Analysis of passive scalar advection in parallel shear flows: Sorting of modes at intermediate time scales

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(Received 15 April 2010; accepted 9 August 2010; published online 4 November 2010)

The time evolution of a passive scalar advected by parallel shear flows is studied for a class of rapidly varying initial data. Such situations are of practical importance in a wide range of applications from microfluidics to geophysics. In these contexts, it is well-known that the long-time evolution of the tracer concentration is governed by Taylor's asymptotic theory of dispersion. In contrast, we focus here on the evolution of the tracer at *intermediate* time scales. We show how intermediate regimes can be identified before Taylor's, and in particular, how the Taylor regime can be delayed indefinitely by properly manufactured initial data. A complete characterization of the sorting of these time scales and their associated spatial structures is presented. These analytical predictions are compared with highly resolved numerical simulations. Specifically, this comparison is carried out for the case of periodic variations in the streamwise direction on the short scale with envelope modulations on the long scales, and show how this structure can lead to "anomalously" diffusive transients in the evolution of the scalar onto the ultimate regime governed by Taylor dispersion. Mathematically, the occurrence of these transients can be viewed as a competition in the asymptotic dominance between large Péclet (Pe) numbers and the long/short scale aspect ratios ($L_{\text{Vel}}/L_{\text{Tracer}} \equiv k$), two independent nondimensional parameters of the problem. We provide analytical predictions of the associated time scales by a modal analysis of the eigenvalue problem arising in the separation of variables of the governing advection-diffusion equation. The anomalous time scale in the asymptotic limit of large k Pe is derived for the short scale periodic structure of the scalar's initial data, for both exactly solvable cases and in general with WKB analysis. In particular, the exactly solvable sawtooth flow is especially important in that it provides a short cut to the exact solution to the eigenvalue problem for the physically relevant vanishing Neumann boundary conditions in linear-shear channel flow. We show that the life of the corresponding modes at large Pe for this case is shorter than the ones arising from shear free zones in the fluid's interior. A WKB study of the latter modes provides a longer intermediate time evolution. This part of the analysis is technical, as the corresponding spectrum is dominated by asymptotically coalescing turning points in the limit of large Pe numbers. When large scale initial data components are present, the transient regime of the WKB (anomalous) modes evolves into one governed by Taylor dispersion. This is studied by a regular perturbation expansion of the spectrum in the small wavenumber regimes. © 2010 American Institute of Physics. [doi:[10.1063/1.3491181](https://doi.org/10.1063/1.3491181)]

I. INTRODUCTION

The advection-diffusion of a passive scalar is a pivotal problem in mathematical physics, the intense efforts spent on the subject are witnessed by the large amount of literature (an overview of theoretical developments with applications can be found, for instance, in Ref. 1, see also the recent survey² on turbulent mixing). A number of factors can characterize the complexity of the problem (e.g., dimensionality, structure of the velocity field, and boundary conditions) but much insight can be gained by focusing on simplified flow configurations, where essential mechanisms can be isolated and made amenable to complete mathematical analysis. In this work, we focus on simple steady parallel shear flows, where we manage to characterize the interplay between arbitrary tracer scales, advection, and diffusion.

An example of flows in this class is of course the one considered in the seminal work by Taylor.³ Since then, only some attention has been paid to the full evolution from initial

data to the long-time limiting behavior, which is governed by a one-dimensional renormalized diffusion equation and thus allows for a concise description of the evolution. The finite-time features of the problem have been considered by some authors focusing on the identification of transient stages acting on intermediate time scales. Transient dynamics can be physically relevant in many situations. For example, the dispersion of pollutants in rivers¹ can occur at very large values of Péclet number, thus delaying the onset of the Taylor regime beyond those times that are physically relevant for, e.g., monitoring purposes. Furthermore, passive scalar dynamics can show up in more general contexts where intermediate time evolution becomes the focus of interest. Examples include the studies by Spiegel and Zalesky⁴ and Doering and Horsthemke⁵ that recognize eigenmodes of the advection-diffusion problem to be a basic ingredient in the stability analysis of an advection-diffusion-reaction system.

By using a free-space solution introduced by Lighthill,⁶

Latini and Bernoff⁷ have studied the complete evolution of δ -function initial data in axially symmetric parabolic shears, and compared this solution with short-time asymptotics and stochastic simulations. These authors have shown that the solution exhibits two different time scales, marking the separation between three different regimes of dispersion: bare molecular diffusivity, anomalous superdiffusion, and Taylor dispersion. The first time scale is well-known to be very dependent on initial conditions, as Camassa *et al.*⁸ have rigorously shown for pipe flows; the second one is often close to the cross-stream diffusive time r^2/D (where r is the pipe diameter and D the diffusivity). Since one focus of our investigation is the questioning of r^2/D as the universal time scale that marks the transition into the Taylor regime, we will refer to the time scale in which the homogenized equation becomes a good approximation to the evolution as the “Taylor regime time scale,” to be distinguished from the above diffusive time scale in the cross-stream direction.

The behavior is very different if the passive scalar possesses some intrinsic scale, such as that arising by imposing periodic boundary conditions. The coupling between convection and bare molecular diffusion in such setups can still result in overall anomalous diffusion, but distinguished from the classical Taylor regime due to the existence of long-lived modes⁹ (see also Ref. 10 for scaling arguments). Camassa *et al.*⁹ have recently considered this category of flows in a study aimed at investigating the effect of shear on the statistical evolution of a random, Gaussian, and small scale distribution of dye. They observed that the probability distribution function (PDF) migrates toward an intermittent regime (stretched-exponential tailed PDF). The physical picture that emerged was as follows. The scalar was first seen to experience an initial phase of stretching and filamentation, with fluctuations most efficiently suppressed within regions of high shear. This is the “rapid expulsion” mechanism in Rhines and Young.¹⁰ In a subsequent stage, the longest-lived concentration of dye was near shear-free regions, where some equilibrium between stretching and diffusion limits further distortion. This stage of the evolution was attributed to be the collapse of the system onto a ground-state eigenmode of an associated spectral problem. This suggests that such a “modal phase” of the evolution could play a role in nonperiodic problems on intermediate time scales, and we explore such scenario in the bulk of this paper. We remark that this viewpoint is also used by Sukhatme and Pierrehumbert,¹¹ who described the scalar evolution with more complex velocity fields in terms of emerging self-similar eigenmodes.

Our study of the modal evolution of an advected passive tracer at intermediate time scales is organized as follows. In Sec. II, the formulation of the eigenvalue problem derived from the advection-diffusion equation is presented. This will lead to a periodic second order nonself-adjoint operator. While the spectral theory for second order self-adjoint periodic equations (Floquet theory) is rather complete,¹² for the more general case the full characterization of the spectrum is in general an open question (which has recently been examined in the context of the so-called $\mathcal{PT}$ -symmetry in quantum theory, where however most of the attention is focused only on the real part of the spectrum, see for example,

Bender *et al.*,¹³ and some existence results for complex spectrum have been obtained by Shin¹⁴). Here we derive simple bounds for the complex spectrum, while in Sec. III, we characterize the ordering of modes in three classes depending on the interplay of advection with diffusion dictated by the limits $\epsilon \rightarrow \infty$ and $\epsilon \rightarrow 0$, where $\epsilon = 1/(k \text{ Pe})$. The limit $\epsilon \rightarrow 0$ is further classified into two categories depending on the relative ordering with respect to the balance $k = O(\text{Pe}^\alpha)$ where the exponent α is shown to depend on the smoothness properties of the velocity profile. In the first limit ($\epsilon \rightarrow \infty$), a straightforward regular perturbation expansion suffices to compute the spectrum, spanning the Taylor regime. In the second limit ($\epsilon \rightarrow 0$), for the simplest cases such as piecewise linear shear layers, the analysis can be worked using exact techniques (presented in Appendix B), while for more general cases, we use WKB asymptotics (such method has proved to be useful in self adjoint problems, such as those arising in quantum mechanics). We further discuss how this exactly solvable, piecewise-linear shear actually provides a shortcut to the exact solution for the physically relevant case involving vanishing Neumann boundary conditions, and gives rise to thin boundary layers and decay rates scaling such as $\epsilon^{1/3}$ as $\epsilon \rightarrow 0$. In contrast, we establish the different scalings of $\epsilon^{1/4}$ and $\epsilon^{1/2}$ for the spatial internal layers and their decay rates, respectively, for generic locally quadratic shear flows.

In Sec. IV, we present a study of the passive scalar evolution comparing the theoretical predictions with numerical simulations. We test the predictive capabilities of the theory on a set of numerical experiments focusing on both single- and multiscale initial data. In particular, the theory identifies new intermediate time scales, which are missed by classical moment analysis, and connects them to the spatial scales of the initial data. By manipulating the initial data, we can extend the transient features associated with these intermediate time scales beyond the Taylor time scale r^2/D .

II. THE EIGENVALUE PROBLEM

The advection-diffusion equation, assuming the velocity field to be a parallel shear, is

$$T_t + u(y)T_x = \text{Pe}^{-1} \nabla^2 T, \quad (1)$$

with $\nabla^2 = (\partial^2/\partial x^2, \partial^2/\partial y^2)$. We consider the problem to be periodic in the cross-flow direction y , and it is understood a nondimensionalization based on the maximum velocity U and on a vertical length scale L_{vel} of the shear in such a way to fix the y period as 2π . The Peclet number Pe is based on such scales and on the molecular diffusivity D , and it measures the relative importance of advection and diffusion. The velocity field is a parallel shear layer with velocity pointing along x and dependent on y .

We assume that the initial data $T(x, y, 0)$ admits a Fourier integral representation with respect to x , linearity and homogeneity in x guarantee the different Fourier components to be uncoupled. A solution of Eq. (1) is expanded as

$$T(x, y, t) = \int_{-\infty}^{\infty} dk \sum_{n=0}^{\infty} a_n(k) \psi_n(y, k) e^{\omega_n t + i k x}, \quad (2)$$

being $\psi_n(y)$, the eigenfunction basis associated with the wavenumber k , and ω_n , the corresponding complex frequency. The freedom in k introduces a second length scale L_{Tracer} , which is connected to the initial data on Eq. (1). Using Eq. (2) into the evolution equation, and projecting onto the adjoints, the eigenfunctions are found to satisfy

$$[\omega + iku(y)]\psi = \text{Pe}^{-1}(-k^2\psi + \psi_{yy}).$$

Introducing

$$\epsilon = 1/(k \text{ Pe}), \quad \lambda = \omega/k + k^2\epsilon,$$

we finally write the periodic eigenvalue problem in normalized form

$$\begin{cases} \epsilon \psi_{yy} = [\lambda + iu(y)]\psi, \\ \psi(-\pi) = \psi(\pi), \end{cases} \quad (3)$$

for the eigenfunction $\psi(y)$ and the eigenvalue λ .

Notice that when the solution of Eq. (1) is real, the eigenvalue-eigenfunction pairs satisfy

$$\lambda(\epsilon) = \lambda^*(-\epsilon), \quad \psi(\epsilon) = \psi^*(-\epsilon),$$

(here superscript $*$ indicates the complex conjugate). Note that without loss of generality ϵ can be regarded as a positive definite quantity.

A. Exact estimates on λ

It is possible to show *a priori* that λ can lie only inside an horizontal strip of the complex plane. Writing separately the real and imaginary parts $\lambda = \lambda_R + i\lambda_I$, we intend to establish that

$$\lambda_R < 0, \quad -1 < \lambda_I < 1. \quad (4)$$

Multiplying both sides of Eq. (3) by ψ^* , and summing each side of the resulting equation to the adjoint part is obtained by the relation

$$(\psi^* \psi_y + \psi \psi_y^*)_y - 2|\psi_y|^2 = 2\epsilon^{-2} \lambda_R |\psi|^2.$$

Integrating over the period P , we have

$$-\int_P |\psi_y|^2 dy = \epsilon^{-2} \lambda_R \int_P |\psi|^2 dy,$$

which implies the first one of Eq. (4). If, otherwise, we repeat the procedure subtracting the adjoint part, we obtain

$$(\psi^* \psi_y - \psi \psi_y^*)_y = 2\epsilon^{-2} (\lambda_I + u) |\psi|^2,$$

and the integration now yields

$$\int_P (\lambda_I + u) |\psi|^2 dy = 0.$$

Such an expression implies that, in order for the integral to vanish, the quantity $\lambda_I + u$ has to change sign within P . Hence $\lambda_I = u(\xi)$ for some $\xi \in P$ and the second one of Eq. (4) follows.

III. THREE CLASSES OF MODES

The problem (3) can be studied in the two possible asymptotic limits $\epsilon \rightarrow 0$ and $\epsilon \rightarrow \infty$. Thinking in terms of Pe , large but fixed, this represents a subdivision of the modes into a high- and a low-wavenumber category with qualitatively different properties. For k small enough we expect to find a class of modes that behave in agreement with the Taylor renormalized-diffusivity theory, and that belongs to the realm of homogenization theory. Within the solutions of Eq. (3) in the $\epsilon \rightarrow \infty$ limit will be found a class referred as Taylor modes. In the opposite limit (as we shall see later), the problem otherwise acquires a WKB structure, in this case we shall use the term WKB- or anomalous modes. We stress that the latter class of modes is more correctly to be considered as an intermediate-asymptotic category. Indeed, letting $k \rightarrow \infty$, diffusivity will, at some point, eventually dominate over the eigenvalue λ . This regime will be discussed as the pure-diffusive mode.

A. The limit $\epsilon \rightarrow \infty$: Taylor modes

In such limit, if the following expansions in ϵ are assumed:

$$\psi_n = \sum_{j=0}^{+\infty} \epsilon^{-j} \psi_{nj}, \quad (5)$$

$$\lambda_n = \sum_{j=0}^{+\infty} \epsilon^{-j+1} \lambda_{nj}, \quad (6)$$

then a regular perturbation problem is found. The use of the above expansion inside the eigenvalue problem (3) leads to a classical recursive system of equations

$$O(\epsilon): \mathcal{L}[\lambda_{n0}] \psi_{n0} = 0,$$

$$O(1): \mathcal{L}[\lambda_{n0}] \psi_{n1} = [\lambda_{n1} + iu(y)] \psi_{n0},$$

$\vdots$

$$O(\epsilon^{1-m}): \mathcal{L}[\lambda_{n0}] \psi_{nm} = (\lambda_{n1} + iu(y)) \psi_{nm-1}$$

$$+ \sum_{p=1}^{m-1} \lambda_{np+1} \psi_{nm-p-1},$$

where $\mathcal{L}[\lambda_n] = d^2/dy^2 - \lambda_n$. The same recursive problem was also derived by Mercer and Roberts,¹⁵ whose starting point was a center manifold approach. At $O(\epsilon)$, and normalizing to unitary L_2 -norm $\|f\|^2 = \int_{-\pi}^{\pi} f^2 dx$, we have

$$\begin{aligned} \psi_{n0} &= \cos ny / \sqrt{\pi}, & \lambda_{n0} &= -n^2, & (n > 0) \\ &= 1/\sqrt{2\pi}, & &= 0, & (n = 0), \end{aligned} \quad (7)$$

for symmetric modes, and

$$\psi_{n0} = \sin ny / \sqrt{\pi}, \quad \lambda_{n0} = -\left(\frac{n+1}{2}\right)^2, \quad (n \geq 0), \quad (8)$$

for the asymmetric ones.

The longest-lived of all the above modes is the $n=0$ element in the symmetric class. This will be referred as the

Taylor mode. The corresponding eigenvalue is smaller than $O(\epsilon)$, hence it requires us to proceed to higher orders to compute it. It turns out also to be the only eigenvalue with nontrivial regularly diffusive scaling.

Corrections to the eigenvalue are given by the solvability condition which the right-hand side is enforced to satisfy at any higher order. At $O(1)$ and $O(\epsilon^{-1})$, these are

$$\lambda_{n1} = -[iu(y), 1],$$

$$\lambda_{n2} = -\{[\lambda_{n1} + iu(y)]\psi_{n1}, 1\},$$

where the notation $(\cdot, \cdot)$ denotes the standard inner product. The first equation expresses the physical fact that Taylor modes travel with the mean flow speed. This corresponds to purely imaginary λ_{n1} that is the phase speed of the mode. The second equation yields a real decay rate. For a cosine profile homogenization theory would yield the renormalized diffusivity $D_{\text{eff}} = (1/2)U^2 L_{\text{vel}}^2 / D$. Here this corresponds to $n=0$, which after some algebra yields $\lambda_{01}=0$ and $\lambda_{02}=-1/2$.

To summarize, in the Taylor modes limit $\epsilon \rightarrow \infty$ eigenvalues are given by

$$\lambda_n \sim \begin{cases} -\epsilon n^2 + O(\epsilon^{-1}), & n > 0 \\ -\frac{1}{2}\epsilon^{-1} + O(\epsilon^{-2}), & n = 0, \end{cases} \quad (9)$$

up to the first nontrivial order.

B. The limit $\epsilon \rightarrow 0$: Anomalous modes

As $\epsilon \rightarrow 0$, we expect to find a class of modes in which the ground-state element reproduces the long-lived structures observed in a periodic domain of $O(1)$ period, at large Pe by Camassa *et al.*⁹ We employ a different approach from the regular perturbation expansion adopted for the Taylor modes. Asymptotics are obtained via WKBJ method. At first, this is done to generalize the classical matched-asymptotics calculation for real, self-adjoint operators (in the classical literature often referred as the two-turning-point problems as seen in Ref. 16). Here, however, the nonself-adjoint character of the problem presents additional complication and a refinement of the technique is required. A second time, a regularized variant of the method is derived and the accuracy of the two approaches is compared. Before developing the asymptotic analysis, we introduce two particular exactly solvable cases.

1. Exactly solvable linear case

The first exactly solvable special case consists in a nonanalytic “sawtooth” shear profile (with full details reported in Appendix B). Eigenfunctions in this case are constructed using piecewise patched Airy functions, and eigenvalues correspond to zeros of certain combinations of these functions that can then be computed with systematic asymptotics. The end result is that the decay rate scales as $O(\epsilon^{1/3})$, a boost over the bare diffusivity $O(\epsilon)$. Such scaling is also obtained by Childress and Gilbert¹⁷ for a linear-shear channel with homogeneous Dirichlet boundary conditions for the scalar (which would correspond to the case of antisymmetric modes in our setup). We emphasize that this scaling differs

FIG. 1. Ground-state mode for $\epsilon=10^{-3}$ ($k=0$, $Pe=1000$, comparison between cosine $u(y)=\cos(y)$ and sawtooth $u(y)=1-|y|$ shear profiles, respectively, top and bottom pictures. For the cosine flow case, the eigenfunction is constructed using Hermite uniform asymptotic approximation, for the sawtooth it is computed exactly using Airy functions (discussed in the text).

from the generic case involving an analytic shear flow, whose decay rate scales as $O(\epsilon^{1/2})$ as we show next. We remark that such differences are physically consistent. As mentioned in Sec. I, shear enhances diffusion and hence the absence of shear-free regions yields, in fact, for large Pe, a stronger damping of the modes. Nonetheless, perhaps surprisingly, even in this case a long-lived mode persists around the corners, which has a counterpart in the analytic case in the near shear-free regions as shown numerically in Ref. 9. However, as also shown in Appendix B, the eigenfunctions localize to a thinner region that scales such as $O(\epsilon^{1/3})$ as opposed to $O(\epsilon^{1/4})$ for the analytic case, confirming previous numerical findings in Ref. 9 (this comparison is depicted in Fig. 1, where the corresponding long-lived modes have the appearance of “chevrons” elongated in the streamwise direction).

While the sawtooth shear profile is amenable to exact analysis, one may think that its physical significance would be per se limited. However, note that the symmetric subclass of the sawtooth eigenfunctions are exact solutions for the problem involving a linear shear between two impermeable walls ($T_y=0$ there), and hence the present analysis is physically relevant. Moreover, the analysis of the sawtooth brings forth the true essence of the boundary conditions’ effect. Generically, all flows near a nonslip flat wall will localize as (weakly nonparallel) linear shear and hence the sawtooth theory predicts the main structures of the scalar’s wall-boundary layer. This emerges clearly in the case of Poiseuille flow in a channel, shown below in Fig. 2, following the asymptotic treatment below.

2. Exactly solvable cosine shear

Our second example of an exactly solvable case is $u(y)=\cos y$. The eigenvalue problem (3) in this case reduces to the complex Mathieu equation

FIG. 2. (Color online) Snapshots of the time evolution governed by Eq. (1) with $u(y)=1-4(y-1/2)^2$ and $Pe=10^3$ from the initial condition $T_0(x,y)=\exp(-(x-L_x/2)^2/\ell_x^2)$, with $\ell_x=10^{-3/2}L_x$, and horizontal Fourier period $L_x=20\pi$, with $n_x=1024$ and $n_y=128$, respectively, for horizontal and vertical Fourier modes. Neumann boundary conditions $T_y(0)=T_y(1)=0$ are enforced by even symmetry with respect to the $y=0$ and $y=1$ horizontal boundaries. The localization of the tracer near the walls and the center of the channel is evident as are the different speeds and decay rates for these two regions (the peaks are normalized by the scalar's maximum).

$$\epsilon \psi_{yy} = (\lambda + i \cos y) \psi, \quad (10)$$

whose eigenfunctions can be written as

$$\psi(y) = S(a, b, y/2),$$

where S is the π -periodic Mathieu function and $b = -2i/\epsilon$, $a = -4\lambda/\epsilon$. However asymptotics in the $\epsilon \rightarrow 0$ limit are not immediately available for these functions, and it is more convenient to resort to WKBJ methods.

3. WKBJ analysis

We next examine analytic shear profiles which can be analyzed approximately with asymptotic WKBJ theory. Since the long-lived structures localize around the extrema of $u(y)$, we shall express the phase velocity of the WKBJ modes as a perturbation about y_e , the location of a maximum/minimum of $u(y)$. Moreover, because for the cosine-flow $u(y_e) = \pm 1$, we seek λ in the form

$$\lambda \sim a\epsilon^p + i(b\epsilon^q - 1), \quad \text{as } \epsilon \rightarrow 0. \quad (11)$$

In our derivation, we use a free-space approximation. Since we are interested in spatially localized eigenmodes, which are rapidly vanishing away from the extrema of $u(y)$, we shall drop the periodic boundary conditions in favor of a decay condition of the eigenfunctions.

a. Eigenvalues from singular WKBJ solution. Turning points play a crucial role in this analysis. These are defined as those points in the complex plane where $[\lambda + i \cos(y)] = q(y; \lambda) = 0$. Since we are concerned with eigenvalues following the scaling given in Eq. (11), as $\epsilon \rightarrow 0$, we will have two turning points approaching $y=0$ symmetrically with respect to the origin, which correspond to simple roots of q , left and right turning points being denoted as y_L and y_R ,

respectively (see Fig. 16).

The eigenvalue condition for complex turning points given by the WKBJ method appears as a natural extension of the well-known result for self-adjoint problems, where the turning points lie on the real line.¹⁶ Since its derivation is quite involved, it is reported separately in Appendix A. The WKBJ approximation of the eigenvalue λ_{WKB} is determined by the integral condition

$$\exp\left(\epsilon^{-1/2} \int_{\gamma} q(\zeta; \lambda_{\text{WKB}})^{1/2} d\zeta\right) = \pm i, \quad (12)$$

where γ is an arbitrary path in the complex plane connecting y_L to y_R without looping around one of them [because of the multivaluedness of $q(\zeta; \lambda)^{1/2}$]. Equation (12) can be rewritten as

$$\int_{\gamma} q(\zeta; \lambda_{\text{WKB}})^{1/2} d\zeta = i\epsilon^{1/2} \pi \left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \dots, \quad (13)$$

which constitutes an implicit relation for a set of eigenvalues λ_{WKB} , corresponding to even (odd) eigenmodes for n even (odd). The left-hand side is a function of λ_{WKB} that involves an integral of the elliptic kind, of which the limits of integration contain themselves a dependence from λ_{WKB} . Such relation can be inverted only numerically.

In order to make any analytical progress one could perform a Taylor expansion of $q(\zeta; \lambda_{\text{WKB}})$, which once truncated would yield an explicitly integrable form. Such possibility will not be pursued here, but in Sec. III B 3 b, it will be related to the result obtained therein. We observe instead that condition (13), even as it stands, unveils the scaling expo-

TABLE I. Approximate and exact eigenvalues, with percentage error on the quantity $\lambda + i$.

		$-\lambda_{\text{WKB}}$ (err %)	$-\lambda_{\text{H}}$ (err %)	$-\lambda_{\text{Exact}}$
$\epsilon = 10^{-1}$	$n=0$	0.154 96+0.841 85 (2)	0.158 11+0.841 89i (4)	0.151 73+0.841 75i
	$n=2$	0.708 81+0.204 48i (2)	0.790 57+0.209 43i (9)	0.724 12+0.208 84i
$\epsilon = 10^{-2}$	$n=0$	0.049 69+0.949 99i (0.6)	0.050 00+0.950 00i (1.2)	0.049 37+0.949 99i
	$n=2$	0.242 07+0.749 87i (0.1)	0.250 00+0.750 00i (3)	0.241 74+0.749 85i
$\epsilon = 10^{-3}$	$n=0$	0.015 78+0.984 19i (0.2)	0.015 81+0.984 19i (0.4)	0.015 75+0.984 19i
	$n=2$	0.078 27+0.920 94i (0.04)	0.079 06+0.920 94i (1)	0.078 24+0.920 94i

nents p and q in Eq. (11). Both the integrand and the measure of the integration path γ are in fact $O(\sqrt{\lambda+i})$, which gives $O[\epsilon^{-1/2}(\lambda+i)]=1$, and it follows $p=q=1/2$.

b. Eigenvalue condition from uniform approximation. The fundamental drawback of WKBJ for eigenvalue problems lies in the lack of asymptoticity for n fixed, although is typically necessary to consider just $n=3$ to 4 to obtain very accurate results and even for the ground state eigenvalue WKBJ is often a fairly good approximation (see Ref. 16, which can also be a suitable reference for some facts used in the rest of this section). The formal failure of WKBJ can be understood in terms of turning points approaching each other too quickly to allow the solution to be fast after a rescaling that fixes the distance between the turning points to be $O(1)$.

The cosine-shear flow, thanks to its local quadratic behavior, allows an alternative route that does not suffer of the latter problem and has the value of giving a simple explicit expression for the eigenvalues.

As $\epsilon \rightarrow 0$ Hermite functions (or, equivalently, parabolic cylinder functions) can be used to obtain a local inner-layer approximation in a region containing both turning points. Using Hermite functions we can express solutions of the equation

$$\varphi'' + \left(\nu + \frac{1}{2} - \frac{1}{4}z^2\right)\varphi = 0, \quad (14)$$

as

$$\varphi = \text{He}_\nu(\pm z/\sqrt{2})e^{-z^2/4}. \quad (15)$$

He_ν represents the Hermite function of (arbitrary and complex) order ν (see Ref. 18, Sec. 10.2). This is exactly the equation one would find expanding Eq. (10) up to second order about $y=0$ and applying the transformations

$$\epsilon^{1/4}z = 2^{1/4}e^{-i\pi/8}y, \quad (16)$$

$$\nu = \frac{1}{\sqrt{2}}(\lambda + i)\epsilon^{-1/2}e^{i\pi/4} - \frac{1}{2}. \quad (17)$$

We essentially can view Eq. (10) as a perturbation problem regularized by the variable rescaling $\epsilon^{-1/4}y$ for $|y| \ll 1$, with leading-order solutions easily constructed from Eq. (15).

Such solutions can eventually be matched with outer WKBJ solutions to construct global approximants. However, the approximate eigenvalues λ_{H} are determined at the level of the inner problem only, imposing asymptotic decay. Hence, the eigenvalues are just related to those of the Hermite Eq. (14) through the transformation (17). Since the ei-

genvalues ν are determined by the condition that $\psi(y)$ be bounded for $|\epsilon^{-1/2}y| \rightarrow \infty$ along the real axes, one has to account for the phase shift involved in the coordinate transformation (16), and to understand the eigenvalues of Eq. (14) as those values that allow φ to vanish for $|z| \rightarrow \infty$ with $\arg(z) = \pi/8$. It is inferred from the large-argument expansion of Hermite functions that within a $\pi/8$ phase shift of the argument from the real line the character at infinity is not altered, hence the eigenvalues of the Hermite equation would be the same if the problem were posed on the real line. Such eigenvalues are known to be just the integers $\nu=0, 1, 2, \dots$, it is then elementary to verify that

$$\lambda_{\text{H}} = -i - \epsilon^{1/2}(1-i)\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \dots \quad (18)$$

We point out that one would obtain the same result expanding up to second order the integrand in Eq. (13) and explicitly solving the integral via standard residue calculation. This confirms that also in case of complex parabolic potential WKBJ provides exact eigenvalues, as well-known for the real self-adjoint Schrödinger equation.

c. Comparison. A comparison of the two approaches described above is given in Table I. Generally, we obtain good accuracy even for moderately small ϵ , bare WKBJ being always more accurate than the uniform approximation. These results, perhaps unexpected, are ultimately due to the boost of accuracy that WKBJ enjoys with locally parabolic potentials. Such accuracy boost absorbs the small- n deficiency. We also observe that the error shows two opposite trends for n growing at ϵ fixed, decreasing for λ_{WKB} and increasing for λ_{H} , respectively. This can be understood observing that while the WKBJ approximation is asymptotic for large n , the second approach is a completely local approximation, hence suffering from the fact that the eigenfunctions widen as n grows.

d. Poiseuille flow in a channel: Intermediate time mode sorting. All the features in the analysis above come together in the classical case of Poiseuille flow in a channel with walls impermeable to the tracer $T_y=0$. The different decay and propagation rates special to the locally linear and quadratic shear and captured exactly by the sawtooth and cosine flow result in a visible mode sorting during the evolution of a generic initial condition. This is illustrated in Fig. 2, generated by a numerical simulation (details of the algorithm are described below in Sec. IV) of the passive scalar evolution initially concentrated in a thin strip (y -independent) in an effectively infinite long channel are advected by the flow

FIG. 3. Schematics of the periodic extension for channel flow: support of interior and wall modes is determined by the scaling of the imaginary part of the eigenvalues of cosine and linear shear, respectively.

$u(y) = 1 - 4(y - 1/2)^2$ with boundary conditions $T_y(0) = T_y(1) = 0$. By even-periodic extension of the flow in y -direction, the ensuing periodic modes of Eq. (3) may be separated between symmetric and antisymmetric with respect to the wall locations, with the symmetric ones automatically satisfying vanishing Neumann boundary conditions at the walls. Tracer initial data symmetric with respect to the channel centerline are spanned by these symmetric modes. This extension of $u(y)$ is schematically depicted in Fig. 3, which shows how the different asymptotic scalings of the (imaginary) component of $\lambda - iu_m = O(\epsilon^{1/2})$ and $\lambda = O(\epsilon^{1/3})$ give rise to modes supported on regions of size $O(\epsilon^{1/4})$ and $O(\epsilon^{1/3})$, respectively, for the interior and wall mode.

The initial stage of the evolution shows the direct imprint of the shear profile, with the initial distribution of tracer deforming accordingly into a parabolic shape. While such behavior can be expected at startup, it soon evolves into a more interesting form of competition between advection and diffusion. The initial (purely advective) mechanism that bends and stretches the tracer isolines is also acted on by diffusion. This mechanism is progressively enhanced until the two effects equilibrate each other. When such nontrivial balance is achieved the chevronlike structures predicted by the asymptotic analysis can be clearly observed near the wall, as well as the fatter, longer-lived interior chevron associated with quadratic (cosine) shear profile at the center. Observe that the tracer distribution near the wall appears to move, even as the local fluid velocity approaches zero. This is predicted by the modal analysis, as the phase speed (determined by imaginary component of the eigenvalue) $\text{Im } \lambda$ is nonzero.

In Fig. 4, the position of the tracer distribution peak near the wall is shown for the simulation depicted in Fig. 2, and compared with an estimate based on the phase speed given by the sawtooth theory. The tangency at short times of the prediction shows accurate comparison with the simulation, while the increase of velocity corresponds to the migration toward smaller k 's as the diffusion decay kills higher wavenumbers. This is in agreement with the dispersion relation, which shows an increasing phase speed of the wall modes as k decreases. (A similar cascade occurs in the interior.) This interplay of modal decay with the modal phase speed is an interesting problem in its own right, which sheds much

FIG. 4. (Color online) Position of the tracer distribution peak near the wall for the simulation depicted in Fig. 2 compared to the wall-mode theoretical prediction for the phase speed based on the characteristic wavenumber of the initial condition ($k \approx \pi$ for the initial data in the simulation).

needed light on the intermediate scales of data evolution toward the Taylor regime. We will report on this in a separate study.

C. The limit $\epsilon \rightarrow 0$, $k \gg \text{Pe}^{1/3}$: Pure-diffusive modes

The ordering of modes that sees straight diffusivity as the dominant effect at wavenumbers beyond the WKBJ range is a consequence of the large-Pe limit we are considering. When this is not true, the time scale of streamwise molecular diffusion ($\text{Pe}^{-1} k^2$) can overcome anomalous diffusion ($k\lambda$) over the whole k -spectrum, including Taylor scales. The threshold between WKBJ and pure-diffusive modes is simply found comparing the time scale $\text{Pe}^{1/2} k^{-1/2}$ from Sec. III B with the streamwise diffusion scale $\text{Pe} k^{-2}$. Equating the two characteristic times we have

$$k\lambda_R \sim \text{Pe}^{-1} k^2 \Rightarrow k = O(\text{Pe}^{1/3}),$$

implying that the condition for pure-diffusive modes is indeed $\epsilon \rightarrow 0$ with $k \gg \text{Pe}^{1/3}$.

Diffusivity in the streamwise (x) direction is not present in the eigenvalue problem, implying that the spatial structure of pure-diffusive modes remains the same as for the WKBJ modes. However, the contraction of the streamwise wavelength eventually overcomes the effect of the gradient along y .

IV. INITIAL VALUE PROBLEMS

In this section, we shall present, guided by the analysis above, numerical simulations of initial-value problems for the passive scalar evolution. We study the nondimensional advection-diffusion Eq. (1), employing the same numerical scheme as Ref. 9. This is a pseudospectral solver based on Fourier modes in both x and y , with an implicit-explicit third-order Runge-Kutta¹⁹ routine for time marching, that combines explicit treatment of the advective part with an implicit one for the diffusive stiff term. The scheme is anti-aliased by the standard 2/3 rule. By proceeding in successive refinements, we have documented that all simulations presented are well resolved. The computational solution enforces doubly periodic boundary conditions. We first explore

FIG. 5. Snapshots of the time evolution from an initial condition $T_0(x, y) = \cos kx$ for $\epsilon = .001$ ($k=1$, $Pe=10^3$). Concentration field is shown at $t \text{ } Pe^{-1/2} k^{1/2} = 0, .032, .095, 1.89$. While this is a single-mode computation in the streamwise direction, the number of Fourier modes used in the cross-flow direction is $ny=256$.

single-scale initial data and then examine nonperiodic (longitudinal) evolutions using a period much larger than the horizontal extent of the initial data.

A. Single-scale initial data

Using the initial condition $T_0(x, y) = \cos kx$, we want to follow the smearing out of initial fluctuations by the shear flow, focusing in particular on the decay rate of the L_2 -norm, and how it depends on ϵ when this parameter spans the whole range of possible regimes. Let the decay rate $\gamma(t)$ be defined as

$$\gamma(t) = -\frac{d}{dt} \log \|T(x, y, t)\|_2,$$

where $\|\cdot\|_2$ is the standard L_2 -norm over the period. For a pure exponential decay γ would be the constant in the exponent.

First we observe in Fig. 5 some snapshots of the time evolution when the wavenumber is chosen to have ϵ small. In the earlier stage the vertical bands are stretched and reduced into thin filaments where the shear is stronger. From the point of view of eigenmodes, this stage in which the vertical structure is built, corresponds to a collapse of the initial superposition of many eigenfunctions on the ground state mode. Owing to the complexity of the physical structure of eigenfunctions, the modal approach is not very informative at this stage. The temporal decay is faster than exponential: the mechanism of this transient enhanced diffusion is essentially the *fast expulsion* explained by Rhines and Young.¹⁰ Such process terminates when fluctuations are completely suppressed by shear, after which two long lived, chevron-shaped structures localize in thin layers around the

FIG. 6. Snapshots of the time evolution from an initial condition $T_0(x, y) = \cos kx$ for $\epsilon = 10$ ($k=10^{-4}$, $Pe=10^3$). Concentration field is shown at $t \text{ } Pe \text{ } k^2 = 0, .08$. Resolution as for Fig. 5.

shear-free regions. At this stage the decay rate settles on a constant value.

The picture is analogous to the one considered in Ref. 9 for random initial data. The long-time behavior is in fact common to a large class of initial condition with streamwise modulation. In striking contrast on the other hand, are the results obtained when a steady source is added (see Ref. 20). In the latter case, the accumulation of the unmixed dye is seen to take place in the high shear region of the flow. The spectral analysis can provide further information on the source problem. Besides being able to show details of the transient evolution out of general initial data to the regime dictated by the source, the eigenvalues and eigenfunctions can be assembled to produce an exact expression of the Green's function, which could then be analyzed by asymptotic methods. In this regard, we note that the asymptotic scaling of the inner layers in the source problem studied in Refs. 20 and 21, while generically of order $O(\epsilon^{1/3})$ would switch over to scalings of order $O(\epsilon^{1/4})$ if the same source $\cos x$ were made to move at a speed sufficiently close to the maximum fluid velocity, an effect not reported by these prior studies.

Shown in Fig. 6 is the opposite limit of ϵ large. The distribution sets on a Taylor mode with weak dependence from y , which is still visible (right picture) because ϵ is only moderately large.

The decay rate γ is shown in Figs. 7 and 8 as obtained from numerical simulations. These two figures report the same data under different rescaling, to emphasize the ϵ dependence in the behavior. Also, in each figure a reference horizontal line marks the asymptotic decay rates of the WKB and Taylor regimes respectively, obtained from the real part of the ground-state eigenvalue given by Eqs. (18) and (9). At large times, the data limits to one of these constant values depending on whether $\epsilon \ll 1$ or $\epsilon \gg 1$, and the different rescaling demonstrates the collapse. Note that the rescaled γ approaches $1/2$ in both limits (this is only a coincidence happening for the shear profile considered).

When $\epsilon = O(1)$ oscillations appear, particularly evident for $\epsilon = 1$. This phenomenon arises through interaction of the two nonorthogonal ground-state modes, with conjugate eigenvalues corresponding to right- and left-traveling chevron-structures. As long as ϵ is small, the two trains of chevrons are each localized in the respective shear-free regions; this

FIG. 7. Decay rates from numerical simulations as a function of time for different values of ϵ obtained setting $\text{Pe}=1000$ and $k=10^{-p}$ ($p=0:1:5$). Axes are rescaled on WKBJ time scale to show the collapse at $\epsilon \ll 1$ on the decay rate predicted by the WKBJ analysis (marked by the horizontal line at $1/2$). The inset contains the exact computation for $\epsilon=1$ (intermediate value between WKBJ and Taylor regimes) obtained using the two ground-state Mathieu functions.

makes the eigenmodes almost orthogonal. As $\epsilon=O(1)$, one can roughly imagine the modes to be made of wide chevron-structures, now with non-negligible overlap. Here nonorthogonality produces oscillations in the decay rate (essentially a constructive-destructive interference depending on the alignment of the two wave trains). The inset in Fig. 7 shows the exact reconstruction of γ using the two Mathieu ground-state functions, confirming this assertion.

The three regimes of modes are represented collectively in Fig. 9. This figure shows a time-averaged value of γ in which we have excluded the initial transient to better approximate the infinite time average. The averaging procedure can be regarded as a device to obtain a measure of “effective” decay rate even in the cases $\epsilon=O(1)$ manifesting unsteadiness. This quantity can be considered essentially equivalent to $\text{Re}[k\lambda_0]$.

B. Multiscale initial data

In Sec. III, we have seen how streamwise variations of different scales behave under shear-distortion. The homog-

FIG. 8. Decay rates from numerical simulations as a function of time for different values of ϵ , as in Fig. 7. Axes are rescaled on the Taylor time scale to show the collapse at $\epsilon \gg 1$ on the decay rate predicted by the regular perturbation analysis (marked by the horizontal line at $1/2$). For the legend, see Fig. 7.

FIG. 9. Averaged decay rate (see text) vs k from numerical simulations. The lines represent the three asymptotic behaviors of $k\Re[\lambda_0]$, including also three simulations from the pure diffusive regime. Results are for $\text{Pe}=1000$.

enization of an initial condition with multiple scales is now discussed and illustrated with some numerical simulations. We consider initial distributions in the form of slowly modulated wave packets

$$T_0 = (A \sin kx + B) e^{-x^2/\ell_x^2}, \quad (19)$$

which perhaps provides the simplest setup to assess the interplay between two length scales with large separation. We remark that such class of initial conditions captures the essential features of those realizable in simple experimental setups currently under study. Through A and B we can tune the relative participation of high- versus low-frequency components. For simplicity we are only considering two longitudinal length scales, given by k and ℓ_x . We shall keep constant k and ℓ_x , and to observe enough scale separation the latter are chosen such as $k \text{Pe} \ll 1$ and $\text{Pe}/\ell_x \gg 1$. In the following, we present four simulations, where all parameters are listed in Table II. Visualizations of the passive scalar fields at different times are reported in Figs. 10–13.

The general physical picture that emerges is as follows. At early times, the high-frequency components of the initial condition govern the main features of evolution, similar to the x -periodic problem discussed in Sec. III (chevron-shaped structures). The interplay between the two wide-separated length scales contained in the initial data adds further physical features that lie in the subsequent phase of evolution; in general, the small scales are wiped out during a global homogenization stage that could not exist in the strictly periodic problem. The time scale of this wipe-out, the “cross-

TABLE II. Parameters used in numerical simulations. For all of them $k=1$, $\ell_x=800$, and $\text{Pe}=50$; the number of (dealiased) Fourier modes used is $n_x=12\,288$ $n_y=64$. The fundamental wavenumbers are $k_{x0}=0.001$, $k_{y0}=1$. The simulations are periodic in x with a domain large enough to mimic an unbounded domain on the time scale of the simulations.

	A	B
Run 1	1	1
Run 2	0	1
Run 3	1	0
Run 4	1	0.001

FIG. 10. (Color online) Snapshots showing the distribution of the passive scalar for run 1. Only a portion of the domain is shown. Colorbar as in Fig. 2, but ranging from -1 to 1 .

FIG. 11. (Color online) Same as Fig. 10 for run 2.

FIG. 12. (Color online) Same as Fig. 10 for run 3.

FIG. 13. (Color online) Same as Fig. 10 for run 4.

over” time, which corresponds to the time when evolution starts to be governed by the homogenized equation (the definition of Taylor time scale used in this paper), and can be different from the nondimensional cross-flow diffusive time scale $\tau_D = \text{Pe}$.

From a spectral perspective, the decay time of the high-frequency spectral bands is estimated by our WKBJ analysis to be $k^{-1/2} \text{Pe}^{1/2}$. While this time scale is in general shorter than τ_D (for large Pe), the initial data can be such that the relative energy of the high versus low frequency bands [e.g., set by the parameters A and B in Eq. (19)] can make the WKBJ modes observable well beyond τ_D . Further, these differences can be seen by comparing the evolution of moments versus norms, as we show below.

Looking at the snapshots for run 1 one can see that by $t=100$ chevronlike structures are completely depleted. We inquire whether this major structural crossover is a benchmark for the transition to the Taylor regime. Figure 15 (top panel) depicts the crossover as the drop at $t \approx 10$ of the L_2 -norm in run 1 to the nearly constant value given by the slowly evolving case in run 2. Note that the oscillations observed in the bottom image are induced by the nonorthogonality of anomalous modes as discussed in Sec. III.

For further comparison, we consider the second moment of the tracer distribution, which sometimes is used as a diagnostic to detect the onset of the Taylor regime. We display in Fig. 14 the variance-gap $\tilde{\sigma}(t) := \sigma_T(t) - \sigma(t)$, where σ is the variance in x of the distribution integrated in y , and $\sigma_T = 2\pi \text{Pe} t$ is the theoretical law for a Gaussian distribution evolving according to Taylor-renormalized pure diffusion. This onset is clearly seen in Fig. 14. Notice that the variance does not capture differences in the structure of the different runs, since fast fluctuations belong to the high-frequency spectrum, and are thus missed by the variance (but are accounted by the L_2 -norm).

We may conclude that in run 1, the crossover transition has occurred earlier ($t \approx 10$) than τ_D , which at $\text{Pe}=50$ is well completed after $t \approx 200$. Perhaps more emphatic on this point is the comparison with the last two runs. In run 3, the initial condition is chosen to have zero mean; thus the decay rate γ [reported in Fig. 15 (bottom)] settles on a constant value (predictable from WKBJ eigenvalues as shown previously),

and the crossover transition to the Taylor regime does not occur at all. In run 4, where the initial data are chosen with a small mean, a clear crossover transition occurs at $t \approx 50$, i.e., deferred respect to run 1 (notice how chevrons are still identifiable in the latest time in Fig. 13).

The difference that stands between the transition at time τ_D and the smearing out of fast scales is further illustrated by looking at run 2. Even at large scales, hence at low wave-numbers, the weak longitudinal variations $O(1/\ell_x)$ combine with the shear to build a weak vertical structure departing from the vertically homogeneous initial condition. The cross-stream diffusion sets this weak variation to a small amplitude $O[(\text{Pe} \ell_x)^{-1}]$ (as given above in the analysis of Taylor modes) once a time scale $O(\text{Pe})$ is reached. In the terminology of homogenization theory, the vertical structure correction to the vertically independent leading-order is dominated by the solution of the *cell problem*.

V. CONCLUDING REMARKS

A number of authors^{3,7-10} have addressed the problem of passive scalar diffusion under simple flow conditions, and nontrivial time scales have been identified and explained in different cases. The present study we believe contributes a more complete global understanding of the various scalings that such problems can exhibit. In particular, with the formu-

FIG. 14. Gap of variance $\tilde{\sigma}$ vs time. All distributions are normalized to unitary mass. The curves level off after the time scale τ_D . Notice that the curves relative to runs 1, 2, and 4 result indistinguishable. Run 3 is not reported because by exact asymmetry the variance is identically zero at all times.

FIG. 15. Time evolution of L_2 norm (top) and decay rate (bottom). Run 2 is not reported in the bottom picture because it would be too low to be visible.

lation of the analysis as an eigenvalue problem we have identified and calculated the explicit long-lived slow modes, and further sorted these modes into two different categories. The first is connected to the Taylor regime, governed by the homogenized evolution equation. The second category is connected to the intermediate- and short-time anomalous evolution. While first computed for idealized periodic flows, we have also shown how such modes provide insight for more physically relevant shears, such as the example of the Poiseuille channel flow. Explicit analysis of a sawtooth shear flow provides the detailed structure and decay properties of the tracer's boundary layer near flat walls, while in the interior shear-free regions [near locations where $u'(y)=0$] more general WKB asymptotic analysis provides the longest lived anomalous modes, which persists well beyond the wall boundary layer modes in the limit $\epsilon \rightarrow 0$.

The analysis characterizes different stages of evolution, each one carrying the signature of a different spectral band. From the spectral point of view of the advection-diffusion problem, the Taylor regime should be regarded as the limiting state in which any component of the spectrum has decayed and become negligible with respect to the $n=0$ modes in the $k \ll \text{Pe}^{-1}$ range. The modes inside the range $k \gg \text{Pe}^{-1}$ characterize the structure of the solution in the super-Gaussian anomalous diffusive regime described, for instance, in the work by Latini and Bernoff. Considering the point source distributions discussed by these authors, the cross-section-averaged distribution is initialized from a flat Fourier spectrum, which necessarily excites all three classes of modes and exhibits three regimes along the evolution. We observe how a simulation in a $L_x \times L_y$ periodic domain would require a fundamental x wavenumber $k_{x0} = 2\pi/L_x \ll 1/\text{Pe}$ in order to observe the Taylor regime. A smaller domain, with lower resolution in the wavenumber domain, leads to a cutoff of the Taylor modes, limiting the possible observable re-

gimes up to the “anomalous diffusion” stage. By adjusting the initial relative energy in the bands we demonstrated how the WKB may in principle be extended well beyond the classical cross-stream-diffusion time scale r^2/D (or τ_D in nondimensional units). Additionally, compared to previous studies, the present investigation provides deeper insight into the geometrical spatial structures arising during time evolution.

It is interesting to consider the implications of our analysis for the case of several superimposed passive scalars with different diffusion coefficients. For example, one can consider a setup consisting of two different chemical species that are injected in the same point within a shear flow. If the molecular diffusivities are different, our analysis indicates that the velocity field acts as a separator for the two scalars, owing to their different interplay with advection. If the scalars are reactive, one could in turn expect the separation to affect reaction, possibly suppressing it, when the time scales of advection- diffusion are comparable to the time scale of reaction. A detailed investigation in this direction is interesting and will be considered for further studies.

Future studies will also include the extension of the concepts presented in this work to the more realistic setups of flows in both two and three dimensions, with open and closed streamlines and physical boundary conditions, where similar phenomena including long-lived modes have been observed. In particular, the axially symmetric geometry naturally merits study for its relevance to pipe flows. Further extensions of the methods presented here should also be directed to addressing time-dependent flows possessing multiple scales and even randomness.

ACKNOWLEDGMENTS

We thank Ray Pierrehumbert for helpful discussions and sharing notes from one of his presentations about strange eigenmodes. We thank Neil Martinsen-Burrell for his initial work on the subject at the end of his post-doctoral appointment at UNC sponsored by NSF CMG Contract No. ATM-0327906. We also thank an anonymous referee for pointing out the consequences of our analysis in the case of reaction between two or more diffusing chemical species with different diffusivities. R.C. was partially supported by NSF Contract No. DMS-0509423 and NSF CMG Contract No. DMS-0620687. R.M.M. was partially supported by NSF CMG Contract No. ATM-0327906, NSF Contract No. DMS-030868, and NSF RTG Contract No. DMS-0502266. C.V. has been partially supported by NSF CMG Contract No. DMS-0620687.

APPENDIX A: DERIVATION OF WKBJ FORMULA

The application of the concepts we are going to use can be traced back to the earlier attempts to solve the Schrödinger equation of quantum mechanics (see, for instance, Ref. 22). In fluid mechanics literature, similar ideas have also been applied to fourth-order operators in the theory of hydrodynamic stability by Lin²³ and others. Unlike the typical quantum mechanics turning-point problems, the present analysis demands additional effort, due to nonself-

FIG. 16. (Color online) Stokes (dashed) and anti-Stokes (continuous) lines for turning points close to the origin. The shaded region is the (open) set $\mathcal{S}$.

adjointness and the existence of complex spectra. Some acknowledgment for complex WKB analysis should be attributed to Wasow,²⁴ in particular for the role of the Stokes phenomenon central to this problem.

In general, we can write a WKB solution of Eq. (10) as a linear combination of two fundamental solutions

$$\phi_{1,2} = q(y; \lambda)^{-1/4} \exp\left(\pm \epsilon^{-1/2} \int_{y_0}^y q(\zeta; \lambda)^{1/2} d\zeta\right), \quad (\text{A1})$$

where so far y_0 is left unspecified. Not yet specified is also the domain of validity of such asymptotic solutions. The breakdown of Eq. (A1) close to turning points is a well-known fact, but moreover WKB solutions fail to hold in a whole annular region looping around a turning point²⁴ (Stokes phenomenon). We point out that a given WKB solution has a full meaning only if the domain of definition is specified. In fact, a single WKB solution could be asymptotic to two different exact solutions depending on the region.

Stokes lines are defined by the property $\text{Re}[\int_{y_0}^y q(\zeta)^{1/2} d\zeta] = 0$. The problem under consideration has simple turning points, hence we have three Stokes lines emanating from y_L and y_R , and the same number of anti-Stokes lines, where the latter are defined by the specular condition $\text{Im}[\int_{y_0}^y q(\zeta)^{1/2} d\zeta] = 0$ with y_0 being y_L or y_R . In Fig. 16 is reported a plot of the complex y -plane with such curves, showing the topology when the turning points y_L and y_R are collapsing at the bottom of the potential $y=0$ from the third and first quadrant (this follows from the ansatz assumed for WKB eigenvalues). On the Stokes and anti-Stokes lines WKB solutions exhibit limiting behaviors, on the first the exponential is purely oscillatory while on the second it is purely growing/decaying without oscillations.

We introduce the four WKB solutions ϕ_{1L} , ϕ_{2L} , ϕ_{1R} , and ϕ_{2R} , where the subscript indicates the specific choice $y_0 = y_L$ or $y_0 = y_R$. The sector of definition of both ϕ_{1L} and ϕ_{2L} is the one contained in between μ_{L2} and μ_{L3} (unshaded left region in Fig. 16). Similarly ϕ_{1R} and ϕ_{2R} are defined in between μ_{R2} and μ_{R3} (unshaded right region in Fig. 16). Also,

the branch choice fixes ϕ_{1L} to be the exponentially small component for y moving to the left along the negative real axis, while ϕ_{2R} will be small for y moving to the right along the positive real axis.

1. Connection formulas

Since we are working under the assumption of free-space condition, in the far field only the vanishing components of the solution (ϕ_{1L} and ϕ_{2R}) are present. To determine the eigenvalues, one has to impose matching in the middle region $\mathcal{S}$ (shaded region in Fig. 16) for the left- and right-hand side solutions, which come as ϕ_{1L} and ϕ_{2R} from the lateral sectors (blank regions in the same picture). Moving from the lateral sectors into $\mathcal{S}$ the two asymptotic solutions ϕ_{1L} and ϕ_{2R} have to be continued inside $\mathcal{S}$ accounting for Stokes phenomenon. In other words, ϕ_{1L} and ϕ_{2R} have to be replaced by different expressions in order to be asymptotic to the same solutions the two functions are asymptotic to outside of $\mathcal{S}$. If the four functions ϕ are extended inside $\mathcal{S}$ by analytic continuation moving in the counterclockwise sense around the turning points, the substitutions to perform are

$$\phi_{1L} \rightarrow \phi_{1L} + i\phi_{2L}, \quad (\text{A2a})$$

$$\phi_{2R} \rightarrow \phi_{2R} + i\phi_{1R}. \quad (\text{A2b})$$

These are analogs of Jefferey's connection formulas, generalized to connect asymptotic solutions valid in different sectors of the complex plane around a turning point, rather than the two parts of the real line divided by a turning point for real self-adjoint problem.

2. Asymptotic matching

After using the connection formulas, we enforce matching inside $\mathcal{S}$. This can be performed in either a symmetric or antisymmetric manner

$$\phi_{1L} + i\phi_{2L} = \pm \phi_{2R} \pm i\phi_{1R}. \quad (\text{A3})$$

For compactness of notation let now $Q_L = \epsilon^{-1/2} \int_{y_L}^y q(\zeta)^{1/2} d\zeta$ and $Q_R = \epsilon^{-1/2} \int_{y_R}^y q(\zeta)^{1/2} d\zeta$, Eq. (A3) (dropping the prefactor $q^{-1/4}$) becomes

$$e^{Q_L} + ie^{Q_L} = \pm e^{-Q_R} \pm ie^{Q_R},$$

where all the integrals now are now path-independent in $\mathcal{S}$. Introducing also $Q_{LR} = \epsilon^{-1/2} \int_{y_L}^{y_R} q^{1/2} d\zeta$, the above equation is equivalent to

$$e^{Q_{LR}+Q_R} + ie^{-Q_{LR}-Q_R} = \pm e^{-Q_R} \pm ie^{Q_R},$$

which can be recombined as

$$e^{Q_R}[e^{Q_{LR}} \mp i] = e^{-Q_R}[-ie^{-Q_{LR}} \pm 1]. \quad (\text{A4})$$

The last relation can be satisfied if the terms in brackets are equal to zero. This yields the eigenvalue condition (12).

APPENDIX B: WKBJ MODES FOR SAWTOOTH SHEAR FLOW

Here we consider the velocity profile to be a piecewise linear shear flow, namely $u(y)=1-|y|$ with $y \in [-2,2]$, and periodic boundary conditions apply. The eigenvalue problem (3), which now reads as

$$\epsilon \psi_{yy} = (\lambda + i - i|y|) \psi, \quad (\text{B1})$$

can be solved in the $\epsilon \rightarrow 0$ limit by a patching method. The starting point is again the assumption of the ansatz (11).

1. Eigenvalue conditions

Before proceeding, the derivation we simplify the problem exploiting the symmetry respect to the origin. Since symmetry implies that all eigenfunctions have to be either symmetric or antisymmetric, we can work on the semi-interval, say $[0,2]$, and impose symmetry [$\psi_y(0)=\psi_y(2)=0$] or antisymmetry [$\psi(0)=\psi(2)=0$] boundary conditions.

The eigenfunction ψ will be in general a linear combination of two independent solutions of Eq. (B1), say ψ_1 and ψ_2 . The boundary conditions require the existence of a non-trivial solution for the linear system

$$\gamma \psi_{1y}(0) + \delta \psi_{2y}(0) = 0,$$

$$\gamma \psi_{1y}(2) + \delta \psi_{2y}(2) = 0,$$

in the symmetric case, or

$$\gamma \psi_1(0) + \delta \psi_2(0) = 0,$$

$$\gamma \psi_1(2) + \delta \psi_2(2) = 0,$$

in the antisymmetric. Setting the determinant equal to zero we obtain the eigenvalue condition, but before writing it, we make ψ_1 and ψ_2 explicit.

We use the change of variable

$$z = -\epsilon^{-1/3} i^{1/3} y + \frac{\lambda + i}{\epsilon^{1/3} i^{2/3}},$$

that transforms Eq. (B1) into an Airy equation in the variable z , hence two base solutions can be chosen as

$$\psi_1(y) = A_1[z(y)], \quad \psi_2(y) = A_2[z(y)],$$

where $A_1(z) = \text{Ai}(z)$ and $A_2(z) = \text{Ai}(\omega z)$, with $\omega = e^{i2\pi/3}$. The two boundary points $y=0$ and $y=2$ map, respectively, into the z -plane as

$$z_+ = \frac{\lambda - i}{\epsilon^{1/3} i^{2/3}}, \quad z_- = \frac{\lambda + i}{\epsilon^{1/3} i^{2/3}},$$

so that the eigenvalue conditions for symmetric and antisymmetric eigenfunctions, respectively, read

$$A'_1(z_+) A'_2(z_-) = A'_1(z_-) A'_2(z_+), \quad (\text{B2})$$

$$A_1(z_+) A_2(z_-) = A_1(z_-) A_2(z_+). \quad (\text{B3})$$

The ansatz for λ implies that we assume the form

$$z_{\pm} \sim 2i^{-5/3} \epsilon^{-1/3}, \quad (\text{B4})$$

$$z_{\pm} \sim i^{-2/3} (a \epsilon^{p-1/3} + i b \epsilon^{q-1/3}), \quad (\text{B5})$$

for z_+ and z_- . Observe that, while the orientation of z_+ in the complex plane is given by $i^{-5/3}$, the orientation of z_- is still to be determined. Representing it as i^α , we have the constraint $\frac{1}{3} \leq \alpha \leq \frac{4}{3}$.

2. Determination of p and q

We first show that assuming either $p < \frac{1}{3}$ or $q < \frac{1}{3}$ (i.e., $z_{\pm} \rightarrow \infty$), then Eqs. (B2) and (B3) cannot be satisfied, hence $p \geq \frac{1}{3}$ and $q \geq \frac{1}{3}$. With little additional effort this condition will be turned in $p=q=\frac{1}{3}$.

We rewrite the eigenvalue conditions separating z_+ from z_- , namely,

$$\frac{A_1(z_+)}{A_2(z_+)} = \frac{A_1(z_-)}{A_2(z_-)}, \quad (\text{B6})$$

$$\frac{A'_1(z_+)}{A'_2(z_+)} = \frac{A'_1(z_-)}{A'_2(z_-)}, \quad (\text{B7})$$

planning to obtain the $\epsilon \rightarrow 0$ asymptotics for left- and right-hand sides of both expressions, and to show that no possibility of matching exists if the above assumption is made. We start from the antisymmetric case.

3. Antisymmetric case

The leading order behavior of $A_1(\rho i^\alpha)$ and $A_2(\rho i^\alpha)$ as $\rho \rightarrow +\infty$ is known to be²⁵

$$\text{for } \alpha \in (-2, 2), \quad (\text{B8})$$

$$A_1(\rho i^\alpha) \sim \rho^{-1/4} \exp\left(-\frac{2}{3} \rho^{3/2} i^{3\alpha/2}\right),$$

$$\text{for } \alpha \in \left(-\frac{10}{3}, \frac{2}{3}\right), \quad (\text{B9})$$

$$A_2(\rho i^\alpha) \sim \rho^{-1/4} \exp\left(\frac{2}{3} \rho^{3/2} i^{3\alpha/2}\right),$$

where the actual constants that should appear in front of these expressions have been omitted, since they are irrelevant for the present investigation. Such simplification will be also assumed in all analogous situations.

The asymptotic behavior of the left-hand side of Eq. (B6) follows directly from the above formulas. In fact from Eq. (B4), we are in the case $\alpha = -\frac{5}{3}$, in which both Eqs. (B8) and (B9) are valid. Using Eq. (B4) and developing the ratio, we obtain

$$\frac{A_1(z_+)}{A_2(z_+)} \sim \exp\left(-\frac{8\sqrt{2}}{3} \epsilon^{-1/2} i^{-5/2}\right). \quad (\text{B10})$$

For the right-hand side, we notice that Eq. (B5) implies that, if z_- is assumed to go to infinity as $\epsilon \rightarrow 0$, it has to belong to the sector S given as $\pi/6 \leq \arg(z_-) \leq 2\pi/3$ (corresponding to $\frac{1}{3} \leq \alpha \leq \frac{4}{3}$). While the asymptotic expansion of A_1 holds in the whole extent of S , the one for A_2 needs to be split in two parts, respectively, valid in the two subsectors S_1 and S_2 , defined by $\pi/3 < \arg(z_-) \leq 2\pi/3$ and $\pi/6 \leq \arg(z_-) < \pi/3$. In sector S_1 , it should be used Eq. (B9) with $\frac{2}{3} < \alpha \leq \frac{4}{3}$, which falls outside the range of validity for that

asymptotic expansion. Hence α has to be taken to belong to $-\frac{10}{3} < \alpha \leq -\frac{8}{3}$. In S_2 both expressions are valid with $\frac{1}{3} \leq \alpha < \frac{2}{3}$ and no change of branch is needed. The case $\alpha = \frac{2}{3}$, the edge between S_1 and S_2 , will be treated separately at the end of this discussion. The resulting asymptotic expressions are as follows:

(1) Sector S_1 , $\frac{2}{3} < \alpha \leq \frac{4}{3}$

$$A_{1,2}(\rho i^\alpha) \sim \rho^{-1/4} \exp\left(-\frac{2}{3}\rho^{3/2}i^{3\alpha/2}\right).$$

It follows

$$\frac{A_1(z_-)}{A_2(z_-)} \sim \text{const.}, \quad \epsilon \rightarrow 0. \quad (\text{B11})$$

(2) Sector S_2 , $\frac{1}{3} \leq \alpha < \frac{2}{3}$

$$A_1(\rho i^\alpha) \sim \rho^{-1/4} \exp\left(-\frac{2}{3}\rho^{3/2}i^{3\alpha/2}\right),$$

$$A_2(\rho i^\alpha) \sim \rho^{-1/4} \exp\left(\frac{2}{3}\rho^{3/2}i^{3\alpha/2}\right).$$

It follows

$$\frac{A_1(z_-)}{A_2(z_-)} \sim \exp\left(-\frac{4}{3}\rho^{3/2}i^{3\alpha/2}\right),$$

hence using Eq. (B5)

$$\frac{A_1(z_-)}{A_2(z_-)} \sim \exp\left(-\frac{4}{3}(a^2 + b^2)^{3/4}\epsilon^{3p-1/2}i^{3\alpha/2}\right), \quad \epsilon \rightarrow 0. \quad (\text{B12})$$

Now it is possible to compare the asymptotics of left- and right-hand side of the eigenvalue condition (B6). It is almost immediate to realize that *no matching is possible*. Indeed, from Eq. (B10), it is clear that left-hand side is asymptotically a growing exponential, while neither Eqs. (B11) and (B12) are in the respective sectors. This fact excludes the possibility $z_- \rightarrow \infty$, and we conclude that z_- has to approach a constant value as $\epsilon \rightarrow 0$ (which so far could be 0). Using Eq. (B5), this immediately implies $p \geq \frac{1}{3}$ and $q \geq \frac{1}{3}$.

4. Symmetric case

Now we have to consider the leading order behavior of $A'_1(\rho i^\alpha)$ and $A'_2(\rho i^\alpha)$ for large ρ , which is²⁵

for $\alpha \in (-2, 2)$,

$$A'_1(\rho i^\alpha) \sim \rho^{1/4} \exp\left(-\frac{2}{3}\rho^{3/2}i^{3\alpha/2}\right), \quad (\text{B13})$$

for $\alpha \in \left(-\frac{10}{3}, \frac{2}{3}\right)$,

$$A'_2(\rho i^\alpha) \sim \rho^{1/4} \exp\left(\frac{2}{3}\rho^{3/2}i^{3\alpha/2}\right). \quad (\text{B14})$$

The same discussion of the sectors of validity for the antisymmetric case applies for the present case as well. We can also note that the structure of the asymptotic expressions is still the same. In particular the exponential term, which essentially determined our conclusions above, is not altered.

Therefore the same result is also established for the symmetric case: the eigenvalue condition (B7) cannot hold unless $p \geq \frac{1}{3}$ $q \geq \frac{1}{3}$.

5. Final step

We first come back to the case $\alpha = 2/3$, which as already mentioned has to be discussed separately. Actually it requires only the observation that along this direction the exponential behavior of A_1 and A_2 vanishes (we are in fact on a Stokes line). Since both A_2/A_1 and A'_2/A'_1 can vanish only algebraically there are no chances, once again, for the eigenvalue conditions (B6) and (B7) to be satisfied.

To turn the inequalities obtained for p and q into equalities we can proceed by showing how the constant which z_- approaches cannot be 0. For the antisymmetric mode it is proven that the ratio $A_1(z_-)/A_2(z_-)$ goes to infinity, we have also to conclude that z_- has to approach a root of A_2 , being this the only possibility allowing $A_1(z_-)/A_2(z_-) \rightarrow \infty$, since Airy functions do not have any finite-range singularity. Moreover, A_2 does not have a root at the origin, and its roots are all aligned along the direction $e^{i(\pi/3)}$ in the first quadrant of the complex plane, so that the constant cannot be 0, hence $p = q = \frac{1}{3}$, and a and b are determined such that $A_2(a + ib) = 0$. The freedom left in the determination of a and b yields a set of eigenvalues, with the one corresponding to the root closer to the origin being the ground state. The same is true for the symmetric modes just replacing A_1 and A_2 with A'_1 and A'_2 .

We can further assess the accuracy of the asymptotic prediction from this analysis. Since $A_2(z_-)$ [and $A'_2(z_-)$] have been shown to vanish exponentially fast as $\epsilon \rightarrow 0$, $O[\exp(-\text{const.}\epsilon^{-1/2})]$, using Eq. (B6) and (B10) and the fact that Airy functions (and their derivatives) have only simple roots, implies that z_- has to approach exponentially fast a root of A_2 (or A'_2). This in turn implies that the form of the remainder in the asymptotic equality (B5) is determined, and the remainder for the leading order expression of λ follows:

$$\lambda = (a + ib)\epsilon^{1/3} - i + O[\exp(-\text{const}\epsilon^{-1/2})],$$

as can be immediately obtained from the definition of z_- .

One may additionally be interested in the eigenvalue for finite ϵ , which may be found by using any root-finding numerical algorithm on Eqs. (B2) and (B3). The above scaling results are confirmed by a numerical approach. Moreover, an additional behavior at fixed value of ϵ merits mention, namely, that the imaginary part of the ground-state eigenvalue vanishes at a critical finite value of ϵ , indicating nonanalytic bifurcations of the eigenvalues. This is essentially in agreement with previous findings by Doering and Horsthemke⁵ in the case of a linear-shear channel (mostly equivalent to our sawtooth.)

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