\tau(z) = G^\infty(z), \quad \forall z \in C(G^\infty),$$

where $C(G^\infty)$ is the set of all points of continuity of G^∞. Also $[C(G^\infty)]^c$ is at most a countable set of points.

Proof: We only need to note that for each sequence $\{\tau_i\}$ such that $\tau_i \to \infty$ when $i \to \infty$, a sequence of functions $(F^{\tau_i}(x) - \bar{f} \cdot n)/\sigma$ is a sequence of random variables converging to

$(f^*(x) - \bar{f})/a$ pointwise almost everywhere. Note that the domain of convergence does not depend on a particular sequence τ_i - it is always Σ. This means that, in the sense of distributions, G^{τ_i} converges to G^∞. As $\{\tau_i\}$ is arbitrary, G^τ converges to G^∞ at z. □

Now, as proofs of the Theorem 3.3.2 and the Proposition 3.3.1 do not involve a limiting process, and the notion of ergodic partition goes through, their statements are the same in the continuous-time case. So, the points of discontinuity of G^∞ are again connected, in the same way as in the Theorem 3.3.2 and the Proposition 3.3.1, with the elements of partitions ξ or ξ_f of nonzero measure.

The analysis of first passage time in 3.1 cannot be extended to a continuous-time case. The reason is that we used Dirichlet's discontinuous integral at each step of the iteration to decide whether a particular point is inside or outside the interval $[-l, l]$, or exactly at l or $-l$. Now, in the case of the continuous time, obviously, we cannot do that. What we can do, though, is state the analogue of the Proposition 3.4.3. We again have the restriction $|f^*(x)| > \delta > 0$, $\forall x \in \Sigma$. Define the first passage time, $\Theta(x, l)$ by

$$\Theta(x,l) = \tau \in \mathbb{R}|\ |F^{\bar{\tau}}(x)| < l\ \forall \bar{\tau} < \tau \text{ and } \ |F^\tau(x)| \geq l.$$

Let the *renormalized first passage time* be defined by

$$\Theta_r(x,l) = \frac{\Theta(x,l)\bar{f}}{l}.$$

Now we have

Proposition 3.5.1

$$\lim_{l\to\infty} \Theta_r(x,l) = \frac{\bar{f}}{f^*(x)}$$

a.e. in A.

Proof: The proof proceeds in the same manner as the proof of the Proposition 3.4.3. □

3.6 Conclusions

Let us now summarize, and discuss certain restrictions of this theory and possible improvements. Firstly, let us discuss the requirements of the boundedness of the functions we consider, and the compactness of A. Note that we were working with a class of bounded measurable functions throughout the chapter. The boundedness served us in showing that the statistical properties, like the mean value and the dispersion, exist, and in providing different estimates. We used compactness only to assure that the ergodic partition can be obtained as the product of the partitions induced by the time averages of continuous functions on A. Furthermore, this fact (proved in chapter 4 and Mezić and Wiggins [M-W2]) was used in in the chapter only in the connection between the ergodic partition and the partition induced by the time averages of bounded, measurable functions (through the Proposition 3.2.1). For all other results it is enough that A is a probability space (and thus of finite measure). Note that in the case when space A has infinite measure, and a measure-preserving map T is such that there is no T-invariant subset of finite measure, the theory developed here is vacuous: in that case the time average of any integrable function is zero almost everywhere (see Rudolph [Ru]). Obviously, if there exists an invariant subset for T, which is of finite measure, we can restrict consideration to that subset and apply our theory. On the other hand, our results really depend only on the existence of time averages. There might be some nonintegrable function for which the time averages on a support of the initial distribution exist, in which case the whole theory goes through.

In this chapter, we have taken the point of view which in the fluid dynamical literature is often called *Lagrangian*: we give some initial condition, and then consider its dynamics under the mapping T. The point samples values of the function f during its motion, and we can show some of the statistical properties of this process. Let us take another point of view, called *Eulerian* in the fluid dynamical context. We can imagine having a probe at a position x in the space A. Let the initial distribution of some scalar-valued quantity be called f_0. Suppose that we are interested in how is this initial distribution transported by T. In the space of bounded, measurable functions, measure-preserving transformation T induces the Koopman operator U defined by

$$Uf = f \circ T.$$

Let $f(x,i)$ be the value of the scalar field at x at time i. Then, $f(x,i) = f_0(T^{-i}x)$. Consider the time average $f^*_-(x)$ of the scalar field at x as sampled by the probe:

$$f^*_-(x) = \frac{1}{n}\sum_{i=1}^{n} f(x,i) = \frac{1}{n}\sum_{i=1}^{n} f_0(T^{-i}x) = (f_0^*)^-(x).$$

Now, $(f_0^*)^-(x) = f_0^*(x)$ (see e.g., Mañe [M]), and the considerations in the sections on distributions, can be applied to deduce the properties of distributions of time averages of passive scalars. In particular, the time average of a passive scalar quantity is constant on the elements of ξ_{f_0}. In connection with this observation, suppose that A is the closure of an open subset of $\mathbb{R}^n$. As is well known, the evolution of the passive scalar function $f(x,t)$ $x \in A$, $t \in \mathbb{R}$, in the case of a continouus flow on A generated by a vector field $\mathbf{v}$, is governed by

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = 0. \qquad (3.6.81)$$

Thus, in the case of a continuous flow, the above considerations allow us to analyze statistical properties of (3.6.81). Besides the well-known application to non-diffusive transport of particle concentration and temperature, (3.6.81) is, as shown recently by Pasmanter [Pas2], related to some types of Schrödinger equation. Of course, the question of how the ergodic properties of $\mathbf{v}$ affect the asymptotic behaviour of the convection-diffusion equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = \nu \triangle f, \tag{3.6.82}$$

appears most naturally here. We pursue this study in chapter 6.

Finally, let us discuss the relationship of this theory to the theory of strictly stationary stochastic processes. As is well-known, every measure-preserving point transformation T on A defines a class of strictly stationary stochastic processes through the Koopman operator defined above (see e.g., Doob [D]). In particular, let f be a function on A or a random variable, in probability theory terminology. Then $f_n = f \circ T^n$. $\{f_n\}$ is is a strictly stationary stochastic process. More interestingly, there is the following partial converse: Let $\{f_n\}$ be a strictly stationary stochastic process. Then there is a measure-preserving set transformation T such that $f_i = f_0 \circ T^i$. It is not hard to realize that all the theorems we have developed are true in the context of measure-preserving set transformations instead of measure-preserving point transformations. In particular, there is a version of the B.E.T. for measure-preserving set transformations (see Doob [D]). Note also that all analogies with probability theory that we used (e.g., in section 3) stem from the above explained connection between dynamical systems theory and stochastic processes. Important early work using this connection was done by Sinai [S1],[S2],[S3].

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Chapter 4

A new characterization of the ergodic partition

4.1 Introduction

The notion of the ergodic partition [1] of automorphisms of Lebesgue spaces originates in the works of von Neumann [7], Halmos [3], [4], and Rokhlin [9]. More modern presentations of the ergodic partition can be found in Denker *et al.* [2], Mañé [5] or Rudolph [11]. It has been shown in chapter 3 and Mezić and Wiggins [6] that the ergodic partition can play a role in the analysis of certain statistical properties of non-ergodic measure-preserving dynamical systems. In the same work, another type of partition of the space A was shown to be important: namely, the partition into sets on which the time averages of bounded, measurable functions are constant. In this chapter we connect these two types of partitions by showing how the ergodic partition can be constructed from the measurable partitions induced by the time averages of continuous functions. This approach provides a constructive way of forming the ergodic partition and, potentially, this

[1] Note that the term *ergodic decomposition* is used usually when the decomposed (or partitioned) object is a measure. In this work we are mainly concerned with the partition of the space A into disjoint ergodic components (or ergodic fibres, as in Denker *et al.* [2]). As this is more of a topological subject matter, the term *partition* would be more appropriate.

can lead to numerical algorithms for constructing ergodic partitions. Our construction of the ergodic partition uses the *product* operation on the space of measurable partitions. The ergodic partition turns out to be just the product of measurable partitions induced by the time averages of functions which are elements of a countable, dense subset of the space of continuous functions on the phase space. Our approach provides an easy way of characterizing uniquely ergodic components. In particular, it is shown that if C is an closed ergodic component, then C is uniquely ergodic. Also, we make connection between the partitions induced by the time averages of measurable, bounded functions, and the ergodic partition.

This work can, in a certain sense, be regarded as a bridge between the two different approaches to the presentation of the ergodic partition: that of Mañé [5] (which is based on the work of Denker *et al.* [2]), and Rokhlin [9]. Rokhlin's work is based on the notion of measurable partitions. He develops his theory around the ergodic theory of functions on $L^2(A)$. The space A is required to be a Lebesgue measure space. He is interested in how the space A splits into ergodic components under the dynamics of T. The ergodic partition is shown to be the measurable hull of the decomposition of the phase space into orbits of T. Mañé's approach uses the Riesz representation theorem on a compact, metric space A. His work is more directed towards understanding the interplay between invariant and ergodic measures on A (as, it seems, is common in modern ergodic theory). He (as well as Denker *et al.*) does not use the Lebesgue structure of the space. We show that it is fruitful (with an view towards the applications to the theory of chaotic dynamical systems) to join these two approaches.

4.2 Set up and definitions

Let (A, μ) be a compact metric space, such that μ is a complete measure defined on a Borel σ-algebra $\mathcal{A}$, and T a measure-preserving continuous automorphism on A. A thus has the structure of a Lebesgue measure space (see Denker *et al.* [2]). We denote the space of all integrable functions on A by $L^1(A)$, the set of all real continuous functions on A by $C^0(A)$, and a dense countable subset of $C^0(A)$ by S. Following the definitions in Rokhlin [9][2], we have the following:

Definition 4.2.1 (Partition, Measurable Partition) *A family ζ of disjoint sets C_α, (α element of some, arbitrary, index set) whose union is all of A is called a* partition *of A. We call C_α* an element *of ζ. Unions of elements of ζ are called* ζ-sets. *A partition is called* measurable *if there exists a countable family $\triangle$ of measurable sets $\{D_i\}$ such that every D_i is a union of elements of ζ , and for every pair C_1, C_2 of elements of ζ there exists $D_j \in \triangle$ such that $C_1 \subset D_j$, $C_2 \subset D_j^c$. We call $\triangle$ a* basis *for the partition ζ.*

We shall omit the index from the notation for the element of the partition, where that does not cause confusion. A partition ζ_1 is said to be finer than a partition ζ_2 if every component of ζ_2 is a ζ_1-set.

Given a partition ζ of A, and a set A/ζ whose elements are the elements of the partition, we can define a projection map $\pi : A \to A/\zeta$, by the rule $\pi(x) = C_\alpha$, where $x \in C_\alpha$. It can be shown (Rokhlin [8]) that the space A/ζ is a Lebesgue measure space, with the measure $\mu_\zeta(C) = \mu(\pi^{-1}(C))$, for any ζ-set C. We now define a *product* operation on the set of measurable partitions of A.

[2]Note that our definition of $\triangle$ is somewhat different from Rokhlin's, but it is easily seen that they are equivalent. Also, note that both in Mañé [5], and in Denker *et al.* [2] the index set in Definition 4.2.1 is allowed to be at most countable.

Definition 4.2.2 (Product) *Let ζ_1 and ζ_2 be two measurable partitions. Denote the element of ζ_1 by C_1 and the element of ζ_2 by C_2. Let ζ be the family of all sets of the form*

$$C = C_1 \cap C_2.$$

Then we call the measurable partition ζ a product *of ζ_1 and ζ_2, and write*

$$\zeta = \zeta_1 \bigvee \zeta_2.$$

For a finite or countable product, we may write

$$\zeta = \bigvee_{i=1}^{n} \zeta_i, \ n \textit{ finite or } \infty$$

meaning

$$\zeta = \zeta_1 \bigvee \zeta_2 ... \bigvee \zeta_n.$$

in the case of finite n, and

$$\zeta = \zeta_1 \bigvee \zeta_2 ... \bigvee \zeta_i ...$$

in the case $n = \infty$.

Finite and countable products of measurable partitions are measurable partitions themselves, so the product operation is well-defined (see Rokhlin [8], pg 33). Now we turn to the proof of the main theorem.

4.3 Proof of the theorem

We start with the following definitions:

Definition 4.3.1 (Stationary partition, Ergodic partition) . *A measurable partition ζ is called* stationary *if every element of ζ is invariant under T. The stationary* *partition ζ is called* ergodic *if, for almost every (with respect to μ_ζ) element C of ζ, there is an invariant measure μ_C on C such that the restriction of T to C, denoted T_C is an ergodic automorphism on C, with respect to some probability measure μ_C on C, and, for every $f \in L^1(A)$,*

$$\int_A f d\mu = \int_{A/\zeta} \left[\int_C f|_C d\mu_C \right] d\mu_\zeta, \tag{4.3.1}$$

where $f|_C$ denotes the restriction of f to the ergodic component C.

We shall call the function f^* the time average of a function f under T if

$$f^*(x) = \lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n-1} f(T^i(x))$$

almost everywhere (a.e.) with respect to μ. Note that by Birkhoff's pointwise ergodic theorem, f^* exists for every function $f \in L^1(A)$, except, possibly, on a set of measure zero. Denote by Σ the set of all $x \in A$ such that f^* exists for every $f \in C^0(A)$, and by $\Sigma(f)$ the set of all $x \in A$ such that f^* exists for a particular $f \in C^0(A)$. The following lemma appears as a statement in the course of the proof of the Theorem 6.1, chapter 2 in Mañé [5], with just a hint for the proof provided. We include the proof for completeness:

Lemma 4.3.1

$$\Sigma = \cap_{f\in S} \Sigma(f),$$

where S is some dense, countable subset of $C^0(A)$.

Proof: We need to prove $\Sigma \subset \cap_{f\in S}\Sigma(f)$ and $\cap_{f\in S}\Sigma(f) \subset \Sigma$. Clearly, if some x is in Σ, it is in $\cap_{f\in S}\Sigma(f)$. So, we need to prove that for every $x \in A$ such that $f^*(x)$ exists for every $f \in S$, $(f')^*$ exists for every $f' \in C^0(A)$.

Now for every f' there exists, by denseness of S a sequence of functions $\{f_n\}$ in S such that $\lim_{n\to\infty} f_n = f'$ in the norm on C^0, given by $||f|| = \max_{x\in A}|f(x)|$. Consider $\lim_{j\to\infty} a_j$, where

$$\begin{aligned} a_j &= \left[\lim_{n\to\infty}\frac{1}{n}\sum_{i=0}^{n-1} f_j(T^i(x)) - \lim_{n\to\infty}\frac{1}{n}\sum_{i=0}^{n-1} f'(T^i(x))\right] \\ &= \lim_{n\to\infty}\frac{1}{n}\left(\sum_{i=0}^{n-1}(f_j - f')(T^i(x))\right). \end{aligned} \tag{4.3.2}$$

If we can prove that $\lim_{j\to\infty} a_j = 0$, and $\lim_{j\to\infty} f_j^*$ exists, than $(f')^*$ exists and is equal to $\lim_{j\to\infty} f_j^*$, as

$$a_j = f_j^*(x) - \lim_{n\to\infty}\frac{1}{n}\sum_{i=0}^{n-1} f'(T^i(x)).$$

To prove $\lim_{j\to\infty} a_j = 0$, consider

$$a_{jn} = \frac{1}{n}\left(\sum_{i=0}^{n-1}(f_j - f')(T^i(x))\right).$$

If we show

$$\lim_{\substack{j\to\infty \\ n\to\infty}} a_{jn} = 0,$$

we are done. To do this, by Courant [1], pg. 101, we need only to show that $\forall\epsilon > 0$, there exists N such that $\forall j, n > N$,

$$\left|\frac{1}{n}\left(\sum_{i=0}^{n-1}(f_j - f')(T^i(x))\right)\right| < \epsilon.$$

We know that, $\forall\delta > 0$, there exists J such that $\forall j > J$,

$$\max_{x\in A}|(f_j - f')(x)| < \delta.$$

Thus, choose ϵ. Pick $\delta < \epsilon$. Choose $N = J$. Then, $\forall n \in \mathbf{N}, j > J$,

$$\left|\frac{1}{n}\left(\sum_{i=0}^{n-1}(f_j - f')(T^i(x))\right)\right| \le \frac{1}{n}\left(\sum_{i=0}^{n-1}|(f_j - f')(T^i(x))|\right)$$

$$\begin{aligned} &\leq \frac{1}{n}(n \max_{x\in A} |(f_j - f')(x)|) \\ &\leq \frac{\delta n}{n} \\ &\leq \epsilon. \end{aligned} \tag{4.3.3}$$

Therefore, $\lim_{j\to\infty} a_j = 0$.

Now we prove that $\lim_{j\to\infty} f_j^*$ exists. Pick $\epsilon > 0$. We show that there exists J such that $j_1, j_2 \geq J \Rightarrow |f_{j_1}^*(x) - f_{j_2}^*(x)| < \epsilon$, which implies that the limit of the sequence exists. Pick $\delta > 0$. As $\{f_l\}$ converges to f' $\exists L \mid l \geq L \Rightarrow \max_{x\in A} |f_j - f'| < \delta$. This means that $\forall\ l_1, l_2 > L$

$$\begin{aligned} \max_{x\in A} |f_{l_1} - f_{l_2}| &= \max_{x\in A} |f_{l_1} - f' - (f_{l_2} - f')| \\ &\leq \max_{x\in A} |f_{l_1} - f'| + \max_{x\in A} |f_{l_2} - f'| \\ &\leq 2\delta. \end{aligned} \tag{4.3.4}$$

Now choose $\delta = \epsilon/2$ and $J = L$. Then

$$\begin{aligned} |f_{j_1}^*(x) - f_{j_2}^*(x)| &= |\lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n-1} (f_{j_1} - f_{j_2})(T^i(x))| \\ &\leq \lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n-1} |(f_{j_1} - f_{j_2})(T^i(x))| \\ &\leq \lim_{n\to\infty} \frac{1}{n} \left(n \max_{x\in A} |f_{j_1} - f_{j_2}|\right) \\ &\leq \frac{2\delta n}{n} = \epsilon, \end{aligned} \tag{4.3.5}$$

for every $j_1, j_2 > J$. Therefore, the limit $\lim_{j\to\infty} f_j^*(x)$ exists, and the proof is complete.

□

Now we have a set Σ such that the time averages of all continuous functions on A exist on Σ. Σ^c is of measure zero, as by Birkhoff's Ergodic Theorem, each $\Sigma(f)^c$ is of measure zero, and thus Σ^c is a countable union of measure zero sets, which is again of measure zero. Thus, Σ is a Lebesgue measure space. The proof of the following lemma stems from one of the remarks in Rokhlin [8]. The lemma shows that the time averages of measurable, bounded functions induce measurable partitions on Σ.

Lemma 4.3.2 *Let f be a measurable, bounded function on Σ. The family of sets C_α, $\alpha \in \mathbb{R}$ such that $C_\alpha = (f^*)^{-1}(\alpha)$ is a measurable, stationary partition of Σ. We denote this partition by ζ_f and call it the* partition induced by f.

Proof: As $F_n = \frac{1}{n}\sum_{i=0}^{n-1} f(T^i(x))$ is a measurable function on A, and $\lim_{n\to\infty} F_n = f^*$, f^* is a measurable function, too. The fact that ζ_f is a measurable partition follows by taking $\triangle_f$ to be the collection of preimages under f^* of open intervals with rational endpoints in $\mathbb{R}$. As f^* is measurable, each $(f^*)^{-1}[a,b]$ is measurable. Sets of this type, where a and b are rational, clearly separate sets of the form $(f^*)^{-1}\{c\}$, $c \in \mathbb{R}$. The fact that the partition is stationary follows immediately from the definition of the time average of f. $\square$

Note that every continuous function on A is measurable and bounded. Now we can prove our main theorem:

Theorem 4.3.1 *Let*

$$\zeta_e = \bigvee_{f \in S} \zeta_f.$$

be a measureble partition on Σ. Then ζ_e together with Σ^c is an ergodic partition of A with respect to T.

Proof: Let C be an element of ζ_e. Define a bounded linear functional L_C on $C^0(A)|_C$ by

$$L_C(f) = \lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n-1} f(T^i(x)), \quad \text{where } x \in C$$

L_C is well-defined by Lemma 4.3.1. Now by the Riesz representation theorem, there exists a measure μ_C on A, such that

$$L_C(f) = \int_A f d\mu_C.$$

Moreover, for the function $\tilde{f} = 1$ we have $L_C(\tilde{f}) = 1$. This implies that

$$\mu_C(A) = 1.$$

Note that μ_C is invariant under T. To prove this, we have for every continuous f,

$$\int_A f \circ T \, d\mu_C = L_C(f \circ T) = L_C(f) = \int_A f d\mu_C. \tag{4.3.6}$$

Note that for the above operation we needed continuity of T. As continuous functions are dense in L^1, μ_C is invariant under T.

Now we show that μ_C is a probability measure on C. We can find a sequence of compact sets C_n^c, subsets of C^c, such that

$$C_1^c \subset C_2^c \subset ...,$$

and

$$\mu_C(C^c \setminus \cup_{n\geq 1} C_n^c) = 0. \tag{4.3.7}$$

Further, we can show that for every C_n^c, $\mu_C(C_n^c) = 0$. To do this, note that, by Urysohn's Lemma, for every C_n^c there is a continuous function f_n equal to one on C_n^c, and equal to zero outside of C_{n+1}^c. Clearly, as C_i^c's are subsets of C^c, $f_n = 0$ on C. Therefore,

$$\mu_C(C_n^c) \leq \int_A f_n d\mu_C = L_C(f_n) = 0 \Rightarrow \mu_C(C_n^c) = 0.$$

As the measure of a union of the countable number of sets of measure zero is zero,

$$\mu_C(\cup_{n\geq 1} C_n^c) = 0. \tag{4.3.8}$$

Therefore, by (4.3.7) and (4.3.8), $\mu_C(C^c) = 0$, and we are done with the proof of the fact that μ_C is a probability measure on C.

We have shown that μ_C is a probability measure when restricted to C. Let us show that it is an ergodic measure on C. Observe that the set of all restrictions of functions in $C^0(A)$ to C, denoted $C^0(A)|_C$ forms a dense set in the set of all integrable (with respect to μ_C) functions on C. To show this, note that $C_0(A)$ is dense in $L^1(A)$. Let f be an element of $L^1(C)$. Consider its extension to all of A, $\bar{f}$, such that $\bar{f} = f$ on C and $\bar{f} = 0$ elsewhere. As

$$\int_A \bar{f} d\mu_C = \int_C f d\mu_C,$$

exists, $\bar{f} \in L^1(A)$. Therefore, there is a sequence of functions in $C^0(A)$, $\{f_n\}$ converging to $\bar{f}$. But then the corresponding sequence of restrictions, $\{f_n|_C\}$ converges to f.

Now, for every $f \in C^0(A)|_C$ we have

$$L_c(f) = \int_C f d\mu_C = f^*(x). \tag{4.3.9}$$

Recalling (Mañé [5] Proposition 2.2) that if (4.3.9) holds for a dense subset of $L^1(C)$, then T_C is ergodic, this completes the proof that μ_C is an ergodic measure, for every C.

What is left is to show that equality (4.3.1) holds. We need the following two lemmas:

Lemma 4.3.3 *Let* $B = \{x \in A | x \in C \Rightarrow \int_C f d\mu_C = f^*(x)\}$, *where* f *is a measurable, bounded function on* A. *Then* $\mu(B) = 1$.

Proof: This follows using Lemma 6.2. in chapter 2 of Mañé [5], by observing that μ is an invariant measure, and $\int_A f d\mu_C = \int_C f d\mu_C$, as we have shown that $\mu_C(C) = 1$. □

Lemma 4.3.4 *Let* $f \in L^1(A)$. *Then*

$$\int_A f d\mu = \int_A \left[\int_C f|_C d\mu_C \right] d\mu. \tag{4.3.10}$$

Proof: This follows from the Theorem 6.4, Chapter 2 in Mañé [5], using Lemma 4.3.3.

□

Now we complete the proof of the theorem. From Rokhlin [8], as ζ_e is an measurable decomposition, there exists a canonical system of measures $\{\mu_C\}$, such that

$$\int_A f d\mu = \int_{A/\zeta} \left[\int_C f|_C d\mu_C \right] d\mu_\zeta = \int_{A/\zeta} \left[\int_C f|_C d\mu_C \right] d\mu_\zeta, \tag{4.3.11}$$

which is unique (mod 0). So, we are done with the proof of the theorem. □

4.4 Some consequences

As we already mentioned, our interest in the problem of ergodic partitioning of the phase space stems from the fact that the ergodic partition plays a major role in the statistical analysis of non-ergodic systems. Rokhlin [9] already characterized the ergodic partition as the finest of all stationary partitions. Note that every partition ζ_f, induced by some bounded, measurable f is a stationary partition, by Birkhoff's ergodic theorem. The following proposition provides a link between ζ_f and ζ_e:

Proposition 4.4.1 *Let $B_c = \{x \in A | f^*(x) = c\}$ be the components of ζ_f, and B'_c a union of all elements C of ζ_e such that*

$$\int_C f_C d\mu_C = c.$$

Then $\mu((B_c - B'_c) \cup (B'_c - B_c)) = 0$, i.e. every B_c is a ζ_e-set (mod 0).

Proof: Let $Z = \{x \in A | \int_{C_\beta} f_{C_\beta} d\mu_{C_\beta} \neq f^*(x)\}$. From Lemma 4.3.3, we have $\mu(Z) = 0$. Now, set of all x in B'_c such that $f^*(x)$ is not equal to the spatial average over the ergodic component associated with x (which is c) has μ-measure zero, as that set is just a subset of a μ-measure zero set, and μ is complete. This means that $\mu(B'_c \backslash B_c) = 0$. By almost the same argument, almost every point in B_c is in B'_c, so $\mu(B_c \backslash B'_c) = 0$ □

Another interesting consequence of our main theorem (or rather, the method of the proof of our main theorem) is the following:

Proposition 4.4.2 *Let $C \in \zeta_e$ be closed. Then it is uniquely ergodic.*

Proof: First observe that the restrictions of all functions continuous on A are continuous functions on C. By Tietze's extension theorem, as C is compact, the converse is also true: any continuous function f on C admits an extension g which is a continuous function $g : A \rightarrow \mathbb{R}$, and $g|_C = f$. Therefore, by the definition of C, and the Lemma 4.3.1, for each continuous $f : C \rightarrow \mathbb{R}$, $f^*(x) = const.$, $\forall x \in C$. As T is continuous on C, by the Theorem 9.2, in chapter 2 of Mañé [5], it is uniquely ergodic. □

4.5 An example

Consider the automorphism of the two-dimensional torus given by

$$\begin{aligned} x &\rightarrow x+\omega, \\ y &\rightarrow y. \end{aligned} \tag{4.5.12}$$

It is clear that the solutions are given by $x_j = x_0 + \omega j, y_n = y_0$. Consider the countable family of harmonic (complex) functions on the torus, $H(m_1, m_2) = \exp(i(m_1 x + m_2 y))$, where i denotes the imaginary number, and $m_1, m_2 \in \mathbb{Z}$. For the time averages of harmonic functions, we have

$$\begin{aligned} H^*(m_1, m_2) &= \lim_{n\to\infty} \frac{1}{n} \sum_{j=0}^{n-1} \exp(i(m_1(x_0+\omega j) + m_2 y_0)) \\ &= \exp(i(m_1 x_0 + m_2 y_0)) \lim_{n\to\infty} \frac{1}{n} \sum_{j=0}^{n-1} \exp(i m_1 \omega j). \end{aligned} \tag{4.5.13}$$

The limit in the above expression is 0 for all m_1, m_2, except for $m_1 = 0$, when its value is 1. Therefore,

$$H^*(0, m_2) = \exp(i m_2 y_0).$$

Note that the time averages of $H(0, m_2)$ are constant on the sets $C = \{(x, y) \in \mathbb{T}^2 | y_0 = const.\}$. As rational linear combinations of harmonic functions form a countable dense subset of a set of all real integrable functions on $\mathbb{T}^2$, it is clear from the above calculation, and the Theorem 4.3.1 that the sets C defined above are the ergodic components.

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Chapter 5

Maximal effective diffusivity for time periodic incompressible fluid flows

5.1 Introduction

In this chapter we study effective diffusivity for time periodic velocity fields. Most of our work deals with spatially periodic, two-dimensional velocity fields. However, we also consider the effective diffusivity for three-dimensional velocity fields admitting a volume-preserving symmetry (see chapter 2). Our approach combines recently developed methods for the analysis of the statistical properties of nondiffusive motion of a passive tracer (chapter 3 and [17]) with homogenization theory ([3], [9]).

Most previous rigorous studies of the effective diffusivity for laminar, deterministic velocity fields have been focused on steady two-dimensional, spatially periodic velocity fields. This case already exhibits a variety of interesting behavior. To emphasize similarities and differences between our analysis and the analysis in the steady case, we first need to define some terminology. We call (in the spirit of Khinchin's [11] statistical mechanics terminology) a velocity field *ergodic in a certain direction* if the time average along the Lagrangian trajectories of the velocity component in that direction is constant almost everywhere on the basic cell defined by the spatial periods. Note that the velocity component in a certain direction is a function on a domain on which the velocity field is defined. In the dynamical systems literature, *ergodicity* of a velocity field means that *all* integrable functions have Lagrangian time averages which are constant almost everywhere. Thus, ergodicity is sufficient but not necessary for ergodicity in a certain direction. It was shown in [9], [14] that, provided certain technical conditions are satisfied, the effective diffusivity behaves like Pe^2 in the large Peclet number Pe limit for steady spatially periodic flows. Using our results in section 3.1, we can conclude that velocity fields that are nonergodic in a certain direction give rise to Pe^2 behavior of the effective diffusivity in that direction, in the limits $Pe \to \infty$, $Pe \to 0$. Also, the dependence of the effective diffusivity in a certain direction on the Peclet number in the large Pe limit is different from Pe^2 if the velocity field is ergodic in that direction. In particular, nonergodicity in a certain direction is equivalent to conditions for Pe^2 effective diffusivity in previously mentioned works. It is quite straightforward to derive conditions for Pe^2 behavior of effective diffusivity in time-periodic flows, but it is not clear how these conditions, analogous to the ones for steady flows derived in [9], [14], could be used for analysis of *specific* unsteady flows. The new condition of non-ergodicity in a certain direction allows us to analyze effective diffusivity in specific time-periodic velocity fields and time-periodic velocity fields with specific kinematical properties, as it is done in section 4.

The addition of time periodicity brings in a qualitatively new feature: the motion of the passive, nondiffusive tracer can be chaotic (for a precise meaning and examples see [25]). There have been many studies of the motion of a nondiffusive passive scalar in spatially and time-periodic velocity fields recently (see the references in [17]). These studies are mostly numerical. What is typically observed is that the motion of a particle can be either chaotic or regular, depending on initial conditions. Thus, some particles visit large portions of the physical space without diffusion being present, while others move along regular trajectories, much as in the steady case. Much attention has been devoted to the determination of the large time asymptotic behavior of the dispersion in certain directions for an ensemble of nondiffusive particles, which is often shown to be proportional to the square of time (ballistic behavior), as opposed to the diffusive case where the dependence on time is linear. It is shown rigorously in this chapter, based on the arguments in chapter 3 (see also [17] and [18]) that the ballistic behavior of the dispersion in a certain direction is a consequence of the non-ergodicity of the velocity component in that direction. Thus, a clear analogy arises between the above conditions for the Pe^2 behavior of the effective diffusivity in the steady case, and the conditions for t^2 behavior of the nondiffusive dispersion. We exploit that analogy in our study of effective diffusivity in time-periodic velocity fields. Our results show that, as soon as we include diffusive effects in the description of motion, the fact that the nondiffusive motion is chaotic does not necessarily change the dependence of the effective diffusivity on the Peclet number. Just as in the steady case, it is the *ergodicity in a certain direction* of the nondiffusive motion that determines the effective diffusivity.

The amount of previous work on effective diffusivity in time-periodic velocity fields is not large, although there is a significant number of natural phenomena which can be modeled by a convection-diffusion equation with time-periodic coefficients (for a list of these natural phenomena, see [6], [7]). Dill and Brenner studied effective diffusivity in time-periodic flows both in spatially periodic [7]) and Taylor dispersion [6] settings, using the moments method. A specific class of velocity fields that they analyze is, in our terminology, ergodic in all directions, and thus does not have Pe^2 enhancement of maximal diffusivity, although an enhancement exists. In these works, references to prior work on effective diffusivity in time-periodic velocity fields are listed. Fannjiang and Papanicolaou [9] developed variational principles which determine effective diffusivity for both steady and time-periodic flows. We use their variational principle for time-periodic flows in section 3.1. Their Theorem 8.16 on flows which are *nonballistic in a certain direction* is a special case of our result on flows which are *ergodic in a certain direction.*

This chapter is organized as follows: in section 2 we introduce concepts and methods from homogenization theory that are required to describe the effective equation of motion of a passive scalar, and the expression for the effective diffusivity. In section 3 we derive conditions for Pe^2 behavior of the effective diffusivity in a particular direction in terms of the Lagrangian time average of the velocity field component in that direction. We make the above described connection with the nondiffusive motion. We also show how these results can be applied when one considers the associated Poincaré map of the velocity field. In section 4 we discuss several examples of velocity fields for which the derived conditions for the Pe^2 behavior of the effective diffusivity are applied. At the end of this section we discuss the so-called *duct velocity fields*, which are three-dimensional velocity fields admitting a volume-preserving symmetry. We study the effective diffusivity for these velocity fields, thus generalizing the standard Taylor-Aris dispersion theory for unidirectional steady shear velocity fields.

5.2 Homogenization of the convection-diffusion equation

5.2.1 Definitions and notation

The convection-diffusion equation

$$\frac{\partial c}{\partial t} + \mathbf{v}(\mathbf{x}, t) \cdot \nabla c = D \Delta c, \tag{5.2.1}$$

describes the conservation of a passive tracer in a moving fluid. In the above equation, $c(\mathbf{x}, t)$ is a scalar field (e.g., temperature or concentration), $\mathbf{v}(\mathbf{x}, t)$ is an incompressible velocity field obtained by solving the Navier-Stokes equation, and D is a constant depending on physical properties of a passive tracer. In what follows, we shall assume that $\mathbf{v}(\mathbf{x}, t)$ is periodic in time with the period $\tau = 2\pi/\omega$. With the exception of the example on duct velocity fields in Section 4, $\mathbf{v}(\mathbf{x}, t)$ will be assumed to be a spatially periodic, two-dimensional vector field. In that case, $\mathbf{x} = (x, y)$, and the period in the direction of x and y is denoted by l (for simplicity, we assume a square cell). Because of the spatial and temporal periodicity, we can *suspend* the vector field $\mathbf{v}(\mathbf{x}, t)$ over $A = T^2 \times S^1$, where T^2 denotes a 2-torus, and S^1 a circle. This can be done by redefining $\mathbf{v}(\mathbf{x}, t)$ to be a three-dimensional velocity field with a component in the direction of time being constant. For example, if $\mathbf{v}(\mathbf{x}, t)$ is given by

$$\begin{aligned} \dot{x} &= u(x, y, t), \\ \dot{y} &= v(x, y, t), \end{aligned}$$

then the suspended, three-dimensional velocity field is

$$\begin{aligned} \frac{dx}{ds} &= u(x, y, t), \\ \frac{dy}{ds} &= v(x, y, t), \end{aligned}$$

$$\frac{dt}{ds} = 1,.$$

where s is a new "time-like" variable. Thus, the phase space on which we analyze properties of $\mathbf{v}(\mathbf{x},t)$ is A. We assume that $\mathbf{v}(\mathbf{x},t)$ is Lipschitz continuous on A. Note that $\mathbf{v}(\mathbf{x},t)$ is immediately bounded and integrable on A. The average of any object defined on this phase space is denoted by $\langle\cdot\rangle$

$$\langle\cdot\rangle = \frac{1}{l^2\tau}\int_0^\tau \int_0^l \int_0^l (\cdot)dxdyd\tau.$$

The average over the unit cell be will be denoted by $\langle\cdot\rangle_s$,

$$\langle\cdot\rangle_s = \frac{1}{l^2}\int_0^l \int_0^l (\cdot)dxdy.$$

The time average of any integrable function f on A under the flow $\phi^t : A \to A$ generated on A by $\mathbf{v}(\mathbf{x},t)$ is given by

$$f^*(\mathbf{x},t) = \lim_{T\to\infty}\frac{1}{T}\int_0^T f(\phi^{\bar{t}}(\mathbf{x},t))d\bar{t},$$

where $(\mathbf{x},t)$ denotes a point on A. When we use the term "time average" in this chapter, it will always mean the time average along a Lagrangian particle trajectory.

The reader will notice that we use the term "velocity field" where a fluid dynamics term would be "flow," e.g., "duct velocity fields" instead of "duct flows." This is introduced in order to preserve the precise meaning of the term "flow" customary in dynamical systems literature.

We shall often state that some statement is valid "almost everywhere" on A. This is always meant in the sense of measure theory. A *measure* on A is a function from a certain subset $\mathcal{A}$ of all sets on A to $\mathbb{R}$, which assigns to each set in $\mathcal{A}$ a number in $\mathbb{R}$.

In our case, for any $B \in \mathcal{A}$, $\mu(B)$ reads

$$\mu(B) = \frac{1}{l^2 T} \int_B dx dy dt,$$

where the integration is meant in the Lebesgue sense. μ is a positive function on $\mathcal{A}$, i.e., $\mu(B) \geq 0$ for every $B \in \mathcal{A}$. Also, μ is a *probability measure*, i.e., $\mu(A) = 1$. Now, the validity of the statement "almost everywhere" on A will always mean that the measure of the set in A on which that statement is not valid is zero, or, equivalently, that the measure of the set on which the statement is valid is 1. Thus, A and the set on which that statement is valid are the same, in the sense of measure theory.

5.2.2 Homogenization

In this section, we introduce the necessary results from homogenization theory that we shall use in our analysis. General references are [3] and [9].

The velocity field can be decomposed into its average and fluctuating parts as

$$\mathbf{v}(\mathbf{x}, t) = \langle \mathbf{v} \rangle + \mathbf{v}'(\mathbf{x}, t).$$

Since $\mathbf{v}'(\mathbf{x}, t)$ is a zero-mean, spatio-temporally periodic vector field, there exists a skew-symmetric, spatio-temporally periodic matrix

$$\mathbf{H} = \begin{bmatrix} 0 & H \\ -H & 0 \end{bmatrix} \tag{5.2.2}$$

such that $\mathbf{v}' = \nabla \cdot \mathbf{H}$ (see [9]). Equation (5.2.1) can then be written as

$$\frac{\partial c}{\partial t} + \langle \mathbf{v} \rangle \cdot \nabla c = \nabla \cdot \mathbf{A}(\mathbf{x}, t) \nabla c. \tag{5.2.3}$$

In the above equation $\mathbf{A} = (D\mathbf{I} - \mathbf{H})$, where $\mathbf{I}$ is the identity operator. We assume that the spatial size of the domain in $\mathbb{R}^2$ on which the velocity field is defined is characterized by a constant L, while a time-scale for the observation of the flow is given by T. Let $\delta_t = \tau/T, \delta_l = l/L$, and $\delta = \sqrt{\delta_t^2 + \delta_l^2}$. Let us rescale time and spatial scales as $(\mathbf{x}, t) \to (\mathbf{x}/\delta, t/\delta^2)$. Thus, (5.2.3) becomes

$$\frac{\partial c}{\partial t} + \delta^{-1} \langle \mathbf{v} \rangle \cdot \nabla c = \nabla \cdot \mathbf{A}(\frac{\mathbf{x}}{\delta}, \frac{t}{\delta^2}) \nabla c. \tag{5.2.4}$$

It can be shown, using homogenization theory for parabolic differential operators (see e.g., [3]) that, on large temporal and spatial scales, i.e., when $\delta \to 0$, and with the initial condition $c(\mathbf{x}, 0) = c_0(\mathbf{x})$ varying on large spatial scales compared with the velocity field, $c(\mathbf{x}, t)$ converges weakly in L^2 to $\bar{c}(\mathbf{x}, t)$, where $\bar{c}$ satisfies

$$\frac{\partial \bar{c}}{\partial t} + \langle \mathbf{v} \rangle \cdot \nabla \bar{c} = \mathbf{D} \Delta \bar{c}, \tag{5.2.5}$$

(for details of a procedure leading to (5.2.5), see [16]). In (5.2.5), $\mathbf{D}$ is the constant *effective diffusivity tensor* given by

$$\mathbf{D} = \langle D\mathbf{I} - \mathbf{H} + (D\mathbf{I} - \mathbf{H}) \nabla \chi \rangle, \tag{5.2.6}$$

with the spatially and temporally periodic vector field χ satisfying the *cell equation*

$$\frac{\partial \chi}{\partial t} + (\langle \mathbf{v} \rangle \ + \ \mathbf{v}') \cdot \nabla \chi - D \Delta \chi = -\mathbf{v}'. \tag{5.2.7}$$

In [7] an equation analogous to (5.2.7) was developed. In that work, χ is denoted by $\mathbf{B}$ and called the $\mathbf{B}$-field.

Equation (5.2.7) is the basis for our analysis of the relationship between the effective diffusivity and ergodicity of the flow generated by the vector field $\mathbf{v}(\mathbf{x}, t)$ on A. We shall restrict our attention to the symmetric part of the effective diffusivity tensor (5.2.6). This restriction is common in the literature (see e.g., [14], [13]), and also there is a large class of velocity fields for which it can be proven that $\mathbf{D}$ actually is symmetric (see [9]).

For a discussion of velocity fields having nonsymmetric effective diffusivity tensors, see [12]. The symmetric part of $\mathbf{D}$ is given by

$$\mathbf{D}_{sym} = D(\mathbf{I} + \langle \nabla\chi \cdot \nabla\chi \rangle). \tag{5.2.8}$$

It is convenient for analysis to put the cell equation (5.2.7) in integral form. First notice that the effective diffusivity in the direction of a unit vector $\mathbf{e}$ is given by

$$\mathbf{D}_{sym}\mathbf{e} \cdot \mathbf{e} = D(1 + \langle \nabla\chi^{\mathbf{e}} \cdot \nabla\chi^{\mathbf{e}} \rangle), \tag{5.2.9}$$

where $\chi^{\mathbf{e}} = \chi \cdot \mathbf{e}$. Let us introduce the operator $\mathbf{\Gamma} = \nabla\Delta^{-1}\nabla$. Then it is easy to show that, in the direction of $\mathbf{e}$, (5.2.7) becomes

$$(D - \mathbf{\Gamma}\Delta^{-1}\frac{\partial}{\partial t} - \mathbf{\Gamma}\Delta^{-1}\langle \mathbf{v} \rangle \cdot \nabla - \mathbf{\Gamma}\mathbf{H}\mathbf{\Gamma})\nabla\chi^{\mathbf{e}} = \mathbf{\Gamma}\mathbf{H} \cdot \mathbf{e}. \tag{5.2.10}$$

5.3 Ergodic theory and effective diffusivity

5.3.1 Conditions for the maximal effective diffusivity

In the previous section, we derived the equation that needs to be solved in order to obtain the effective diffusivity for a time-periodic, spatially periodic velocity field in the direction of the unit vector $\mathbf{e}$. Following [14] we call the effective diffusivity in the direction of $\mathbf{e}$ *maximal* if

$$\mathbf{D}\mathbf{e} \cdot \mathbf{e} \sim \frac{1}{D}.$$

In this section we shall be interested in determining the conditions on a time periodic, spatially periodic velocity field in order that it has a maximal enhanced diffusivity.

Let us define a new operator $\mathbf{G}$ as

$$\mathbf{G} = -\mathbf{\Gamma}\Delta^{-1}\frac{\partial}{\partial t} - \mathbf{\Gamma}\Delta^{-1}\langle \mathbf{v} \rangle \cdot \nabla - \mathbf{\Gamma}\mathbf{H}\mathbf{\Gamma}.$$

The operator $\mathbf{G}$ is compact (see [9]), and it is clearly related to the purely convective part of (5.2.1). Equation (5.2.10) now becomes

$$(D\mathbf{I} - \mathbf{G})\nabla\chi^{\mathbf{e}} = \mathbf{\Gamma}\mathbf{H} \cdot \mathbf{e}. \tag{5.3.11}$$

Let $\mathcal{H}$ be the Hilbert space of all square-integrable, curl-free, time periodic, spatially periodic, zero mean vector fields. More precisely

$$\mathcal{H} = \{\mathbf{F} \in L^2(A) \mid \mathbf{F} = \nabla f, f \in H^1(A)\}.$$

So, for any function f in the Sobolev space $H^1(A)$ of all square integrable functions on A with square integrable distributional derivatives, its generalized derivative ∇f is in $\mathcal{H}$. Let us decompose $\mathcal{H}$ as $\mathcal{H} = \mathcal{N} \oplus \mathcal{N}^{\perp}$, where $\mathcal{N}$ is the null space of $\mathbf{G}$, and $\mathcal{N}^{\perp}$ its complement in $\mathcal{H}$. Now, using the same type of calculations as in the demonstration of Lemmas 8.2 and 8.4 in [9] (in particular, using a variational principle for time-periodic velocity fields developed there), we can conclude that

$$\mathbf{De} \cdot \mathbf{e} \sim \frac{1}{D} \quad \text{as } D \to 0 \text{ if and only if } \mathbf{\Gamma}\mathbf{H} \cdot \mathbf{e} \text{ has a non-zero component in } \mathcal{N}.$$

Note that exactly the same result is obtained by using the formalism developed in [1], [2], based on the Stieltjes integral representation for the effective diffusivity.

In what follows, we shall interpret the condition

$$\mathbf{\Gamma}\mathbf{H} \cdot \mathbf{e} \text{ has a non-zero component in } \mathcal{N} \tag{5.3.12}$$

in terms of the time average, $(\mathbf{v}' \cdot \mathbf{e})^*$, of the function $\mathbf{v}' \cdot \mathbf{e}$, which is just the time average of the velocity in the direction of $\mathbf{e}$. We assume $(\mathbf{v}' \cdot \mathbf{e})^* \in H^1(A)$.

First, note that for (5.3.12) to be satisfied, $\mathcal{N}$ has to be non-empty. It is not hard to show (cf. Section 8.2 of [9]) that this means that there must exist a nontrivial (i.e., f is not a constant almost everywhere) $f \in H^1(A)$ such that f is constant on orbits. This means that such an f satisfies

$$\frac{\partial f}{\partial t} + \mathbf{v}(\mathbf{x},t) \cdot \nabla f = 0, \tag{5.3.13}$$

in a generalized sense.

Second, let $\mathcal{M}$ be the Hilbert space of functions $f \in L^1(A)$ such that $f = g^*$ for some $g \in L^1(A)$. It is clear that the space of all functions in $H^1(A)$ which are constant on orbits is a subset of $\mathcal{M}$. For $\mathbf{\Gamma H} \cdot \mathbf{e}$ to have a component in $\mathcal{N}$, we need

$$\langle (\mathbf{\Gamma H} \cdot \mathbf{e}) \cdot \nabla f \rangle \neq 0$$

for some $f \in H^1(A)$. Integrating by parts, we get

$$\langle f\mathbf{v}' \cdot \mathbf{e} \rangle \neq 0 \text{ for some } f \in H^1(A). \tag{5.3.14}$$

Now we show that (5.3.13) and (5.3.14) are satisfied if and only if the time average of $\mathbf{v} \cdot \mathbf{e}$ is not a constant almost everywhere on A. As $(\langle \mathbf{v} \rangle \cdot \mathbf{e})^*$ is a constant, it is enough to show that (5.3.13) and (5.3.14) are satisfied if and only if $(\mathbf{v}' \cdot \mathbf{e})^*$ is not a constant almost everywhere on A.

Suppose first

$$(\mathbf{v}' \cdot \mathbf{e})^* \quad \text{is not a constant almost everywhere.} \tag{5.3.15}$$

Then, take $f = (\mathbf{v}' \cdot \mathbf{e})^*$. By Birkhoff's ergodic theorem, $(\mathbf{v}' \cdot \mathbf{e})^*$ satisfies (5.3.13). For (5.3.14) let us first note that the projection operator $\Pi : L^1 \to \mathcal{M}$, which takes every function in L^1 to its time average, is orthogonal ([15]). Then, we have the following calculation:

$$\langle (\mathbf{v}' \cdot \mathbf{e})^* \mathbf{v}' \cdot \mathbf{e} \rangle = \langle (\mathbf{v}' \cdot \mathbf{e})^* ((\mathbf{v}' \cdot \mathbf{e})^* + z) \rangle$$

$$
\begin{aligned}
&= \left\langle ((\mathbf{v}'\cdot\mathbf{e})^*)^2 \right\rangle \\
&\neq 0, \qquad (5.3.16)
\end{aligned}
$$

where $z = \mathbf{v}'\cdot\mathbf{e} - (\mathbf{v}'\cdot\mathbf{e})^*$ is a function in $\mathcal{M}^\perp$.

To prove the converse, assume there exists some, nontrivial, f in H^1 which is constant on orbits such that

$$\langle f\mathbf{v}'\cdot\mathbf{e}\rangle \neq 0.$$

Then, as $\langle \mathbf{v}'\rangle = 0$,

$$\langle (f - \langle f\rangle)\mathbf{v}'\cdot\mathbf{e}\rangle = \langle f\mathbf{v}'\cdot\mathbf{e}\rangle \neq 0.$$

Note that $(f - \langle f\rangle) \in \mathcal{M}$. Now suppose $(\mathbf{v}'\cdot\mathbf{e})^* = c$, $c \in \mathbb{R}$ almost everywhere. Then, $\mathbf{v}'\cdot\mathbf{e} = c + z$ where $z = \mathbf{v}'\cdot\mathbf{e} - (\mathbf{v}'\cdot\mathbf{e})^*$ is a function in $\mathcal{M}^\perp$, so

$$
\begin{aligned}
\langle (f - \langle f\rangle)\mathbf{v}'\cdot\mathbf{e}\rangle &= \langle (f - \langle f\rangle)(c + z)\rangle \\
&= c\langle (f - \langle f\rangle)\rangle + \langle (f - \langle f\rangle)z)\rangle \\
&= c\langle (f - \langle f\rangle)\rangle = 0
\end{aligned}
$$

and we are done by contradiction.

Thus, we have proved that the maximal enhanced diffusivity in a certain direction will exist if and only if the time average of the velocity in that direction is not a constant almost everywhere. Following Khinchin [11] we call functions whose time average under the velocity field $\mathbf{v}$ is constant almost everywhere *ergodic functions*. Thus, the effective diffusivity in a certain direction $\mathbf{e}$ is not maximal, i.e.,

$$\mathbf{De}\cdot\mathbf{e} << \frac{1}{D} \text{ as } D \to 0,$$

if and only if $\mathbf{v} \cdot \mathbf{e}$ is an ergodic function, or as defined in the introduction, if $\mathbf{v}$ is not ergodic in the direction of $\mathbf{e}$. Theorem 8.16 in ([9]) is a special case of the "if" part of this statement.

In the convection-diffusion equation (5.2.1) there exists only one nondimensional parameter, the Peclet number $Pe = Vl/D$, where V is the maximal velocity on A. Letting $(x, y, t) \to (x/l, y/l, tV/l)$, we obtain the nondimensional equation

$$\frac{\partial c}{\partial t} + \mathbf{v}(\mathbf{x}, t) \cdot \nabla c = \frac{1}{Pe} \Delta c. \tag{5.3.17}$$

Now we see that all the above analysis comes through for equation (5.3.17). In particular, the above conclusions are valid in the limit $Pe \to \infty$. In terms of the Peclet number, we have

$$\frac{\mathbf{De} \cdot \mathbf{e}}{D} \sim Pe^2 \text{ as } Pe \to \infty.$$

The point of writing (5.2.1) in the form (5.3.17) here is twofold: firstly, we do not have to decrease molecular diffusivity, which is awkward experimentally, but we can increase the velocity or spatial scale to achieve maximal enhanced diffusivity. Secondly, in what follows we analyse the limit $Pe \to 0$: to achieve that limit, it is more natural to let U or l go to zero, rather than let $D \to \infty$.

In particular, suppose again that $\mathbf{\Gamma H} \cdot \mathbf{e}$ has a non-zero component in $\mathcal{N}$. We can decompose $\nabla \chi^{\mathbf{e}}$ into the components in $\mathcal{N}$ and $\mathcal{N}^{\perp}$ as $\nabla \chi^{\mathbf{e}} = \nabla \chi^{\mathbf{e}}_{\mathcal{N}} + \nabla \chi^{\mathbf{e}}_{\mathcal{N}^{\perp}}$. The effective diffusivity tensor becomes

$$\mathbf{D}_{sym} \mathbf{e} \cdot \mathbf{e} = D + D \left\langle \nabla \chi^{\mathbf{e}}_{\mathcal{N}} \cdot \nabla \chi^{\mathbf{e}}_{\mathcal{N}} \right\rangle + D \left\langle \nabla \chi^{\mathbf{e}}_{\mathcal{N}^{\perp}} \cdot \nabla \chi^{\mathbf{e}}_{\mathcal{N}^{\perp}} \right\rangle.$$

From (5.3.11), using the fact that $\nabla \chi^{\mathbf{e}}_{\mathcal{N}}$ is in the null space of $\mathbf{G}$, it satisfies

$$\frac{1}{Pe} \nabla \chi^{\mathbf{e}}_{\mathcal{N}} + \mathbf{\Gamma H} \cdot \mathbf{e}_{\mathcal{N}} = 0. \tag{5.3.18}$$

Clearly,

$$\langle \nabla \chi^{\mathbf{e}}_{\mathcal{N}} \cdot \nabla \chi^{\mathbf{e}}_{\mathcal{N}} \rangle = Pe^2 \langle \mathbf{\Gamma H} \cdot \mathbf{e}_{\mathcal{N}} \cdot \mathbf{\Gamma H} \cdot \mathbf{e}_{\mathcal{N}} \rangle = cPe^2,$$

where $c = \langle \mathbf{\Gamma H} \cdot \mathbf{e}_{\mathcal{N}} \cdot \mathbf{\Gamma H} \cdot \mathbf{e}_{\mathcal{N}} \rangle$. This derivation does not depend on the value of Pe. Now, again from (5.2.10),

$$\frac{1}{Pe} \nabla \chi^{\mathbf{e}}_{\mathcal{N}^\perp} + \mathbf{G} \nabla \chi^{\mathbf{e}}_{\mathcal{N}^\perp} + \mathbf{\Gamma H} \cdot \mathbf{e}_{\mathcal{N}^\perp} = 0. \tag{5.3.19}$$

For small Pe, solving (5.3.19) for $\nabla \chi^{\mathbf{e}}_{\mathcal{N}^\perp}$ gives

$$\nabla \chi^{\mathbf{e}}_{\mathcal{N}^\perp} = Pe(\mathbf{I} - Pe\mathbf{G})^{-1} \mathbf{\Gamma H} \cdot \mathbf{e}_{\mathcal{N}^\perp} = \mathcal{O}(Pe).$$

Therefore, if $\mathbf{\Gamma H} \cdot \mathbf{e}$ has a non-zero component in $\mathcal{N}$,

$$\frac{\mathbf{De} \cdot \mathbf{e}}{D} \sim Pe^2 \quad \text{as } Pe \to 0.$$

For an equivalent result in the steady case, and numerical simulation of some interesting crossover phenomena between small Pe and large Pe limits of Pe^2 behavior of the effective diffusivity divided by the molecular diffusivity, see [14]. In fact, all the results in this subsection carry over to the steady case.

5.3.2 Connection to nondiffusive motion

In the previous section we concluded that, for $\mathbf{v}(\mathbf{x}, t)$ to have maximal effective diffusivity in the direction $\mathbf{e}$ in the limit $D \to 0$ (or $Pe \to \infty$), it is necessary and sufficient that

$$(\mathbf{v} \cdot \mathbf{e})^* \text{ is not a constant almost everywhere.} \tag{5.3.20}$$

As the Peclet number measures the ratio between convective and diffusive effects, convective motion dominates in that limit. It is natural to ask what (if anything) the condition (5.3.20) means in the case of nondiffusive motion. Statistical properties of the motion of a nondiffusive passive scalar have been investigated in chapter 3 with an additional application to dispersion in fluid velocity fields provided in [18]. We shall now establish, as a corollary of that work, the meaning of (5.3.20) for the nondiffusive case.

The motion of nondiffusive passive scalar in a two dimensional, time periodic and spatially periodic incompressible fluid velocity field is governed by the ordinary differential equations

$$
\begin{aligned}
\dot{x} &= u(x, y, t), \\
\dot{y} &= v(x, y, t).
\end{aligned}
\tag{5.3.21}
$$

Let us assume that at $t = 0$, tracer particles are uniformly distributed over the unit cell. The nondiffusive dispersion in the direction of $\mathbf{e}$, denoted by $D^n_{\mathbf{e}}(t)$:

$$
\begin{aligned}
D^n_{\mathbf{e}}(t) &= \left\langle [(\mathbf{x}\cdot\mathbf{e} - \mathbf{x}_0\cdot\mathbf{e}) - \langle(\mathbf{x}\cdot\mathbf{e} - \mathbf{x}_0\cdot\mathbf{e})\rangle_s]^2 \right\rangle_s, \\
&= \left\langle [\int_0^t \mathbf{v}(\mathbf{x}(\bar{t}), \bar{t})\cdot\mathbf{e}\, d\bar{t} - \left\langle \int_0^t \mathbf{v}(\mathbf{x}(\bar{t}), \bar{t})\cdot\mathbf{e}\, d\bar{t} \right\rangle_s]^2 \right\rangle_s .
\end{aligned}
\tag{5.3.22}
$$

Dividing (5.3.22) by t^2 and letting $t \to \infty$, we obtain

$$
\begin{aligned}
\lim_{t\to\infty} \frac{D^n_{\mathbf{e}}(t)}{t^2} &= \lim_{t\to\infty} \frac{1}{t^2} \left\langle [\int_0^t \mathbf{v}(\mathbf{x}(\bar{t}), \bar{t})\cdot\mathbf{e}\, d\bar{t} - \left\langle \int_0^t \mathbf{v}(\mathbf{x}(\bar{t}), \bar{t})\cdot\mathbf{e}\, d\bar{t} \right\rangle_s]^2 \right\rangle_s, \\
&= \lim_{t\to\infty} \left\langle [\frac{1}{t}\int_0^t \mathbf{v}(\mathbf{x}(\bar{t}), \bar{t})\cdot\mathbf{e}\, d\bar{t} - \left\langle \frac{1}{t}\int_0^t \mathbf{v}(\mathbf{x}(\bar{t}), \bar{t})\cdot\mathbf{e}\, d\bar{t} \right\rangle_s]^2 \right\rangle_s, \\
&= \left\langle [(\mathbf{v}\cdot\mathbf{e})^* - \langle(\mathbf{v}\cdot\mathbf{e})^*\rangle_s]^2 \right\rangle_s, \\
&\equiv a.
\end{aligned}
\tag{5.3.23}
$$

The passage from the first to the second line is justified using boundedness and integrability of $\mathbf{v}\cdot\mathbf{e}$ and Lebesgues bounded convergence theorem. The existence of the infinite time limit is proved as follows: $\mathbf{v}(\mathbf{x}, t)$ induces a flow on A, as discussed in section 2. Thus, by Birkhoff's ergodic theorem, the time average of $\mathbf{v} \cdot \mathbf{e}$ exists almost everywhere on A. We need to show that it exists almost everywhere on the basic cell, which is a cross-section $t = 0$ of A. To prove this, suppose there exists a set of positive measure B, $\mu(B) > 0$, where $\mu(B) = \int_B dx dy$ on the basic cell such that the time average of $\mathbf{v} \cdot \mathbf{e}$ does not exist. By the volume preservation of the flow on A, the set B' which consists of trajectories emanating from B is of positive measure on A. Then by Birkhoff's ergodic theorem the time average of $\mathbf{v} \cdot \mathbf{e}$ does not exist anywhere on B'. Thus we are done by contradiction.

Using the positivity of the integrand in a, we conclude that $a = 0$ if and only if $(\mathbf{v} \cdot \mathbf{e})^*$ is constant almost everywhere (see chapter 3). As $a < \infty$ by the boundedness of $\mathbf{v}$ we reach the following conclusion:

$$\frac{\mathbf{De} \cdot \mathbf{e}}{D} \sim Pe^2 \text{ as } Pe \to \infty \text{ if and only if } D^n_{\mathbf{e}}(t) \sim t^2 \text{ as } t \to \infty.$$

Thus, the Pe^2 behavior of the effective diffusivity is a consequence of the fact that the diffusing particle visits regions in the phase space where the convective motion takes place with different average velocities. In a purely convective case, there is a linear growth of the separation of particles starting in regions with different average velocities and quadratic growth of the dispersion of such particles. This physical mechanism for Pe^2 behavior of the effective diffusivity in the steady case was proposed in [13].

5.3.3 Formulation of the results in the context of Poincaré maps

In the past 10 years the techniques and approach of dynamical systems theory have been applied to many issues associated with fluid transport and mixing. In this setting much of the analysis has been carried out using the Poincaré map associated with the time periodic velocity field. We now discuss a relationship between the ergodic properties of the velocity field $\mathbf{v}(\mathbf{x},t)$ needed in the analysis of the effective diffusivity, and the associated Poincaré map P.

The Poincaré map of a time-periodic, spatially periodic flow on A induced by $\mathbf{v}(\mathbf{x},t)$ is a map $P : T^2 \rightarrow T^2$ defined by

$$P(x_0, y_0) = (x(\tau, x_0, y_0, 0), y(\tau, x_0, y_0, 0)),$$

where $(x(t, x_0, y_0, 0), y(t, x_0, y_0, 0))$ is the solution of (5.3.21) with initial conditions

$$\begin{aligned} x(0, x_0, y_0, 0) &= x_0, \\ y(0, x_0, y_0, 0) &= y_0. \end{aligned}$$

The time average f_P^* of any function $f \in L^1(T^2)$ under P is given by

$$f_P^*(\mathbf{x}) = \lim_{n\rightarrow\infty} \frac{1}{n} \sum_{i=0}^{n-1} f(P^i(\mathbf{x})).$$

Let us define a *jump function* $\mathbf{j} : T^2 \rightarrow \mathbb{R}$ as

$$\mathbf{j}(\mathbf{x}) = \int_0^\tau \mathbf{v}(\phi^{\bar{t}}(\mathbf{x}, 0))d\bar{t}.$$

It is not hard to show that $(\mathbf{j}\cdot\mathbf{e})_P^* = \tau(\mathbf{v}\cdot\mathbf{e})^*$. Therefore, we have that, in terms of the Poincaré map P, (5.3.20) becomes

$$(\mathbf{j}\cdot\mathbf{e})_P^* \text{ is not a constant almost everywhere.} \tag{5.3.24}$$

5.4 Some examples

In this section we apply the conditions for the maximal effective diffusivity to a number of specific velocity fields, or velocity fields posessing some specific dynamical property.

In particular, we discuss the relationship of the so-called "accelerator modes" in Poincaré maps to the maximal enhanced diffusivity. We analyze small, time-periodic perturbations of a steady cellular velocity field, which can produce a discontinuous transition in the effective diffusivity coefficient. A velocity field which exhibits such a discontinuous transition is an example due to Zeldovich, which we discuss in terms of the concepts introduced above. The analysis in previous sections can be extended to three-dimensional, time-periodic duct velocity fields, the study of which closes this section.

5.4.1 Accelerator modes

In the dynamical systems literature an accelerator mode is an invariant region surrounding an elliptic fixed point p of the map P, such that all initial conditions in that invariant region have the same, nonzero time average of the jump function $\mathbf{j} \cdot \mathbf{e}$ in some direction $\mathbf{e}$. Physically, particles starting in the region called accelerator mode move to infinity with the same average speed, while their mutual distance stays bounded.

Let us be more precise about the above definition of an accelerator mode in the case when P is a Poincaré map derived from a time periodic, spatially periodic $\mathbf{v}(\mathbf{x}, t)$. Let p be an elliptic fixed point for P. Let $(\mathbf{j} \cdot \mathbf{e})(p) \neq 0$, for some $\mathbf{e}$. Then, using the fact that $\mathbf{v}(\mathbf{x}, t)$ is Lipschitz continuous, and the result proven in [19] for a general continuous area preserving map P, we deduce that there is an invariant region D, of a positive measure, around p such that

$$(\mathbf{j} \cdot \mathbf{e})^*_P(p_1) = (\mathbf{j} \cdot \mathbf{e})^*_P(p) = (\mathbf{j} \cdot \mathbf{e})(p) \;\; \forall \, p_1 \, \in \, D.$$

This means that all the particles starting in D have the same time average of the jump in the direction of $\mathbf{e}$, and that time average is equal to the value of $\mathbf{j} \cdot \mathbf{e}$ at p, which is not zero. Therefore, D is an accelerator mode.

We shall show that, assuming the existence of an elliptic fixed point p such that $(\mathbf{j}\cdot\mathbf{e})(p) \neq 0$ (so, as argued above, an accelerator mode exists), and assuming that

$$\langle(\mathbf{j}\cdot\mathbf{e})\rangle_s \neq (\mathbf{j}\cdot\mathbf{e})(p), \tag{5.4.25}$$

the velocity field $\mathbf{v}(\mathbf{x},t)$ posesses a maximal effective diffusivity in the direction of $\mathbf{e}$. By Birkhoff's ergodic theorem

$$\langle(\mathbf{j}\cdot\mathbf{e})\rangle_s = \langle(\mathbf{j}\cdot\mathbf{e})^*_P\rangle_s \,.$$

Thus, using the condition (5.4.25), there must be a region E in T^2/D of positive measure such that $(\mathbf{j}\cdot\mathbf{e})^*_P \neq (\mathbf{j}\cdot\mathbf{e})(p)$ in E. Therefore, $(\mathbf{j}\cdot\mathbf{e})^*_P$ is not a constant almost everywhere. So, by the condition (5.3.24) there is a maximal enhanced diffusivity in the direction of $\mathbf{e}$. Note that (5.4.25) is easily checked if $\mathbf{v}$ is explicitly given:

$$\langle(\mathbf{j}\cdot\mathbf{e})\rangle_s = \tau\,\langle(\mathbf{v}\cdot\mathbf{e})\rangle \,.$$

In chapter 3 and [17] Mezić and Wiggins numerical evidence was presented that showed that the conditions above are satisfied for certain parameter values in a model of Rayleigh-Benard convection. Additional numerical evidence, for a different model of the same problem, is presented in [22]. These authors also make a connection between the accelerator mode islands and lobe dynamics, as developed in [23]. Karney et al. in [10] used heuristic methods to derive the above result for the special case in which P is the standard map.

5.4.2 Small, time periodic perturbations of a steady cellular velocity field

In this subsection we analyze time-dependent perturbations of a class of velocity fields which are usually called *cellular*. These are spatially periodic velocity fields for which the streamlines $x = nl$ and $y = ml$, $m, n \in \mathbf{N}$ separate cells inside which the velocity field is composed of closed streamlines surrounding an elliptic fixed point (see figure (5.1). A particular example of such a velocity field, shown in figure 1, is given by the streamfunction

$$\psi = \sin(2\pi x)\sin(2\pi y).$$

It is a well-known result (see [9] and the references therein) that for such a velocity field

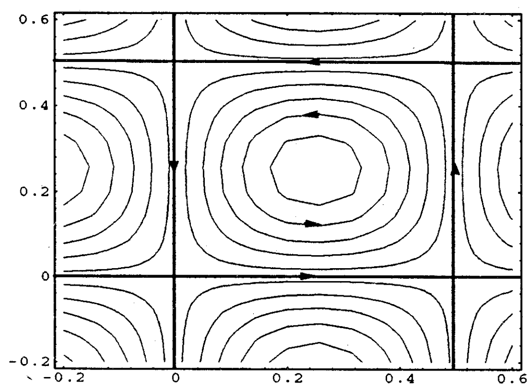

Figure 5.1: Cellular flow.

$$\frac{\mathbf{De}\cdot\mathbf{e}}{D} \sim \sqrt{Pe} \text{ as } Pe \rightarrow \infty.$$

We now show how a discontinuous change of the dependence of the effective diffusivity on the Peclet number can appear if we perturb $\mathbf{v}(\mathbf{x})$ by a time-dependent perturbation. Such a time-dependent perturbation can appear if, by increasing the Rayleigh number, the velocity field undergoes a Hopf bifurcation.

Let

$$\mathbf{v}(\mathbf{x}, t) = \mathbf{v}(\mathbf{x}) + \epsilon\mathbf{v}^p(\mathbf{x}, t)$$

where the dependence of $\mathbf{v}^p(\mathbf{x},t)$ on time is periodic, and ϵ is a small parameter. Also, assume $\mathbf{v}(\mathbf{x})$ is cellular, and satisfies the assumptions above. Let P be the Poincaré map associated with $\mathbf{v}(\mathbf{x},t)$. By Moser's version of the KAM theorem (see [21]) we know that, for small enough ϵ, and under nondegeneracy, "twist" condition, there are invariant circles surrounding the elliptic fixed point. Assume

$$\langle \mathbf{v}^p(\mathbf{x},t)\cdot\mathbf{e}\rangle \neq 0, \tag{5.4.26}$$

for some $\mathbf{e}$. Pick one of the invariant circles surrounding the elliptic fixed point, and denote the region that it surrounds by D. Then,

$$(\mathbf{j}\cdot\mathbf{e})^*_P = 0,$$

for all points inside D, as suppose that $(\mathbf{j}\cdot\mathbf{e})^*_P \neq 0$ for some point. Then that point can not stay inside a bounded region for all times, which gives us a contradiction. But then, there must be a region E of a positive measure in T^2/D such that $(\mathbf{j}\cdot\mathbf{e})^*_P \neq 0$ in E. Because, suppose this is not true. By Birkhoff's ergodic theorem,

$$\langle \mathbf{j}\cdot\mathbf{e}\rangle_s = \langle (\mathbf{j}\cdot\mathbf{e})^*_P\rangle_s .$$

Then by condition (5.4.26) and the fact that $\langle \mathbf{v}(\mathbf{x})\rangle_s = 0$, $\langle (\mathbf{j}\cdot\mathbf{e})^*_P\rangle_s \neq 0$, and $(\mathbf{j}\cdot\mathbf{e})^*_P$ must be different from zero on a set of positive measure in T^2/D. This means that $(\mathbf{j}\cdot\mathbf{e})^*_P$ is not a constant almost everywhere, and so, by (5.3.24)

$$\frac{\mathbf{De}\cdot\mathbf{e}}{D} \sim Pe^2 \quad \text{as } Pe \to \infty. \tag{5.4.27}$$

Note that at $\epsilon = 0$ the effective diffusivity in the large Peclet number limit exhibits the transition from $\sqrt{Pe}$ behavior to Pe^2 behavior.

According to the above result, a $\log(\mathbf{De}\cdot\mathbf{e}/D) - Pe$ diagram should have a discontinuity at the Peclet number corresponding to $\epsilon = 0$. It would be interesting to provide a numerical or experimental evidence for this situation. A model velocity field is easy to construct: let

$$\mathbf{v}(\mathbf{x},t) = (\sin y + \epsilon(\sin^2 y \sin^2 \omega t), \cos x + \epsilon(\sin^2 x \sin^2 \omega t).$$

This velocity field is two-dimensional, spatially and time periodic perturbation of a cellular velocity field, satisfying (5.4.26). The time scales for integration of (5.2.1) such that the scaling in (5.4.27) is obtained should typically be very long ($\mathcal{O}(1/\epsilon)$) for ϵ small.

5.4.3 Zeldovich's example

In ([28]) Zeldovich considers the following velocity field:

$$\mathbf{v}(\mathbf{x},t) = (2v \cos ky \cos \omega t, 0), \tag{5.4.28}$$

where v, k and ω are constants. This velocity field is in the form appropriate for the analysis developed above. Zeldovich finds for the effective diffusivity in the direction of x:

$$\frac{\mathbf{D}\mathbf{e}_x \cdot \mathbf{e}_x}{D} = D(1 + \frac{v^2k^2}{\omega^2 + D^2k^4}). \tag{5.4.29}$$

Because of the simplicity of the velocity field (5.4.28), the above result for the effective diffusivity is exact. Note that for $\omega = 0$, (5.4.28) is a shear velocity field, with a time average of the velocity in the direction of x clearly not a constant almost everywhere. Therefore, by the results in the subsection 3.2, $D^n_{\mathbf{e}_x} \sim t^2$ when $t \to \infty$ and so, a priori

$$\frac{\mathbf{D}\mathbf{e}_x \cdot \mathbf{e}_x}{D} \sim \frac{1}{D} \sim Pe^2 \text{ as } Pe \to \infty.$$

Consider the $\omega \neq 0$ case. We can solve (5.4.28) exactly:

$$\begin{aligned} y(t) &= y_0, \\ x(t) &= x_0 + \int_0^t 2v \cos ky_0 \cos \omega \bar{t} d\bar{t}. \end{aligned}$$

The time average of the velocity in the direction of x for any particle is zero. Therefore, we know

$$\frac{\mathbf{D}\mathbf{e}_x \cdot \mathbf{e}_x}{D} << \frac{1}{D} \sim Pe^2 \text{ as } Pe \to \infty.$$

Indeed, from the exact formula (5.4.29) we see that there is no enhancement of the effective diffusivity in the case $\omega \neq 0$. There is again a discontinuous transition in the behavior of the effective diffusivity at $\omega = 0$, where Pe^2 dependence is changed to Pe^0.

It is seen that our methods provide an elegant way of deriving a priori scalings of the effective diffusivity (a priori in the sense that we only have to compute the time averages of the velocity field, without having to analyze the convection-diffusion equation).

Zeldovich's example is a shear velocity field with bounded velocity. The question arises: what would happen in a linear shear velocity field, of the type $\mathbf{v}(\mathbf{x}) = (ky, 0)$. It is well-known that motion of a passive tracer is not diffusive in this example. In particular, the size of the cloud of tracer particles grows like t^3. No homogenization in the above presented sense is possible. This example establishes the optimality of the condition that the velocity be bounded. The boundedness of the velocity is a technical condition needed both in studies of nondiffusive and diffusive motions (see [4], chapter 3 and [17]).

5.4.4 Duct velocity fields

As a final example, we analyse the fluid mechanically important class of three-dimensional velocity fields called *duct velocity fields* $\mathbf{v}(\mathbf{x}, t)$, where $\mathbf{x} = (x, y, z)$ now, of the form

$$\begin{aligned} v_x &= \frac{\partial \psi(x, y, t)}{\partial y}, \\ v_y &= -\frac{\partial \psi(x, y, t)}{\partial x}, \end{aligned}$$

$$v_z = f(x, y, t)$$

(5.4.30)

(see [8] for examples of steady duct velocity fields). In chapter 2 we have proved that any incompressible velocity field admitting a volume-preserving symmetry can be transformed to the above form. In particular, every Euler velocity field admits a volume-preserving symmetry, which is generated by the vorticity field. We shall assume that the $x-y$ components of (5.4.30) satisfy the conditions on two-dimensional velocity fields imposed in previous sections, but the analysis can be extended to velocity fields which are bounded, but not periodic in x and y. We shall refer to the $x-y$ components of (5.4.30) as the *cross-section.*

We are interested in finding the effective diffusivity in the direction of z,

$$\mathbf{D}_{sym}\mathbf{e}_z \cdot \mathbf{e}_z = D(1 + \langle \nabla \chi^{\mathbf{e}_z} \cdot \nabla \chi^{\mathbf{e}_z} \rangle), \tag{5.4.31}$$

and $\chi^{\mathbf{e}_z}$ satisfies

$$\frac{\partial \chi^{\mathbf{e}_z}}{\partial t} + (\langle \mathbf{v} \rangle + \mathbf{v}') \cdot \nabla \chi^{\mathbf{e}_z} - D\Delta \chi^{\mathbf{e}_z} = -\mathbf{v}' \cdot \mathbf{e}_z = v_z', \tag{5.4.32}$$

where $\langle \cdot \rangle$ still denotes an average over A, and fluctuating quantities are denoted by $(\cdot)'$. (5.4.32) is of the same form as (5.2.7), and it is easily seen that the condition for maximal diffusivity in the direction of z reads

$$(v_z)^* \text{ is not a constant almost everywhere,} \tag{5.4.33}$$

where $*$ denotes the time average under the flow on A generated by the suspension of the $x-y$ components of (5.4.30) over A. In terms of the Poincaré map, (5.4.33) becomes

$$(j_z)^* \text{ is not a constant almost everywhere,} \tag{5.4.34}$$

where j_z denotes a distance in z that a particle traverses during one period of the velocity field.

Now we can discuss the difference between steady velocity fields of the form (5.4.30), with $f(x,y) = \psi(x,y)$, discussed in [14], and time-periodic velocity fields. In particular, it was concluded in [14] that steady velocity fields of the type

$$\mathbf{v} = (\frac{\partial\psi(x,y)}{\partial y}, -\frac{\partial\psi(x,y)}{\partial x}, \psi(x,y))$$

always have maximal enhanced diffusivity in the direction of z, under the assumption that the mean value of the spatially periodic part is zero. In terms of (5.4.33) the maximal effective diffusivity in this case can be understood through the fact that ψ partitions the cross section $(x-y)$ of the duct velocity field into streamlines (i.e., the $x-y$ components of the velocity field are integrable), and the time average of $v_z = \psi$ is not the same on all streamlines (in a measure-theoretic sense). In the time-dependent case this does not have to be so. If the cross section is ergodic, then the diffusivity in the direction of z is not maximal. Now, a typical scenario for fluid velocity fields is the following: a steady duct velocity field undergoes a Hopf bifurcation, and the resulting velocity field has the form

$$\mathbf{v}(x,y,t) = \mathbf{v}(x,y) + \epsilon\mathbf{v}^p(x,y,t),$$

where ϵ is a small parameter. The cross section of the unperturbed duct velocity field $\mathbf{v}(x,y)$ might possess some separating streamlines (see figure (5.1)). Under the time-dependent perturbations these streamlines can break. It is widely believed that there is a neighborhood of these streamlines for small ϵ such that the perturbed cross section is ergodic in that neighborhood (this has been proven for some very simple cases, see [26], [27]). But, as the whole cross section is not ergodic, the effective diffusivity in the direction of z is still maximal, i.e., $\mathbf{D}_{sym}\mathbf{e}_z \cdot \mathbf{e}_z \sim Pe^2$. As the strength of the perturbation, ϵ is increased, a larger portion of A might become ergodic, ultimately leading to the ergodicity on the whole A. At that point the effective diffusivity in the direction of z is not maximal. So, the time dependence of the cross sectional velocity field provides a mechanism for the transition in the behavior of the effective diffusivity for duct velocity fields which have cross-sectional velocity field with zero mean. This was not possible in the steady velocity fields of the type considered in [14].

5.5 Conclusions

We have provided tools for the study of maximal effective diffusivity in two-dimensional, time and space-periodic flows, and in three-dimensional, time dependent flows admitting a volume-preserving symmetry. Of course, the analysis of maximal effective diffusivity in three-dimensional, space and time periodic flows can be done along the same lines. But, there is much less knowledge of a kinematical structure for three-dimensional maps and flows, then for two-dimensional ones. Our study could be extended to more general time dependences upon establishment of the relevant homogenization theory (however, see [3] for a "weak" homogenization theorem for flows with the almost periodic time dependence).

It would be interesting to provide numerical or experimental evidence for the "phase transition" phenomena predicted in section 4.

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Chapter 6

Chaotic transport and dispersion near a helical vortex filament in a time-periodic strain rate field

6.1 Introduction

In the past years there has been much work in applying concepts of dynamical systems theory to fluid transport and mixing issues. The reason for this is as follows. For two-dimensional, incompressible time-periodic fluid flows the equations for fluid particle paths are given by

$$\begin{aligned} \dot{x} &= \frac{\partial \psi}{\partial y}(x, y, t), \\ \dot{y} &= -\frac{\partial \psi}{\partial x}(x, y, t), \end{aligned}$$

where $\psi(x, y, t)$ is the stream function, which we will consider to be periodic in t. From the dynamical systems viewpoint, these are Hamilton's equations where $\psi(x, y, t)$ is the Hamiltonian function and the phase space of this dynamical system is actually the physical space where the fluid flows. Through time periodicity the study of these equations can be reduced to the study of a two-dimensional area preserving Poincaré map and once the problem has been cast in this setting a variety of techniques and ideas from dynamical systems theory can be applied for the purpose of studying fluid transport and mixing issues. For example, KAM tori represent barriers to fluid transport and mixing, chaotic dynamics should act to enhance mixing, and invariant manifolds, such as the stable and unstable manifolds of hyperbolic periodic points, are manifested as "organized structures" in the fluid flow. See Ottino [15] and volume 3 (1991), number 5 of the Physics of Fluids A for recent reviews.

Because of the analogy with two-dimensional area preserving maps described above, most of the theoretical work has been in the context of two dimensional time periodic flows, or for three-dimensional flows that have some property that allows a reduction to a two-dimensional area preserving map. For example, the ABC flow is a three-dimensional steady Euler flow that has received much attention in recent years (see, e.g., Dombre *et al.* [9]).

In recent years there has been some progress in extending the dynamical systems approach to flows with more general time dependence and to three dimensions. Beigie *et al.* [5], [6] have developed methods for studying transport and mixing in quasiperiodically time dependent flows. MacKay [11] and Mezić and Wiggins [12] (or chapter 2 of this thesis) have developed methods for studying transport and mixing in certain classes of three-dimensional flows.

In this chapter we present a study of convective transport in a three-dimensional time periodic flow from the point of view of dynamical systems theory. In particular, we study the flow induced by a helical vortex filament in an axisymmetric time-dependent strain field. The dynamics of vortex filaments in three-dimensional flows is an area of continuing activity with many open problems remaining. We want to emphasize that the purpose of this chapter is *not* to develop models for the dynamics of vortex filaments. Rather, we wish to take a specific model that is physically realistic in certain situations, and study the fluid particle kinematics and transport properties resulting from the flow induced by the vortex filament. Therefore, we will not present a literature survey of the various theories of the dynamics of vortex filaments. Rather, we will only describe results that are relevant for our particular model, as well as discussions of its validity. We refer the reader to the recent monograph of Saffman [16] for general background on the dynamics of vortex filaments.

This chapter is organized as follows. In section 2 we derive the velocity field induced by a helical vortex filament in a time periodic, axisymmetric strain rate field, under certain assumptions based on the structure of the vortex core and the self-induced motion of the helix. The axisymmetric strain rate field is considered as a perturbation of the flow induced by the helix. We then transform the flow into a special system of "helical coordinates" based on the symmetries of the unperturbed flow. These coordinates play an important role in our analysis of global kinematics and transport. In section 3 we analyze the structure of the unperturbed flow and use this as a framework to analyze the structure of the perturbed flow in section 4. For the perturbed flow we show the existence of invariant two-dimensional helical cylinders in the flow that act as barriers to the transport of fluid, as well as the existence of regions of chaotic fluid particle motions. In the same section we discuss a mechanism for the Ranque effect which appears in swirling flows in pipes (increase of the temperature of certain regions and decrease of the temperature in others) provided by the chaoticity of the motion. In section 5 we discuss shear dispersion of an ensemble of perfect tracer.

6.2 The velocity field of a helical vortex filament in an axisymmetric time-periodic strain rate field

In this section we will derive an approximate expression for the velocity field induced by a helical vortex filament in an axisymmetric time-periodic strain rate field. The derivation involves several steps, and will be broken down and distributed through several subsections.

6.2.1 The velocity field induced by a helical vortex filament

Consider a vorticity distribution along a space curve that is given parametrically by $\mathbf{x}'(\phi, t) = (x'(\phi, t), y'(\phi, t), z'(\phi, t))$, where ϕ denotes the parameter along the curve at each instant of time. The time dependence of $\mathbf{x}'(\phi, t)$ comes from the fact that the vortex filament may move in time. The velocity induced by this vorticity distribution is given by the Biot-Savart integral as follows (see Batchelor [4])

$$\mathbf{u}(\mathbf{x}, t) = -\frac{\Gamma}{4\pi} \int_{\alpha} \frac{\mathbf{s}(\mathbf{x}, \phi, t) \times \frac{d\mathbf{x}'(\phi,t)}{d\phi}}{s^3(\mathbf{x}, \phi, t)} d\phi, \tag{6.2.1}$$

where α denotes the space curve or *filament* under consideration, and Γ is the circulation of the vortex filament.

Let us consider the situation of a helical vortex filament *fixed in space*, i.e., it does not move in time. The filament is represented parametrically in Cartesian coordinates as

$$\begin{aligned} x' &= a_0 \cos\phi, \\ y' &= a_0 \sin\phi, \end{aligned}$$

$$z' = k_0\phi, \tag{6.2.2}$$

or, in cylindrical coordinates

$$r' = a_0, \tag{6.2.3}$$

$$\theta' = \phi, \tag{6.2.4}$$

$$z' = k_0\phi, \tag{6.2.5}$$

where a_0 is the radius of the cylinder circumscribed by the helix and $2\pi k_0$ is the pitch of the helix.

Hardin [10] was the first to derive the velocity field for this situation, although he followed a procedure that is slightly different, but equivalent, to that described above. Rather than evaluate the Biot-Savart integrals directly he derived a vector velocity potential

$$\mathbf{A}(\mathbf{x},t) = -\frac{\Gamma}{4\pi}\int_\alpha \frac{\frac{d\mathbf{x}'(\phi)}{d\phi}}{s(\mathbf{x},\phi)}d\phi, \tag{6.2.6}$$

whose curl gives the velocity field. In cylindrical coordinates, the components of the velocity potential are given by

$$\begin{pmatrix} A_r \\ A_\theta \\ A_z \end{pmatrix} = -\frac{\Gamma}{4\pi}\int_{-\infty}^{\infty} \frac{\begin{pmatrix} a_0\sin(\theta-\phi) \\ a_0\cos(\theta-\phi) \\ k_0 \end{pmatrix} d\phi}{(r^2+a_0^2-2a_0 r cos(\theta-\phi)+(z-k_0\phi)^2)^{1/2}}. \tag{6.2.7}$$

Hardin evaluated these integrals and used the results to construct the following velocity field

$$\begin{aligned}
\dot{r}^{in}_{BS}(a_0,k_0,r,\theta,z) &= \frac{\Gamma}{\pi}\frac{a_0}{k_0^2}\sum_{m=1}^{\infty} mK'_m(ma_0/k_0)I'_m(mr/k_0)\sin(m(\theta - z/k_0)),\\
\dot{\theta}^{in}_{BS}(a_0,k_0,r,\theta,z) &= \frac{\Gamma}{\pi}\frac{a_0}{k_0\, r^2}\sum_{m=1}^{\infty} mK'_m(ma_0/k_0)I_m(mr/k_0)\cos(m(\theta - z/k_0)),\\
\dot{z}^{in}_{BS}(a_0,k_0,r,\theta,z) &= \frac{\Gamma}{2\pi k_0} - \frac{\Gamma}{\pi}\frac{a_0}{k_0^2}\sum_{m=1}^{\infty} mK'_m(ma_0/k_0)I_m(mr/k_0)\cos(m(\theta - z/k_0)),
\end{aligned} \tag{6.2.8}$$

for the region $r < a_0$, and

$$\begin{aligned}
\dot{r}^{out}_{BS}(a_0,k_0,r,\theta,z) &= \frac{\Gamma}{\pi}\frac{a_0}{k_0^2}\sum_{m=1}^{\infty} mK'_m(mr/k_0)I'_m(ma_0/k_0)\sin(m(\theta - z/k_0)),\\
\dot{\theta}^{out}_{BS}(a_0,k_0,r,\theta,z) &= \frac{\Gamma}{2\pi r^2} + \frac{\Gamma}{\pi}\frac{a_0}{k_0\, r^2}\sum_{m=1}^{\infty} mK_m(mr/k_0)I'_m(ma_0/k_0)\cos(m(\theta - z/k_0)),\\
\dot{z}^{out}_{BS}(a_0,k_0,r,\theta,z) &= -\frac{\Gamma}{\pi}\frac{a_0}{k_0^2}\sum_{m=1}^{\infty} mK_m(mr/k_0)I'_m(ma_0/k_0)\cos(m(\theta - z/k_0))).
\end{aligned} \tag{6.2.9}$$

for the region $r > a_0$. In these expressions K_m, I_m denote m-th order modified Bessel functions of the second kind , with K'_m, I'_m denoting their derivatives with respect to the argument. Different expressions for the velocity field in the two regions in $\mathbb{R}^3$ arise due to the fact that $\mathbb{R}^3 - \alpha$ is not simply connected.

However, this velocity field is not physically realistic. This is because the helical vortex filament will not remain fixed in space. Rather, the filament experiences a self-induced velocity. If one uses this velocity field to calculate the self-induced velocity, one obtains an infinite velocity, i.e., the velocity field is singular on the helix. However, if we consider a helix with nonzero thickness, it is known that under this self-induced velocity the helix remains a helix and convects in the direction of the z axis with constant speed and rotates at a constant angular velocity about the z axis ([8], [14]).

With these features in mind, we now describe our model of the velocity field due to a helical vortex filament. Let V_T denote the translational velocity of the helix in the direction of the z axis and let Ω denote the rotational velocity about the z axis. We then transform to a frame moving with the helix as follows

$$\begin{aligned} r &\rightarrow r, \\ \theta &\rightarrow \theta + \Omega t, \\ z &\rightarrow z + V_T t. \end{aligned} \tag{6.2.10}$$

In this frame the helix is fixed. Therefore, as an approximate velocity field, in this moving frame we use the velocity field obtained by Hardin. Thus, we have

$$\begin{aligned} \dot{r}^{in,out} &= \dot{r}_{BS}^{in,out}(a_0, k_0, r, \theta, z), \\ \dot{\theta}^{in,out} &= \dot{\theta}_{BS}^{in,out}(a_0, k_0, r, \theta, z) - \Omega, \\ \dot{z}^{in,out} &= \dot{z}_{BS}^{in,out}(a_0, k_0, r, \theta, z) - V_T. \end{aligned} \tag{6.2.11}$$

Now we must find V_T and Ω.

The self-induced velocity of the helical vortex filament–the local induction approximation

The simplest theory describing the self-induced motion of a vortex filament is the so-called *local induction approximation* developed by da Rios [8]. In this approximation the velocity of the helix is given by

$$\mathbf{v}_{hel} = \kappa \frac{\Gamma}{4\pi}(\ln \frac{1}{\delta})\mathbf{b},$$

where κ is the curvature, δ is the core radius and $\mathbf{b}$ is the unit binormal vector. This expression is valid up to $\mathcal{O}(1)$ terms in δ (the most precise derivation of this is given in da Rios [8]). Letting

$$\gamma = \frac{1}{4}(\ln \frac{1}{\delta}),$$

we have

$$\mathbf{v}_{hel} = \frac{\Gamma}{\pi}\kappa\gamma\mathbf{b}.$$

In Fig. 6.1 we show the coordinate systems and geometry for the velocity of the helical vortex filament. From the geometry in Fig. 6.1, we see that the rotational and translational velocities are given, respectively, as

$$\begin{aligned} V_R &= |\mathbf{v}_{hel}| \cos\beta = \frac{\Gamma}{\pi}\kappa\gamma\cos\beta, \\ V_T &= |\mathbf{v}_{hel}| \sin\beta = \frac{\Gamma}{\pi}\kappa\gamma\sin\beta, \end{aligned} \tag{6.2.12}$$

where β is the pitch angle of the helix, defined by

$$\tan\beta = \frac{a}{k}. \tag{6.2.13}$$

The angular velocity of the helix, Ω is then given by

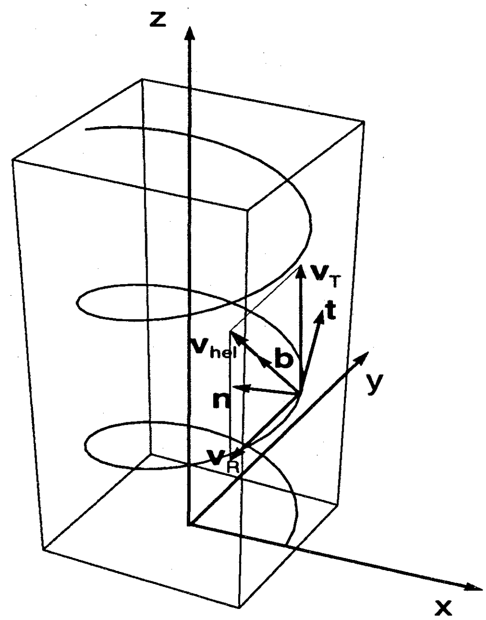

Figure 6.1: Geometry and coordinate systems associated with the helix.

$$\Omega = -V_R/a = -\frac{\Gamma}{\pi}\frac{\kappa\gamma\cos\beta}{a}. \tag{6.2.14}$$

Using trigonometric identities and the expression for the curvature of the helix in terms of the helix parameters given by

$$\kappa = \frac{a}{a^2 + k^2}, \tag{6.2.15}$$

from (6.2.12), (6.2.13), (6.2.14), and (6.2.15) we deduce that

$$\begin{aligned} V_T &= \frac{\Gamma}{\pi}\gamma\frac{a^2}{(a^2+k^2)^{3/2}}, \\ \Omega &= -\frac{\Gamma}{\pi}\gamma\frac{k}{(a^2+k^2)^{3/2}}. \end{aligned} \tag{6.2.16}$$

Note that we have dropped the subscript "0" from the notation for the helix parameters a_0 and k_0. This is because the helix may vary in time, without affecting the application of the local induction approximation.

6.2.2 The motion of the helical vortex filament in an axisymmetric time-periodic strain rate field

We now consider the helical vortex filament embedded in an axisymmetric time-periodic strain rate field expressed in cylindrical coordinates as follows

$$\begin{aligned} \dot{r}_{str} &= \epsilon r \cos \omega t, \\ \dot{\theta}_{str} &= 0, \\ \dot{z}_{str} &= -2\epsilon z \cos \omega t. \end{aligned} \tag{6.2.17}$$

It is well-known (see, e.g., Batchelor [4]) that the total velocity field can be expressed as a superposition of the vortical and potential velocity fields. However, first we need to address the issue of whether or not the helical vortex filament remains a helix in this axisymmetric time-periodic strain rate field.

The equations for the motion of particles under the influence of the axisymmetric strain rate field on the vortex filament are given by

$$
\begin{aligned}
\dot{r}' &= \epsilon r' \cos(\omega t), \\
\dot{\theta}' &= \Omega(t), \\
\dot{z}' &= V_T(t) - 2\epsilon z' \cos(\omega t).
\end{aligned}
\tag{6.2.18}
$$

$V_T(t)$ and $\Omega(t)$ are given by the local induction approximation expression in (6.2.16) where the parameters a and k may vary in time under the action of the axisymmetric strain rate field, and the relationship between the helix parameters and the Cartesian coordinates is given in (6.2.5). We will not write this latter relationship out explicitly as it will not be needed in our arguments. From the solution of these equations we want to argue that if the filament is a helix at $t = 0$, then it remains a helix for all later times, though the parameters of the helix my change in time. Hence, we seek a solution of these equations with initial conditions $r'(t = 0) = a_0, \theta'(t = 0) = \phi, z'(t = 0) = k_0\phi$ (i.e., at $t = 0$ the vortex filament is a helical curve defined by (6.2.2). The solution is easily found to be

$$
\begin{aligned}
r'(t) &= a_0 \exp\left(\frac{\epsilon}{\omega} \sin(\omega t)\right), \\
\theta'(\phi, t) &= \phi + \int_0^t \Omega(s) ds,
\end{aligned}
$$

$$z'(\phi, t) = \exp(-2\frac{\epsilon}{\omega}\sin(\omega t))(k_0\phi + \int_0^t V_T(s)\exp(2\frac{\epsilon}{\omega}\sin(\omega s)ds). \quad (6.2.19)$$

It is clear that equations (6.2.19) represent a helical vortex filament where the parameters of the helix vary periodically in time as follows,

$$a = a_0 \exp(\frac{\epsilon}{\omega}\sin(\omega t)),$$

$$k = k_0 \exp(-2\frac{\epsilon}{\omega}\sin(\omega t)).$$

6.2.3 The complete velocity field

Assembling the pieces from the previous subsections, we now can write down the velocity field of a helical vortex filament in the axisymmetric time-periodic strain rate field given by (6.2.17). First, we need to make some preliminary coordinate transformations. Let

$$\begin{aligned} I_1 &= \int_0^t \Omega(s)ds, \\ I_2 &= \exp(-2\frac{\epsilon}{\omega}\sin(\omega t))\int_0^t V_T(s)\exp(2\frac{\epsilon}{\omega}\sin(\omega s)ds. \end{aligned} \quad (6.2.20)$$

As in (6.2.10) we make a time-dependent change of coordinates

$$\begin{aligned} r &\rightarrow r, \\ \theta &\rightarrow \theta + I_1, \end{aligned}$$

$$z \rightarrow z + I_2.$$

(6.2.21)

Note that

$$\begin{aligned} \dot{I}_1 &= \Omega(t), \\ \dot{I}_2 &= V_T(t) - 2\epsilon\cos(\omega t)\exp(-2\frac{\epsilon}{\omega}\sin(\omega t)) \int_0^t V_T(s)\exp(2\frac{\epsilon}{\omega}\sin(\omega s) ds. \end{aligned}$$

(6.2.22)

The helix is given parametrically by $r' = a, \theta' = k\phi + I_1, z' = k\phi + I_2$. Using (6.2.21), (6.2.11), (6.2.22), and the expression for the strain rate field in cylindrical coordinates (6.2.17), the velocity field induced by a helical vortex filament embedded in a three-dimensional, axisymmetric time-periodic strain field is given as follows

$$\begin{aligned} \dot{r}^{in,out} &= \dot{r}_{BS}^{in,out}(a,k,r,\theta,z) + \epsilon r\cos(\omega t), \\ \dot{\theta}^{in,out} &= \dot{\theta}_{BS}^{in,out}(a,k,r,\theta,z) - \Omega(t), \\ \dot{z}^{in,out} &= \dot{z}_{BS}^{in,out}(a,k,r,\theta,z) - V_T - 2\epsilon z\cos(\omega t). \end{aligned}$$

(6.2.23)

Note that the frame in which (6.2.23) is valid is the one in which the helical curve has oscillating parameters a and k, but it does not translate or rotate.

By another change of coordinates, we can simplify the velocity field further. Let

$$r \rightarrow r\exp(\frac{\epsilon}{\omega}\sin(\omega t)),$$

$$z \quad \rightarrow \quad z\exp(-\frac{2\epsilon}{\omega}\sin(\omega t)). \tag{6.2.24}$$

Then

$$\begin{aligned}
\dot{r}^{in,out} &= \exp(-\frac{\epsilon}{\omega}\sin(\omega t))\dot{r}_{BS}^{in,out}(a,k,r\exp(\frac{\epsilon}{\omega}\sin(\omega t)),\theta,z\exp(-\frac{2\epsilon}{\omega}\sin(\omega t))). \\
\dot{\theta}^{in,out} &= \dot{\theta}_{BS}^{in,out}(a,k,r\exp(\frac{\epsilon}{\omega}\sin(\omega t)),\theta,z\exp(-\frac{2\epsilon}{\omega}\sin(\omega t))) - \Omega(t), \\
\dot{z}^{in,out} &= \exp(\frac{2\epsilon}{\omega}\sin(\omega t))\dot{z}_{BS}^{in,out}(a,k,r\exp(\frac{\epsilon}{\omega}\sin(\omega t)),\theta,z\exp(-\frac{2\epsilon}{\omega}\sin(\omega t))) \\
&\quad - \exp(\frac{2\epsilon}{\omega}\sin(\omega t))V_T(t).
\end{aligned} \tag{6.2.25}$$

Next we nondimensionalize (6.2.25). Let

$$z = Zk_0, \quad r = Ra_0, \quad t \rightarrow t\frac{a_0 k_0 \pi}{\Gamma}, \quad \epsilon \rightarrow \epsilon\frac{a_0 k_0 \pi}{\Gamma}, \quad \omega \rightarrow \omega\frac{a_0 k_0 \pi}{\Gamma}. \tag{6.2.26}$$

We will continue to denote derivatives with respect to the dimensionless time T with overdots. We introduce the following nondimensional parameter

$$\lambda = \frac{a}{k} = \frac{a_0}{k_0}\exp(3\frac{\epsilon}{\omega}\sin(\omega t)). \tag{6.2.27}$$

Using (6.2.8) and (6.2.9), the velocity field (6.2.25) in nondimensional coordinates becomes

$$\dot{R}^{in} \quad = \quad [\lambda S_{in}(R,\theta - Z,\lambda)]\exp(\frac{\epsilon}{\omega}\sin(\omega t)),$$

$$\begin{aligned}
\dot{\theta}^{in} &= \left[\gamma\frac{\lambda}{(1+\lambda^2)^{3/2}} + \frac{1}{R^2}C_{in}(J,\theta - Z,\lambda)\right]\exp(\frac{\epsilon}{\omega}\sin(\omega t)),\\
\dot{Z}^{in} &= \left[-\gamma\frac{\lambda^3}{(1+\lambda^2)^{3/2}} + \frac{\lambda}{2} - \lambda^2 C_{in}(J,\theta - Z,\lambda)\right]\exp(\frac{\epsilon}{\omega}\sin(\omega t)),
\end{aligned} \tag{6.2.28}$$

$$\begin{aligned}
\dot{R}^{out} &= [\lambda S_{out}(R,\theta - Z,\lambda)]\exp(\frac{\epsilon}{\omega}\sin(\omega t)),\\
\dot{\theta}^{out} &= \left[\gamma\frac{\lambda}{(1+\lambda^2)^{3/2}} + \frac{1}{2R^2\lambda^2} + \frac{1}{R^2}C_{out}(R,\theta - Z,\lambda)\right]\exp(\frac{\epsilon}{\omega}\sin(\omega t)),\\
\dot{Z}^{out} &= \left[-\gamma\frac{\lambda^3}{(1+\lambda^2)^{3/2}} - \lambda^2 C_{out}(R,\theta - Z,\lambda)\right]\exp(\frac{\epsilon}{\omega}\sin(\omega t)),
\end{aligned} \tag{6.2.29}$$

where

$$\begin{aligned}
C_{in}(R,\theta - Z,\lambda) &= \sum_{m=1}^{\infty} mK'_m(\lambda m)I_m(R\lambda m)\cos(m(\theta - Z)),\\
S_{in}(R,\theta - Z,\lambda) &= \sum_{m=1}^{\infty} mK'_m(\lambda m)I'_m(R\lambda m)\sin(m(\theta - Z)),
\end{aligned} \tag{6.2.30}$$

and

$$\begin{aligned}
C_{out}(R,\theta - Z,\lambda) &= \sum_{m=1}^{\infty} mK_m(R\lambda m)I'_m(\lambda m)\cos(m(\theta - Z)),\\
S_{out}(R,\theta - Z,\lambda) &= \sum_{m=1}^{\infty} mK'_m(R\lambda m)I'_m(\lambda m)\sin(m(\theta - Z)).
\end{aligned} \tag{6.2.31}$$

6.2.4 Validity of the approximations

In the derivation of the velocity field we used the Localized Induction Approximation (LIA) twice: to approximate the velocity of the helical vortex filament and to derive the equations of motion of the helical vortex filament in the external stain rate field given in (6.2.17). The equations of motion of an arbitrary vortex filament in an external potential flow might be seriously affected by the use of LIA. For a helical vortex filament, though, this is not the case. The only component of velocity besides the binormal one is a component in the direction of the tangent vector. So, the same derivation of the motion of the vortex filament goes through, with only the expressions for time dependent radius and k changing. Starting the derivation of the equations of motion of the vortex filament from the expression for the velocity of the type

$$\dot{\mathbf{x}} = \kappa \mathbf{b} + f(\kappa, \tau)\mathbf{t} + \mathbf{v},$$

one finds out that these new equations still admit the same solution (oscillating helix) when the perturbation velocity $\mathbf{v}$ is a strain rate field. As we are interested in the qualitative, kinematic description of the motion of fluid particles, and not in a precise description of the motion of a helical vortex filament, we proceed by analyzing the flow obtained above.

6.2.5 Coordinates that exploit the symmetry of the flow

In Mezić and Wiggins [12] (or chapter 2 of this thesis) it was shown that a three-dimensional divergence-free velocity field admitting a volume-preserving, spatial symmetry group can be transformed to the following form

$$\begin{aligned} \dot{x} &= \frac{\partial H(x,y,t)}{\partial y}, \\ \dot{y} &= -\frac{\partial H(x,y,t)}{\partial x}, \end{aligned}$$

$$\dot{z} = f(x, y, t). \tag{6.2.32}$$

In the case of a steady velocity field, the function H is an integral of motion. It was also shown that sufficient and necessary conditions for a velocity field $\mathbf{v}$ to admit a volume-preserving spatial symmetry group are that the infinitesimal generator of the action of the symmetry group, $\mathbf{w}$ satisfies

$$\begin{aligned} \frac{\partial \mathbf{w}}{\partial t} &= 0, \\ [\mathbf{v}, \mathbf{w}] &= 0, \\ \nabla \cdot \mathbf{w} &= 0, \end{aligned} \tag{6.2.33}$$

where $[\mathbf{v}, \mathbf{w}]$ is a Lie bracket of vector fields (for more background on this issue, see Mezić and Wiggins [12]) or chapter 2 of this thesis. Coordinates of this type are very nice because the velocity field assumes the form of an "almost Hamiltonian" dynamical system. We want to show that the velocity field we have derived can be transformed into this form since it will greatly facilitate the global analysis of transport properties.

Let the candidate for the action of the symmetry group of (6.2.28), (6.2.29) be

$$\begin{aligned} R &\to R, \\ \theta &\to \theta + \lambda, \\ Z &\to Z + \lambda. \end{aligned} \tag{6.2.34}$$

Its infinitesimal generator, a vector field in $\mathbb{R}^3$, is given in (R, θ, Z) coordinates by $\mathbf{w} = (0, 1, 1)$. A straightforward calculation shows that the velocity field (6.2.28), (6.2.29) and $\mathbf{w}$ commute (i.e., their Lie bracket is zero). Further, $\mathbf{w}$ is steady and divergence free, therefore (6.2.34) is a spatial, volume-preserving symmetry group for the velocity field (6.2.28), (6.2.29).

To transform the velocity field into the form (6.2.32), we follow the procedure described in chapter 2. To obtain the first two coordinates, in which the system is of Hamiltonian form, we first need to find two integrals of motion for $\mathbf{w}$. These are easily found to be R and $\psi = \theta - Z$. We choose the third coordinate to be $\vartheta = \theta + a_0^2 Z/k_0^2 = \theta + Z/\lambda_0^2$ instead of Z, which we would do in following the procedure in chapter 2, as it simplifies the velocity field induced by the helical vortex filament, in the sense that the velocity of the helix in the $\epsilon = 0$ case has a contribution only in the direction of ψ. Finally, to achieve a canonical Hamiltonian form in two of the variables, we introduce the new variable $J = R^2/2$.

Performing these transformations of coordinates, we have

$$
\begin{aligned}
\dot{J}_{in} &= \left[\lambda\sqrt{2J}\,S_{in}(\sqrt{2J},\psi,\lambda)\right]\exp(\frac{\epsilon}{\omega}\sin(\omega t))\\
\dot{\psi}_{in} &= \left[-\frac{1}{2}\lambda+\gamma\frac{\lambda}{\sqrt{1+\lambda^2}}+\frac{1+2J\lambda^2}{2J}C_{in}(\sqrt{2J},\psi,\lambda)\right]\exp(\frac{\epsilon}{\omega}\sin(\omega t)),\\
\dot{\vartheta}_{in} &= \left[\gamma\frac{\lambda}{(1+\lambda^2)^{3/2}}(1-\exp(\frac{6\epsilon}{\omega}\sin(\omega t)))+\frac{1}{2\lambda}\exp(\frac{6\epsilon}{\omega}\sin(\omega t))\right.\\
&\left.+\frac{1-2J\exp(\frac{6\epsilon}{\omega}\sin(\omega t))}{2J}C_{in}(\sqrt{2J},\psi,\lambda)\right]\exp(\frac{\epsilon}{\omega}\sin(\omega t)),
\end{aligned}
\tag{6.2.35}
$$

$$\begin{aligned}
\dot{J}_{out} &= \left[\lambda\sqrt{2J}S_{out}(\sqrt{2J},\psi,\lambda)\right]\exp(\frac{\epsilon}{\omega}\sin(\omega t))\\
\dot{\psi}_{out} &= \left[\frac{1}{4\lambda J}+\gamma\frac{\lambda}{\sqrt{1+\lambda^2}}+\frac{1+2\lambda^2 J}{2J}C_{out}(\sqrt{2J},\psi,\lambda)\right]\exp(\frac{\epsilon}{\omega}\sin(\omega t)),\\
\dot{\vartheta}_{out} &= \left[\gamma\frac{\lambda}{(1+\lambda^2)^{3/2}}(1-\exp(\frac{6\epsilon}{\omega}\sin(\omega t)))+\frac{1}{4\lambda J}\right.\\
&\left.+\frac{1-2J\exp(\frac{6\epsilon}{\omega}\sin(\omega t))}{2J}C_{in}(\sqrt{2J},\psi,\lambda)\right]\exp(\frac{\epsilon}{\omega}\sin(\omega t)).
\end{aligned}$$

For later geometrical interpretation it is important to note that

$$(J,\psi,\vartheta)\in \mathbb{R}^+\times S^1\times\mathbb{R}.$$

As discussed above, the $J-\psi$ components of the velocity induced by the helical vortex filament can be written in the form

$$\begin{aligned}
\dot{J}_{in,out} &= \frac{\partial H_{in,out}}{\partial\psi}(J,\psi,t;\epsilon),\\
\dot{\psi}_{in,out} &= -\frac{\partial H_{in,out}}{\partial J}(J,\psi,t;\epsilon),
\end{aligned} \tag{6.2.36}$$

where

$$\begin{aligned}
H_{in}(J,\psi,t;\epsilon) &= \exp(\frac{\epsilon}{\omega}\sin(\omega t))(\frac{1}{2}\lambda J-\gamma\frac{\lambda}{\sqrt{1+\lambda^2}}J\\
&-\lambda\sqrt{2J}\sum_{m=1}^{\infty}K_m'(\lambda m)I_m'(\sqrt{2J}\lambda m)\cos(m\psi)), \qquad (6.2.37)\\
H_{out}(J,\psi,t;\epsilon) &= \exp(\frac{\epsilon}{\omega}\sin(\omega t))(-\frac{1}{2\lambda}\ln\sqrt{2J}-\gamma\frac{\lambda}{\sqrt{1+\lambda^2}}J-\\
&-\lambda\sqrt{2J}\sum_{m=1}^{\infty}mK_m'(\sqrt{2J}\lambda m)I_m'(\lambda m)\cos(m\psi). \qquad (6.2.38)
\end{aligned}$$

Thus, the velocity field for ϵ small can be Taylor expanded as

$$\begin{aligned}
\dot{J}_{in,out} &= \frac{\partial H^0_{in,out}}{\partial \psi}(J,\psi) + \epsilon \frac{\partial H^1_{in,out}}{\partial \psi}(J,\psi,t) + \mathcal{O}(\epsilon^2), \\
\dot{\psi}_{in,out} &= -\frac{\partial H^0_{in,out}}{\partial J}(J,\psi) - \epsilon \frac{\partial H^1_{in,out}}{\partial J}(J,\psi,t) + \mathcal{O}(\epsilon^2), \\
\dot{\vartheta}_{in,out} &= h^0_{in,out}(J,\psi) + \epsilon h^1_{in,out}(J,\psi,t) + \mathcal{O}(\epsilon^2),
\end{aligned} \tag{6.2.39}$$

where

$$H^0_{in,out}(J,\psi) = H_{in,out}(J,\psi,t;0), \qquad H^1_{in,out}(J,\psi,t) = \frac{\partial H_{in,out}}{\partial \epsilon}(J,\psi,t;0),$$

and

$$\begin{aligned}
h^0_{in}(J,\psi) &= \frac{1}{4\lambda_0 J} + \frac{1-2J}{2J} C_{in,out}(\sqrt{2J},\psi,\lambda_0), \\
h^0_{out}(J,\psi) &= \frac{1}{2\lambda_0} + \frac{1-2J}{2J} C_{in,out}(\sqrt{2J},\psi,\lambda_0), \\
h^1_{in}(J,\psi,t) &= \frac{\partial}{\partial \epsilon}\Bigg(\Bigg[\gamma \frac{\lambda}{(1+\lambda^2)^{3/2}}(1-\exp(\frac{6\epsilon}{\omega}\sin(\omega t))) + \frac{1}{2\lambda}\exp(\frac{6\epsilon}{\omega}\sin(\omega t)) \\
&\quad + \frac{1-2J\exp(\frac{6\epsilon}{\omega}\sin(\omega t))}{2J} C_{in}(\sqrt{2J},\psi,\lambda)\Bigg]\exp(\frac{\epsilon}{\omega}\sin(\omega t))\Bigg)\Big|_{\epsilon=0}, \\
h^1_{out}(J,\psi,t) &= \frac{\partial}{\partial \epsilon}\Bigg(\Bigg[\gamma \frac{\lambda}{(1+\lambda^2)^{3/2}}(1-\exp(\frac{6\epsilon}{\omega}\sin(\omega t))) + \frac{1}{4\lambda J} \\
&\quad + \frac{1-2J\exp(\frac{6\epsilon}{\omega}\sin(\omega t))}{2J} C_{in}(\sqrt{2J},\psi,\lambda)\Bigg]\exp(\frac{\epsilon}{\omega}\sin(\omega t))\Bigg)\Big|_{\epsilon=0}.
\end{aligned} \tag{6.2.40}$$

We remark that all higher order terms in ϵ of the Taylor expansion of the velocity field are functions only of J, ψ, and t.

6.3 Analysis of the unperturbed velocity field: the geometry of invariant surfaces and particle paths

For this discussion we will work in the R, ψ, ϑ coordinates. The expression for the velocity field in these coordinates can be obtained from (6.2.28) and (6.2.29), where $\vartheta = \theta + a_0^2 Z/k_0^2$. This coordinate system is nonorthogonal except at $R = 1$. The coordinate system is depicted in Fig 6.2.

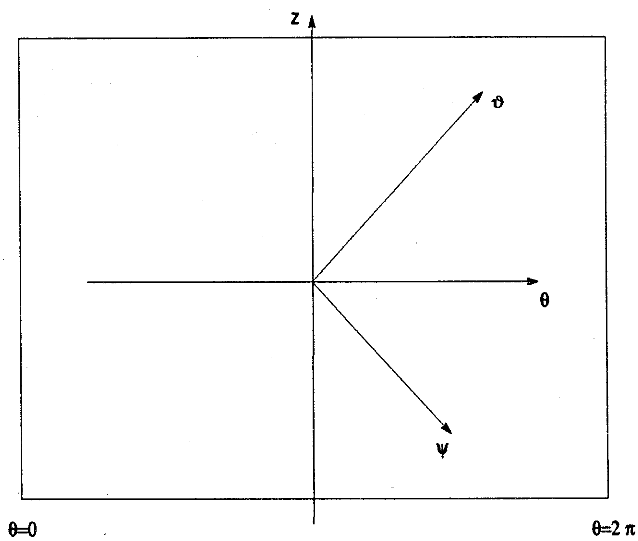

Figure 6.2: $\psi - \vartheta$ coordinate system.

We first consider the velocity field for $R < 1$. This velocity field for $\epsilon = 0$ is given by (note that $\lambda = \lambda_0$ for $\epsilon = 0$)

$$\dot{R} = \lambda S_{in}(R, \psi, \lambda)$$

$$\begin{aligned}\dot{\psi} &= -\frac{1}{2}\lambda + \gamma\frac{\lambda}{(1+\lambda^2)^{1/2}} + \frac{1+R^2\lambda^2}{R^2}C_{in}(R,\psi,\lambda), \\ \dot{\vartheta} &= \frac{1}{2\lambda} + \frac{1-R^2}{R^2}C_{in}(R,\psi,\lambda),\end{aligned} \tag{6.3.41}$$

where the function $C_{in}(R,\psi,\lambda)$ is defined in (6.2.30). Since the ϑ component decouples from the $R-\psi$ components (as a result of the helical symmetry), we can analyze separately the particle trajectories of the velocity field associated with the $R-\psi$ components, and then use this information to build up the complete picture in three dimensions.

6.3.1 Analysis of the $R-\psi$ component of the unperturbed velocity field

We first consider the existence of fixed points and their bifurcations. Since the $R-\psi$ component of the unperturbed velocity field is a one-degree-of-freedom Hamiltonian system, this basic informaton will enable us to easily infer the nature of the global orbit structure. Using a combination of Fourier analysis and numerical analysis one can argue that $\dot{R}=0$ is possible only for $\psi=0$ or $\psi=\pi$ (details of this analysis are presented in Appendix 1). This gives us the following condition that must be satisfied by fixed points in the $R-\psi$ plane:

$$\dot{\psi} = -\frac{1}{2}\lambda + \gamma\frac{\lambda}{(1+\lambda^2)^{1/2}} + \frac{1+R^2\lambda^2}{R^2}C_{in}(R, 0 \text{ or } \pi, \lambda) = 0.$$

Using the following properties of Bessel functions

$$\begin{aligned} K_m(x) &> 0, \\ I_m(x) &> 0, \\ K_m'(x) &< 0, \end{aligned}$$

$$I_m'(x) \;>\; 0, \qquad \text{for every } x, m, \tag{6.3.42}$$

one can argue that at $\psi = 0$ $C_{in} < 0$, and therefore that $-1/2 + \gamma/\sqrt{(1+\lambda^2)}$ must be bigger than zero in order for $\dot{\psi} = 0$. This gives the following conditions on the parameters in order to have fixed points at $\psi = 0$

$$\lambda < \sqrt{(2\gamma)^2 - 1}.$$

Next we consider fixed points with $\psi = \pi$. Using the fact that the coefficients in the Fourier series for for C_{in} are monotonically increasing, and (6.3.42), we conclude that for $\psi = \pi$ we have $C_{in} > 0$. Therefore in order to have fixed points at $\psi = \pi$ we have the following condition on the parameters

$$-\frac{1}{2}\lambda + \gamma\frac{\lambda}{\sqrt{1+\lambda^2}} < 0 \Rightarrow \lambda > \sqrt{(2\gamma)^2 - 1}.$$

However, these conditions do not tell us the exact number of fixed points. For this we have had to numerically solve (6.3.1). We have solved for the roots of this equation for the parameter ranges $\lambda \in [0.2, 10]$, $\gamma \in [2, 15]$ with increments in each parameter of 0.01. The results are presented in Fig. 6.3. In this figure we show two curves, denoted C1, and C2, on which Hamiltonian saddle-node bifurcations of fixed points occur as indicated. The possible phase portraits are also indicated in this figure. These follow very naturally from the Hamiltonian structure of the $R - \psi$ component of the vector field once the fixed points and their stability are known.

Carrying out the same kind of analysis for the part $R > 1, (J > 1/2)$, we find that there are no additional bifurcations. For the outer velocity field the fixed points can

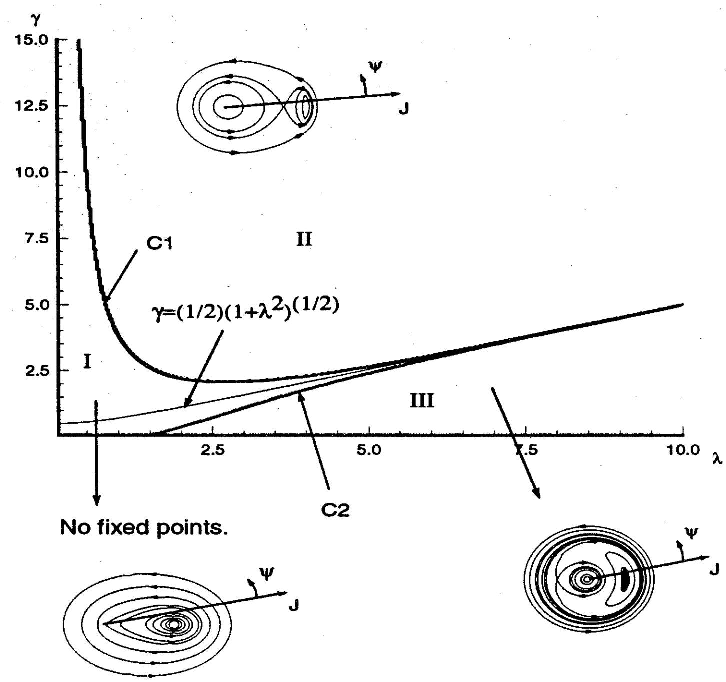

Figure 6.3: Trajectories of the $R - \psi$ component of the unperturbed velocity field in different regions of the $\lambda - \gamma$ parameter plane.

exist only for $\psi = \pi$, as

$$\frac{1}{4\lambda J} + \gamma \frac{\lambda}{\sqrt{1+\lambda^2}} > 0.$$

Therefore $C_{out}(R, \psi, \lambda)$ must be less than zero in order that zeros are possible, but this is the case for $\psi = \pi$. Thus we see that the $R - \psi$ component of the velocity field, depending on the parameters λ and γ, has elliptic and hyperbolic fixed points, periodic orbits, and homoclinic orbits connecting the hyperbolic fixed points.

Before leaving this secion it is instructive to consider two limiting cases. In the limit $\lambda \to 0$ we have the case of a straight vortex filament, for which the phase portrait consists of circular closed orbits in the $R - \psi$ plane, i.e., there are no fixed points. In the limit $\lambda \to \infty$ we have a densely wound helix, or a cylinder whose surface is a vortex surface, corresponding to a jet of infinite velocity.

6.3.2 Geometry of invariant surfaces and particle paths in three dimensions

We have seen that in the $R - \psi$ phase plane (or $J - \psi$ phase plane) we have fixed points (both hyperbolic and elliptic), periodic orbits, and homoclinic orbits, or separatrices, that connect hyperbolic fixed points and separate regions of qualitatively different periodic orbits. Our coordinates allow a simple interpretation of these structures in terms of invariant surfaces for the full three-dimensional flow. We summarize these results in the following table.

Orbit in the R- ψ Phase Plane	Corresponding Orbit or Invariant Surface for the 3-d Flow in R- ψ - ϑ coordinates, $\vartheta \in R^1$
elliptic fixed point	elliptic, unbounded invariant curve
hyperbolic fixed point	hyperbolic, unbounded invariant curve
periodic orbit	invariant 2-cylinder
homoclinic orbit	2-dimensional separatrices

Now we want to determine the nature of fluid particle trajectories on these invariant manifolds, which can be characterized entirely in terms of the sign of $\dot{\vartheta}$. We examine each invariant manifold individually.

Invariant curves

Consider a fixed point (J_f, ψ_f) for the $J - \psi$ components of the velocity field. For $\dot{\vartheta}(J_f, \psi_f) \neq 0$ invariant manifolds in three dimensions are unbounded invariant curves on which the magnitude of the ϑ component of trajectories increases without bound. However, if $\dot{\vartheta} = 0$ then these are invariant curves of fixed points.

Invariant cylinders

The trajectories on these invariant manifolds can be most easily studied by using the $J - \psi - \vartheta$ coordinates given in (6.2.39). In these coordinates the $J - \psi$ component is Hamiltonian. As a result of this, in a region where the level curves of the Hamiltonian are closed, i.e., they are periodic orbits, we can transform the $J - \psi$ system to action-angle coordinates I, ϕ_1 (see Wiggins [17] or Arnold [2]). From the fluid dynamical context, these are just the familiar streamline coordinates. The action-angle transformation is given explicitly by

$$I = \frac{1}{2\pi} \int_{H=h} J d\psi, \tag{6.3.43}$$

while the angle variable is given by

$$\phi_1 = \frac{2\pi}{T(H)} t, \tag{6.3.44}$$

where $T(H)$ is the period on the closed orbit in the $J - \psi$ plane (which is a level set of H), and t denotes the time of flight along the orbit measured from a reference point on the orbit. This transformation satisfies the following properties.

1. $I = I(h)$, i.e., I is constant on the closed orbits.

2. $\oint_{H=h} d\phi_1 = 2\pi$.

3. $\dot{\phi}_1 = \Omega_1(I)$.

We assume that the action-angle transformation on the $J-\psi$ component of the velocity field has been carried out so that the velocity field now takes the form

$$\begin{aligned} \dot{I} &= 0, \\ \dot{\phi}_1 &= \Omega_1(I), \\ \dot{\vartheta} &= h(I,\phi_1). \end{aligned} \tag{6.3.45}$$

It was shown in chapter 2 that the following additional transformation

$$\phi_2 = \vartheta + \frac{\Delta\vartheta}{2\pi}\phi_1 - \int \frac{h(I,\phi_1)}{\Omega_1(I)} d\phi_1,$$

where

$$\Delta\vartheta = \int_0^{2\pi} \frac{h(I,\phi_1)}{\Omega_1(I)} d\phi_1,$$

transforms the velocity field into the following form

$$\dot{I} = 0,$$

$$\begin{aligned}\dot{\phi}_1 &= \Omega_1(I),\\ \dot{\phi}_2 &= \Omega_2(I), \qquad (I,\phi_1,\phi_2) \in \mathbb{R}^+ \times S^1 \times \mathbb{R},\end{aligned} \tag{6.3.46}$$

where

$$\Omega_2 = \frac{\Delta\vartheta}{2\pi}\Omega_1(I).$$

In these coordinates we can easily determine the nature of the fluid particle trajectories on these two-dimensional invariant manifolds.

If $\Omega_2 = 0$ then the trajectories are closed orbits. For $\Omega_2 \neq 0$ the magnitude of the ϕ_2 component of the trajectories increases without bound.

In the original coordinates these two types of behaviour are determined by the increase in ϑ coordinate when the particle encircles a closed orbit in $J - \psi$ plane once. If this increase is positive, the particle will for large times tend to $\vartheta = +\infty$, while if it is negative, the particle will ultimately tend to $\vartheta = -\infty$. In the figure (6.4) we present a numerical calculation of the curve on which the velocity in the direction of ϑ vanishes. This curve is denoted by C on the figure. Note from the expression for the velocity field that C is independent of γ. The phase portrait in the figure (6.4) is that for $\lambda = 3.0, \gamma = 6.0$. Computations are done with 23 terms of the Fourier series for $C_{in,out}$. Outside of C $\dot{\vartheta} > 0$, so for any cylinder entirely contained in that region $\Delta\vartheta > 0$. For such cylinders, particles tend to $\vartheta = +\infty$ as time goes to infinity. As our analysis is done in the frame moving together with the helix, physically $\dot{\vartheta} > 0$ means that the particles on these cylinders move faster than the helix itself at all times. For some other values of parameters (e.g., $\lambda = 6.0$) $\dot{\vartheta}$ is uniformly bigger than zero.

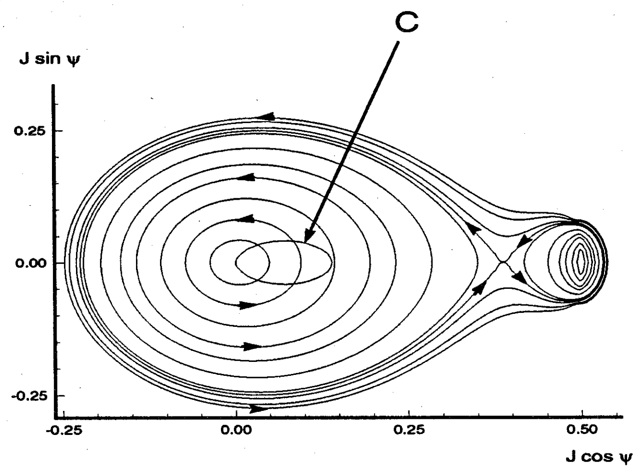

Figure 6.4: Curve on which $\dot{\vartheta}$ vanishes

Two-dimensional separatrices

We recall the general form of the unperturbed equations for particle paths in the $J-\psi-\vartheta$ coordinates

$$\begin{aligned} \dot{J} &= \frac{\partial H}{\partial \psi}(J,\psi), \\ \dot{\psi} &= -\frac{\partial H}{\partial J}(J,\psi), \\ \dot{\vartheta} &= h(J,\psi), \end{aligned} \tag{6.3.47}$$

where the explicit form of the unperturbed Hamiltonian $H(J,\psi)$ and the general form of $h_3(J,\psi)$ can be obtained from (6.2.39). Trajectories in the two dimensional separatrices are forward and backwards asymptotic to the normally hyperbolic invariant curve, denoted Γ_0, defined by

$$\Gamma_0 = \left\{(J,\psi,\vartheta) \,|\, J = J^h,\ \psi = \psi^h, \vartheta \in \mathbb{R}^1\right\},$$

where (J^h, ψ^h) denotes the hyperbolic fixed point of the $J - \psi$ component of the velocity field. If we denote the homoclinic trajectory of the $J - \psi$ component of the velocity field by $J^h(t), \psi^h(t)$. Then the orbits on the homoclinic manifold are given by

$$(J^h(t-t_0), \psi^h(t-t_0), \int_{t_0}^{t} h(J^h(\hat{t}-t_0), \psi^h(\hat{t}-t_0))d\hat{t}.$$

When $t \to \pm\infty$ we have

$$\left(J^h(t-t_0), \psi^h(t-t_0), \int_{t_0}^{t} h(J^h(\hat{t}-t_0), \psi^h(\hat{t}-t_0))d\hat{t}\right) \to \left(J^h, \psi^h, \vartheta(\pm\infty) - \vartheta(0)\right), \tag{6.3.48}$$

where we have used the fact that

$$\dot{\vartheta}(\hat{t}-t_0) = h(J^h(\hat{t}-t_0), \psi^h(\hat{t}-t_0)).$$

We define the *phase shift* of trajectories in the two-dimensional separatrice as follows

$$\Delta\vartheta = \vartheta(+\infty) - \vartheta(-\infty) = \int_{-\infty}^{\infty} h(J^h(\hat{t}), \psi^h(\hat{t}))d\hat{t}. \tag{6.3.49}$$

There are two distinct cases to consider that give rise to qualitatively different dynamics: $h(J^h, \psi^h) \neq 0$ and $h(J^h, \psi^h) = 0$.

$\boxed{h(J^h, \psi^h) \neq 0}$

In this case we see from (6.3.49) that the phase shift of trajectories in the two-dimensional separatrices is infinite. This indicates that the ϑ components of trajectories approach $\pm\infty$ when $t \to \pm\infty$ if

$$h(J^h, \psi^h) > 0,$$

and they approach $\pm\infty$ when $t \to \mp\infty$ if

$$h(J^h, \psi^h) < 0.$$

$\boxed{h(J^h, \psi^h) = 0}$

In this case the phase shift of a trajectory is finite, since the function under the integral sign in (6.3.49) decreases exponentially when $t \to \infty$. Therefore, if $\Delta\vartheta \neq 0$, every fixed point is conected to some other fixed point on Γ_0 through a heteroclinic orbit. If the phase shift is zero, every fixed point on Γ_0 is connected to itself by a homoclinic orbit.

6.4 Geometry and dynamics of invariant manifolds and particle paths for the perturbed velocity field

We will refer to the velocity field induced by the helical vortex filament as the *unperturbed velocity field.* In the analysis of the kinematics of the unperturbed velocity field induced by the helical vortex filament, we have shown that the flow is foliated by two dimensional invariant surfaces or manifolds, apart from isolated elliptic and hyperbolic one-dimensional invariant manifolds. These two-dimensional invariant manifolds are essentialy of two types: one-parameter families of invariant cylinders and manifolds homoclinic to normally hyperbolic invariant curves. When the velocity field is perturbed and the amplitude of the perturbation ϵ is small, for each of these invariant manifolds there is a global perturbation theory allowing us to analyze the effect of the perturbation on these invariant manifolds. In the case of cylinders, the special form of the velocity field in the $J - \psi - \vartheta$ coordinates allows us to use the classical KAM theory to show that certain types of invariant cylinders persist under the perturbation. In the case of homoclinic manifolds the perturbative theory is a Melnikov-type theory as developed in Wiggins [18] and chapter 2 (or Mezić and Wiggins [12]).

6.4.1 The persistence of two-dimensional invariant cylinders : KAM theory

Since the velocity field is periodic in t, we will study the fluid particle kinematics in the perturbed velocity field by studying the associated three-dimensional Poincaré map. Moreover, in studying the persistence of the cylinders the coordinates developed in chapter 2 (or Mezić and Wiggins [12]) and discussed in Sect. 6.3.2 are most appropriate. Applying this coordinate transformation to the perturbed vector field given in (6.2.39) transforms the perturbed velocity field to the following form

$$\begin{aligned} \dot{I} &= \epsilon F_0(I,\phi_1,t) + \mathcal{O}(\epsilon^2), \\ \dot{\phi}_1 &= \Omega_1(I) + \epsilon F_1(I,\phi_1,t) + \mathcal{O}(\epsilon^2), \\ \dot{\phi}_2 &= \Omega_2(I) + \epsilon F_2(I,\phi_1,t) + \mathcal{O}(\epsilon^2), \end{aligned} \tag{6.4.50}$$

where the $\mathcal{O}(\epsilon^2)$ are functions only of I, ϕ_1, and t. Explicit formulae for the functions $F_i(I,\phi_1,t)$ are given in Appendix 2. The velocity field is periodic in t with period $T = \frac{2\pi}{\omega}$. In chapter 2 (or Mezić and Wiggins [12]) the Poincaré map associated with (6.4.50) is constructed explicitly using regular perturbation theory and is shown to have the form

$$\begin{aligned} I &\mapsto I + \epsilon \widetilde{F}_0(I, \phi_1) + \mathcal{O}(\epsilon^2), \\ \phi_1 &\mapsto \phi_1 + 2\pi \frac{\Omega_1(I)}{\omega} + \epsilon \widetilde{F}_1(I, \phi_1) + \mathcal{O}(\epsilon^2), \\ \phi_2 &\mapsto \phi_2 + 2\pi \frac{\Omega_2(I)}{\omega} + \epsilon \widetilde{F}_2(I, \phi_1) + \mathcal{O}(\epsilon^2), \end{aligned} \tag{6.4.51}$$

where explicit formulae for $\widetilde{F}_i(I, \phi_1)$ in terms of $F_i(I, \phi_1, t)$ are given in Appendix 2. The important point in our discusion now is the form of (6.4.51). In particular, the $I - \phi_1$ component of (6.4.51) decouples from the ϕ_2 component. The $I - \phi_1$ component has the form of a two-dimensional area-preserving twist map, to which the standard KAM theory can be applied to determine the existence of invariant circles in the $I - \phi_1$ plane. In the full three-dimensional space these are then interpreted as invariant cylinders.

6.4.2 The effect of the perturbation on the two-dimensional homoclinic manifold: Melnikov's method

From the general persistence theory for normally hyperbolic invariant manifolds, the normally hyperbolic invariant curve and its two-dimensional stable and unstable manifolds persist under perturbation. However, the stable and unstable manifolds need not coincide. Indeed, they may intersect in an extremely complicated fashion and give rise to chaotic fluid particle motions. A Melnikov type method is described in chapter 2 (or Mezić and Wiggins [12]) for measuring the distance between these manifolds. The Melnikov function in this case is given by

$$M(t_0,\vartheta_0;\phi_0) = \int_{-\infty}^{+\infty} \Big(\tfrac{\partial H^0_{in}}{\partial \psi} \tfrac{\partial H^1_{in}}{\partial J}((J^h(t),\psi^h(t)),\omega t+\omega t_0) \\ + \tfrac{\partial H^0_{in}}{\partial J} \tfrac{\partial H^1_{in}}{\partial \psi}((J^h(t),\psi^h(t)),\omega t+\omega t_0) \Big)\, dt \tag{6.4.52}$$

where

$$\vartheta^h(t) \equiv \int_0^{t+t_0} h^0_{in}(J^h(s),\psi^h(s))ds + \vartheta_0,$$

and it does not depend on ϑ_0. We can-not calculate the Melnikov function explicitly because even the homoclinic trajectory in the unperturbed case is known only numerically. But, using the symmetry properties of the velocity field and the perturbation with respect to $\psi = 0$, we obtain the following form for the Melnikov function, choosing $\vartheta_0 = 0$:

$$M(t_0) = F(\lambda_0,\gamma,\omega)\cos(\omega t_0), \tag{6.4.53}$$

(see Appendix 3).

So, for a particular value of parameters of the problem for which $F(\lambda_0,\gamma,\omega) \neq 0$, the Melnikov function will have an infinite number of zeros which corespond to infinity of points at which the unstable and stable manifolds of the hyperbolic fixed point intersect transversally.

6.4.3 Poincaré maps

We calculated Poincaré maps for our flow using the velocity field (6.2.39) expressed in terms of Fourier series. This posed a difficulty around $R = 1$ as the terms in the Fourier series converge very slowly. Therefore, in a typical calculation we used 11 terms of Fourier series when a point was such that $R < 0.9$ or $R > 1.1$, and 23 terms otherwise. This caused the calculation time to be excessive. For that reason, we present Poincaré maps only for two sets of parameters. Still, these Poincaré maps are quite representative, as they correspond to two different phase portraits of the unperturbed motion presented in the bifurcation diagram.. In each of the two Poincaré maps, the largest chaotic zones are around the place where in the unperturbed phase portraits separatrices existed. This occurs because of the breakup of separatrices analyzed above.

Figure (6.5) represents a Poincaré map of the flow for $\lambda = 3.0, \gamma = 6.0, \epsilon = 0.5, \omega = 10.0$. We used such a large ω, as it reduced the time of computation. λ and γ are for this case in the zone **II** in the unperturbed bifurcation diagram. The largest chaotic zone is aruond the unperturbed separatrices, whose breakup for small ϵ can be predicted using the above described Melnikov theory.

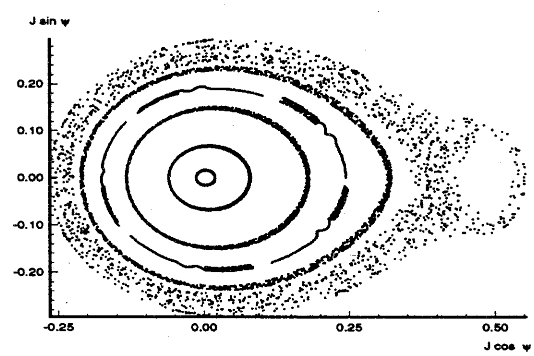

Figure 6.5: Poincaré map for the perturbed flow. $\lambda = 3.0, \gamma = 6.0, \epsilon = 0.5, \omega = 10.0$

The Poincaré map for the other value of parameters, $\lambda = 6.0, \gamma = 2.0, \epsilon = 0.1, \omega = 4.0$ (λ and γ are for this case in the zone **III** in the unperturbed bifurcation diagram) is presented in figure **??**. In that Poincaré map we see that there is a large chaotic region around the place where there were separatrices in the unperturbed phase portrait. That part of the plot is actually produced by a single particle starting at $J = 0.93, \psi = \vartheta = 0.0$.

6.5 Shear dispersion

In this section we want to consider the dispersion of a distribution of perfect tracer particles in the ϑ direction. The work in chapter 3 of this thesis (or Mezić and Wiggins [12], [13]) gives necessary and sufficient conditions for the dispersion to grow asymptotically in time like t^2. We will show how these conditions may be obtained in this flow. The geometrical structure of the flow developed thus far will play an important role in these considerations.

For ease of reference, we rewrite the velocity field given in (6.2.39),

$$
\begin{aligned}
\dot{J}_{in,out} &= \frac{\partial H^0_{in,out}}{\partial \psi}(J,\psi) + \epsilon \frac{\partial H^1_{in,out}}{\partial \psi}(J,\psi,\theta) + \mathcal{O}(\epsilon^2), \\
\dot{\psi}_{in,out} &= -\frac{\partial H^0_{in,out}}{\partial J}(J,\psi) - \epsilon \frac{\partial H^1_{in,out}}{\partial J}(J,\psi,\theta) + \mathcal{O}(\epsilon^2), \\
\dot{\vartheta}_{in,out} &= h^0_{in,out}(J,\psi) + \epsilon h^1_{in,out}(J,\psi,\theta) + \mathcal{O}(\epsilon^2), \\
\dot{\theta} &= \omega,
\end{aligned}
\tag{6.5.54}
$$

where we have rewritten (6.2.39) as a time independent velocity field in one higher dimension by including the phase of the time periodic strain field (θ) explicity as a dependent variable. $(J, \psi, \vartheta, \omega) \in A \times \mathbb{R} \times S^1$ denotes the domain of (6.5.54), where A is a subset of $\mathbb{R} \times S^1$. Up to this point, it has not been necessary for us to place any restrictions on the flow domain. However, some restriction on the domain of the $J - \psi$ component of the flow will be important for dispersion. $\phi_t(J, \psi, \theta)$ denote the flow generated by the $J - \psi - \omega$ component of (6.5.54).

We rewrite the ϑ component of (6.5.54) in integral equation form as follows

$$\vartheta(t) - \vartheta(0) = \int_0^t \left(h^0_{in,out} + \epsilon h^1_{in,out} + \mathcal{O}(\epsilon^2)\right)(\phi_\tau(J,\psi,\theta))\,d\tau,$$

or, for notational convenience (for which we also drop the subscripts "*in, out*")

$$\vartheta(t) - \vartheta(0) = \int_0^t \dot{\vartheta}\,(\phi_\tau(J,\psi,\theta))\,d\tau.$$

The mean square displacement or *dispersion* of the ϑ component of (6.5.54) of an ensemble of points in the flow is given by

$$D_\vartheta(t) \equiv \langle(\vartheta(t) - \vartheta(0) - \langle\vartheta(t) - \vartheta(0)\rangle)^2\rangle,$$

where the average indicated by the angle brackets is given by

$$\langle\cdot\rangle \equiv \int_{A\times S^1} (\cdot)p(J,\psi,\theta)d\mu,$$

$p(J,\psi,\theta)$ denotes the initial distribution of points (assumed to be bounded and integrable on $A \times S^1$) and $d\mu$ denotes the measure of "volume element" on $A \times S^1$.

We are interested in determining the asymptotic behavior of the dispersion. This can be deduced from the following calculations:

$$\begin{aligned}
\lim_{t\to\infty} \frac{D_\vartheta(t)}{t^2} &= \lim_{t\to\infty} \langle\left(\frac{1}{t}\int_0^t \dot{\vartheta}\,(\phi_\tau(J,\psi,\theta))\,d\tau - \langle\frac{1}{t}\int_0^t \dot{\vartheta}\,(\phi_\tau(J,\psi,\theta))\,d\tau\rangle\right)^2\rangle,\\
&= \langle\left(\lim_{t\to\infty}\frac{1}{t}\int_0^t \dot{\vartheta}\,(\phi_\tau(J,\psi,\theta))\,d\tau - \langle\lim_{t\to\infty}\frac{1}{t}\int_0^t \dot{\vartheta}\,(\phi_\tau(J,\psi,\theta))\,d\tau\rangle\right)^2\rangle,\\
&= \langle\left(\dot{\vartheta}^*(J,\psi,\theta) - \langle\dot{\vartheta}^*(J,\psi,\theta)\rangle\right)^2\rangle \equiv a.
\end{aligned}$$

The mathematical manipulations in these calculations are justified as follows:

1. The passage from the first to the second line is justified by the fact that the function $\dot{\vartheta}$ is bounded and integrable on $A \times S^1$. This will be true if A is a bounded subset of $\mathbb{R} \times S^1$ that is also an invariant subset for the $J - \psi$ component of (6.5.54). For ϵ sufficiently small such an invariant subset A can always be found as a result of the persistence of KAM tori, which form the boundary of invariant sets. In the original $x - y - z$ physical coordinates these give rise to infinitely long helically twisted cylinders.

2. In the second line the limit

$$\lim_{t \to \infty} \frac{1}{t} \int_0^t \dot{\vartheta}\left(\phi_\tau(J, \psi, \theta)\right) d\tau \equiv \dot{\vartheta}^*(J, \psi, \theta)$$

exists for all points in $A \times S^1$ by Birkhoff's ergodic theorem (see [1]), *with the possible exception of a set of μ-measure zero.* Birkhoff's ergodic theorem applies since the flow is incompressible and A is bounded. This limit is the time average of the function $\dot{\vartheta}$ along the fluid particle trajectory that starts at the point (J, ψ, θ). Moreover, Birkhoff's ergodic theorem also guarantees that this limit is integrable. This, together with the boundedness of $\dot{\vartheta}$, implies that the quantity a defined above is finite, and if it is nonzero, we can conclude that the dispersion of the ensemble of particles in the ϑ direction behaves asymptotically like t^2.

The nature of the coefficient a gives some insight into the dynamical mechanism giving rise to t^2 dispersion. It is easy to see that since the expression inside the angle brackets defining a is nonnegative, $a = 0$ if and only if $\dot{\vartheta}^* = \langle \dot{\vartheta}^* \rangle$ on the support of p, i.e., on the set of points for which $p(J, \psi, \theta)$ is *nonzero*, with the possible exclusion of sets of measure zero. However, $\langle\dot{\vartheta}^*\rangle$ is a constant. Therefore, we can make the following conclusion. Let $C \subset A \times S^1$ denote the support of $p(J,\psi,\theta)$. Then, if $\dot{\vartheta}^*(J,\psi,\theta)$ is not constant almost everywhere on C, $D_\vartheta(t) \sim t^2$ as $t \to \infty$. Now assume that the flow due to the $J-\psi-\theta$ component of (6.5.54) restricted to $A \times S^1$ is ergodic. Then $\dot{\vartheta}^* = \langle\dot{\vartheta}^*\rangle = \langle\dot{\vartheta}\rangle$ almost everywhere. Therefore, $a = 0$. Hence, a necessary condition for t^2 dispersion is the non-ergodicity of the flow.

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6.6 Appendix 1

In this appendix we show the details of the analysis of the fixed points of the unperturbed velocity field. We shall present the analysis only for the case $R < 1$, but the analysis for $R > 1$ follows a similar route. The velocity field for $R < 1$ is given by

$$\begin{aligned} \dot{R} &= \lambda S_{in}(R, \psi, \lambda) \\ \dot{\psi} &= -\frac{1}{2}\lambda + \gamma \frac{\lambda}{(1+\lambda^2)^{1/2}} + \frac{1+R^2\lambda^2}{R^2} C_{in}(R, \psi, \lambda), \\ \dot{\vartheta} &= \frac{1}{2\lambda} + \frac{1-R^2}{R^2} C_{in}(R, \psi, \lambda). \end{aligned} \tag{6.6.55}$$

As this velocity field involves functions S_{in} and C_{in} which are represented in terms of Fourier series, it is not completely amenable to analytic analysis. Still, something can be said about the behaviour of C_{in} and S_{in}. Let us first note that we shall use the following conjecture:

Conjecture 6.6.1 *The sequence of coefficients in Fourier series of* C_{in} *,* $\{a_m\}$*, where*

$$a_m = mK'_m(\lambda m)\, I_m(R\lambda m),$$

is monotonically strictly increasing, i.e.,

$$\Delta a_m = a_{m+1} - a_m > 0, \quad \forall m \in \mathbf{N}.$$

The sequence of coefficients in Fourier series of S_{in}*,* $\{b_m\}$*, where*

$$b_m = mK'_m(\lambda m) I'_m(R\lambda m),$$

is strictly convex, i.e.,

$$\Delta^2 b_m = b_m - 2b_{m+1} + b_{m+2} > 0, \quad \forall m \in \mathbf{N}. \tag{6.6.56}$$

We checked this only numerically, by calculating the functions $\Delta a_m, \Delta^2 b_m$. The conjecture appears to be true for $0.2 < \lambda < 10$ which is also the range in which we studied bifurcations numerically. We shall continue the analysis under the assumption that the conjecture holds. Using Abel's transformation familiar from the analysis of Fourier series, and the above conjecture, one can show that S_{in} has only two zeros at $\psi = 0$ and $\psi = \pi$ (the fact that the zeros are there is obvious from the Fourier representation of S_{in}, but the fact that these are the only ones is not). Our proof follows that given by [3] in the similar context. We shall need the following well-known lemma:

Lemma 6.6.1 (Abel's Transformation)

$$\sum_{k=0}^{n} u_k v_k = \sum_{k=0}^{n-1} (u_k - u_{k+1}) V_k + u_n V_n,$$

where

$$V_n = \sum_{k=0}^{n} v_k.$$

Proof: This is just an easy rearangement of terms which can be checked by direct computation. □

Theorem 6.6.1 *Suppose*

$$\sum_{i=1}^{\infty} a_j \sin jx,$$

Is a Fourier series for a function $f(x)$. Suppose further that $a_j \to 0$ as $j \to \infty$ and that the sequence a_j is strictly convex, i.e.,

$$\Delta^2 a_j = a_j - 2a_{j+1} + a_{j+2} > 0, \quad \forall j.$$

Then $f(x) > 0$ for $0 < x < \pi$ and $f(x) < 0$ for $\pi < x < 2\pi$.

Proof: Let

$$S_n(x) = \sum_{i=1}^{n} a_j \sin jx.$$

Using Abel's transformation, we obtain

$$S_n = \sum_{k=0}^{n-1} (a_k - a_{k+1})\tilde{D}_k + a_n\tilde{D}_n,$$

where $\tilde{D}_k$ is a conjugate Dirichlet kernel of order k. Using Abel's transformation once again, we obtain

$$S_n = \sum_{k=0}^{n-2} (\Delta a_k - \Delta a_{k+1}) \sum_{i=0}^{k} \tilde{D}_i + \Delta a_{n-1} \sum_{i=0}^{n-1} \tilde{D}_i + a_n\tilde{D}_n,$$

where $\Delta a_j = a_j - a_{j+1}$. Note that

$$\tilde{K}_k = \frac{1}{k+1} \sum_{i=0}^{k} \tilde{D}_i,$$

is usually called the conjugate Fejér kernel. Using this, we have

$$S_n = \sum_{k=0}^{n-2} (\Delta^2 a_k)(k+1)\tilde{K}_k + \Delta a_{n-1} n \tilde{K}_{n-1} + a_n\tilde{D}_n.$$

Since a_n is convex, $n\Delta a_n \to 0$ as $n \to \infty$ (see [3], pg. 5). Also, by assumption $a_n \to 0$ as $n \to \infty$. Using this and expressions for $\tilde{K}_j$ and $\tilde{D}_j$, the last two terms go to zero when $n \to \infty$, except possibly at $x = 0$. Therefore

$$S_n = \sum_{k=0}^{\infty} (\Delta^2 a_k)(k+1)\tilde{K}_k.$$

But $\Delta^2 a_k$ is strictly positive by assumption, and $\tilde{K}_k(x) > 0$ for $0 < x < \pi$, $\tilde{K}_k(x) < 0$ for $\pi < x < 2\pi$ so we are done. □

The conjecture (6.6.1) was used because it is much easier numerically to check for the requirements on a_m and b_m given in (6.6.1), then to compute zeros numerically.

6.7 Appendix 2

Here we give the formulae for F_i and $\widetilde{F}_i$ needed in section 4.1

$$\begin{aligned}
F_0 &= \frac{\partial I}{\partial J}\frac{\partial H^1_{in,out}}{\partial \psi}(J,\psi,t) - \frac{\partial I}{\partial \psi}\frac{\partial H^1_{in,out}}{\partial J}(J,\psi,t),\\
F_1 &= \frac{\partial \phi_1}{\partial J}\frac{\partial H^1_{in,out}}{\partial \psi}(J,\psi,t) - \frac{\partial \phi_1}{\partial \psi}\frac{\partial H^1_{in,out}}{\partial J}(J,\psi,t),\\
F_2 &= \frac{\partial \phi_2}{\partial J}\frac{\partial H^1_{in,out}}{\partial \psi}(J,\psi,t) - \frac{\partial \phi_2}{\partial \psi}\frac{\partial H^1_{in,out}}{\partial J}(J,\psi,t) + h^1_{in,out}(J,\psi,t).
\end{aligned} \tag{6.7.57}$$

Further, we have

$$\widetilde{F}_0(I^0,\phi_1^0,\phi_2^0) = \int_0^T F_0(I^0,\Omega_1(I^0)t+\phi_1^0,\Omega_2(I^0)t+\phi_2^0,t)dt,$$

$$\widetilde{F}_1(I^0,\phi_1^0,\phi_2^0) = \tfrac{\partial\Omega_1}{\partial I}|_{I=I^0}\int_0^T\int_0^t F_0(I^0,\Omega_1(I^0)\xi+\phi_1^0,\Omega_2(I^0)\xi+\phi_2^0,\xi)d\xi dt$$

$$+\int_0^T F_1(I^0,\Omega_1(I^0)t+\phi_1^0,\Omega_2(I^0)t+\phi_2^0,t)dt. \tag{6.7.58}$$

$$\widetilde{F}_2(I^0,\phi_1^0,\phi_2^0) = \tfrac{\partial\Omega_2}{\partial I}|_{I=I^0}\int_0^T\int_0^t F_0(I^0,\Omega_1(I^0)\xi+\phi_1^0,\Omega_2(I^0)\xi+\phi_2^0,\xi)d\xi dt$$

$$+\int_0^T F_2(I^0,\Omega_1(I^0)t+\phi_1^0,\Omega_2(I^0)t+\phi_2^0,t)dt.$$

(see chapter 2).

6.8 Appendix 3

In this appendix we show how the expression for the Melnikov function accepts the form (6.4.53). This is due to the reflectional symmetry of the Hamiltonian part of the flow in $J-\psi$ coordinates. Recall that the Melnikov function is given by

$$M(t_0) = \int_{-\infty}^{+\infty}\Big(\tfrac{\partial H^0_{in}}{\partial\psi}\tfrac{\partial H^1_{in}}{\partial J}((J^h(t),\psi^h(t)),\omega t+\omega t_0)$$

$$+\tfrac{\partial H^0_{in}}{\partial J}\tfrac{\partial H^1_{in}}{\partial\psi}((J^h(t),\psi^h(t)),\omega t+\omega t_0)\Big)\,dt, \tag{6.8.59}$$

where the expressions for the partial derivatives of Hamiltonian functions are given in 2.5. From the expressions for the unperturbed J and ψ components of the velocity,

$$(J^0(t), \psi^0(t)) = (J^0(-t), -\psi^0(-t)), \qquad (6.8.60)$$

where the superscript "0" denotes the unperturbed orbit. We can expand (6.2.35) for small ϵ, up to $\mathcal{O}(\epsilon)$ terms. Then, the only time-dependent term in the above expression for the Melnikov function is

$$\sin(\omega t + \omega t_0) = \sin\omega t \cos\omega t_0 + \cos\omega t \sin\omega t_0.$$

Also, note that S_{in} is odd in ψ, while C_{in} even in ψ. Now, using these observations and (6.8.60), we find that, in the $\mathcal{O}(\epsilon)$ expression for $\dot{J}$, all of the terms multiplying $\sin\omega t$, and the unperturbed terms are odd in t. Moreover, analogous terms in $\dot{\psi}$ are even in t. This means that the part of the Melnikov function multiplying $\sin\omega t_0$ is zero, and therefore the Melnikov function is of the form $F(\lambda_0, \gamma, \omega) cos\omega t_0$. Actually, the Melnikov function can be explicitly written as

$$\begin{aligned} M(t_0) = {} & \cos\omega t_0 \int_{-\infty}^{+\infty} \Bigg(\lambda_0 \left[\sqrt{2J^h(t)} S_{in}(J^h(t), \psi^h(t), \lambda_0)\right] \qquad (6.8.61) \\ & \left[-\frac{3\lambda_0}{2\omega} - \frac{3\gamma(\lambda_0^3 - \lambda_0)}{\omega\sqrt{1+\lambda_0^2}} + \frac{6\lambda_0^2}{\omega} C_{in}(J^h(t), \psi^h(t), \lambda_0) + \right. \\ & \left. \frac{3\lambda_0(1 + 2J^h(t)\lambda_0^2)}{2J^h(t)} \frac{\partial C_{in}}{\partial \lambda}(J^h(t), \psi^h(t), \lambda_0) \right] \\ & + \left[-\frac{1}{2}\lambda_0 + \frac{1 + 2J^h(t)\lambda_0^2}{2J^h(t)} C_{in}(J^h(t), \psi^h(t), \lambda_0) \right] \\ & \left[\sqrt{2J^h(t)} \Big(\frac{4\lambda_0}{\omega} S_{in}(J^h(t), \psi^h(t), \lambda_0) \right. \\ & \left. \left. + \frac{3\lambda_0^2}{\omega} \frac{\partial S_{in}}{\partial \lambda}(J^h(t), \psi^h(t), \lambda_0) \right] \right) sin\omega t dt. \end{aligned}$$