0.1. Mixing and Transport in Dynamical Systems[1]

Mixing is a widely observed phenomenon in nature. Among other areas, it is well known to occur in fluid mechanics, biology, chemistry, atmospheric science and celestial mechanics. Because of its complexity, there is no single accepted approach or definition for this phenomenon. Physically speaking, mixing is a process that tends to reduce nonuniformities or gradients in composition, properties, or temperature of material in bulk (definition from Uhl and Gray [9]). Geometrically speaking, mixing is a reduction of length scales accomplished by stretching and folding of designated material lines or surfaces. (definition from Ottino [6]). Mathematically speaking, mixing is a concept from ergodic theory that roughly requires a transformation to distribute measurable sets of initial conditions fairly evenly in the phase space (definition from de Vries [10]; see more precise definition below). Despite the different language and tools used in different disciplines, describing, understanding, predicting and influencing mixing is one of the most important objectives in various fields of applied science.

The systematic mathematical treatment of mixing is not an old subject and has been developed mainly over the past four decades. The reason for this is twofold; first, the underlying physical phenomenon was believed to be hopelessly complicated for a long time, and hence experimental description and statistical assessment was the preferred tool over analysis. Second, the modern concepts of dynamical systems, ergodic theory and probability that can successfully bear on mixing problems were not available before the 1950's.

These notes survey the most important tools of applied mathematics that can be used to study physical mixing problems. The emphasis is on fluid mixing, the approach is primarily geometric and applied, and the overall level of the text is introductory. The subject itself is far from being well established, as one might guess from the number of textbooks having "mixing" in their title. It is therefore our hope that the reader, having seen the basic ideas and available tools, will synthesize the material and make new contributions to this dynamically emerging and exciting field.

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1. Main physical ideas

1.1. Fluid mixing

The most easily illustrated example of mixing is "mechanical mixing" in fluids, where an initial, coherent blob of *tracers* extends over a larger spatial domain. This can be viewed as the result of three main factors:

1. *Advection:* The tracer set is viewed as continuum of material points which are transported under the action of the velocity field $\mathbf{v}(\mathbf{x},t)$ in the space of $\mathbf{x}$ coordinates.. In this process, the initial tracer set is stretched and folded into streaks accumulating on each other (see Fig. 1.1). We consider the tracer well-mixed if the average width of the layers, the *striation thickness*[1] d_s is small enough. Needless to say, this is only relevant measure of advective mixing if the blob remains confined to a bounded region, a requirement that emerges in all different approaches to mixing.

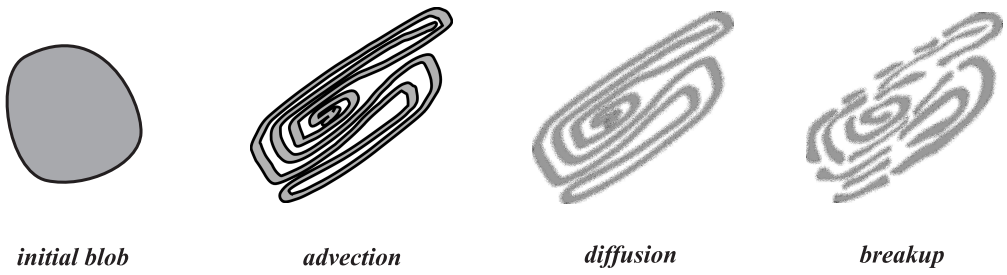

Figure 1.1: The three main components of fluid mixing.

The concept of advective mixing relies on the basic continuum hypothesis that the macroscopic properties of a fluid can also be defined for its arbitrarily small subsets. This enables one to define velocity, temperature, pressure for *fluid particles,* i.e., limits of volumes shrinking to a point, as the limit of averages

[1] If d_T denotes the width of a typical tracer treak, and d_A is the average length of ambient fluid streaks, then the striation thickness can be defined as $d_s = \frac{1}{2}(d_T + d_A)$.

over molecules contained in a small volume. This fluid particles are then tagged forever by the initial value of some *nondiffusive scalar* c whose mixing is of interest. However, one has to remember that a fluid particle does not consist of the same set of molecules while it travels in space. As a result, purely advective mixing of nondiffusive tracers is an idealization.

2. *Diffusion:* The interchange of molecules between fluid particles can be taken into account by tracing the evolution of diffusive properties in the fluid. Tracking the mixing of diffusive quantities, e.g., temperature, one does not tag individual fluid particles any more with a constant material property. Rather, one follows the evolution of the concentration $c(x,t)$ of an initial blob. If this *diffusive scalar* follows *Fick's diffusion law*
$$\frac{\partial c}{\partial t} = \mathcal{D}\nabla^2 c,$$
then a simple dimension analysis suggest that diffusion becomes important on time scales of the order of $d_s^2/\mathcal{D}$ (Here d_s is the striation thickness introduced above and $\mathcal{D}$ is the diffusivity coefficient). Below these time scales mixing is dominated by advection, and diffusion is only seen to create a "fuzzy" interface between the tracer and the ambient fluid (see Fig. 1.1). For larger time scales, however, the global characteristics of mixing become uncorrelated with pure advection. In that case the mixing of c is determined by the *advection-diffusion equation*
$$\frac{Dc}{Dt} \equiv \frac{\partial c}{\partial t} + \nabla c \cdot \mathbf{v} = \mathcal{D}\nabla^2 c,$$
in which the advection and diffusion terms are comparable.

3. *Breakup:* In our discussion of advection and diffusion, we have assumed that c is *passive scalar,* i.e., it does *not* affect the underlying velocity field $\mathbf{v}(\mathbf{x},t)$. In the present context this means that the two fluids have been assumed perfectly *miscible,* producing thinner and thinner streaks as time increases. In reality, there is an end to this process. Below a certain striation thickness, the fluids become immiscible and the tracer blob breaks up into smaller fragments (see Fig. 1.1). The resulting new interfaces modify the velocity field due to surface tension, and hence the observed quantity, c, becomes an *active scalar* (see, e.g., Aref and Tryggvason [3]).

We shall primarily be concerned with the advective mixing of passive scalars which is the most accessible to geometric methods. This implies that our discussion is primarily aimed at fluids. In contrast, gases typically admit high molecular diffusion and the dominance of advection is lost in very short times.

1.2. The basic equations of fluid mechanics

Since these notes have an emphasis on mixing in fluid mechanics, it is appropriate here to recollect the fundamental equations governing the dynamics of fluid. It also

gives us an opportunity to fix the basics of our notation.

1.2.1. The Navier-Stokes equations and a word on notation

The velocity field associated with a moving fluid is of the form

$$\mathbf{v}(\mathbf{x},t) = (u(\mathbf{x},t),v(\mathbf{x},t),w(\mathbf{x},t)), \quad \mathbf{x} = (x,y,z),$$

where $\mathbf{x}$ denotes the location of a material element of the fluid or a *fluid particle and* t refers to the time. For two-dimensional flows it will be understood that $\mathbf{v}$ and $\mathbf{x}$ have only two components. The first basic set of equations expresses incompressibility, and is usually referred to as the mass conservation equations:

$$\nabla \cdot \mathbf{v} = 0.$$

The second set of equations is the *Navier-Stokes* (or *momentum*) *equation*, given by

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{v} + \mathbf{f}, \tag{1.1}$$

where $\rho(\mathbf{x})$ is the density, $p(\mathbf{x},t)$ is the pressure, $\mathbf{f}(\mathbf{x},t)$ is the resultant of the volume forces per unit mass, and ν is the kinematic viscosity. For vanishing viscosity, i.e., for an *inviscid* fluid, the Navier-Stokes equation is called *Euler's equation.*

While, for the most part, we shall use the usual notational convention for the operator $\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$, we will occasionally also use the modern notation from dynamical systems, where appropriate. For instance, in terms of the accepted notation in dynamical systems, the Navier-Stokes and the conservation of mass equations could be rewritten as

$$\begin{aligned} D_t\mathbf{v} + (D_{\mathbf{x}}\mathbf{v})\,\mathbf{v} &= -\frac{1}{\rho}D_{\mathbf{x}}p + \nu\Delta\mathbf{v} + \mathbf{f}, \\ \operatorname{div}\mathbf{v} &= 0, \end{aligned}$$

with D referring to differentiation with respect to its subscript, and with the dimension of the outcome depending on the context. While many results in geometric mixing theory are easier to drive or explain in this alternative notation, the reader more used to the classical notation of fluid mechanics may find it confusing initially. For this reason we enclose a table below that shows the most frequently used operations in both notations[2]:

[2]Of course, in the literature one often sees a mixture of the two types of nomenclature.

Equivalent notation		
	Fluid mechanics	Dynamical systems
Jacobian	$\nabla \mathbf{v}$	$D_{\mathbf{x}} \mathbf{v}$
partial time-derivative	$\frac{\partial \mathbf{v}}{\partial t}$	$D_t \mathbf{v}$ or $\dot{\mathbf{v}}$
gradient of scalar	∇s	$D_{\mathbf{x}} s$ or $\operatorname{grad} s$
total (material) derivative	$\frac{D}{Dt} s = \frac{\partial s}{\partial t} + \mathbf{v} \cdot \nabla s$	$\frac{d}{dt} s = D_t s + D_{\mathbf{x}} s \cdot \mathbf{v}$
divergence	$\nabla \cdot \mathbf{v}$	$\operatorname{div} \mathbf{v}$
Laplacian	$\nabla^2 \mathbf{v}$	$\Delta \mathbf{v}$
curl	$\nabla \times \mathbf{v}$	$\operatorname{curl} \mathbf{v}$
Jacobian acting on a vector	$\mathbf{v} \cdot \nabla \mathbf{v}$	$(D_{\mathbf{x}} \mathbf{v})\, \mathbf{v}$

1.2.2. The vorticity equations

A quantity of central important is the curl of the velocity field, i.e., the *vorticity* field $\boldsymbol{\omega} = \nabla \times \mathbf{v}$. Vorticity characterizes the amount of local rotation in the fluid; in particular, at any point the vorticity vector is twice the local angular velocity associated with the fluid element. We note that locally circular motion of fluid elements by itself does not create vorticity in the fluid. Nonzero vorticity indicates change in orientation, i.e., rigid body rotation for fluid elements.

Taking the curl of both sides of the Navier-Stokes equation (1.1), and using $\nabla \cdot \mathbf{v} = 0$ and $\nabla \cdot \boldsymbol{\omega} = 0$, one obtains

$$\frac{\partial \boldsymbol{\omega}}{\partial t} = -\mathbf{v} \cdot \nabla \boldsymbol{\omega} + \boldsymbol{\omega} \cdot \nabla \mathbf{v} + \nu \nabla^2 \boldsymbol{\omega} + \nabla \times \mathbf{f}.$$

For potential forces $\nabla \times \mathbf{f} = \nabla \times \nabla U = 0$, the above equation can be rewritten as the *vorticity equation*

$$\frac{D\boldsymbol{\omega}}{Dt} = \boldsymbol{\omega} \cdot \nabla \mathbf{v} + \nu \nabla^2 \boldsymbol{\omega}, \tag{1.2}$$

where D/Dt refers to the material derivative (cf. the table on notation above). For two-dimensional, inviscid flows, we therefore have

$$\frac{D\boldsymbol{\omega}}{Dt} = 0, \tag{1.3}$$

since $\boldsymbol{\omega} \cdot \nabla \mathbf{v} = (D_{\mathbf{x}} \mathbf{v})\, \boldsymbol{\omega}$, and $\boldsymbol{\omega}$ lies in the kernel of the operator $D_{\mathbf{x}} \mathbf{v}$. In other words, in two-dimensional inviscid flows $\boldsymbol{\omega}$ is conserved along fluid particle motions. A similar result hold for three-dimensional inviscid flows with circular symmetry.

1.3. Applicability of dynamical systems to fluid mixing

The modern theory of dynamical systems, the study deterministic evolutionary processes, has a strong geometric flavor. One of its most basic concepts, the idea of a *flow,* gives a natural geometric tool to study the evolution of sets of initial conditions in phase space. For this reason the advective component of *laminar mixing*, i.e., mixing in

a velocity field $\mathbf{v}(\mathbf{x}, t)$ with known time-dependence is accessible to dynamical systems methods, as we shall see below. The structures identified in laminar mixing also suggest paradigms for *turbulent mixing,* i.e., mixing induced by a velocity field with random time dependence. In fact, mixing between isolated coherent structures and their surroundings in a turbulent flow appear to follow the geometric templates identified for laminar mixing.

While dynamical systems theory has significantly changed the way mixing is viewed in applied science, there are still limitations of its applicability to "real-life" problems.

- Dynamical systems theory assumes that the velocity field $\mathbf{v}(\mathbf{x}, t)$ is at ones disposal at arbitrary $\mathbf{x}$ and t. In reality, $\mathbf{v}$ is typically known experimentally or numerically, i.e., at discrete spatial and temporal locations, and on a *finite* time interval. At the same time, the most important concepts in dynamical systems, such as attractors, invariant manifolds, hyperbolicity, are defined for infinite time intervals.

- There exists a conceptual difference between the classical theory of dynamical systems, focused primarily on asymptotic behavior, and engineering applications, where one typically wants to accelerate mixing on short time scales.

- Inspired by classical mechanics, many dynamical systems results have been developed for systems that are small perturbations of an *integrable* one. While in rigid body dynamics near-integrable systems are often good models for a physical phenomenon (e.g., planetary motion), recent results indicate that two- and three-dimensional integrable fluid flows are typically unstable: Their small perturbations will grow rapidly in time (see, e.g., Lifshitz and Hameiri [5], Friedlander and Vishik [4], and the references cited in these papers). This questions the relevance of dynamical systems results obtained for small, bounded perturbations of steady flows. While an abundance of such results exists in the literature, one has to be aware of their limited validity in time.

In these notes we first survey the most important classical results of dynamical systems pertaining to mixing. In addition, we discuss recent developments that enable the theory to bear on real-life problems. These developments include techniques for aperiodic numerical or experimental velocity fields that are only known for a finite time, and are far from integrable.

2. Geometric concepts

2.1. Phase space and trajectories

Assuming that a velocity field $\mathbf{v}$ is given, the equation governing the motion of fluid particles is

$$\dot{\mathbf{x}} = \mathbf{v}(\mathbf{x}, t), \tag{2.1}$$

where $\mathbf{x} \in X$, with X denoting either $\mathbb{R}^2$ or $\mathbb{R}^3$, and t denotes the time. The set X is typically called the *phase space,* while its product with the time axis, $X \times \mathbb{R}$ is called the *extended phase space.*

By fundamental results from the theory of ordinary differential equations, any initial location $\mathbf{x}_0$ and initial time t_0, the above equation admits a unique solution $\mathbf{x}(t; t_0, \mathbf{x}_0)$ provided that $\mathbf{v}$ is a differentiable function of $\mathbf{x}$ and a continuous function of t.[1] While the solution does not automatically exist for all times, we shall assume that it makes sense to write $\mathbf{x}(t; t_0, \mathbf{x}_0)$ for any t. This is certainly the case if the fluid motion is known to be bounded a priori (see, e.g., Arnold [2]). By classic results, the solution $\mathbf{x}(t; t_0, \mathbf{x}_0)$ is also known to be as many times continuously differentiable in its arguments as the velocity field $\mathbf{v}$.

When visualized in the phase space X, a solution $\mathbf{x}(t; t_0, \mathbf{x}_0)$ appears as a curve which is parametrized with t. This curve, the set of positions occupied by the particle as time increases, is called an *pathline, particle path*, or *orbit*. In general, a pathline can intersect itself; an intersection simply means that the fluid particle crosses at the same physical point at different times. However, pathlines cannot intersect if the right-hand side of (2.1) has no explicit time dependence, i.e., we have a *steady* velocity field $\mathbf{v}(\mathbf{x})$. In such a case it is easy to verify that

$$\mathbf{x}(t + \tau; t_0 + \tau, \mathbf{x}_0) \equiv \mathbf{x}(t; t_0, \mathbf{x}_0) \tag{2.2}$$

for any choice of τ, i.e., the evolution of the solution is independent of the initial time chosen. As a result, orbits in the phase space cannot intersect, since that would violate their uniqueness. To eliminate intersections in the unsteady case, one can also visualize solutions in the extended phase space $X \times \mathbb{R}$, in which case the corresponding curve, shown in Fig. 2.1, is called a *trajectory.* One can also think of trajectories as orbits for the extended, time-independent velocity field $\dot{\mathbf{x}} = \mathbf{v}(\mathbf{x}, s)$, $\dot{s} = 1$ on the phase space $X \times \mathbb{R}$.

[1] In fact, it is enough if $\mathbf{v}(\mathbf{x},t)$ is *locally Lipschitz* near $(\mathbf{x}_0,t_0)$ (see, e.g., Arnold [2]).

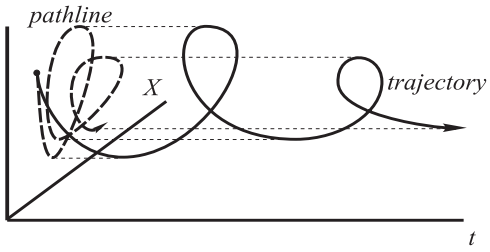

Figure 2.1: Pathline in the phase space X, and the corresponding trajectory in the extended phase space $X \times \mathbb{R}$.

Exercise 2.1.1. Verify the identity (2.2).

2.2. Streamlines and streaklines

There are two other techniques to visualize the fluid flow associated with (2.1). First, for any fixed t one can look for lines that are tangent to the velocity field at every point. Such curves are called *streamlines*, and they satisfy the differential equation

$$\frac{d}{ds}\mathbf{x}(s) = \mathbf{v}(\mathbf{x}(s), t),$$

where s is a parameter along individual curves. For steady velocity fields, streamlines coincide with orbits as they both satisfy the same differential equation. For unsteady velocity fields, streamlines are time-dependent and generally differ from particle paths (see Fig. 2.2).

The second technique of flow visualization is the experimentally preferred one, obtained by releasing dye into the flow at a fixed point. A *streakline* through $\mathbf{x}_0$ is the defined as the curve spanned by all fluid particles released from $\mathbf{x}_0$ on the time interval $[t_0, t_1]$. Classic examples of streaklines include the line of smoke emanating from the tip of a cigar or a chimney. Again, for steady velocity fields streaklines coincide with streamlines and pathlines, but for unsteady flows they are generally all different objects.

Exercise 2.2.1. Find expressions for the trajectories, streamlines and pathlines associated with the velocity field $\mathbf{v} = \mathbf{x} + t$.

2.3. Time-t maps, flows, and Poincaré maps

A convenient way to describe the evolution of initial conditions is through the map

$$\mathbf{F}_{t_0}^{t} : \mathbf{x}_0 \mapsto \mathbf{x}(t; t_0, \mathbf{x}_0),$$

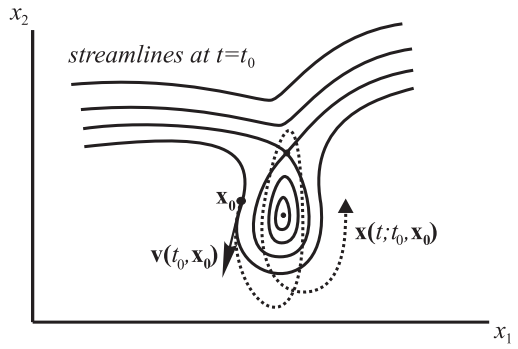

Figure 2.2: Streamlines and pathlines for an unsteady flow.

that relates initial particle positions at time t_0 to their later location at time t. Clearly, we have

$$\mathbf{F}_{t_0}^{t_0} \equiv I,$$

where I denotes the identity map. The action of $\mathbf{F}_{t_0}^{t}$ on an initial "blob" is shown in Fig. 2.3 in the extended phase space. By the properties of the solution $x(t; t_0, \mathbf{x}_0)$,

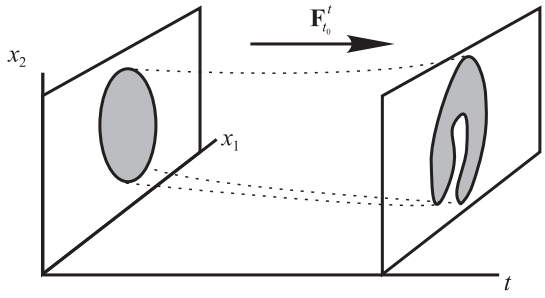

Figure 2.3: The map $F_{t_0}^{t}$ in the extended phase space.

the mapping $\mathbf{F}_{t_0}^{t}$ is well-defined, differentiable, and one-to-one with a differentiable inverse

$$\left(\mathbf{F}_{t_0}^{t}\right)^{-1} = \mathbf{F}_{t}^{t_0},$$

i.e., it is a *diffeomorphism*. In fact, $\mathbf{F}_{t_0}^{t}$ is a family of mappings, depending smoothly on the parameters t and t_0. By uniqueness of solutions, it also satisfies

$$\mathbf{F}_{t_0}^{t} \circ \mathbf{F}_{\tau}^{t_0} = \mathbf{F}_{\tau}^{t},$$

where $\circ$ denotes the composition of two maps. To simplify notation, we may fix the initial time $t_0 \equiv 0$, and define the *time-t map* as

$$\mathbf{F}^t \equiv \mathbf{F}_0^t,$$

which will then describe evolution of particles with respect to the fixed initial time $t = 0$.

The time-t map has additional properties in the case where the vector field $\mathbf{v}$ is steady. Namely, in such a case we have

$$\mathbf{F}^{t+\tau} = \mathbf{F}^t \circ \mathbf{F}^\tau \tag{2.3}$$

for any choice of t and τ. Together with this last property, $\mathbf{F}^t$ satisfies the definition of a *flow:* a one-parameter family of diffeomorphisms which satisfy the group property (2.3).

For a flow, we can fix a time $T > 0$ and track the evolution of particles at time $T, 2T, 3T, \ldots$ by applying the iterates of $\mathbf{F}^T$, i.e., $\left[\mathbf{F}^T\right]^2 = \mathbf{F}^{2T}, \left[\mathbf{F}^T\right]^3 = \mathbf{F}^{3T}, \ldots$. Such an iterated map or *discrete dynamical system* provides us with a stroboscopic picture of the fluid motion, and, in many cases, simplifies the geometric study of the motions considerably, since one only has to keep track of a single map $\mathbf{F}^T$, often called the *advance-T mapping*. This mapping is also well-defined for T-periodic unsteady velocity fields, i.e., for the case where $\mathbf{v}(\mathbf{x}, t) = \mathbf{v}(\mathbf{x}, t + T)$ for all $\mathbf{x}$ and t. Intuitively, this should be clear since for such periodic velocity fields the evolution rule determining fluid particle motions repeats itself periodically in time.

Exercise 2.3.1. Verify that $\mathbf{x}(t + T; t_0 + T, \mathbf{x}_0) \equiv \mathbf{x}(t; t_0, \mathbf{x}_0)$ for a T-periodic velocity field.

For T-periodic velocity fields the advance-T mapping is called the *Poincaré map.* Because of periodic t-dependence, the velocity field can be imagined on cylindrical extended phase space $X \times S^1$, where S^1 denotes a circle of perimeter $2\pi/T$. The geometry of the Poincaré map is then shown in Fig. 2.4. We stress that the motion of fluid particles in an aperiodic velocity field *cannot* be tracked via the iteration of a single Poincaré map since such velocity fields do not give rise to a flow. As a result, the stroboscopic images of an initial condition $\mathbf{x}_0$ can only be followed by subsequently applying the members of the infinite map family $\mathbf{F}_{t_0}^{t_0+T}, \mathbf{F}_{t_0+T}^{t_0+2T}, \mathbf{F}_{t_0+2T}^{t_0+3T}, \ldots$. These maps are all different, and hence passing to a map description does not bring simplification in the general aperiodic case.

We must point out that there is considerable confusion in terminology in the literature, since in fluid mechanics the velocity field itself is often referred to as the flow. In addition, people often call $\mathbf{F}^t$ (i.e., $\mathbf{F}_0^t$) a flow for a general unsteady flow, although in such a case (2.3) is not satisfied. The fluid mechanical notion of the flow predates its mathematical definition given above, and also agrees with ones intuition about the meaning of the word. For this reason, we will also use this term quite freely, pointing out its strict mathematical meaning only when necessary.

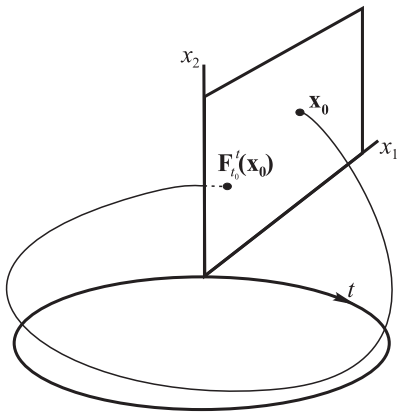

Figure 2.4: The Poincaré map.

2.4. The Eulerian and Lagrangian points of view

The two main approaches to the description of the velocity field (2.1) are known as the Eulerian and the Lagrangian point of view. The *Eulerian* point of view is concerned with the "global picture", i.e., with the properties of the velocity field $\mathbf{v}$ as it changes in space and time. At the same time, the *Lagrangian* approach is to monitor the evolution of individual particles, i.e., solutions of (2.1). This duality can be extended to any scalar or vector quantity $c(\mathbf{x}, t)$ associated with a given physical problem. Accordingly, the Eulerian time derivative of c is $\partial c/\partial t$, while the Lagrangian or *material* derivative is defined as

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + \nabla c \cdot \mathbf{v},$$

which is the time derivative of $c(\mathbf{x}(t), t)$. The quantity $c(\mathbf{x}, t)$ is called a *first integral,* an *integral of the motion,* or an *invariant*, if

$$\frac{Dc}{Dt} \equiv 0, \tag{2.4}$$

i.e., c does not change along fluid particle motions.

Example 1. As we recalled in Section 1.2.2, for two-dimensional flows the single not-identically-zero component of the vorticity is a first integral.

Example 2. For steady, inviscid flows without forcing, the Navier-Stokes equation takes the form

$$\mathbf{v}\cdot\nabla\mathbf{v} = -\frac{1}{\rho}\nabla p.$$

Integrating this equation along a particle path $x(t)$, we obtain the well-known Bernoulli theorem

$$\left[\frac{1}{2}\rho\left|\mathbf{v}\right|^2 + p\right]_{x(t)} = const,$$

i.e., the Bernoulli sum or dynamic pressure is a first integral.

2.5. Invariant manifolds

For geometric mixing theory, the basic point of view is Lagrangian. The main reason for this is that the advective part of mixing will turn out to be governed by distinguished invariant surfaces (or manifolds) in the extended phase space $X \times \mathbb{R}$. An *invariant manifold* for the dynamical system (2.1) is a smooth set of trajectories in $X \times \mathbb{R}$. By definition, a solution starting on an invariant manifold stays on it, as shown in Fig. 2.5. For a three-dimensional velocity field, invariant manifolds can be of dimension one (a single trajectory), two (trajectories starting from a curve), three (trajectories starting from a two-dimensional surface), or four (trajectories starting from a three-dimensional blob). For two-dimensional velocity fields, only one, two, and three-dimensional invariant manifolds are possible. The $t = const$ slices of an invariant manifold are called *material lines* and *material surfaces,* respectively, in fluid mechanics. These are time-dependent lines and surfaces that always consist of the same fluid particles (see Fig. 2.5).

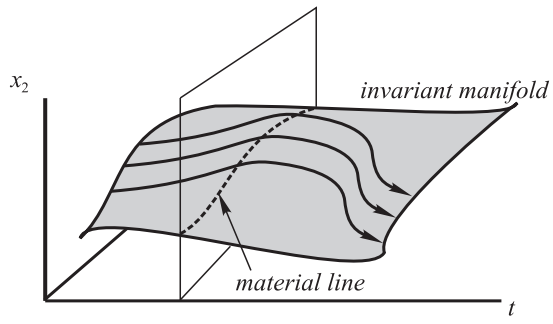

Figure 2.5: An invariant manifold and a material line.

Note that a curve or surface Γ of initial conditions always generates an invariant manifold through the trajectories passing through it. However, most of these manifolds have no special significance. Below is an example of invariant manifolds that are dynamically distinguished: they separate regions of different qualitative behavior.

Example 3. Consider the steady velocity field $\mathbf{v}(\mathbf{x}) = A\mathbf{x}$ with the constant matrix

$$A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The phase portrait of the system $\dot{\mathbf{x}} = \mathbf{v}(\mathbf{x})$ is shown in Fig. 2.6a, from which one can reconstruct the geometry in the extended phase space, as shown in Fig. 2.6b. Two invariant manifolds, $\mathcal{M}_1$ and $\mathcal{M}_2$, emanating from the line $x_1 = x_2 = 0$ at $t = 0$, have special significance. They divide the plane into four regions. The regions differ from each other in the forward or backward asymptotic behavior of trajectories. Also, the four regions do not mix with each other: they themselves are three-dimensional invariant manifolds in $X \times \mathbb{R}$. Note that nearby trajectories are either attracted to, or repelled from, $\mathcal{M}_1$ and $\mathcal{M}_2$,which will be a characteristic feature of manifolds with dynamical significance for mixing.

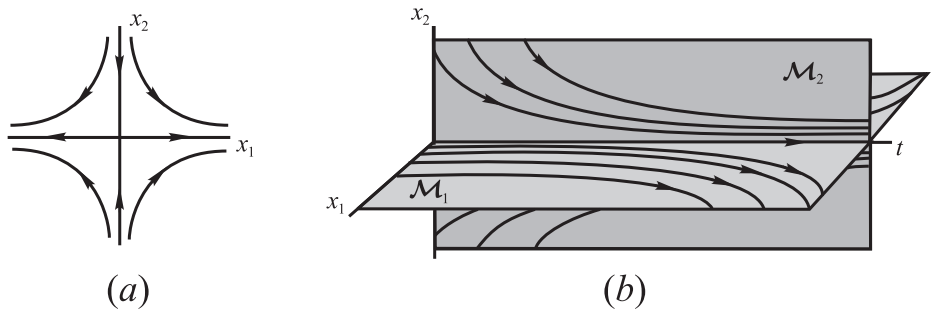

Figure 2.6: (a) Saddle point in the phase space. (b) The corresponding invariant manifolds in the extended phase space.

An important class of invariant manifolds is generated by first integrals. If $c(\mathbf{x}, t)$ is a first integral (see (2.5)), then individual trajectories are confined to level sets of c.

Example 4. *As follows from Example 1, for two-dimensional inviscid velocity fields, fluid particle motions are confined to the level sets of the vorticity $\boldsymbol{\omega}(\mathbf{x},t)$ in the extended phase space.*

Example 5. *As follows from Example 2, for steady, inviscid velocity fields, the trajectories lie in the level sets of the Bernoulli sum $\frac{1}{2}\rho\left|\mathbf{v}\right|^2 + p$.*

By the implicit function theorem of real analysis, such a level set is locally a smooth surface around a point $(\mathbf{x}_0, t_0)$ if

$$\left(\nabla c(\mathbf{x}, t), \frac{\partial c}{\partial t}\right) \neq 0,$$

with ∇ referring to the gradient with respect to $\mathbf{x}$. In three-dimensional vector-fields the above conditions assures that the level set of the integral is locally a three-dimensional manifold in $X \times \mathbb{R}$. For two-dimensional $\mathbf{v}$ the level set is locally two-dimensional manifold in the extended phase space. Such manifolds, with their dimension being one less than that of the ambient space, are called *codimension one manifolds* or *hypersurfaces.*

2.6. Change of volume

Perhaps the simplest question one might ask about the geometry of mixing is the following: How does, if at all, the measure of a blob D_0 of initial conditions change in time? By *measure* here we simply mean area if $\mathbf{x}$ is two-dimensional, and volume if $\mathbf{x}$ is three-dimensional. The most convenient answer to this question can be given in terms of the instantaneous rate of change of the volume (or area) $V(t)$ of the evolving blob $D(t) = \mathbf{F}_{t_0}^t(D(t_0))$ (see Fig. 2.7).

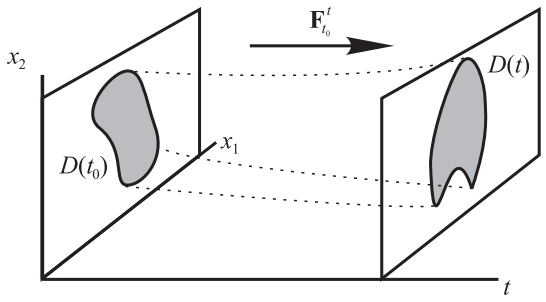

Figure 2.7: The geometry of Liouville's theorem.

Theorem 6 (Liouville's Theorem). *The rate of change of V obeys the formula*

$$\dot{V}(t_0) = \int_{D_0} \nabla \cdot \mathbf{v}(\mathbf{x}, t_0)\, dx.$$

Proof: Since the volume of $D(t)$ is given by the formula $V(t) = \int_{D(t)} dx$, by the change of variables formula from multivariable calculus we have $V(t) = \int_{V_0} \det\left[\nabla \mathbf{F}_{t_0}^t(\mathbf{x})\right]\, dx$, from which we obtain

$$\dot{V}(t) = \int_D \frac{d}{dt}\left[\det \nabla \mathbf{F}_{t_0}^t(\mathbf{x})\right]\, dx. \tag{2.5}$$

To calculate the integrand, we first Taylor-expand $F_{t_0}^t(\mathbf{x})$ around t_0 :

$$\mathbf{F}_{t_0}^t(\mathbf{x}) = \mathbf{x} + \mathbf{v}(\mathbf{x},t_0)(t - t_0) + \mathcal{O}((t - t_0)^2).$$

From this we obtain

$$\nabla \mathbf{F}_{t_0}^t(\mathbf{x}) = I + \nabla \mathbf{v}(\mathbf{x},t_0)(t-t_0) + \mathcal{O}((t-t_0)^2).$$

By direct calculation, for any matrix A,

$$\det(\mathbf{I} + \mathbf{A}\tau + \mathcal{O}(\tau^2)) = 1 + \operatorname{tr} \mathbf{A} + \mathcal{O}(\tau^2),$$

and hence

$$\det \nabla \mathbf{F}_{t_0}^t(\mathbf{x}) = 1 + \nabla \cdot \mathbf{v}(\mathbf{x},t_0)(t-t_0) + \mathcal{O}((t-t_0)^2).$$

Therefore, differentiating of this last equation with respect to t, setting $t = t_0$, and substituting into (2.5), we obtain the statement of the theorem.□

Liouville's theorem identifies the basic action of the flow on volume elements without using actual trajectories of velocity field. Namely, a vector field with negative divergence compresses volume, while one with positive divergence expands volume. Typical fluid velocity fields are closer to the case of $\nabla \cdot \mathbf{v} = 0$, i.e., they are *incompressible*.

2.7. Two-dimensional incompressible fluids

2.7.1. Hamiltonian structure: the streamfunction

For a two-dimensional velocity field $\mathbf{v}(\mathbf{x},t) = (u(x,y,t), v(x,y,t))$, the incompressibility condition $\nabla \cdot \mathbf{v} = 0$ takes the form

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0.$$

This implies, that for the three-dimensional velocity field $\mathbf{w} = (-v, u, 0)$, we have $\nabla \times \mathbf{w} = 0$. Then, by a well-known result from potential theory, the irrotational field $\mathbf{w}$ admits a potential function ψ on a simply connected domain, i.e., $\mathbf{w} = \nabla\psi$. The last component of this equation gives $\partial\psi/\partial z = 0$, (ϕ does not depend on z), while the first two components give

$$\begin{aligned} \dot{x} &= u(x,y,t) = \frac{\partial \psi(x,y,t)}{\partial y}, \\ \dot{y} &= v(x,y,t) = -\frac{\partial \psi(x,y,t)}{\partial x}. \end{aligned} \tag{2.6}$$

In classical mechanics, an equation of this kind is called a *one-degree-of-freedom Hamiltonian system* with the *Hamiltonian* ϕ. In fluid mechanics the Hamiltonian is called the *streamfunction.*[2] The name refers to the fact that for any fixed t, the

[2]It is equally common in the literature to call $-\psi$ the streamfunction, in which case the velocity field is of the form

$$\dot{x} = -\frac{\partial \psi(x,y,t)}{\partial y}, \quad \dot{y} = \frac{\partial \psi(x,y,t)}{\partial x}.$$

level curves of ψ coincide with streamlines. This can be seen by noting that $\mathbf{v}\cdot\nabla\psi \equiv 0$, i.e., the velocity field is everywhere perpendicular to a vector that is normal to the level curves of ψ.

In dynamical systems theory, it is customary to use a more compact notation for system (2.6). Let us introduce the skew-symmetric matrix[3]

$$J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Using this matrix, we can rewrite (2.6) as

$$\dot{\mathbf{x}} = J\nabla\psi(\mathbf{x},t),$$

which makes it easier to discuss the structure of the velocity field. For instance, the velocity field is easily seen to be tangent to streamlines since the inner product of the gradient $\nabla\psi$ and $J\nabla\psi$ must be zero[4].

The streamfunction is only unique up to an additive function of time. For steady velocity fields, one can choose ψ time-independent, in which case its level curves coincide with fluid particle trajectories. In other words, ψ is a first integral in the steady case.

2.7.2. Basic topology of streamlines

For incompressible, two-dimensional fluids the streamlines are level sets of ψ. Their geometry changes in time, but for any fixed t, it must obey some basic properties.

1. Any boundary is necessarily a streamline (see Fig. 2.8a)
2. A streamline can end on a boundary, but not away from the boundary (see Fig. 2.8a).
3. Any streamline on which $\nabla\psi \neq \mathbf{0}$ is a smooth curve. As a consequence, non-smooth streamlines, including self-intersecting streamlines, always contain a *stagnation point,* i.e., a point where the velocity field vanishes (see Fig. 2.8c). In case of no-slip boundary conditions, the whole boundary is filled with stagnation points.
4. At any stagnation point $\mathbf{p}$ the trace of the Jacobian $\nabla\mathbf{v} = J\nabla^2\psi$ is zero, which implies that for any t, the eigenvalues λ_1 and λ_2 of $J\nabla^2\psi(\mathbf{p},t)$ add up to zero. As a result, any stagnation point is one of the following four types:
   (a) $\lambda_1 < 0 < \lambda_2$: *Hyperbolic stagnation point* or *saddle*. In this case $\mathbf{p}$ is at the intersection of two streamlines, that asymptote to the eigenvectors of the matrix $J\nabla^2\psi(\mathbf{p},t)$. As a result, they always intersect at a nonzero angle

[3] This matrix is usually referred to as the two-dimensional canonical symplectic matrix in the theory of Hamiltonian systems.

[4] $\nabla\psi \cdot J\nabla\psi \equiv 0$ since J is skew-symmetric.

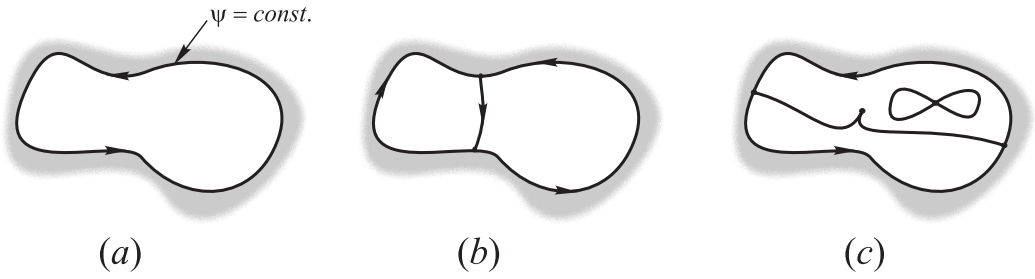

Figure 2.8: Basic streamline topology in two-dimensional incompressible flows.

(b) $\lambda_{1,2} = \pm i\omega$: *Elliptic stagnation point* or *center.* The point $\mathbf{p}$ is surrounded by closed streamlines with nonvanishing velocity.

(c) $\lambda_1 = \lambda_2 = 0$, and $J\nabla^2\psi(\mathbf{p},t)$ has only one linearly independent eigenvector. The stagnation point $\mathbf{p}$ may or may not be isolated in this case. In the former case we have a *cusp* and the latter case involves most frequently a *boundary point* on a boundary with no-slip boundary condition.

(d) $\lambda_1 = \lambda_2 = 0$, and $J\nabla^2\psi(\mathbf{p},t)$ has two linearly independent eigenvector. In this case, the velocity field at $\mathbf{p}$ has no linear component. The geometry of streamlines depends on the given problem. One extreme case is where $\mathbf{p}$ is just a point in a flow at rest. A more common case is where $\mathbf{p}$ is a *distinguished boundary point* on a boundary with no-slip boundary conditions. A distinguished stagnation point, such as a separation point or reattachment point, is one where a streamline emanating from the interior connects to the boundary.

The four main types of stagnation points are shown in Fig. **??**. Geometrically, stagnation points are local extrema of the level surfaces of $\psi(\mathbf{x},t)$ for fixed t. Hyperbolic stagnation points indicate a saddle on a level surface, while elliptic stagnation points correspond to local maxima or minima (see Fig. 2.10).

5. Hyperbolic and elliptic stagnation points are called *nondegenerate,* as they correspond to $\det\left[J\nabla^2\psi(\mathbf{p},t)\right] \neq 0$. Typical stagnation points away from boundaries are nondegenerate. By the implicit function theorem, they are *structurally stable,* i.e., they may move as ψ changes in time, but will persist for forward and backward times close enough to t. In contrast, degenerate stagnation points away from the boundary are not structurally stable: as t is changed, they either disappear or turn into one or more nondegenerate stagnation points, which will in turn be robust in time. The latter case is called a *bifurcation* of stagnation points. The structural stability of nondegenerate stagnation points also

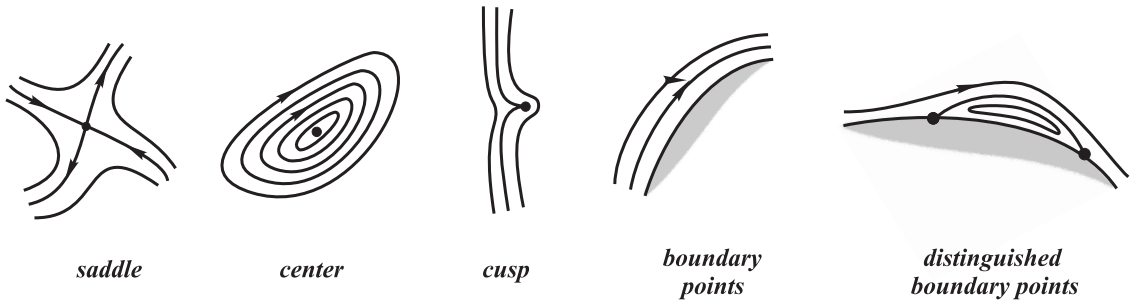

Figure 2.9: The four basic stagnation points in two dimensional, incompressible velocity fields.

involves another property: they will also persist under small perturbations of the streamfunction.

6. A stagnation point may be connected to itself through a *homoclinic*[5] streamline. Homoclinic streamlines attached to hyperbolic stagnation points are structurally stable in the sense described above: they might deform but will persist for nearby times and for small perturbations of the streamfunction. This readily follows if one pictures the of the corresponding contour line on a $\psi = const$ surface, as shown in Fig. 2.11. Indeed, a nearby, similar contour line will clearly exist under small smooth deformations of ψ.

7. Streamlines connecting different stagnation points are called *heteroclinic.* Unlike homoclinic streamlines, heteroclinic streamlines are not robust with respect to changes of ψ in time, or with respect to perturbations of $\psi(\mathbf{x},t)$, unless some special symmetry is present. The reason is that at two distinct stagnation points ψ will typically have different value, in which case they cannot be connected by level curves of ψ. In the absence of some special symmetry, such a connection is seen only at isolated time instances. Figure 2.12 shows the typical fate of an instantaneous heteroclinic streamline as t is varied.

2.7.3. Flux across a curve

There is another meaning of the streamfunction, related to mixing, which also holds in the unsteady case. Consider a smooth curve Γ joining two points A and B. The

[5]The term *homoclinic* is originally due to Poincaré, and was introduced to describe solutions of differential equations that approach the same equilibrium point in forward and backward time. Solutions connecting different equilibria are called *heteroclinic.*

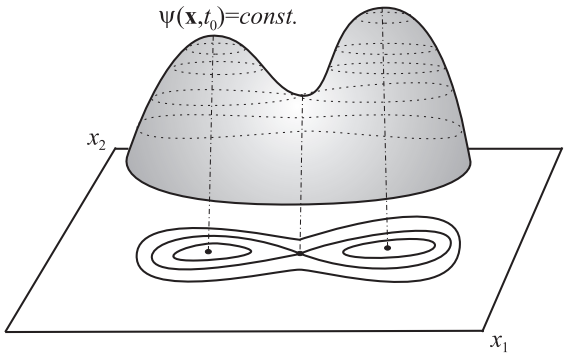

Figure 2.10: Nondegenerate extrema of a level set of the stream function, and the corresponding stagnation points.

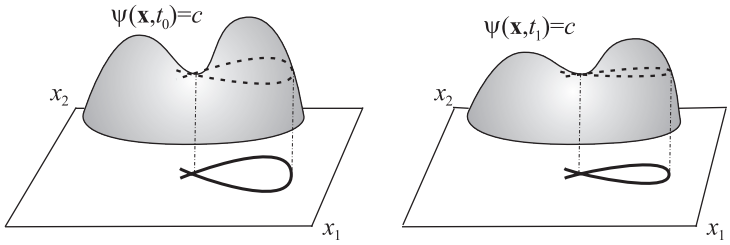

Figure 2.11: Persistence of a homoclinic streamline for times near t_0.

instantaneous flux of the velocity field across Γ is defined as

$$\text{Flux}(t) = \int_A^B \mathbf{v}(\mathbf{x},t)\, d\mathbf{n},$$

where $\mathbf{n}$ denotes the normal direction to Γ . Using (2.6), we can actually compute this flux by introducing the unit normal $\mathbf{N}$ to Γ and writing

$$\begin{aligned}
\text{Flux}(t) &= \int_A^B \mathbf{v}(\mathbf{x},t)\, d\mathbf{n} = \int_A^B \mathbf{v}(\mathbf{x},t) \cdot\ \mathbf{N}(\mathbf{x},t)\, d\mathbf{x} \\
&= \int_A^B u dy - v dx = \int_A^B \frac{\partial \psi}{\partial y} dy + \frac{\partial \psi}{\partial x} dx \\
&= \int_A^B \nabla \psi\, d\mathbf{x} = \psi(B,t) - \psi(A,t).
\end{aligned}$$

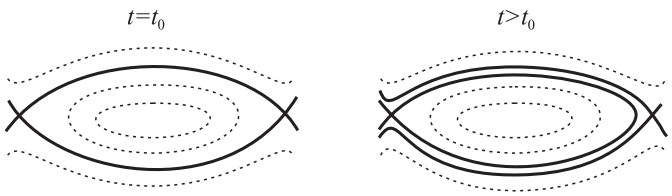

Figure 2.12: Breakdown of a heteroclinic streamline as time is varied.

Thus, we obtain that *the flux through a curve* Γ *is equal to the difference in the values of the streamfunction at the endpoints of* Γ. This also implies that the flux is the same for any two oriented curves connecting A to B. That, in turn implies, that the flux with respect to a closed curve is zero (see Fig. 2.13), which is of course no surprise by incompressibility.

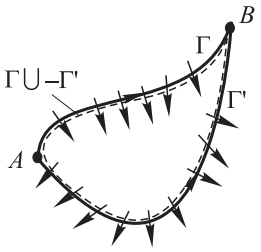

Figure 2.13: The flux across Γ is the sam as the flux across Γ', which in turn implies zero flux across $\Gamma \cup -\Gamma'$.

It is important to note that a zero *net* flux across a curve does not imply that there is not fluid mixing through the curve. In fact, mixing can be quite intense through Γ and is independent of the value of the net instantaneous flux relative to Γ.

2.7.4. Flux into a ring

In some cases one is interested in the instantaneous flux of fluid particles relative to a structure that changed its shape in time. For instance, in geophysical fluid dynamics a set of closed streamlines is often referred to as a *ring* (Fig. 2.14). A ring may grow or shrink in time, i.e., the closed streamline Γ_t that one selects as a ring boundary at time t will be time-dependent. Even though the velocity field is always tangent to the ring

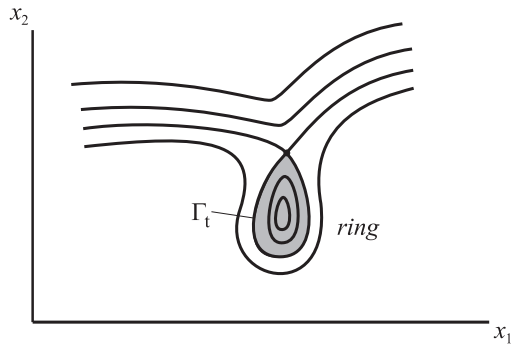

Figure 2.14: A ring with time-dependent boundary Γ_t.

boundary by definition, the flux of particles into a growing ring is clearly positive.[6] The flux of trajectories can then be better visualized in the extended phases space, where the growing ring boundary appears as a two-dimensional cylindrical surface. Between two fixed times, the flux through this surface must be equal to the difference of ring areas. As a result, the instantaneous flux is obtained as

$$\text{Flux}(t) = \frac{dA(t)}{dt},$$

where $A(t)$ denotes the time-dependent area of the ring.[7]

Example 7. A singular example of a ring is the "corner eddy" indicated in Fig. 2.15. From an Eulerian point of view, the boundary of the eddy is defined by the streamline

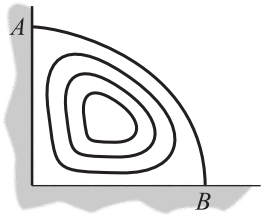

Figure 2.15: Instantaneous streamline configuration for a corner eddy.

[6] The fluid is incompressible, so the mass of fluid enclosed by a larger ring boundary must be larger.

[7] We assumed that the are function is continuously differebtiable in time.

connecting the stagnation points A and B. If the velocity field is unsteady, the points A and B will typically move along the walls, and the time dependence of the area of the eddy may not be known. However, the instantaneous net flux into the eddy must be zero regardless of its size The reason is that the walls are always streamlines, and hence, by the continuity of the streamfunction, A and B are contained in the same level set of ψ, implying

$$Flux(t) = \int_A^B \mathbf{v}(\mathbf{x},t)\, d\mathbf{n} = \psi(B,t) - \psi(A,t) \equiv 0.$$

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