# MAXIMAL EFFECTIVE DIFFUSIVITY FOR TIME-PERIODIC INCOMPRESSIBLE FLUID FLOWS\*

IGOR MEZIĆ<sup>†</sup>, JOHN F. BRADY<sup>‡</sup>, AND STEPHEN WIGGINS<sup>§</sup>

Abstract. In this paper we establish conditions for the maximal,  $Pe^2$ , behavior of the effective diffusivity in time-periodic incompressible velocity fields for both the  $Pe \rightarrow \infty$  and  $Pe \rightarrow 0$  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 the velocity field. The connection between the  $Pe^2$  asymptotic behavior of the effective diffusivity and  $t^2$  asymptotic dispersion of a nondiffusive tracer is established. Several examples are analyzed: we relate the existence of 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 an effective diffusivity with Peclet number dependence other than  $Pe^2$  in time-dependent flows is established.

Key words. effective diffustivity, homogenization, ergodic theory

AMS subject classifications. 76R50, 60H25, 35R60, 58F

1. Introduction. In this paper we study the problem of a spreading of a diffusive passive tracer in incompressible fluid flows. Being a problem of a great interest in both engineering and physics, it has attracted a lot of attention in both of these fields (see the reference list). A physical problem is the following: an initial distribution of passive, diffusive particles is placed in an incompressible velocity field and allowed to evolve. The second moment of the distribution of convecting and diffusing particles is a particularly interesting quantity: it gives the average size of the cloud of particles. Of course, the second moment is dependent on time, and at large times it grows linearly with time if the diffusive limit is reached. The constant obtained by dividing the second moment by time and taking the limit when time goes to infinity is the quantity we are interested in. It is called the effective diffusivity (see the precise definition in §2). The effective diffusivity naturally depends on the nondimensional number in the problem, called the Peclet number, which is defined as

$$Pe = \frac{Ul}{D},$$

where U is the characteristic velocity, l is the characteristic lengthscale, and D is the molecular diffusivity of particles.

Most previous studies of the effective diffusivity for laminar, deterministic velocity fields have 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 [12] statistical mechanics terminology) a velocity field *ergodic in a certain direction* if the time average along the

<sup>\*</sup> Received by the editors June 29, 1994; accepted for publication (in revised form) January 5, 1995. This research was partially supported by an NSF Presidential Young Investigator Award, ONR grant N00014-89-J-3023, and AFOSR grant AFOSR910241.

<sup>&</sup>lt;sup>†</sup> Department of Mechanical and Environmental Engineering, University of California, Santa Barbara, CA 93106-5070.

<sup>&</sup>lt;sup>‡</sup> Chemical Engineering 210-41, California Institute of Technology, Pasadena, CA 91125.

<sup>&</sup>lt;sup>§</sup> Applied Mechanics 104-44, California Institute of Technology, Pasadena, CA 91125.

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 that are constant almost everywhere. Thus, ergodicity is sufficient but not necessary for ergodicity in a certain direction. It was shown in [10], [15] that, provided certain technical conditions are satisfied, the effective diffusivity behaves like  $Pe^2$  in the large Peclet number limit for steady spatially periodic flows. Using our results in  $\S3.1$ , 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  $Pe \to \infty$  and  $Pe \to 0$ . 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 the effective diffusivity in time-periodic flows, but it is not clear how these conditions, analogous to the ones for steady flows derived in [10], [15], could be used for analysis of *specific* unsteady flows. The new condition of nonergodicity in a certain direction allows us to analyse effective diffusivity in specific time-periodic velocity fields and time-periodic velocity fields with specific kinematical properties, as it is done in  $\S4$ .

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 [26]). 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 [18]). 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 paper, based on the arguments in [18] and [19], that the ballistic behavior of the dispersion in a certain direction is a consequence of the nonergodicity 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 the effective diffusivity in time-periodic velocity fields is not large, although there is a significant number of natural phenomena that can be modeled by a convection-diffusion equation with time-periodic coefficients (for a list of these natural phenomena, see [7], [8]). Dill and Brenner studied the effective diffusivity in time-periodic flows both in spatially periodic [8] and Taylor dispersion [7] settings, using the method of moments. A specific class of velocity fields that they analyse 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 [10] developed variational principles which determine effective diffusivity for both steady and time-periodic flows. We use their variational principle for time-periodic flows in §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.

The formalism that we use follows from the work of Avellaneda and Majda [1], [2]. In particular, they used the ideas of homogenization theory and Peclet number expansions for effective diffusivity, following the previous work of Milton, Bergman and Golden and Papanicolaou on permittivity of two-phase composites. A similar approach can also be found in the work of Brenner [6] on Taylor dispersion.

This paper is organized as follows: in §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 §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 §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 threedimensional 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.

### 2. Homogenization of the convection-diffusion equation.

### 2.1. Definitions and notation. The convection-diffusion equation

(1) 
$$\frac{\partial c}{\partial t} + \mathbf{v}(\mathbf{x}, t) \cdot \nabla c = D \triangle c$$

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 §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

$$\begin{array}{rcl} \frac{dx}{ds} &=& u(x,y,t),\\ \frac{dy}{ds} &=& v(x,y,t),\\ \frac{dt}{ds} &=& 1, \end{array}$$

where s is a new "time-like" variable. Thus, the phase space on which we analyse 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  $\langle \cdot \rangle$ ,

$$\langle \cdot \rangle = \frac{1}{l^2\tau} \int_0^\tau \int_0^l \int_0^l (\cdot) dx dy d\tau.$$

The average over the unit cell be will be denoted by  $\langle \cdot \rangle_s$ ,

$$\left<\cdot\right>_s = \frac{1}{l^2} \int_0^l \int_0^l (\cdot) dx dy$$

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 paper, it will always mean the time average along a Lagrangian particle trajectory.

The reader will note 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 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

$$\mu(B) = \frac{1}{l^2 \tau} \int_B dx dy dt,$$

where the integration is meant in the Lebesgue sense.  $\mu$  is a positive function on  $\mathcal{A}$ , i.e.,  $\mu(B) \geq 0$  for every  $B \in \mathcal{A}$ . Also,  $\mu$  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 is 1. Thus, A and the set on which that statement is valid is 1.

**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 [10].

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

(2) 
$$\mathbf{H} = \begin{bmatrix} 0 & H \\ -H & 0 \end{bmatrix}$$

such that  $\mathbf{v}' = \nabla \cdot \mathbf{H}$  (see [10]). Equation (1) can then be written as

(3) 
$$\frac{\partial c}{\partial t} + \langle \mathbf{v} \rangle \cdot \nabla c = \nabla \cdot \mathbf{A}(\mathbf{x}, t) \nabla c.$$

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, (3) becomes

(4) 
$$\frac{\partial c}{\partial t} + \delta^{-1} \langle \mathbf{v} \rangle \cdot \nabla c = \nabla \cdot \mathbf{A} \left( \frac{\mathbf{x}}{\delta}, \frac{t}{\delta^2} \right) \nabla c.$$

It can be shown, using homogenization theory for parabolic differential operators (see, e.g., [3]) that, after subtracting the mean drift, 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, the resulting process is diffusive. In that limit,  $c(\mathbf{x}, t)$  converges weakly in  $L^2$  to  $\bar{c}(\mathbf{x}, t)$ , where  $\bar{c}$  satisfies

(5) 
$$\frac{\partial \bar{c}}{\partial t} + \langle \mathbf{v} \rangle \cdot \nabla \bar{c} = \mathbf{D} \triangle \bar{c}$$

(for details of a procedure leading to (5), see [17]). In (5),  $\mathbf{D}$  is the constant *effective* diffusivity tensor given by

(6) 
$$\mathbf{D} = \langle D\mathbf{I} - \mathbf{H} + (D\mathbf{I} - \mathbf{H})\nabla\chi\rangle,$$

with the spatially and temporally periodic vector field  $\chi$  satisfying the *cell equation* 

(7) 
$$\frac{\partial \chi}{\partial t} + (\langle \mathbf{v} \rangle + \mathbf{v}') \cdot \nabla \chi - D \Delta \chi = -\mathbf{v}'.$$

In [8] an equation analogous to (7) was developed. In that work,  $\chi$  is denoted by **B** and called the **B**-field.

Equation (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 (6). This restriction is common in the literature (see, e.g., [15], [14]), and also there is a large class of velocity fields for which it can be proven that  $\mathbf{D}$  actually is symmetric

(see [10]). For a discussion of velocity fields having nonsymmetric effective diffusivity tensors, see [13]. The symmetric part of  $\mathbf{D}$  is given by

(8) 
$$\mathbf{D}_{sym} = D(\mathbf{I} + \langle \nabla \chi \cdot \nabla \chi \rangle).$$

It is convenient for analysis to put the cell equation (7) in integral form. First note that the effective diffusivity in the direction of a unit vector  $\mathbf{e}$  is given by

(9) 
$$\mathbf{D}_{sym}\mathbf{e}\cdot\mathbf{e} = D(1 + \langle \nabla\chi^{\mathbf{e}}\cdot\nabla\chi^{\mathbf{e}}\rangle),$$

where  $\chi^{\mathbf{e}} = \chi \cdot \mathbf{e}$ . Let us introduce the operator  $\Gamma = \nabla \triangle^{-1} \nabla$ . Then it is easy to show that, in the direction of  $\mathbf{e}$ , (7) becomes

(10) 
$$\left( D - \mathbf{\Gamma} \triangle^{-1} \frac{\partial}{\partial t} - \mathbf{\Gamma} \triangle^{-1} \langle \mathbf{v} \rangle \cdot \nabla - \mathbf{\Gamma} \mathbf{H} \mathbf{\Gamma} \right) \nabla \chi^{\mathbf{e}} = \mathbf{\Gamma} \mathbf{H} \cdot \mathbf{e}_{\mathbf{v}}^{\mathbf{e}}$$

The operator  $\Gamma$  was used by Avellaneda and Majda in [1].

## 3. Ergodic theory and effective diffusivity.

**3.1. Conditions for the maximal effective diffusivity.** In the previous section, we derived the equation that needs to be solved to obtain the effective diffusivity for a time-periodic, spatially periodic velocity field in the direction of the unit vector **e.** Following [15] we call the effective diffusivity in the direction of **e** maximal if

$$\mathbf{De} \cdot \mathbf{e} \sim \frac{1}{D}.$$

In this section we shall be interested in determining the conditions on a time-periodic, spatially periodic velocity field so that it has a maximal enhanced diffusivity.

Let us define a new operator  $\mathbf{G}$  as

$$\mathbf{G} = -\mathbf{\Gamma} \triangle^{-1} \frac{\partial}{\partial t} - \mathbf{\Gamma} \triangle^{-1} \langle \mathbf{v} \rangle \cdot \nabla - \mathbf{\Gamma} \mathbf{H} \mathbf{\Gamma}.$$

The operator **G** is compact (see [10]), and it is clearly related to the purely convective part of (1). Equation (10) now becomes

(11) 
$$(D\mathbf{I} - \mathbf{G})\nabla\chi^{\mathbf{e}} = \mathbf{\Gamma}\mathbf{H} \cdot \mathbf{e}.$$

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  $\nabla f$  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 [10] (in particular, using a variational principle for time-periodic velocity fields developed there), we can conclude that

$$\mathbf{De} \cdot \mathbf{e} \sim \frac{1}{D}$$
 as  $D \to 0$  if and only if  $\mathbf{\Gamma} \mathbf{H} \cdot \mathbf{e}$  has a nonzero 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

(12) 
$$\Gamma \mathbf{H} \cdot \mathbf{e}$$
 has a nonzero component in  $\mathcal{N}$ 

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  $\mathbf{e}$ . For simplicity of presentation, we assume  $(\mathbf{v}' \cdot \mathbf{e})^* \in H^1(A)$ . This condition is very restrictive and we relax it at the end of the subsection.

First, note that for (12) to be satisfied,  $\mathcal{N}$  must be nonempty. It is not hard to show (cf. [10, §8.2]) 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

(13) 
$$\frac{\partial f}{\partial t} + \mathbf{v}(\mathbf{x}, t) \cdot \nabla f = 0$$

in a generalized sense.

Second, let  $\mathcal{M}$  be the Hilbert space of functions  $f \in L^2(A)$  such that  $f = g^*$  for some  $g \in L^2(A)$ . It is clear that the space S of all functions in  $H^1(A)$  that are constant on orbits is a subset of  $\mathcal{M}$ . For  $\Gamma \mathbf{H} \cdot \mathbf{e}$  to have a component in  $\mathcal{N}$ , we need

$$\langle (\mathbf{\Gamma}\mathbf{H}\cdot\mathbf{e})\cdot\nabla f\rangle \neq 0$$

for some  $f \in H^1(A)$ . Integrating by parts, we get

(14) 
$$\langle f \mathbf{v}' \cdot \mathbf{e} \rangle \neq 0 \text{ for some } f \in H^1(A).$$

Now we show that (13) and (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 (13) and (14) are satisfied if and only if  $(\mathbf{v}' \cdot \mathbf{e})^*$  is not a constant almost everywhere on A.

Suppose first

(15) 
$$(\mathbf{v}' \cdot \mathbf{e})^*$$
 is not a constant almost everywhere.

Then, take  $f = (\mathbf{v}' \cdot \mathbf{e})^*$ . By Birkhoff's ergodic theorem,  $(\mathbf{v}' \cdot \mathbf{e})^*$  satisfies (13). For (14) let us first note that the projection operator  $\Pi : L^2 \to \mathcal{M}$ , which takes every function in  $L^2$  to its time average, is orthogonal [16]. Then, we have the following calculation:

(16)  
$$\langle (\mathbf{v}' \cdot \mathbf{e})^* \mathbf{v}' \cdot \mathbf{e} \rangle = \langle (\mathbf{v}' \cdot \mathbf{e})^* ((\mathbf{v}' \cdot \mathbf{e})^* + z) \rangle$$
$$= \langle ((\mathbf{v}' \cdot \mathbf{e})^*)^2 \rangle$$
$$\neq 0,$$

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  $H^1$  that 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

$$\begin{array}{lll} \langle (f - \langle f \rangle) \mathbf{v}' \cdot \mathbf{e} \rangle &=& \langle (f - \langle f \rangle) (c + z) \rangle \\ &=& c \left\langle (f - \langle f \rangle) \right\rangle + \left\langle (f - \langle f \rangle) z \right) \rangle \\ &=& c \left\langle (f - \langle f \rangle) \right\rangle = 0 \end{array}$$

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 [12] 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.,

$$\mathbf{De} \cdot \mathbf{e} \ll \frac{1}{D}$$
 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 [10] is a special case of the "if" part of this statement.

As we have already mentioned, the requirement that the time average of the velocity in the direction of  $\mathbf{e}$  is in  $H^1$  is very restrictive. The time averages of smooth velocity fields that have sufficiently complicated (e.g., chaotic) dynamics can be discontinuous functions, thus certainly not having the distributional derivatives in  $L^2$ . We shall now prove that the above result on the condition for the maximal effective diffusivity is true under much weaker assumption on  $(\mathbf{v}' \cdot \mathbf{e})^*$ . In particular, we require only that  $(\mathbf{v}' \cdot \mathbf{e})^*$  is not orthogonal to the space S of all functions in  $H^1$  that are constant on orbits. S is clearly a closed linear subspace of M. Denote by  $\Pi_S : M \to S$ the orthogonal projection. Let  $f = \Pi_S((\mathbf{v}' \cdot \mathbf{e})^*)$  be the function in S that is, by assumption, nonzero. Similar to the previous calculation, we have

$$\langle \Pi_{S}((\mathbf{v}' \cdot \mathbf{e})^{*})\mathbf{v}' \cdot \mathbf{e} \rangle = \langle \Pi_{S}((\mathbf{v}' \cdot \mathbf{e})^{*})((\mathbf{v}' \cdot \mathbf{e})^{*} + z) \rangle$$

$$= \langle \Pi_{S}((\mathbf{v}' \cdot \mathbf{e})^{*})(\mathbf{v}' \cdot \mathbf{e})^{*} \rangle$$

$$= \langle \Pi_{S}((\mathbf{v}' \cdot \mathbf{e})^{*})(\Pi_{S}((\mathbf{v}' \cdot \mathbf{e})^{*}) + w) \rangle$$

$$= \langle (\Pi_{S}((\mathbf{v}' \cdot \mathbf{e})^{*}))^{2} \rangle$$

$$\neq 0,$$

where  $z = \mathbf{v}' \cdot \mathbf{e} - (\mathbf{v}' \cdot \mathbf{e})^*$  is a function in  $\mathcal{M}^{\perp}$ , and  $w = (\mathbf{v}' \cdot \mathbf{e})^* - \Pi_S((\mathbf{v}' \cdot \mathbf{e})^*)$  is a function in  $S^{\perp}$  (with respect to  $\Pi_S$ ). Note that if  $\Pi_S((\mathbf{v}' \cdot \mathbf{e})^*)$  is not zero, then it is not a constant a.e., either. Suppose  $\Pi_S((\mathbf{v}' \cdot \mathbf{e})^*) = c \neq 0$ . Then

(18) 
$$\langle ((\mathbf{v}' \cdot \mathbf{e})^* - c)c \rangle = -\langle c^2 \rangle$$
$$\neq 0,$$

which gives a contradiction, by orthogonality.

(17)

**3.2. Small Peclet number limit.** In the convection-diffusion equation (1) there exists only one nondimensional parameter, the Peclet number Pe = Vl/D, where V is the maximal velocity on A. Letting  $(x, y, t) \rightarrow (x/l, y/l, tV/l)$ , we obtain the nondimensional equation

(19) 
$$\frac{\partial c}{\partial t} + \mathbf{v}(\mathbf{x}, t) \cdot \nabla c = \frac{1}{Pe} \triangle c.$$

Now we see that all the above analysis comes through for (19). In particular, the above conclusions are valid in the limit  $Pe \to \infty$ . In terms of the Peclet number, we have

$$\frac{\mathbf{D}\mathbf{e}\cdot\mathbf{e}}{D} \sim Pe^2 \quad \text{as } Pe \to \infty.$$

The point of writing (1) in the form (19) here is twofold: first, 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. Second, 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  $\Gamma \mathbf{H} \cdot \mathbf{e}$  has a nonzero 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

$$\mathbf{D}_{sym}\mathbf{e}\cdot\mathbf{e} = D + D\left\langle\nabla\chi_{\mathcal{N}}^{\mathbf{e}}\cdot\nabla\chi_{\mathcal{N}}^{\mathbf{e}}\right\rangle + D\left\langle\nabla\chi_{\mathcal{N}^{\perp}}^{\mathbf{e}}\cdot\nabla\chi_{\mathcal{N}^{\perp}}^{\mathbf{e}}\right\rangle.$$

From (11), using the fact that  $\nabla \chi^{\mathbf{e}}_{\mathcal{N}}$  is in the null space of **G**, it satisfies

(20) 
$$\frac{1}{Pe}\nabla\chi_{\mathcal{N}}^{\mathbf{e}} + \mathbf{\Gamma}\mathbf{H}\cdot\mathbf{e}_{\mathcal{N}} = 0.$$

Clearly,

$$\langle \nabla \chi_{\mathcal{N}}^{\mathbf{e}} \cdot \nabla \chi_{\mathcal{N}}^{\mathbf{e}} \rangle = P e^2 \left\langle \mathbf{\Gamma} \mathbf{H} \cdot \mathbf{e}_{\mathcal{N}} \cdot \mathbf{\Gamma} \mathbf{H} \cdot \mathbf{e}_{\mathcal{N}} \right\rangle = c P e^2,$$

where  $c = \langle \mathbf{\Gamma} \mathbf{H} \cdot \mathbf{e}_{\mathcal{N}} \cdot \mathbf{\Gamma} \mathbf{H} \cdot \mathbf{e}_{\mathcal{N}} \rangle$ . This derivation does not depend on the value of *Pe*. Now, again from (10),

(21) 
$$\frac{1}{Pe}\nabla\chi^{\mathbf{e}}_{\mathcal{N}^{\perp}} + \mathbf{G}\nabla\chi^{\mathbf{e}}_{\mathcal{N}^{\perp}} + \mathbf{\Gamma}\mathbf{H}\cdot\mathbf{e}_{\mathcal{N}^{\perp}} = 0.$$

For small Pe, solving (21) for  $\nabla \chi^{\mathbf{e}}_{\mathcal{N}^{\perp}}$  gives

$$\nabla \chi^{\mathbf{e}}_{\mathcal{N}^{\perp}} = Pe(\mathbf{I} - Pe\mathbf{G})^{-1}\mathbf{\Gamma}\mathbf{H} \cdot \mathbf{e}_{\mathcal{N}^{\perp}} = \mathcal{O}(Pe).$$

Therefore, if  $\mathbf{\Gamma} \mathbf{H} \cdot \mathbf{e}$  has a nonzero component in  $\mathcal{N}$ ,

$$\frac{\mathbf{D}\mathbf{e}\cdot\mathbf{e}}{D} \sim Pe^2 \quad \text{as } Pe \to 0.$$

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 [15]. In fact, all the results in this subsection carry over to the steady case. **3.3. 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

(22) 
$$(\mathbf{v} \cdot \mathbf{e})^*$$
 is not a constant almost everywhere.

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 (22) means in the case of nondiffusive motion. Statistical properties of the motion of a nondiffusive passive scalar have been investigated in [18] with an additional application to dispersion in fluid velocity fields provided in [19]. We shall now establish, as a corollary of that work, the meaning of (22) 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

$$\dot{x} = u(x, y, t),$$
  
 $\dot{y} = v(x, y, t).$ 

(23)

(24)

Let us assume that at t = 0, tracer particles are uniformly distributed over the unit cell. The nondiffusive dispersion in the direction of **e**, denoted by  $D_{\mathbf{e}}^{n}(t)$ :

$$D_{\mathbf{e}}^{n}(t) = \left\langle \left[ \left( \mathbf{x} \cdot \mathbf{e} - \mathbf{x}_{0} \cdot \mathbf{e} \right) - \left\langle \left( \mathbf{x} \cdot \mathbf{e} - \mathbf{x}_{0} \cdot \mathbf{e} \right) \right\rangle_{s} \right]^{2} \right\rangle_{s}, \\ = \left\langle \left[ \int_{0}^{t} \mathbf{v}(\mathbf{x}(\bar{t}), \bar{t}) \cdot \mathbf{e} \ d\bar{t} - \left\langle \int_{0}^{t} \mathbf{v}(\mathbf{x}(\bar{t}), \bar{t}) \cdot \mathbf{e} \ d\bar{t} \right\rangle_{s} \right]^{2} \right\rangle_{s}.$$

Dividing (24) by  $t^2$  and letting  $t \to \infty$ , we obtain

$$\lim_{t \to \infty} \frac{D_{\mathbf{e}}^{n}(t)}{t^{2}} = \lim_{t \to \infty} \frac{1}{t^{2}} \left\langle \left[ \int_{0}^{t} \mathbf{v}(\mathbf{x}(\bar{t}), \bar{t}) \cdot \mathbf{e} \ d\bar{t} - \left\langle \int_{0}^{t} \mathbf{v}(\mathbf{x}(\bar{t}), \bar{t}) \cdot \mathbf{e} \ d\bar{t} \right\rangle_{s} \right]^{2} \right\rangle_{s},$$

$$= \lim_{t \to \infty} \left\langle \left[ \frac{1}{t} \int_{0}^{t} \mathbf{v}(\mathbf{x}(\bar{t}), \bar{t}) \cdot \mathbf{e} \ d\bar{t} - \left\langle \frac{1}{t} \int_{0}^{t} \mathbf{v}(\mathbf{x}(\bar{t}), \bar{t}) \cdot \mathbf{e} \ d\bar{t} \right\rangle_{s} \right]^{2} \right\rangle_{s},$$

$$= \left\langle \left[ (\mathbf{v} \cdot \mathbf{e})^{*} - \left\langle (\mathbf{v} \cdot \mathbf{e})^{*} \right\rangle_{s} \right]^{2} \right\rangle_{s},$$
(25)
$$\equiv a.$$

The passage from the first to the second line is justified using boundedness and integrability of  $\mathbf{v} \cdot \mathbf{e}$  and Lebesgue's 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 §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  $\mu(B) = \int_B dxdy$  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 [18]). As  $a < \infty$  by the boundedness of  $\mathbf{v}$  we reach the following conclusion:

$$\frac{\mathbf{De} \cdot \mathbf{e}}{D} \sim Pe^2 \text{ as } Pe \to \infty \text{ if and only if } D_{\mathbf{e}}^n(t) \sim t^2 \text{ as } t \to \infty.$$

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 [14].

**3.4.** 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  $P: T^2 \to T^2$  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 (23) with initial conditions

$$\begin{array}{rcl} x(0,x_0,y_0,0) &=& x_0, \\ y(0,x_0,y_0,0) &=& y_0. \end{array}$$

The time average  $f_P^*$  of any function  $f \in L^1(T^2)$  under P is given by

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

Let us define a jump function  $\mathbf{j}: T^2 \to \mathbb{R}$  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, (22) becomes

(26)  $(\mathbf{j} \cdot \mathbf{e})_P^*$  is not a constant almost everywhere.

4. Some examples. In this section we apply the conditions for the maximal effective diffusivity to a number of specific velocity fields, or general velocity fields possessing 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 that exhibits such a discontinuous transition is an example due to Zeldovich [30] and Young, Rhines, and Garrett [29], 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.

**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 referred to as an 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 [20] for a general continuous area preserving map P, we deduce that there is an invariant region D, of positive measure, around p such that

$$(\mathbf{j} \cdot \mathbf{e})_P^*(p_1) = (\mathbf{j} \cdot \mathbf{e})_P^*(p) = (\mathbf{j} \cdot \mathbf{e})(p) \quad \forall p_1 \in D.$$

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

(27) 
$$\langle (\mathbf{j} \cdot \mathbf{e}) \rangle_s \neq (\mathbf{j} \cdot \mathbf{e})(p),$$

the velocity field  $\mathbf{v}(\mathbf{x}, t)$  possesses a maximal effective diffusivity in the direction of  $\mathbf{e}$ . By Birkhoff's ergodic theorem

$$\langle (\mathbf{j} \cdot \mathbf{e}) \rangle_s = \langle (\mathbf{j} \cdot \mathbf{e})_P^* \rangle_s.$$

Hence, using the condition (27), 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 (26) there is a maximal enhanced diffusivity in the direction of  $\mathbf{e}$ . Note that (27) is easily checked if  $\mathbf{v}$  is explicitly given:

$$\langle (\mathbf{j} \cdot \mathbf{e}) \rangle_s = \tau \langle (\mathbf{v} \cdot \mathbf{e}) \rangle_s$$

In [18] 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 [23]. These authors also make a connection between the accelerator mode islands and lobe dynamics, as developed in [24]. Karney, Rechester, and White in [11] used heuristic methods to derive the above result for the special case in which P is the standard map.

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 that are usually called *cellular*. These are spatially periodic velocity fields for which the streamlines  $x = nL_x$  and  $y = mL_y$ ,  $m, n \in \mathbb{N}$  separate cells inside which the velocity field is composed of closed streamlines surrounding an elliptic fixed point. A particular example of such a velocity field is given by the streamfunction

$$\psi = \sin(2\pi x)\sin(2\pi y).$$

It is a well-known result (see [10] and the references therein) that for such a velocity field

$$\frac{\mathbf{D}\mathbf{e}\cdot\mathbf{e}}{D}\sim\sqrt{Pe} \quad \text{as } Pe\to\infty.$$

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  $\epsilon$  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 [22]) we know that, for small enough  $\epsilon$ , and under the nondegeneracy "twist" condition, there are invariant circles surrounding the elliptic fixed point. Assume

(28) 
$$\langle \mathbf{v}^p(\mathbf{x},t) \cdot \mathbf{e} \rangle \neq 0,$$

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 cannot 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. 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 (28) 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 (26)

(29) 
$$\frac{\mathbf{D}\mathbf{e}\cdot\mathbf{e}}{D} \sim Pe^2 \quad \text{as } Pe \to \infty.$$

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

52

provide 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 a two-dimensional, spatially and time-periodic perturbation of a cellular velocity field, satisfying (28). The time scales for integration of (1) such that the scaling in (29) is obtained should typically be very long  $(\mathcal{O}(1/\epsilon))$  for  $\epsilon$  small.

**4.3.** An oscillatory shear flow. Zeldovich [30] and Young, Rhines, and Garrett [29] consider the following velocity field:

(30) 
$$\mathbf{v}(\mathbf{x},t) = (2v\cos ky\cos\omega t,0),$$

where v, k, and  $\omega$  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:

(31) 
$$\frac{\mathbf{D}\mathbf{e}_x \cdot \mathbf{e}_x}{D} = D\left(1 + \frac{v^2 k^2}{\omega^2 + D^2 k^4}\right).$$

Because of the simplicity of the velocity field (30), the above result for the effective diffusivity is exact. Note that for  $\omega = 0$ , (30) 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 subsection 3.2,  $D_{\mathbf{e}_x}^n \sim t^2$  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 (30) exactly:

$$y(t) = y_0,$$
  

$$x(t) = x_0 + \int_0^t 2v \cos ky_0 \cos \omega \bar{t} d\bar{t}.$$

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 (31) 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 analyse the convection-diffusion equation).

This 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], [18]). **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*, where  $\mathbf{x} = (x, y, z)$  now, and  $\mathbf{v}(\mathbf{x}, t)$  is of the form

$$v_x = \frac{\partial \psi(x, y, t)}{\partial y},$$
  

$$v_y = -\frac{\partial \psi(x, y, t)}{\partial x},$$
  

$$v_z = f(x, y, t).$$

(32)

(see [9] for examples of steady duct velocity fields). Mezić and Wiggins [21] 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 (32) 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 (32) as the cross-section.

We are interested in finding the effective diffusivity in the direction of z,

(33) 
$$\mathbf{D}_{sym}\mathbf{e}_{z}\cdot\mathbf{e}_{z} = D(1 + \langle \nabla\chi^{\mathbf{e}_{z}}\cdot\nabla\chi^{\mathbf{e}_{z}}\rangle),$$

and  $\chi^{\mathbf{e}_z}$  satisfies

(34) 
$$\frac{\partial \chi^{\mathbf{e}_z}}{\partial t} + (\langle \mathbf{v} \rangle + \mathbf{v}') \cdot \nabla \chi^{\mathbf{e}_z} - D \triangle \chi^{\mathbf{e}_z} = -\mathbf{v}' \cdot \mathbf{e}_z = v'_z,$$

where  $\langle \cdot \rangle$  still denotes an average over A, and fluctuating quantities are denoted by  $(\cdot)'$ . Equation (34) is of the same form as (7), and it is easily seen that the condition for maximal diffusivity in the direction of z reads

(35) 
$$(v_z)^*$$
 is not a constant almost everywhere,

where \* denotes the time average under the flow on A generated by the suspension of the x - y components of (32) over A. In terms of the Poincaré map, (35) becomes

(36) 
$$(j_z)^*$$
 is not a constant almost everywhere,

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 (32), with  $f(x,y) = \psi(x,y)$ , discussed in [15], and time-periodic velocity fields. In particular, it was concluded in [15] that steady velocity fields of the type

$$\mathbf{v} = \left(rac{\partial\psi(x,y)}{\partial y}, -rac{\partial\psi(x,y)}{\partial x}, \psi(x,y)
ight)$$

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 (35) the maximal effective diffusivity in this case can be understood through the fact that  $\psi$  partitions the cross section (x - y) of the duct velocity field into streamlines (i.e., the x - y

54

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  $\epsilon$  is a small parameter. The cross section of the unperturbed duct velocity field  $\mathbf{v}(x, y)$  might posess some separating streamlines. Under the time-dependent perturbations these streamlines can break. It is widely believed that there is a neighborhood of these streamlines for small  $\epsilon$  such that the perturbed cross section is ergodic in that neighborhood (this has been proven for some very simple cases, see [27], [28]). 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,  $\epsilon$  is increased, a larger portion of A might become ergodic, ultimately leading to 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 [15].

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 §4.

Acknowledgments. We thank Albert Fannjiang for useful discussions.

#### REFERENCES

- M. AVELLANEDA AND A. J. MAJDA, Stieltjes integral representation and effective diffusivity bounds for turbulent transport, Phys. Rev. Lett., 62 (1989), pp. 753–755.
- [2] —, An integral representation and bounds on the effective diffusivity in passive advection by laminar and turbulent flows, Comm. Math. Phys., 138 (1991), pp. 339–391.
- [3] A. BENSOUSSAN, J. L. LIONS, AND G. C. PAPANICOLAOU, Asymptotic Analysis for Periodic Structures, North-Holland, Amsterdam, 1978.
- [4] R. BHATTACHARYA, A central limit theorem for diffusions with periodic coefficients, Ann. Probab., 13 (1978), pp. 385–396.
- [5] R. N. BHATTACHARYA, V. K. GUPTA AND, H. F. WALKER, Asymptotics of solute dispersion in periodic porous media, SIAM J. Appl. Math., 49 (1989), pp. 86–98.
- [6] H. BRENNER, Dispersion resulting from flow through spatially periodic porous media, Philos. Trans. Roy. Soc. London Ser. A, A297 (1980), pp. 81–133.
- [7] L. H. DILL AND H. BRENNER, A general theory of Taylor dispersion phenomena. V. Timeperiodic convection, PhysicoChemical Hydrodynamics, 3 (1982), pp. 267–292.
- [8] ——, Dispersion resulting from flow through spatially periodic porous media-III. Timeperiodic processes, PhysicoChemical Hydrodynamics, 4 (1983), pp. 279–302.

- [9] J. G. FRANJIONE AND J. M. OTTINO, Stretching in duct flows, Phys. Fluids A, 3 (1991), pp. 2819–2821.
- [10] A. FANNJIANG, AND G. C. PAPANICOLAOU, Convection enhanced diffusion for periodic flows, SIAM J. Appl. Math., 54 (1994), pp. 333–408.
- [11] C. F. F. KARNEY, A. B. RECHESTER, AND R. B. WHITE, Effect of noise on the standard mapping, Physica D, 4 (1982), pp. 425–438.
- [12] A. I. KHINCHIN, Mathematical Foundations of Statistical Mechanics, Dover, New York, 1949.
- [13] D. L. KOCH AND J. F. BRADY, The symmetry properties of the effective diffusivity tensor in anisotropic porous media, Phys. Fluids, 30 (1987), pp. 642–650.
- [14] D. L. KOCH, R. G. COX, H. BRENNER, AND J. F. BRADY, The effect of order on dispersion in porous media, J. Fluid Mech., 200 (1989), pp. 173–188.
- [15] A. J. MAJDA AND R. M. MCLAUGHLIN, The effect of mean flows on enhanced diffusivity in transport by incompressible periodic velocity fields, Stud. Appl. Math. 89 (1993), pp. 245– 279.
- [16] R. MAÑE, Ergodic Theory and Differentiable Dynamics, Springer-Verlag, New York, Heidelberg, Berlin, 1987.
- [17] R. MAURI, Dispersion, convection and reaction in porous media, Phys. Fluids A, 3 (1991), pp. 743–756.
- [18] I. MEZIĆ AND S. WIGGINS, Birkhoff's ergodic theorem and statistical properties of dynamical systems with applications to fluid mechanical dispersion and mixing, preprint, California Institute of Technology, Pasadena, CA.
- [19] —, On the dynamical origin of asymptotic t<sup>2</sup> dispersion of a non-diffusive tracer in incompressible laminar flows, Phys. Fluids A, 6 (1994), pp. 2227–2229.
- [20] —, On the dynamical Origin of Asymptotic n<sup>2</sup> Diffusion in a Class of Volume Preserving Maps, Phys. Rev. E., accepted for publication.
- [21] —, On the integrability and perturbation of three-dimensional fluid flows with symmetry, J. Nonlinear Sci., 4 (1994), pp. 157–194.
- [22] J. MOSER, Stable and Random Motions in Dynamical Systems, Princeton University Press, Princeton, NJ, 1973.
- [23] K. OUCHI AND H. MORI, Anomalous diffusion and mixing in an oscillating Rayleigh-Benard flow, Progress Theoret. Phys., 88 (1992), pp. 467–484.
- [24] V. ROM-KEDAR AND S. WIGGINS, Transport in two-dimensional maps, Arch. Rat. Mech. Anal., 109 (1989), pp. 239–298.
- [25] A. M. SOWARD AND S. CHILDRESS, Large magnetic Reynolds number dynamo action in a spatially periodic flow with mean motion, Philos. Trans Roy. Soc. London Ser. A, 331 (1990), pp. 649–733.
- [26] S. WIGGINS, Introduction to Applied Nonlinear Dynamical Systems and Chaos, Springer-Verlag, New York, Heidelberg, Berlin, 1990.
- [27] M. WOJTKOWSKI, A model problem with the coexistence of stochastic and integrable behaviour, Comm. Math. Phys., 80 (1981), pp. 453–464.
- [28] ——, On the ergodic properties of piecewise linear perturbations of the twist map, Ergodic Theory Dynamical Systems, 2 (1982), pp. 525-542
- [29] W. R. YOUNG, P. B. RHINES, AND C. J. R. GARRETT, Shear-flow dispersion, internal waves and horizontal mixing in the ocean, Journal of Physical Oceanography, 12 (1982), pp. 515– 527.
- [30] I. B. ZELDOVICH, Exact solution of the diffusion problem in a periodic velocity field and turbulent diffusion, Dokl. Akad. Nauk SSSR, 266 (1982), pp. 821-826.